32nd International Conference on Defects in Semiconductors

Program for the 32nd ICDS

Rehoboth Beach, Delaware, USA

September 10–15th, 2023

Sunday, September 10th

Special Plenary Perspectives Session – Swan Ballroom

Chairperson: Anderson Janotti, University of Delaware

6:15-6:30 PM Opening remarks

6:30-7:15 PM "Using Light to Understand – and Change – Defects"

Matthew McCluskey

Washington State University

The optical properties of semiconductors are inextricably linked to their electronic and vibrational properties. Electronic transitions from hydrogenic impurities and vibrational modes of mass defects lead to well-defined peaks in the infrared (IR) spectrum that provide information about the symmetry and chemical composition of the defects. Optical techniques such as photoluminescence (PL) provide researchers with a (mostly) nondestructive method for identifying defects. Light can also *change* defects, especially those that undergo large relaxation when their charge state changes. The *DX* center, for example, can absorb a photon and move to its shallow-donor site, leading to persistent photoconductivity (PPC) at low temperatures. In certain oxide semiconductors, substitutional hydrogen can be optically excited, causing the proton and electrons to leave. This leads to large *room temperature* PPC. Similar processes may cause photochromism, which is a change in sample color after exposure to light.

7:15-8:00 PM "From Color Centers to Quantum Emitters: A Century of Point Defects"

Chris Van de Walle

University of California, Santa Barbara

The term "defects" connotes trouble. Indeed, defects can cause carrier trapping, nonradiative recombination, and device degradation, and thus need to be beaten into submission. But defects can also provide functionality: Point defects in semiconductors and insulators provide a platform for quantum technologies that combines the environmental isolation necessary to maintain coherence with the ability to perform electrical and optical manipulation. Accurate knowledge of how and why defects form, and how they affect the electronic and optoelectronic properties, is essential. I will outline how characterization of defects in semiconductors has historically progressed, with a focus on theoretical understanding and the insights that can be gained from accurate computations.

Following the talks **Reception at Kiwi's Kove**

Monday, September 11th

Plenary Session – Swan Ballroom

Chairperson: Chris G. Van de Walle, University of California, Santa Barbara

8:30-9:15 AM “Shallow donor defects in ZnO for quantum information applications”

Kai-Mei Fu

University of Washington

Donors in semiconductors have been studied as a qubit platform for over 20 years. Here we present our work on synthesizing and isolating single donors in zinc oxide (ZnO). The direct band gap nature of ZnO enables efficient access to the donor electron via the donor-bound exciton. Here we demonstrate synthesis of indium (In) donors via ion implantation and annealing with properties on par with In donors incorporated *in situ* during growth including: a narrow inhomogeneous linewidths (< 10 GHz), spin initialization, and long longitudinal spin relaxation (> 100 ms). Next we demonstrate single In donor isolation for *in situ* doped In via plasma-enhanced focused ion beam milling. An outlook toward single implanted In isolation, access to the In nuclear spin, and applications in quantum quantum networks, memories and transduction will also be presented.

This presentation is based upon work supported by the Army Research Office MURI Grant on Ab Initio Solid-State Quantum Materials: Design, Production and Characterization at the Atomic Scale (18057522), National Science Foundation under Grant 2212017, and U.S. Department of Energy, Office of Science, National Quantum Information Science Research Centers, Co-design Center for Quantum Advantage (C2QA) under contract number DE-SC0012704.

9:15-10:00 AM “Charged defects in semiconductors and beyond”

Jörg Neugebauer

Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Designing key functionality of semiconductor materials and devices requires a deep understanding and accurate description of fundamental defect properties such as their formation energies, charge states or charge transition levels. For more than half a century electronic structure calculations had and still have a tremendous impact in providing an accurate description of these fundamental properties. This enabled the discovery of new materials or the design of new strategies in doping or growth. However, the accurate description of charged defects with ab initio methods turned out to be challenging and stimulated computational scientists to invent ingenious approaches and algorithms.

A prime example is the description of charged defects with their long-ranged Coulomb interaction in supercells that are rather small due to the large computational effort required by ab initio calculations. While semiconductor physicists took the lead in developing these approaches, charged defects are a key component also in research fields commonly not connected to semiconductor physics such as corrosion science or electrochemistry. In the presentation, we will provide a brief overview of recent breakthroughs in describing charged defects in dimensionally reduced systems, such as 2D materials, surfaces, or electrified interfaces, and how these approaches helped in understanding semiconductor materials. We will show how these developments opened an efficient transfer of ideas and concepts between defect semiconductor physics and these research fields, providing interesting new perspectives on long-standing issues such as doping limitations or degradation.

10:00-10:20 AM **Coffee break**

Parallel Sessions

Gallium oxide (I) – Swan Ballroom

Chairperson: Matthew McCluskey, Washington State University

10:20-10:40 AM “Kinetics of Compensation in Sn-doped Ga_2O_3 During O_2 Annealing Revealed by FTIR and Modelling”

Jacob High, Haobo Yang, Nathan Rock, Mike Scarpulla
University of Utah

It is well known that annealing n-type doped β-Ga_2O_3 in air or O_2 produces insulating surface layers on the micron scale; however the microscopic mechanisms by which this occurs remain a mystery. Over time, assumed mechanisms have evolved from elimination of V_O to the introduction of V_{Ga}, but in fact multiple hypotheses involving elementary native defects and complexes can reproduce the same phenomenology (transition to insulating and increased positron trapping). Besides the identity of the defects involved, the locations of generation and transport are unknown.

At this time, V_{Ga}, V_O and their complexes are believed to be the dominant stable native defects but the mechanisms of their formation are unknown. Do V_{Ga} form at structural defects and interfaces then diffuse to permeate the material, or do Frenkel pairs nucleate homogeneously and the Ga_i diffuse away to sinks? How is the information about oxygen richness imposed transmitted from the surfaces inwards to the bulk; do O_i play any transient role in mediating these processes? Such details still have not been addressed, and can not be distinguished by their effects on net charge alone; some orthogonal data such as formation or migration barriers must also constrain hypotheses in order to determine the most likely.

We have been utilizing FTIR transmission through wafers approximately 500 um thick to reveal the kinetics of the conducting-to-insulating transition during annealing. In thick samples, a mechanism with diffusion constant many orders of magnitude faster than that found near the surface using electrical methods would be required. Put more concretely, if only the previously determined mechanism is present, the insulating transition would take centuries in wafers while only days to weeks are required near 1000 C in pure O_2.

We developed a coupled defect diffusion, carrier density, dielectric function, multilayer optics model of the samples with which we can test hypotheses for the kinetics of compensating defect formation and transport. Our model spans from the bandgap near 5 eV to the limiting 2-phonon absorption at 1500 cm^{-1} and, after inclusion of POP phonon-limited momentum scattering lifetime in the Drude component, reproduces the data extremely well. With this level of modelling, we show with high confidence that at least two diffusion-mediated processes are required to reproduce the data. We review possible mechanisms and provide evidence on the kinetic barriers for what is presumably a native defect driven process. Fortunately, the fidelity and predictiveness of computations of defect energetics and migration barriers now allow differentiation between possible mechanisms; we hope that these experiments will motivate detailed studies to uncover the detailed mechanisms of defect processes in Ga_2O_3 and beyond.

10:40-11:20 AM "Classes of O-H centers in β-Ga_2O_3 and their effect on the concentration of free carriers" *(invited presentation)*

Michael Stavola[1], Amanda Portoff[1], Andrew Venzie[1], W. Beall Fowler[1], Evan Glaser[2], Stephen Pearton[3]

[1]Lehigh University, [2]U.S. Naval Research Laboratory, [3]University of Florida

β-Ga_2O_3 has attracted much recent attention as a promising ultrawide bandgap semiconductor. Hydrogen can affect the conductivity of β-Ga_2O_3 through the introduction of shallow donors and the passivation of deep acceptors. The introduction of hydrogen or deuterium into β-Ga_2O_3 by annealing in an H_2 or D_2 ambient at elevated temperature produces different classes of O-H or O-D centers. This presentation describes a study of the interaction of hydrogen with V_{Ga1} and V_{Ga2} deep acceptors as well as other impurities and native defects in Ga_2O_3, using infrared spectroscopy and complementary theory. O-H centers in β-Ga_2O_3 evolve upon annealing in an inert ambient and are transformed from one type of O-H center into another. These reactions affect the compensation of unintentional shallow donors by deep acceptors that are passivated by hydrogen. Defects involving additional impurities in β-Ga_2O_3 compete with deep acceptors for hydrogen and modify the hydrogen-related reactions that occur. The defect reactions that occur when hydrogen is introduced by annealing in an H_2 ambient appear to be simpler than those observed for other introduction methods and provide a foundation for understanding the hydrogen-related reactions that can occur in more complicated situations.

Work supported by NSF Grant 1901563.

11:20-11:40 AM “Metastable cation vacancies in semiconducting oxides”

W. Beall Fowler, Michael Stavola, Andrew Venzie, Amanda Portoff

Department of Physics, Lehigh University, Bethlehem, PA 18015 USA

Theoretical and experimental evidence has emerged [1-7] over the past decade that the simple cation vacancy in a number of semiconducting oxides is metastable, and that the lowest-energy configuration may have the form of cation vacancy - cation interstitial - cation vacancy. This situation may occur in crystal structures for which such a configuration has high symmetry and in which the cation interstitial forms tetrahedral or octahedral bonds with adjacent oxygens. Such structures include the Ga(1) vacancy in the β phase of Ga_2O_3, the cation vacancy in the α phase of Ga_2O_3, Al_2O_3 and In_2O_3, and the Cu vacancy in Cu_2O, among others. We review and (using the CRYSTAL17 code [8]) add to the knowledge of these families of defects, and we note that it is critical that the significance of the “split” structure as *the* equilibrium configuration be fully recognized in calculations of electronic properties, level positions, cation diffusion, interactions with hydrogen, and other properties of these and similar systems.

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11:40-12:00 PM

"Vacancy defects in Si doped β-$(Al,Ga)_2O_3$"

Iuliia Zhelezova[1], Ilja Makkonen[1], Zbigniew Galazka[2], Filip Tuomisto[1]

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The science and technology of β-Ga_2O_3 materials synthesis and (opto-)electronic device development has progressed at a fast pace in the past decade [1]. Thanks to the ultra-wide band gap of about 4.85 eV and the availability of large-area single crystals for substrates, the diversity of applications is high. In particular, power switching devices are aimed at, and further increasing the band gap by alloying with Al_2O_3 that has even wider band gap is expected to bring important benefits [2]. While n-type doping is routinely achieved for β-Ga_2O_3, it is not a straightforward question for its wider band gap alloys. Cation vacancies are archetypical compensating defects for n-type dopants in compound semiconductors. In this work, we study their formation in Si-doped single crystals of β-$(Al,Ga)_2O_3$ with positron annihilation spectroscopy [3].

We present results obtained in 8 different (16 pieces) Czochralski-grown β-$(Al,Ga)_2O_3$ single crystals with Al content 0, 10, 20, and 25%, in both undoped and n-type doped form [2]. The unintentional Si content in the undoped crystals is $2 - 3 \times 10^{17}$ cm^{-3}, and in the doped crystals the Si content is $3 - 6 \times 10^{18}$ cm^{-3} as measured by secondary ion mass spectrometry. Hall measurements show that the undoped crystals are n-type for all Al mole fractions with the carrier concentration roughly matching the unintentional Si content, but in the Si doped crystals the doping efficiency is reduced at higher Al content, and the doped 25% alloy is electrically insulating [2]. The overall 3D anisotropy of the Doppler broadening signals [4] is significantly smaller for all Si doped samples irrespective of the Al content. The undoped samples show the usually high anisotropy observed in β-Ga_2O_3 for all Al contents. In addition, the average positron lifetime is significantly longer in the Si-doped samples for all Al contents, in the 207-

214 ps range, compared to 176-185 ps in the undoped samples. Importantly, the positron data do not depend on the Al content in the Si doped samples.

The results indicate that Si doping generates unrelaxed Ga vacancy related defects as opposed to the split Ga vacancies that typically dominate the positron annihilation signals in β-Ga_2O_3 [4-6]. However, these unrelaxed Ga vacancies do not appear to be the key to understanding to the sudden strong passivation of the Si dopants at higher Al content, as there appear to be no significant differences between the Si doped samples across the Al content range in our preliminary experiments. Further work is required to resolve this issue.

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2D Materials (I) – Sanibel

Chairperson: Michael Swift, Naval Research Lab

10:20-10:40 AM “Benchmarking and applying quantum embedding methods for defects”

Cyrus Dreyer[1, 2]

[1]Department of physics and astronomy, Stony Brook University, [2]Center for Computational Quantum Physics, Flatiron Institute

Point defects, including vacancies, interstitials, antisites, and impurity atoms, are ubiquitous in all materials and can have a profound influence on their properties. Density-functional theory (DFT) calculations have proven to be a crucial tool for defect identification and characterization. However, such calculations have fundamental limitations, e.g., for excited electronic states that may have correlated, multireference nature. This motivates the application of many-body methods to treat such cases. However, the large system sizes necessary to treat isolated defects in their bulk host constitutes a challenge for many-body methods because of their computational cost. Recently, quantum embedding approaches, where a small set of states is treated via many-body methods as a correlated active space, while the weakly-correlated bulk is treated with DFT, have shown promise for defects. In this talk, I will describe one such approach, based on

Wannierization of defect orbitals and constrained random-phase approximation calculation of screened Coulomb interactions. I will discuss work on benchmarking this approach via comparison to variational and diffusion Monte Carlo calculations for transition metal impurities, and how it can be used to gain insight into the the effect of the environment on the properties of defects in 2D materials. Finally, I will report on progress on using embedding to obtain optical properties for the rare-earth impurity Er in 2D WS2.

10:40-11:00 AM “High-throughput computationally-driven discovery and experimental realization of a new quantum defect in WS_2”

Geoffroy Hautier[1], John Thomas[2], Bradford Barker[3], Wei Chen[4], Yihuang Xiong[1], Junze Zhou[2], Weiru Chen[1], Antonio Rossi[2], Nolan Kelly[3], Zhuohang Yu[5], Da Zhou[5], Shalini Kumari[5], Joshua Robinson[5], Mauricio Terrones[5], Adam Schwartzberg[2], D. Frank Ogletree[2], Eli Rotenberg[2], Marcus Noack[2], Sinéad Griffin[2], Archana Raja[2], David Strubbe[3], Alexander Weber-Bargioni[2]

[1]Dartmouth College, [2]Lawrence Berkeley National Laboratory, [3] University of California, Merced, [4]Université catholique de Louvain, [5]The Pennsylvania State University, University Park

Point defects in semiconducting hosts have been proposed as building blocks for future quantum technologies. Two dimensional hosts such as boron nitride or the transition metal dichalogenides are especially attractive as they promise accessible surface for quantum sensing and long spin coherence time. Among all possible defects in a 2D host (e.g., WS_2), it is still unclear which point defects will lead to the most promising opto-electronic and spin properties. In this talk, we will show how searching for quantum defects in WS_2 can be accelerated through high-throughput computational screening. Building a database of more than 700 charged defects in WS_2 (tungsten and sulfur substitutions) combining DFT and hybrid functionals techniques, we will present what defects show the most promising properties. We will discuss the general trends in our data set that will serve as a guideline for further computational and experimental work. Importantly, we will report on the synthesis and scanning tunneling microscopy and spectroscopy of one of our quantum defect candidates; demonstrating good agreement with the theoretical high-throughput prediction and confirming the discovery of an entirely new quantum defect with high potential for applications in WS_2.

11:00-11:20 AM “Chalcogen vacancies as paramagnetic deep acceptors in 2D transition-metal dichalcogenides”

Shoaib Khalid[1], Anderson Janotti[2], Bharat Medasani[1]

[1]Princeton Plasma Physics Laboratory, NJ, USA, [2]University of Delaware, Newark, DE

Monolayer (ML) transition-metal dichalcogenides (TMDs) have attracted great attention due to their features as single-photon emitters for quantum communication. Defects are expected to drastically alter their electronic and optical properties, and add functionality. However, the identification and characterization of defects in these materials remain puzzling. For example, the sulfur vacancy in MoS_2 has often been invoked as a source of the observed unintentional n-type conductivity. And, first-principles calculations are plagued by large errors in predicting the defect thermodynamic transition levels due to the use of optical band gap instead of the fundamental band gap, which differs by ~0.7 eV. In this work, we report the defect energetics computing with a hybrid functional tuned to reproduce the experimentally observed values of the fundamental band gaps of a series of chalcogenides, that include MoS_2, $MoSe_2$, $MoTe_2$, WS_2, and WSe_2 in the 2H semiconducting phases. We find that both (0/-1) and (-1/-2) levels occur in the gap, leading to paramagnetic charge states S=1/2 and S=1 respectively. The results are discussed in terms of the band alignments between the TMDs considering the fundamental band gaps, serving as a guide to future experimental observations.

11:20-12:00 PM “Native defects, electronic inhomogeneities, and charge density waves in 1T-TaS_2” *(invited presentation)*

Shawna Hollen

University of New Hampshire

Two-dimensional semiconductors now form the basis for a broad and rich field of research bristling with exciting possible applications from photonics to quantum computing. In many cases, these opportunities are enabled by material tunability via defects and electrostatic environment. Here we report a series of scanning tunneling microscopy (STM) experiments on 1T-TaS_2 at 10 K that show nanometer-scale electronic inhomogeneities in addition to the commonly observed commensurate charge density wave (C-CDW). These inhomogeneities are observed as variations in the apparent height in STM topographs and as variations in the local density of states. They are prevalent in images over a large set of samples and result in shifts of the band edges by up to 50 mV while the C-CDW lattice remains intact. Atomic resolution images suggest that atomic defects, likely S vacancies, are a source of the electronic inhomogeneities. These results highlight the importance of defects to the electronic properties of 1T-TaS_2 and contribute toward a broad understanding of the role of defects, disorder, and interlayer interactions in determining the electronic properties of 2D semiconductors.

12:20-1:40 PM Lunch (on your own)

Parallel Sessions

Gallium nitride (I) – Swan Ballroom

Chairperson: Cyrus Dreyer, Stony Brook University

1:40-2:20 PM "Radiation-induced deep-level traps in homoepitaxial GaN layers"
(invited presentation)

Jun Suda[1], Keito Aoshima[1], Masahiro Horita[1]

[1]Nagoya University

We have carried out studies on radiation-induced point defects (deep-level traps) in homoepitaxial GaN layers with threading dislocation density (TDD) of 3x10^{6} cm^{-2}. Among them, we have investigated electron-beam-induced traps extensively. Several traps were observed. Production rates, trap parameters for each trap were studied in detail. Displacement energies are the most important values to discuss displacement damage. Since nitrogen (N) is lighter than Ga, displacement of N occurs at lower electron beam energy. By changing electron beam energy, we successfully obtained the displacement energy of N in GaN of 21.8 eV. We have also investigated gamma-ray-induced traps. Common trap level at E_c-0.14 eV were observed for both electron beam-irradiated and gamma-ray-irradiated GaN . From literatures, similar traps were observed for energetic particles (such as proton or alpha-ray)-irradiated GaN. We calculated non-ionizing energy loss (NIEL) for various particles in GaN by using SR-NIEL calculator. We used the experimentally obtained nitrogen displacement energy. For Ga, we employed a value of theoretical calculation (22 eV) since there was no reliable experimental results. It was found that production rates of E_c-0.14 eV trap were proportional to NIEL for various particles (10 different irradiation conditions). It means that predict production rate of E_c-0.14 eV trap for any irradiation conditions can be predicted by NIEL calculations. To confirm it, we performed proton beam irradiation to homoepitaxial GaN. The obtained production rate showed very good agreement with prediction by NIEL calculation.

2:20-2:40 PM "Controllable incorporation of dopant and dilute alloy elements in nitrides"

Yujie Liu[1], Ishtiaque Navid[1], Zetian Mi[1], Emmanouil Kioupakis[1]

[1]University of Michigan, Ann Arbor

The fascinating realm of nitride semiconductors is significantly transformed by the dilute incorporation of dopants and alloying elements. Dilute concentrations of antimony (Sb) doping in GaN induce large band gap-bowing and tunable photoluminescence (PL) at room temperature from the UV to the green spectral regions. Previous experimental works investigated the PL spectra of GaSbN nanostructures and found a band gap tuning from 3.4 eV to 2 eV, consistent with Sb incorporated as an anion (SbN3-) into the N sublattice. However, the incorporation of Sb into the host nitride material, both within the bulk and on the surface, may adopt other possible configurations. In addition, the n-type doping of AlN and Al-rich AlGaN by Si donors is limited by the formation of DX centers, where the bond between the Si donor atom and one of its neighboring N atoms is severed, leading to the creation of a deep defect level. In this work, we use first-principles calculations to understand the incorporation of Si dopants in AlN and Sb alloying atoms in GaN. For Sb-alloyed GaN, we explore the possibility that Sb may also be incorporated as cations (SbGa3+/SbGa5+) into the metal sublattice of GaN. The analysis of bulk defect thermodynamics demonstrates that SbGa is energetically preferable compared to SbN under both N-rich and Ga-rich conditions in n-type samples. Thermodynamics of surface defects is also investigated, revealing the site-selective nature of Sb incorporation for various crystallographic orientations. Specifically, strong preference of Sb to incorporate on non-polar GaN surfaces is demonstrated, together with selectivity of Sb replacing Ga or N by controlling the N-rich or Ga-rich conditions during growth. For Si-doped AlN, we apply predictive atomistic calculations to understand the formation of shallow Si donors in AlN. We discovered that while the DX center is mostly stable when the Fermi level is near conduction band, mid-gap Fermi energies result in a shallow donor geometry for SiAl without structural changes. Hence, Fermi-level engineering during growth or annealing can stabilize this Si geometry, averting DX center formation. Moreover, once equilibrium is reestablished in n-type AlN and the Fermi level shifts closer to the conduction band, the severance of the Si-N bond is inhibited by an energy barrier on the order of 1 eV. A barrier of this magnitude prevents conversion of these metastable shallow Si donors to DX centers over sufficiently long timescales. Overall, our results explain the selective incorporation of Sb into GaN, and uncover the incorporation mechanism of metastable shallow Si donors in AlN.

2:40-3:00 PM “Dual nature of acceptors in semiconductors: Evidence from photoluminescence experiments”

Michael Reshchikov

Department of Physics, Virginia Commonwealth University

First-principles calculations predicted the dual nature of acceptors in semiconductors [1]. In particular, the Be_{Ga} acceptor in GaN is expected to have a deep (polaronic) state at 0.45 eV and a shallow state at 0.15 eV above the valence band maximum [1]. Our experimental studies of Be-doped GaN by photoluminescence (PL) confirmed theoretical predictions for the Be_{Ga} acceptor. The deep state of this defect is associated with the broad yellow luminescence band. Analysis of PL dependences on temperature reveals two deep states, labeled Be1 and Be2: at 0.30 and 0.35 eV above the valence band. The Be1-related luminescence transforms into Be2-related luminescence at a critical temperature of about 100 K. The shallow state of the Be_{Ga} (Be3) is found at 0.2 eV above the valence band. The related ultraviolet PL band emerges at $T > 130$ K, after it is activated by transitions of holes from state Be2 to Be3 over a potential barrier. The activation energy of this process (0.14 eV) is the same in a large number of Be-doped GaN samples grown by MOCVD and MBE techniques. A simple phenomenological model explains the experimental results. Similar behavior of PL was found for the Li_{Zn} acceptor in ZnO. The orange luminescence band is caused by electron transitions via deep polaronic states of the Li_{Zn}. Two deep polaronic states of the Li_{Zn} acceptor, separated by 34 meV, were studied by luminescence and electron paramagnetic resonance [2,3]. However, no reliable data about the shallow state of the Li_{Zn} acceptor existed so far. We have found that, very similar to the case of Be_{Ga} in GaN, an ultraviolet luminescence band from the shallow Li_{Zn} state emerges with increasing temperature with an activation energy of 0.18 eV. The Be_{Ga} in GaN and Li_{Zn} in ZnO are the first confirmed cases of acceptors with dual nature. However, we do not find experimental evidence for the dual nature of the Zn_{Ga} and Mg_{Ga} acceptors in GaN predicted by theory [1]. The rate equations model indicates that the observation of both states (shallow and deep) in PL experiments may be hampered by too high or too low potential barriers between the two defect configurations.

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3:00-3:20 PM “Surface Defect Electronic Properties in Gallium Nitride Epitaxial Layers on Different Substrates”

Andrew Winchester[1], Michael Mastro[2], Travis Anderson[2], Jennifer Hite[2], Sujitra Pookpanratana[1]

[1]National Institute of Standards and Technology, [2]Naval Research Laboratory

The wide bandgap material GaN is desired for next-generation high power electronics. However, the vertical structures needed for scalable devices suffer from issues related to dislocations and defects, which propagate from the substrate into the epitaxially grown device area. Much work has gone into substrate development, such as strain patterning on foreign seeds to coalesce dislocation bundles[1], and alternate scalable growth methods such as the ammonothermal process to produce higher structural quality substrates[2]. However, in both cases, the remaining dislocations and defects are still a major concern for high power device performance and reliability. For example, threading dislocations with screw components are known to exhibit leakage current[3] and are predicted to have mid-bandgap states[4], while newer ammonothermal GaN substrates may exhibit different defect densities and distributions compared to GaN grown on foreign substrates[2]. Therefore, determining the electronic properties of dislocations and defects at the microscale will provide valuable information for identifying "killer" defects.

Here, we use a combination of laser-based photoemission electron microscopy (PEEM) and conductive atomic force microscopy (cAFM) to investigate the local surface electronic properties of defects and dislocations in GaN epitaxially grown via MOCVD on two different substrates. In the epitaxy on dot-core patterned substrates, we identify surface defects located near the strain centers that have a star-shaped appearance with central pits and extending cracks. These star defects exhibit a larger work function and a shifted valence band maximum, and further, show increased reverse bias leakage current compared to the surrounding GaN. For epitaxy on ammonothermal GaN substrates, we instead observe elongated triangular patches using PEEM that occur on a particular face of certain growth step ridges. These regions also show altered electronic structure compared to the surrounding GaN, but are instead more resistive under both forward and reverse bias conditions. Our results provide evidence for defective sites likely related to extended dislocations that will lead to degraded device performance.

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Halide Perovskites (I) – Sanibel

Chairperson: Vladan Stevanovic, Colorado School of Mines

1:40-2:00 PM “Deep Levels and Acceptor Dopants in Lead Halide Perovskites”

Michael Swift and John Lyons

US Naval Research Laboratory

Lead halide perovskites such as methylammonium lead iodide are attractive solar cell materials, and others such as cesium lead bromide are expected to be high-performing optoelectronic materials with potential applications including lighting, displays, and quantum information. Their potential is due in large part to their good performance despite significant defect densities, i.e., “defect tolerance”, which has often been explained by hypothesizing that none of the dominant defects give rise to deep levels in the gap. We refer to this as the “shallow defect hypothesis”. In this work [1], we reject the shallow defect hypothesis for $CsPbBr_3$. *Via* a thorough first-principles inventory of native defects and hydrogen impurities using a hybrid functional with spin-orbit coupling, we show that a number of relevant defects do in fact have deep levels, most notably the bromine interstitial and hydrogen interstitial. This adds to a growing body of evidence against the shallow defect hypothesis, suggesting that the observed defect tolerance may be due instead to relatively low recombination rates at deep levels. Guided by the theoretical identification of these defects, experiments can take steps to mitigate trap-assisted non-radiative recombination, further boosting the efficiency of lead halide perovskite optoelectronics.

All of the applications of lead halide perovskites will benefit from having fully controlled electrical conductivity, but it has proven difficult to achieve high hole concentrations in these materials *via* impurity doping. In this work, possible acceptor dopants for the halide perovskites (including Ag, Na, and Cu) are evaluated [2,3]. We assess which dopants can act as shallow acceptors on the proper substitutional site, whether other configurations of these impurities cause self-compensation, and whether native defects might ultimately compensate *p*-type doping attempts. We show that *p*-type doping is difficult because of two related effects: the moderately high formation energies of acceptor impurities and compensation from native defects, particularly lead-cesium antisites and halogen interstitials. Among the dopants considered, sodium is consistently the most promising acceptor for overcoming these obstacles and achieving *p*-type conductivity in the halide perovskites.

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2:00-2:20 PM "Extrinsic doping and compensating defects in the 2D hybrid perovskite phenethylammonium lead iodide"

Gabrielle Koknat[1], Haipeng Lu[2, 3], Yi Yao[1], Ji Hao[2], Xixi Qin[1], Chuanxiao Xiao[2], Ruyi Song[4], Florian Merz[5], Markus Rampp[6], Sebastian Kokott[7], Christian Carbogno[7], Tianyang Li[1], Glenn Teeter[2], Matthias Scheffler[7], Joseph J. Berry[2], David B. Mitzi[1, 4], Jeffrey L. Blackburn[2], Volker Blum[1, 4], Matthew C. Beard[2]

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2D hybrid organic-inorganic perovskites (HOIPs) are exciting materials for optoelectronic device applications due to their high degree of structural tunability. We here present a systematic study of n-type and p-type doping of the 2D perovskite phenylethylammonium lead iodide (PEA_2PbI_4), using Bi and divalent Sn as dopants, respectively. Both Bi and Sn are expected to be incorporated as substituents on the Pb site. Using spin-orbit coupled hybrid density functional theory and supercell models up to 3,383 atoms in size, we pinpoint the expected positions of the electronic levels associated with different dopants in the bandgap. Bi as a substitution for Pb is a deep donor (0.55 eV below the conduction band). Sn is isovalent with Pb but creates a shallow acceptor state if combined with a neighboring Pb vacancy. Indeed, we find that the Pb vacancy formation energy is lowered by approximately 0.3 eV next to a substitutional Sn defect, compared to a Pb vacancy in an otherwise defect-free PEA_2PbI_4 crystal. A complementary experimental study shows that Bi incorporation does lead to weak n-type doping whereas Sn incorporation leads to weak p-type doping. For Bi substitution, measurements of the Fermi level point to a population of compensating acceptors that limit the n-type doping efficiency. For Sn

substitution, we surmise that the creation of vacancies adjacent to Sn sites may be the factor that limits the p-type doping efficiency.

2:20-3:00 PM "Optoelectronic and phase stability impacts of interstitial defects in halide perovskite semiconductors" *(invited presentation)*

Ross Kerner[1], John Lyons[2], Kai Zhu[1], Joseph Berry[1]

[1]National Renewable Energy Laboratory, [2]Naval Research Laboratory

Many density functional theory (DFT) calculations predict low formation and migration energies for various +1 interstitial defects in metal halide perovskite materials (e.g. methylammonium [MA] lead iodide or $MAPbI_3$) meaning they should be an important defect in this emerging class of semiconductors. However, there is a dearth of studies designed to test these theoretical predictions. Here, we present our experimental investigation, supported by first-principles calculations, into the impacts of several types of interstitial defects on the optoelectronic properties and halide phase stability of halide perovskites. In part one, we present a device level study designed to electrochemically induce Au and Ag +1 interstitial formation under anodic conditions, and observe them to induce *n*-type doping compensating the charge of the intercalating cations. These results provide some of the most compelling evidence in support of extrinsic interstitial defects moving throughout the halide perovskite and influencing the optoelectronic properties. In part two, we describe our proposed model to explain how homogeneously mixed iodide (I):bromide (Br) perovskite alloys (e.g. $MAPbBr_xI_{1-x}$) phase separate into I-rich and Br-rich regions under bias or illumination. The model predicts iodine +1 interstitials may play a critical role giving rise to unequal fluxes of halide species - the origin of voltage- or photo-induced compositional instabilities. We briefly review our recent experimental results testing the model, and further present DFT computations comparing the relative formation enthalpies of I versus Br interstitial defects in different halide compositions which serves to verify the validity of our model's core assumptions. Overall, this body of work brings a level of clarity to interstitial defect chemistry and physics in halide perovskites, advancing our understanding a step closer to that of more conventional semiconductors.

3:00-3:20 PM "Origins of photoluminescence instabilities at halide perovskite/organic hole transport layer interfaces"

Zhaojian Xu[1], Daniel Astridge[2], Ross Kerner[3], Xinjue Zhong[1], Junnan Hu[1], Jisu Hong[1], Jesse Wisch[1], Kai Zhu[3], Joseph Berry[3], Antoine Kahn[1], Alan Sellinger[2, 3], Barry Rand[1]

[1]Princeton University, [2]Colorado School of Mines, [3]National Renewable Energy Laboratory

Metal halide perovskites have been widely implemented in various optoelectronic devices, but their poor stability associated with defect formation under solar illumination remains a primary concern. While the intrinsic photostability of isolated neat perovskite samples has been widely discussed, it is important to explore how charge transport layers - employed in most devices - impact defect formation and thus photostability. In this study, we investigate the effect of organic hole transport layers (HTLs) on the stability of the perovskite photoluminescence (PL) spectrum and interfacial defect formation, and demonstrate that the HTL ionization energy dictates PL behavior. Furthermore, we reveal the key role of halogen loss from the perovskite and subsequent permeation into organic HTLs, where it acts as an interfacial defect causing PL quenching and introduces additional mass transport pathways to facilitate halide phase separation. These findings reveal the microscopic mechanism of non-radiative recombination at perovskite/organic HTL interfaces and detail the chemical rationale for closely matching the perovskite/organic HTL energetics to maximize solar cell efficiency and stability.

Poster Session (I) – Kiwi's Kove

4:00-5:30 PM

Corbett Prize finalists

C1. Chitraleema Chakraborty, **Univ. Delaware:** "Defects in atomically thin semiconductors for optical quantum technologies"

Chitraleema Chakraborty

University of Delaware

Although defects in semiconductors can often be detrimental to device performance, they are also responsible for the breadth of functionality exhibited by modern optoelectronic devices. For example, defect centers in solids and quantum dots are currently being investigated for an ideal single photon emitter (SPE) platform for applications ranging from quantum information science to high-resolution sensing. However, despite the rapid progress in recent years, existing material platforms face several challenges, some of which are intrinsic to their host materials, motivating the search for SPEs in alternative platforms. For instance, self-assembled InAs quantum dots (QDs) are considered state-of the-art in terms of purity and indistinguishability, yet spatial and spectral inhomogeneity has prevented the development of large-scale arrays of identical emitters. On the other hand, defect-based emitters in wide bandgap insulators like diamond offer a more direct route toward site-controlled placement using defect engineering techniques, but they are more challenging to integrate with available photonic technologies, tend to have low photon extraction efficiencies, and are challenging to address electrically[1].

To this date, no SPE technology has met all the metrics required for scalable optical quantum information applications thereby prompting the need for exploring alternative material platforms[2]. In parallel to existing 3D platforms, optically active defects in two-dimensional (2D) semiconductors have unique advantages like atom-scale proximity for photonic and sensing applications, potential atom-scale imaging and deterministic placement using surface probe techniques and efficient electrical addresibility[3]. Their brightness and purity are comparable to more established solid-state emitters such as Indium Arsenide QDs and Nitrogen Vacancy (NV) centers in diamond. For example, 2D semiconductor SPEs generally emit photons in the tens to hundreds of kHz range, which is comparable to some of the reported rates of NV centers in diamond[2]. Additionally, recent efforts on integrating WSe_2 SPEs with photonic and plasmonic cavities promise brighter emission with tens of MHz count rates, which would make them competitive with their QD-based SPEs counterparts in terms of brightness and purity[2] with the added advantage of electrical and strain control[4-8].

In this talk, I will share the story of the discovery and control of quantum emitters in two-dimensional materials defects and lattice deformations. The possibility of leveraging van der Waals heterostructure for charging these emitters with a single electron will be discussed. This lays the foundation for optically addressable spin qubits in flatland materials. Further, I will also discuss their potential in deterministic generation and scalable growth of 2D semiconductors, and integration with photonic and magnetic devices, which offers a compelling solution to scalable solid-state quantum photonics and sensing. This work opens the frontier of quantum optics in two-dimensional materials with the potential to revolutionize solid-state quantum devices.

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C2. Ross Kerner, NREL: "Optoelectronic and phase stability impacts of interstitial defects in halide perovskite semiconductors"

Ross Kerner[1], John Lyons[2], Kai Zhu[1], Joseph Berry[1]

[1]National Renewable Energy Laboratory, [2]US Naval Research Laboratory

Many density functional theory (DFT) calculations predict low formation and migration energies for various +1 interstitial defects in metal halide perovskite materials (e.g. methylammonium [MA] lead iodide or $MAPbI_3$) meaning they should be an important defect in this emerging class of semiconductors. However, there is a dearth of studies designed to test these theoretical predictions. Here, we present our experimental investigation, supported by first-principles calculations, into the impacts of several types of interstitial defects on the optoelectronic properties and halide phase stability of halide perovskites. In part one, we present a device level study designed to electrochemically induce Au and Ag +1 interstitial formation under anodic conditions, and observe them to induce *n*-type doping compensating the charge of the intercalating cations. These results provide some of the most compelling evidence in support of extrinsic interstitial defects moving throughout the halide perovskite and influencing the optoelectronic properties. In part two, we describe our proposed model to explain how homogeneously mixed iodide (I):bromide (Br) perovskite alloys (e.g. $MAPbBr_xI_{1-x}$) phase separate into I-rich and Br-rich regions under bias or illumination. The model predicts iodine +1 interstitials may play a critical role giving rise to unequal fluxes of halide species - the origin of voltage- or photo-induced compositional instabilities. We briefly review our recent experimental results testing the model, and further present DFT computations comparing the relative formation enthalpies of I versus Br interstitial defects in different halide compositions which serves to verify the validity of our model's core assumptions. Overall, this body of work brings a level of clarity to interstitial defect chemistry and physics in halide perovskites, advancing our understanding a step closer to that of more conventional semiconductors.

C3. Brendan McCullian, Cornell University: "Coherent Orbital Control of Diamond NV Center Excited States Using Strain"

Brendan McCullian[1], Huiyao Chen[1], Johnny Crossman[1], Gregory Fuchs[1]

[1]School of Applied and Engineering Physics, Cornell University

The spectrally narrow, spin-dependent optical transitions of solid-state defects can be leveraged for quantum networking applications. The best-characterized defect in this field is the nitrogen-vacancy (NV center) in diamond, however, NV centers exhibit spectral diffusion that limits the entanglement generation rate that lies at the heart of this application. The largest source of spectral diffusion is electric field fluctuations that couple to the excited-state orbital doublet. To better understand potential mechanisms of dynamically engineering NV center optical transitions, we investigate quantum control of the excited state orbitals via dynamic strain-orbital driving with an acoustic wave resonator. We demonstrate nanosecond, multi-phonon orbital Rabi oscillations in the time domain, where the orbital states are resonantly driven by GHz frequency acoustic waves. The Rabi oscillation frequencies agree well with the spectroscopic splitting that we observe by probing the driven orbital states of the NV center using a tunable laser. Such resonant orbital quantum control can enable strategies for dynamically decoupling the NV center orbital states from spectral diffusion, thus protecting optical transitions from decoherence sources.

C4. Yihuang Xiong, Dartmouth College: "High-throughput identification of spin-photon interfaces in silicon"

Yihuang Xiong[1], Weiru Chen[1], Diana Dahliah[2], Céline Bourgois[2], Sinéad Griffin[3], Alp Sipahigil[4], Geoffroy Hautier[1]

[1]Dartmouth College, [2]Université catholique de Louvain, [3]Lawrence Berkeley National Laboratory, [4]University of California, Berkeley

Color centers in semiconducting hosts have become an emerging candidate for spin-photon interfaces. Silicon is a technologically mature material that provides an attractive platform for realizing defect-based qubits that can be manufactured at scale. In this talk, we will present our work on a high-throughput search for promising spin-photon interfaces using first-principles computations. We will report on the challenges in ensuring an accurate enough electronic structure while building a large enough data set and discuss our approach using single-shot hybrid computations. By building a database that documents thousands of quantum defects in silicon, we will discuss strategies for designing defects that could emit at technologically relevant wavelengths, especially considering silicon's relatively narrow band gap. Our results suggest promising candidates and highlight the designing strategies for novel spin-photon interfaces.

C5. Fangzhou Zhao, UCSB: "Trap-assisted Auger-Meitner recombination from first principles"

Fangzhou Zhao[1], Mark Turiansky[1], Audrius Alkauskas[2], Chris Van de Walle[1]

[1]Materials Department, University of California, Santa Barbara, [2]Center for Physical Sciences and Technology (FTMC)

Trap-assisted nonradiative recombination is a key mechanism limiting the efficiency of optoelectronic devices such as light-emitting diodes. Trap-assisted recombination via multiphonon emission (MPE) has been studied from first principles [1]; its rate was found to become negligibly low in materials with band gaps larger than about 2.5 eV [2, 3] since the rate of the MPE process decreases exponentially as the energy difference between the trap state energy level and the band edge increases. Experimentally, however, trap-assisted recombination is observed to persist at larger band gaps [4]. We propose that trap-assisted Auger-Meitner (TAAM) recombination can resolve the puzzle.

We have developed a practical first-principles methodology to calculate the TAAM rate for defects and impurities in semiconductors [5]. As a case study, we applied our formalism to a calcium substitutional impurity in GaN and InGaN. We found that for band gaps larger than 2.5 eV, the combination of hole capture by MPE and electron capture by TAAM results in recombination rates orders of magnitude larger than the recombination rate governed by MPE alone.

Our computational formalism is general and can be applied to any defect or impurity in any semiconducting or insulating material. The results provide insight into the physics of nonradiative recombination processes and elucidate why TAAM processes are key to describing defect-assisted recombination in wider-band-gap materials, where MPE alone fails to explain efficiency loss.

This work is supported by the Department of Energy Office of Science.

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T. Mates, and J. Speck, Appl. Phys. Lett. 109, 212103 (2016).[5] F. Zhao, M. E. Turiansky, A. Alkauskas, and C. G. Van de Walle, arXiv:2211.08642 (2022).

Haller Prize finalists

H1. Piyush Kumar, ETH Zurich: “Interface and bulk defects induced by the thermal oxidation and post-oxidation annealing in SiO_2-SiC system”

Piyush Kumar[1], Maria Martins[1, 2], Marianne Bathen[1], Thomas Prokscha[2], Ulrike Grossner[1]

[1]Advanced Power Semiconductor Laboratory, ETH Zurich, [2]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute

Thermal oxidation at high temperatures is one of the crucial steps in the fabrication of a SiC metal oxide semiconductor field effect transistor (MOSFET). SiO_2 is used as gate oxide for the MOSFET which offers the benefits of high thermal stability and ease of fabrication. However, despite high temperature oxidation and post-oxidation annealing (POA) treatments, the devices suffer from low mobility due to high concentration of defects at and near the SiO_2-SiC interface. In this work, we have explored the impact of thermal oxidation and POA in nitric oxide (NO) and argon (Ar) environment on the resulting structure. We have performed capacitance-voltage (CV) and conductance measurements to study the defects at the SiO_2-SiC interface, low-energy muon spin rotation (LE-μSR) spectroscopy and positron annihilation spectroscopy (PAS) to study the near-interface region, deep level transient spectroscopy (DLTS) and minority carrier transient spectroscopy (MCTS) to study defects in the bulk of the semiconductor, and above bandgap optical excitation to study the near interface oxide traps (NIOTs).

The DLTS measurements reveal the generation of several bulk defects in SiC: $E_{0.23}$ at 0.23 eV, $C_{1/2}$ at 0.36/0.39 eV, ON1 at 0.85 eV, $ON2_{a/b}$ at 1.05/1.167 eV and ON3 at 1.76 eV below the conduction band (E_C) edge. The injection of carbon interstitials during thermal oxidation is predicted to be responsible for several of the above-mentioned defects. Additionally, the defect concentration is substantially increased after annealing in NO environment at 1300 °C. MCTS measurements further reveal the generation of the $O_{0.17}$ and B levels, which are located 0.17 eV and 0.28 eV above the valence band edge (E_V). Measurements of the defect depth profiles reveal a reduction in the defect concentration with depth, allowing us to estimate the diffusivity and the migration barrier of the defects.

Using LE-μSR measurements, we have observed signatures of silicon vacancies (V_{Si}) in the SiC near the interface after thermal oxidation. We have also observed a substantial increase in the carrier concentration in the near interface region (up to 100 nm from the interface) due to the incorporation of nitrogen (N) after NO annealing in the SiC crystal. Transmission electron microscopy (TEM) and PAS measurements also bolster the hypothesis of V_{Si} generation during thermal oxidation. CV measurements confirm a high concentration of defects at the interface which are reduced by post oxidation annealing in the NO/Ar environment whereas the conductance measurements help extract the emission time constants and the capture cross section of these defects. Further, we have also carried out optical excitation experiments with above bandgap light to probe the NIOTs at the valence band. Charging and discharging of these defects during device operation could lead to threshold voltage instability.

In the final contribution, we discuss the results in detail and attempt to build a scenario of the defects created in several regions of the oxide-semiconductor system due to thermal oxidation and POA in NO and Ar at different temperatures.

H2. Yujie Liu, Univ. Michigan: "Controllable incorporation of dopant and dilute alloy elements in nitrides"

Yujie Liu, Ishtiaque Navid, Zetian Mi, Emmanouil Kioupakis

University of Michigan, Ann Arbor

The fascinating realm of nitride semiconductors is significantly transformed by the dilute incorporation of dopants and alloying elements. Dilute concentrations of antimony (Sb) doping in GaN induce large band gap-bowing and tunable photoluminescence (PL) at room temperature from the UV to the green spectral regions. Previous experimental works investigated the PL spectra of GaSbN nanostructures and found a band gap tuning from 3.4 eV to 2 eV, consistent with Sb incorporated as an anion (SbN3-) into the N sublattice. However, the incorporation of Sb into the host nitride material, both within the bulk and on the surface, may adopt other possible configurations. In addition, the n-type doping of AlN and Al-rich AlGaN by Si donors is limited by the formation of DX centers, where the bond between the Si donor atom and one of its neighboring N atoms is severed, leading to the creation of a deep defect level. In this work, we use first-principles calculations to understand the incorporation of Si dopants in AlN and Sb alloying atoms in GaN. For Sb-alloyed GaN, we explore the possibility that Sb may also be incorporated as cations (SbGa3+/SbGa5+) into the metal sublattice of GaN. The analysis of bulk defect thermodynamics demonstrates that SbGa is energetically preferable compared to SbN under both N-rich and Ga-rich conditions in n-type samples. Thermodynamics of surface defects is also investigated, revealing the site-selective nature of Sb incorporation for various crystallographic orientations. Specifically, strong preference of Sb to incorporate on non-polar GaN surfaces is demonstrated, together with selectivity of Sb replacing Ga or N by controlling the N-rich or Ga-rich conditions during growth. For Si-doped AlN, we apply predictive atomistic calculations to understand the formation of shallow Si donors in AlN. We discovered that while the DX center is mostly stable when the Fermi level is near conduction band, mid-gap Fermi energies result in a shallow donor geometry for SiAl without structural changes. Hence, Fermi-level engineering during growth or annealing can stabilize this Si geometry, averting DX center formation. Moreover, once equilibrium is reestablished in n-type AlN and the Fermi level shifts closer to the conduction band, the severance of the Si-N bond is inhibited by an energy barrier on the order of 1 eV. A barrier of this magnitude prevents conversion of these metastable shallow Si donors to DX centers over sufficiently long timescales. Overall, our results explain the selective incorporation of Sb into GaN, and uncover the incorporation mechanism of metastable shallow Si donors in AlN.

H3. Igor Prozheev, Univ. Oslo: "Defects in aluminum rich Si-doped 90% AlGaN determined by positron annihilation and X-ray absorption spectroscopy"

Igor Prozheev[1], Frank Mehnke[2], Marcel Schilling[2], Tim Wernicke[2], Michael Kneissl[2], Rene Bès[1], Filip Tuomisto[1]

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The performance of devices based on AlGaN alloys emitting light shorter than 240 nm suffers from limited *n*-type conductivity of the Si-doped current spreading layers due to the high Al content >80%. The conductivity is limited not only by the increasing dopant ionization energy and formation of a stable DX center but probably also by the formation of cation vacancy defects that are known to act as compensating acceptors in *n*-type GaN and AlN. Here we present results obtained in Si-doped $Al_{0.90}Ga_{0.10}N$ layers grown by metal-organic vapor phase epitaxy on AlN/sapphire. [1 - 3] Doppler broadening of positron annihilation radiation experiments are employed for studying the cation vacancy related defects [4], and x-ray absorption spectroscopy gives information on the immediate surroundings of the Si dopants. In our samples, the Si doping is varied in the range from 9×10^{17} cm^{-3} to 1.7×10^{19} cm^{-3}, and the employed growth conditions resulted in two different carbon impurity concentrations (2×10^{17} cm^{-3} and 2×10^{18} cm^{-3}).

We observe positron saturation trapping at cation vacancy defects present above 5.0×10^{18} cm^{-3} for all studied Si doping levels in low-carbon samples. Interestingly, these vacancy defects do not appear to play a role in the electrical compensation of this material. In the high carbon content samples, the concentration of negatively charged cation vacancies increases with the Si concentration from less than 1×10^{16} cm^{-3} to above 2×10^{18} cm^{-3}, with these vacancies becoming important from the compensation point of view only at Si concentrations approaching 1×10^{19} cm^{-3}. At the highest Si doping levels, above 1×10^{19} cm^{-3}, the positron data exhibit a transition from the dominant positron trap being a cation vacancy to negatively charged non-open volume defect with a concentration exceeding 5×10^{18} cm^{-3}. The only impurity with sufficient concentration is the Si dopant, strongly suggesting that Si DX centers become an important limiting factor for *n*-type doping when the Si content is sufficiently high. [3] This behavior of the positron data coincides with the Si doping range where the electrical resistivity of the samples increases with increasing Si doping. At lower Si doping concentrations the resistivity decreases with increasing Si doping. X-ray absorption data in these two regimes show that the Si surroundings change from GaN-like in the range of decreasing resistivity to AlN-like in the range of increasing resistivity. This strongly suggests that the local chemical environment and might reveal important information on achieving lower resistivity in high Al content AlGaN.

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H4. Muhammad Hassan Shaikh, Univ. Delaware: "Magnetic proximity coupling to defects in two-dimensional semiconductors"

Muhammad Hassan Shaikh[1] , Matt Whallen[3],Aqiq Ishraq[2], Collin Maurtua[2], John Xiao[1,3], Chitraleema Chakraborty [1,2,3]

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Magnetically active defects have been extensively employed in quantum sensing applications, with nitrogen-vacancy (NV) centers in diamond and silicon-vacancy (SiV) in silicon carbide (SiC) being the most commonly used examples. These defects have played a crucial role in characterizing the magnetic behavior of three-dimensional (3D) magnetic materials. However, their applicability to two-dimensional (2D) magnetic materials is limited due to the challenges associated with accessibility and interaction with surfaces. Conversely, defects in 2D materials, particularly transition metal dichalcogenides (TMDCs), have garnered significant attention. TMDCs are semiconductor materials that exhibit optical activity with valley-dependent optical selection rules. In the presence of a magnetic field, the energy degeneracy within these valleys can be lifted. Optically active defects in TMDCs are highly sensitive to magnetic fields, providing an opportunity for direct probing of the layer-dependent 2D magnet's magnetic properties at the nanoscale. Layer-dependent 2D magnets, such as Chromium triiodide (CrI_3) and Chromium thiophosphate ($CrPS_4$), which display ferromagnetic (FM) and antiferromagnetic (AFM) properties depending on the layer count, have emerged as promising candidates for next-generation advanced spintronics devices. These materials offer improved speed (ranging from GHz to THz), electromagnetic interference immunity, and enhanced memory density due to their net-zero magnetization. However, their potential for future devices is hindered by challenges related to air stability and magnetic degradation of a few layers. While previous studies have classified the bulk form of these materials as AFM using the Magnetic Optical Kerr Rotation (MOKE) technique, the magnetic behavior of the surface layer of bulk $CrPS_4$ remains unexplored.

To investigate the FM and AFM responses of the surface layers of bulk in these materials, we utilize magnetic proximity coupling with optically active defects in TMDCs, These defect-based quantum emitters offer higher spectral resolution compared to 2D exciton transitions, which suffer from broad linewidths, thereby enabling increased magnetic field sensitivity.

In this study, we examine the magneto-photoluminescence of a heterostructure composed of $CrPS_4$ and WSe_2, utilizing defect-based quantum emitters as optically active probes at low temperatures. The surface layer of bulk $CrPS_4$ is found to exhibit a detectable net magnetic moment (NMM) via the Degree of Circular Polarization (DOP) of photoluminescence (PL) from the defect-based quantum emitters. We also performed X-ray photoelectron microscopy on bulk $CrPS_4$ revealing no signs of oxidation or hydration in the bulk material.

These findings provide valuable insights into the potential applications of next-generation AFM-based spintronics and advanced memory-based devices. By harnessing the unique properties of AFM materials and defect-based quantum emitters, this study contributes to the ongoing exploration of novel magnetic phenomena in heterostructures, facilitating advancements in spintronics and memory technology.

H5. Sarah Thompson, Univ. Pennsylvania: "R-Cu Color Centers in ZnS:Cu Colloidal Nanocrystals and Potential Applications for Quantum Information Science"

Sarah Thompson[1], Cüneyt Şahin[2], Shengsong Yang[1], Michael Flatté[3], Christopher Murray[1], Lee Bassett[1], Cherie Kagan[1]

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Colloidal ZnS:Cu nanocrystals (NCs) are widely used in bio-imaging and optoelectronic applications due to their bio-inertness and their ability to emit light across a wide range of wavelengths. In this context, we explore the potential of ZnS:Cu colloidal NCs containing red-emitting, "R-Cu" color centers for defect discovery in quantum information science. Previous approaches to identifying point defects suitable for quantum spin-light interfaces in semiconductors have relied on ad hoc observations in bulk crystals. In contrast, we propose a deliberate process that involves synthesizing, modifying, and assembling lightly-doped colloidal nanocrystals to systematically identify and evaluate promising defect-host combinations. We have identified the R-Cu center in ZnS as one such combination, and we have reported a synthesis method for obtaining colloidal NCs with photoluminescence emission dominated by R-Cu [1]. ZnS, as the host material, possesses a wide optical bandgap and a low concentration of nuclear spins, enabling the operation of an electronically isolated spin-light interface with low magnetic background noise. The R-Cu center, as the point defect of interest, is believed to possess a C3V-symmetric impurity-vacancy structure, which results in favorable orbital and spin characteristics for several known defect qubits. We have conducted first principles calculations that verify the electronic structure and thermodynamic stability of this proposed defect complex in ZnS:Cu. Additionally, we have employed ensemble time- and temperature-resolved luminescence spectroscopy to gain a deeper understanding of the R-Cu emission mechanism and electronic structure. We find that the R-Cu emission arises from thermally activated carrier transfer between two radiative manifolds, producing an anomalous plateau in the thermal quenching profile and blueshifted luminescence upon increasing temperature. Understanding of these characteristics and their relationship to the charge and spin states of the R-Cu center can inform the development of protocols for operating the center as a quantum spin-light interface.

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H6. Zhaojian Xu, Princeton Univ.: "Origins of photoluminescence instabilities at halide perovskite/organic hole transport layer interfaces"

Zhaojian Xu[1], Daniel Astridge[2], Ross Kerner[3], Xinjue Zhong[1], Junnan Hu[1], Jisu Hong[1], Jesse Wisch[1], Kai Zhu[3], Joseph Berry[3], Antoine Kahn[1], Alan Sellinger[2, 3], Barry Rand[1]

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Metal halide perovskites have been widely implemented in various optoelectronic devices, but their poor stability associated with defect formation under solar illumination remains a primary concern. While the intrinsic photostability of isolated neat perovskite samples has been widely discussed, it is important to explore how charge transport layers - employed in most devices - impact defect formation and thus photostability. In this study, we investigate the effect of organic hole transport layers (HTLs) on the stability of the perovskite photoluminescence (PL) spectrum and interfacial defect formation, and demonstrate that the HTL ionization energy dictates PL behavior. Furthermore, we reveal the key role of halogen loss from the perovskite and subsequent permeation into organic HTLs, where it acts as an interfacial defect causing PL quenching and introduces additional mass transport pathways to facilitate halide phase separation. These findings reveal the microscopic mechanism of non-radiative recombination at perovskite/organic HTL interfaces and detail the chemical rationale for closely matching the perovskite/organic HTL energetics to maximize solar cell efficiency and stability.

H7. Iuliia Zhelezova, Univ. Oslo: "Vacancy defects in Si doped β-$(Al,Ga)_2O_3$"

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The science and technology of β-Ga_2O_3 materials synthesis and (opto-)electronic device development has progressed at a fast pace in the past decade [1]. Thanks to the ultra-wide band gap of about 4.85 eV and the availability of large-area single crystals for substrates, the diversity of applications is high. In particular, power switching devices are aimed at, and further increasing the band gap by alloying with Al_2O_3 that has even wider band gap is expected to bring important benefits [2]. While n-type doping is routinely achieved for β-Ga_2O_3, it is not a straightforward question for its wider band gap alloys. Cation vacancies are archetypical compensating defects for n-type dopants in compound semiconductors. In this work, we study their formation in Si-doped single crystals of β-$(Al,Ga)_2O_3$ with positron annihilation spectroscopy [3].

We present results obtained in 8 different (16 pieces) Czochralski-grown β-$(Al,Ga)_2O_3$ single crystals with Al content 0, 10, 20, and 25%, in both undoped and n-type doped form [2]. The unintentional Si content in the undoped crystals is $2 - 3 \times 10^{17}$ cm^{-3}, and in the doped crystals the Si content is $3 - 6 \times 10^{18}$ cm^{-3} as measured by secondary ion mass spectrometry. Hall measurements show that the undoped crystals are n-type for all Al mole fractions with the carrier concentration roughly matching the unintentional Si content, but in the Si doped crystals the doping efficiency is reduced at higher Al content, and the doped 25% alloy is electrically insulating [2]. The overall 3D anisotropy of the Doppler broadening signals [4] is significantly smaller for all Si doped samples irrespective of the Al content. The undoped samples show the usually high anisotropy observed in β-Ga_2O_3 for all Al contents. In addition, the average positron lifetime is significantly longer in the Si-doped samples for all Al contents, in the 207-214 ps range, compared to 176-185 ps in the undoped samples. Importantly, the positron data do not depend on the Al content in the Si doped samples.

The results indicate that Si doping generates unrelaxed Ga vacancy related defects as opposed to the split Ga vacancies that typically dominate the positron annihilation signals in β-Ga_2O_3 [4-6]. However, these unrelaxed Ga vacancies do not appear to be the key to understanding to the sudden strong passivation of the Si dopants at higher Al content, as there appear to be no significant differences between the Si doped samples across the Al content range in our preliminary experiments. Further work is required to resolve this issue.

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Poster presentations

1. Giovanni Alfieri, Hitachi Energy: "Deep levels in epitaxially grown 4H-SiC p+-i-n diodes"

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The use of homoepitaxial p^+-i-n 4H-SiC wafers, plus reactive ion etching (RIE) for the delimitation of the anodes areas, is often preferred to Al^+ ion implantation for anode fabrication in n-type 4H-SiC bipolar diodes. The reason is that implantation leads to the formation of rather high concentrations of electrically active levels at the implant tail, like lifetime killer defects, e.g. carbon vacancy (V_C).

Several techniques for the removal of V_C have been proposed in the past. However, their integration in the process flow of bipolar devices, either epitaxial or ion implanted, is still challenging. An alternative is tuning the parameters of 4H-SiC epitaxial growth in order to achieve low [V_C] in the bipolar diodes drift layer.

In this study, we analyze the presence of those point defects controlling the electrical performances of epitaxial 4H-SiC p^+-i-n diodes of recent production. We have used epitaxial 4H-SiC p^+-i-n vertical diodes fabricated using very thick (around hundreds of microns) and very low doped ($\sim 10^{14}$ cm^{-3}) drift layer. No V_C removal process was employed. The characterization of the electrically active defects was carried out by deep levels transient spectroscopy (DLTS).

DLTS measurements were carried out in the 100-650 K temperature range using a reverse bias of -3V and a pulse voltage in the +3 V for 1 ms for the detection of majority carriers traps while a pulse voltage of 8 V was employed for the detection of minority charge carrier traps.

DLTS measurements reveal the presence of several electrically active levels in the 0.3-1.6 eV energy range, below the conduction band edge E_C. In particular, we observe the presence of the $Z_{1/2}$ level (the doubly negative charge state of V_C), with a concentration of $8x10^{11}$ cm^{-3}. Another level, visible as a shoulder DLTS peak next to that of the $Z_{1/2}$, is also detected (E_C-0.7 eV, 10^{12} cm^{-3}), similarly to other epitaxially grown 4H-SiC p^+-i-n diodes. This level might be associated to the one found in dry etched n-type 4H-SiC epilayers. Two major DLTS peak at 0.38 and 0.5 eV below E_C, that have not been reported elsewhere, are also found. Such traps do not show any electric field dependence of the emission rates, meaning that they can be associated to acceptor traps. Further investigations are being carried out in order to understand their nature.

Analysis of the minority carrier traps show the presence of the shallow B-acceptor and of the D-center, which has been recently identified as a deep B-acceptor. Both levels show rather high concentrations in the 10^{13} cm^{-3} range. In addition, two minor levels are also found close to both the shallow and deep B levels, with concentrations in the 10^{12} cm^{-3} range. One in particular can be associated to the IP1 level found in dry etched p-type 4H-SiC which, in turn, was found to be the same as the UK1 level detected in electron irradiated material.

2. Pejk Amoroso, Univ. Helsinki: “Point Defects in Ga-doped Ge”

Pejk Amoroso[1], Waldemar Särs[1], Jonatan Slotte[1, 2], Filip Tuomisto[1], Radhakrishnan Sumathi[3], Kenichiro Mizohata[1], Aravind Subramanian[3]

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P-type Ge has been researched very little using Positron Annihilation Spectroscopy due to the low sensitivity of the method to positively charged defects. Here, we studied highly Ga-doped bulk Ge, with the doping concentration ranging from 10^{18} to 10^{20} cm^{-3}. The bulk crystals were grown by the Czochralski method. The samples were irradiated with 6 MeV protons at room temperature with a fluence of 1×10^{14} cm^{-3} and upwards, thus introducing vacancy defects into the lattice. The vacancy defect distribution was studied using both Positron Annihilation Lifetime Spectroscopy and Doppler Broadening Spectroscopy. The lifetime setup consisted of two collinear detectors with BaF_2-scintillators and quartz-windowed photomultiplier tubes, with a resolution of 282 ps, and the Doppler broadening was measured using a high-purity Ge detector. A conventional ^{22}Na positron source was used. The positron lifetime and Doppler broadening results will be presented in this poster.

3. João P. Castelo-Branco, Univ. Coimbra: “Role of the interfacial defect layer in chalcopyrite solar cells studied through electrical modelling”

João P. Castelo-Branco[1], Helena V. Alberto[1], Rui C. Vilão[1], João M. Gil[1], André F. Violas[2, 3], Jennifer P. Teixeira[2], Paulo A. Fernandes[2, 3, 4], Pedro M. P. Salomé[2, 5], Alois Weidinger[6]

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Solar cell modelling is a valuable tool to obtain insight on the relation between microscopic physical parameters and macroscopic measurements, namely efficiency and current-voltages J-V curve parameters.

Predefined, baseline parameters for electrical modeling of $Cu(In,Ga)Se_2$ (CIGS) solar cells have been proposed [1,2] using the Solar Cell Capacitor Simulator (SCAPS) software. The development of these baseline models confirms the need to include an interfacial defect layer (SDL) in CIGS, near the p-n interface. However, many of the parameter values used in the proposed models are not well known. Updates using new experimental data are necessary for the continuous improvement of these models.

Recent experimental results, using a probe sensitive to structural disorder [3] indicate that the width of the surface defect layer at the CIGS near-interface region is larger than considered in the existing baseline models. In addition, the interpretation of the experimental results suggests that charge mobility and density of some defects may be key factors for the role of the interface defect layer in the solar cell performance.

In this work, simulations using SCAPS software were performed, using as a starting point the baseline for ultrathin CIGS solar cells proposed by Violas et al. [2]. The effect of selected physical parameters in the SDL on the solar cell efficiency and I-V curve parameters is presented and discussed.

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4. Weiru Chen, Dartmouth College: "First-principles investigations of quantum defects in two-dimensional transition metal dichalcogenides"

Weiru Chen[1], Yihuang Xiong[1], John Thomas[2], Archana Raja[2], Alexander Weber-Bargioni[2], Geoffroy Hautier[1]

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The availability of reliable quantum defects is a key component towards realizing quantum information science applications. Two-dimensional (2D) materials such as transition metal dichalcogenides (TMDs) emerge as a promising platform to host such defects owing to their intrinsic quantum confinement nature, long expected spin coherence time and strong spin-orbit coupling (SOC). Here we present our study on two common point defects in monolayer tungsten disulfide (WS_2): vacancies and carbon substitutions. By taking into account the nonunique exact exchange fraction in low dimensional materials[1], we employ hybrid functionals with SOC to examine the thermodynamic stabilities and the electronic structures of these two defects. Our results on their optical properties, combined with experimental characterizations, shed light on future endeavors towards studying and fabricating quantum defects in TMDs.

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5. Henry Fried, Univ. Luxembourg: "Tight-Binding Modeling of Point Defects: A Machine Learning Approach for Predicting Parameters"

Henry Fried[1], Daniel Barragan-Yani[1], Christoph Schattauer[2], Florian Libisch[2], Ludger Wirtz[1]

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In recent years, there has been significant progress in calculating the optical properties of defects. Ab-initio calculations in the supercell approach offer valuable insights, even within the single-particle framework. Moreover, ab-initio many-body perturbation theory is feasible for simple systems and small supercells. However, these approaches still struggle to capture complex questions such as the strain dependence of optical properties. Tight-binding models can address this limitation. Nevertheless, accurate modelling of defect levels and their optical signature requires many parameters and a detailed understanding of the distance-dependence of hopping parameters. Our work takes the first step towards developing a machine learning algorithm that predicts defect tight-binding parameters. By utilizing the Green's function and local density of states obtained from pristine crystal tight-binding parameters, we are able to describe the local potential induced by the defect and its impact on the neighboring atoms and their parameters. Our algorithm predicts parameters based on the ab-initio local density of states on the defect site and its neighbors. This offers two key advantages over current methods. Firstly, scalability: the use of density of states (instead of folded band structures) allows for larger supercell sizes and systems with complex band structures, eliminating the need for band disentanglement. Secondly, once trained, the machine learning algorithm can predict tight-binding parameters for different point defects within the same material. This opens up new possibilities for understanding the optical properties of point defects.

6. Helton Goncalves de Medeiros, ETH Zurich: "Raman spectroscopy study of defects near the SiO_2-SiC interface and their correlation to electrically active defects"

Helton G. de Medeiros[1], Marianne E. Bathen[1], Piyush Kumar[1], Maria I. M. Martins[1, 2], Ulrike Grossner[1]

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Silicon carbide (SiC) is a wide band gap (WBG) material with material properties that make it a suitable candidate to replace silicon (Si) devices in power semiconductor applications [1]. One of the advantages of 4H-SiC over other WBG materials is that it has SiO_2 as its native oxide. However, the different stoichiometry of SiO_2/SiC compared to SiO_2/Si causes the SiC counterpart to contain more interface defects. The nature of such interface defects is still heavily discussed and silicon vacancies [2], dangling bonds, and carbon-based precipitates [3] are some of the candidates. These interface defects have been related to a reduction in the electron mobility in 4H-SiC MOSFETs. Therefore, understanding the nature of interface defects is important for further improvement of the SiO_2/SiC based interface system.

In the present work, a series of four samples with similar oxidation processes and distinct post-oxidation annealing (POA) parameters is used to investigate the defects created at and near the SiC/SiO2 interface. All samples were thermally oxidized at 1300 ◦C and exposed to either no POA, POA in NO at 1150 ◦C or 1300 ◦C, or POA in Ar at 1300 ◦C. A comparable sample set showed a reduction in Dit after NO annealing that was associated with a passivation of Si vacancies [2].

We will present transmission electron microscopy (TEM) data that shows extended regions (some nm) in the SiC lattice where Si atoms are missing after thermal oxidation. In other words, carbon-rich regions are formed in the SiC lattice. Carbon species are commonly studied with Raman Spectroscopy where their vibrational states such as sp^2 and sp^3 can be investigated [4]. The 4H-SiC presents first and second-order Raman features, where the second-order features are located in the same spectral region as commonly observed Raman signatures for carbon species. This makes the study of such signatures a challenge. Previous works have used confocal Raman and Surface Enhanced Raman Spectroscopy (SERS) and subtracted the spectra of the thermally oxidized SiC/SiO_2 sample from spectra from a reference 4H-SiC sample to identify interface-related features [3].

Since Raman Spectroscopy is a surface-sensitive technique, the majority of the thermally grown oxide will be removed to leave only a few nanometers, enabling the study of interface near defects. Raman spectra from the reference sample will be compared to the thermally oxidized samples at different excitation wavelengths. In addition, gold thin films will be deposited and annealed to form nanoparticles that will act as nanoantennas that locally enhance the electric field, which will enable the identification of species present at low concentrations such as carbon species. The results from this study are expected to build up the understanding of the interface defects created during the thermal oxidation process.

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7. Ylva Hommedal, Univ. Oslo: "Diffusion of Ge in β-Ga_2O_3"

Ylva Knausgård Hommedal[1], Ymir Kalmann Frodason[1], Lasse Vines[1], Klaus Magnus Johansen[1]

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The unique combination of and ultra-wide bandgap (high breakdown field), inherent *n*-type conductivity through doping, and availability of high-quality melt-grown substrates has made beta-phase gallium oxide (β-Ga_2O_3) highly interesting as a semiconductor for high-power electronics with reduced power loss compared to current technology. To fulfill this potential and develop β-Ga_2O_3, it is important to understand and predict the diffusion of impurities that can be utilized as dopants, such as Sn and Si (donors) or Fe, Mg, and Zn (acceptors).

In a recent study by Frodason *et al.,* diffusion of Sn in β-Ga_2O_3 was studied using both experimental and computational techniques. [1] The Ga-substitutional Sn (Sn_{Ga}) was found to bind to a Ga vacancy (V_{Ga}) and form a mobile complex that diffuses with a migration barrier of 3.0±0.4 eV. V_{Ga} is thus needed for Sn to diffuse and because the fermi level influences the concentration of V_{Ga} in β-Ga_2O_3, the diffusion of Sn in β-Ga_2O_3 is fermi-level dependent. Ge is a single donor like Sn, and we expect Ge to diffuse with a similar mechanism that can be explained with a fermi level-dependent vacancy-mediated reaction-diffusion (RD) model. In the present work, we have studied the diffusion of Ge, which substitutes on the Ga site (Ge_{Ga}) and acts as a shallow single donor in β-Ga_2O_3 [2].

Ge was introduced to unintentionally doped (UID) and Sn-doped (-201) β-Ga_2O_3 by ion implantation with a dose of 1×10^{16} cm^{-2} and an energy of 450 keV. The samples were then heat treated to temperatures of 900-1050°C in air. Using Secondary Ion Mass Spectrometry (SIMS), we measured the Ge concentration as a function of depth. The concentration profiles show that Ge diffused up to 5 μm in this temperature range. The diffusion length is the same in the UID and Sn-doped samples, however, the shapes of the diffusion profiles are slightly different. The Ge profiles in the UID samples resemble an error function while the Sn-doped samples have less curved profiles compared to the UID samples.

We simulated the concentration profiles using the RD model to extract the diffusivity and in turn find migration barriers and binding energies for the two types of samples. Migration energy, binding energies, and formation energies for relevant defects were calculated using first-principles calculations with hybrid functionals and compared to the experimental values. The results were compared to the results on Sn diffusion in β-Ga_2O_3.

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8. Jesse Huso, Klar Scientific: “Photoluminescence mapping of defects in semiconductors”

Jesse Huso[1], Violet Poole[1], Rick Lytel[1], Matthew McCluskey[2]

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Photoluminescence (PL) spectra with high spatial resolution provide insight into semiconductor defects, inhomogeneous composition, and surface imperfections. The method serves as a valuable tool for failure analysis. Typical PL spectroscopy is not spatially resolved. Excitation photons impinge on a sample; emitted light is collected by a spectrometer. Spatial variations get averaged into one overall spectrum. This approach is adequate for a homogeneous sample but there are many instances where one requires a spectrum at each (x,y) point on the surface as well as the ability to visualize the data.

This poster presents PL mapping of several key semiconductor materials, with excitation wavelengths ranging from 266 to 975 nm. The sample is scanned in the x-y plane and emitted light is collected by an Ocean Optics spectrometer (detection ranges encompass 200 to 1700 nm). This system yields a map that covers an area as large as 100 × 100 mm. Analysis software performs rapid peak fitting on each spectrum and displays the data in a false-color image. An autofocusing routine analyzes the laser spot and adjusts the objective height to keep the laser spot in-focus on the sample surface, ensuring diffraction-limited resolution.

9. Grace McKnight, Univ. Illinois: “Investigation of oxygen interstitial diffusion pathways in β-Ga_2O_3”

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Monoclinic β-Ga_2O_3 is a highly stable wide band gap semiconductor that exhibits a wide spectrum of complex defects. Understanding the diffusion of these defects may help elucidate some active degradation pathways and understand degradation mechanisms in high-performance power electronics based on Ga_2O_3. While recent computational studies have investigated the diffusion of intrinsic defects including Ga interstitials and Ga and O vacancies as well as extrinsic defects like Si and Sn interstitials, the diffusion of O interstitials has received comparatively less attention. This is because, in many oxide semiconductors, O and H interstitials are believed to exhibit faster diffusion than other types of cation interstitials or vacancies, owing to their low diffusion barriers and small ionic sizes, making them highly mobile within the material. However, high anisotropy of the monoclinic crystal structure of β-Ga_2O_3 implies significant variations in the diffusion coefficients along different crystallographic directions. In this study, we aim to (1) understand the complete diffusion mechanism of oxygen interstitials and (2) predict directionality in diffusivity of oxygen interstitials in β-Ga_2O_3 from first principles calculations based on total energy density functional theory. We first explore all possible configurations of oxygen interstitials including extended structures, such as O interstitials split into two or three O sites, and their respective formation energies. Interstitial structures for both charged and neutral β-Ga_2O were identified by the Voronoi tessellation method and from literature of anion defects in monoclinic crystals. We then grouped the sites of identified O interstitials based on their bonding environment and space configurations within the unit cell, resulting in several groups of unique sites where split interstitials are stable. After identifying preferred sites for split interstitials, we construct a three-dimensional diffusion network by connecting these sites via hops, resulting in a total of 16 unique hops. The migration barriers of these unique hops are obtained by the climbing image-nudged elastic band method (CI-NEB). Additional low-energy configurations discovered along the migration path are incorporated into the network for further analysis, allowing us to isolate and investigate each elementary jump between the lowest-energy configurations.The migration paths and barriers of the diffusion network are used to construct and then solve the master diffusion equations, resulting in highly anisotropic Onsager transport coefficients, which illuminate the most dominant pathways in each crystallographic direction. Our study provides valuable insights into the migration of O interstitials, which contributes to the further development and characterization of β-Ga_2O_3 based applications.

10. Michael Reshchikov, Virginia Commonwealth Univ.: "Dual nature of the Li_{Zn} acceptor in ZnO"

Michael Reshchikov[1]

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First-principles calculations predict the dual nature of acceptors in semiconductors [1]. In particular, the Li_{Zn} acceptor in ZnO is expected to have a deep (polaronic) state at 0.64 eV and a shallow state at 0.21 eV above the valence band maximum (VBM) [1]. In photoluminescence (PL) experiments, the orange luminescence (OL) band with a maximum at 2.0 eV is attributed to the Li_{Zn} defect. Two deep polaronic states of the Li_{Zn} acceptor, separated by 34 meV, were studied by

luminescence and electron paramagnetic resonance [2,3]. From the analysis of the OL band shape and from its quenching with temperature, the -/0 level of the deep Li_{Zn} state was found with a large uncertainty (0.4-0.86 eV above the VBM [4]). In addition, Li-doped ZnO samples showed PL from a shallow acceptor, with the main peak at 3.05 eV at $T = 4.2$ K, attributed to a hydrogen-containing complex such as Li_{Zn}-H-Li_{Zn} [5].

We studied PL from ZnO grown by hydrothermal method. The OL1 band was quenched above 250 K, similar to its behavior in other ZnO:Li samples. Interestingly, at $T > 150$ K a shoulder at the high-energy side (up to 3.1 eV) of the OL1 band emerged. The ratio of PL intensities at 3.0 eV and 2.0 eV increased exponentially (over two orders of magnitude) with temperature and revealed an activation energy of 0.18 eV. We attribute the PL signal at 3.0 eV to transitions from the conduction band to the shallow state of the Li_{Zn} acceptor. A phenomenological model for a dual-nature acceptor suggests that the found activation energy is equal to the energy difference between the deep and shallow states of the Li_{Zn} (predicted to be 0.43 eV in [1]). The shallow state is located at 0.3-0.4 eV above the VBM and two deep polaronic states are at 0.5-0.6 eV above the VBM. The phenomenological model also predicts that PL from the shallow state may be observed at very low temperatures, and the band observed in [5] could be caused by this state. This PL may disappear at elevated temperatures ($T > 10$ K) due to the transition of captured holes from the shallow state to a deep state over a low potential barrier. At $T > 150$ K it emerges thanks to the thermal excitation of holes from a deep state to the shallow state. We observed very similar transformations in PL from Be-doped GaN, where Be_{Ga} has been proven to be a dual-nature acceptor, in agreement with theoretical predictions [1].

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11. Michael Reshchikov, Virginia Commonwealth Univ.: "Photoluminescence from GaN implanted with Be, F, and Cl ions"

Michael Reshchikov[1], Oleksandr Andrieiev[1], Mykhailo Vorobiov[1], Denis Demchenko[1], Benjamin McEwen[2], Shadi Shahedipour-Sandvik[2]

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Point defects in GaN are still not well understood. We used photoluminescence (PL) to identify defects in GaN implanted with various impurities. Undoped and Si-doped GaN wafers were grown by hydride vapor phase epitaxy on sapphire substrates. Alternatively, GaN unintentionally doped with carbon was grown on sapphire by metalorganic chemical vapor deposition. The as-grown GaN wafers were implanted with Be, F, and Cl ions. In addition, sequential implantation of Be and F ions at 600 °C was conducted. After the implantation, the samples were annealed at temperatures between 900 and 1000 °C. PL spectra from Be-implanted GaN contained the yellow band (YL_{Be}) assigned to the isolated Be_{Ga} acceptor. This defect has characteristic properties, namely, two deep states at about 0.3 eV and a shallow state at 0.2 eV above the valence band (VBM), that determine the behavior of the PL. Another Be-related shallow acceptor (0.113 eV above the VBM) causes a relatively narrow PL band at 3.38 eV followed by a few LO phonon replicas. In GaN samples co-doped with Be and F, two new PL bands appeared when the concentration of F exceeded that of Be. The orange luminescence (OL1) band with a maximum at 1.9 eV was observed in semi-insulating GaN:Be,F samples. The red luminescence (RL5) band with a maximum at 1.6 eV appeared in conductive n-type GaN:Be,F samples. The OL1 and RL5 bands were also found in GaN implanted with only F, semi-insulating and conductive n-type samples, respectively. PL bands from GaN implanted with Cl ions significantly overlapped. However, deconvolution using known shapes of PL bands indicates the presence of PL bands similar to the OL1 and RL5. We conclude that the OL1 and RL5 bands are not related to Be and are unlikely caused by F or Cl defects. These bands could be caused by some native defects or complexes created by ion implantation.

12. Rokas Silkinis, Center for Phys. Sci. & Tech., Vilnius, Lithuania: “Theoretical modeling of vibrationally resolved optical lineshapes of a carbon-oxygen pair defect in silicon”

Rokas Silkinis[1], Marianne Etzelmüller Bathen[2], Audrius Alkauskas[1], Lukas Razinkovas[1]

[1]Center for Physical Sciences and Technology (FTMC), Vilnius, Lithuania, [2]Advanced Power Semiconductor Laboratory, ETH Zürich, Zürich, Switzerland

In recent years, quantum technologies have been at the forefront of scientific interest due to various possible applications in quantum sensing, communication, and computing. Given its history of commercial and practical success as an essential part of solid-state devices, silicon is a rational choice as a host material for future quantum technologies. Optically active point defects are of particular interest as single-photon emitters that could be used for short- and long-distance exchange of information. The C-center, composed of a carbon-oxygen interstitial pair (C_iO_i), is one such defect. It emits light at telecom wavelengths of 1570 nm (0.789 eV) and is thus a suitable candidate for a telecom-range single-photon source that is compatible with fiber-optic technology.

This work presents a first-principles computational study of the luminescence and absorption lineshapes associated with the C-center in silicon. We perform density functional theory (DFT) calculations with a semilocal functional based on the meta-generalized gradient approximation (meta-GGA), in particular, the recently developed SCAN (Strongly-Constrained and Appropriately-Normed) functional. Using a novel embedding methodology, we obtain optical emission and absorption lineshapes of the defect in the dilute limit. Our results show a close agreement to the experimentally observed luminescence lineshape, while the absorption lineshape data could be used as a guide for further experimental analysis of the C-center. Finally, we discuss the calculated vibrational features in light of the C-center being a Rydberg-like center.

13. Vytautas Žalandauskas, Center for Phys. Sci. & Tech., Vilnius, Lithuania: “Ab initio study of vibrational properties of divacancy defects in 4H-SiC”

Vytautas Žalandauskas[1], Marianne Etzelmüller Bathen[2], Lukas Razinkovas[1]

[1]Center for Physical Sciences and Technology (FTMC), Vilnius, Lithuania, [2]Advanced Power Semiconductor Laboratory, ETH Zürich, Zürich, Switzerland

Silicon carbide (SiC) is a wide bandgap material with great potential for high-power and high-frequency electronic devices. Furthermore, certain deep-level semiconductor defects have potential applications as qubits and single photon emitters for quantum technologies (QT). SiC hosts a wide variety of defects with QT-compatible properties. In multi-component semiconductors, such as SiC, these defects can often inhabit several configurations with different characteristics. Therefore, a detailed characterization of different defect configurations and their electro-optical properties is essential.

Our study employed first-principles calculations to study four neutral divacancy configurations (*hh*, *kk*, *hk*, and *kh*) and their vibrational properties in the 4H-SiC polytype. The labels *h* and *k* refer to the distinct hexagonal and pseudo-cubic lattice sites in 4H-SiC, respectively. Using the r^2SCAN density functional, we have determined the zero-phonon line (ZPL) energies and zero-field splitting (ZFS) values, which are in close agreement with experimental data. Furthermore, we calculated the spectral functions of electron-phonon coupling using a novel embedding methodology. The calculated luminescence lineshapes provide excellent agreement with the experimental data. Additionally, the obtained absorption cross-sections give a comprehensive picture of the contributions of each neutral divacancy defect configuration to the observed photoluminescence spectra.

14. Shimin Zhang, Univ. Wisconsin-Madison: "Advanced Simulations of Spin defect in hBN: Strain and substrate effect, ODMR and Quantum Embedding theory"

Shimin Zhang[1], Kejun Li[1], Yuan Ping[2]

[1]University of California, Santa Cruz, [2]University of Wisconsin, Madison

Advanced Simulations of Spin defect in hBN: Strain and substrate effect, ODMR and Quantum Embedding theory

Shimin Zhang, Kejun Li, Yuan Ping

University of California, Santa Cruz

Spin defects in hexagonal boron nitride (hBN) have been proposed as promising spin qubits, which are fundamental components for quantum information technologies. We have applied advanced simulation methodologies to explore the optoelectronic properties of these defects. In first part we study the impact of strain and substrate on optoelectronic properties of single-photon emitters (SPEs) in hBN. The second part focuses on the spin-photon interface, where we have developed a methodology for simulating Optically Detected Magnetic Resonance (ODMR) processes, specifically the ODMR contrast. In the third part, we apply the advanced Quantum Defect Embedding Theory (QDET) to simulate the correlated excited state of spin defects. Our research on these three important aspects of the spin defects provides critical guidelines for the future experimental investigation in the field of quantum spin defects.

Tuesday, September 12th

Plenary Session – Swan Ballroom

Chairperson: Kai-Mei Fu, University of Washington

8:30-9:15 AM “Defects and diffusion in β-Ga_2O_3”

Lasse Vines[1], Ymir K Frodason[1], Ylva K. Hommedal[1], Klaus Magnus Johansen[1], Augustinas Galeckas[1], Joel Varley[2], Chris G. Van de Walle[3]

[1]University of Oslo, [2]Lawrence Livermore National Laboratory, [3]University of California, Santa Barbara

Gallium oxide (Ga_2O_3) is an ultra-wide bandgap semiconductor that is currently under intensive investigations due its intriguing fundamental properties with potential prospects in power electronics and UV devices. Essential to this development is defect control and precise dopant distributions, which relies on a solid understanding of the role of defects in dopant diffusion. In particular, the gallium vacancy (V_{Ga}) plays a key role in diffusion of several important dopants. We recently showed that V_{Ga} can transform between its different split configurations, where an intermediate state that consists of a vacancy split between three Ga sites, a three-split vacancy, enables passage over a significantly lower energy barrier compared to what has previously been reported[1]. Moreover, the strong Fermi level dependence of the formation energy of V_{Ga} has a strong impact on the diffusivity of dopants.

In this contribution, we will discuss the interplay between defects and diffusion of dopants in β-Ga_2O_3, where we combine first-principles defect calculations with diffusion modeling to describe the concentration vs depth of the dopants measured by secondary ion mass spectrometry (SIMS). For example, migration of Sn, a typical donor, was studied in an epitaxially grown layer using the bulk Sn doped substrate as a source [2]. Calculated formation energies of Sn-related and intrinsic defects show that the migration of Sn is mediated by V_{Ga} through the formation and dissociation of intermittent mobile $V_{Ga}Sn_{Ga}$ complexes. Building upon this we can construct a reaction-diffusion model that well describes the evolution of the Sn concentration with depth after heat treatments.

Zn has been proposed as a potential acceptor dopant, and can be introduced into β-Ga_2O_3 by exposing samples to vaporized Zn in a sealed quartz ampules[3]. Based on comparison between our diffusion model parameters and values obtained from first-principles calculations, we propose a physical model for the diffusion of Zn in β-Ga_2O_3, where Zn diffuses through a split interstitial mechanism and is limited by trapping through the formation of a Zn_iZn_{Ga}-donor complex. The donor complex can dissociate into the acceptor state Zn_{Ga} and the mobile donor state Zn_i. Further dissociation of Zn_{Ga} is effectively prevented by a large binding energy. This model is further supported by photoluminescence measurements, where a signature around 2.5 eV is proposed to be associated with Zn_{Ga} in samples first treated in Zn vapor to introduce the Zn_iZn_{Ga}-donor, and later annealed at high temperature in an oxygen ambient to convert the donor complex into Zn_{Ga}. Diffusion and complex formation of other dopants will also be discussed.

[1] Frodason et al., Phys. Rev. B, 107, 024109 (2023)
[2] Frodason et al., APL Mater. 11, 041121 (2023)
[3] Hommedal et al., Phys. Rev. Mater. 7, 035401 (2023)

9:15-10:00 AM

"Piecewise Linearity Condition for Addressing the Self-Interaction of Polarons"

Alfredo Pasquarello

École Polytechnique Fédérale de Lausanne

The piecewise linearity condition is a property satisfied by the exact density functional and has been found to yield band gaps in accord with experiment [1,2] when imposed to hybrid functionals. Here, we address the self-interaction in relation to polarons in density functional theory. The self-interaction can be corrected focusing on its one-body form like it appears in Hartree-Fock theory or through the enforcement of the piecewise linearity condition, also referred to as the correction of the many-body self-interaction. We develop a unified theoretical framework encompassing one-body and many-body forms of self-interaction [3,4]. In this way, we establish a quantitative connection between the two forms of self-interaction, by which the many-body form is seen to account for the effect of electron screening [3,4]. In our investigation, we consider widely used functionals such as the global hybrid functional PBE0(α) [3-6], and the Hubbard-corrected functional DFT+*U* [5,6], as well as a newly developed semilocal scheme, called γ-DFT, which involves the use of a weak localized potential [3,4,6]. The enforcement of the piecewise linearity condition is achieved by imposing the generalized Koopmans' condition to the neutral and charged states of the polaron upon proper consideration of finite-size effects induced by the lattice polarization [7]. The polaron properties are found to be robust upon variation of the functional, including charge densities [3-6], structural distortions [3-6], formation energies [3-6], energy barriers [6], hyperfine and superhyperfine parameters [6], and charge hopping rates [6].

Work done in collaboration with S. Falletta.
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[4] S. Falletta and A. Pasquarello, Polarons free from many-body self-interaction in density functional theory, *Phys. Rev. B* **106,** 125119 (2022).
[5] S. Falletta and A. Pasquarello, Hubbard *U* through polaronic defect states, *npj Comput. Mater.* **8**, 265 (2022).
[6] S. Falletta and A. Pasquarello, Polaron hopping through piecewise-linear functionals, *Phys. Rev. B* **107**, 205125 (2023).
[7] S. Falletta, J. Wiktor, and A. Pasquarello, Finite-size corrections of defect energy levels involving ionic polarization, *Phys. Rev. B* **102**, 041115(R) (2020).

10:00-10:20 AM **Coffee break**

Parallel Sessions

2D materials (II) – Swan Ballroom

Chairperson: Shawna Hollen, University of New Hampshire

10:20-10:40 AM “Optical and structural characterization of electron-beam treatments of hexagonal boron nitride”

Jordan Gusdorff[1, 2], Rachael Keneipp[3], Pia Bhatia[3], Marija Drndić[3], Lee Bassett[1]

[1]Quantum Engineering Laboratory, Department of Electrical and Systems Engineering, University of Pennsylvania, [2]Department of Materials Science and Engineering, University of Pennsylvania, [3]Department of Physics and Astronomy, University of Pennsylvania

Hexagonal boron nitride (hBN) hosts quantum emitters that exhibit bright single photon emission and spin-dependent fluorescence at room temperature. These features make hBN a promising platform for quantum sensing and photonics. Despite many investigations of their optical properties, the emitters’ chemical nature remains unclear. We use confocal photoluminescence (PL) microscopy and aberration corrected scanning transmission electron microscopy (AC-STEM) to analyze fluorescent emission and atomic structure, respectively. In addition to providing atomic-resolution imaging, AC-STEM enables defect creation down to the nanometer scale through targeted electron-beam drilling. PL imaging is used to characterize changes in the optical signal—both localized and extended—following the material’s exposure to the electron beam. Both PL and AC-STEM imaging can be employed to monitor the effects of treatments, such as annealing. These characterization methods advance our understanding of the material’s morphology and defect chemistry, while

providing insight into the controllable creation of desirable defects in hBN.

10:40-11:00 AM “Room-temperature optical and spin dynamics of a single quantum emitter in hexagonal boron nitride”

Rebecca Fishman[1], Raj Patel[1], Tzu-Yung Huang[1], Jordan Gusdorff[1], David Hopper[1], S. Alex Breitweiser[1], Benjamin Porat[1], Lee Bassett[1]

[1]University of Pennsylvania

Hexagonal boron nitride (hBN) is a wide bandgap, two-dimensional van der Waals material that is known to host pure, single-photon emitters. Recent observations of ODMR and spin resonance in hBN and efforts to understand hBN emitters' optical dynamics [1] have represented progress toward hBN spin defects as a platform for quantum devices. We report on a single spin defect in hBN exhibiting optically detected magnetic resonance, and we propose a model for its electronic structure and optical dynamics. Using photon emission correlation spectroscopy in conjunction with time-domain optical and microwave experiments, we establish key features of the electronic model. Specifically, we propose a spinless optical ground and excited state along with a metastable spin-½ state and an additional dark state. We then employ optical dynamics simulations to constrain and quantify various transition rates in the model in accordance with the observed experimental results. By establishing a potential model, we take a necessary step toward quantum control of spin states in hBN.

[1] Patel et al. PRX Quantum 3, 030331 (2022)

11:00-11:20 AM “Defect spins and qubits in hexagonal boron nitride from first principles theory guiding experiments”

Song Li[1], Anton Pershin[1], Péter Udvarhelyi[1], Viktor Ivády[2], Ádám Gali[1]

[1]Wigner Research Centre for Physics, Budapest, Hungary, [2]Eötvös Loránd Science University, Budapest, Hungary

We have recently developed first principles techniques for theoretical microscopy and spin control of point defects in semiconductors and insulators [1]. We have applied these techniques to several point defects in hexagonal boron nitride (hBN) that are relevant in real hBN materials. We proposed to apply the negatively charged boron-vacancy to realize qubits [2,3]. This center was indeed later observed in experiments [4]. We have recently simulated the coherence time and Rabi-oscillation of this center with showing an entanglement between the electron spin and the first three neighbor ^{14}N spins [5,6]. We have recently identified the coupling of the electric field and the strain to the electron spin in the ground state of the center with quantifying the theoretical sensitivity limits and interpreting the optically detected magnetic resonance (ODMR) spectrum of ensembles [7,8]. We identified an oxygen-related electron paramagnetic resonance center in hBN which produces 2-eV emission with relatively small phonon sideband [9]. Furthermore, we proposed two types of ultraviolet (UV) emitters in hBN: (i) the 5-7 Stone-Wales defects [10] and (ii) the carbon-pair defect structures with the most stable form of a carbon ring [11]. We shall show how the optical properties of the UV emitters may drastically change upon stacking sequences of hBN layers.

[1] Á. Gali, Nanophotonics, 8, 1907 (2019); *ibid* 12, 359 (2023).
[2] M. Abdi *et al.*, ACS Photonics 5, 1967 (2018).
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[4] A. Gottscholl *et al.*, Nature Materials, 19, 540 (2020).
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[6] W. Liu *et al.*, Nature Communications 13, 5713 (2022).
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[8] A. Durand *et al.*, arXiv:2304.12071 (2023).
[9] S. Li & A. Gali, The Journal of Physical Chemistry Letters 13, 9544-9551 (2022).
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[11] S. Li *et al.*, The Journal of Physical Chemistry Letters 13, 3150 (2022).

This work was supported by the National Research, Development, and Innovation Office of Hungary (NKFIH) grant No. KKP129866 of the National Excellence Program of Quantum-coherent materials project and the Quantum Information National Laboratory supported by the Cultural and Innovation Ministry of Hungary (grant No. 2022-2.1.1-NL-2022-00004).

11:20-11:40 PM “Controlled generation of spin defects in hexagonal boron nitride for quantum sensing applications”

Aqiq Ishraq[1], Muhammad Hassan Shaikh[2], Collin Maurtua[1], Shahidul Asif[1], Saurabh Lamsal[2], Mark Ku[1, 2], Chitraleema Chakraborty[1, 2]

[1]Department of Materials Science and Engineering, University of Delaware, [2]Department of Physics and Astronomy, University of Delaware

Quantum sensing allows us to understand how we interact with the world around us by detecting small changes in electric or magnetic fields and other physical quantities with superior accuracy over classical sensing techniques. This is possible as quantum sensors utilize quantum resources to analyze data at the atomic level, whereas classical sensors can only extract data from a large collection of atomic systems. The capability to sense subtle changes at the atomic level makes quantum sensors significantly more reliable and accurate. Until recently, quantum sensors were mostly restricted to the bulk of solid state materials, which included the bright NV^- centers in diamond and SiV in Silicon Carbide. Unlike bulk

solids, 2D materials have extremely high flexibility which will allow the device to conform to the shape of any subject - be it a human brain for bioimaging or a spintronics material platform thereby improving the resolution. Hexagonal boron nitride (hBN) is a wide band gap 2D material which can house color centers consisting of the negatively charged boron vacancy (V_B^-) defect which is optically active even at room temperature, and is biocompatible, making them very desirable especially for biomedical technologies. In this work we explore different techniques for fabricating and characterizing optically active spin defects in hBN as deterministic quantum emitters. We utilize a high energy electron beam of a standard e^- beam lithography system and high energy Xe ions from a standard focused ion beam source to bombard the surface of a few nm thick hBN flake to generate localized spin defects, particularly the V_B^- defects.

11:40-12:20 PM "Defects in atomically thin semiconductors for optical quantum technologies" *(invited presentation)*

Chitraleema Chakraborty

University of Delaware

Although defects in semiconductors can often be detrimental to device performance, they are also responsible for the breadth of functionality exhibited by modern optoelectronic devices. For example, defect centers in solids and quantum dots are currently being investigated for an ideal single photon emitter (SPE) platform for applications ranging from quantum information science to high-resolution sensing. However, despite the rapid progress in recent years, existing material platforms face several challenges, some of which are intrinsic to their host materials, motivating the search for SPEs in alternative platforms. For instance, self-assembled InAs quantum dots (QDs) are considered state-of the-art in terms of purity and indistinguishability, yet spatial and spectral inhomogeneity has prevented the development of large-scale arrays of identical emitters. On the other hand, defect-based emitters in wide bandgap insulators like diamond offer a more direct route toward site-controlled placement using defect engineering techniques, but they are more challenging to integrate with available photonic technologies, tend to have low photon extraction efficiencies, and are challenging to address electrically[1]. To this date, no SPE technology has met all the metrics required for scalable optical quantum information applications thereby prompting the need for exploring alternative material platforms[2]. In parallel to existing 3D platforms, optically active defects in two-dimensional (2D) semiconductors have unique advantages like atom-scale proximity for photonic and sensing applications, potential atom-scale imaging and deterministic placement using surface probe techniques and efficient electrical addresibility[3]. Their brightness and purity are comparable to more established solid-state emitters such as Indium Arsenide QDs and Nitrogen Vacancy (NV) centers in diamond. For example, 2D semiconductor SPEs generally emit photons

in the tens to hundreds of kHz range, which is comparable to some of the reported rates of NV centers in diamond[2]. Additionally, recent efforts on integrating WSe_2 SPEs with photonic and plasmonic cavities promise brighter emission with tens of MHz count rates, which would make them competitive with their QD-based SPEs counterparts in terms of brightness and purity[2] with the added advantage of electrical and strain control[4-8].
In this talk, I will share the story of the discovery and control of quantum emitters in two-dimensional materials defects and lattice deformations. The possibility of leveraging van der Waals heterostructure for charging these emitters with a single electron will be discussed. This lays the foundation for optically addressable spin qubits in flatland materials. Further, I will also discuss their potential in deterministic generation and scalable growth of 2D semiconductors, and integration with photonic and magnetic devices, which offers a compelling solution to scalable solid-state quantum photonics and sensing. This work opens the frontier of quantum optics in two-dimensional materials with the potential to revolutionize solid-state quantum devices.

[1] *Nature Photonics* **10**, 631-641 (2016).
[2] *Applied Physics Letters* **118**, 240502 (2021).
[3] *Nanophotonics* **8**, 2017-2032 (2019).
[4] *Nat. Nanotechnology* **10**, 507-511 (2015).
[5] *Nano Letters* (2018).
[6] *Nano Letters* **17**, 2253-2258 (2017).
[7] *Physical Review B* **99**, 045308 (2019).
[8] *Optica* **7**, 580-585 (2020).

Silicon carbide (I) – Sanibel

Chairperson: Evan Glaser, US Naval Research Laboratory

10:20-11:00 AM "Doping-induced color centers in silicon carbide" *(invited presentation)*

Marianne E. Bathen[1, 2], Brett C. Johnson[3], Augustinas Galeckas[2], Maria I. M. Martins[1], Piyush Kumar[1], Lukas Razinkovas[4], Lasse Vines[2], Ulrike Grossner[1]

[1]ETH Zurich, [2]University of Oslo, [3]RMIT, [4]FTMC

Point defects acting as color centers are receiving broad attention for applications within quantum computing, sensing, and communication. Single-photon emitters (SPEs) with emission energies in the near-infrared or telecommunication bands are of particular interest because of their compatibility with fiber optic technology. Silicon carbide (SiC) is a promising host platform for quantum emitters considering its favorable properties, including a wide band gap and availability of spin-zero isotopes, in combination with scalable fabrication. The continued growth of the SiC device industry, targeted towards energy-efficient power devices, can be beneficial for the future development of scalable SiC quantum devices.

SiC hosts a wide variety of intrinsic and extrinsic SPEs. Perhaps most studied are the silicon vacancy (V_{Si}) [1] and its counterpart, the carbon antisite-vacancy pair ($C_{Si}V_C$) [2], the divacancy ($V_{Si}V_C$) [3], and the nitrogen-vacancy or NV center (N_CV_{Si}) in the 4H polytype of SiC [4]. The NV center is intriguing because of zero phonon line (ZPL) energies in the near-infrared (1252-1291 nm) and the fact that nitrogen impurities, commonly used as n-type dopants in SiC, are involved.

Dopants in SiC exhibit different lattice site preferences. Nitrogen donors strongly prefer the C site over the Si site [5], while boron acceptors can occupy both atomic sites but act as shallow dopants only in the case of B_{Si} [6]. Phosphorous can occupy either the C or Si site from the energetic point of view, but the Si site is preferred [7].

In this work, we investigate the formation of optically active defects due to n-type doping by ion implantation in 4H-SiC epitaxial layers ($N_D \sim 3\times10^{15}$ cm^{-3}). The samples are prepared by implantation of N and P. One set of samples experienced single N or P implantations (N: 300 keV, P: 500 keV) to different fluences and subsequent annealing at 1000 °C for 30 min. The other set of samples underwent box profile formation by N or P doping to approximately 300 nm depth and $N_D \sim 10^{18}$ cm^{-3} doping density. The samples then underwent activation annealing at 1600 °C, followed by 1.8 MeV He irradiation to different fluences and 1100 °C annealing for 1 h for defect creation.

The resulting defects are monitored by photoluminescence (PL) measurements in the UV and infrared and confocal Raman spectroscopy. Different defect species are observed in the different samples. We observe new sharp emission signatures that are compared to density functional theory (DFT) calculations of different point defect complexes focusing on formation energies and optical and spin properties.

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11:00-11:20 AM

“Investigation of unintentional aggregation of impurity-related defects within 4H-SiC and at the (11-20) 4H-SiC/SiO_2 interface”

Niamh Smith[1], Alexander Shluger [1], Teofilo Cobos Freire[1]

[1]UCL (University College London)

To create p-doped regions within 4H-SiC MOSFET devices, 4H-SiC is bombarded with high energy Al^+ ions from gaseous AlH_3, during ion implantation. However, recent experimental studies have found shallow electron and hole donor states affecting channel mobility, whose densities are directly proportional to the Al-implantation dose even after post oxidation anneal in NO atmospheres. This suggests that Al-related defects present after the creation of the -4H-SiC/SiO_2 interface could be unintentionally interacting via aggregation with N- and O-related passivation defects at the interface.

We investigate the possibility of Al-O and Al-N complex formation within SiC devices, as well as whether such complexes can be correlated with the experimentally found mobility reducing states. In accordance with the charge compensation and site-competition theories, the $Al_{Si}N_{C}Al_{Si}$ and $Al_{Si}O_{C}Al_{Si}$ complexes have been examined using density functional theory (DFT) calculations. For each complex, four different geometry configurations corresponding to impurity substitution at different hexagonal (HEX) and cubic (CUB) lattice sites, derived using the Site-Occupancy Disorder package, were studied. Incorporation and binding energies, and charge transition levels (CTL) of these complexes in four different charge states were calculated in bulk 4H-SiC using DFT with the PBE0 functional. Within bulk 4H-SiC, negative binding energies were obtained for all configurations, indicating that, if Al_{Si} and N_C/O_C are separately present within 4H-SiC, it is more energetically favourable for them to form aggregates. Negative incorporation energies were also obtained for all eight configurations when the impurity chemical potential sources were taken to be AlH_3, NH_3, and NO, in correspondence to the device creation process. Within the 4H-SiC bandgap, the -1/0 charge transition is found to be the only stable transition for both complexes. The -1/0 charge transition levels of three out of four $Al_{Si}N_{C}Al_{Si}$ geometry configurations were found to occur within the activation range of the I_D-DLTS identified trap state. Using NH_3, rather than NO, for the chemical potential of N resulted in even lower incorporation energies for the $Al_{Si}N_{C}Al_{Si}$ configurations, implying the formation of the $Al_{Si}N_{C}Al_{Si}$ complex is easier under anneal in NH_3. This aligns extremely well with experimental measurements which find the density of the shallow hole donor interface state to be higher after annealing with NH_3 than with NO. For the $Al_{Si}O_{C}Al_{Si}$ complex, the total and incorporation energies of each charge state were found to be lowest for the $Al_{Si(HEX)}O_{C(HEX)}Al_{Si(CUB)}$ configuration. The -1/0 transition level of this configuration was found to be at E_c-0.004 eV, within the activation energy range of the shallow electron donor state observed experimentally. These results demonstrate how Al-O and Al-N complexes, can be responsible for channel mobility degradation in SiC devices.

We plan to have also further investigated the four complex configurations with 0/-1 transition levels that coincide with the activation energies of the experimentally found mobility reducing states at the (11-20) 4H-SiC/SiO_2 interface.

11:20-11:40 AM “Assessing the potential of perfect screw dislocations in SiC for solid-state quantum technologies”

Ludger Wirtz[1], Daniel Barragan-Yani[1]

[1]University of Luxembourg

Although point defects in solids are one of the most promising physical systems to build functioning qubits, it remains challenging to position them in a deterministic array and to integrate them into large networks. By means of advanced ab initio calculations we show that undissociated screw dislocations in cubic 3C-SiC, and their associated strain fields, could be used to create a deterministic pattern of relevant point defects. Specifically, we present a detailed analysis of the formation energies and electronic structure of the divacancy in 3C-SiC when located in the vicinity of this type of dislocations. Our results show that the divacancy is strongly attracted towards specific and equivalent sites inside the core of the screw dislocations, and would form a one-dimensional arrays along them. Furthermore, we show that the same strain that attracts the divacancy allows the modulation of the position of its electronic states and of its charge transition levels. In the case of the neutral divacancy, we find that these modulations result in the loss of its potential as a qubit. However, these same modulations could transform defects with no potential as qubits when located in bulk, into promising defects when located inside the core of the screw dislocations. Since dislocations are still mostly perceived as harmful defects, our findings represent a technological leap as they show that dislocations can be used as active building blocks in future defect-based quantum computers.

11:40-12:00 PM “Optical and electrical characterization of potential single photon emitters in 6H silicon carbide”

Erlend Ousdal[1], Marianne Bathen[1], Lasse Vines[1], Andrej Kuznetsov[1]

[1]University of Oslo

Point defects in semiconductors are a highly anticipated platform for quantum technology (QT) with the advantage of being scalable, potentially operative at room temperature, and relatively inexpensive to make and maintain. Moreover, for some of the material platforms where quantum friendly defects have been demonstrated, such as silicon (Si) and silicon carbide (SiC), there already exists a mature infrastructure for the fabrication of components.

Several point defects in SiC have proven to be single photon sources (SPEs) [1], which is of great interest in quantum applications. The majority of research on SiC has been done on the 4H polytype, where several SPEs have been identified, including the silicon vacancy (V_{Si}) [2], the carbon antisite-carbon vacancy (CAV) pair [3] and the divacancy ($V_{Si}V_C$) [4].A limited focus, however, has been given to other polytypes such as 6H SiC, which is of similar crystal structure as 4H.

In this work, we study 6H SiC for the purpose of increasing the knowledge

and understanding of properties that can be exploited for QT. In particular, the configuration and energy difference of relevant defects are compared between the 4H and 6H polytypes.
We characterize a highly doped epi-layer of 6H SiC having free carrier density of $N_D \sim 6\times10^{17}\mathrm{cm}^{-3}$ both optically and electrically, using photoluminescence (PL) and deep-level transient spectroscopy (DLTS) measurements. The samples were subjected to irradiation of protons at an energy of 1.8 MeV with different fluences and annealing at varying temperatures in inert atmospheres. The result is a mapping of how the point defects behave with the purpose of increased control of defect manipulation.
So far, all the three abovementioned point defects have been identified optically, with clear dependencies of both fluence and annealing temperature. Indeed, defect levels are observed to be different in the two polytypes, and comparison between processing dependencies is in progress.
In addition, DLTS measurements have been able to prove the existence of a defect level in an as-received sample of the 6H polytype, however there is still a need to identify the source of this signal, and to compare it with the PL data.
In the complete work, a full mapping of quantum defect dependencies on fluence and annealing temperature in 6H SiC, and a comparison with 4H SiC, will be presented. The results will mainly concern optical identification from PL with complementary electrical measurements.

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[2] Widmann, M., Lee, SY., Rendler, T. *et al.* Coherent control of single spins in silicon carbide at room temperature. *Nature Mater* **14**, 164-168 (2015). https://doi.org/10.1038/nmat4145.

[3] Castelletto, S., Johnson, B., Ivády, V. *et al.* A silicon carbide room-temperature single-photon source. *Nature Mater* **13**, 151-156 (2014). https://doi.org/10.1038/nmat3806.
[4] Christle, D., Falk, A., Andrich, P. *et al.* Isolated electron spins in silicon carbide with millisecond coherence times. *Nature Mater* **14**, 160-163 (2015). https://doi.org/10.1038/nmat4144.

12:00-12:20 PM “Defects and compensation centers in group-V doped CdTe for enhanced solar cell efficiency”

Intuon Chatratin, Igor Evangelista, and Anderson Janotti

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Cadmium Telluride is at the core of an important thin-film technology for photovoltaics that is already commercially available, yet the CdTe-based solar cell efficiency remains limited at 22%, well below the theoretical limit of ~30%. Increasing the hole concentration is crucial for higher efficiency, and group-V elements such as As, P, and Sb are potential dopants as they are shallow acceptors. Nevertheless, group-V doped p-type CdTe often exhibits low doping activation, and the compensation source remains debated. Here, we performed hybrid density functional calculations with spin-orbit coupling to investigate possible sources of hole compensation in group-V doped CdTe. First, regarding possible self-compensation of the group-V dopants, we find that the formation of AX centers is unlikely since they are found to be unstable relative to the shallow acceptor forms. However, if the group-V dopants come in during growth (such as dimer molecules As_2 , P_2 , and Sb_2), we find that the impurity atoms, which would occupy nearest neighbor sites, maintain the V-V bonds, limiting the hole density. For the native defects, our study reveals that Cd interstitial is the lowest energy donor defect in p-type CdTe. Still, it has a small migration barrier of 0.5 eV, making it highly mobile and unstable at room temperature. Te vacancy is the next lowest formation energy donor. The migration barrier of 1.4 eV indicates that the Te vacancy is stable at room temperature. The antisite Cd Te is also a donor, with low formation energy and stable at room temperature, potentially limiting the hole concentration. Our results, therefore, shed light on possible compensation centers and some guidance on how to avoid them.

This work was supported by the EERE Solar Energy Technologies Office, DOE grant number DE-EE0009344, and used resources of the National Energy Research Scientific Computing Center (NERSC), a U.S. Department of Energy Office of Science User Facility located at Lawrence Berkeley National Laboratory, operated under Contract No. DE-AC02-05CH11231, using NERSC award BES-ERCAP0021133. I.C. acknowledges the support from Development and Promotion of Science and Technology Talents Project (DPST) administered by the Institute for the Promotion of Teaching Science and Technology (IPST), Thailand, for funding a Ph.D. studentship.

12:20-1:40 PM **Lunch (on your own)**

Parallel Sessions

Gallium oxide (II) – Swan Ballroom

Chairperson: Michael Stavola, Lehigh University

1:40-2:20 PM

“Magneto-optical spectroscopy of transition metal impurities in β-Ga_2O_3” *(invited presentation)*

Jan Stehr[1], Mattias Jansson[1], Stephen Pearton[2], Weimin Chen[1], Irina Buyanova[1]

[1]Linköping University, [2]University of Florida

Owing to its large bandgap, β-Ga_2O_3 is currently considered as a promising material for numerous applications, including power electronics, solar blind UV photodetectors and sensors with capabilities superior to existing technologies. Transition-metal ions represent common contaminants in this material affecting its electrical and optical properties. They could also be potential candidates for spin qubits and quantum light emitters serving as spin-photon interface in future quantum spintronics. To control and explore transition-metal ions for future applications, a good understanding of their electronic, optical and spin properties is required but is largely lacking so far. In this talk we will review our recent results on spin resonance signatures of Co^{2+} and Cu^{2+} [1], as well as magneto-optical properties of Cr in the Cr^{3+} [2] and Cr^{4+} charge states. Through these detailed studies, we are able to obtain in-depth information on the properties of the ground and excited states of Cr^{3+} and Cr^{4+}, as well as their associated intracenter optical transitions. Prospects of Cr^{4+} centers for applications as spin qubits will also be discussed.

[1] J.E. Stehr, D.M. Hofmann, J. Schörmann, M. Becker, W.M. Chen, and I.A. Buyanova, Appl. Phys. Lett. **115**, 242101 (2019).
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2:20-2:40 PM

“Quantitative Modelling of Defect Concentrations in β-Ga_2O_3”

Khandakar Aaditta Arnab[1], Isaac Maxfield[1], Channyung Lee[2], Elif Ertekin[2, 3], Joel B. Varley[4], Ymir K. Frodason[5], Michael A. Scarpulla[1, 6]

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β-gallium oxide (β-Ga_2O_3) is of intense current interest because of its ultra-wide bandgap, high critical field, and availability of melt-grown substrates.

Point defects and complexes determine the properties of bulk crystals as well as epitaxial layers, thus, predictive models of defect concentrations under various impurity and processing scenarios are of very high value. First-principles calculations of defect energetics have provided critical insights into the defect system in β-Ga_2O_3, but translating computed enthalpies into defect concentrations corresponding to real-world crystal growth requires additional steps. Material processing in terms of growth or annealing typically controls the sample's thermochemical trajectory in terms of temperatures and partial pressures, while computational papers frequently present results holding chemical potentials constant.

Here we report quantitative modelling of equilibrium defect concentrations in Ga_2O_3, considering especially the temperature dependence of the bandgap and temperature-dependent chemical potentials from the Ga-O binary system's known thermochemistry. Additionally, we compute results for realistic sample types such as Fe- or Sn-doped wafers accounting for the fixed concentrations of these impurities as opposed to their fixed chemical potentials. Results are presented for various background n-type doping and for equilibrium and quenching, corresponding respectively to 0 or infinite cooling rates. We find significant departures from prior simpler predictions, especially in the case of the bandgap temperature dependence which tends to suppress V_{Ga}. We also explore the inclusion of H, Ir and transition metals like Fe and Cr explicitly. We compare our predicted results to experimental cases such as annealing in O_2 or Ga_2O vapors.

2:40-3:00 PM "Phase stability of $(Al_xGa_{1-x})_2O_3$ polymorphs: a first-principles study"

Sai Mu[1]

[1]University of South Carolina

Monoclinic-Ga_2O_3 and its Al alloy $(Al_xGa_{1-x})_2O_3$ are wide-bandgap materials and are of active interest due to their promising applications in power electronics. Several polymorphs (monoclinic, corundum, spinel, orthorhombic) are known and are being pursued due their potential advantages for applications. A thorough understanding of the stability of the competing phases in Ga_2O_3 and $(Al_xGa_{1-x})_2O_3$ is needed to promote the formation of the desired phase for device applications. We employ density functional theory to investigate the phase stability of Ga_2O_3 and $(Al_xGa_{1-x})_2O_3$ at both zero temperature and finite temperature. Strain is found to have a weak effect on relative phase stability. At finite temperature, we found that the lattice vibrations tend to stabilize the orthorhombic phase and destabilize the corundum and spinel phase, referenced to monoclinic phase. Importantly, we find that a unique configurational entropy is present in the spinel phase due to cation vacancy disorder, and that it substantially contributes to stabilizing the spinel phase in $(Al_xGa_{1-x})_2O_3$ at finite temperature. Our study offers insights into phase control of these important alloys.

This work was supported by AFOSR. Work performed in collaboration with Prof. Chris G. Van de Walle.

3:00-3:20 PM **Break**

3:20-3:40 PM “Controlling defects in wide-bandgap oxides for memristor applications”

Hartwin Peelaers[1], Sierra Seacat[1]

[1]Department of Physics and Astronomy, University of Kansas, Lawrence, KS 66045

Memristors, with proposed applications for logic gates, non-volatile memory, and neuromorphic computing, typically consist of an oxide sandwiched between two metal contacts. When a voltage is applied, oxygen vacancies diffuse through the material and form a conducting filament, causing the memristor to switch from a high resistance state (HRS) to a low resistance state (LRS). Increasing the concentration of oxygen vacancies can improve the performance of memristors in critical areas such as switching speed and on/off ratio (HRS/LRS). Using density functional theory with hybrid functionals, we investigated if Mg doping in Al_2O_3 can increase the performance of memristors. We found that Mg defects act as deep acceptors that will lower the Fermi level compared to undoped Al_2O_3. This creates a more resistive HRS, while at the same time lowering the formation energy of oxygen vacancies, thus promoting their formation. These findings were used to guide experiments in tuning the performance of ultrathin memristors by stacking ALD grown Al_2O_3 and MgO layers. Adding MgO layers to the stack increased both the HRS and the on/off ratio, as predicted by our calculations [1].

Alloying or replacing the Al_2O_3 with Ga_2O_3 has the potential to further tune the properties of memristors, as Ga_2O_3 has a smaller bandgap and Ga has different coordination preferences (e.g., in the monoclinic ground state 50% of the cation are tetrahedrally coordinated), which can impact the oxygen vacancy mobility. We will discuss doping of Ga_2O_3 [2], the properties of Ga_2O_3 and Al_2O_3 alloys [3-4], and of oxygen vacancies, and their impact on memristor performance.

[1] R. Goul *et al.*, “Atomic-Scale Tuning of Ultrathin Memristors”, Commun. Phys. **5**, 1 (2022).
[2] H. Peelaers, J. L. Lyons, J. B. Varley, and C. G. Van de Walle “Deep Acceptors and Their Diffusion in Ga_2O_3”, APL Mater. **7**, 022519 (2019).
[3] S. Seacat, J. L. Lyons, and H. Peelaers, “Properties of Orthorhombic Ga_2O_3 Alloyed with In_2O_3 and Al_2O_3”, Appl. Phys. Lett. **119**, 042104 (2021).

[4] H. Peelaers, J. B. Varley, J. S. Speck, and C. G. Van de Walle "Structural and Electronic Properties of Ga_2O_3-Al_2O_3 Alloys", Appl. Phys. Lett. **112**, 242101 (2018).

3:40-4:00 PM "Excited-state properties of oxygen vacancies near α-Al_2O_3(0001) surfaces from first principles and quantum defect embedding"

Vijaya Begum-Hudde[1], Barbara Jones[2], André Schleife[1]

[1]University of Illinois, Urbana-Champaign, [2]IBM

Density functional theory (DFT) has proven to be a successful mean-field approach to calculate structural properties of bulk materials as well as their surfaces, however, it fails to correctly describe excited-state properties. Since defect states are often confined to a small space comprising of only a few correlated states, recently, a quantum defect embedding theory (QDET) [1,2] was proposed to study such correlated defect states in solids. It treats the defect states at a high level of theory, for example, with Full Configuration Interaction (FCI), or on a Quantum computer. The defect is coupled to a host material that is solved within the mean-field approach that allows to simulate systems with hundreds of atoms.
We present a detailed analysis of the electronic and structural properties of O vacancies near the surface of α-Al2O_3(0001). This material is a widely studied system as it hosts a range of important technological applications such as catalysis, and natural occurring processes such as corrosion. Oxygen vacancies near the surface of α-Al2O_3(0001) are of significant interest as they aid in understanding the hydration of the surface which is critical to the aforementioned processes. Our first-principles calculations reveal large inward relaxation of the surface Al monolayer (~88% of the unrelaxed configuration) accompanied by the reconstruction of the Al ions. The vertical relaxation of the subsequent layers is concurrent with previous density-functional theory studies and experimental results from X-ray diffraction. Upon introducing the O defect, emergence of defect states is observed. These defect states are characterized to describe an active space to perform QDET calculations. An effective Hamiltonian is constructed for the active space, and we subsequently obtain excitation energies for the correlated defect states by employing FCI. Our results confirm that QDET is a reliable approach to study excited-state properties of large surfaces with correlated defect states. Furthermore, with the ongoing implementation to solve the effective Hamiltonian on a quantum computer, we aim to predict the ground- and excited-state properties of defects on a noiseless simulator and extend our study to include error-mitigation techniques to obtain accurate results on actual quantum hardware.

We wish to acknowledge funding by the IBM-Illinois Discovery Accelerator Institute.

[1] H. Ma, M. Govoni, and G. Galli,*npj Computational Materials***6**, 85 (2020).
[2] N. Sheng,C. Vorwerk, M. Govoni, and G. Galli,*J. Chem. Theory Comput.* **18**, 3512 (2022).

Silicon (I) – Sanibel

Chairperson: Marianne Bathen, University of Oslo

1:40-2:00 PM "High-throughput identification of spin-photon interfaces in silicon"

Yihuang Xiong[1], Weiru Chen[1], Diana Dahliah[2], Céline Bourgois[2], Sinéad Griffin[3], Alp Sipahigil[4], Geoffroy Hautier[1]

[1]Dartmouth College, [2]Université catholique de Louvain, [3]Lawrence Berkeley National Laboratory, [4]University of California, Berkeley

Color centers in semiconducting hosts have become an emerging candidate for spin-photon interfaces. Silicon is a technologically mature material that provides an attractive platform for realizing defect-based qubits that can be manufactured at scale. In this talk, we will present our work on a high-throughput search for promising spin-photon interfaces using first-principles computations. We will report on the challenges in ensuring an accurate enough electronic structure while building a large enough data set and discuss our approach using single-shot hybrid computations. By building a database that documents thousands of quantum defects in silicon, we will discuss strategies for designing defects that could emit at technologically relevant wavelengths, especially considering silicon's relatively narrow band gap. Our results suggest promising candidates and highlight the designing strategies for novel spin-photon interfaces.

2:00-2:20 PM "Photoluminescence spectra of the G center in silicon: comparison between first principles computations and experiment"

Jiongzhi Zheng[1], Lukas Komza[2], Yihuang Xiong[1], Alp Sipahigil[2], Geoffroy Hautier[1]

[1]Thayer School of Engineering, Dartmouth College, Hanover, New Hampshire 03755, USA ,

[2]Department of Electrical Engineering and Computer Sciences, University of California, Berkeley, California 94720, USA

The G center in silicon is a complex carbon-based defect that has been reinvestigated lately due to its promises for applications in quantum technologies. Here we use report on an experimentally measured high quality photoluminescence spectra of the G center and compare with first principles results. We focus on the phonon sideband and use a compressive

sensing technique [1,2] to obtain the vibrational spectra of the defect with Density Functional Theory (DFT) in the generalized gradient approximation (GGA) and the hybrid HSE functional. This approach is significantly cheaper than the traditional finite-difference approach for phonon computations. The computed spectrum agrees very well with experiment and shows a Debye-Waller factor of 54%. We identify specific features in the vibrational spectra (e.g., the E line) and use our first principles computations to resolve their atomic nature. Our work confirms that the G center forms in the so-called configuration B. We also study the effect of isotopes on the phonon sidebands and compare with previous experiments.

[1] F. Zhou, W. Nielson, Y. Xia, and V. Ozoliņš, Physical Review B **100**, 184308 (2019).

[2] E. J. Candès and M. B. Wakin, IEEE Signal Process. Mag. **25**, 21 (2008).

2:20-3:00 PM "Defect Spectroscopy of Erbium Implanted Silicon for Quantum Technologies" *(invited presentation)*

Jeffrey McCallum[1], Christopher Lew[1], Aochen Duan[1], Elijah Foster-McLachlan[1], S. Q. (Qi) Lim[1], Brett Johnson[2]

[1]University of Melbourne, School of Physics, Melbourne, Australia,
[2]RMIT University, Melbourne, Australia

Erbium is an attractive optically-addressable spin-centre for applications in quantum technologies including quantum memories, repeaters, and quantum computers.[1] The features that make Er in Si particularly attractive for applications in quantum technologies include the fact that it possesses spin states with low decoherence rates, optical addressable transitions to interface solid-state qubits with flying qubits, and a potentially scalable device engineering platform. While early ion implantation studies of Er:Si focussed on implantation of Er at relatively high fluences for possible applications in optical amplification and lasing, more recently research has generally been concerned with low fluence implants to produce populations of relatively isolated spin-centres suitable for quantum computing applications.[2-4] Er is a heavy ion that creates considerable damage upon implantation into Si and deep level transient spectroscopy, DLTS, offers a sensitive method of exploring the defect evolution and damage recovery that occurs during subsequent thermal processing and hence is well-suited and directly relevant to this low-fluence implant regime. DLTS studies of Er implanted Si have highlighted the fact that the dense collision cascades of these heavy ions produce strain in the lattice that tends to broaden and distort the DLTS features when compared with DLTS spectra for lighter ions. [5, 6] Defects can also be projected well beyond the projected range of the ions. The defects produced by heavy ion implantation are also stable up to higher temperatures than those introduced by electron irradiation and low mass ions and this can be an important consideration for quantum devices fabrication since in some cases available thermal budgets for removal of the implantation damage are quite limited and it is possible that detectable levels of electrically active defects are still present in the devices in their fully-processed state. [1, 2, 4] While most studies have focussed on Er implantation of n-type Si there have been fewer studies of p-type Si and this has been a particular focus of our recent research since many of the Er implanted FinFET devices in our quantum measurement program have B-doped channels. In this presentation, a broad introduction to the attributes of Er in Si for quantum device development will be given along with details of how the companion DLTS studies are used to complement the quantum device development and measurement programs.

[1] G. Hu et al. Quantum Sci. Technol. **7** (2022) 025019; https://doi.org/10.1088/2058-9565/ac56c7.
[2] C. Yin et al. Nature, 497 (2013) 91; doi:10.1038/nature12081.
[3] M. A. Hughes et al. Appl. Phys. Lett. 118, 194001 (2021); doi: 10.1063/5.0046904.
[4] A. Gritsch et al. PHYS. REV. X 12, (2022) 041009; doi: 10.1103/PhysRevX.12.041009.
[5] C. T.-K. Lew et al., J. Appl. Phys. 124, (2018) 125701; https://doi.org/10.1063/1.5047534.
[6] J. H. Evans-Freeman et al., J. Appl. Phys. 92, (2002) 3755-3760; https://doi.org/10.1063/1.1497721.

3:00-3:20 PM **Break**

3:20-3:40 PM “Atomic scale analysis of N dopants in InAs”

Tom Verstijnen[1], Douwe Tjeertes[1], Edoardo Banfi[1], Qiandong Zhuang[2], Paul Koenraad[1]

[1]Eindhoven University of Technology, [2]Lancaster University

The band gap of most III-V semiconductors is strongly reduced with the introduction of only a few percent of N, even if the III-N alloy has a much bigger band gap. N impurities in InAs introduce an impurity state around 1 eV above the conduction band minimum, much deeper in the band than in other III-V materials. Topographic scanning tunneling spectroscopy measurements (STS) and areal spectroscopy measurements performed on N atoms up to two layers below the (110) surface of InAs show a reduction of the resonance energy of the N atom with increasing depth. This is attributed to tip induced band bending, pulling the N states up at positive bias and acting most strongly on surface N atoms. STS measurements obtained on undoped InAs and N-doped InAs show a similar band gap, due to band bending and electron accumulation effects at the InAs-vacuum interface. Spectroscopy maps of N atoms up to two layers below the surface provide a high resolution spatial and spectroscopic view of the N atoms. Here the characteristic shape of the N atoms in different layers below the surface is observed as an enhancement of the dI/dV signal compared to the InAs background. At energies above the enhancement a reduction of the dI/dV is observed, which has the same shape and size as the enhancement. This shows that the redistribution of density of states caused by the N impurities is mainly energetic in nature.

3:40-4:00 PM “Characterization of carbon-13 T centers in silicon”

M. Mehdi Keshavarz[1, 2], Nicholas Brunelle[1, 2], Chloe Clear[1, 2], Joshua Kanaganayagam[1, 2], Amirhossein AlizadehKhaledi[1, 2], Ian R. Kennedy[1, 2], Yehudah Ackermann[1, 2], Melanie SL Gascoine[1, 2], Myles Ruether[1, 2], Michael L. W. Thewalt[1], Daniel B. Higginbottom [1, 2], Stephanie Simmons[1, 2]

[1]Simon Fraser University, [2]Photonic Inc.

Spin-photon interfaces are a promising platform for quantum network technologies. They simultaneously possess the advantages of long-lived spin qubits and the ability to transmit information and distribute entanglement through photons. In addition to an optical interface, a networkable solid-state spin-photon interface should host a register of multiple individually addressable memory spins constituting a small quantum processor for local operations. The T center is a spin-photon interface in silicon with optical emission in the low-loss telecommunications O-band and can be integrated with the mature silicon nanophotonic and nanoelectronic commercial foundry processes [1, 2]. The T center consists of two nonequivalent carbon atoms, one hydrogen atom, and one electron. In its most common isotopic configuration, the electron spin and the hydrogen nuclear spin serve as two local spin qubits but the carbon atoms are spinless carbon-12 [3]. Prior work has focused on this configuration almost exclusively. If, instead, the carbon sites are occupied by carbon-13 atoms, their nuclear spin can also be used as two extra memory qubits providing a four-spin register. In this work we measure the ground state structure of two isotopic variations of T centers, each containing one carbon-13 and one carbon-12 atom, and we characterize the hyperfine interactions between the electron spin and the carbon nuclear spins and explore using carbon nuclear spins in T centers as local memory resources for networked quantum technologies.

Poster Session (II) – Kiwi’s Kove

4:00-5:30 PM

Poster presentations

1. Giovanni Alfieri, Hitachi Energy: "Electrical characterization of 4H-SiC MOS interfaces with an ion implanted thermal oxide"

Giovanni Alfieri[1], Sami Bolat[1], Yulieth Arango[1], Piyush Kumar[2], Ulrike Grossner[2]

[1]Hitachi Energy, Switzerland, [2]ETH, Switzerland

The effects of pre-oxidation ion implantation (POI) on the electrical characteristics of SiO_2/SiC interfaces have been studied, in recent years. For instance, it was found that Sb POI improves the flat-band voltage (V_{FB}) due to the passivation of carbon dimers ($(C_O)_2$) in the oxide. However, the effects of ion implantation on SiO_2/SiC interfaces, when implantation is performed in the thermal oxide, are not known.

To shed light on this topic, we carried out ion implantation of C, N or O in a 50 nm thick thermal oxide grown on n-type 4H-SiC epilayer samples (~10^{16} cm^{-3}). After implantation, samples were annealed in vacuum in the 100-1000°C temperature range, for 15 min. Ni was deposited on the oxide in order to electrically characterize the samples by both C-V (at RT) and constant capacitance deep level transient spectroscopy (CC-DLTS), in the 77-650 K temperature range. CC-DLTS measurements (1 MHz) were performed by keeping the reverse voltage at -10V and a constant pulse voltage height of 30 V.

C-V measurements show V_{FB} of ~10 V in the as-grown SiO_2/SiC MOS. After implantation, the C implanted samples show ~2 V lower V_{FB} values than those implanted by either N or O. Such difference (DV_{FB}) is also found after heat treatments up to 700°C, whereas DV_{FB} is reduced to <0.4 V after annealing at 800°C.

CC-DLTS measurements, in as-grown and as-implanted samples, show the presence of two levels, previously labeled as O1 and O2, located at 0.14 and 0.24 eV below the conduction band edge of SiC (E_C) and typically associated to $(C_O)_2$ and silicon interstitial (Si_i), respectively. In the present study, we do not observe any significant increase in concentration for both O1 and O2, after implantation and annealing, with [O2] ranging between 7 and 9x10^{14} cm^{-3}. Unlike the as-grown samples and C-implanted sample, a ~200 K broad DLTS peak and a level at E_C-1.39 eV are observed in the N and O implanted samples. The broad peak is due to the overlap of several contributions ranging between 0.7-0.8 eV, below E_C. After annealing at 800°C, when DV_{FB} is reduced among all of the implanted samples, most of these contributions and the E_C-1.39 level are not detectable anymore, except for a level at ~E_C-0.73 eV.

The nature of such detected levels is currently under investigation. It is known that open volume defects are present in the oxide side of the SiO_2/SiC interface, e.g. silicon vacancies (V_{Si}) surrounded by oxygen atoms. It can be suggested that, after implantation, different types of V_{Si}-related complexes are formed in the oxide. However, unlike the case of either N or O implantation, the implanted C atoms might occupy such V_{Si} thus making such complexes electrically inactive.

In summary, 4H-SiC MOS were implanted with either C, N or O. N or O implanted MOS give worse V_{FB} values than C implantation and this is attributed to the presence of levels arising in the 0.7-1.4 eV energy range, below E_C.

2. Nikolay Arutyunov, IKZ Berlin: “Bismuth impurity centers in silicon: microstructure of bismuth-related defects produced by proton irradiation”

Nikolay Arutyunov[1, 2, 3], V Emtsev[2], R. Krause-Rehberg[1], M. Elsayed[2], N. Abrosimov[3], G. Oganesyan[2], V. Kozlovski[4]

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In search of a high-performance interface between telecom photons and matter qubits, bismuth (Bi) centers and their radiation complexes are being scrutinized in floating zone (FZ) silicon of n-type, mostly, by the resonance and optical methods. Meanwhile, beyond narrow zones of resonance and optical transitions, data on electron and micro-structural properties of Bi centers in silicon is scarce. To gain deeper insight into properties of both the spin system and open volume related to the Bi donor center, we have probed the microstructure of the Bi center by positrons registering their two-quantum annihilation with electrons. The samples were irradiated with 15 MeV protons at room temperature. To characterize the investigated material, low-temperature Hall’s measurements were carried out on the samples-satellites.For the first time, an inhibition and a delay of emission of two annihilation quanta has been revealed at the declining temperature, when the electron density contacting positron at the Bi center increases. This observation performed by high-resolution positron annihilation lifetime spectroscopy and looking paradoxically is suggested to be caused by non-local interaction between the nuclear and electron spins of atoms of magnetic isotope 29Si(J = 1/2) and Bi(J = 9/2) centers [1]. Interestingly, this interaction does not manifest itself in the enriched 28Si(Bi) material (i.e., in so-called 28Si “semiconductor vacuum" where the residual concentration of atoms of 29Si (J=1/2) isotope ambient Bi impurity center is as low as 50 ppm). We believe that the data obtained demonstrate for the first time the influence of a non-local interaction of the spin systems of Bi(J = 9/2) and 29Si (J=1/2) centers on the essentially local phenomenon of emission of the two-quantum electron-positron annihilation radiation.The Bi center acquires an open volume Vop as a result of interaction with the point defects created by the proton irradiation. It is argued that the thermally stable complex [Vop - Bi] possesses D3d symmetry [1]; this comes into line with the data on the electrical properties of the electron-irradiated n-FZ-Si(Bi) material [2].The [Vop - Bi] center is decomposing during a fast stage of isochronal annealing over the temperature range ΔTann.= 320 to 470 °C [1]; the estimated activation energy is equal to Ea = 0.89 ± 0.08 eV and is surprisingly close to the energy ~0.92 eV characterizing structural stability of the center where Bi donor impurity atom is coupled with the modeled vacancy (see [1] and references therein). It is worth mentioning that the thermally stable radiation complexes related to the phosphorus (P) impurity centers in the proton-irradiated material are annealed during a somewhat broader stage, ΔTann.= ~ 430 to ~ 650 °C (Ea = 1.05 ± 0.21 eV [3, 4]).The results available for the Bi and P centers of radiation origin in FZ silicon are briefly discussed in the light of reconsideration of a whole conception of formation of point radiation defects in moderately doped n-type silicon subjected to irradiation with protons and electrons (see [5] and references therein).

3. Hayley Austin, Lehigh Univ.: "Carrier Confinement for Improved Color Tunability of Eu-doped GaN LEDs"

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GaN-based materials whose active layers are doped with rare-earth (RE) ions provide precise emission wavelengths in LEDs. In particular, Eu^{3+} ions can be excited electrically and emit red light due to relaxation from the $^5D_0$ excited state. In addition, we have found that Eu^{3+} ions can emit green, yellow, and orange light from the $^5D_1$ state. The ratio of the red and green emission can be adjusted through carrier-mediated re-excitation and energy shuffling between a local defect and different excited states of Eu^{3+} ions. This color tunability exploits the distinct lifetimes of the $^5D_0$ and $^5D_1$ states, allowing for controlled color tunability in proof-of-concept LEDs. Simulations have provided insights into how different excitation conditions impact the populations of the different Eu^{3+} states, which can be interpreted to predict the nature of the color tunability under current injection. In these simulations, the local defect is considered as the mitigator of energy transfer, where the carriers are captured and then recombine and transfer energy to the Eu^{3+} ions. Furthermore, by considering the local defect as a co-dopant that serves as a blue emitter, our model can predict tunability parameters within a larger color space due to the mixing of the primary colors: red, green, and blue. This model can also be tailored to predict color mixing, where samples designed utilizing various enhancements, provided by heterostructures and nanostructures, can shift the ratios of emitted colors, filter out various colors completely, or shorten emission lifetimes. In particular, carrier confinement that benefits the majority site, the source of the desired emission, would help increase the efficiency of the re-excitation for color tuning. To explore such confinement, multiple layered structure (MLS) samples were studied. Beyond the pursuit of color tunability, these findings also contribute to our understanding of how other REs can be integrated into different semiconductor hosts, designed to confine carriers in ways that will benefit the wider semiconductor community.

4. Brittany Baker, Francis Marion Univ.: "Analysis of Positively Charged Muonium in Tin Oxide"

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Tin oxide is a transparent conducting oxide (TCO) that has many applications in optoelectronic devices, such as solar cells and LED's. Tin oxide is naturally n-type, with hydrogen acting as a shallow donor. Zero Field Muon Spin Relaxation (ZF-MuSR) measurements were completed on a single crystal sample from 2 K to 710 K in a closed cycle refrigerator and from 300 K to 1080 K in an optical furnace. In ZF-MuSR measurements, muons (Mu+; spin ½, positive charge; 1/9 mass of a proton) are implanted in a sample and the evolution of the Mu spin polarization is tracked as the Mu interacts with the local fields within the sample. Implanted muons can take on a positive (Mu+), neutral (Mu0: attached to one e-) or negative (Mu-: attached to 2 electrons) states. Because of its similarity to isolated hydrogen, Mu serves as an experimentally accessible analogue to isolated H impurities in materials. In the ZF technique, the sample under study is in an environment where the magnetic field at the sample site is controlled to be zero so that the implanted Mu (c.f. H) behaves in a material close to its natural state, directly measure the local fields (e.g. dipolar fields for a static Mu center) and characterize dynamics that result from either Mu+/- motion between sites or fluctuations in the local field itself. Our analysis of these data reveals two positive muonium states with hints of an additional state at temperatures below 300 K. The current model shows a high occupancy positive muonium state and a low occupancy positive muonium state with a slow migration of muonium from the high occupancy state to the low occupancy state above 300 K. We will present details of an updated model and the muonium sites, energies barriers, and diffusion processes of the positively charged muonium determined from the model.

5. Abdelhamid El Kaaouachi, Univ. Ibn Zohr: "Electrical conduction mechanisms on both sides of the Metal-Insulator Transition in dilute p-Si/SiGe/Si in the presence of the magnetic field"

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In this work we highlight the electrical conduction mechanisms on the both sides of the Metal-Insulator (Metallic and insulating sides of the MIT) in 2D p-Si/SiGe/Si system. We show by using a numerical technique that on theinsulating side, we are witnessing a Variable Range Hopping (VRH) conduction regime according to EfrosShklovskii (ES) indicating the existence of a Coulomb Gap (GC) at the Fermi level EF. On the other hand, on the metallic side, we show that the electrical conductivity follows an empirical law due to electron-electron interaction effects and to the weak localization effect. We re-used in our investigation the experimental measurements of p-Si/SiGe/Si obtained by I. L Drichko et al. [1].

6. Emily Garrity, Colorado School of Mines: "Point Defects and Doping of Ultra-wide Band Gap (III)BO Oxides for Power Electronics"

Emily Garrity[1], Cheng-Wei Lee[1], Andriy Zakutayev[2], Vladan Stevanovic[1]

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New wide band gap semiconductors are needed to reach higher power, voltage, and switching-frequency in power electronics. A recent computational search identified a group of promising ultra-wide band gap (4.8-7.8 eV), calcite-type, orthoborates, assuming *n*-type doping could be attained. In this work, we test this assumption and investigate the point defect chemistry and dopability of $AlBO_3$, $GaBO_3$, and $InBO_3$ using first-principles calculations. Of the three, we find $InBO_3$ to have the most capacity for *n*-type doping without significant compensation by native acceptor defects. Furthermore, Zr is predicted to readily substitute for In and behave as a shallow donor with maximal net donor concentrations exceeding 10^{18} cm^{-3} under growth conditions typical for this class of material. We also perform hybrid functional calculations to confirm the presence of small hole polarons in $InBO_3$ which will limit achievable *p*-type conductivity. Ultimately, our results confirm the promise of $InBO_3$ as an *n*-type power semiconductor and suggest alloying with $GaBO_3$ and $AlBO_3$ for further optimization of band gap, performance, and electron concentration.

7. Akira Kiyoi, Mitsubishi Electric: "Effect of oxygen on trap-limited diffusion of hydrogen in proton-irradiated n-type silicon for power devices"

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Defect engineering plays an important role in the development of semiconductor devices. In particular, methods associated with the modification of semiconductor properties using irradiation-induced defects has been actively developing for a variety of applications.[1] In Si-based power devices, applications of defect engineering are seen in the lifetime control of nonequilibrium charge carriers and doping in the structures of switching devices (e.g., diodes, IGBT). This is accompanied with the formation of local energy levels in the bandgap of Si, which act either as recombination centers for nonequilibrium charge carriers and as an electron source, or as a hole source (donor or acceptor), according to their energy levels in the bandgap. It is worth mentioning that, in addition to recombination centers (i.e., deep-level defects), hydrogen-related shallow donors (HDs) have been observed in Si that have been subjected to proton irradiation and post-implantation annealing at temperatures ranging between 300 and 550 °C. [2] This process can realize *n*-type doping with an advantage in controlling the depth of doping areas. [3,4] In addition, the recently growing demand for the devices has led to the use of magnetic field-applied Czochralski (m:Cz) wafers owing to the limited production capacity and available diameters of the traditionally used floating zone (FZ) wafers. Consequently, the influence of oxygen impurities in the wafers on the electrical properties of devices, regardless of the growth method, needs to be investigated to achieve a stable fabrication process for devices. In connection with doping process using proton irradiation, we evaluated the effective diffusion coefficient (D_{eff}) related to trap-limited diffusion of hydrogen and the effects of impurities on hydrogen diffusivity. We irradiated *n*-type silicon wafers, which have different carbon, oxygen, and phosphorus concentrations, with 2 MeV protons and annealed them at 300-400 °C. By analyzing the width of the *n*-type region, where HDs are induced, we estimated D_{eff} to be five to six orders of magnitude lower than the intrinsic diffusion coefficient, indicating that hydrogen motion is highly trap-limited. Moreover, D_{eff} was significantly dependent on the oxygen concentration, and the activation energy of hydrogen diffusion varied from 0.57 ± 0.15 eV (pure epitaxial wafer) to 2.19 ± 0.15 eV (m:Cz wafer). This trend suggests that oxygen-related defects preferentially trap the mobile hydrogen released from thermally dissociated HDs. These information is essential because we can treat m:Cz and FZ wafers equivalently during the doping process.

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8. Amelia Klein, Univ. Pennsylvania: “Designing a collimating metasurface photon extractor for solid-state color centers through many-body adjoint shape optimization”

Amelia Klein[1], Nader Engheta[1], Lee Bassett[1]

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Point defects in solid-state substrates are of great interest as spin qubits for emerging quantum technologies including quantum computing, quantum communication, and quantum sensing. Readout of these color centers is typically performed optically, and it is crucial to efficiently collect their single-photon emission. In this work, we design a nanophotonic collection optic for the diamond nitrogen-vacancy (NV) center, the prototypical solid-state color center. We use nanophotonic inverse design techniques to perform a many-body shape optimization on a diamond nanopillar array while respecting fabrication constraints. This metastructure improves photon transmission through the diamond surface by overcoming total internal reflection, while simultaneously directing the emitted photons for collection by the narrow numerical aperture of an optical fiber, circumventing the need for bulky, expensive free-space optics. In contrast to other nanophotonic structures, the metastructure modifies only the far field of the NV center such as to maximally preserve the optical and spin coherence of an isolated defect. While the design shown here is tailored for the NV center, the technique is readily applicable to other defects and materials.

9. Amanda Langørgen, Univ. Oslo “A metastable defect center in β-Ga_2O_3”

Amanda Langørgen[1], Ingvild Julie Thue Jensen[2], Lasse Vines[1], Ymir Kalmann Frodason[1]

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Monoclinic gallium oxide (β-Ga_2O_3) is a semiconductor material receiving considerable research interest as a promising material for power electronics applications, owing to its ultrawide-band gap of ~ 4.9eV, melt-based bulk growth and a widely tunable *n*-type conductivity, [1-3] offering the potential for high-performance devices at a low cost.[1] To unlock the potential offered by $\beta$$Ga_2O_3$-based devices, a mature understanding and control of the defect structure in the material is imperative.

Consequently, defect levels have been studied to a great extent in β-Ga_2O_3 by a range of characterization techniques, such as deep-level transient spectroscopy (DLTS)[4-8] and also through theoretical predictions using density functional theory.[9, 10] With a view towards devices, metastable defects are especially interesting as they can form or alter configuration under device operation when exposed to elevated temperatures and/or electric fields. Several metastable defects have already been reported, including the E_2^* and E center.[5, 7]

Here, we report on the observation of a new metastable defect level in β-Ga_2O_3 with an activation energy of $E_A \sim 1.6$ eV and an apparent capture cross-section of $\sigma_{na} \sim 2\times10^{-13}$ cm^2. The sample studied herein is a halide vapor-phase epitaxy (HVPE) grown, (001)-oriented β-Ga_2O_3 thin film with a carrier concentration of $N_d \sim 7\times10^{15}$ cm^{-3}. The level is introduced after He-implantation with a kinetic energy of 500 keV and a fluence of 3×10^{10} cm^{-2} and subsequent exposure to elevated temperatures above 500K while under reverse bias conditions. The level is not observed in as-received samples, and a depth profile indicates a clear correlation between the defect concentration and the implantation distribution, hinting toward an intrinsic defect origin. Further experimental probing of the defect level, such as zero-bias annealing and capture cross-section measurements, is conducted, and different models for the defect origin are discussed based on the combination of experimental findings and hybrid functional calculations.

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10. Channyung Lee, Univ. Illinois: "Investigation of split vacancy and interstitial Defects and ionic diffusion mechanisms in β-Ga_2O_3: A direct approach via master diffusion equations"

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The low symmetry of the monoclinic structure of β-Ga_2O_3 has led to interesting discoveries of a variety of complex configurations of intrinsic defects, such as Ga vacancies split into two or three different Ga sites. These complex defects contribute to the fast, yet highly anisotropic, diffusion of ions in β-Ga_2O_3, making it challenging to understand the dominant diffusion mechanisms. While previous computational studies have analyzed some migration pathways between these complex split defects, a comprehensive understanding of the overall diffusion mechanism, and predictions of the components of the full diffusivity tensor accounting for the full spectrum of intrinsic defects, is not yet achieved. In this work, we calculate from the first principles the 3D diffusion tensors for Ga interstitial and vacancy self-diffusion via a direct approach based on the solution of the master diffusion equations. To achieve this, we first explore the maximum extent of "N"-split defects with large configurational complexity, including their formation energies. With the dominant low-energy defects identified, we then construct the complete diffusion network taking into account all stable split defects and all possible hops connecting them (including via the interstitialcy mechanism). The nudged elastic band method is used to accurately determine hopping barriers, and the barriers and diffusion pathways are used to construct the complete master diffusion equations for Ga cations. Finally, the solution to these equations yields the Onsager transport coefficients, resulting in the 3d diffusion tensors and identification of the most active diffusion paths along three different crystallographic directions. Our analysis includes the identification of over 32 unique interstitial and interstitialcy hops between 20 different configurations of Ga interstitials and more than 31 unique vacancy hops between 15 different configurations of Ga vacancies. Extended N-split Ga defects are remarkably more stable than simple point defects, and play a critical role in creating low-energy pathways for both interstitial and vacancy diffusion. Furthermore, we found that selecting the appropriate supercell size is crucial for accurately describing the formation energies of N-split defects and calculating their associated migration energy barriers. Our findings reveal that Ga interstitial diffusion coefficients are higher in the c, b, and a* crystal orientations, whereas Ga vacancy diffusion coefficients are greater in the c, a*, and b orientations. We estimate effective activation barrier energies for each diffusion direction, which lie within an order of magnitude to previous experimental measurements. Notably, the predicted c-axis effective activation energy of V_{Ga}^{-3} of 0.79 is in good agreement with the experimental observation of 0.8 ± 0.1 eV by Azarov et al. [1] measured in the temperature range of 25-250 °C. Our study provides a clear understanding of the migration mechanisms of native Ga species in β-Ga_2O_3 and the origin of its anisotropic diffusion, which can contribute to further developments in the design and optimization of β-Ga_2O_3-based electronics.

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11. Marek Maciaszek, Center for Phys. Sci. & Tech., Vilnius, Lithuania: “The application of the SCAN density functional to color centers for quantum applications”

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Detailed characterization of deep-level color centers requires understanding their electronic and atomic structure, which is most commonly investigated utilizing the Kohn-Sham density functional theory. Standard semilocal functionals based on the generalized-gradient approximation (GGA) are inclined to an imprecise quantitative description of defects’ electronic structure. Hybrid functionals provide an improved prediction of electronic properties, albeit at a much increased computational cost. In this work, we test the newly developed SCAN family of meta-GGA density functionals for selected color centers in diamond and 4H-SiC. In particular, we study nitrogen-, silicon-, germanium-, and tin-vacancy centers in diamond as well as four neutral divacancy configurations in silicon carbide that have been recently investigated for their use in future quantum technologies. We show that SCAN and its derivatives rSCAN and r^2SCAN functionals significantly improve the calculated energies of optical transitions, almost reaching the accuracy of the hybrid HSE functional. Moreover, we also show that the SCAN family of functionals improves the description of the adiabatic potential energy surfaces, compared to both GGA and hybrid functionals, leading to an improvement in calculated luminescence lineshapes. In these applications, SCAN seems to be the best choice providing better precision than GGA and also hybrid functionals. As a result of these findings, we recommend using the SCAN family of functionals as a promising alternative for studying color centers in solids, in particular in calculations of the properties involving electron-phonon interactions.

12. Erlend Ousdal, Univ. Oslo: “Optical and electrical characterization of potential single photon emitters in 6H-SiC”

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Point defects in semiconductors are a highly anticipated platform for quantum technology (QT) with the advantage of being scalable, potentially operative at room temperature, and relatively inexpensive to make and maintain. Moreover, for some of the material platforms where quantum friendly defects have been demonstrated, such as silicon (Si) and silicon carbide (SiC), there already exists a mature infrastructure for the fabrication of components. Several point defects in SiC have proven to be single photon sources (SPEs) [1], which is of great interest in quantum applications. The majority of research on SiC has been done on the 4H polytype, where several SPEs have been identified, including the silicon vacancy (V_{Si}) [2], the carbon antisite-carbon vacancy (CAV) pair [3] and the divacancy ($V_{Si}V_C$) [4].A limited focus, however, has been given to other polytypes such as 6H SiC, which is of similar crystal structure as 4H.

In this work, we study 6H SiC for the purpose of increasing the knowledge and understanding of properties that can be exploited for QT. In particular, the configuration and energy difference of relevant defects are compared between the 4H and 6H polytypes.

We characterize a highly doped epi-layer of 6H SiC having free carrier density of $N_D \sim 6\times10^{17}cm^{-3}$ both optically and electrically, using photoluminescence (PL) and deep-level transient spectroscopy (DLTS) measurements. The samples were subjected to irradiation of protons at an energy of 1.8 MeV with different fluences and annealing at varying temperatures in inert atmospheres. The result is a mapping of how the point defects behave with the purpose of increased control of defect manipulation.

So far, all the three abovementioned point defects have been identified optically, with clear dependencies of both fluence and annealing temperature. Indeed, defect levels are observed to be different in the two polytypes, and comparison between processing dependencies is in progress. In addition, DLTS measurements have been able to prove the existence of a defect level in an as-received sample of the 6H polytype, however there is still a need to identify the source of this signal, and to compare it with the PL data.

In the complete work, a full mapping of quantum defect dependencies on fluence and annealing temperature in 6H SiC, and a comparison with 4H SiC, will be presented. The results will mainly concern optical identification from PL with complementary electrical measurements.

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13. Houwei Pang, Zhejiang Univ.: "Oxygen vacancies in gallium oxide and its sensitizing luminescence effect on rare earth ions"

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Recently, as an emerging widegap semiconductor, gallium oxide (Ga_2O_3) has aroused extensive interest in the fields of power devices, solar-blind detectors, and transparent conductors, due to its ultrawide bandgap, high breakdown field, as well as outstanding stability [1]. For the most stable β-Ga_2O_3 phase, progresses in the aspects of the bulk crystal growth, film epitaxy, and the demonstration of the electronic devices have been made. However, in view of the frequent deviation of the composition from the stoichiometry, together with the considerable inequivalent sites of Ga and O in the monoclinic crystal structure, abundant native point defects exist in β-Ga_2O_3. Among all the point defects, oxygen vacancies which serve as main donors seem to play significant roles in the electrical properties of β-Ga_2O_3 [2]. Nevertheless, because of the relative low concentration ($<10^{19}$ cm^{-3}), the oxygen vacancies are hard to detect and manipulate, which hinders the development of high-performance Ga_2O_3 related devices. Principally, the donor oxygen vacancies can also act as the luminescence centers via the donor-acceptor pair recombination, which can be transferred to other activators, such as the common rare earth ions, sensitizing the intense luminescence in various wavelengths. As a result, oxygen vacancies can be indirectly identified from the photoluminescence (PL) of Ga_2O_3 hosts, while the concentration can be compared with the help of the emission intensity of the rare earth ion activators.

Herein, we deposited Ga_2O_3 and erbium (Er) doped Ga_2O_3 films on silicon substrates by sputtering. The existence of oxygen vacancies in Ga_2O_3 was identified by means of PL, and the energy transfer between oxygen vacancies and Er^{3+} ions was demonstrated [3]. We fabricated light-emitting devices based on the Er doped Ga_2O_3 films and realized the Er^{3+} ions related electroluminescence in the visible and communication wavelengths assisted by oxygen vacancies. For the purpose of enhancing the concentration of oxygen vacancies, we changed the annealing atmosphere and modulated the sputtering ambient. It is found that annealed in N_2, the concentration of oxygen vacancies could be maintained, while sputtering in pure argon atmosphere made the composition of Ga and O deviate from the stoichiometry, resulting in extra oxygen vacancies. Such sensitizing effect of oxygen vacancies could also be found in europium (Eu) and thulium (Tm) doped Ga_2O_3 systems.

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14. Christian Pederson, Univ. Washington: "Imaging Surface Transfer Doping of Quantum Point Defects in Diamond Using Electrical Atomic Force Microscopy Techniques"

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Quantum technologies based on point defects in diamond, either as sensors or qubits, require maintaining a desired defect charge state nanometers from a surface. Typically the charge state is controlled by chemically modifying the surface and detected by analyzing the spectra of optically active defects. However, only a small fraction of defects possess charge states with bright optical transitions, their spectra provide limited information about the nature of the charge transfer, and the measurement is complicated by photoionization due to optical excitation. Here we demonstrate that electric-based atomic force microscopy techniques such as conductive atomic force microscopy (C-AFM) and Kelvin probe force microscopy (KPFM) can be used directly to image the charge of quantum point defects formed by ion implantation and annealing in diamond with high spatial resolution. Furthermore, these measurements provide a way to differentiate between similar surface termination methods, such as hydrogenated surfaces prepared via plasma processing versus high-temperature annealing in forming gas, as well as detect spatial inhomogeneity within the same passivation method. We demonstrate that by combining these electrical measurements with the optical measurements of a desired charge state, surfaces with desired fermi levels can now be identified and characterized with the future potential to study arbitrary optical excitation conditions.

15. Amanda Portoff, Lehigh Univ: “Hydrogen centers as a probe of V_{Ga2} in β-Ga_2O_3”

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While a number of O-H and O-D lines have been observed for hydrogen and deuterium in β-Ga_2O_3, it has been commonly reported that there is no absorption for the polarization with **E**//[010] [1,2]. This experimental result has led to O-H and O-D defect structures that involve split configurations of a vacancy at the tetrahedrally coordinated Ga(1) site and have ruled out structures that involve a vacancy at the octahedrally coordinated Ga(2) site because these structures are predicted to show absorption for **E**//[010] [1,2].

Weak O-D lines at 2467, 2475 and 2493 cm^{-1} with components of their polarization with **E**//[010] have been discovered for β-Ga_2O_3 grown by the Czochralski method that was annealed in a D_2 ambient [3]. SIMS results show that these samples contain high concentrations of Fe and Ir impurities. Theory has considered O-D defect structures involving an unsplit V_{Ga2} defect and also the “a” configuration of V_{Ga} that includes V_{Ga1} and V_{Ga2} half vacancies as possible assignments for these O-D lines. An estimate is made for a lower limit of the concentration of V_{Ga2} defects in the samples from the intensities of the IR absorption lines.

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16. Michael Reshchikov, Virginia Commonwealth Univ.: “Effect of ion implantation damage on photoluminescence from GaN”

Michael Reshchikov[1], Oleksandr Andrieiev[1], Mykhailo Vorobiov[1], Kacper Sierakowski[2], Rafal Jakiela[3], Piotr Jaroszynski[2], Akira Uedono[4], Michal Bockowski[2]

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Ion implantation is used for selective area doping of n- and p-type regions of GaN-based devices. In particular, there have been many attempts to fabricate p-type GaN by implanting Mg, Zn, and Be acceptors. Post-implantation annealing at temperatures higher than 1000 °C is needed to recover the implantation-induced damage. Since GaN decomposes at these temperatures, ultra-high-pressure annealing (UHPA) with nitrogen ambient pressure up to 1 GPa can be used [1]. While the impurities for p-type doping diffuse well at $T_a > 1200$ °C, significant concentrations of point defects may remain in the implanted region. In this work, we study defects created in GaN after implantation with Be and Zn ions and their effect on photoluminescence (PL). Zinc ions were implanted in c-plane GaN with an energy of 230 keV and fluence 10^{16} cm^{-2}. According to implantation profile simulations and secondary-ion mass-spectrometry (SIMS) measurements, the concentration of Zn is between 10^{20} and 10^{21} cm^{-3} in ~0.2 mm-thick near-surface region and then abruptly drops. After 30 min of UHPA at T_a = 1250-1400°C Zn diffuses by up to ~ 1 mm, where [Zn] = 10^{18}-10^{19} cm^{-3}. However, the concentration of Zn in the implanted 0.2 mm-thick layer remains unchanged. Positron annihilation spectroscopy (PAS) studies indicate that complex defects involving gallium and nitrogen vacancies (V_{Ga} and V_N) are abundant near the surface, and their concentrations decrease substantially after UHPA in the region beyond the implantation. Similarly, after UHPA of Be-implanted GaN (with the energy of 200 keV and a dose of 2.9×10^{15} cm^{-2}) a near-surface peak in Be concentration (~10^{19} cm^{-3} in top 1 mm) remained [2]. We studied PL from GaN implanted with Zn and Be and annealed with UHPA. In addition, to get PL signal from regions beyond the implantation peak, the samples were mechanically lapped and polished. After the lapping, strong and narrow exciton lines were observed in GaN:Zn and GaN:Be, indicating high optical quality. Bright blue luminescence (BL_{Zn}) band in GaN:Zn is attributed to the Zn_{Ga} acceptor, and a broad yellow band (YL_{Be}) in GaN:Be is assigned to the Be_{Ga} acceptor. The latter is confirmed by the characteristic behavior of PL, including two-step quenching. PL spectra from the implanted region (before lapping) contained additional features. Namely, for both GaN:Zn and GaN:Be, a red-yellow band spread from 1.5 to 2.3 eV. It red-shifted by more than 0.1 eV with decreasing excitation intensity, and no separate PL bands could be resolved by changing the measurement conditions. We propose that this band (or a superposition of PL bands) is related to complexes containing the V_{Ga}. Broad PL bands in this spectral region were previously observed in ammonothermally grown GaN and attributed to complexes containing V_{Ga}, H, and O_N [3]. This assumption also agrees with our PAS results.

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17. Connor Roncaioli, Army Research Lab.: “All In One Quantum Diamond Microscope for Rapid Sample Characterization”

Connor Roncaioli[1], Don Fahey[1], Connor Hart[2]

[1]Army Research Laboratory, [2]University of Maryland

Nitrogen Vacancy (NV) defects in diamond host optically pumpable spin-1 states with long coherence times which are ideal for room temperature magnetometry. Samples can be engineered to have part-per-million NV density, creating robust, portable, vectorized magnetic sensors with high spatial resolution. We present an all-in-one apparatus which can simultaneously measure NV ensemble quantum coherence properties across mm-scale regions, as well as classical properties such as diamond substrate and active layer strain and NV charge state, allowing us to characterize NV diamond samples rapidly for magnetometry applications.

18. Michael Scarpulla, Univ. Utah: “Defect Quasi Fermi Levels in Photoluminescence: Are they true thermodynamic potentials?”

Henry Silverman[1], Eric Klossner[1], Nathan Rock[1], Gerald Stringfellow[1], Mike Scarpulla[1]

[1]University of Utah

In this work, we investigate defect-related photoluminescence in semiconductors using two parallel well-established frameworks: detailed rate laws for bands and defect states conserving electrons, and the generalized Planck's law built upon photon statistics. Within this effort, we also examine two fundamental questions with further-reaching implications:

1) Under what conditions do defect Quasi-Fermi Levels (dQFLs) behave as thermodynamic chemical potentials for localized electrons and holes and thus the potentials driving carrier transitions?

2) Are band to band and defect-related photoluminescence transitions governed by the same or different chemical potential difference in the generalized Planck Law?

The answers to these questions are not well established, and certainly understood by even fewer than the thermodynamic roles of band quasi-Fermi levels. Answering these questions will allow better understanding of how to interpret defect-related luminescence and e.g. relate it to quasi-Fermi level splitting in PV absorber materials. Additionally, establishing when dQFLs are thermodynamic potentials helps to address unanswered questions about semiconductor defects' energetics under non-equilibrium processing or operation.

We build the carrier model conventionally, assuming the rates of all transitions whether phonon- or photon-mediated are proportional to the available electrons in the initial state and empty final states. We consider both defect-to-band transitions (and thus band tails as a sub-case) and donor-acceptor-pair (DAP) transitions. Such a system of equations allows the occupations of defects to be calculated and from those, dQFLs. Using the same assumed densities of states, we compare to predictions from generalized Planck law, with and without resorting to the van Roosbroeck-Shockley relation. As expected, since both capture and emission are rapid, we find that shallow dopants share QFLs with their bands. In this situation, it is clear that the dQFL acts as a proper chemical potential that can be used for calculating energy fluxes. However once emission transitions become limited by Boltzmann success factors as defects become deep, the situation becomes more complex. We discuss our results and the implications for issues like formation of defects during material processing and device operation.

19. Michael Scarpulla, Univ. Utah: "Measuring the Static and Dynamic Disorder in β-Ga_2O_3 Using Optical Transmission"

Ariful Islam[1], Nathan Rock[2], Michael Scarpulla[1, 2]

[1]Department of Electrical and Computer Engineering, University of Utah, Salt Lake City, USA,
[2]Department of Materials Science and Engineering, University of Utah, Salt Lake City, USA

Gallium oxide (Ga_2O_3) has an extremely wide bandgap, predicted high breakdown field, and can be produced from melt crystal growth techniques making it attractive for next-generation high-power electronics. It is well-known that the optical transitions in monoclinic β-Ga_2O_3 are anisotropic; the threshold energies for carrier generation using linearly polarized light depend on crystallographic direction. Using transmission optical spectroscopy, which probes subtly differently than e.g., ellipsometry, we have investigated the optical transitions of Fe doped [100] β-Ga_2O_3 as a function of elevated temperature, and have documented the dramatic bandgap narrowing with temperature, which was recently explained using density functional theory [1]. In addition, we have done the optical transmission of Sn doped [010], [001], [-201] at room temperature and liquid nitrogen temperature. We elucidate the differences between ellipsometric and transmission measurements and demonstrate that transmission measurements in the literature have determined erroneous values for the bandgap because of very strong Urbach tails. We report on the anisotropy and doping dependencies of the disorder-induced tails in the optical absorption coefficient for β-Ga_2O_3 and separate the tails into static and dynamic disorder induced by phonons. Given the low symmetry of β-Ga_2O_3 and its strong electron-phonon coupling, we observed that the Urbach energy increases at elevated temperature due to the contribution of static and dynamic disorder and exhibit significant anisotropy. However, at liquid nitrogen temperature (77K), the Urbach energy for Fe-doped crystals decreases as dynamic disorder is suppressed but at elevated temperatures, it increases. We also show that in the case of room temperature and liquid nitrogen temperature for Sn doped crystal. We analyze the dynamic and static components within the model of Cody et al., [2] and find that the static disorder is actually dominant. We discuss the possible microscopic origins in terms of point and extended defects; interestingly at low absorption coefficients, even imperfect surface polishing may contribute. We combine the temperature dependences of the Urbach tails from our measurements with those of the optical transitions from ellipsometry [3], [4] to extract the mean square displacement-deformation potential product for Ga2O3 along different crystal directions. These parameters play roles in optical transitions and carrier scattering and are thus critical to measure. We elucidate open questions and opportunities especially for further theory and calculation to predict the implications on multiple properties of wider interest than the Urbach tails per-se.

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20. Andrew Venzie, Lehigh Univ.: “Diffusion of Interstitial Hydrogen in SnO_2”

Andrew Venzie[1], Michael Stavola[1], W. Beall Fowler[1], Lynn A. Boatner[2]

[1]Lehigh University, [2]Oak Ridge National Laboratory

Hydrogen impurities give rise to n-type conductivity in the well-known transparentconducting oxide, SnO_2 [1]. Interstitial H (H_i) and H at an oxygen vacancy (H_O) are both shallowdonors in SnO_2 [2,3]. An O-H vibrational line at 3155 cm^{-1} has been assigned to the H_i centerand is unstable at room temperature on a timescale of weeks. An IR absorption study of thedecay kinetics of the 3155 cm^{-1} center has been performed to determine the activation energyfor H_i diffusion.

SnO_2 samples for our experiments were bulk, rutile-phase, single crystals grown by thevapor transport method [4]. As-grown crystals contained a sufficient concentration of H for ourexperiments, and no further H had to be added.

Annealing H-containing samples at $500^{\circ C}$ in an inert ambient followed by a rapid quenchto room temperature in water produced the 3155 cm^{-1} line due to H_i . The decay of H_i was thenstudied for a range of temperatures from room temperature to $120^{\circ C}$. After a sequence ofisothermal anneals, the 3155 cm^{-1} line could then be recovered by another anneal at 500°C andquench without significant loss of H from the sample.

The disappearance of H_i upon annealing has been found to follow second order kinetics. Measurements of the decay rate for a range of temperatures have determined an activationenergy for the diffusion of interstitial H in SnO_2 .

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21. Tom Verstijnen, Eindhoven Univ.: “Atomic scale analysis of N dopants in InAs”

Tom Verstijnen[1], Douwe Tjeertes[1], Edoardo Banfi[1], Qiandong Zhuang[2], Paul Koenraad[1]

[1]Eindhoven University of Technology, [2]Lancaster University

The band gap of most III-V semiconductors is strongly reduced with the introduction of only a few percent of N, even if the III-N alloy has a much bigger band gap. N impurities in InAs introduce an impurity state around 1 eV above the conduction band minimum, much deeper in the band than in other III-V materials. Topographic scanning tunneling spectroscopy measurements (STS) and areal spectroscopy measurements performed on N atoms up to two layers below the (110) surface of InAs show a reduction of the resonance energy of the N atom with increasing depth. This is attributed to tip induced band bending, pulling the N states up at positive bias and acting most strongly on surface N atoms. STS measurements obtained on undoped InAs and N-doped InAs show a similar band gap, due to band bending and electron accumulation effects at the InAs-vacuum interface. Spectroscopy maps of N atoms up to two layers below the surface provide a high resolution spatial and spectroscopic view of the N atoms. Here the characteristic shape of the N atoms in different layers below the surface is observed as an enhancement of the dI/dV signal compared to the InAs background. At energies above the enhancement a reduction of the dI/dV is observed, which has the same shape and size as the enhancement. This shows that the redistribution of density of states caused by the N impurities is mainly energetic in nature.

22. Darshana Wickramaratne, Naval Research Lab.: "Assessing the SCAN functional for point defects and polarons"

Darshana Wickramaratne[1], John Lyons[1]

[1]US Naval Research Laboratory

Accurate first-principles calculations of point defects in semiconductors are now possible due in part to the ability to reliably describe the electronic structure of semiconductors using hybrid functionals (eg. HSE06). However, the large computational cost of hybrid functionals severely limits their use when performing a comprehensive investigation of defect properties across a wide range of materials.
Here we assess the performance of the recently developed strongly-constrained and appropriately-normed (SCAN) functional to describe the properties of native point defects, impurities and polarons across a diverse range of semiconductors (III-nitrides, oxides, alkali halides). The SCAN functional has recently been extensively used to study a wide range of semiconductors since it overcomes deficiencies associated with conventional functionals (GGA, LDA) without any additional computational cost. We use the SCAN functional to calculate formation energies, thermodynamic transitions levels and optical transition levels and compare these results against those obtained using a hybrid functional. Based on this analysis we discuss potential advantages and pitfalls when applying the SCAN functional to describe defects in semiconductors.

Wednesday, September 13th

Parallel Sessions

Silicon carbide (II) – Swan Ballroom

Chairperson: Chitraleema Chakraborty, University of Delaware

8:20-9:00 AM "Laser Writing' of Silicon Vacancy Qubits in 4H SiC"
(invited presentation)

Evelyn Hu, Aaron Day, Jonathan Dietz, Madison Sutula, Matthew Yeh

Harvard School of Engineering and Applied Sciences

In recent years, “defects” in materials such as diamond and SiC hold promise as possible quantum mechanical bits (qubits). The power of such defects lies in their ability to manifest coherent spin states which can be initialized and read-out by optical signals. The focus of this talk will be on Silicon Vacancies in 4H SiC. The engineered creation of such defects has principally used techniques that direct the kinetic energy of charged beams (ion implantation, electron irradiation) to break bonds to create the defects. We will discuss a recently developed process that uses a laser to “write” Silicon Vacancies directly into photonic crystal cavities. The laser utilizes a frequency corresponding to photon energies above the bandgap of the 4H SiC, and the photonic crystal cavity has been designed to selectively amplify the photon signature of the Silicon Vacancy. The technique provides near real-time, direct feed back on the defect creation process, allowing us to ultimately understand the minimum energies and the optimal conditions required to form such qubits.

9:00-9:20 AM “Magnetometry using point defect ensembles in isotopically pure 4H-SiC”

Ignas Lekavicius[1], Samuel Carter[1], Rachael Myers-Ward[1], Kurt Gaskill[1], Samuel White[2], Daniel Pennachio[1], Jenifer Hajzus[3], Andrew Purdy[1], Andrew Yeats[1]

[1]US Naval Research Laboratory, [2]NRC Research Associate at NRL, [3]ASEE Research Associate at NRL

Optically active spin defects in solid state materials are promising systems in the fields of quantum information, communications and sensing. Particular to sensing, defects with coherent spin transitions are highly suited for magnetic sensing with high spatial resolution and low working distances at ambient conditions. Applications involving magnetic sensing with point defects have mostly been dominated by the nitrogen vacancy center in diamond, which possesses an excellent combination of spin coherence at room temperature as well as spin initialization and readout. However, spin defects in other materials have been explored as alternatives, especially in industrially mature materials such as silicon carbide. In this work we report on the improved sensitivity of a magnetic sensor system utilizing an ensemble of silicon vacancies in silicon carbide due to isotopic purification [1] of the host crystal. A near dc sensitivity of 4 nT/rt(Hz) is demonstrated in our system with a calculated shot noise limited sensitivity of 200 pT/rt(Hz) [2]. In addition, the S=3/2 ground state of the defect allows for highly broadband ac magnetic sensing from 10 MHz up to ~1 GHz with moderate applied magnetic fields.

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9:20-9:40 AM “Depth-resolved investigation of N and P ion-implantation induced defects in 4H-SiC”

Maria Mendes Martins[1], Piyush Kumar[2], Marianne Bathen[2], Ulrike Grossner[2], Thomas Prokscha[1]

[1]1Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, Switzerland, [2]Advanced Power Semiconductor Laboratory, ETH Zurich, Switzerland

Selective doping of silicon carbide (4H-SiC) is necessary to obtain well defined regions with precise doping concentrations. In SiC, this is only possible with ion implantation due to the low diffusivity of the material. The n-type regions require implantation of N or P [1]. Importantly, the implantation process leads to the formation of point defects, such as vacancies and interstitials [2]. A follow-up post-implantation annealing (PIA) treatment at high temperatures is needed to electrically activate the dopants and recover the lattice damage. Such high temperatures could also be expected to lead to complex formation between the primary point defects.

N- and P-implanted 4H-SiC samples, with doping concentrations of 10^{17} and 10^{18} cm^{-3}, were investigated with low-energy muon spin-rotation spectroscopy (LE-µSR), deep level transient spectroscopy (DLTS) and minority carrier transient spectroscopy (MCTS). Implantation was performed with different ion energies to obtain a uniform box-like implantation profile in the first 250 nm of SiC and was followed by PIA at 1700 °C for 30 minutes.

With LE-µSR and DLTS/MCTS, it is possible to study defects created due to ion implantation in a wide depth range. The implanted positive muon is sensitive to the presence of defects and charge carriers in its environment and can probe SiC with nanometer depth resolution from near the surface and up to ~150 nm depth [3, 4]. With LE-µSR, information about the activation of donors can be extracted as a function of depth in the implanted region, and electrically active defects can be identified. DLTS/MCTS provides information about concentration and energetic position of defects present in SiC at larger depths in the region of 500 nm to 1 µm, where DLTS/MCTS shows the presence of defects well beyond the implantation profile of 200-300 nm, where the concentration of the dopant species is reduced. To probe the region beyond the implantation profile, additional

LE-μSR measurements will be performed to extract the distribution of defect concentration in the implantation tale, after etching the 200 nm implanted region of SiC. In the final contribution, a detailed analysis of the DLTS/MCTS results and the distribution of defects created during implantation will be presented.

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[2] A. Hallén, *et al.*, Nucl. Instrum. Methods Phys. Res. B 186:186-94 (2002)
[3] J. Woerle, *et al.*, Phys. Rev. Applied 14, 054053 (2020)
[4] P. Kumar, *et al.,* Phys. Rev. Applied 19, 054025 (2023)

9:40-10:00 AM

“Interface and bulk defects induced by the thermal oxidation and post-oxidation annealing in SiO_2-SiC system”

Piyush Kumar[1], Maria Martins[1, 2], Marianne Bathen[1], Thomas Prokscha[2], Ulrike Grossner[1]

[1]Advanced Power Semiconductor Laboratory, ETH Zurich, [2]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute

Thermal oxidation at high temperatures is one of the crucial steps in the fabrication of a SiC metal oxide semiconductor field effect transistor (MOSFET). SiO_2 is used as gate oxide for the MOSFET which offers the benefits of high thermal stability and ease of fabrication. However, despite high temperature oxidation and post-oxidation annealing (POA) treatments, the devices suffer from low mobility due to high concentration of defects at and near the SiO_2-SiC interface. In this work, we have explored the impact of thermal oxidation and POA in nitric oxide (NO) and argon (Ar) environment on the resulting structure. We have performed capacitance-voltage (CV) and conductance measurements to study the defects at the SiO_2-SiC interface, low-energy muon spin rotation (LE-μSR) spectroscopy and positron annihilation spectroscopy (PAS) to study the near-interface region, deep level transient spectroscopy (DLTS) and minority carrier transient spectroscopy (MCTS) to study defects in the bulk of the semiconductor, and above bandgap optical excitation to study the near interface oxide traps (NIOTs).

The DLTS measurements reveal the generation of several bulk defects in SiC: $E_{0.23}$ at 0.23 eV, $C_{1/2}$ at 0.36/0.39 eV, ON1 at 0.85 eV, $ON2_{a/b}$ at 1.05/1.167 eV and ON3 at 1.76 eV below the conduction band (E_C) edge. The injection of carbon interstitials during thermal oxidation is predicted to be responsible for several of the above-mentioned defects. Additionally, the defect concentration is substantially increased after annealing in NO environment at 1300 °C. MCTS measurements further reveal the generation of the $O_{0.17}$ and B levels, which are located 0.17 eV and 0.28 eV above the valence band edge (E_V). Measurements of the defect depth profiles reveal a reduction in the defect concentration with depth, allowing us to estimate the diffusivity and the migration barrier of the defects.

Using LE-μSR measurements, we have observed signatures of silicon vacancies (V_{Si}) in the SiC near the interface after thermal oxidation. We have also observed a substantial increase in the carrier concentration in the near interface region (up to 100 nm from the interface) due to the incorporation of nitrogen (N) after NO annealing in the SiC crystal. Transmission electron microscopy (TEM) and PAS measurements also bolster the hypothesis of V_{Si} generation during thermal oxidation. CV measurements confirm a high concentration of defects at the interface which are reduced by post oxidation annealing in the NO/Ar environment whereas the conductance measurements help extract the emission time constants and the capture cross section of these defects. Further, we have also carried out optical excitation experiments with above bandgap light to probe the NIOTs at the valence band. Charging and discharging of these defects during device operation could lead to threshold voltage instability.

In the final contribution, we discuss the results in detail and attempt to build a scenario of the defects created in several regions of the oxide-semiconductor system due to thermal oxidation and POA in NO and Ar at different temperatures.

10:00-10:20 AM **Coffee break**

Oxides (I) – Sanibel

Chairperson: Mary Ellen Zvanut, University of Alabama-Birmingham

8:20-8:40 AM “Properties of Donor Qubits in ZnO Formed by Indium-Ion Implantation”

Xingyi Wang[1], Christian Zimmermann[1], Michael Titze[2], Lasse Vines[3], Vasileios Niaouris[1], Samuel H. D’Ambrosia[1], Ethan Hansen[1], Edward S. Bielejec[1], Kai-Mei C. Fu[1, 4]

[1]University of Washington, [2]Sandia National Laboratories, [3]University of Oslo, [4]Pacific Northwest National Laboratory

The indium substitutional donor (In^0_{Zn}) in ZnO is an emerging semiconductor spin qubit with optical access via the donor-bound exciton ($In^0_{Zn}X$). The optical and spin properties of in ZnO formed via indium ion implantation and subsequent annealing are on par with those of *in situ*-doped donors [1]. The inhomogeneous linewidth of the donor-bound-exciton transition is less than 10 GHz, comparable to the optical linewidth of *in situ* In ensembles in commercially-available ZnO single crystals. The longitudinal spin relaxation time (T_1) of implanted is measured to be 4 ms at 7 T, four times longer than what has been found for in-grown Ga donors in our previous work [2], indicating that residual In-implantation damage does not degrade T_1. T_1 increases with decreasing magnetic field following the expected inverse power-law [3]. Optical pumping and coherent population trapping (CPT) of the implanted In^0_{Zn} is shown using two resonant lasers at 7 T. Two-laser Raman spectroscopy of the donor spin reveals the hyperfine interaction of the donor electron with the spin-9/2 In nuclei. This work is an important step toward the deterministic formation of In-donor qubits in ZnO with optical access to a long-lived nuclear-spin memory. We are experimenting with obtaining ZnO substrates free of indium defects for ion implantation, and progress has been made towards formation of single In^0_{Zn} with extra low implantation fluences and focused ion beam implantation.

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[2] Xiayu Linpeng, et. al., Phys. Rev. Appl. 10, 064061 (2018).
[3] Vasileios Niaouris, et. al., Phys. Rev. B 105, 195202 (2022).

8:40-9:00 AM

“Ti^{3+} centers in nonstoichiometric $KTiOPO_4$ from DFT calculations”

Adriana Bocchini[1], Wolf Gero Schmidt[1], Uwe Gerstmann[1]

[1]University of Paderborn, 33095 Paderborn, Germany

Potassium titanyl phosphate ($KTiOPO_4$, KTP) is a largely utilized ferroelectric crystal. Unfortunately, its application in nonlinear optical devices is limited by its characteristic photochromic damage, i.e., so-called gray tracking, which strongly impairs its transmission properties. Gray tracking is discussed to be related with the reduction of Ti atoms (i.e., Ti^{3+} centers) upon the charge compensation of different point defects. Four different Ti^{3+} centers have been resolved by magnetic resonance, whereby the thermally stable center is assumed to be related to oxygen vacancies [1]. On the other hand, empirical treatments reducing the number of potassium vacancies (e.g., a potassium-nitrate treatment [2]) or the ionic conductivity in KTP (e.g., a small rubidium doping [3]) are beneficial to enhance its resistivity against gray tracking. The microscopic mechanism behind gray-tracking, however, is still far from being completely understood. Neither the effects arising from the rubidium doping nor the interplay between potassium and oxygen vacancies have been systematically investigated, yet.

In the present study, we use density functional theory (DFT) to unravel the impact of these application-relevant nonstoichiometries on the Ti^{3+} centers and by this on gray tracking in KTP. Oxygen vacancies are modeled in rubidium-doped KTP (RKTP) as well as in potassium-deficient KTP ($K_{1-x}TiOPO_4$). We discuss the energetics as well as the electronic, optical [4], and magnetic [5] properties of the O-vacancy-related Ti^{3+} centers in these different chemical environments, whereby the defect models are validated by comparing their DFT-calculated hyperfine structure with the experimentally resolved hyperfine splittings [1]. This allows us to establish a complex picture of the gray-tracking formation mechanisms, where many second order effects can influence and trigger the actual origin behind Ti^{3+} centers reduced by nearby O-vacancies.

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9:00-9:20 AM

"Defect Identification in Atomic Layer Deposited Aluminum Oxide using Kelvin Probe Force Microscopy"

Leah Tom, University of Wisconsin-Madison

Leah Tom[1], Zachary Krebs[1], Joel Varley[2], Emily Joseph[1], Mark Eriksson[1], Keith Ray[2], Vincenzo Lordi[2], Victor Brar[1], Susan Coppersmith[3], Mark Friesen[1]

[1]University of Wisconsin-Madison, [2]Lawrence Livermore National Laboratory, [3]University of New South Wales

Kelvin Probe Force Microscopy (KPFM) measurements combined with Density Functional Theory (DFT) calculations are used to identify individual charged defects in an amorphous aluminum oxide layer grown via atomic layer deposition (ALD) atop bulk silicon. Charged defects in the oxide, especially those supporting multiple charge states, are an important source of charge noise in silicon-based quantum dot qubits, and thus defect characterization and identification are key to noise mitigation. Local variations in the work function found using KPFM reveal a high density of charged defects in the aluminum oxide layer. Sweeping the AFM tip-to-sample bias induces charging and discharging events near the surface, allowing us to probe the defects' different charge states. With the aid of electrostatic simulations, we extract the charging and discharging energies as a function of voltage bias. The sign and magnitude of a charge state can also be determined from KPFM measurements. Combining information about the charging energies with the sign and magnitude of the charged

states allows us to identify individual defects with high confidence, by comparison with DFT calculations. This work represents a unique and novel approach to imaging and identifying point defect distributions down to individual defects and can even distinguish multiple overlapping defects in some cases. Prepared by LLNL under Contract DE-AC52-07NA27344

9:20-10:00 AM “Migration of nitrogen impurity in titanium dioxide and perovskite titanates” *(invited presentation)*

Naoki Ohashi[1], Isao Sakatuchi[1], Hiroyo Segawa[1], Takeo Ohsawa[1], Yoshio Matsui[1]

[1]National Institute for Materials Science, Japan

Defects in oxide is an important issue in electronic and optical devices, such as dielectric capacitors, sensors, phosphors and semiconductors. Indeed, defects are sometimes source of functionality and, on the other hand, cause of properties degradation. It must be very important that defect structures must be investigated simultaneously with unintentional impurities as both are interacting through charge compensation.

In this paper, we focus on interaction between defects and impurities from the viewpoint of mass transport and charge compensation. At first, we re-visit defects in zinc oxide to discuss if native defects, such as oxygen vacancy, are the cause of electric conductivity. Then, this paper will focus on nitrogen impurity in oxides. Recently, a lot of studies on nitrides and oxynitride as well as nitrogen doping into oxide are conducted aiming to explore new functional materials and functionalization by nitrogen doping. For instance, nitrogen doping into titania is a technique to improve photocatalytic activity to visible light illumination, and some studies indicated that oxynitride exhibits very high dielectric permittivity.

In this study, we performed thermal treatment to oxides in ammonia containing atmosphere to know the behavior of nitridation and nitrogen insertion into oxides. Absolutely, usage of pure ammonia for thermal treatment often induces formation of nitrides or oxynitrides. Hence, we used not pure ammonia but oxygen/ammonia mixture for thermal treatment to see the nitrogen doping behavior in oxides. During such investigation, we happened to find very strange phenomena, that was oxide crystals were crushed into nano-sized powders by thermal treatment [1,2]. We performed analytical studies including STEM-EELS analyses, and finally concluded that crystals were crushed by deposition of nitrogen molecule (N2) in oxide induced by thermal treatment in oxygen containing ammonia. We will discuss mass transport in oxide crystals heated in ammonia containing atmosphere using the models constructed using DFT calculations.

N. Ohashi et al., J. Am. Ceram. (2022) [DOI:10.1111/jace.18200]

A. Noviyanto et al., J. Euro. Ceram. Soc. (2016)
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10:00-10:20 AM **Coffee break**

Parallel Sessions

Diamond (I) – Swan Ballroom

Chairperson: Jeffrey McCallum, University of Melbourne

10:20-10:40 AM “First-principles calculation of the Stark shift for the NV center in diamond”

Louis Alaerts[1], Yihuang Xiong[1], Sinéad Griffin[2], Alp Sipahigil[3], Geoffroy Hautier[1]

[1]Dartmouth College, [2]Lawrence Berkeley National Laboratory,
[3]University of California, Berkeley

Color centers in semiconductors are promising candidates for several applications in quantum information sciences such as quantum computing, communication or sensing. Acting as single-photon sources, they provide the robust spin-photon interface needed for the distribution of entanglement in quantum networks. However, this requires a high level of indistinguishability between emitted photons, which is limited by the sensitivity of defects to the environment. Mechanical and electrical fluctuations in the vicinity of the defects will cause a shift of their optical zero-phonon-line (ZPL), an effect known as spectral diffusion. Spectral diffusion is a major technological issue in the deployment of high-performance quantum defects. Stark shift caused by stray electric field is usually considered as the main cause of spectral diffusion. Here, I will present the results of our first principles computation of the Stark shift on the negatively charged nitrogen-vacancy (NV) center in diamond. Using a slab model, we monitor the Stark shift by calculating the energy difference between the ground-state and the excited-state as a function of an applied electric field. We discuss the methodological challenges involved with charged slabs and compare our results with our own and previous computations using Modern theory of polarization. We discuss the advantages of the slab approach and issues with the Modern theory of polarization approach. We also compare the effect of different functionals including hybrids, compare to experimental data and provide a perspective of Stark shift computations on other quantum defects.

10:40-11:00 AM “Coherent Orbital Control of Diamond NV Center Excited States Using Strain”

Brendan McCullian[1], Huiyao Chen[1], Johnny Crossman[1], Gregory Fuchs[1]

[1]School of Applied and Engineering Physics, Cornell University

The spectrally narrow, spin-dependent optical transitions of solid-state defects can be leveraged for quantum networking applications. The best-characterized defect in this field is the nitrogen-vacancy (NV center) in diamond, however, NV centers exhibit spectral diffusion that limits the entanglement generation rate that lies at the heart of this application. The largest source of spectral diffusion is electric field fluctuations that couple to the excited-state orbital doublet. To better understand potential mechanisms of dynamically engineering NV center optical transitions, we investigate quantum control of the excited state orbitals via dynamic strain-orbital driving with an acoustic wave resonator. We demonstrate nanosecond, multi-phonon orbital Rabi oscillations in the time domain, where the orbital states are resonantly driven by GHz frequency acoustic waves. The Rabi oscillation frequencies agree well with the spectroscopic splitting that we observe by probing the driven orbital states of the NV center using a tunable laser. Such resonant orbital quantum control can enable strategies for dynamically decoupling the NV center orbital states from spectral diffusion, thus protecting optical transitions from decoherence sources.

11:00-11:20 PM “Ab-initio theory of spin-lattice relaxation for NV center and other spin-1 defects by means of ab-initio calculations”

Gergo Thiering[1], Matthew C. Cambria[2], Ariel Norambuena[3], Yanfei Li[2], Hossein Dinani[3], Aedan Robert H. Gardill[2], Ishita Kemeny[2], Vincenzo Lordi[4], Jeronimo R. Maze[5], Shimon Kolkowitz[2], Adam Gali[1]

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[5]Instituto de Física, Pontificia Universidad Católica de Chile, Casilla 306, Santiago, Chile

Certain defects in diamond are promising candidates as building blocks for quantum computing. In particular, the nitrogen-vacancy (NV) center in diamond has become one of the leading contenders in solid-state quantum information processing due to its favorable properties. One of its particular property is its remarkably long spin coherence time: it can be 1 ms at room temperature and can even exceed the second regime at cryogenic temperatures. The remarkable spin properties of NV originates from its electronic structure because a S=1 spin embedded on an orbitally nondegenerate ($|^3A_2\rangle$) state can interact with phonons only perturbatively. In our present work, we will describe the spin-lattice interaction between S=1 electronic spin of NV and lattice phonons by means of DFT ab-initio tools and experimental measurements of temperature from 9 to 474 K in high-purity samples[1].

While the decoherence (T_2) and relaxation (T_1) induced by naturally abundant (1.1%) ^{13}C spins can be suppressed by means of ^{12}C purification the above mentioned spin-lattice relaxation can not be avoided this way as it is an intrinsic property of the defect center. However, the effect of phonon bath is heavily temperature dependent thus can be quenched on sufficiently low temperature. Therefore, we will review the first and second order (Raman) spin-lattice relaxation processes acting between NV's $|ms = 0\rangle \leftrightarrow |ms = +1\rangle \leftrightarrow |ms = -1\rangle$ spin sublevels. In our best knowledge only the cryogenic regime below 1 K were discussed for NV by ab-initio tools succesfully[2]. On the other hand, the spin-phonon relaxation recipe were already applied for small molecular spin magnets[3], thus the discussion of phonon continuum can be avoided. Consequently, in the present work we will describe the second order Raman transitions that dominate relaxation at high temperatures. Informed by the full ab-initio spin-phonon spectral function $F(\hbar\omega,\hbar\omega')$, we propose a novel analytic model in which NV spin-phonon relaxation is characterized by interactions with two distinct groups of quasi-localized phonons centered at 68.2(17) and 167(12) meV. We also discuss the symmetry requirements for such processes where the spin moment is transferred ($\Delta S=\pm1,\pm2$) towards the lattice by two Raman phonons with either the same "$e_\pm$, $e_\pm$" or different "$a_{1,2}$, $e_\pm$" symmetry of point group C_{3v}. The latter process is accessible only upon sampling all offdiagonal $\hbar\omega\neq\hbar\omega'$ and requires dense (8×8×8) sampling on a q-point mesh to fulfill the $\hbar\omega\approx\hbar\omega'$ requirement appropriately.

In summary, we developed an ab-initio framework that can predict the spin-lattice relaxation and coherence times that can be applied on orbitally nondegenerate spin-1,3/2... qubit centers.

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[2] J. Gugler et al. Phys. Rev. B 98, 214442 (2018)[3] A. Lunghi, Sci. Advances 8, 31 (2022)

11:20-12:00 PM "Photoionization spectroscopy of the long-lived 1E singlet state of NV centers in diamond" *(invited presentation)*

Sean Blakley[1], Thuc Mai[1], Stephen Moxim[1], Jason Ryan[1], Adam Biacchi[1], Angela Hight Walker[1], Robert McMichael[1]

[1]National Institute of Standards and Technology, Gaithersburg MD

The nitrogen-vacancy (NV) center in diamond is valued for its accessible quantum properties and for quantum sensing applications. The NV's basic energy level diagram and optical cycle explain the NV's key characteristics and are well-understood. For applications, there are significant efforts to improve optical and electrical readout by controlling ionization and recombination between NV^- and NV^0 charge states. In this work, we use photoionization spectroscopy to determine the ionization energy of the long-lived ^1E singlet state, the final energy level in the optical cycle yet to be determined. In our measurement, we modulate the populations of the optical cycle states by applying and removing a 100 mT magnetic field, while observing the resulting amplitude changes in the NV^0 and NV^- photoluminescence spectra. The extensive measurements cover a region of parameter space spanning 488 nm to 560 nm in excitation wavelength, 1.5 μW to 40 μW in excitation power, and 1.6 K to 295 K in temperature. Ionization from ^1E indicated by field-induced increases in NV^0 photoluminescence is observed for excitation wavelengths 532 nm and below but not 550 nm and above. From this data, we conclude that the ionization threshold from the singlet is between 2.25 eV and 2.33 eV, in agreement with theoretical predictions based on of singlet-triplet transition rates. Subtle narrowing of the NV^0 zero-phonon line with the applied field is consistent with a reduction in charged defects. In addition to the ^1E ionization, the NV^- ground state $^3A_2$ ionization threshold near 2.7 eV shows an apparent temperature dependence. At the same time, a strong, zero-field, spin-mixing phenomenon between 10 K and 100 K is revealed.

[2301.10383v1] Spectroscopy of photoionization from the 1E singlet state in nitrogen-vacancy centers in diamond (arxiv.org)

12:00-12:20 PM "Predicting Defect Concentrations from Stark Shift Measurements"

Rodrick Kuate Defo[1], Alejandro W. Rodriguez[1], Efthimios Kaxiras[2], Steven L. Richardson[2, 3]

[1]Princeton University, [2]Harvard University, [3]Howard University

Nitrogen, the most common element in the atmosphere, is difficult to detect reliably in materials using the standard energy-dispersive spectroscopy (EDS) method. Employing wavelength-dispersive spectroscopy (WDS) improves detection at the cost of being a more destructive method. Our work enables non-invasive high-accuracy determination of nitrogen concentrations in diamond by evaluating the leading-order contributions to the Stark shifts of the optical frequencies of NV^- centers measured using optically detected magnetic resonance experiments. Our results have the potential to aid in predicting the potential for failure of semiconductor devices and in predicting and correcting the spectral diffusion that frequently hinders the generation of indistinguishable photons from single-photon emitters in crystals.

Other Materials (I) – Sanibel

Chairperson: Ross Kerner, National Renewable Energy Laboratory

10:20-11:00 AM “Excitation Power- and Temperature-Dependent Photoluminescence Studies of Cubic Boron Arsenide Bulk Crystals” *(invited presentation)*
Evan Glaser, US Naval Research Laboratory

Evan R. Glaser[1], Pawan Koirala[2], Sam White[3], J.A. Freitas, Jr.[1], J.C. Culbertson[1], John L. Lyons[1], Wenhao Liu[2], Aswin Kondusamy[2], Geethal Amila Gamage[4], Haoran Sun[4], Zhifeng Ren[4], Bing Lv[2]

[1]Naval Research Laboratory, [2]Dept. of Physics, U. of Texas at Dallas, [3]NRC Research Associate at the Naval Research Laboratory, [4]Dept. of Houston and the Texas Center for Superconductivity, U. of Houston

There is current interest in cubic BAs due to its high room temperature thermal conductivity (>1300 $Wm^{-1}K^{-1}$) [1] and the recently revealed high ambipolar (i.e., electron and hole) mobility values (1500-1600 $cm^2V^{-1}s^{-1}$) [2]. Given the thermal and electrical properties are expected to depend strongly on the concentrations of residual impurities and intrinsic lattice defects, it is imperative to obtain as much of an understanding as possible on the roles of these defects in this material system. We have employed photoluminescence (PL) to reveal defects participating in various radiative recombination processes. A variety of sharp and broad emission bands were observed in the PL spectra at 4K between 1.2 and 1.8 eV from multiple c-BAs bulk crystals grown by chemical vapor transport. Likely dependent on the concentrations of residual impurities (including silicon and carbon), the PL at 4K exhibited mainly excitonic recombination, donor - acceptor pair (DAP) recombination, or both of these processes. Detailed excitation power ($P_{exc.}$) and temperature dependent (4-300 K) studies were performed to provide more information on the nature and origin of these PL bands. Highlights include the large shifts (~100 meV) in the peak energies of two broad PL bands observed for one sample with $P_{exc.}$ density varied over six orders of magnitude. The peak energies (1.335 eV and 1.494 eV, respectively) found under very low $P_{exc.}$ are in excellent agreement with those predicted for C- and Si-related DAP recombination processes using a low temperature bandgap of ~1.80 eV [3] and the donor and acceptor binding energies calculated for these amphoteric impurities in c-BAs [3,4]. In addition, detailed fits made to these spectra revealed a third DAP-like emission band that also exhibited large shifts as a function of $P_{exc.}$ With a peak energy of 1.421 eV under low $P_{exc.}$, we tentatively assign this PL band to recombination between residual sulfur impurities and Si_B and/or C_B shallow acceptors due to the good agreement with the S_{As} energy level using hybrid density functional theory. Two more recently grown c-BAs samples exhibited a pair of previously unreported very sharp (FWHM ~0.4 meV) near bandgap PL lines with excitonic-like behavior (based on an excitation power study) at 1.7954 eV and 1.7962 eV, respectively. The temperature behavior of these lines and their possible origin(s) will also be discussed.

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The work at NRL was supported by the Office of Naval Research. The work at UT-Dallas was supported by the Office of Naval Research by grants N00014-19-1-2061 and N00014-22-1-2755. The work performed at the University of Houston was supported by the Office of Naval Research under Multidisciplinary University Research Initiative grant N00014-16-1-2436.

11:00-11:20 AM “Muons in semiconductor research: Recent review and looking forward”
Rick (P.W.) Mengyan, Northern Michigan University

Brittany Baker[1], Rick (P.W.) Mengyan[2]

[1]Francis Marion Univesrity, [2]Northern Michigan Unviersity

There has been a long history of contributions to the defect in ICDS community centered around utilizing muons as an experimentally accessible analogue to isolated hydrogen (H) impurities in materials. Specifically, in semiconductors, muons provide insight on the characteristics and behavior of isolated H impurity centers and complexes. These implanted muons can also be used to probe carrier distribution and dynamics.

Here we present an overview of the Muon Spin Research techniques relevant to studying isolated H impurities in semiconductors (including a technique in development to study excited states and carrier dynamics) as well as an overview of past and current works. Ordinarily, these recent works would have been presented in greater detail at the ICDS conferences; however, due to COVID and some significant changes in our research group we have not been able to make our usual turnout to recent conferences and would like the opportunity to share an overview of where we are at and where we are heading.

Materials our group has been working on over the last two decades relating to understanding the behavior and characteristics of isolated H impurities include those such as SiGe alloys, GaP, GaN, ZnO, CdO, II-IV-V2 Chalcopyrites including Mn doped $ZnGeP_2$ [room temp FM]), Ga_2O_3, 6H-SiC, CdO, In_2O_3, TiO_2 (rutile, brookite and anatase), VO_2, GaAs, SnO, CIGS compounds, CZTS compounds, BeO, Al_2O_3 and others.

11:20-11:40 AM “Electron-Spin-Resonance and Optical Signature of a V^{4+} center in Halide Double Perovskites $Cs_2NaInCl_6$”
Yuttapoom Puttisong, Linköping University

Yuttapoom Puttisong[1], Kunpot Mopoung[1], Anna David[1], Xianjie Liu[1], Mats Fahlman[1], Irina A. Buyanova[1], Weimin Chen[1]

[1]Linköping University

Doping of halide double perovskite (HDP) by metal ions has recently emerged as new revenue to tailor physical properties of lead-free and solution-processed semiconducting perovskites, highlighting target applications in optoelectronics and spintronics. Incorporating transition-metal ions such as Fe, Cr, and V into a B’-site of $A_2B(+1)B'(+3)X_6$ HDP host has led to many interesting properties such as bandgap tuning [1,2], highly efficient broadband near-infrared light emissions [3], and magnetic response [4]. However, introducing metal ions into the HDP can also lead to the formation of thermodynamically stable point defects that can impact the target applications either positively by e.g. introducing spin qubits and quantum emitters or negatively by e.g. reducing internal quantum efficiency. In this study, we show that doping of Vanadium (V) into $Cs_2NaInCl_6$ not only leads to a targeted V^{3+} isoelectronic substitution of In but also promotes the formation of a new V^{4+} defect. such center is unambiguously identified from our detailed electron spin resonance (ESR) studies of $Cs_2NaInCl_6$ single crystals, exhibiting a rich ESR spectrum arising from an effective electron spin S =1/2 and a nuclear spin I=7/2 (corresponding to ^{51}V with nearly 100% natural abundance). The determined electron g-factor and the hyperfine parameters are $g_x=g_y=1.973$, $g_z=1.945$, $A_x=A_y=180$ MHz and $A_z=504$MHz, with the principal axis z along a <001> crystallographic axis. Closely linked to the presence of the V^{4+} center, we also observed a broadband near-infrared light emission over

the spectral range of 815-1100 nm. Through a complementary and correlative analysis of the results from ESR, photoluminescence and photoluminescence excitation, we suggest the chemical origin of the studied V^{4+} center to an axial V^{4+}-O^{-2} complex where V^{4+} replaces In^{3+} at the B' site of the octahedral lattice and one of its nearest-neighbor Cl^{-1} is replaced by O^{-2}. We will also briefly present our ongoing study of other transition-metal ion doping (i.e., Fe and Cr) of $Cs_2NaInCl_6$, and highlight a potentially rich library of the spin- and optical-active centers in HDP that can be explored for quantum light and spin functionality beyond the presently known potential of semiconducting perovskites.

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11:40-12:00 PM "R-Cu Color Centers in ZnS:Cu Colloidal Nanocrystals and Potential Applications for Quantum Information Science"
Sarah Thompson, University of Pennsylvania

Sarah Thompson[1], Cüneyt Şahin[2], Shengsong Yang[1], Michael Flatté[3], Christopher Murray[1], Lee Bassett[1], Cherie Kagan[1]

[1]University of Pennsylvania, [2]Bilkent University, TR, [3]University of Iowa

Colloidal ZnS:Cu nanocrystals (NCs) are widely used in bio-imaging and optoelectronic applications due to their bio-inertness and their ability to emit light across a wide range of wavelengths. In this context, we explore the potential of ZnS:Cu colloidal NCs containing red-emitting, "R-Cu" color centers for defect discovery in quantum information science. Previous approaches to identifying point defects suitable for quantum spin-light interfaces in semiconductors have relied on ad hoc observations in bulk crystals. In contrast, we propose a deliberate process that involves synthesizing, modifying, and assembling lightly-doped colloidal nanocrystals to systematically identify and evaluate promising defect-host combinations. We have identified the R-Cu center in ZnS as one such combination, and we have reported a synthesis method for obtaining

colloidal NCs with photoluminescence emission dominated by R-Cu [1]. ZnS, as the host material, possesses a wide optical bandgap and a low concentration of nuclear spins, enabling the operation of an electronically isolated spin-light interface with low magnetic background noise. The R-Cu center, as the point defect of interest, is believed to possess a C3V-symmetric impurity-vacancy structure, which results in favorable orbital and spin characteristics for several known defect qubits. We have conducted first principles calculations that verify the electronic structure and thermodynamic stability of this proposed defect complex in ZnS:Cu. Additionally, we have employed ensemble time- and temperature-resolved luminescence spectroscopy to gain a deeper understanding of the R-Cu emission mechanism and electronic structure. We find that the R-Cu emission arises from thermally activated carrier transfer between two radiative manifolds, producing an anomalous plateau in the thermal quenching profile and blueshifted luminescence upon increasing temperature. Understanding of these characteristics and their relationship to the charge and spin states of the R-Cu center can inform the development of protocols for operating the center as a quantum spin-light interface.

[1] Sarah M. Thompson, Cüneyt Şahin, Shengsong Yang, Michael E. Flatté, Christopher B. Murray, Lee C. Bassett, and Cherie R. Kagan, Red Emission from Copper-Vacancy Color Centers in Zinc Sulfide Colloidal Nanocrystals. ACS Nano 2023 *17* (6), 5963-5973

12:00-12:20 PM

"Electronic and structural properties of rare-earth mono-pnictide (RE-V) nanoparticles in III-V semiconductors"

Ruiqi Hu1 , Dai Q. Ho[1,2] , Quang To[1] , Garnett W. Bryant[3] , and Anderson Janotti[1]
[1]Department of Materials Science and Engineering, University of Delaware, Newark, DE 19716, USA, [2] Faculty of Natural Sciences, Quy Nhon University, Quy Nhon 590000, Vietnam, [3]Nanoscale Device Characterization Division, Joint Quantum Institute, National Institute of Standards and Technology, Gaithersburg, Maryland 20899-8423, USA and the University of Maryland, College Park, Maryland 20742, USA

Embedding semi-metallic rare-earth mono-pnictide (RE-V) nanoparticles into III-V semiconductors enables nanocomposites with a wide range of optical, electrical, and thermoelectric properties. It decreases carrier lifetime and increases the phonon scattering, leading to lower thermal conductivity but enhanced electrical conduction through electron filtering mechanisms. The common group-V sublattice offers an interestin matching

across the interface of the rock-salt semimetal RE-V (e.g. ErAs) to the zinc-blende semiconductor III-V (e.g. GaAs, and AlAs) matrices with similar lattice parameters. Density functional theory (DFT) calculations with the modified Becke-Johnson meta-GGA (MBJ functional are used to describe the electronic properties of ErAs nanoparticles embedded in GaAs, AlAs, InAs and their alloys. We investigate the stability of different nanoparticle shapes and sizes, from cubic to spherical, deriving a direct correlation between the electron density and atomic density associated with excess metal atoms at the interface. Four different sizes of spherical ErAs nanoparticle embedded in different sizes of two III-V matrices are studied. According to the formation energy calculations, a spherical shape is the most energetic favorable among all shapes considered. We discuss the band alignment between the RE-V and the III-Vs, finding the Fermi level is pinned
near mid-gap of GaAs for the 1.73 nm size ErAs nanoparticle, explaining previous experimental measurements. Our predictions serve to guide the design of nanocomposite materials with targeted properties.

This work was supported by the NSF through the UD-CHARM University of Delaware Materials Research Science and Engineering Center (No. DMR-2011824). We also acknowledge the use of Bridges-2 at PSC through allocation DMR150099 from the Advanced Cyberinfrastructure Coordination Ecosystem: Services & Support (ACCESS) program, which is supported by National Science Foundation grant No. 2138259, 2138286, 2138307, 2137603, and 2138296, and the DARWIN computing system at the University of Delaware, which is supported by the NSF grant No. 1919839.

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12:20-6:30 PM Lunch (on your own)/free time

6:30-9:00 PM Banquet (Swan Ballroom)

Thursday, September 14th

Parallel Sessions

Recombination at defects (I) – Swan Ballroom

Chairperson: John Lyons, US Naval Research Laboratory

8:20-9:00 AM "Understanding the behavior of vacancies and complexes in Ga_2O_3 through atomistic simulations" *(invited presentation)*

Joel Varley

Lawrence Livermore National Laboratory

Gallium oxide (Ga_2O_3) is rapidly developing as one of the most promising ultra-wide bandgap platforms for next-generation power electronics due to its high breakdown field, controllable electrical conductivity, and commercially-available single-crystal substrates that can be produced using several scalable growth processes. Despite the progress and regular reporting of record-setting Ga_2O_3 devices, a number of open questions remain on the nature of fundamental defects and the role of impurities and dopants and how they may influence the electronic and optical characteristics. Of particular importance are cation vacancies, which have been identified to be present in significant concentrations in donor-doped material, are quite mobile within the lattice, and associated with a variety of luminescence lines and electronic transition levels. These vacancies become even more problematic in wider-band gap alloys like $(Al_xGa_{1-x})_2O_3$ (AGO), where they can compensate any attempts at donor-doping in the limit high Al-contents. Here we summarize the optical and electronic behaviour predicted for cation vacancies in Ga_2O_3 under different processing conditions, and discuss their propensity for interacting with other defects like oxygen vacancies. These results provide guidance for controlling defect populations and the electrical conductivity in Ga_2O_3 and related alloys and for facilitating next-generation power electronics based on this ultra-wide bandgap semiconductor family.

This work draws on collaborations with Ymir Frodason, Lasse Vines, John Lyons, Darshana Wickramaratne, Hartwin Peelaers, Becky Peterson, Martin Albrecht, Matt McCluskey and Chris Van de Walle, among others, and was partially performed under the auspices of the U.S. DOE by Lawrence Livermore National Laboratory (LLNL) under contract DE-AC52-07NA27344 and partially supported by LLNL Laboratory Directed Research and Development funding under project number 22-SI-003 and by the Critical Materials Institute, an Energy Innovation Hub funded by the

U.S. DOE, Office of Energy Efficiency and Renewable Energy, Advanced Materials and Manufacturing Office.

9:00-9:20 AM

"Defect migration energies in Ga$_2$O$_3$ polymorphs measured by variations of temperature and flux under irradiation"

Alexander Azarov[1], Ji-Hyeon Park[2], Dae-Woo Jeon[2], Edouard Monakhov[1], Andrej Kuznetsov[1]

[1]University of Oslo, Centre for Materials Science and Nanotechnology, PO Box 1048 Blindern, N-0316 Oslo, Norway, [2]Korea Institute of Ceramic Engineering & Technology, Jinju 52851, South Korea

Ga$_2$O$_3$ is an ultra-wide bandgap semiconductor which can be crystallized in different polymorphs and the monoclinic β-Ga$_2$O$_3$ phase is the most stable under normal conditions. In its turn, the rhombohedral phase conventionally labeled as a-Ga$_2$O$_3$ exhibits the widest bandgap of ~5.3 eV, making it particularly interesting for applications in power electronics and deep ultra-violet optoelectronics. However, despite the steadily growing interest on Ga$_2$O$_3$, the experimental data reported in literature on the intrinsic defects energetics are rare. In this work, in order to estimate migration properties of the intrinsic defects in β- and a-Ga$_2$O$_3$ polymorphs, we interpreted the residual disorder in the implanted samples as a function of the defect generation and annihilation rates in balance, reached by variations of the ion flux and irradiation temperature, keeping the ion dose constant. Specifically, the ion flux determines the time intervals between neighboring collision cascades, while the defect migration rates between the cascades obviously depend on temperature. In literature, this concept is also known as the dose-rate effect [1].

In this work we used bulk (010) β-Ga$_2$O$_3$ single crystals and ~1um thick a-Ga$_2$O$_3$ films grown by halide vapor phase epitaxy on sapphire substrates. The samples were implanted with 400 keV ^{58}Ni^{+} ions, applying a wide range of ion doses (6×10^{13} - 2×10^{16} cm^{-2}), ion fluxes (8×10^{10} - 5×10^{12} at.cm^{-2}s^{-1}) and irradiation temperatures (25-500 °C). Arrhenius analysis of the data revealed that the dose-rate effect in a-Ga$_2$O$_3$ occurs with an activation energy of 0.33±0.04 eV [2]. In contrast to α-Ga$_2$O$_3$, in β-phase the dose-rate effect occurs with an activation energy of 0.8±0.1 eV [3]. By setting these results in the context of the theoretical data available in literature [4], we argued that the obtained energies may be attributed to the migration activation of the Ga self-interstitials.

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9:20-9:40 AM “Quantum embedding methods for carbon dimer defects in hexagonal boron nitride”

Woncheol Lee[1, 2, 3], Cyrus Dreyer[2, 4], Emmanouil Kioupakis[5]

[1]Materials Department, University of California, Santa Barbara, [2]Center for Computational Quantum Physics, Flatiron Institute, [3]Department of Electrical and Computer Engineering, University of Michigan, [4]Department of Physics and Astronomy, Stony Brook University, [5]Department of Materials Science and Engineering, University of Michigan

The carbon dimer defect present in hexagonal boron nitride (h-BN) has captured considerable attention recently due to its potential association with the 4.1 eV zero-phonon line single-photon emitter observed within h-BN [1]. The pursuit of a comprehensive theoretical understanding of the electronic excited states of such defects led to the development and application of quantum embedding methods based on Kohn-Sham density functional theory [2]. Nevertheless, the imprecise definition of the double counting term, a pivotal aspect of embedding methodologies, emerged as a primary constraint in these approaches, subsequently constraining the precision of calculations.
In the context of this research, we employ the G_0W_0-level quantum embedding technique [3], which encompasses an accurate double counting correction term, to examine carbon dimer defects within h-BN. Our results indicate that the G-$_0$W$_0$ double counting correction effectively addresses the tendency to overestimate the energy of excited states as calculated through the Hartree correction. Furthermore, our G_0W_0-level embedding outcomes exhibit good agreement with the analytically derived dimer model.

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9:40-10:00 AM “Optical signatures of defects in hBN: comparing different calculation methods”

Henry Fried[1], Daniel Barragan-Yani[1], Ludger Wirtz[1]

[1]University of Luxembourg

Hexagonal boron nitride, both in its monolayer and bulk form, is recently receiving a lot of attention, not only as a flat and insulating substrate for other 2D materials, but also for its intrinsic optical properties in the UV range. The intrinsic luminescence spectrum of bulk hBN comprises four phonon-assisted peaks around 5.9 eV. However, various peaks at lower energy have been observed as well. These are, most likely, related to the presence of defects. Besides, hBN is also being discussed as a material for single-photon emission. Again, the exact nature of the responsible defects is not known.

We are pursuing different routes towards the calculation of optical signatures of defects in hBN. One route is the use of the GW+Bethe Salpeter approach, using sufficiently large supercells [1,2]. Another route is the calculation of charge transition levels, which can be done by comparing total energies (which are reliable quantities within density functional theory). We analyze the difference between charge transition levels, optical transition levels, the position of defect related quasi-particle states, and we present preliminary results for the case of hBN.

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10:00-10:20 AM **Coffee break**

10:20-11:00 AM “Theoretical Modeling of Vibrationally Resolved Optical Lineshapes of Semiconductor Deep-Level Defects” *(invited presentation)*

Lukas Razinkovas[1], Audrius Alkauskas[1]

[1]Center for Physical Sciences and Technology (FTMC)

Optically active semiconductor deep-level defects have emerged as essential building blocks for various quantum technologies, including quantum computing, quantum sensing, and quantum communication. Theoretical modeling and characterization of their optical properties are pivotal in chemical identification, understanding their fundamental properties, and harnessing their potential for quantum applications.

This talk aims to explore the theoretical modeling techniques employed to unravel the vibrationally resolved optical signatures of deep-level defects. The presentation will begin by overviewing the established theory for optical transitions between two non-degenerate electronic states. Practical computational methodologies to obtain high-resolution optical emission and absorption lineshapes will be presented with examples of defects in diamond, silicon, and silicon carbide.

Next, the talk will explore the theoretical modeling approaches employed to simulate and interpret optical spectra associated with transitions involving degenerate electronic states. Such electronic degeneracy commonly gives rise to the dynamical Jahn-Teller effect, which emerges from the intricate coupling between electronic and vibrational degrees of freedom. The presentation will examine practical computational methodologies that enable the analysis of multimode Jahn-Teller coupling and its impact on optical lineshapes.

11:00-11:20 AM “Ab initio modeling of the photoionization of negatively charged NV centers in diamond”

Marek Maciaszek[1], Lukas Razinkovas[1], Friedemann Reinhard[2], Marcus W. Doherty[3], Audrius Alkauskas[1]

[1]Center for Physical Sciences and Technology (FTMC), Vilnius LT-10257, Lithuania, [2]Institute of Physics, University of Rostock, 18059 Rostock, Germany, [3]Laser Physics Centre, Research School of Physics, Australian National University, Australian Capital Territory 2601, Australia

In this contribution, we present theoretical analysis and *ab initio* calculations of the photoionization processes of the negatively charged nitrogen-vacancy (NV) center in diamond. Photoionization thresholds and cross-sections are determined for the ionization from the triplet ground state $^3A_2$, triplet excited state ^3E, and singlet state ^1E. Moreover, the stimulated emission from ^3E and intra-defect absorption from $^3A_2$ to ^3E are also considered. Technical difficulties related to calculations of smooth photoionization cross-sections are discussed. The presented results provide a comprehensive picture of the interaction mechanisms of NV^- with light, which can serve as a “guide” for designing future optical experiments on

NV centers. Finally, we discuss obtained results in light of existing experimental data: we propose an explanation of the signal observed in electron paramagnetic resonance experiments attributed to the $^4A_2$ state, and we interpret data on the wavelengths corresponding to the efficient photoionization obtained using the dual-beam excitation technique.

11:20-11:40 AM “Optical transitions in Mg-doped Ga_2O_3”

Darshana Wickramaratne[1], John Lyons[1], Suman Bhandari[2], Mary Ellen Zvanut[2]

[1]US Naval Research Laboratory, [2]University of Alabama-Birmingham

We use first-principles calculations based on density functional theory to model the optical properties of magnesium (Mg) in monoclinic gallium oxide (b-Ga_2O_3). Doping b-Ga_2O_3 with Mg leads to semi-insulating material which is useful for power electronic devices. We compare our calculations against the photo-EPR measurements on Mg-doped Ga_2O_3, and establish the position of the Mg_{Ga} (0/-) level. For the photo-EPR measurements, we will discuss how first-principles calculations are instrumental in guiding the use of different analytical models that are fit to experimental photoionization cross sections to extract defect ionization energies.

11:40-12:20 PM “Trap-assisted Auger-Meitner recombination from first principles”
(invited presentation)

Fangzhou Zhao[1], Mark Turiansky[1], Audrius Alkauskas[2], Chris G. Van de Walle[1]

[1]Materials Department, University of California, Santa Barbara, [2]Center for Physical Sciences and Technology (FTMC)

Trap-assisted nonradiative recombination is a key mechanism limiting the efficiency of optoelectronic devices such as light-emitting diodes. Trap-assisted recombination via multiphonon emission (MPE) has been studied from first principles [1]; its rate was found to become negligibly low in materials with band gaps larger than about 2.5 eV [2, 3] since the rate of the MPE process decreases exponentially as the energy difference between the trap state energy level and the band edge increases. Experimentally, however, trap-assisted recombination is observed to persist at larger band gaps [4]. We propose that trap-assisted Auger-Meitner (TAAM) recombination can resolve the puzzle.

We have developed a practical first-principles methodology to calculate the TAAM rate for defects and impurities in semiconductors [5]. As a case study, we applied our formalism to a calcium substitutional impurity in GaN and InGaN. We found that for band gaps larger than 2.5 eV, the combination of hole capture by MPE and electron capture by TAAM results in recombination rates orders of magnitude larger than the recombination rate governed by MPE alone.

Our computational formalism is general and can be applied to any defect or impurity in any semiconducting or insulating material. The results provide insight into the physics of nonradiative recombination processes and elucidate why TAAM processes are key to describing defect-assisted recombination in wider-band-gap materials, where MPE alone fails to explain efficiency loss.

This work is supported by the Department of Energy Office of Science.

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Other materials (II) – Sanibel

Chairperson: Kirstin Alberi, National Renewable Energy Laboratory

8:20-8:40 AM “DFT study of B-Si-defects for modelling light-induced degradation (LID) in silicon”

Aaron Flötotto[1], Wichard Beenken[1], Kevin Lauer[1, 2], Erich Runge[1]

[1]Technische Universität Ilmenau, [2]CiS Forschungsinstitut für Mikrosensorik GmbH

Acceptor atoms and corresponding defects in silicon are of utmost importance for the functionality of many silicon devices. For example, boron-doped silicon was vitally important for the photovoltaics industry but has recently been replaced by gallium-doped silicon due to a boron-related defect causing light-induced degradation (LID). Similarly, silicon detectors based on boron-doping such as those used in the large hadron collider at CERN suffer from boron related defects, which degrade the detector efficiency. The longstanding research on LID in silicon has been reviewed recently by Lindroos and Savin [1]. Among other point defects such as boron-oxygen defects [2], the so-called A_{Si}-Si_i defect has also been linked to LID in silicon. This defect consists of a substitutional acceptor atom, in this case boron, on a silicon lattice site (A_{Si}) and a nearby silicon self-interstitial (Si_i). In addition to the A_{Si}-Si_i defect itself, related configurations also consisting of one acceptor atom and one silicon atom which share one lattice site need to be considered in order to explain LID in the A_{Si}-Si_i defect model. This model has recently been reviewed by us [3].

Here, we present the first DFT study of the A_{Si}-Si_i defect and its transition states in relation to LID in boron-doped silicon. Using DFT, we determined all neutral and charged metastable configurations related to the A_{Si}-Si_i defect and compared their formation energies by constructing a phase diagram. Using the Nudged Elastic Band algorithm, we calculated the minimal-energy pathways between relevant meta-stable configurations. The corresponding barrier heights and resulting conversion rates will be discussed within the A_{Si}-Si_i model for LID and compared with the existing, qualitative model of LID caused by the A_{Si}-Si_i defect. We will model the lifetime decay of boron-doped silicon by calculation of the nonradiative carrier capture coefficients using the procedure proposed by Alkauskas et al. [4]. This procedure will enable us to compare ab-initio predicted properties of the A_{Si}-Si_i defect with previous experimental findings on LID and discuss whether the A_{Si}-Si_i defect is likely to cause LID in boron-doped silicon.

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8:40-9:00 AM “Experimental Study on Defect Behavior during Crystal Growth of Phosphorus Heavily Doped Czochralski-Silicon”

Masataka Hourai[1], Yasuhito Narushima[2], Koutaro Koga[2], Kazuhisa Torigoe[1], Hiroshi Horie[1], Toshiaki Ono[1], Naoya Nonaka[1], Koji Sueoka[3]

[1]Production and Technology Division, SUMCO Corporation, [2]Product & Technology Division, SUMCO TECHXIV Corpation, [3]Dept. of Communication Engineering, Okayama Pref. University

Phosphorus (P) heavily doped Czochralski-Silicon (P:Cz-Si) crystals are widely used in power devices. To reduce the power consumption, reduction of the crystal resistivity to the utmost limit is required. Currently, the most advanced crystals can be manufactured with a resistivity of down to 0.6 mΩcm ([P]=1.3E20/cm^3). However, such P:Cz-Si crystals have dislocation defects including staking faults (SF), which degrade device characteristics. The purpose of this paper is to investigate experimentally the defect behavior during P:Cz-Si crystal growth.

P:Cz-Si crystals with a diameter of 200mm and a resistivity of about 0.6 mΩcm were grown. Defects in as-grown wafers taken from the bottom and middle portions of the crystals and annealed wafers taken from the bottom portion, which were annealed at 500°C to 600°C for 5hr to 720hr, were observed using transmission electron microscopy (TEM). In addition, the photoelectron spectra of P1s were measured by hard X-ray photoelectron spectroscopy (HAXPES) at SPring-8 (BL46XU).

In the bottom portion, a high density of micro interstitial-type dislocation loops of several 10 nm was observed. In contrast, in the middle portions, large dislocations of several 100nm, tangled inside of them, and P segregation with a few atomic percent were observed on the SF planes of the defects. Similarly, the growing and tangling of dislocations and P segregation were also observed in annealed wafers for short time from 5h to 20h.

HAXPES showed that at least two P states (P1 and P2) exist in the P:Cz-Si, P1 being the valence +1 substitutional P (Ps), and P2 being the valence 0 state, although the atomic structure and charge state of P2 were unknown. P2 ratio to P1+P2 in the as-grown wafers were almost constant at about 20-30% independent of crystal position. However, the P2 ratio in annealed wafers increased to about 40% during annealing at 600°C or lower for long time from 240h to 720h. Carrier concentrations in the annealed wafers measured by a Hall effect were decreased with annealing time, while in the as-grown wafers, they were almost consistent with the total P concentrations. This indicates that the P2 existing in the as-grown state is electrically active, while the P2 formed during annealing is inactive and in different states from each other. In fact, there is a small shift of binding energies of P2 in HAXPES spectra of both wafers.

It was previously reported that positron lifetime increases and P-Vacancy (V) clusters form in electron-irradiated P:Si with the P concentration of 1e20/cm^3. To investigate the attribution of P2, as-grown P:Cz-Si wafers were also irradiated with electron beams at a maximum dose of 1.3E18e/cm2 and evaluated by HAXPES. As with long annealed wafers, P1 decreased and P2 increased. Therefore, it was inferred that the newly formed P2 by long-time annealing was a P-V cluster.

These results suggest that in P:Cz-Si crystal growth, supersaturated Ps transforms into P-V clusters at crystal positions with long residence time below 600°C, and the interstitial Si produced simultaneously in this reactin is absorbed by the micro-dislocation loops, causing defects growth and tangle.

9:00-9:20 AM

"Density Functional Theory Study on Peculiar Defect Behavior during Crystal Growth of Phosphorus Heavily Doped Silicon"

Koji Sueoka[1], Yasuhito Narushima[2], Koutaro Koga[2], Kazuhiro Torigoe[3], Hiroshi Horie[3], Toshiaki Ono[3], Naoya Nonaka[3], Masataka Hourai[3]

[1]Okayama Prefectrural University, [2]SUMCO TECHXIV Corpation,
[3]SUMCO Corporation

Phosphorus (P) heavily doped silicon (Si) crystals are applied for low-voltage power MOSFETs. Crystals with a resistivity down to 0.6 mΩcm ([P] = 1.3×10^{20}/cm^3) are currently being manufactured. In P-doped Si crystals with a conventional concentration ([P] < 5×10^{19}/cm^3), vacancy (V) becomes dominant and the size of void defects increases during Si crystal growth. However, recent studies including our own (presented at this conference) have revealed that P heavily doped Si exhibits peculiar defect behaviors such as interstitial-type stacking fault (SF) formation during crystal growth. The purpose of this paper is to clarify what causes the defect behavior in P heavily doped Si through theoretical calculations.

We carried out the density functional theory (DFT) calculations within the generalized gradient approximation (GGA) for electron exchange and correlation using the CAmbridge Serial Total Energy Package (CASTEP) code. Periodic boundary conditions were set with cubic supercells of 512 Si atoms for the total energy calculation of Si crystals containing substitutional P (Ps), interstitial P (Pi), Ps_nV (n = 1-4) clusters, or Ps-Ps dimers. The cut-off energy of the plane waves was 340 eV. We carried out k-point sampling at Γ point. Note that if the model with 512 Si atoms contains one P atom, [P] = 1×10^{20}/cm^3, which is close to the actual concentration of the P heavily doped Si crystal. The formation energy of these P defects was obtained after geometry optimization. Finally, the thermal equilibrium concentration C_{eq} of the P defects was determined as $C_{eq,\mathrm{Ps}} = 1.8\times10^{22}\exp(-0.4\ \mathrm{eV}/kT)$ for Ps and $C_{eq,\mathrm{Pi}}$ = 2.7×10^{22} exp(-1.51 eV/kT) for Pi.

On the basis of these calculated results, the equilibrium P defect concentrations as a function of the total P concentration and the temperature are obtained. In the case of [P] = 1×10^{20}/cm^3 doping, (1) Pi is incorporated with [Pi] = 1×10^{17}/cm^3 at the melting point and supersaturates at around 1100 °C, (2) Ps supersaturates at around 600 °C, and (3) the formation energy of Ps_4V is negative (-0.81 eV) and [Ps_4V] increases to 4×10^{18}/cm^3 at around 600 °C.

We propose the following defect model during Si crystal growth that takes the concentration and diffusion barrier of P defects into consideration.

1) Melting point: Pi with [Pi] = 1×10^{17}/cm^3 is incorporated by Ps heavily doping around [Ps] = 1×10^{20}/cm^3.

2) 1100 °C - 600 °C: The supersaturated Pi interacts with Si atom to be Ps with the emission of self-interstitial Si atom (I). The emitted Is agglomerate and form SFs.

3) Less than 600 °C: The supersaturated Ps becomes P_4V with the emission of I. The SFs absorb Is and become more complex defects. The supersaturated Pi also precipitates on the defects.

Finally, we theoretically analyzed hard X-ray photoelectron spectroscopy (HAXPES) spectra for P heavily doped Si. The experimentally obtained peak energies of active Ps and inactive Ps_4V were well reproduced by DET calculations.

9:20-10:00 AM

"Influence of Solute Incorporation Mechanisms on the Properties of Highly Mismatched Semiconductors" *(invited presentation)*

Rachel Goldman

University of Michigan

Highly mismatched "designer" alloys contain chemical elements with large differences in atomic sizes and abilities to attract nearby electrons. When a few atoms with larger or smaller atomic sizes are added to a host material, its physical properties often change dramatically. A well-known example is the controlled incorporation of C and Mn into Fe (i.e. steel), leading to mechanical properties which differ from the pure form of Fe. A more recent example is the controlled incorporation of H into transition metal and rare earth alloys for hydrogen storage. In the case of semiconductors, incorporation of ultra-dilute mole fractions of solute atoms result in dramatic reductions in energy band gaps (ex: GaAs:N,Bi), transitions from indirect to direct band gaps (ex: GeSn:C), and transformations from pyroelectric to piezoelectric (ex: AlN:Sc). In this talk, we discuss combined computational-experimental studies of non-substitutional solute incorporation in highly mismatched alloys, with an emphasis on understanding the relationships between local atomic environments and physical properties of GaAsN, GaAsNBi, GeSnC, and AlScN alloys.

10:00-10:20 AM **Coffee break**

Gallium nitride (II) – Sanibel

Chairperson: Jun Suda, Nagoya University

10:20-10:40 AM "Sub-Bandgap Optical Absorption and Hydrogenated Gallium Vacancies in Ammonothermal GaN"

Siddha Pimputkar[1, 2], Sami Suihkonen[3], Mamoru Imade[4], Yusuke Mori[4], James Speck[2], Shuji Nakamura[2]

[1]Lehigh University, [2]University of California, Santa Barbara, [3]Aalto University, [4]Osaka University

Gallium nitride (GaN) has achieved widespread adoption as the material of choice for visible light emitters in the white and green to violet spectrum. High-power and high-efficiency devices commonly require low defect densities necessitating GaN substrates of high crystal quality. The ammonothermal method has demonstrated the ability to produce at least 2-inch diameter wafers of high quality, though they continue to exhibit coloration due to absorption of light below the bandgap of GaN.[1] In optical applications where light may pass through the substrates, light absorption can lead to unnecessary loss of generated light and hence efficiency.

Two absorption mechanisms were investigated and will be discussed in this contribution. The first investigates the limits of transparency for n-type doped GaN substrates by measuring optical absorption at sub-bandgap wavelengths for thick ammonothermal, sodium-flux, and hydride vapor phase epitaxy (HVPE) GaN substrates. The results clearly indicate that highly conductive GaN substrates will simultaneously become highly absorbing due to phonon-assisted free carrier absorption.[2]

The second absorption mechanism investigates the origin of the orange-yellow coloration of basic ammonothermal GaN substrates. Hydrogenated gallium vacancies were identified to be the origin of this coloration. The study was able to quantify the concentration of hydrogenated gallium vacancy using Fourier transform infrared (FTIR) spectroscopy for the first time. Use of non-polar substrates allowed for the determination of the type of hydrogen gallium vacancies present (V_{Ga}-H, V_{Ga}-H_2, V_{Ga}-H_3). Absorption peaks in the FTIR spectrum were tentatively assigned to different hydrogenated gallium vacancy types. [3]

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10:40-11:00 AM “Defects in aluminum rich Si-doped 90% AlGaN determined by positron annihilation and X-ray absorption spectroscopy”
Igor Prozheev, University of Helsinki

Igor Prozheev[1], Frank Mehnke[2], Marcel Schilling[2], Tim Wernicke[2], Michael Kneissl[2], Rene Bès[1], Filip Tuomisto[1]

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The performance of devices based on AlGaN alloys emitting light shorter than 240 nm suffers from limited *n*-type conductivity of the Si-doped current spreading layers due to the high Al content >80%. The conductivity is limited not only by the increasing dopant ionization energy and formation of a stable DX center but probably also by the formation of cation vacancy defects that are known to act as compensating acceptors in *n*-type GaN and AlN. Here we present results obtained in Si-doped $Al_{0.90}Ga_{0.10}N$ layers grown by metal-organic vapor phase epitaxy on AlN/sapphire. [1 - 3] Doppler broadening of positron annihilation radiation experiments are employed for studying the cation vacancy related defects [4], and x-ray absorption spectroscopy gives information on the immediate surroundings of the Si dopants. In our samples, the Si doping is varied in the range from 9×10^{17} cm^{-3} to 1.7×10^{19} cm^{-3}, and the employed growth conditions resulted in two different carbon impurity concentrations (2×10^{17} cm^{-3} and 2×10^{18} cm^{-3}).

We observe positron saturation trapping at cation vacancy defects present above 5.0×10^{18} cm^{-3} for all studied Si doping levels in low-carbon samples.

Interestingly, these vacancy defects do not appear to play a role in the electrical compensation of this material. In the high carbon content samples, the concentration of negatively charged cation vacancies increases with the Si concentration from less than 1×10^{16} cm^{-3} to above 2×10^{18} cm^{-3}, with these vacancies becoming important from the compensation point of view only at Si concentrations approaching 1×10^{19} cm^{-3}. At the highest Si doping levels, above 1×10^{19} cm^{-3}, the positron data exhibit a transition from the dominant positron trap being a cation vacancy to negatively charged non-open volume defect with a concentration exceeding 5×10^{18} cm^{-3}. The only impurity with sufficient concentration is the Si dopant, strongly suggesting that Si DX centers become an important limiting factor for *n*-type doping when the Si content is sufficiently high. [3] This behavior of the positron data coincides with the Si doping range where the electrical resistivity of the samples increases with increasing Si doping. At lower Si doping concentrations the resistivity decreases with increasing Si doping. X-ray absorption data in these two regimes show that the Si surroundings change from GaN-like in the range of decreasing resistivity to AlN-like in the range of increasing resistivity. This strongly suggests that the local chemical environment and might reveal important information on achieving lower resistivity in high Al content AlGaN.

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11:00-11:40 AM “First Principles Studies on the Defect States in the Gate Dielectrics in GaN MOSFET” *(invited presentation)*

Kenji Shiraishi[1]

[1]Nagoya University

We report first-principles molecular-dynamics calculations with the simulated annealing technique that clarify the atomic and electronic structures of the semiconductor-insulator interfaces consisting of GaN (0001) and (0001$^-$) faces and the amorphous (Al2O3)1-x(SiO2)x. We confirm that the obtained interfaces are free from dangling bonds, irrespective of the thickness of the amorphous (Al2O3)1-x(SiO2)x layer. This is due to the high atomic density and large mean coordination number near the interfaces caused by atomic diffusion from inside of the insulator to the interfaces. The calculated local density of states of the $(Al_2O_3)_{1-x}(SiO_2)_x$/GaN system quantitatively shows clear band offsets and, more importantly, the absence of deep states in the GaN energy gap. Interestingly, we find that the band alignment causing the offset is not abrupt at the interface but varies gradually near the interface, predicting the existence of transition layers. We determine the thicknesses of the transition layers in the $(Al_2O_3)_{1-x}(SiO_2)_x$/GaN system to be about 10 Å. We argue that those structural characteristics prevent the formation of the dangling-bond origin carrier traps at the interface, and this is a superior feature of the $(Al_2O_3)_{1-x}(SiO_2)_x$ as a gate dielectrics for the GaN-based metal-oxide-semiconductor devices.

Moreover, we also discuss the physical origin of hole trap defects which are expermentally observed in p-type GaN MOSFET.

11:40-12:00 PM “Thermal annealing behavior of nitrogen-displacement-related defects in homoepitaxial n-type GaN”

Meguru Endo[1], Masahiro Horita[1], Jun Suda[1]

[1]Nagoya University

GaN-based power-switching devices have attracted considerable attention. Understanding point defects in GaN is essential for superior device performance since various kinds of point defects may be introduced in GaN through the device fabrication process. However, most of the origins of deep levels are still unclear.

Intentional introduction of point defects by electron beam (EB) irradiation is an effective method to investigate the deep levels originating from intrinsic defects. We have reported 137-401 keV EB-irradiation to n-type GaN to selectively displace nitrogen (N) atoms. We observe two electron traps, EE1 (E_C-E_T=0.13 eV) and EE2 (E_C-E_T=0.98 eV), that could be attributed to V_N and N_I. However, the trap density of EE2 was several times higher than that of EE1 for the 137-keV EB-irradiated sample. If the origins of EE1 and EE2 are V_N and N_I, respectively, the trap densities should be the same. The difference in trap densities indicates that they are not simple Frankel pairs. In this study, we have investigated the thermal-annealing behavior of EE2 and estimated the activation energy of the annealing rate of EE2 in MOVPE-grown n-type GaN with 137-keV EB irradiation in order to acquire knowledge of the origin of the traps. The samples of GaN p^+-n^- diodes (PNDs) with mesa structure were used. The Si concentrations of the n-GaN layer of PNDs were 5.0×10^{16} cm^{-3}. EB irradiation was carried out after ohmic contact formation of PNDs to prevent annealing of the EB-induced traps. The EB irradiation was performed at the energy of 137 keV and the fluence of 2×10^{16} cm^{-2}. Isothermal capacitance transient spectroscopy (ICTS) measurements were performed to investigate electron traps.

In the ICTS spectra at 420 K, electron trap EE2 (activation energy E_a of 1.1 eV) was observed. The trap density of EE2 was 1×10^{15} cm^{-3}. This value was higher by two orders of magnitude than the trap density of EE1 (3×10^{13} cm^{-3}) which was predicted by the production rate of EE1 (1.6×10^{-3} cm^{-1}). We evaluated the annealing behavior of EE2 at the temperature range from 500 to 555 K in a vacuum. Following first-order kinetics, annealing dependence of ICTS intensity $\Delta C(t)$ can be expressed $\Delta C_0\exp(-A(T)\times t)$, assuming the net donor density does not change by annealing. Here, ΔC_0, t, and T are ICTS intensity before annealing, annealing time, and temperature, respectively. From the Arrhenius plots obtained from the temperature dependence of $A(T)$, which were acquired through the sequence of ICTS measurements and thermal annealing, an activation energy of 1.9 eV for EE2 was determined. The origin of EE2 is likely to be N_I (0/−1) since the activation energy of EE2 matched well with the migration barrier of N_I (−1) of 1.9 eV in GaN crystal, which was predicted by the First-principle calculation. The result that the trap density of EE1 was higher by two orders of magnitude indicates that the origin of EE1 might be the complex of nitrogen-displacement-related defects. These results are useful for the device fabrication process such as thermal-anneal after ion implantation for n-type GaN.

12:00-12:20 PM "Vacancy complexes in H-implanted AlN"

Igor Prozheev[1], Tanja Heikkinen[2], Ilja Makkonen[1], Filip Tuomisto[1]

[1]University of Helsinki, [2]Aalto University

Aluminium nitride (AlN) is an ultra-wide band-gap semiconductor with applications in, for example, deep ultraviolet (UV) optoelectronics or power electronics, in particular when alloyed with GaN. In spite of high quality single crystals and thin films being available already for more than a decade, the identification of native point defects and their possible complexes with impurities is still in its infancy.

Positron annihilation spectroscopy is a powerful, nondestructive technique for studying neutral and negative vacancy type defects in semiconductors [1]. The method is based on the observation of changes in the positron lifetime and the positron-electron momentum distribution due to positron trapping at vacancies. In this work, we present results obtained by combining H ion implantation, positron annihilation measurements and theoretical calculations to identify Al vacancies and their complexes with N vacancies and/or the implanted hydrogen.

100 keV H^+ ions were implanted at room temperature into AlN single crystal samples at fluences ranging from 5×10^{14} cm^{-2} to 2×10^{18} cm^{-2}. Depth-resolved experiments of the Doppler broadening of the positron-electron annihilation radiation were performed with a slow positron beam with positron implantation energies varied from 0.5 to 35 keV, corresponding to depths up to 4 µm. State-of-the-art theoretical calculations [1] of the positron states and annihilation parameters were performed for various defects for direct comparison with experiments.

We find isolated Al vacancies on the H^+ ion track and Al vacancy - (multi-)N vacancy complexes, possibly decorated by hydrogen, at the projected range of the H^+ ions. Note that the pre-existing vacancy defects in these crystals are Al vacancy - O impurity complexes [2]. Extremely high H implantation fluences are required to detect vacancy defects in the crystals, manifesting the high concentration of negative non-open volume defects present in the crystals before irradiation [2]. The fact that the Al to N vacancy balance in the complexes is on the side of N vacancies suggests that the latter are present at high concentrations already before irradiation. It is hence likely that N vacancies are in the negative charge state in AlN when the Fermi level is in the upper half of the band gap.

[1] F. Tuomisto and I. Makkonen, Rev. Mod. Phys. 85, 1583 (2013).
[2] J.-M. Mäki et al., Phys. Rev. B 84, 081204(R) (2011).

12:20-1:40 PM **Lunch (on your own)**

Parallel Sessions

Recombination at defects (II) – Swan Ballroom

Chairperson: Joel Varley, Lawrence Livermore National Laboratory

1:40-2:20 PM "Unveiling Defects at the Semiconductor/Oxide Interface: A Multiscale Modeling Approach" *(invited presentation)*

Dominic Waldhoer[1], Christian Schleich[1], Jakob Michl[1], Markus Jech[1], Tibor Grasser[1]

[1]TU Wien

Defects at the semiconductor/oxide interface, so-called border traps, play a crucial role in the performance and reliability of modern nanoelectronic devices. These defects can lead to significant issues such as bias temperature instability (BTI), hot carrier degradation (HCD), trap-assisted tunneling (TAT), and random telegraph noise (RTN). While these effects are observable in experiments, the microscopic nature of the involved defects often remains elusive. This work aims to bridge this gap by combining insights from electrical characterization methods, theoretical ab-initio calculations based on density functional theory (DFT), and compact device models.

Our investigations leverage the capabilities of our recently published compact device simulator *Comphy* [1], which is based on a physical description of charge trapping within the nonradiative multiphonon (NMP) theory. This physical model allows us to extract various defect parameters from electrical device characterizations and compare them to theoretical predictions from ab-initio methods for specific defect candidates.

We demonstrate the effectiveness of this multiscale approach by applying it to several technologically relevant problems. We identify hydrogen-related defects like the hydrogen bridge or the hydroxyl-E' center as a plausible cause for BTI in common Si transistors [2]. Furthermore, our analysis of the temperature-activation of gate-leakage currents suggests that the defects responsible for TAT currents must have unusually small relaxation energies, ruling out many typical oxide defects. However, the extracted parameters suggest a conduction mechanism via polarons, which is further supported by ab-initio simulations of intrinsic charge trapping in amorphous SiO_2 and ZrO_2 dielectrics [3].

We further explore the origin of RTN in CMOS devices for controlling solid-state qubits at cryogenic temperatures. Reducing the noise level is critical here to increase the coherence time of the quantum states. By comparing our model parameters extracted from measurements at cryogenic temperatures to ab-initio calculations of explicit atomistic models of the Si/SiO_2 interface, we propose that the canonical P_b-center is a likely source for noise in the cryogenic temperature regime [4].In our final showcase, we study the effect of electric fields and heated carriers on passivated P_b-centers at the Si/SiO_2 interface within a density matrix based framework for open quantum systems. Our studies suggest that the depassivation of Si-H bonds and the subsequent creation of new electrically active P_b-centers at the interface are the root cause of hot carrier degradation in Si-based electronic devices [5].

This work provides a framework for understanding defects at the semiconductor/oxide interface. Using a multi-scale modeling approach allows us to link those defects to macroscopically observable effects on electronic devices and thus to gain valuable insights on the underlying physics of various degradation mechanisms.

[1] D. Waldhoer et al, Microelectronics Reliability 146, 115004 (2023)
[2] D. Waldhoer et al, IEEE Trans. Electron Devices 68, 8, 4057-4063 (2021)
[3] C. Schleich et al, IEEE Trans. Electron Devices 69, 8, 4486-4493 (2022)
[4] J. Michl et al, IEEE IEDM, 31.3.1-31.3.4 (2021)[5] M. Jech et al, Physical Review Applied 16 (1), 014026 (2021)

2:20-2:40 PM “Telecom-wavelength quantum defects in cubic boron nitride”
Mark Turiansky, University of California, Santa Barbara

Mark Turiansky, Chris Van de Walle

University of California, Santa Barbara

The nitrogen vacancy (NV) center in diamond is the prototype quantum defect and has been used to demonstrate a variety of feats of quantum information science. However alternatives to the NV center with an improved optical interface are desired. Using first-principles computational techniques, we predict that $(V_B\text{-}C_B)^0$ and $(V_B\text{-}Si_B)^0$ in cubic boron nitride are NV-center analogues with a telecom-wavelength optical interface. Specifically, both centers possess a triplet ground-state spin, which enables them to be utilized as spin qubits. The zero-phonon line of the main optical transition falls within O-band telecom wavelengths, and the strength of electron-phonon coupling for the transition is quantified by a Huang-Rhys factor of 1.51. We also investigate the role of nonradiative processes in the dynamics of these centers.

This work was supported by the DOE and NSF.

2:40-3:00 PM “Proton irradiation-induced point defects acting as Shockley-Read-Hall recombination centers in homoepitaxial GaN p+/n- and p-/n+ junctions”

Tetsuo Narita[1], Masakazu Kanechika[2], Kazuyoshi Tomita[2], Yoshitaka Nagasato[3], Takeshi Kondo[2], Tsutomu Uesugi[2], Satoshi Ikeda[3], Masayoshi Kosaki[4], Tohru Oka[4], Jun Suda[2]

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An understanding of the properties of point defects is an important aspect of the engineering of *p*-*n* junctions in semiconductor devices. Unlike silicon-based and silicon carbide-based devices, point defects acting as Shockley-Read-Hall (SRH) recombination centers for gallium nitride (GaN) are not well understood. An intentional creation of point defects using particle irradiation is helpful to survey the characters of point defects. For this aim, point defects were intentionally introduced into homoepitaxial GaN *p*-*n* junctions having dislocation densities on the order of 10^6 cm^{-2} using proton irradiation with varying doses in the present study. Then, the effect of the conduction type was examined using GaN specimens having p^+/n^- and p^-/n^+ junctions.

The *p*-*n* junction layers were formed by a metalorganic vapor phase epitaxy method on freestanding GaN substrates. By changing the magnesium (Mg) acceptor and the silicon (Si) donor concentrations, both p^+/n^- and p^-/n^+ junctions were produced. The Mg and Si concentrations in the p^+/n^- junction were 3.5×10^{17} and 4.5×10^{16} cm^{-3}, respectively, while those in the p^-/n^+ junctions were 6.5×10^{16} and 2.1×10^{17} cm^{-3}. After the device fabrication composed of the mesa isolation and the electrode formation, these samples were irradiated with 4.2 MeV protons (H^+) at varying doses through anode electrodes. Positron annihilation spectroscopy (PAS) was also used to assess the reference *n*-type specimen, and the data indicated that the vacancies in this sample comprised gallium vacancy and divacancy types and were present at comparable levels, which corresponded to the implantation simulation.

Based on the analysis of the recombination current in the forward bias characteristics, these defects evidently served as SRH recombination centers such that the SRH lifetimes were reduced to several picoseconds from several hundred picoseconds prior to irradiation [1]. The compensation for holes in the p^-/n^+ junctions was almost double that for electrons in the p^+/n^- junctions. Furthermore, the SRH lifetimes associated with p^-/n^+ junctions were shorter than those for p^+/n^- junctions for a given proton dose [1]. These differences can be explained by variations in the charge state and/or the formation energy of intrinsic point defects in the *p*-type and *n*-type GaN layers. The results of the present work indicate the asymmetry of defect formation in GaN based on the fact that intrinsic point defects in *p*-type GaN readily compensate for holes.

The authors thank Mr. Takahide Yagi and Mr. Joji Ito of SHIATEX Co., Ltd., for performing proton irradiation and irradiation simulations. The authors thank Dr. Akira Uedono of Tsukuba Materials Research Co., Ltd., who is also a professor at the University of Tsukuba, for assisting in the assessment of vacancy types using positron annihilation spectroscopy.

[1] T. Narita et al., Appl. Phys. Lett.122, 113505 (2023).

3:00-3:20 PM **Break**

3:20-4:00 PM “Defect and dopant ab-initio Simulation Package (DASP) and Carrier Lifetime Calculation based on Non-adiabatic Molecular Dynamics (NAMD)” *(invited presentation)*

Shiyou Chen

Fudan University, China

In order to perform automated calculations of defect and dopant properties in semiconductors and insulators, we developed a software package, Defect and Dopant ab-initio Simulation Package (DASP), which is composed of four modules for calculating: (i) elemental chemical potentials, (ii) defect (dopant) formation energies and transition energy levels, (iii) defect and carrier densities and (iv) carrier dynamics properties of high-density defects. DASP uses the materials genome database for quick determination of competing secondary phases and calculation of the energy above convex hull when calculating the elemental chemical potential that stabilizes compound semiconductors, so it can perform high-throughput prediction of thermodynamic stability of multinary compounds. DASP calls the ab-initio softwares to perform the total energy, structural relaxation and electronic structure calculations of the defect supercells with different structure configurations and charge states, based on which the defect formation energies and transition energy levels are calculated and the corrections for electrostatic potential alignment and image charge interaction can be included. Then DASP can calculate the equilibrium densities of defects and electron and hole carriers as well as the Fermi level in semiconductors under different chemical potential conditions and different growth/working temperature. For high-density defects, DASP can calculate the carrier dynamics properties such as the photoluminescence (PL) spectrum, defect-related radiative and non-radiative carrier capture cross sections, and recombination lifetime of non-equilibrium carriers. In the talk, I will demonstrate the applications of DASP in studying the undoped GaN, C-doped GaN, SbSeI, CdTe, $ZnGeP_2$ and HfO_2.

On the other hand, recently the non-adiabatic molecular dynamics (NAMD) method was widely used for calculating the lifetime of non-equilibrium carriers in semiconductors. However, the carrier lifetimes calculated using NAMD often differ from experimental results by orders of magnitude. By revisiting the definition of carrier lifetime, we report a systematic procedure for calculating the effective carrier lifetime in semiconductor crystals under realistic conditions based on NAMD calculations. We found that the consideration of all recombination mechanisms and the use of appropriate carrier densities and recombination-center defect densities are crucial to bridging the gap between NAMD calculations and measurements. Our calculated effective carrier lifetime of $CH_3NH_3PbI_3$ agrees with experiments, and is limited by the band-to-band radiative recombination and Shockley-Read-Hall (SRH) defect-assisted non-radiative recombination, while the band-to-band non-radiative recombination is found to be negligible. The procedure is further validated by application to the compound semiconductors CdTe and GaAs, and thus, can be applied in carrier lifetime simulations in other material systems. Through combining the DASP and NAMD calculations, we can calculate the densities of defects and equilibrium carriers as well as the density and lifetime of non-equilibrium carriers in semiconductors under realistic conditions.

References:

[1] Menglin Huang, Zhengneng Zheng, Zhenxing Dai, Xinjing Guo, Shanshan Wang, Lilai Jiang, Jinchen Wei, Shiyou Chen, DASP: Defect and Dopant ab-initio Simulation Package, Journal of Semiconductors, 4, 042101 (2022).
[2] Shanshan Wang, Menglin Huang, Yu-Ning Wu, Weibin Chu, Jin Zhao, Aron Walsh, Xin-Gao Gong, Su-Huai Wei, Shiyou Chen, Effective lifetime of non-equilibrium carriers in semiconductors from non-adiabatic molecular dynamics simulations, Nature Computational Science 2, 486 (2022).

4:00-4:40 PM “An all-optical approach for comprehensive operando analyses of radiative and nonradiative recombination processes in semiconductors” *(invited presentation)*

Yong Zhang

The University of North Carolina at Charlotte

Photoluminescence (PL) is typically used as a qualitative probe for assessing the material quality, such as the general idea of the effectiveness of defects to the nonradiative recombination of the free carriers. To obtain quantitative information of the defects, one would then use electrical techniques, such as, current-voltage (I-V) characteristics, deep level transient spectroscopy (DLTS), and deep-level optical spectroscopy

(DLOS). We have developed an all-optical approach that can surprisingly offer the possibility of yielding much more information than one would expect, pertinent to the carrier recombination dynamics via both radiative and nonradiative processes when only one dominant deep defect level is present in a semiconductor material [1]. By applying a band-defect state coupling model that explicitly treats the inter-band radiative recombination and Shockley-Read-Hall (SRH) recombination via the deep defect states on an equal footing for any defect center occupation fraction, and analyzing PL as a function of excitation density over a wide range of the excitation density (e.g., 5-6 orders in magnitude), in conjunction with Raman measurements of the LO-phonon plasmon (LOPP) coupled mode, nearly all of the key parameters relevant to the recombination processes can be obtained. They include internal quantum efficiency (IQE), minority and majority carrier density, inter-band radiative recombination rate (Wr), minority carrier nonradiative recombination rate (Wnr), defect center occupation fraction (f), defect center density (Nt), and minority and majority carrier capture cross-sections (σt and σtM). While some of this information is thought to be obtainable optically, such as IQE and the Wr/Wnr ratio, most of the other parameters are generally considered to be attainable only through electrical techniques, such as DLTS or DLOS. In contrast to DLOS where light is used for exciting the trapped carriers back to the band states while monitoring the changes in the depletion region capacitance, the new approach does not involve electrical measurement at all, thus, might be termed as optical deep-level spectroscopy (ODLS) to distinguish them. This approach has been successfully applied to GaAs double-heterostructures that exhibit two distinctly different nonradiative recombination characteristics at room temperature. The method greatly enhances the usefulness of the simple PL technique to an unprecedented level, facilitating comprehensive material and device characterization without the need for any device processing.

[1] Zhang et al. Light: Science & Applications (2022) 11:137, https://doi.org/10.1038/s41377-022-00833-5

Gallium nitride (III) – Sanibel

Chairperson: Qimin Yan, Northeastern University

1:40-2:00 PM “Enhanced light output of Eu,O-codoped GaN caused by luminescent site reconfiguration during post-growth thermal annealing”

Takenori Iwaya[1], Shuhei Ichikawa[1, 2], Dolf Timmerman[1], Jun Tatebayashi[1], Yasufumi Fujiwara[1]

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Micro-light-emitting diode (μ-LEDs) is a promising candidate for the realization of next-generation display technique, such as smartphones/watches and wearable glasses for virtual/augmented reality. There has been a great demand on III-nitride-based red LEDs for the integration of the three primary colors LEDs. We have demonstrated III-nitride-based red LEDs using Eu,O-codoped GaN (GaN:Eu,O) grown by organometallic vapor phase epitaxy (OMVPE) [1]. It was shown that the luminous efficiency of GaN:Eu,O does not decrease as the size of the device is reduced [2], thus is expected to achieve high-efficient ultra-small (< 10μm) μ-LEDs.

Eu^{3+} ions doped in GaN form several luminescent sites with different local atomic structures around the Eu^{3+} ions. In particular, OMVPE7,8, which are believed to have an oxygen atom in the vicinity of the Eu^{3+} ion, are known to be excited with much higher efficiency as opposed to other sites [3]. However, their small existence ratio (~1%) has been the bottleneck to improve the luminous efficiency. For the growth of GaN:Eu,O by the OMVPE method, a relatively low growth temperature (960°C) is employed as compared to typical growth conditions for undoped GaN because high temperature growth (> 1000°C) results in a rough surface and limited Eu incorporation. However, such low temperature growth preferentially creates luminescent sites with small excitation cross sections (designated as OMVPE1,2). In this research, we perform post-growth thermal annealing to reconstruct the luminescent site and decrease the amount of OMVPE1,2 while increasing that of OMVPR7,8.

The sample is constructed by ud-GaN (2 μm), $Al_{0.19}In_{0.81}N$ (600 nm) and GaN:Eu,O (200 nm) layer. A 50-nm-thick SiO_2 film was deposited on samples to prevent the thermal decomposition of GaN. Thermal annealing was performed at 1000°C and 1100°C in N_2+NH_3 atmosphere for 10 minutes.

We performed combined excitation-emission spectroscopy (CEES) technique at 10 K using a wavelength-tunable dye-laser. The CEES technique allows us to selectively excite specific luminescence sites by resonantly exciting them, making it possible to quantify the number of each luminescent site. The CEES shows that the emission from OMVPE1,2 is dominant, while that from OMVPE7,8 is negligible for the as-grown sample. In contrast, for the sample annealed at 1100°C, the emission from OMVPE1,2 almost disappeared, while OMVPE4,7,8 became dominant. The sample annealed at 1100°C showed a 7.7-fold increase in the amount of OMVPE7 and 0.13-fold decrease in that of OMVPE1,2 compared to the as-grown sample.

Subsequently, we performed photoluminescence measurements at room temperature using a He-Cd laser. The sample annealed at 1100°C shows the highest integrated PL intensity, with the maximum enhancement factor of 5.1 compared to the as-grown sample at 0.18 mW/cm^2 [4]. These results suggest that the post-growth thermal annealing is an effective method to preferentially form OMVPE7,8.

[1] A. Nishikawa *et al.*, *Appl. Phys. Express* **2**, 071004 (2009). [2] D.D. Gon *et al.*, *Opt. Lett.* **45**, 3973 (2020). [3] D. Timmerman *et al.*, *Phys. Rev. Appl.* **13**, 014044 (2020). [4] T. Iwaya *et al.*, *Appl. Phys. Lett.* **122**, 032102 (2023).

This work was partially supported by JSPS KAKENHI (Grant No.18H05212, No.22K14614 and No.23H05449).

2:00-2:20 PM “Ultrafast carrier dynamics in GaN:Eu LED structures studied by terahertz emission spectroscopy”

Fumikazu Murakami[1], Atsushi Takeo[2], Brandon Mitchell[3], Volkmar Dierolf[4], Yasufumi Fujiwara[2], Masayoshi Tonouchi[1]

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Europium (Eu)-doped gallium nitride (GaN:Eu) is attracting much attention as the most promising candidate to realize the GaN-based red LEDs, due to its superior spectral properties such as extremely sharp peak and no peak shift with various current densities. It was reported several years ago that introducing a multilayer structure (MLS) of alternating undoped and Eu-doped GaN layers into the emitting layer of the LEDs enhanced Eu related luminescence efficiency significantly; however, the enhance mechanism is still standing as a long term question. To understand it, we studied the carrier dynamics within the LED structures using terahertz emission spectroscopy (TES). Terahertz (THz) emissions are generated from transient photocurrent induced by femto second (fs) optical pule excitation, and TES observes the THz emissions which reflects the carrier mobility, material bandgap, and electric field dispersion. In this work, we found that the carrier mobility in the MLS was smaller than that in the bulk GaN:Eu and directly observed the bandgap reduction in GaN due to Eu doping.

We used three types of samples, the bulk undoped GaN (ud-GaN), bulk GaN:Eu, and MLS grown by organometallic vapor-phase epitaxy on c-sapphire substrates. The MLS consisted of 40 pairs of 10 nm GaN layer and 3 nm GaN:Eu layer. The GaN:Eu layers in bulk GaN:Eu and MLS were expected to have an Eu doping density of . Optical pulses (center wavelength: 355-370 nm, pulse width: ~200 fs, repetition rate: 80 MHz) were employed to excite the GaN samples. The samples were excited with a pump power of 6 mW and a spot diameter of 300 μm at an incident angle of 45. THz waves were detected using a dipole-type photoconductive antenna fabricated on low-temperature-grown gallium arsenide.

We first measured the THz emissions from bulk GaN:Eu and MLS samples. The emission amplitude from the MLS was smaller than that from bulk GaN:Eu. This suggested the smaller carrier mobility in MLS than bulk GaN:Eu since the THz emission electric field emitted from GaN is proportional to the carrier mobility. The smaller carrier mobility in MLS can increase the carrier recombination within the active layers, and consequently enhance the LED emissions. To discuss the band structure in MLS, we evaluated the bandgap energy of ud-GaN and GaN:Eu by the excitation wavelength dependence of the THz emissions. The bandgap of ud-GaN was estimated to be 3.43 eV which is the same as reported value. On the other hand, measured value of bandgap of GaN:Eu was about 40 meV smaller than that of ud-GaN. The bandgap difference between ud-GaN and GaN:Eu should make energy band discontinuity in the MLS, which can enhances the carrier capture within the active layers. Therefore, we attributed the LED improvement to the potential barriers induced in MLS. To gain further insight, we will discuss the influence of potential barriers on the carrier behavior in MLS using the temperature dependence of THz emissions.

2:20-3:00 PM “Rare-earth defects for quantum information applications” *(invited presentation)*

Khang Hoang

North Dakota State University

Rare-earth (RE) doped semiconductors have long been of interest for optoelectronics and spintronics. More recently, they have also been considered for quantum information applications. The materials can offer features similar to those found in RE-doped complex oxide insulators that have often been used in quantum computing and quantum memory experiments. These include sharp optical transitions and excellent coherence properties. The advantage of using semiconducting hosts is that the materials can be controlled electrically, as opposed to just optically. To support progress in this direction, one needs to identify RE-related quantum defects that can be efficient luminescent centers via current injection. In this talk, I discuss recent results for RE defects in semiconductor platforms such as GaN, GaAs, and Si, obtained from hybrid density-functional calculations. The focus will be on erbium (Er) related defects, as trivalent Er with its optical transitions in the telecom C-band is of particular interest for quantum networking.

3:00-3:20 PM **Break**

3:20-3:40 PM "Probing the interfacial defect layer in chalcopyrite solar cells"

Helena V. Alberto[1], Rui C. Vilão[1], Eduardo F.M. Ribeiro[1], João M. Gil[1], Marco A. Curado[1, 2], Jennifer P. Teixeira[2, 3, 4], Paulo A. Fernandes[2, 3, 4], José M. V. Cunha[2, 3, 5], Pedro M. P. Salomé[2, 5], Marika Edoff[6], Maria I. Martins[7, 8], Thomas Prokscha[8], Zaher Salman[8], Alois Weidinger[9]

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It is well known that $Cu(In,Ga)Se_2$ (CIGS) films used in solar cells exhibit a cupper poor defect layer at its front surface. However, the nature of this surface defect layer (SDL) and its role in solar cell performance is still a matter of debate. The muon spin technique is used to study the defect layer near the p/n interface in chalcopyrite solar cells, obtaining depth-resolved information at the nanometer scale. The amplitude of the measured signal (diamagnetic muon fraction) is sensitive to structural disorder at the SDL and is measured as a function of film depth. A particularly strong lattice disorder is found in a layer about 50 nm wide at CIGS surface and can be reduced by applying a buffer layer. The muon probe can be used to determine quantitatively which materials are more effective in reducing this structurally disturbed region [1]. We find that the best results are obtained with CdS, whereas other buffer layers such as ZnSnO, Al_2O_3 or SiO_2 show weaker or no restorative effects. Results also indicate that the post deposition alkali treatment produces a healing effect that extends deeper into the absorber.

[1] Alberto H. V. et al., Characterization of the interfacial defect layer in chalcopyrite solar cells by depth resolved muon spin spectroscopy, Adv. Mater. Interfaces 2200374 (2022).

3:40-4:00 PM “First-principles study of intrinsic point defects and hydrogen impurities in the earth-abundant photovoltaic absorber Zn_3P_2”

Zhenkun Yuan, Yihuang Xiong, Geoffroy Hautier

Dartmouth College

The light-absorbing semiconductor Zn_3P_2 has had a long interest largely because of its potential for earth-abundant photovoltaics. To realize high-efficiency Zn_3P_2 solar cells, it is critical to understand and control point defects in the absorber material. Using hybrid-functional calculations, we assess the energetics and electronic behavior of intrinsic point defects in Zn_3P_2. Comparing our results with experiments, we address the open questions concerning the shallow or deep nature of the intrinsic defects in Zn_3P_2. Our work clarifies the likely defects leading to *p*-type doping in Zn_3P_2 and the possible deep-level defects which could act as detrimental nonradiative carrier recombination centers. We also study hydrogen impurities, which are frequently present in the growth or annealing environment of Zn_3P_2, and examine their impact on the electrical properties of Zn_3P_2.

4:00-4:40 PM “Defects in Arsenic doped CdSeTe Absorbers and their Impact to Current Collection Efficiency” *(invited presentation)*

Mariana Bertoni

Arizona State University

Copper and arsenic have been used as primary dopants in CdTe photovoltaic absorbers. However, both atomic species suffer from very low dopant activation. Arsenic concentration in these devices are on the order of 10^{16} cm^{-3}, which makes it notoriously difficult to correlate nanoscale distributions to the local charge transport properties. To measure and correlate these properties, measurement techniques require high sensitivity to elemental concentration, large penetration depth, and operando compatibility. In this work, we use nanoscale X-ray microscopy to correlate chemical distribution - structure - electrical properties through X-ray Fluorescence, X-ray Absorption Near edge spectroscopy, and X-ray Beam Induced Current at a pixel-to-pixel level (50-120nm).

Our cross-section studies unveil the segregation of As and the transition of the maximum charge-collection efficiency from the back interface to the front interface as a function of processing conditions, which is correlated to the balance of acceptors and donors, and thus the activation of the dopants.

We will show linear combination fitting of XANES and the presence of active species as well as inactive species through the absorber.

Friday, September 15th

Parallel Sessions

Other materials (III) – Swan Ballroom I

Chairperson: Rachel Goldman, University of Michigan

8:20-9:00 AM "Data-driven discovery and design of quantum defects in two-dimensional materials" *(invited presentation)*

Qimin Yan
Northeastern University

Being atomically thin and amenable to external controls, two-dimensional (2D) materials offer a new paradigm for the realization of patterned qubit fabrication and operation at room temperature for quantum information sciences and technologies. In this talk, I will discuss how data-driven material science can be combined with symmetry-based physical principles to guide the search for quantum defects in 2D materials for quantum information processing and quantum computing. In our initial work, the use of local bonding symmetry (irreducible representations) as a material design hypothesis enables the identification of anion antisite defects as promising spin qubits and quantum emitters in six monolayer transition metal dichalcogenides. The expansion of the high-throughput search in all known binary 2D materials led to the identification of more than 45 quantum defect candidates in a large set of host systems that can be utilized as qubits and/or quantum emitters. The work creates a technically accessible 2D platform for the fabrication of defect-based multi-qubit systems for quantum computing and quantum information technologies. At the end of the talk, I will discuss the development of machine learning models specially designed for defect properties, which will greatly accelerate the discovery of the "defect genome" in a vast space of material systems.

9:00-9:20 AM "Defect assisted triplet exciton transfer across the tetracene-Si(111):H interface"

<u>Marvin Krenz</u>[1], Uwe Gerstmann[1], Wolf Gero Schmidt[1]

[1]Lehrstuhl für Theoretische Materialphysik Universität Paderborn

Exciton transfer is highly relevant for many physical, chemical, and biological processes. The transfer of triplet excitons across the tetracene-silicon interface in sensitized solar cells is a recent example in this context [1]: The excitons, generated by singlet fission in tetracene (Tc), promise to increase the cell efficiency from the single-junction limit of 29% to as high as 35% [2]. While the atomistic details of the Tc-Si interface are decisive for maximizing the triplet transfer, the transfer mechanism is essentially unknown. Here, we present *ab initio* molecular dynamics (AIMD) calculations that provide a microscopic understanding of the exciton transfer across the Tc-Si(111):H interface. The transfer characteristics is found to depend strongly on the presence of Si dangling bond defects. Such interface defects are often considered detrimental to material performance, because they accelerate charge and energy losses [3]. Here, however, we find them to be instrumental for excitation transfer: The Si dangling bonds give rise to interface states energetically close to the Tc valence band edge. They assist the hole transfer into Si bulk either directly - for low-density Tc layers - or upon thermal activation, in case of high-density Tc layers. The time scale of this activation process is highly dependent on the starting configuration and the temperature with over 85% occurring within 1 ps at room temperature. The exciton electron is found to follow the hole within a few femtoseconds.

[1] M. Einzinger, T. Wu, J. Kompalla, H. Smith, C. Perkin- son, L. Nienhaus, S. Wieghold, D. Congreve, A. Kahn, M. Bawendi, and M. Baldo, Nature 571, 90-94 (2019).
[2] A. Rao and R. Friend, Nat. Rev. Mater. 2, 17063 (2017).
[3] D. C. Moritz, *et al*., Solar RRL 2201063 (2023).

9:20-9:40 AM

"Magnetic proximity coupling to defects in two-dimensional semiconductors"

Muhammad Hassan Shaikh[1] , Matt Whallen[3],Aqiq Ishraq[2], Collin Maurtua[2], John Xiao[1,3], Chitraleema Chakraborty [1,2,3]

[1]*Department of Physics and Astronomy, University of Delaware,* [2]*Department of Materials Science and Engineering, University of Delaware,* [3]*Department of Quantum Science and Engineering, University of Delaware*

Magnetically active defects have been extensively employed in quantum sensing applications, with nitrogen-vacancy (NV) centers in diamond and silicon-vacancy (SiV) in silicon carbide (SiC) being the most commonly used examples. These defects have played a crucial role in characterizing the magnetic behavior of three-dimensional (3D) magnetic materials.

However, their applicability to two-dimensional (2D) magnetic materials is limited due to the challenges associated with accessibility and interaction with surfaces. Conversely, defects in 2D materials, particularly transition metal dichalcogenides (TMDCs), have garnered significant attention. TMDCs are semiconductor materials that exhibit optical activity with valley-dependent optical selection rules. In the presence of a magnetic field, the energy degeneracy within these valleys can be lifted. Optically active defects in TMDCs are highly sensitive to magnetic fields, providing an opportunity for direct probing of the layer-dependent 2D magnet's magnetic properties at the nanoscale. Layer-dependent 2D magnets, such as Chromium triiodide (CrI_3) and Chromium thiophosphate ($CrPS_4$), which display ferromagnetic (FM) and antiferromagnetic (AFM) properties depending on the layer count, have emerged as promising candidates for next-generation advanced spintronics devices. These materials offer improved speed (ranging from GHz to THz), electromagnetic interference immunity, and enhanced memory density due to their net-zero magnetization. However, their potential for future devices is hindered by challenges related to air stability and magnetic degradation of a few layers. While previous studies have classified the bulk form of these materials as AFM using the Magnetic Optical Kerr Rotation (MOKE) technique, the magnetic behavior of the surface layer of bulk $CrPS_4$ remains unexplored.

To investigate the FM and AFM responses of the surface layers of bulk in these materials, we utilize magnetic proximity coupling with optically active defects in TMDCs, These defect-based quantum emitters offer higher spectral resolution compared to 2D exciton transitions, which suffer from broad linewidths, thereby enabling increased magnetic field sensitivity.

In this study, we examine the magneto-photoluminescence of a heterostructure composed of $CrPS_4$ and WSe_2, utilizing defect-based quantum emitters as optically active probes at low temperatures. The surface layer of bulk $CrPS_4$ is found to exhibit a detectable net magnetic moment (NMM) via the Degree of Circular Polarization (DOP) of photoluminescence (PL) from the defect-based quantum emitters. We also performed X-ray photoelectron microscopy on bulk $CrPS_4$ revealing no signs of oxidation or hydration in the bulk material.

These findings provide valuable insights into the potential applications of next-generation AFM-based spintronics and advanced memory-based devices. By harnessing the unique properties of AFM materials and defect-based quantum emitters, this study contributes to the ongoing exploration of novel magnetic phenomena in heterostructures, facilitating advancements in spintronics and memory technology.

9:40-10:00 AM “Alloying-related changes in electronic properties of common grown-in and radiation-induced defects in $Al_xGa_{1-x}N$ layers grown by MOVPE on Ammono-GaN substrates”

Piotr Kruszewski[1], Jerzy Plesiewicz[1], Pawel Prystawko[1], Ewa Grzanka[1], Szymon Grzanka[1], Vladimir P. Markevich[2], Lijie Sun[2], Matthew P. Halsall[2], Sylwester Bulka[3], Anthony R. Peaker[2]

[1]Institute of High Pressure Physics Polish Academy of Sciences, Poland, [2]Photon Science Institute and Department of Electrical and Electronic Engineering, the University of Manchester, [3]Institute of Nuclear Chemistry and Technology, Poland

Deep level transient spectroscopy (DLTS) and high-resolution Laplace-DLTS have been used for studying alloying-related changes in electronic signatures of common grown-in and radiation-induced traps with energy levels in the upper half of the gap in $Al_xGa_{1-x}N$ ($0 < x \leq 0.05$) layers grown by MOVPE on Ammono-GaN substrates and doped with Si during growth. In the conventional DLTS spectra, broadening and shifts to higher temperatures have been observed for the detected electron emission signals (known as the E1, E3, and EE1 traps in GaN) with the increase in Al content. The rates of alloying-induced increases in mean ionization enthalpies of the above-mentioned traps relative to the conduction band edge have been determined. Electric-field dependencies of electron emission rates from the traps have been analysed and taken into account. No significant changes in the values of electron capture cross sections and entropy of electron ionization with the changes in Al content have been observed. Laplace-DLTS measurements have been further used for deconvolution of the observed emission signals to components related to the defects with different atomic compositions in the first and second nearest neighbour shells. Origins of the observed traps and possible reasons of the alloying-induced changes in their electronic properties are discussed.

10:00-10:20 AM **Coffee break**

10:20-10:40 AM “Role of Nitrogen Vacancies in Obtaining Semi-Insulating Properties of Ammonothermal GaN:Mg”

Marcin Zajac[1], Leszek Konczewicz[1], Elzbieta Litwin-Staszewska[1], Ryszard Piotrzkowski[1], Robert Kucharski[1], Pawel Kaminski[2], Roman Kozlowski[2]

[1]Institute of High Pressure Physics, Polish Academy of Sciences, Warsaw, Poland , [2]Lukasiewicz Research Network - Institute of Microelectronics and Photonics, Warsaw, Poland

Precise knowledge on point defects properties in bulk GaN substrates is essential for two reasons: 1) shaping the crystal electrical properties, 2) improving the performance of devices made using these substrates. In basic ammonothermal method semi-insulating (SI) properties are achieved by the compensation of unintentional donors by Mg acceptors. It was suggested that in case of SI-GaN:Mg, Ga vacancy (V_{Ga}) and V_{Ga}-related complexes determine the character of the temperature dependence of resistivity and carrier concentration [1]. However, the participation of other intrinsic point defects in Mg compensation has not been investigated, especially for various Mg concentrations. In this communication we demonstrate the first experimental observation of the presence of N-vacancies (V_N) in addition to V_{Ga} in ammonothermal GaN:Mg crystals for various compensation regimes.

The SI-GaN:Mg crystals with Mg concentrations ranging from 5×10^{18} cm^{-3} to 4×10^{19} cm^{-3} and a fixed oxygen concentration (1×10^{18} cm^{-3}) were thoroughly studied by Hall effect measurements vs temperature in the range 300°C-800°C. These studies were completed with investigations of defects energy levels and concentrations performed by High Resolution Photo-induced Transient Spectroscopy (HRPITS). This method allows for determining the activation energies of charge carrier traps from the photocurrent relaxation waveforms induced by the thermal emission of excess carriers (generated by UV laser pulses) from defect levels.

It is shown that the activation energy (E_A), determined from the slope of the carrier density dependence vs. temperature, can be tuned from 1.6 eV, through 1-1.2 eV, to 0.5 eV with increasing the Mg concentration. High-temperature Hall effect data revealed *p*-type conductivity for all the Mg-doped crystals. At the same time HRPITS results revealed a complex defect structure of SI GaN:Mg, showing the presence of a number of traps with activation energies ranging from 0.2-1.6 eV. One of the distinguished group of traps is the family of V_{Ga}, $V_{Ga}H_n$, $V_{Ga}O_N$ and $V_{Ga}V_N$ defects of closely-spaced (+/0) transition energies in the range 0.7 eV-1.1 eV above the valence band maximum (vbm). The higher transition energies (0/-) and (-/2-) of V_{Ga} at 1.5-1.6 eV above the vbm were also detected. The other group of defects were identified with the activation energies around 0.5 eV. They were found to be dominant for the highest Mg concentration and were attributed to the transition energies (2+/+) and (3+/2+) of V_N according to theoretical predictions [2]. Obtained data are interpreted in terms of the compensation dependent Fermi level pinning to different energy levels of V_{Ga}-related (1.6 eV and 1 eV above vbm) and V_N defects (0.5 eV above vbm). In addition, the solution of the charge neutrality equation allowed to describe the compensation mechanism quantitatively. The participation of other traps (like antisite defects) will be discussed. The presented results indicate a crucial role of V_{Ga} and V_N in optimizing the resistivity of ammonothermal GaN:Mg by the material non-stoichiometry control.

[1] M.Zajac et al., Prog. Cryst. Growth Charact. Mat. **64**, (2018) 63-74.
[2] I.C.Diallo et al., Phys. Rev. Appl. 6 (2016) 064002.

This work was supported by the Polish National Science Center through Project No. 2020/37/B/ST5/03746.

10:40-11:00 AM "Hydrogen Passivation of Acceptor Defects in delafossite $CuMO_2$ (M=Ga, In, Al): Insights for Enhanced p-Type Conductivity"

Aroon Ananchuensook[1], Intuon Chatratin[2], Anderson Janotti[2], Pakpoom Reunchan[1]

[1] Department of Physics, Faculty of Science, Kasetsart University, Bangkok 10900, Thailand, [2] Department of Materials Science and Engineering, University of Delaware, Newark, Delaware 19716, USA

Transparent conducting oxides with *p*-type conductivity hold immense potential for diverse electronic applications. The role of native point defects in α-$CuMO_2$ as the source of *p*-type conductivity has been widely acknowledged. However, understanding the primary defects governing the electrical properties and devising strategies for their improvement remains a critical challenge. In this study, we employ range-separated hybrid density functional calculations to elucidate the impact of acceptor defects and their interactions with hydrogen on electrical conductivity. Our findings demonstrate that hydrogen plays a pivotal role in controlling the *p*-type conductivity in these oxides.

Our investigation reveals that hydrogen can form stable complexes with acceptor defects V_{Cu}, resulting in effective passivation. Notably, the interactions between hydrogen and V_{Cu} defects facilitate the formation of stable complexes, rendering the defects electrically inactive. Considerable binding energies are observed for H_i-V_{Cu} complexes, indicating their thermodynamic stability and the likelihood of high concentrations under both O-rich and O-poor conditions. A second hydrogen can be bound to H_i-V_{Cu} to form $2H_i$-V_{Cu} complexes, which are thermodynamically stable and function as a single donor. Furthermore, hydrogen can bind with another acceptor defect, Cu_{Ga}, forming H_i-Cu_{Ga} complexes. However, the smaller binding energies associated with these complexes suggest their potential dissociation into isolated H_i and Cu_{Ga} at relatively low temperatures.

By shedding light on the profound influence of hydrogen on *p*-type conductivity, this study offers valuable insights into the hydrogen passivation of acceptor defects in delafossite $CuMO_2$ (M=Ga, In, Al). These findings have significant implications for designing and developing

transparent conducting oxides, leading to enhanced electrical properties and the realization of advanced electronic devices.

11:00-11:40 PM "Optical absorption of point defects in ultrawide bandgap semiconductors AlN and Ga_2O_3 as measured by photo-induced electron paramagnetic resonance" *(invited presentation)*

Mary Zvanut[1], Shafiqul Mollik[1], Mackenzie Siford[1], Suman Bhandari[1]

University of Alabama at Birmingham

Ultrawide bandgap semiconductors are actively pursued as a substrate for high power electronics due to the high critical fields achievable as well as for the potential for optical devices active in the ultraviolet. In either application, point defects play a critical role - either by limiting the effectiveness of dopants or by causing absorption well-below the bandgap. Many optically-induced techniques provide convenient ways for assessing the role of point defects; however, the photo-induced electron paramagnetic resonance (photo-EPR) method offers an advantage over other techniques because the defect itself is monitored, rather than the material as a whole.

The talk will focus on defects in as-grown bulk hexagonal AlN and β-Ga_2O_3 crystals. All measurements were performed 10 GHz electron paramagnetic resonance (EPR) spectrometer at temperatures from 4-300 K. Illumination is provided by a series of LEDs.

The sole EPR signal observed in the amber-tinted AlN crystals is thought to be due to either a nitrogen vacancy (V_N^0) or substitutional oxygen (O_N^0) [1]. Preliminary steady-state photo-EPR results indicate that the EPR signal is activated at 3.8 eV and subsequently quenched at about 1.8 eV. Neither threshold is within a reasonable range of those expected for the neutral to positive defect level of O_N, we therefore suggest that V_N^0 is the dominant defect in these substrates.

The true power of photo-EPR comes from defects with well-defined EPR spectra such as the compensating impurities, Fe^{3+} and Mg^0 in Ga_2O_3. When the amount of Fe^{3+} is monitored during illumination, analysis of the time dependence yields a defect level of 0.6 eV below the conduction band edge for the 2+ to 3+ transition of Fe and a relaxation energy of 0.7 eV [2]. The defect level is consistent with values obtained by less direct methods and supports the results of density functional theory [2,3]. Similarly, the values for the defect level and relaxation energy for the neutral-to-negative transition of $Mg^{-/0}$, 1.35 eV above the valence band maximum and 1.1 eV, respectively, are consistent with theory [4]. However there remains some

conflict with other experimental work which places the $Mg^{-/0}$ closer to the valence band edge [5].

The talk will begin by discussing the significance of ultrawide bandgap material and briefly outline the use of photo-EPR to study defect levels. The bulk of the presentation will focus on a controversial defect assignment in AlN and the determination of the defect level for $Fe^{2+/3+}$ and $Mg^{-/0}$ in β-Ga_2O_3.

[1] V.A. Soltamov et al, J. Appl. Phys. **107**, 113515 (2010).
[2] Suman Bhandari, et al, J. Appl. Phys. **126**, 165703 (2019).
[3] M. E. Ingebrigtsen, et al, Appl. Phys. Lett. **112**, 042104 (2018).
[4] Bhandari, S., et al, APL Materials **10**, 021103 (2022).
[5] C. A. Lenyk et al, Appl. Phys. Lett. **116**, 142101 (2020).

This AlN work was supported by the Ultra Materials for a Resilient Energy Grid, an Energy Frontier Research Center funded by the DOE, Basic Energy Sciences under Award # DE-SC0021230. The Ga_2O_3 work is supported by NSF Grant: DMR-1904325.

Theory of defects – Swan Ballroom II

Chairperson: Khang Hoang, North Dakota State University

8:20-8:40 AM

"Hardware Bayesian Machine Learning for Quantum Sensing with Solid State Defects"

Sean Blakley[1, 2, 3], Robert McMichael[2]

[1]DEVCOM Army Research Laboratory, Adelphi, MD, USA, [2]National Institute of Standards and Technology, Gaithersburg, MD, USA, [3]University of Maryland, College Park, MD, USA

Bayesian machine learning methods have been used in optically detected magnetic resonance (ODMR) measurements with nitrogen--vacancy (NV) diamond sensors to improve measurement efficiency in both pulsed [J. Appl. Phys. 130, 144401 (2021)] and continuous wave regimes [Phys. Rev. Appl. 14, 054036 (2020)]. One such method, known as Bayesian experiment design, is well suited to situations where it is favorable to trade an increase in computational complexity for a reduction in time or resources spent during data collection. In a swept-frequency ODMR measurement, most of the acquisition time is spent on system settings corresponding to measurements yielding no useful data. Bayesian experiment design uses Bayesian statistics to adaptively predict which system settings correspond to measurements with important results. However, the computational complexity of Bayesian experiment design methods results in increased time spent collecting each datapoint. A hardware optimized Bayesian experiment design architecture implemented in a field-programmable gate array (FPGA) can reduce computation time by orders of magnitude, further improving the performance, versatility, and utility of Bayesian experiment design methods. In this work, a simplified, adaptive, general use Bayesian algorithm for high speed quantum sensing is described and simulated for measurements with NV centers. This algorithm is implemented with fixed-point arithmetic and parallel execution of the Bayesian inference, optimization, and resampling subroutines for use in a FPGA platform. This results in a projected 1000 fold reduction in processing time compared to the software implementation of this algorithm, potentially speeding up quantum sensing with solid state defects by orders of magnitude.

8:40-9:00 AM "Evaluating finite size effects for hybrid functional defect calculations"

Tammo van der Heide[1], Bálint Aradi[1], Ben Hourahine[2], Thomas Frauenheim[3, 4, 5], Thomas Niehaus[6]

[1]Bremen Center for Computational Materials Science, University of Bremen, 28359 Bremen, Germany, [2]Department of Physics, SUPA, University of Strathclyde, John Anderson Building, 107 Rottenrow, Glasgow G4 0NG, United Kingdom, [3]Constructor University, School of Science, Campus Ring 1, 28759 Bremen, Germany, [4]Computational Science and Applied Research Institute (CSAR), 518110 Shenzhen, China, [5]Beijing Computational Science Research Center (CSRC), 100193 Beijing, China, [6]Univ Lyon, Université Claude Bernard Lyon 1, CNRS, Institut Lumière Matière, F-69622 Villeurbanne, France

Point defect studies with density functional theory have begun to increasingly rely on hybrid density functionals, due to the improved band gap and reduction of self-interaction problems. However, compared to earlier generations of DFT, these are somewhat more expensive calculations, but are closer to GW-type theories in terms of predictive power (particularly for the range-separated functionals) with the additional advantage of improved thermochemistry. biut they are computationally limitated to relatively small simulation cells for the usual supercell geometries, and hence have increased hybridization, electrostatic and elastic defect-defect interactions.

Using our recent implementation of general hybrid functionals [1], within the framework of density-functional-based tight binding, multi-thousand atom systems are readily accessible for modest computational resources. Hence we can perform systematic convergence studies of the properties of point defects to bulk-like concentration limits.

The behavior of deep and shallow level defect systems in both wide and narrow gap materials with a range of elastic constants are investigated. leading to recommendations for cases where smaller cells can be employed and estimates for corrections to the results evaluated.

[1] Hybrid functionals for periodic systems in the density functional tight-binding methodTammo van der Heide, Bálint Aradi, Ben Hourahine, Thomas Frauenheim, and Thomas A. NiehausPhys. Rev. Materials 7, 063802 (2023).

9:00-9:40 AM "Defects in Topological Semimetals" *(invited presentation)*

Kirstin Alberi

National Renewable Energy Laboratory, Golden, CO

Three-dimensional topological semimetals (TSM) exhibit phenomena that have the potential to extend device functionality beyond what is possible with semiconductors today. These materials are characterized by linear band touching nodes near their Fermi levels, and they have demonstrated the ability to support very high electron mobilities, linear magnetoresistance and non-equilibrium electron spin populations. To access and tailor these properties in devices, we must first learn to master the details of defects and disorder in TSMs the same way we have in semiconductors. In this talk, I will discuss our work to uncover the relationships between defects and electron transport in the Dirac semimetal Cd_3As_2. We use molecular beam epitaxy to systematically vary point and extended defects in thin films. Combining magnetotransport measurements of these materials with density functional theory provides a greater understanding of the impact of defects on electron scattering, magnetoresistance and the Fermi level. I will also discuss our investigation of extrinsic doping and alloying as routes for altering transport behavior.

9:40-10:00 AM "Defect Analysis at Database Scale"

Jimmy-Xuan Shen and Joel B. Varley

LLNL Lawrence Livermore National Laboratory

A requirement for building large-scale, persistent, materials databases is the ability to group calculations that represent the same physical concept together regardless of the computational details. The major challenge for codifying point defect data is the fact that atomic structures used to represent a defect are not unique, so grouping and aggregation are essentially impossible. We have developed a structure-only definition of point defects, allowing us to use standard structure analysis techniques to aggregate defects calculations. Doing this also allows us to side-step a major challenge of automated defect analysis: DFT codes not finding the global energy minimum for a particular charge state, since we can now revisit a defect at a later time to find the actual energy minum. We have designed a full defect analysis package around this core concept and added many features that make defect analysis more accessible to Python users. The code is distributed as an add-on to the popular PYMATGEN materials analysis code. Additionally, our code is fully integrated with the ATOMATE2 automation framework so scaling up to hundreds of thousands of calculations is now possible.

10:00-10:20 AM **Coffee break**

10:20-11:00 AM “On a quest for novel wide gap semiconductors” *(invited presentation)*

Vladan Stevanovic, Emily Garitty, Cheng-Wei Lee

Colorado School of Mines & NREL

Increased electrification, smart grid technology, and renewable power generation has brought to light the need for new wide-gap semiconductors for power electronics applications. Currently used or explored wide-gap systems are costly (GaN), difficult to synthesize as high-quality single crystals (SiC) and at scale (diamond, BN), have low thermal conductivity (β-Ga_2O_3), or cannot be suitably doped (AlN). In this talk I will describe our recent efforts in using modern computational techniques to identify promising wide gap systems for power applications beyond those currently explored. As power applications demand relatively high doping levels to achieve good electric conductivity, predicting dopability when searching for new wide gap systems is of utmost importance. I will discuss the approach we developed to integrate defect calculations within the wide-gap materials discovery workflow and how it addresses challenges associated with accurate dopability predictions for: (a) compounds whose properties have not been characterized experimentally except for chemical composition and crystal structure, and (b) possibly tens of such systems that emerge from the materials screening efforts that are based solely on the relevant intrinsic properties (e. g. band gap, effective masses, thermal conductivity, etc.). The focus will be on two classes of oxide systems, (III)BO_3 borates and $In_2(IV)_2O_7$ pyrochlores, members of which emerge from our search as having favorable combination of relevant properties including n-type dopability to technologically relevant charge carrier concentrations. Lastly, I will discuss a model description of the semiconductor dopability that is based on the tight-binding Hamiltonian, and the intrinsic properties suggested by tight-binding as governing the doping tendencies and doping limits of semiconductors.

11:00-11:20 AM “Modelling device degradation by hydrogen-related hole trapping defects at the c-Si/a-SiO2 and c-Si/a-SiO2/a-HfO2 interface

Teo Cobos
University College London

The performance metal-oxide-semiconductor field-effect transistors (MOSFETs) is affected by random telegraph noise and bias temperature instability. These effects are caused by the trapping and release of holes and electrons in the dielectric oxide layer, but the atomistic nature of these processes is unclear. This research is focused on the DFT modelling of the effect of Negative Bias Temperature Instability (NBTI) in c-Si/a-SiO_2/a-HfO_2 devices. We aim to evaluate the accuracy of the Reaction Diffusion Drift (RDD) model, which suggests that the hole-induced dissociation of hydrogen-passivated defects can explain the trap generation kinetics in many types of devices.

We investigate how H-related defects in amorphous SiO_2 can be involved in hole trapping and hydrogen release, making them possible candidates for NBTI. Using non-local density functional we investigate how H-passivated oxygen vacancies and 3-coordinated silicon centres trap holes and release protons in bulk a-SiO_2 by reporting barriers for proton dissociation and defect charge transition levels with respect to the Si/SiO_2 interface using the rigid band approximation. We also probe the effect of trap levels of pre-existing defects with respect to the distance to the interface using models of c-Si/a-SiO_2/a-HfO_2 stacks to simulate both thick and thin film devices. Distributions of one-electron levels are calculated for oxygen vacancy centres and H-induced defects as a function of the distance to the interface. The thermodynamic nature of interstitial hydrogen is studied with respect to its position in the Si/SiO_2/HfO_2 stacks to assess its behaviour according to the RDD model. The charge state of interstitial H depends on the material in which it is present, and it can drift toward HfO_2 with a low energy barrier, as proposed by the RDD model.

11:20-11:40 AM “Adiabatic energy surfaces for charge carrier trapping in NiO and MnO”

Hannes Raebiger

Yokohama National University

NiO and MnO are described as charge transfer and Mott insulators, respectively. This implies that upon carrier doping, split-off deep states should be formed inside the band gap. These split-off states are not simply small polaron states, as by inserting one electron or hole carrier, more than one gap states are introduced forming e.g. Zhang-Rice like states. These gap states have typically been discussed based on the electronic degrees of freedom and strong correlation effects, and the role of ionic relaxation and displacements have received little attention. Hence we investigate the microscopic mechanisms and adiabatic energy surfaces of carrier doping in these strongly correlated materials by density-functional calculations. To correctly describe strong correlation effects, we extend density-functional theory to comply with Koopmans' linearity. In addition to the antiferromagnetic (AF) ground states, we also consider paramagnetic (PM) phases described by special quasirandom spin configurations.

For NiO, we find that both electron and hole carriers prefer delocalized host band like states instead of deep small polaron states, in both AF and PM phases. We also find several deep small polaron states, for both electrons and holes, higher in energy than the delocalized ground states, well in agreement with experimental observations. For MnO, there is a clear asymmetry between electron and hole doping: holes get trapped in split-off deep gap states, whereas electrons are delocalized in conduction band states, and electron polarons remain absent. In the PM phase of MnO, the energy difference between delocalized and trapped holes becomes very small, indicating a co-existence of polaron hopping and band conductivity. For the split-off polaronic states in both MnO and NiO, the charge trapping changes the on-site screening, which via a charge self-regulation mechanism not only induces new gap states akin to Zhang-Rice states, but also induces ultra-deep states that lie below the valence band.

The multifarious small polaron states are associated with structural deformations, namely, axial, planar, or volumetric deformations of the octahedron surrounding polaron site. The type of deformation is determined by the orbital the polaron is trapped in, with hole polarons contracting the octahedron and electron polarons expanding it. While the various observed polaron states are close in energy, the adiabatic energy landscapes vary significantly. Some polarons are connected with smooth adiabatic transitions with free carrier states, and some have no adiabatic connection at all. These differences will be discussed in detail.

Acknowledgment: This work is done in collaboration with S. Bae, O. Malyi, and A. Zunger.

11:20-11:40 AM	Open
11:40-12:00 PM	**Concluding remarks and departure**