



**32<sup>nd</sup> International Conference  
on Defects in Semiconductors**

**Program for the 32<sup>nd</sup> ICDS**

**Rehoboth Beach, Delaware, USA**

**September 10–15<sup>th</sup>, 2023**

**Sunday, September 10<sup>th</sup>**

**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
7:15-8:00 PM	“From Color Centers to Quantum Emitters: A Century of Point Defects” Chris G. Van de Walle, University of California, Santa Barbara

***Following the talks    Reception***

## **Monday, September 11<sup>th</sup>**

### **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
- 9:15-10:00 AM    “Charged defects in semiconductors and beyond”  
Jörg Neugebauer, Max Planck Institute
- 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<sub>2</sub>O<sub>3</sub> During O<sub>2</sub> Annealing  
Revealed by FTIR and Modelling”  
Michael Scarpulla, University of Utah
- 10:40-11:20 AM    “Classes of O-H centers in β-Ga<sub>2</sub>O<sub>3</sub> and their effect on the concentration  
of free carriers” (*invited presentation*)  
Michael Stavola, Lehigh University
- 11:20-11:40 AM    “Metastable cation vacancies in semiconducting oxides”  
W. Beall Fowler, Lehigh University
- 11:40-12:00 PM    “Oxygen vacancies in gallium oxide and its sensitizing luminescence  
effect on rare earth ions”  
Houwei Pang, Zhejiang University
- 12:00-12:20 PM    “Vacancy defects in Si doped β-(Al,Ga)<sub>2</sub>O<sub>3</sub>”  
Iuliia Zhelezova, University of Helsinki

## **2D Materials (I) – Sanibel**

***Chairperson:***

- 10:20-10:40 AM “Benchmarking and applying quantum embedding methods for defects”  
Cyrus Dreyer, Stony Brook University and Flatiron CCQ
- 10:40-11:00 AM “High-throughput computationally-driven discovery and experimental realization of a new quantum defect in WS<sub>2</sub>”  
Geoffroy Hautier, Dartmouth College
- 11:00-11:20 AM “Magnetoelectricity (MC) behavior due to electron-electron interaction, Weak localization, and Zeeman effects in 2D layered WS<sub>2</sub>”  
Abdelhamid El Kaaouachi, University Ibn Zohr
- 11:20-11:40 AM “Chalcogen vacancies as paramagnetic deep acceptors in 2D transition-metal dichalcogenides”  
Shoaib Khalid, University of Delaware
- 11:40-12:20 PM “Native defects, electronic inhomogeneities, and charge density waves in 1T-TaS<sub>2</sub>” (*invited presentation*)  
Shawna Hollen, University of New Hampshire

## ***12:20-1:40 PM Lunch***

### **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, Nagoya University
- 2:20-2:40 PM “Analysis of Carbon Concentrations in GaN Epilayers by Cathodoluminescence”  
Kagiso Loeto, University of Cambridge

- 2:40-3:00 PM “Selective incorporation of antimony into gallium nitride”  
Yujie Liu, University of Michigan
- 3:00-3:20 PM** *Coffee break*
- 3:20-3:40 PM “Dual nature of acceptors in semiconductors: Evidence from photoluminescence experiments”  
Michael Reshchikov, Virginia Commonwealth University
- 3:40-4:00 PM “Surface Defect Electronic Properties in Gallium Nitride Epitaxial Layers on Different Substrates”  
Andrew Winchester, National Institute of Standards and Technology

### **Halide Perovskites (I) – Sanibel**

*Chairperson: Vladan Stevanovic, Colorado School of Mines*

- 1:40-2:00 PM “Experimentally observed defect tolerance in the electronic structure of lead bromide perovskites”  
Gabriel Man, MAX IV Laboratory
- 2:00-2:20 PM “Deep Levels and Acceptor Dopants in Lead Halide Perovskites”  
Michael Swift, US Naval Research Laboratory
- 2:20-3:00 PM “Optoelectronic and phase stability impacts of interstitial defects in halide perovskite semiconductors” (*invited presentation*)  
Ross Kerner, National Renewable Energy Laboratory
- 3:00-3:20 PM** *Coffee break*
- 3:20-3:40 PM “Extrinsic doping and compensating defects in the 2D hybrid perovskite phenethylammonium lead iodide”  
Gabrielle Koknat, Duke University
- 3:40-4:00 PM “Origins of photoluminescence instabilities at halide perovskite/organic hole transport layer interfaces”  
Zhaojian Xu, Princeton University

## Poster Session (I) – Kiwi's Kove

4:00-5:30 PM

**C1. Chitraleema Chakraborty**, “Defects in atomically thin semiconductors for optical quantum technologies”

**C2. Ross Kerner**, “Optoelectronic and phase stability impacts of interstitial defects in halide perovskite semiconductors”

**C3. Brendan McCullian**, “Coherent Orbital Control of Diamond NV Center Excited States Using Strain”

**C4. Yihuang Xiong**, “High-throughput identification of spin-photon interfaces in silicon”

**C5. Fangzhou Zhao**, “Trap-assisted Auger-Meitner recombination from first principles”

**H1. Piyush Kumar**, “Interface and bulk defects induced by the thermal oxidation and post-oxidation annealing in SiO<sub>2</sub>-SiC system”

**H2. Yujie Liu**, “Selective incorporation of antimony into gallium nitride”

**H3. Igor Prozheev**, “Defects in aluminum rich Si-doped 90% AlGaN determined by positron annihilation and X-ray absorption spectroscopy”

**H4. Muhammad Hassan Shaikh**, “Magnetic proximity coupling to defects in two-dimensional semiconductors”

**H5. Sarah Thompson**, “R-Cu Color Centers in ZnS:Cu Colloidal Nanocrystals and Potential Applications for Quantum Information Science”

**H6. Zhaojian Xu**, “Origins of photoluminescence instabilities at halide perovskite/organic hole transport layer interfaces”

**H7. Iuliia Zhelezova**, “Vacancy defects in Si doped  $\beta$ -(Al,Ga)<sub>2</sub>O<sub>3</sub>”

**1. Giovanni Alfieri**, “Deep levels in epitaxially grown 4H-SiC p+-i-n diodes”

**2. Pejk Amoroso**, “Point Defects in Ga-doped Ge”

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

**4. Weiru Chen**, “First-principles investigations of quantum defects in two-dimensional transition metal dichalcogenides”

5. **Henry Fried**, “Tight-Binding Modeling of Point Defects: A Machine Learning Approach for Predicting Parameters”
6. **Helton Goncalves de Medeiros**, “Raman spectroscopy study of defects near the SiO<sub>2</sub>-SiC interface and their correlation to electrically active defects”
7. **Ylva Hommedal**, “Diffusion of Ge in  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>”
8. **Jesse Huso**, “Photoluminescence mapping of defects in semiconductors”
9. **Grace McKnight**, “Investigation of oxygen interstitial diffusion pathways in  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>”
10. **Michael Reshchikov**, “Dual nature of the Li\_Zn acceptor in ZnO”
11. **Michael Reshchikov**, “Photoluminescence from GaN implanted with Be, F, and Cl ions”
12. **Rokas Silkinis**, “Theoretical modeling of vibrationally resolved optical lineshapes of a carbon-oxygen pair defect in silicon”
13. **Vytautas Žalandauskas**, “Ab initio study of vibrational properties of divacancy defects in 4H-SiC
14. **Shimin Zhang**, “Advanced Simulations of Spin defect in hBN: Strain and substrate effect, ODMR and Quantum Embedding theory”

## **Tuesday, September 12<sup>th</sup>**

### **Plenary Session – Swan Ballroom**

***Chairperson: Kai-Mei Fu, University of Washington***

- |                              |  |
|------------------------------|--|
| 8:30-9:15 AM                 | “Defects and diffusion in $\beta$ -Ga <sub>2</sub> O <sub>3</sub> ”<br>Lasse Vines, University of Oslo   |
| 9:15-10:00 AM                | “Piecewise Linearity Condition for Addressing the Self-Interaction of Polarons”<br>Alfredo Pasquarello, École Polytechnique Fédérale de Lausanne |
| <b><i>10:00-10:20 AM</i></b> | <b><i>Coffee break</i></b>   |

### **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”<br>Jordan Gusdorff, University of Pennsylvania                  |
| 10:40-11:00 AM | “Room-temperature optical and spin dynamics of a single quantum emitter in hexagonal boron nitride”<br>Rebecca Fishman, University of Pennsylvania               |
| 11:00-11:20 AM | “Defect spins and qubits in hexagonal boron nitride from first principles theory guiding experiments”<br>Ádám Gali, Wigner Research Centre for Physics, Budapest |
| 11:20-11:40 PM | “Controlled generation of spin defects in hexagonal boron nitride for quantum sensing applications”<br>Aqiq Ishraq, University of Delaware                       |
| 11:40-12:20 PM | “Defects in atomically thin semiconductors for optical quantum technologies” ( <i>invited presentation</i> )   |



Chitraleema Chakraborty, University of Delaware

### **Silicon carbide (I) – Sanibel**

***Chairperson: Evan Glaser, US Naval Research Laboratory***

- |                |   |
|----------------|---|
| 10:20-11:00 AM | “Doping-induced color centers in silicon carbide” <i>(invited presentation)</i><br>Marianne Bathen, University of Oslo  |
| 11:00-11:20 AM | “Investigation of unintentional aggregation of impurity-related defects within 4H-SiC and at the (11-20) 4H-SiC/SiO <sub>2</sub> interface”<br>Niamh Smith, University College London |
| 11:20-11:40 AM | “Assessing the potential of perfect screw dislocations in SiC for solid-state quantum technologies”<br>Daniel Barragan-Yani, University of Luxembourg                                 |
| 11:40-12:00 PM | “Nitrogen-dependent electronic and kinetic properties of dislocations in 4H silicon carbide”<br>Rong Wang, Zhejiang University  |
| 12:00-12:20 PM | “Optical and electrical characterization of potential single photon emitters in 6H silicon carbide”<br>Erlend Ousdal, University of Oslo  |

***12:20-1:40 PM Lunch***

## 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 b-Ga<sub>2</sub>O<sub>3</sub>”  
(invited presentation)  
Irina Buyanova, Linköping University
- 2:20-2:40 PM “Measuring the Static and Dynamic Disorder in  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> Using Optical Transmission”  
Ariful Islam, University of Utah
- 2:40-3:00 PM “Phase stability of (Al<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub> polymorphs: a first-principles study”  
Sai Mu, University of South Carolina
- 3:00-3:20 PM** ***Coffee break***
- 3:20-3:40 PM “Controlling defects in wide-bandgap oxides for memristor applications”  
Hartwin Peelaers, University of Kansas
- 3:40-4:00 PM “Excited-state properties of oxygen vacancies near  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>(0001) surfaces from first principles and quantum defect embedding”  
Vijaya Begum-Hudde, University of Illinois, Urbana-Champaign

### 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, Dartmouth College
- 2:00-2:20 PM “Photoluminescence spectra of the G center in silicon: comparison between first principles computations and experiment”  
Jiongzhi Zheng, Dartmouth College
- 2:20-3:00 PM “Defect Spectroscopy of Erbium Implanted Silicon for Quantum Technologies” (invited presentation)  
Jeffrey McCallum, University of Melbourne

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

***Coffee break***

3:20-3:40 PM

“Atomic scale analysis of N dopants in InAs”  
Tom Verstijnen, Eindhoven University of Technology

3:40-4:00 PM

“Characterization of carbon-13 T centers in silicon”  
M. Mehdi Keshavarz, Simon Fraser University

## **Poster Session (II) – Kiwi’s Kove**

**4:00-5:30 PM**

- 1. Giovanni Alfieri**, “Electrical characterization of 4H-SiC MOS interfaces with an ion implanted thermal oxide”
- 2. Khandakar Aaditta Arnab**, “Generalized Quenching as a Method for Predicting Defect Concentrations Resulting from Crystal Growth or Annealing”
- 3. Nikolay Arutyunov**, “Bismuth impurity centers in silicon: microstructure of bismuth-related defects produced by proton irradiation”
- 4. Hayley Austin**, “Carrier Confinement for Improved Color Tunability of Eu-doped GaN LEDs”
- 5. Brittany Baker**, “Analysis of Positively Charged Muonium in Tin Oxide”
- 6. Abdelhamid El Kaaouachi**, “Electrical conduction mechanisms on both sides of the Metal-Insulator Transition in dilute p-Si/SiGe/Si in the presence of the magnetic field”
- 7. Emily Garrity**, “Point Defects and Doping of Ultra-wide Band Gap (III)BO Oxides for Power Electronics”
- 8. Akira Kiyoi**, “Effect of oxygen on trap-limited diffusion of hydrogen in proton-irradiated n-type silicon for power devices”
- 9. Amelia Klein**, “Designing a collimating metasurface photon extractor for solid-state color centers through many-body adjoint shape optimization”
- 10. Amanda Langørgen**, “A metastable defect center in  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>”

- 11. Channyung Lee**, “Investigation of split vacancy and interstitial Defects and ionic diffusion mechanisms in  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>: A direct approach via master diffusion equations”
- 12. Lorenzo Maserati**, “Photo-Induced Current Transient Spectroscopy on Metal Halide Perovskites”
- 13. Marek Maciaszek**, “The application of the SCAN density functional to color centers for quantum applications”
- 14. Erlend Ousdal**, “Optical and electrical characterization of potential single photon emitters in 6H-SiC”
- 15. Houwei Pang**, “Oxygen vacancies in gallium oxide and its sensitizing luminescence effect on rare earth ions”
- 16. Christian Pederson**, “Imaging Surface Transfer Doping of Quantum Point Defects in Diamond Using Electrical Atomic Force Microscopy Techniques”
- 17. Amanda Portoff**, “Hydrogen centers as a probe of VGa<sub>2</sub> in  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>”
- 18. Michael Reshchikov**, “Effect of ion implantation damage on photoluminescence from GaN”
- 19. Connor Roncaioli**, “All In One Quantum Diamond Microscope for Rapid Sample Characterization”
- 20. Abdul Saboor**, “Electronic structure and band alignment of dilute III-V1-xBix alloys”
- 21. Michael Scarpulla**, “Defect Quasi Fermi Levels in Photoluminescence: Are they true thermodynamic potentials?”
- 22. Andrew Venzie**, “Diffusion of Interstitial Hydrogen in SnO<sub>2</sub>”
- 23. Tom Verstijnen**, “Atomic scale analysis of N dopants in InAs”
- 24. Darshana Wickramaratne**, “Assessing the SCAN functional for point defects and polarons”

## Wednesday, September 13<sup>th</sup>

### 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, Harvard University
- 9:00-9:20 AM “Magnetometry using point defect ensembles in isotopically pure 4H-SiC”  
Ignas Lekavicius, US Naval Research Laboratory
- 9:20-9:40 AM “Depth-resolved investigation of N and P ion-implantation induced defects in 4H-SiC”  
Maria Mendes Martins, Paul Scherrer Institute
- 9:40-10:00 AM “Interface and bulk defects induced by the thermal oxidation and post-oxidation annealing in SiO<sub>2</sub>-SiC system”  
Piyush Kumar, ETH Zurich
- 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, University of Washington
- 8:40-9:00 AM “Ti<sup>3+</sup> centers in nonstoichiometric KTiOPO<sub>4</sub> from DFT calculations”  
Adriana Bocchini, University of Paderborn
- 9:00-9:20 AM “Investigation of the structural, optical, and electrical properties of indium-doped TiO<sub>2</sub> thin films grown by pulsed laser deposition technique on low and high index GaAs planes”

Faisal Al Mashary, Qassim University

9:20-10:00 AM “Migration of nitrogen impurity in titanium dioxide and perovskite titanates” (*invited presentation*)  
Naoki Ohashi, National Institute for Materials Science, Japan

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

## **Parallel Sessions**

### **Diamond (I) – Swan Ballroom**

***Chairperson: Jeffrey McCallum, University of Melbourne***

10:20-10:40 AM “Photoexcitation dynamics of NV centers in diamond”  
Ronald Ulbricht, Max-Planck Institute for Polymer Research

10:40-11:00 AM “First-principles calculation of the Stark shift for the NV center in diamond”  
Louis Alaerts, Dartmouth College

11:00-11:20 AM “Coherent Orbital Control of Diamond NV Center Excited States Using Strain”  
Brendan McCullian, Cornell University

11:20-11:40 PM “Ab-initio theory of spin-lattice relaxation for NV center and other spin-1 defects by means of ab-initio calculations”  
Gergo Thiering, Wigner Research Centre for Physics, Budapest, Hungary

11:40-12:00 PM “Photoionization spectroscopy of the long-lived 1E singlet state of NV centers in diamond”  
Robert McMichael, National Institute of Standards and Technology

12:00-12:20 PM “Predicting Defect Concentrations from Stark Shift Measurements”  
Rodrick Kuate Defo, Princeton University

### **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
- 11:00-11:20 AM      “Muons in semiconductor research: Recent review and looking forward”  
Rick (P.W.) Mengyan, Northern Michigan University
- 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
- 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
- 12:00-12:20 PM      “Defect Identification in Atomic Layer Deposited Aluminum Oxide using Kelvin Probe Force Microscopy”  
Leah Tom, University of Wisconsin-Madison

***12:20-6:30 PM Lunch/free time***

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

## Thursday, September 14<sup>th</sup>

### 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 <sub>2</sub> O <sub>3</sub> through atomistic simulations” ( <i>invited presentation</i> )<br>Joel Varley, Lawrence Livermore National Laboratory |
| 9:00-9:20 AM          | “Defect migration energies in Ga <sub>2</sub> O <sub>3</sub> polymorphs measured by variations of temperature and flux under irradiation”<br>Alexander Azarov, University of Oslo                              |
| 9:20-9:40 AM          | “Quantum embedding methods for carbon dimer defects in hexagonal boron nitride”<br>Woncheol Lee, University of California, Santa Barbara   |
| 9:40-10:00 AM         | “Optical signatures of defects in hBN: comparing different calculation methods”<br>Ludger Wirtz, University of Luxembourg  |
| <b>10:00-10:20 AM</b> | <b><i>Coffee break</i></b>   |
| 10:20-11:00 AM        | “Theoretical Modeling of Vibrationally Resolved Optical Lineshapes of Semiconductor Deep-Level Defects” ( <i>invited presentation</i> )<br>Lukas Razinkovas, Center for Physical Sciences and Technology       |
| 11:00-11:20 AM        | “Ab initio modeling of the photoionization of negatively charged NV centers in diamond”<br>Marek Maciaszek, Center for Physical Sciences and Technology  |
| 11:20-11:40 AM        | “Optical transitions in Mg-doped Ga <sub>2</sub> O <sub>3</sub> ”<br>Darshana Wickramaratne, US Naval Research Laboratory  |



11:40-12:20 PM      “Trap-assisted Auger-Meitner recombination from first principles”  
(*invited presentation*)  
Fangzhou Zhao, University of California, Santa Barbara

### **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, Technische Universität Ilmenau

9:00-9:20 AM      “Experimental Study on Defect Behavior during Crystal Growth of  
Phosphorus Heavily Doped Czochralski-Silicon”  
Masataka Hourai, SUMCO Corporation

9:00-9:20 AM      “Density Functional Theory Study on Peculiar Defect Behavior during  
Crystal Growth of Phosphorus Heavily Doped Silicon”  
Koji Sueoka, Okayama Prefectural University

9:00-9:20 AM      “Influence of Solute Incorporation Mechanisms on the Properties of  
Highly Mismatched Semiconductors” (*invited presentation*)  
Rachel Goldman, University of Michigan

**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, Lehigh University

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

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

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

12:00-12:20 PM “Vacancy complexes in H-implanted AlN”  
Filip Tuomisto, University of Helsinki

### ***12:20-1:40 PM Lunch***

#### **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, TU Wien

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

2:40-3:00 PM “Proton irradiation-induced point defects acting as Shockley-Read-Hall recombination centers in homoepitaxial GaN p<sup>+</sup>/n<sup>-</sup> and p<sup>-</sup>/n<sup>+</sup> junctions”  
Tetsuo Narita, Toyota Central R&D Labs., Inc.

***3:00-3:20 PM Coffee 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)*  
Shiyu Chen, Fudan University
- 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, University of North Carolina at Charlotte

### **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, Osaka University
- 2:00-2:20 PM “Ultrafast carrier dynamics in GaN:Eu LED structures studied by terahertz emission spectroscopy”  
Fumikazu Murakami, Osaka University
- 2:20-3:00 PM “Rare-earth defects for quantum information applications” *(invited presentation)*  
Khang Hoang, North Dakota State University
- 3:00-3:20 PM Coffee break***
- 3:20-3:40 PM “Probing the interfacial defect layer in chalcopyrite solar cells”  
Helena V. Alberto, University of Coimbra
- 3:40-4:00 PM “First-principles study of intrinsic point defects and hydrogen impurities in the earth-abundant photovoltaic absorber Zn<sub>3</sub>P<sub>2</sub>”  
Zhenkun Yuan, Dartmouth College
- 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

## Friday, September 15<sup>th</sup>

### 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” ( <i>invited presentation</i> )<br>Qimin Yan, Northeastern University  |
| 9:00-9:20 AM          | “Native Point Defects in Transition Metal Dichalcogenides - Experimental Verification of Theoretical Prediction”<br>Łukasz Gelczuk, Wrocław University of Science and Technology  |
| 9:20-9:40 AM          | “Defect assisted triplet exciton transfer across the tetracene-Si(111):H interface”<br>Marvin Krenz, University of Paderborn  |
| 9:40-10:00 AM         | “Magnetic proximity coupling to defects in two-dimensional semiconductors”<br>Muhammad Hassan Shaikh, University of Delaware  |
| <b>10:00-10:20 AM</b> | <b><i>Coffee break</i></b>  |
| 10:20-10:40 AM        | “Alloying-related changes in electronic properties of common grown-in and radiation-induced defects in $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layers grown by MOVPE on Ammono-GaN substrates”<br>Piotr Kruszewski, Inst. High Pressure Phys. Polish Academy of Sciences |
| 10:40-11:00 AM        | “Role of Nitrogen Vacancies in Obtaining Semi-Insulating Properties of Ammonothermal GaN:Mg”<br>Marcin Zajac, Inst. of High Pressure Phys. Polish Academy of Sciences   |
| 11:00-11:40 AM        | “Optical absorption of point defects in ultrawide bandgap semiconductors AlN and $\text{Ga}_2\text{O}_3$ as measured by photo-induced electron paramagnetic resonance” ( <i>invited presentation</i> )<br>Mary Ellen Zvanut, University of Alabama at Birmingham      |

11:40-12:00 PM      “Role of Nitrogen Vacancies in Obtaining Semi-Insulating Properties of Ammonothermal GaN:Mg”  
Pakpoom Reuchan, Kasetsart University

### **Theory of defects (I) – Sanibel**

*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, DEVCOM Army Research Laboratory

8:40-9:00 AM      “Evaluating finite size effects for hybrid functional defect calculations”  
Ben Hourahine, University of Strathclyde

9:00-9:40 AM      “Defects in Topological Semimetals” (*invited presentation*)  
Kirstin Alberi, National Renewable Energy Laboratory

9:40-10:00 AM      “Defect Analysis at Database Scale”  
Jimmy-Xuan Shen, Lawrence Livermore National Laboratory

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

10:20-11:00 AM      “On a quest for novel wide gap semiconductors” (*invited presentation*)  
Vladan Stevanovic, Colorado School of Mines

11:00-11:20 AM      “Adiabatic energy surfaces for charge carrier trapping in NiO and MnO”  
Hannes Raebiger, Yokohama National University

11:20-11:40 AM      “Small Electron Polarons in Tantalum Oxynitride: Formation and Hopping Transport”  
Manoj Dey, Indian Institute of Science

11:40-12:00 PM      “Modelling device degradation by hydrogen-related hole trapping defects at the c-Si/a-SiO<sub>2</sub> and c-Si/a-SiO<sub>2</sub>/a-HfO<sub>2</sub> interface”  
Teo Cobos, University College London

**12:00-12:15 PM      *Concluding remarks and departure***