IMEC2021

19th Israel Materials Engineering Conference

December 13-14, 2021

The international Convention Center –
ICC Jerusalem

Welcome letter

Dear Colleagues,

On behalf of the Local Organizing and Scientific Committees, it is our great pleasure to invite you to participate in the 19th Israel Materials Engineering Conference (IMEC2021).

The broad coverage by IMEC2021 should provide scientific inspiration and stimulation to an interdisciplinary audience, including materials, mechanical, electrical, chemical, biomedical, environmental, and nuclear engineers, as well as chemists, physicists, professionals in life sciences and medicine.

This meeting, the first IMEC to be held after the Corona crisis, includes more than 120 talks, 230 posters, 17 commercials booths and ~ 700 participants (all locals) which reflects the emerging importance of the Materials Science community in Israel.

Looking forward to meet you at IMEC2021!

Sincerely

Prof. Shachar Richter

Dr. Noa Lachman Senesh

Prof. Brian Rosen

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Program

DAY 1 - December 13, 2021

TIME	ACTIVITY
08:00 - 09:00	Registration
09:00 - 09:45	Plenary 1 - Noam Eliaz - Tel Aviv Univesity | Towards Additive Manufacturing of Novel Aluminum-Based Self-Healing Metal Matrix Composites by Directed Energy Deposition (DED)
09:45 - 10:30	Plenary 2 - Gitty Frey - Technion | Organic electronics: An interface user
10:30 - 11:00	Coffee break
11:00 - 13:00	**Sessions 1-5**

Session 1	**Teddy A**	
Session name	**Materials for Energy I**	
Session chairs	**Lioz Etgar, Doron Urbach**	
TIME	**Speaker**	**Title**
11:00 - 11:20	Omer Yaffe Weizmann Institute of Science	Anharmonic semiconductors - Lessons Learned from Halide perovskites
11:20 - 11:40	Yehonadav Bekenstein Technion	Buckling and tolerance in semiconductors perovskite CsPbBr_3 nanostructures
11:40 - 11:55	Mor Fiegenbaum-Raz Tel Aviv University	Spatial External Luminescence Efficiency of Perovskite Solar Cells
11:55 - 12:10	Oded Nahor Technion	Coexisting multiple glassy phases with different compositions in NFA-based Organic solar cells
12:10 - 12:25	David Zitoun Bar-Ilan University	Hydrogen-Bromine Redox-Flow Batteries
12:25 - 12:45	Lioz Etgar The Hebrew University of Jerusalem	Low dimensional perovskite and their applications in photovoltaic cells, nanostructures and semitransparency
12:45 - 13:05	Ines Zucker Tel Aviv University	MoS2-based Nanocomposites for Water Decontamination

Session 2	**Teddy B**	
Session name	**2D Materials I**	
Session chairs	**Doron Naveh, Ariel Ismach**	
TIME	**Speaker**	**Title**
11:00 - 11:20	Maya Bar-Sadan Ben-Gurion University of the Negev	A place where everyone matters – interfaces in functional nanostructures
11:20 - 11:40	Elad Koren Technion	Interlayer electronic transport in bilayer graphene systems
11:40 - 11:55	Daniel Gilbert Nessim Bar Ilan University	Spaghetti and lasagne: the cooking of 1D and 2D nanomaterials

11:55 - 12:10	Assael Cohen Tel Aviv University	Metal-Organic Chemical Vapor Deposition of Wafer-Scale and Carbon- Free WS2 Atomic Layers
12:10 - 12:25	Avia Ohayon-Lavi Ben-Gurion University of the Negev	Graphene-based Conformal Coating: How to Avoid Hot Spots?
12:25 - 12:45	Assaf Ya'akobovich Ben-Gurion University of the Negev	Heat transfer in Graphene foams
12:45 - 13:05	Oded Hod Tel Aviv University	The Fascinating Frictional Properties of Layered Materials

Session 3	**Teddy C**	
Session name	**Additive Manufacturing I (Metals)**	
Session chairs	**Amnon Shirizly, Eitan Tiferet**	
TIME	**Speaker**	**Title**
11:00 - 11:20	Gennady Ziskind Ben-Gurion University of the Negev	A study of pre-heating stages in electron beam melting
11:20 - 11:40	Elad Caspi	Residual stress and texture characterization of curved parts in SLM and EBM additive manufactured Ti-6wt%Al-4wt%V tubes
11:40 - 12:00	Shmuel Osovski Technion	Effect of roughness on energy absorption in AM Ti6Al4V thin walled cylinders
12:00 - 12:15	Roman Bendersky RAFAEL	Leveraging additive manufacturing process simulation to meet contradicting geometrical requirements
12:15 - 12:30	Noa Lulu-Bitton Tel Aviv University / NCRN	The influence of Electrochemically Charged Hydrogen on the Mechanical behavior of Electron Beam Melting (EBM) and Wrought Ti-6Al-4V using the Small Punch Test (SPT)
12:30 - 12:45	Yaron Ganor Rotem	Novel Thermotopographic Analysis of Electron Beam Additive Manufacturing Process Using Stock Arcam Q20 Plus
12:45 - 13:00	Daniel Moreno Beth Shemesh Engines LTD	Mechanical Properties, Metallurgical Characteristics and Anisotropy of Additive Manufacturing of 316L

Session 4	**Oren 2**	
Session name	**Analytical Techniques**	
Session chairs	**Yaron Kauffmann, Atzmon Vakahi**	
TIME	**Speaker**	**Title**
11:00 - 11:20	Hagai Cohen Weizmann Institute of Science	Combined Chemical & Electrical Analyses of Hetero-Structures: Past, Present, Future

11:20 - 11:40	Louisa Meshi Ben-Gurion University of the Negev	Unambiguous structure determination of intermetallics using electron crystallography methods
11:40 - 11:55	Aleksei Solomonov Weizmann Institute of Science	Spiky Gold Nanostructures
11:55 - 12:10	Assaf Dana Technion	Unraveling the rate of the reverse martensitic transformation: A microsecond-scale time-resolved X-ray diffraction study
12:10 - 12:25	Maya Barzilay Technion	Advanced Imaging and Analysis of Inorganic-Organic Hybrid Nano-Structures Fabricated via Sequential Infiltration Synthesis
12:25 - 12:45	Arik Kreisel Nuclear research center	Opportunities at the new Soreq accelerator facility neutron source
12:45 - 13:05	Inna Popov The Hebrew University of Jerusalem	Characterization of Nanostructured Alloys with FIB Tomography

Session 5	**Oren 3**	
Session name	**Corrosion & Coating**	
Session chairs	**Yair Ein Eli, Tal Kaufman**	
TIME	**Speaker**	**Title**
11:00 - 11:20	Brian Rosen Tel Aviv University	Corrosion resistance and catalytic activity of nanocrystalline alloys of molybdenum and tantalum carbide
11:20 - 11:40	Alec Groysman Technion	A fascinating journey into the world of corrosion: New book “Corrosion: monitoring, control, and prevention”
11:40 - 12:00	Nissim Navi NCRN	Hydrogen Induced Degradation of Electrochemically Charged Electron Beam Melted (EBM) and Wrought Ti-6Al-4V Alloys
12:00 - 12:15	Barbara Kazanski Azrieli College of Engineering	Effect of Plasma electrolytic oxidation treatment on corrosion behavior of AZ91D, AM50, AE42 and MRI 230D magnesium alloys
12:15 - 12:30	Sharon Waichman Rotem/NCRN	A systematic deposition parameters study of boron carbide coatings onto aluminum substrates
12:30 - 12:45	Tal Kaufman Simtal	A breakthrough technological solution in the nano-conformal coating world

13:00 - 14:30 Lunch and poster session

TIME	ACTIVITY
14:30 - 16:30	Sessions 6-10

Session 6	Teddy A	
Session name	Materials for Energy II	
Session chairs	Lioz Etgar	
TIME	**Speaker**	**Title**
14:30 - 14:50	Daniel Grave Ben-Gurion University of the Negev	Metal-oxide photoelectrodes for solar water splitting
14:50 - 15:10	Lior Elbaz Bar Ilan University	Design of Aerogel-based Electrocatalysts for Oxygen Reduction Rection in Fuel Cells
15:10 - 15:25	Adi Lavi Ben-Gurion University of the Negev	Graphite-GnP-salt composite: Thermal properties enhancement for energy storage applications
15:25 - 15:40	Roey Ben David Weizmann Institute of Science	Methanol conversion to hydrogen on copper surfaces: A molecular level study
15:40 - 15:55	Subhabrata Mukhopadhyay Ben-Gurion University of the Negev	Assembly of a MOF Membrane on Solid Electrocatalyst: Molecular-Level Control Over Heterogeneous CO2 Reduction
15:55 - 16:15	Menny Shalom Ben-Gurion University of the Negev	Carbon Nitride Layers as Light-Harvesting Semiconductors for Photoelectrochemical Cells
16:15 - 16:35	Elad Gross The Hebrew University of Jerusalem	IR Nanospectroscopy Measurements Uncover Structure-Reactivity Correlations in Catalytic Nanostructures

Session 7	Teddy B	
Session name	2D Materials II	
Session chairs	Doron Naveh, Ariel Ismach	
TIME	**Speaker**	**Title**
14:30 - 14:50	Efrat Lifshitz Technion	The influence of global and local magnetism on optical properties of two-dimensional semiconductors
14:50 - 15:10	Moshe Haratz Ben-Gurion University of the Negev	Effects of non-uniform strain in transition-metal dichalcogenides
15:10 - 15:25	M.B. Sreedhara Weizmann Institute of Science	Asymmetric "misfit" nanotubes: Chemical affinity outwits the entropy at high-temperature solid-state reactions
15:25 - 15:40	Efrat Ruse Nuclear Research Center	Molten Salt-Assisted Exfoliation of Graphite to Graphene: A Mechanistic Study

15:40 - 15:55	Michal Poplinger Bar Ilan University	Study of 2D Alloys Bi2Se(3-x)Sx Optical and Optoelectronic Properties
15:55 - 16:15	Eilam Yalon Technion	Electrical Contact Resistance to Atomically Thin Semiconductors
16:20 - 16:40	Moshe Ben-Shalom Tel Aviv University	"Slide-Tronics"

Session 8	**Teddy C**	
Session name	**Oxides and Engineered Quantum Materials**	
Session chairs	**Yoram Dagan, Shmulik Hayun**	
TIME	**Speaker**	**Title**
14:30 - 14:50	Muntaser Naamneh Ben-Gurion University of the Negev	Surface state at BaSnO3 evidenced by angle-resolved photoemission spectroscopy and ab initio calculations
14:50 - 15:10	Beena Kalisky Bar Ilan University	Imaging the magnetic landscape in a superconductor-correlated insulator alternate stacking 4Hb-TaS2
15:10 - 15:25	Anna Lavie Weizmann Institute of Science	Strain glass properties in Sm doped ceria
15:25 - 15:40	Lee Shelly Ben-Gurion University of the Negev / NCRN	Water adsorption and oxidation in the Th1-xUxO2 system
15:40 - 16:00	Maxim Sokol Tel Aviv University	On the stability of MXene in aqueous colloidal suspensions
16:00 - 16:15	Barak Ratzker Tel Aviv University	Processing and properties of transparent ceramics by high-pressure spark plasma sintering
16:15 - 16:35	lior kornblum Technion	Oxide interfaces and device building blocks for oxide electronics
16:35 - 16:50	Inbal Segev Gavish Technion	MeV Proton induced radiation damage in tungsten and tantalum

Session 9	**Oren 2**	
Session name	**Metallurgy and Processing**	
Session chairs	**Louisa Meshi, Nachum Frage**	
TIME	**Speaker**	**Title**
14:30 - 14:50	Shmulik Hayun Ben-Gurion University of the Negev	Thermochemistry of High Entropy Alloys
14:50 - 15:10	Eugen Rabkin Technion	The role of grain and interphase boundaries in nucleation-controlled plasticity
15:10 - 15:25	Mor Levi Technion	Solid-state dewetting synthesis of Nickel-Platinum nanoparticles

15:25 - 15:40	Einat Strumza Ben-Gurion University of the Negev	Comprehensive study of phase transitions in Al0.5CoCrFeNi high-entropy alloy at intermediate temperatures (400 ≤ T ≤ 900°C)
15:40 - 16:00	Itamar Gutman Rafael	Emerging Opportunities in the Fields of Metallurgy and Processing
16:00 - 16:20	Eyal Yahel Kamag	Phase diagrams under pressure: Experiments and thermodynamic modelling
16:20 - 16:35	Ofer Burg The Hebrew University of Jerusalem	Periodic Nanowire Arrays with Alternating Compositions and Structures Fabricated using a Simultaneous Nanowire Formation Step

Session 10	**Oren 3**	
Session name	**Additive Manufacturing II (metals)**	
Session chairs	**Amnon Shirizly**	
TIME	**Speaker**	**Title**
14:30 - 14:50	Eitan Tiferet NRCN, Rotem Ind, AEAI	Development of generic parameters for additive manufacturing (AM) of Ti-alloys and 316L SS by powder bed electron beam melting (EBM) method
14:50 - 15:10	Galit Katarivas Levy Ben-Gurion University of the Negev	Additive Manufacturing in Biomedical Applications
15:10 - 15:30	Adi Ben-Artzy Ben-Gurion University of the Negev / Berekely	Compositionally graded SS316 to C300 Maraging steel using additive manufacturing
15:30 - 15:45	Tomer Ron Ben-Gurion University of the Negev	Additive manufacturing of high entropy alloy WTaMoNbV produced by SLM process using elemental powder mixture
16:00 - 16:15	Noa Gabay Ben-Gurion University of the Negev	Additively manufactured Ti-6Al-4V lattice infiltrated with biodegradable Zn-base alloy as a hybrid structure for osseointegrated implants
16:15 - 16:30	Yuval Gale IAI	Pushing LPBF the the edge - the boundaries between design and manufacturing

16:30 - 18:00 Happy hour and poster session

DAY 2 - December 14, 2021

TIME	ACTIVITY
08:00 - 09:00	Registration
09:00 - 09:45	Plenary 3 - Uri Banin - The Hebrew University | Colloidal Semiconductor Nanocrystals: From Artificial Atoms to Artififfical Molecules
09:45 - 10:30	Plenary 4 - Lia Addadi - Weizmann Institute of Science | Biogenic nano-scale mirrors and light scatterers, built of organic crystals, and engineered to fulfill optical functions
10:30 - 11:00	Coffee break
11:00 - 13:00	**Sessions 11-15**

Session 11	**Teddy A**	
Session name	**Soft matter and Bio materials I**	
Session chairs	**Jacob Klein, Alejandro Sosnik**	
TIME	**Speaker**	**Title**
11:00 - 11:20	Hanna Rapaport Ben-Gurion University of the Negev	Peptides assemblies as a versatile platform for enhancing the functionality of biomaterials
11:20 - 11:40	Filipe Natalio Weizmann Institute of Science	Where plants meet material science: "bio-facturing" cellulose fibers with tailored properties
11:40 - 11:55	Gerardo Byk Bar Ilan University	Tuning the size and composition of nanohydrogels using a "Phantom monomer" for biological applications
11:55 - 12:10	Yael Levi-Kalisman The Hebrew University of Jerusalem	Hierarchical Assembly Pathways of Spermine-Induced Tubulin Conical-Spiral Architectures
12:10 - 12:25	Lital Mordechay Bar Ilan University	Mechanical Regulation of the Cytotoxic Activity of Natural Killer Cells
12:25 - 12:45	Eyal Golub Bar Ilan University	Dynamic and stimuli-responsive protein constructs via interfacial engineering
12:45 - 13:05	Luai Khoury Technion	Proteins as a Gamechanger in Biomaterials

Session 12	**Teddy B**	
Session name	**Polymers and Composites**	
Session chairs	**Roy Shenhar, Shmuel Kenig**	
TIME	**Speaker**	**Title**
11:00 - 11:20	Oren Regev Ben-Gurion University of the Negev	Compression-enhanced thermal conductivity of polymer composites

11:20 - 11:35	Yuval Vidavskyn Nuclear research center	Enhancing the mechanical properties of polymers via metal-ligand interactions
11:35 - 11:55	Tamar Segal-Perets Technion	Polymer- metal oxide nanocomposites and nanostructures via vapor-phase based growth within polymers
11:55 - 12:10	Omri Yannay Ansys	Short Fibers Polymer Matrix Composites (PMCs) Micro-Thermo-Mechanical Material Parametric Optimization
12:10 - 12:30	Elizabeth Amir Shenkar handesaim	Surface functionalization of textile as a tool for fabrication of smart fabrics
12:30 - 12:45	Ronen Verker Nuclear research center	Infrared Irradiated Reversible Shape Memory Polymer Mechanisms
12:45 - 13:05	Noy Cohen Technion	On the swelling of hydrogen-bond dominated polymer networks

Session 13	**Teddy C**	
Session name	**Surfaces of Materials**	
Session chairs	**Ilan Goldfarb**	
TIME	**Speaker**	**Title**
11:00 - 11:20	Igor Rahinov The Open University	Tracking the microscopic pathways of molecule's accommodation on a metal surface
11:20 - 11:40	Edward Bormashenko Ariel University	Bioinspired and Meta-Materials - the Nearest Future of the Materials Science and Engineering
11:40 - 11:55	Shaked Caspi Technion	Capping layers for SrVO3 films and their influence on the near-surface region
11:55 - 12:10	David Ehre Weizmann Institute of Science	Surface Pyroelectricity and Piezoelectricity of Centrosymmetric Crystals
12:10 - 12:25	Ran Eitan Abutbul Ben-Gurion University of the Negev	Stability of cubic tin sulphide nanocrystals: role of ammonium chloride surfactant headgroups
12:25 - 12:45	Dvir Gur Weizmann Institute of Science	The physical and cellular mechanism of nano-crystals based color change in zebrafish
12:45 - 13:05	Eren Baran Weizmann Institute of Science	Observing Electrochemical Reactions on Suspended Graphene: An Operando Kelvin Probe Force Microscopy Approach

Session 14	Oren 2	
Session name	Additive Manufacturing (General)	
Session chairs	Noam Eliaz	
TIME	**Speaker**	**Title**
11:00 - 11:20	Noa Lachamn Tel Aviv University	The perks of using fused filament fabrication in polymer matrix composites processing
11:20 - 11:40	Diana golodnitzki Tel Aviv University	Towards Smart Flexible Batteries
11:40 - 12:00	Rotem Almany Elbit	THE GUTENBERG-WRITE FUTURE With 3D composite printing into aerospace structures
12:00 - 12:15	Hadar Shaked Technion	Long-term stabilized amorphous calcium carbonate (ACC) as an ink for bio-inspired 3D printing
12:15 - 12:30	Doron Kam The Hebrew University of Jerusalem	Additive Manufacturing of 3D Wooden Structures
12:30 - 12:45	Tamar Rozental The Hebrew University of Jerusalem	Particle-Free inks for 3D printing Dense Ceramic Structures by DLP

Session 15	Oren 3	
Session name	Computationa and Theory	
Session chairs	Leeor Kronik, Maytal Caspary Toroker	
TIME	**Speaker**	**Title**
11:00 - 11:20	Tamar Goldzak Mizrachi Bar Ilan University	Performance of modified MP2 methods for solids
11:20 - 11:40	Ilya Grinberg Bar Ilan University	Approaches for controlling the mechanism of molecular catalysts towards ORR
11:40 - 12:00	Guy Makov Ben-Gurion University of the Negev	Materials Modelling of π-Phase Monochalcogenide semiconductors
12:00 - 12:20	Tamar Stein Hebrew University	The Effect of Cluster Size on the Intra-Cluster Ionic Polymerization Process
12:20 - 12:40	Oswaldo Dieguez Tel Aviv University	Flexoelectricity and Ferroelectric Domain Walls: Landau Theory from Density-Functional Theory Calculations
12:40 - 13:00	Dan thomas major Bar Ilan University	Computational studies of structure, composition, and electrochemical behavior of Li-ion battery components

13:00 - 14:30 Lunch and poster session

TIME	ACTIVITY
14:30 - 16:30	Sessions 16-20

Session 16	Teddy A	
Session name	Soft matter and Bio materials II	
Session chairs	Jacob Klein, Alejandro Sosnik	
TIME	**Speaker**	**Title**
14:30 - 14:50	Ulyana Shimanovich Weizmann Institute of Science	Self-assembly phenomenon in biomaterials science
14:50 - 15:10	Liraz Chai The Hebrew University of Jerusalem	A multiscale study of bacterial biofilms. From isolated components to multicellular organisms
15:10 - 15:25	Daniela Dobrynin Technion	A study of the SARS CoV-2 Spike protein adsorption on to various surfaces
15:25 - 15:40	Guillaume Le Saux Ben-Gurion University of the Negev	Dynamic Surface-Layer Coiled Coil Proteins Processing Analog-to-Digital Information
15:40 - 16:00	Michal Levin Technion	The influence of flexible mechanical constraints on the swelling of gels
16:00 - 16:20	Lihi Adler-Abramovich Tel Aviv University	Designing New Bioinspired 3D Nanostructure for Biological Applications
16:20 - 16:40	Ofra Benny The Hebrew University of Jerusalem	Cell Mechanomics for Precision Nanomedicine in Cancer

Session 17	Teddy B	
Session name	Magnetic and Electronic Materials	
Session chairs	Rakefet Ofek Almog, Alexander Strikovsky	
TIME	**Speaker**	**Title**
14:30 - 14:50	Yoav Kalcheim Technion	Tuning resistive switching in engineeres mott insulators
14:50 - 15:10	Ori Gidron The Hebrew University of Jerusalem	Controlling the Helicity of Aromatic Materials
15:10 - 15:30	Yonatan Calahorra Technion	Nanostructure effects in piezoelectric semiconductors and related magneto-semiconductor composites
15:30 - 15:50	Igor Lubomirsky Weizmann Institute of Science	Non-classical electrostriction: current understanding and potential applications

15:50 - 16:05	Rakefet Ofek Almog Azrieli College of Engineering	Characterization of ZnO Nanostructures Decorated with Noble Metal Nano Particles
16:05 - 16:25	Ran Manor NVIDIA	Package Materials & Processes for High-Speed IO – A Review
16:25 - 16:40	Anjan Bhukta Tel Aviv University	Exploiting compositional variations in epitaxial Permalloy-silicide nanostructures on silicon to affect their magnetic properties

Session 18	**Teddy C**	
Session name	**Mechanical and Structural Materials**	
Session chairs	**Mirit Sharabi, Dan Mordehai**	
TIME	**Speaker**	**Title**
14:30 - 14:50	Daniel Wagner Weizmann Institute of Science	Hierarchical interfaces as fracture propagation traps in natural layered composites
14:50 - 15:10	Dov Sherman Tel Aviv University	Macro to micro in fracture – from macroscopic cleavage energy to atomistic bond breaking mechanisms
15:10 - 15:25	XiaoMeng Sui Weizmann Institute of Science	A polarized micro-Raman study of necked epoxy fibers
15:25 - 15:45	Joshua M. Grolman Technion	Extracellular Matrix Mechanics and Disease States
15:45 - 16:00	Emil Bronstein Technion	Tracking twin boundary jerky motion at nanometer and microsecond scales
16:00 - 16:20	Benny Bar on Ben-Gurion University of the Negev	Plant wings as biocomposites
16:20 - 16:35	Emanuel Avrahami Weizmann Institute of Science	Complex hierarchical biominerals are the result of differential facet growth of a simple habit
16:35 - 16:50	Carol Rodricks Weizmann Institute of Science	Polymer beads as interfacial obstacles in fibre composites

Session 19	**Oren 2**	
Session name	**Materials for Optics**	
Session chairs	**Tal Ellenbogen, Rami Cohen**	
TIME	**Speaker**	**Title**
14:30 - 14:50	Dan Oron Weizmann Institute of Science	Heralded spectroscopy reveals exciton-exciton correlations in single colloidal nanocrystals

14:50 - 15:05	Cecile Saguy Technion	Polarization Origin of Photoconductivity in MAPbI3 Thin Films
15:05 - 15:20	Orr Be'er Technion	Correlated emission in self assembled CsPbBr3 perovskite superlattices
15:20 - 15:40	Adi Salomon Bar Ilan University	Cathodoluminescence Nanoscopy of Plasmonic Structures
15:40 - 16:00	Ido Hadar The Hebrew University of Jerusalem	Broadband Emission from Metal-Halide Perovskites – Towards Light Emitting Diodes
16:00 - 16:20	Yoav Dias Elbit	Challenges in the design of Electro-Optics parts, using AM (additive manufacturing) of aluminum
16:20 - 16:35	Ora Bitton Weizmann Institute of Science	Plasmonic cavities and individual quantum emitters in the strong coupling limit

Session 20	**Oren 3**	
Session name	**Materials for Defense and Security**	
Session chairs	**Orna Breuer, Michael Gozin**	
TIME	**Speaker**	**Title**
14:30 - 14:50	Ehud Galun	Materials for Defense
14:50 - 15:10	Yinon Yavor Afeka College of Engineering	Combustion of Boron-Water-AN Solid Propellants
15:10 - 15:30	Oded Shoseyov The Hebrew University of Jerusalem	The Plant Age; Materials for the future
15:45 - 16:05	Daniel Rittel Technion	Impact response of thermoreversible methylcellulose hydrogels
16:05 - 16:25	Eran Tuval IDF/Aegisium	Design Considerations in Energetic Materials Compatibility: Imbuing Service-Long Robustness of Weapon System Attributes
16:25 - 16:40	Matan Levin Technion/Rafael	Compounding and 3D Printing of a Tailored Electromagnetic Radiation Absorber

16:30 - 17:00 Coffee break and poster session

17:00 - 18:00 Plenary 5 - Yaniv Geblstein - Ben Gurion University | Development of highly efficient thermoelectric materials and devices

Plenary Lectures

Plenary 1

Towards Additive Manufacturing of Novel Aluminum-Based Self-Healing Metal Matrix Composites by Directed Energy Deposition (DED)

Noam Eliaz
Tel Aviv Univesity

Noam Eliaz,a David Svetlizky,a Baolong Zheng,b Sen Jiang,b Yizhang Zhou,b Lorenzo Valdevit,b Julie M. Schoenung,b Enrique J. Laverniac

a Department of Materials Science and Engineering, Tel-Aviv University, Ramat Aviv, Tel Aviv 6997801, Israel

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c US National Academy of Engineering, Irvine, CA 92617, USA

The concept of metallic-based self-healing materials has attracted a rapid increase of interest in recent years, yet it is in its infancy. Here, we review our collaborative work towards additive manufacturing using Laser Engineered Net Shaping (LENS®) directed energy deposition (DED) of novel aluminum-based self-healing metal-matrix composites (SHMMCs). The challenges to be discussed include: (1) Deposition of Al 5xxx matrix with mechanical properties comparable to those of the wrought alloy; (2) An in-depth understanding of the influence of the dominant processing parameters (laser power, scan speed, powder mass flow rate, and hatch spacing) on the characteristics of the deposits by means of design of experiments (DOE); (3) Processing of custom-made low melting point ZnAl core powder and its electrochemical encapsulation by either metallic or ceramic shells as both thermal and diffusion barriers; (4) Numerical simulation of heat transfer and phase transformation for a core-shell powder particle floating in the Al-based alloy molten pool to determine the DED process windows for retaining the coated ZnAl particles in the final builds; and (5) Processing by spark plasma sintering (SPS), as a proof-of-concept, of a composite material composed of the Al 5xxx matrix and a core-shell powder, and demonstration of a crack liquid-assisted healing process under external force.

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Plenary 2

Organic electronics: An interface user

Gitty Frey

Technion

"Organic electronics" utilizes conjugated polymers and small molecules as the active components in electronic and opto-electronic devices. The semiconducting character of these materials is inherent to their chemical structure, but the device performance often reflects not the materials, but rather interfaces in the device. For example, injection of charge carriers from the contacts into the semiconducting channel in organic transistors is modulated by the metal/organic interface, while the photogeneration of charges in organic solar cells depends on organic/organic interfaces. In this presentation we'll discuss the challenges of directing and studying such interfaces and demonstrate approaches for their design, processing, and imaging towards improved performance and new applications.

Plenary 3

Colloidal Semiconductor Nanocrystals: From Artificial Atoms to Artififical Molecules

Uri Banin

The Hebrew University

Colloidal semiconductor Quantum Dots (CQDs) that contain hundreds to thousands of atoms have reached an exquisite level of control, side by side with gaining fundamental understanding of their size, composition and surface controlled properties leading to their technological applications in displays and in bioimaging. Inspired by molecular chemistry, in which functionality of molecules depends on how atoms couple, we apply similar concepts to enrich CQDs based materials. If CQDs were deemed as artificial atom building blocks, how plentiful would be the selection of composition, properties and functionalities of the analogous artificial molecules? Herein we introduce the utilization of CQDs as basic elements in nanocrystal chemistry for construction of coupled colloidal nanocrystals molecules focusing on homodimer quantum dots (QDs), in analogy to homonuclear diatomic molecules.

The coupled CQD molecules are synthesized via a facile and powerful strategy with precise control over the composition and size of the barrier in between the artificial atoms to allow for tuning the electronic coupling characteristics and their optical properties. Our approach entails fusing two core/shell CQDs yielding a dimer with a tailored barrier dictated by the shell composition, thickness and fusion reaction conditions. The artificial molecules manifest various coupling effects and unique characteristics owing to the presence of two emission centers within one nanosystem. This sets the stage for nanocrystals chemistry to yield a diverse selection of coupled CQD molecules utilizing the rich collection of ubiquitous artificial atom core/shell CQD building blocks. Such CQD molecules are of direct relevance for numerous applications including in displays, sensing, biological tagging, electric field sensing and quantum technologies.

Plenary 4

Biogenic nano-scale mirrors and light scatterers, built of organic crystals, and engineered to fulfill optical functions

Lia Addadi
Weizmann Institute of Science

Organisms construct optical 'devices' based on assemblies of organic crystals. The constituent molecules are mostly purines and pteridines. All the crystals have unusually high refractive indexes in the directions along which the light penetrates the crystal. The crystals form mirrors and light scattering layers that function to increase light sensitivity in the eyes of scallops [1], of crustaceans such as shrimps and crayfish [2], of some fish [3], and so far, in one case of terrestrial insects, the jumping bristletails [4]. Scallops contain in their eyes a concave multi-layered mirror perfectly tiled with a mosaic of square guanine crystals, reflecting the light to form images onto the overlying retinas. The crustaceans and the zander fish have in their image-forming eyes crystals surrounding the light receptors. In the crustaceans, the crystals form densely packed assemblies of highly organized spherulites, composed of layers of isoxanthopterin crystals [5]. In the zander fish, the tissue surrounding the light receptors is densely occupied by block-shaped crystals of 7,8-dihydroxanthopterin. In both the latter cases, the crystals backscatter the direct light missed in the first passage to the light receptors. In the insect, a mirror composed of disordered crystals of xanthine reflects light back onto the scattered retina components, resulting in light sensors that are not image forming. In all these examples, the hierarchical organization is controlled from the crystal structure at the nanoscale to the complex 3D super-structure at the millimeter level. The crystal structure, the size, the crystal morphology and the superstructural arrangement all together determine the optical properties of the material. We have thus a vast choice of molecular components, of structures and superstructures, assembled following precise blueprints to fulfill optical functions. A fascinating heterogeneous source of inspiration for engineering optical materials.

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Plenary 5

Development of highly efficient thermoelectric materials and devices

Yaniv Geblstein

Ben Gurion University

Poster prizes and concluding remarks

In the recent years, demands for energy efficiency have motivated many researchers globe-wide to seek for innovative methods capable of enhancement the efficiency of heat to electricity thermoelectric (TE) energy conversion. Many of these methods incorporated interfaces and sub-micron features, which are much more effective in phonon scattering (rather than electron scattering), for reduction of the lattice contribution to the thermal conductivity, kl, without adversely affecting the other involved electronic properties. Although such an approach resulted in increased TE efficiencies, stabilizing the nano-centers while preventing coarsening under practical operation conditions, combined with an additional electronic optimization, is still required.

The presentation will cover a combination of several novel methods approaching toward a higher technology readiness level (TRL) of TE devices. These methods include:

- Phase separation into the sub-micron scale with an enhanced thermodynamic stability.
- Co-doping of known thermoelectric compounds, while one doping element introduces vacancies which are occupied by another doping element, for optimizing the electronic TE properties.
- Functionally graded materials (FGM) generation, with an optimal ZT envelope over a wide temperature range.

Besides of the listed above approaches for optimizing the TE compositions, the presentation will cover some of the procedures required for development of practical TE devices.

Oral Presentations

Session 1
Materials for Energy

Session chair:
Doron Urbach

Location: Teddy A

Anharmonic semiconductors - Lessons Learned from Halide perovskites

Omer Yaffe

Weizmann Institute of Science

In semiconductor physics, the dielectric response, charge carrier mobility and other electronic material properties at finite temperatures, are always treated within the framework of the harmonic approximation. This approach is very successful in capturing the properties of tetrahedrally bonded semiconductors such as silicon and GaAs.

Buckling and tolerance in semiconductors perovskite CsPbBr_3 nanostructures

Yehonadav Bekenstein

Technion

Flexible semiconductor materials, where structural fluctuations and transformation are tolerable and have a low impact on electronic properties, focus interest for future applications. Two-dimensional thin-layer lead halide perovskites are hailed for efficiency and a high degree of compliance in devices. I will show common structural deformation via thin layer buckling in colloidal CsPbBr3 nanobelts adsorbed on carbon substrates. The microstructure of buckled nanobelts was determined using transmission electron microscopy, using our original selected orientation dark-field imaging (SODFI) technique. This method enabled the collection of scattered electrons from solid angles and traced them back to the specific orientation of the crystal. Albeit attenuated, apparent emission was measured from the buckled nanobelt using cathodoluminescence, signifying tolerance to mechanical deformations of electronic properties. By employing plate buckling theory, we approximate adhesion forces between the buckled nanobelt and the substrate, to be F_{adhesion}~0.12\mu N, marking a limit to sustain such deformations. This work opens possibilities for the fabrication of flexible future devices due to electronic tolerance to mechanical buckling of halide perovskite nanostructures.

Spatial External Luminescence Efficiency of Perovskite Solar Cells

Mor Fiegenbaum-Raz
Tel Aviv University

Lead halide perovskites have recently emerged as one of the most promising future candidates for replacing silicon-based photovoltaics. Their unique optoelectronic properties, such as tunable and direct bandgap and high absorbance coefficient, in combination with a low-cost fabrication process, make them promising candidates for use in next-generation and tandem solar cells. Although their photocurrents are reaching the theoretical maximum, the devices' open-circuit voltage can be improved significantly. Thus, an operando characterization method that can map the contributions to the device's photovoltage is called for.

With the progress in device performance, surface and SRH recombination are suppressed, making radiative recombination more dominant. In this process, electron-hole pairs recombine to generate photons that can be either reabsorbed elsewhere within the device or be emitted through photoluminescence. Since the photoluminescence quantum yield (PLQY) and the harvestable voltage are tightly coupled, mapping the contribution to photoluminescence within the device can inform on the contribution to the buildup of photovoltage within it.

The spatial external luminescence efficiency (SELE) is the probability for a photon absorbed at a specific point in the device to contribute to the measured photoluminescence. The SELE can be extracted by combining wavelength-dependent PLQY measurements with detailed optical modeling. Hence, the SELE maps the contribution of different regions to the device photovoltage. In this contribution, we apply SELE extraction to perovskite solar cells. This spatial information can shed light upon different loss mechanisms, quantify surface recombination at the interfaces between the different layers in the device, and discriminate between radiative and non-radiative recombination processes at the surface and in the bulk of the device

Coexisting multiple glassy phases with different compositions in NFA-based Organic solar cells

Oded Nahor
Technion

Organic solar cell (OSC) bulk heterojunctions (BHJ) comprise a complex mixture of phases, and their compositions, distribution and interplay significantly affect device performance. Of utmost importance are the composition and distribution of the intermixed donor:acceptor phase where the contradictory processes of charge generation and charge recombination occur. To gain insight on these intermixed phases in non-fullerene acceptor (NFA) based BHJs, we focus on blends of the most investigated donor polymer, P3HT, and the prototype NFA, ITIC. We find that, in contrast to fullerene-based BHJs, which typically include one type of amorphous (glassy) phase, two different glassy populations co-exist: an amorphous intermixed phase and an amorphous ITIC-rich phase, each with a different composition. Thermal analysis and GIWAXS measurements show that the relative fractions of the two glassy phases and the degree of crystallinity of the NFA and polymer components can be manipulated by blend composition and film annealing. The observation of multiple glassy phases and their non-trivial multi-scale phase separation demonstrates the complexity of NFA-based BHJs and highlights that advancing this technology towards commercialization requires deeper understanding of the phase behavior of such systems.

Hydrogen-Bromine Redox-Flow Batteries

David Zitoun

Bar-Ilan University

Hydrogen-bromine redox-flow batteries (RFBs) technology offers an economic storage solution and is considered promising as a sustainable electricity storage solution due to its fast kinetics, highly reversible reactions and low chemical costs. The main bottleneck of conventional RFBs is the corrosion due to the bromine species which results in the high cost of systems and the rapid fading of the hydrogen catalyst performance in the highly corrosive environment. Catalyst poisoning is a prominent issue, reducing the lifetime of catalysts and increasing the costs of the processes that rely on them. Current solutions to protect electrocatalysts from harmful species fall short of effective selectivity without inhibiting the required reactions.[1–4] In an attempt to produce a catalyst with increased stability in the presence of HBr and Br_2, a single-wall carbon nanotube (SWCNT) encapsulated Pt catalyst has been synthesized via a simple synthesis. The Pt showed the typical Pt peaks during cyclic voltammetry, and the typical diffusion limited activity for HOR, although some effect on diffusion was observed, showing that diffusion occurred through the SWCNTs. The encapsulated Pt showed a much slower degradation rate than the commercial catalyst when exposed to HBr/Br_2 electrolyte, showing that encapsulation within SWCNTs is a route to protecting catalysts from corrosive species. The diffusion pathway through the SWCNTs selectively blocks bromine species whilst still allowing hydrogen to access the Pt, shown both experimentally and via DFT. This catalyst has the potential give H_2-Br_2 RFBs a longer lifetime and hence more applicability to large scale energy storage. It may also find application in other technologies that require a Pt catalyst. The general platform, of encapsulating the catalyst inside a SWCNT to impose a localized diffusion selectivity, has the potential to solve many poisoning and corrosion problems that occur with other systems.

Low dimensional perovskite and their applications in photovoltaic cells, nanostructures and semitransparency

Lioz Etgar
The Hebrew University of Jerusalem

Recent discoveries have revealed a breakthrough in the field using inorganic-organic hybrid layers called perovskites as the light harvester in the solar cell. The inorganic-organic arrangement is self-assembled as alternate layers, being a simple, low cost procedure. These organic-inorganic hybrids promise several benefits not delivered by the separate constituents. In this lecture I will discusses new directions in low dimensional perovskite and their applications in solar cells.

In low dimensional systems, stability of excitons in quantum wells is greatly enhanced due to the confined effect and the coulomb interaction. The exciton binding energy of the typical 2D organic-inorganic perovskites is up to 300 meV and their self-assembled films exhibit bright photoluminescence at room temperature.

v In this work we will show the dimensionality in the perovskite structure. The 2D perovskite structure should provide stable perovskite structure compare to the 3D structure. The additional long organic cation, which is added to the perovskite structure (in the 2D structure), is expected to provide hydrophobicity, which will enhance the resistivity of the perovskite to humidity. Moreover we will demonstrate the use of 2D perovskite using unique barrier molecultes in high efficiency solar cells.

v Moreover, we will show a highly efficient semitransparent perovskite solar cell. The semitransparency was achieved through an inkjet printing of "holes" in the perovskite film. The "holes" in the perovskite allows to control the semitransparency of the solar cell.

v Organic-inorganic halide perovskite is used mainly in its "bulk" form in the solar cell. Confined perovskite nanostructures could be a promising candidate for efficient optoelectronic devices, taking advantage of the superior bulk properties of organo-metal halide perovskite, as well as the nanoscale properties. In this talk, I will present our recent progress related to the synthesis and characterization of perovskite NPs- i.e. Inorganic and hybrid organic-inorganic NPs. New nanostructures such us: NRs and NWs will be presented and the introduction of other cations such us Rb will be shown.

MoS2-based Nanocomposites for Water Decontamination

Ines Zucker
Tel Aviv University

Contamination of drinking water sources by a variety of organic and inorganic compounds demands more efficacious and reliable treatment technologies. However, conventional water treatment technologies remain chemically demanding, energy intensive, and ineffective in removing key trace contaminants. Nanotechnology-based approaches have been increasingly explored to enhance or replace traditional remediation methods because of the high reactivity and tunable-properties of nanomaterials. In her talk, Dr. Zucker will provide an overview on the current status of nano-enabled water decontamination, including promising opportunities and barriers for implementation. Specifically, the application of molybdenum disulfide (MoS2) for heavy metal removal will be extensively discussed as a case study, where material properties, removal mechanisms, and large-scale applications are optimized.

Session 2
2D Materials I

Session chairs:
Doron Naveh, Ariel Ismach

Location: Teddy B

A place where everyone matters – interfaces in functional nanostructures

Maya Bar-Sadan
Ben-Gurion University of the Negev

Although nanostructures contain tenths of thousands of atoms, the atoms at the interfaces make most of the impact on the functionality, especially regarding the catalytic activity. It is therefore an important mission to control the formation of interfaces at the atomic scale, but that is easier said than done. First, it is hard to characterize and understand what was obtained in the synthesis. Then, relating the specific structures to the macroscopic properties requires overcoming issues of adequate sampling and statistics, reproducibility to the atomic scale features and abundance of similar structures within a synthetic batch. Last, there are confusing cases where we synthesize a certain structure to best of our knowledge and spontaneous rearrangements produce other active particles. Here, I will present a few such cases.

Interlayer electronic transport in bilayer graphene systems

Elad Koren
Technion

Weak interlayer coupling in 2-dimensional layered materials such as graphene gives rise to rich mechanical and electronic properties, in particular in the case where the two atomic lattices at the interface are rotated with respect to one another. The reduced crystal symmetry leads to anti-correlations and cancellations of the atomic interactions across the interface, leading to low friction and low interlayer electrical transport. Using our recent nanomanipulation technology, based on atomic force microscopy, we show that combined electro-mechanical characterization can uniquely address open fundamental questions related to electronic charge transport through stacking faulted structures. To this end, we studied experimentally and theoretically the interlayer charge transport in twisted bilayer graphene systems separately for edges and bulk parts. We find that interlayer edge currents are several orders of magnitude larger than in the bulk and therefore govern the transport up until very large critical diameters depending on the potential across the adjacent layers and the angular mismatch angle. In addition, we show that the strong edge transport across the interface is governed by strong quantum mechanical interference effects as opposed to simple interlayer atomic interactions.

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Spaghetti and lasagne: the cooking of 1D and 2D nanomaterials

Daniel Gilbert Nessim
Bar Ilan University

Chemical Vapor Deposition (CVD) is a powerful tool for synthesizing nanostructured materials. In this talk, I will show how we synthesized carbon-based 1D nanostructures and 2D layered bulk metal chalcogenides and these materials showed promise for many applications in the realms of energy, electronic devices, composites, etc. For both types of materials, there are complex mechanisms at play such heterogenous catalysis, surface reactions, gas phase reactions, thin film dewetting and coarsening, growth mechanisms, etc. This leads to a wide selection of parameters we need to optimize such as the choice and morphology of the catalytic materials, the choice of gases and their flows, the multiple heating temperatures, the duration of each step, etc.

1D: Despite the massive progress achieved in the growth of carbon nanotube (CNT) forests on substrate, apart from lithographic patterning of the catalyst, little has been done to selectively (locally) control CNT height. Varying process parameters, gases, catalysts, or underlayer materials uniformly affects CNT height over the whole substrate surface. We show here how we can locally control CNT height, from no CNTs to up to 4X the nominal CNT height from iron catalyst on alumina underlayer by patterning thin film reservoirs below the alumina layer or by using foil overlayers placed above the catalyst during annealing or growth. I will show examples of growth with patterned regions of CNTs with different CNT heights (or without CNTs) using the reservoir and the overlayer techniques. This modulation of the CNT height is a significant improvement compared to the "CNTs (one height) / no CNTs" patterning that has been achieved using lithography of the catalyst, and moves us closer to building 3D architectures of CNTs that could be useful for future electronic devices or sensors.

2D: Since the excitement about graphene, a monolayer of graphite, with its 2010 Nobel Prize, there has been extensive research in the synthesis of other non-carbon few/mono-layers exhibiting a variety of bandgaps and semiconducting properties. The main approaches to deposit few/monolayers on a substrate are: (a) bottom-up synthesis from precursors using chemical vapor deposition (CVD) or (b) top-down exfoliation (liquid or mechanical) of bulk layered material. Using a Lego approach of superposing monolayers, we can envisage the fabrication of heterojunctions with original electronic behavior. Here I will show a combined bottom-up and top-down approach where (a) we synthesize in one step high yields of bulk layered materials by annealing a metal in the presence of a gas precursor (sublimated selenium from S, P, or Se powder) using chemical vapor deposition (CVD) and (b) we exfoliate and deposited (dropcast or Langmuir Blodgett) few/mono-layers on a substrate from a sonicated mixture of our material. I will present the chemical synthesis, the very extensive characterizations, and the lessons we learned in making multiple metal chalcogenides and their applications for sensors and electrochemical devices.

Metal-Organic Chemical Vapor Deposition of Wafer-Scale and Carbon- Free WS_2 Atomic Layers

Assael Cohen
Tel Aviv University

Two-Dimensional (2D) TMDs materials have attracted extensive attention in many researches due to their unique property their remarkable electronic and optoelectronic properties, which include a unique indirect-to-direct bandgap transition with reducing layer numbers, high carrier mobility, and strong spin-orbital coupling due to broken inversion symmetry. These interesting properties make 2D TMDCs particularly well suited to be used in electronic and optoelectronic devices. Despite the unique proprieties of TMDs it is not easy to get a large area of one or a few layers.

This requires the systematic study of the growth mechanism of such atomic films. Here, I will present the results on the growth of WS_2 and WSe_2, via the metal-organic chemical vapor deposition (MOCVD) approach. One of the major advantages of MOCVD is the use of volatile precursors for both, the metal and the chalcogen sources, in contrast to the more common metal oxide powder-based CVD approach, where the control over the precursor supply is limited. Although the MOCVD method results in large-scale growth, it might include intrinsic carbon contamination arising from the volatile organic-based precursors themselves. This, together with the high rate of precursor decomposition at the growth temperatures, leads to the formation of nano-crystalline films.

Here, a Growth-Etch cycle technique is developed, in which the precursors are sequentially delivered while a small amount of water vapour is introduced to the growth chamber. This causes the re-evaporation of small and defective domains as well as the carbon contaminants from the growth substrate, allowing the highly crystalline domains to expand, resulting in high-quality large domains or continuous atomic layers, depending on growth conditions. This methodology could be further extended to other 2D materials in general and TMDs in particular. Finally, I will describe how the MOCVD approach can be used to study the Van der Waals epitaxy of TMDs.

Graphene-based Conformal Coating: How to Avoid Hot Spots?

Avia Ohayon-Lavi
Ben-Gurion University of the Negev

A printed circuit board (PCB, Figure 1a) is an essential component of nearly all forms of commercial electronics, where conformal coating over the PCB and the attached electronic components is widely used to protect the electronics from the external environment, e.g., moisture, dirt, electromagnetic interference (EMI) and thermal stresses. The highly dense electronic components in modern PCBs result in elevated operating temperatures (hot spots) that directly affect the performance of the device, i.e., reduced operation speed and life-time shortening. Conventional heat removal solutions (e.g., metal-based heat sinks) may partially solve the heat accumulation challenge, but are heavy and large, and do not provide shielding against shocks, vibrations and corrosive agents for the electronic devices when located outdoors. Heat can be removed by coupling the heat source (resistor) to thermally conductive polymer composites, as a replacement for the metallic heat-sink when lighter weight and easier processing (workability) are required. Unfortunately, polymers possess low thermal conductivity (TC, ~0.2 W (m K)-1) and hence cannot provide heat dissipation. Our approach is to employ the existing conformal polymeric coating approach as a platform for solving heat dissipation by loading it with high conductivity filler(s) to form a composite, i.e., graphene nanoplatelets (GnP, Figure 1b) and boron nitride nanoplatelets (BNNP). The GnPs contribute significantly to the TC of the composite while BNNP inhibit the electrical conductivity to avoid short circuits. We showed that GnP-based conformal coating reduced the hot spot temperature drastically (~30°C) by increasing the TC of the coating. The use of a commercially available polymer material, GnP, and BNNP, along with a simple but highly effective dispersion method, constitutes a timely and relevant approach for thermal management applications.

Heat transfer in Graphene foams

Assaf Ya'akobovich

Ben-Gurion University of the Negev

The effective dissipation of heat from electronic devices is essential to enable their long-term operation and their further miniaturization. Graphene foams (GF) is a promising material for thermal applications, including heat dissipation, due to its excellent thermal conduction and low thermal interface resistance. We synthesized GF devices, subjected them to high temperatures, and investigated their thermal behavior using infrared micro-thermography under forced and free convections. Under free convection we found that while the convective area of GF devices is comparable to that of bulk materials (such as metals), its coefficient of free convection of is several orders of magnitude higher than that of metals. In addition, the GF devices showed a reproducible thermal behavior, which we attribute to negligible temperature-induced morphological changes (as confirmed by Raman analysis). Then, we investigated the forced convection characteristics of GF. We applied controlled airflow to heated samples of GF while recording their temperature. Then, we analyzed them using finite-element simulations in conjunction with a genetic optimization algorithm, from which we extracted their heat fluxes in the horizontal and vertical directions. We found that boundary layers have a profound impact on the heat transfer characteristics of our samples, as they reduce the heat transfer in the horizontal direction. The heat transfer in the vertical direction, on the other hand, is dominated by the material conduction and is much higher than the horizontal heat transfer. Taken together, our findings suggest GF as a promising candidate material for advanced cooling applications where efficient heat dissipation is needed, e.g., in electrical circuits.

The Fascinating Frictional Properties of Layered Materials

Oded Hod
Tel Aviv University

Structural superlubricity may provide a viable route for significant reduction of friction and wear. In this talk, I will present results of fully atomistic numerical simulations of unique static and dynamical properties exhibited by graphite/hexagonal boron nitride (h-BN) heterojunctions, performed using a dedicated anisotropic inter-layer potential recently developed in our group. I will demonstrate how structural superlubricity at interfaces formed between graphite and h-BN persists even at aligned microscale contacts sustaining external loads. I will underline the conditions required for achieving negative friction coefficients - a state where friction is reduced upon increasing normal load. Nanoscale demonstrations of the "princess and the pea" problem and the motion of nanosrepents will be briefly discussed. The tribological properties associated with motion over grain boundaries appearing in large-scale polycrystalline surfaces will be presented. Should time permit, I will further show intriguing parity dependence of moiré superstructures occurring at heterogeneous layered materials interfaces and controllable heat flow through twisted layered materials junctions.

Session 3
Additive Manufacturing I (Metals)

Session chairs:
Tbaamnon Shirizly, Eitan Tiferet

Location: Teddy C

A study of pre-heating stages in electron beam melting

Gennady Ziskind
Ben-Gurion University of the Negev

Key Words: EBM, Pre-heating, Additive manufacturing, Thermal history

Additive manufacturing by electron beam melting (EBM) requires careful process thermal management. Particularly, unlike other powder bed fusion methods, significant pre-heating of the powder prior to melting is essential in order to ensure sufficient adhesion between the powder particles (through partial sintering and thermal expansion). This is required in order to avoid kinetic effects (AKA powder smoking) from a concentrated melting electron beam. The pre-heating algorithm used in most EBM machines is material-specific with reliable results only for materials after rigorous testing procedures. Therefore, in order to allow reliable adaptation of new build materials in EB, the pre-heating thermal management must be adequately studied and characterized. In this work, the thermal history of the pre-heated powder is studied using transient numerical simulations in finite elements. The first step in developing reliable pre-heating thermal simulations included a dedicated full-3D model of the ARCAM Q20+ machine build chamber, including all participating components (e.g. start-plate, heat shields, build stage, powder hoppers, etc.) in order to model the thermal boundary conditions. This model included a grey-body radiation cavity space, with several modified gap-conductance interactions tailored to the given geometry, in addition to 3D conduction. Dedicated validation experiments were performed using spatially distributed thermocouple measurements over the start-plate and heat shields over long duration pre-heating, and a good agreement was obtained between the experimental and computed results [1]. In the next step, the boundary conditions were analyzed and implemented in a unique multi-stage additive pre-heating simulation with time-scale resolution of adaptable size. The additive model uses progressive element volume activation to introduce new powder layers, mimicking an actual rake spread, as in an EBM machine. The electron beam energy deposition is modelled using adaptive scaling which adjusts to the required time-incrementation resolution. Since this sort of computation may become too expensive depending on the time-scaling level of the moving heat source (the pre-heating beam travels at ~40-46m/s), the algorithm is adapted so the process may be solved in larger time-increments by scaling the energy deposition into several simultaneous line-blast energy sources. It is then possible to dictate, in any certain portion of the transient, a reduction of the time-incrementation scale for short durations, in order to assess some more local thermal phenomena where they are of interest. This approach enables generating a database of simulation results for different pre-heating cases (e.g. beam current, velocity and scan path) including 1st and 2nd pre-heating. These results can then be examined against complying pre-heating (only) experiments to assess the resulting "melt-safe" level of the pre-heated powder per material.

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Residual stress and texture characterization of curved parts in SLM and EBM additive manufactured Ti-6wt%Al-4wt%V tubes

Elad Caspi

Titanium and its alloys are broadly used in wide range of application, biomedical, aerospace structures, marine environments, and other applications. Ti-6Al-4V alloy is the most popular among Ti alloys. It belongs to a family of α+β alloy combining excellent properties and good producibility. Additive manufacturing (AM) of metals, a relatively new production method, is widespread at both academic and industrial level. However, in general this method results in with different microstructure, and assumably different mechanical properties, compared to that of conventional manufacturing. Of special interest is the difference in properties as a function of location in the built space and orientation relative to the build direction. Roughly five years ago our group embarked on an endeavor to characterize and understand in detail the bulk microstructure of powder bed AM Ti-6Al-4V, and its correlation with parts mechanical properties. In particular, we invested our focus in studying the effect the orientation of printed objects, or parts thereof, relative to the AM build direction, has on bulk microstructure and therefore on their mechanical properties. Our main tool of investigation is thermal neutron diffraction, owing to these particles' high penetrability in most metals that allow for microscopic bulk determination of important microstructure parameters. In continuation of this endeavor, I present here with our most recent results, collected by neutron and x-ray diffraction from curved objects of different AM Ti-6Al-4V tubes. Using mainly these two methods we determined the bulk texture, relative phase fraction and tri-axes residual stress of such tubes manufactured by electron beam melting (EBM), heat treated selective laser melting (HT-SLM), and as made SLM (nHTSLM) tubes of identical geometry and dimensions. Again, we focused on identifying the differences in these properties as a function of relative orientation to the build direction. Results clearly show that although the texture has no significant differences between different parts, and in general is very small for all studied objects, there are substantial differences between residual stress values in different parts. Whereas no such stresses are observed in both EBM and HT-SLM tubes, significant residual stresses, as high as 1000 MPa, are observed in nHT-SLM tubes. In addition, we show that the distribution of these stresses has clear connection with the relative orientation to the build direction. The origin of these differences, and in particular the mechanism by which stresses are eliminated for the HT-SLM or as printed EBM objects are discussed.

Effect of roughness on energy absorption in AM Ti6Al4V thin walled cylinders

Shmuel Osovski

Technion

Thin walled structures are repeatedly being used as energy absorbers in the car industry, aiming to dissipate energy during a collision. The emergence of 3D metal additive manufacturing processes has paved the way to geometrical topology optimization of such structures without the traditional limitations arising from the manufacturing complexity. Metallic components manufactured using additive manufacturing often suffer from poor surface quality, which in turn has a large effect on the ability of a thin walled structure to resist buckling. In this work, the effect of printing parameters on the resulting surface roughness of thin walled tubes with circular cross section is examined under dynamic and static loads. Our results demonstrate that while under static load the energy absorption is strongly influenced by the surface roughness, under dynamic loads, those differences tend to diminish. Moreover, different printing parameters considered in this work, for which very similar surface roughness is obtained, are observed to result in rather different microstructures leading to an increased energy absorption capability.

Leveraging additive manufacturing process simulation to meet contradicting geometrical requirements

Roman Bendersky

RAFAEL

Additive manufacturing (AM) is a workflow of steps rather than a single "press button" print action, more specifically – it can be divided into three main stages: the design for additive manufacturing (DfAM) phase which is a part of the development phase, the AM production phase and the post-processing phase.
In this session, we will dive into the development phase.

There are different design considerations for AM and in some aspects even more so when using selective laser melting (SLM) to produce metal parts.

AM is often the preferable manufacturing method for complex geometries such as lattice structures, internal cavities, etc. This session will focus on the AM process simulation phase and the way to leverage it in order to meet challenging and sometimes contradicting geometrical requirements.

A brief review of the software packages commercially available will be presented using case studies demonstrating the use of simulation tools to benefit real life DfAM. Finally, a review of software's ability to produce an opposite pre-distorted model (OPDM) to achieve a better accurate final geometry will be presented.

The influence of Electrochemically Charged Hydrogen on the Mechanical behavior of Electron Beam Melting (EBM) and Wrought Ti-6Al-4V using the Small Punch Test (SPT)

Noa Lulu-Bitton
Tel Aviv University / NCRN

The influence of electrochemically charged hydrogen (j = –5 mA/cm2, t = 6, 12, 48, and 96 hours) on the mechanical behavior of wrought and electron beam melting (EBM) Ti-6Al-4V alloys with similar beta phase content was studied. After hydrogenation, both alloys had a surface layer that was composed of a combination of delta-a and delta-b hydrides. A combination of higher density of alpha/beta interphase boundaries arranged in a lamellar Widmanstätten microstructure, which acted as a short-circuit path, promoted hydrogen diffusion into the bulk of the EBM alloy. Hydrogen penetration into the EBM alloy resulted in a gradual degradation of mechanical properties over charging time, up to 86% and ~81% in displacement at failure and in pop-in load, respectively. On the other hand, a denser hydride layer at the surface of the wrought alloy surface, which acted as a barrier for hydrogen uptake into the bulk alloy, with a lower density of alpha/beta interphase boundaries, resulted in a stable mechanical degradation after 6 hours of charging, showing a maximum decrease of 11% and ~32% in displacement at failure and maximum load, respectively. The mode of fracture in the EBM alloy changed from mixed-mode (ductile-brittle) to star-like fracture, while in the wrought alloy the mode of fracture changed from ductile to semi-brittle mud-crack fracture for all hydrogenated samples. The results of this study show that EBM Ti–6Al–4V is more prone to hydrogen embrittlement compared to the wrought alloy.

Novel Thermotopographic Analysis of Electron Beam Additive Manufacturing Process Using Stock Arcam Q20 Plus

Y.Ganor

Rotem, NCRN,BGU

The advantages afforded by additive manufacturing such as increased design freedom and reduced waste, can only be utilized after tailoring an intricate matrix of co-dependent parameters that have major effects on the produced part and its properties. Extensive study is dedicated to refine validation and verification processes, improve repeatability, and detect imperfections. Developing tools for monitoring, controlling, and analyzing the increasingly widespread process of AM is thus both an industry and an academic focus. Development requires thorough interdisciplinary research and understanding of the underlying mechanisms that govern a specific AM process. Monitoring the temperature field that develops during the printing process is crucial, since the temperature regime dictates mechanical properties, microstructure, and residual stresses of final parts. Using IR cameras for thermographic imaging is a promising method of measuring temperature regimes in-situ. However, thermographic imaging usually requires expensive equipment, modification of the printer and arduous calibration. This study proves feasibility of using image processing on stock defect detection feature (LayerQam) in an Arcam Q20 Plus to produce thermographic imaging in-situ without modifying the machine. Calibration was achieved for Ti6Al4V using thermocouples heated with the electron beam. Calibration using initial factory settings provided a temperature range of 400°C - 850°C. Changing only software settings can extend the range to higher temperatures. The standard software allows capturing multiple images with varying settings, enabling thermotopographic images of multiple temperature ranges throughout the printing process. This method proves to be a cost-saving way to determine temperature gradients in the process, finding imperfections and areas prone to flawed mechanical properties.

Mechanical Properties, Metallurgical Characteristics and Anisotropy of Additive Manufacturing of 316L

D. Moreno

Beth Shemesh Engines LTD

The alloy IN939 is extensively used in industrial gas turbines as structure material for moderated high temperatures applications in gas turbines for aerospace in additional energy industries, process industry, oil and gas ship building where excellent oxidation resistance and high creep strength at elevated temperatures are needed.

This promising cast alloy is used in combustion turbines up to 850 °C. However, the needed joining technology required for large structural components in aero engines present a challenge, and was investigated elsewhere [1].

The innovative Additive Manufacturing (AM) technology of Nickel-base superalloys avoid major design (geometry, tooling etc.) problems and enables to optimize complexity of engineered parts, while reducing product development and marketing times. Despite the noticeable advantages of AM technology, unacceptable defects as micro-cracks in the bulk and surface oxidation were observed during production capability tests of BSEL sample item. This study investigates the sources of those defects and presents the way how to avoid them.

The study shows that the actual composition and tolerance of elements in the powder, particularly Zr and B, may have an influence on micro-cranks formation in the blank [2]. A comparison of As-Print parts to heat-treated printed parts was carried out. The results shows that the environment during the heat treatment may cause IGA (Inter-Granular Attack) on the surfaces. The surfaces quality (roughness) before heat treatment, make the part susceptible to surface attack and depletion of some of the elements close to the surface.

Addressing these issues lead to printing defect free sample part form the required alloy NI939.

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Session 4
Analytical Techniques

Session chairs:
Yaron Kauffmann, Atzmon Vakahi

Location: Oren 2

Combined Chemical & Electrical Analyses of Hetero-Structures: Past, Present, Future

Hagai Cohen
Weizmann Institute of Science

Nano systems frequently present mutual dependencies between composition, structure and functionality that are not only complex in appearance, but also extremely difficult to be controlled, or even systematically studied. Their characterization requires state of the art technique capabilities, usually achieved upon separated instrumentation, such that consistency between the characterization studies is likely to encounter key unknowns. Typical examples may be found among the electric measurements, known to be highly structure-sensitive, especially with miniaturized systems, while yet the electrical probe is frequently operated as a black-box, with unknown contact-related details and various atomic-scale instabilities that may evolve under applied fields, varied imperfections in particular, to mention just a few.

Fitted into this gap, a promising technique for extracting simultaneously compositional and electrical information is proposed under the template of x-ray photoelectron spectroscopy (XPS). XPS is well acknowledged as a powerful quantitative analytical technique, effective in particular for the study of thin layered heterostructures. Inherently however, XPS is also sensitive to the electrical properties of samples, such that it can be exploited for extracting detailed I-V and V-V characteristics in a top-contact-free mode. A technique dedicated to this type of experiments, termed chemically resolved electrical measurements (CREM), adds to the latter the use of elemental signals as addresses at which electrical characteristics are probed. Thus, unique capabilities as an electrical tool are achieved, already proven very useful with a variety of systems, from standard electronic components and solid-state nanoparticles to organic molecular layers and bio materials. In this talk, description of the CREM principles and examples demonstrating some of its immediate successes will be shown, next to potential developments and applications, promises and some of the intriguing capabilities yet to be explored.

Unambiguous structure determination of intermetallics using electron crystallography methods

Louisa Meshi
Ben-Gurion University of the Negev

Recent advances in the development of electron crystallography (EC) methods allowed their application on structure determination of complex structures, such as metal organic frameworks, zeolites, proteins and intermetallics. In some cases, EC is the only viable tool for structure solution. In current presentation, our contribution to this field will be shown, concentrating on recent structure determination of complex intemetallics performed by members of our research group. In [1], we have suggested a routine for structure solution of aluminides based solely on electron diffraction methods. Using this methodology, 13 structures of intermetallics (having 20-480 atoms in the unit cell) were solved by our group in the last decade. Two recent cases will be presented.

First case is a part of metallurgical study on high entropy alloys (HEAs), during which novel AlCrFeNiNb0.3 alloy was cast and characterized [2]. This alloy solidifies dendritically. The interdendrite region exhibited typical ternary eutectic microstructure, containing Laves phase, BCC and B2. Dendrite cores were found to be of two types containing either BCC particles embedded in the B2 matrix or vice versa - B2 particles embedded in the BCC matrix. Regardless the type of dendrite's microstructure, this area also contained small particles of highly defected Laves phase and additional Nb-rich nanosized particles with an unknown structure. Crystal structure of the unknown phase was investigated by means of EC and was characterized as cubic, Fm3m, with a = 11.61 Å. Structure type was assigned as Th6Mn23.

Second case concentrates on the new Al78Mn17.5Pt4.5 phase (attributed to be isostructural to Al3Mn) revealed in the Al-Mn-Pt system [3]. Despite numerous investigations of the high temperature Al3Mn (T phase) and its ternary extensions, until today, exact space group and atomic positions of transition metals is a matter of dispute. As stated, Al78Mn17.5Pt4.5 phase (quenched from 800 °C) was regarded as ternary extension of the "Al3Mn" T–phase. Using convergent beam electron diffraction (CBED), the space group of this ternary composition was proved to be non-centrosymmetric Pna21, instead of Pnam - which describes the symmetry of the binary T-phase. Atomic model was determined applying direct methods on electron diffraction tomography data. At the Al78Mn17.5Pt4.5 composition, the Pt atoms were not distributed randomly in the Mn/Al sublattices, but adopted two specific Wyckoff sites, therefore, this composition should be regarded as an ordered variant of the T-structure. On the other hand, CBED study of the T-phase samples with a bit different stoichiometry (Al71.3Mn25.1Pt3.6) allowed attribution of the structure to the original T-phase structure type, i.e. centrosymmetric. Using Barnighausen tree [4], these two structures (centrosymmetric and non-centrosymmetric) were found to be related.

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Spiky Gold Nanostructures

Aleksei Solomonov
Weizmann Institute of Science

Surface-Enhanced Spectroscopy (SES) is a broadly applied characterization technique with highly localized chemical sensitivity. Its working principle is based on the plasmonic excitation of light on a rough, or tightly-spaced nanostructured plasmonic metal surface with the adsorbed analyte. It is challenging to develop multipurpose systems that may be used for the enhancement of different types of signals. Moreover, in many cases, the existing systems end up with signal-interfering capping agents, suffer from substrate instability, or insufficient signal enhancement, which still limits the wide applicability of SES technology.

In this work, we present the facile preparation of SES transducers based on the spiky gold-based films on solid-state substrates. The synthesized nanostructures have various sizes and various morphology of nano-star, nano-flower, nano-urchin (or hedgehog) shape or represent uniformly organized spiked surfaces. The developed systems serve as sensitive transducers in localized surface plasmon resonance (LSPR) spectroscopies, surface-enhanced and tip-enhanced Raman (SERS, TERS), surface-enhanced circular dichroism (SECD), surface-enhanced infrared absorbance spectroscopy (SEIRAS), surface-enhanced fluorescence spectroscopy (SEFS) for biological molecules and other compounds with possibilities of integration within microfluidic devices. The advantages of the proposed preparation procedure are: (i) a facile and simple preparation, (ii) capping agent-free surface, (iii) integration with lithographic procedures, (iv) stable in short-cycle reusability, (v) stability in a wide range of pH. These advantages, along with high scalability will further enhance the applicability of SES technology in applications such as the dynamics of biological macromolecules, diagnostics, and catalysis. Performed numerical simulations of the structures show enhanced electromagnetic field distribution around each spike. According to the experiments and simulations, it is possible to design the systems in such a way that will enable selective enhancement of the signal at specific wavelengths.

Unraveling the rate of the reverse martensitic transformation: A microsecond-scale time-resolved X-ray diffraction study

Asaf Dana
Technion

The Martensitic transformation serves as the basic deformation mechanism in many functional materials. The question "how fast can the martensitic transformation be?" is elemental to the field of solid-solid phase transformations. However, the answer to this question remains obscure or experimentally unvalidated as in most studies the transformation rate is restricted by heat or momentum transfer. As a result, the applied driving force slightly exceeds the threshold value required for overcoming the transformation barriers. In addition, a lack of experimental tools prevented tracking the evolution of the martensitic transformation with sufficient spatial and temporal resolutions. Thus, the sequence of transformation stages has not been characterized at the large-driving-force regime. We study the transformation kinetics under a large thermodynamic driving force by inducing a rapid Joule-heating-pulse in a shape memory alloy wire. In these experiments, the temperature of the SMA wire reaches a constant value, above the austenite finish temperature, before the phase transformation begins. The wire was fixed at both ends, preventing motion of masses except for local motions in the wire, and the stress in the wire due to the phase transformation was measured. These experiments provide the desired conditions for measuring the unhindered kinetics of the transformation in the large-driving-force regime. We track the evolution of the transformation by multi-frame time-resolved X-ray diffraction at synchrotron radiation with simultaneous high-bandwidth stress measurements. The diffraction data provides local measures for the austenite content with a temporal resolution of one microsecond. The study identified three stages occurring at different times on the microsecond-scale and at different length scales. Specifically, the transformation was shown to occur initially in a thin layer near the surface, and only later in the bulk of the wire. we explain the obtained experimental results by modeling the evolution of the phase transformation using a continuum approach. Theoretical approaches are discussed and model fitting to experimental results provides insight into the kinetic relation between the velocity of the phase front and the driving force. Results support a scenario in which a cylindrical phase front propagates inward along the wire radius. The propagation of such a high-specific energy front releases energy faster than low-energy fronts forming under low driving forces.

This contribution is based on the following publications:
doi.org/10.1016/j.jallcom.2020.157968
doi.org/10.1007/s40830-021-00326-1

Advanced Imaging and Analysis of Inorganic-Organic Hybrid Nano-Structures Fabricated via Sequential Infiltration Synthesis

Maya Barzilay
Technion

Sequential infiltration synthesis (SIS) is an emerging method for fabricating organic-inorganic hybrid materials and polymer-templated inorganic nanostructures using growth of inorganic materials within polymers. SIS allows for direct conversion of polymer templates into metal oxides with various microstructures and complexities. This unique ability attracts a burgeoning range of technologies, such as advanced lithography, microelectronics, optical coatings, water filtration, and renewable energies.

SIS is based on sequential exposures of the polymer to volatile organometallic precursors and co-reactants. High partial pressure and long exposure time of the precursors drive the precursors diffusion into the polymer free volume, creating organic-inorganic hybrid material at the nanoscale level. If desired, the polymer can be etched away after the SIS process to obtain an inorganic material replica of the polymer template. The reactions between various polymers and the organometallic precursors are unique and significantly affect the growth densities. Hence, it is important to understand the nucleation and growth processes in order to optimize the fabrication of the inorganic-organic hybrid nanostructures.

We used advanced high-resolution scanning transmission electron microscopy (HR-STEM) methods, such as high-angle annular dark-field (HAADF) and energy-dispersive x-ray spectroscopy (EDS) mapping, to investigate ZnO and Al_2O_3 nucleation and growth within different polymers using DEZ, TMA, and H_2O precursors while varying SIS cycles and exposure times. We found that the polymer-precursor interactions dictate ZnO growth densities and growth morphologies resulting in various growth structures such as net-like morphology constructed of small nanocrystals (3-5 nm) to stand-alone larger nanocrystals (5-8 nm). Importantly, we were able to identify ZnO nucleation initiation from random dispersion into ordered nanocrystals with well-defined crystallographic structure.

Opportunities at the new Soreq accelerator facility neutron source

Arik Kreisel
Nuclear research center

Phase II of the Soreq Applied Research Accelerator Facility (SARAF) is under construction in the Soreq Nuclear Research Center at Yavne, Israel. Phase II is planned to be operational in 2024. SARAF will be a user facility for basic and applied physics, based on a 40 MeV, 5 mA CW proton/deuteron superconducting linear accelerator. The high brilliance neutron source target for the full 200 kW beam will be a liquid Gallium-Indium jet target. This neutron source could be used to produce cold neutrons for different measurement technics such as neutron imaging and tomography, Bragg-Edge imaging, quasi elastic neutron scattering, small angle scattering, neutron diffraction and more. SARAF joins a list of new neutron sources based on high current, medium energy, accelerators that use the new development in neutron cooling and neutron guides to compete with the big spallation neutron sources.

Characterization of Nanostructured Alloys with FIB Tomography

Inna Popov
The Hebrew University of Jerusalem

Nanostructured metals acquire properties, which their bulk counterparts do not exhibit. That is why a nanometer size gold cluster became attractive catalyst, and nanometer - thick layer of aluminum patterned at a nanoscale serves as optical plasmonic antenna.

Alloying at a nanoscale is a promising way to get more unconventional properties via synergy of elemental composition and nanoscale dimensionality. But, preparation of nanoscale alloys is fundamentally limited by the intrinsically good conductivity of metals. This same reason prevents straightforward fabrication of nano -porous alloys and metals.

In this talk, I will introduce the synthetic path for fabrication of nano-crystalline nano-porous alloys with controllable elemental and phase composition. FIB tomography results obtained on thus prepared alloys will be discussed as an application case for the materials which surface area could not be measured otherwise.

Session 5
Corrosion & Coating

Session chairs:
Yair Ein Eli, Tal Kaufman

Location: Oren 3

Corrosion resistance and catalytic activity of nanocrystalline alloys of molybdenum and tantalum carbide

Brian Rosen
Tel Aviv University

Catalysts such as platinum are nearly always supported by carbon in fuel cell electrodes. These carbon supports are susceptible to corrosion at operating potentials. Transition metal carbides (TMCs) are a class of material that could be used as catalyst supports to replace carbon as they are electrically conductive and can be resistant to corrosion. TMCs which show promising catalytic activity but have been shown to suffer from oxidation and dissolution, whereas corrosion-resistant carbides tend to have significantly lower activities. Here we used co-reduction carburization and magnetron sputtering to synthesize alloy carbides containing molybdenum and tantalum with the aim of designing a carbide support that was both active and corrosion resistant. The addition of 15 mol% Ta to the precursor mixture used to synthesize the alloy support increased the corrosion potential by nearly 150 mV and decreased the corrosion current to 16% of that observed in the Ta-free support. Such supports also showed promising activity in functional fuel cells. In some systems, synchrotron x-ray adsorption experiments showed that corrosion resistant alloy carbides derive improved catalytic activity via electronic reconfiguration of the active metal. Finally, we show that density functional theory (DFT) calculations can be used to predict corrosion resistance in carbides, and therefore improvements in this field can come from machine learning modules to formulate ideal digitally designed materials.

A fascinating journey into the world of corrosion: New book "Corrosion: monitoring, control, and prevention"

Alec Groysman
Technion

Thinking about the future, will be there a shortage of energy, water, fuels, food? We will clarify that the expectation is for a shortage of experts in all the fields we mentioned just as is happening today when there is a shortage of specialists in the field of corrosion in Israel and in the world.

The idea to write a book in the field of corrosion was born during a course dedicated to the energy industry on "Corrosion, control and monitoring in oil, fuel and natural gas systems" held by the Israel Institute of Energy and the Environment in 2019.

The first book in the field of corrosion was published in England in 1924. Since then, many textbooks on the subject of corrosion have been published in various languages, with the exception of Hebrew. There is currently no book that makes accessible to a Hebrew reader the many important innovations developed in the field in recent decades with the understanding that corrosion causes severe damage to the society and environment due to leakage of hazardous substances, fires, and explosions, when the human factor is responsible for 60-85% of the occurrence of corrosion.

In light of the growing involvement of Israeli industry with metallic structures and equipment, the Israel Institute of Energy and the Environment initiated the idea and execution of writing a contemporary book that includes the entire theory and sheds light on the field of corrosion while presenting practical examples.

In this book, a new approach is given to the theory of corrosion and its causes, corrosion control methods, corrosion monitoring, interaction with the safety of industrial processes, corrosion management, elucidation of terminology, philosophy, and art. Such an approach gives enjoyable reading and learning of the subject of corrosion.

This is the first book of its kind in the Hebrew language that will serve as an aid and knowledge tool for industry, academia, planning, project and design organizations, schools, colleges, universities, regulators and all those involved in the field of infrastructure and industrial facilities, and will provide knowledge and solutions in the field of corrosion in Israel and around the world.

Hydrogen Induced Degradation of Electrochemically Charged Electron Beam Melted (EBM) and Wrought Ti-6Al-4V Alloys

Nissim Navi
NCRN

Additive manufacturing (AM) of Ti alloys allows producing complex geometries and small dimensions with high precision, which are not attainable by traditional processes such as casting or milling. Hydrogen may enter the Ti alloy during processing, post-treatments, or service. While AM of Ti–6Al–4V and the interaction of wrought Ti–6Al–4V alloy with hydrogen have been studied extensively, only few studies have been published on hydrogen interaction with AM Ti–6Al–4V, in most of them gaseous hydrogenation was used. In this study we compare the behavior of electrochemically charged hydrogen in both EBM and wrought Ti–6Al–4V alloys, both with ~6 wt.% β content. Both hydrogenated alloys contain αH (hcp) and βH (bcc) solid solutions, as well as δa (fcc) and δb (fcc) hydrides, and in both – hydrogen-related microvoids are found mainly in vicinity of the surface. The hydrides are found to originate from the α phase. Cracks along interphase boundaries are observed in the EBM alloy after three days of charging. In contrast, no cracks are evident in the hydrogenated wrought alloy. Both the kinetics and products of thermal hydride decomposition are different in the two alloys. The higher susceptibility of the EBM alloy to hydrogen-induced degradation is related to its distinct microstructure, namely a discontinuous arrangement of finer needle-like morphology of β-phase, a smaller lattice constant of the β-phase, and more α/β interphase boundaries. It also seems to inhibit hydrogen diffusion through the β-phase into the bulk alloy at elevated temperatures. Our study shows that the EBM Ti–6Al–4V alloy might be more prone to hydrogen damage, both at room temperature and at elevated temperatures, than its wrought counterpart, when both have a similar β-phase content. This finding is of paramount importance for many applications where AM'ed Ti–6Al–4V is considered.

Effect of Plasma electrolytic oxidation treatment on corrosion behavior of AZ91D, AM50, AE42 and MRI 230D magnesium alloys

Barbara Kazanski
Azrieli College of Engineering

Corrosion behavior of an advanced special magnesium alloy MRI 230D (Magnesium Research Institute, Beer-Sheva) as compared to the commercially available zinc-, manganese- and rare earth- containing alloys was studied. The representatives of the appropriate groups were AZ91D, AM50, and AE42 alloys, respectively.

The applicability of Plasma Electrolytic Oxidation treatment for the corrosion protection of all four of magnesium alloys in 3.0 wt% NaCl aqueous solution saturated with $Mg(OH)_2$, and corrosion behavior of these alloys was studied in this work by several electrochemical and non-electrochemical techniques. The corrosion process of all the alloys before and after PEO treatment was evaluated by open circuit potential (OCP) measurements, electrochemical impedance spectroscopy (EIS), linear polarization tests, linear sweep voltammetry (Tafel extrapolation) and chemical methods, namely mass loss and hydrogen evolution. Corrosion rates for each method were calculated and compared, and the morphology of corroded surface studied. According to the tests results, the protection by the PEO lowers the rate of corrosion and shifts the corrosion potential to a more noble value for all four alloys. An attempt to explain the influence of the PEO process on the corrosion behavior of the alloys was made. However, the localized character of corrosion causes some deviations in the results obtained even by the same method.

A systematic deposition parameters study of boron carbide coatings onto aluminum substrates

Sharon Waichman
NRCN/Rotem Industries

Boron has a big cross section for neutron absorption which makes it suitable for nuclear based applications including homeland security, accelerators and more. Here, we established a several microns sized (2-3.5 μm) boron carbide coating on an aluminum substrate using a pulsed-DC magnetron sputtering technique in an argon atmosphere. The efficient attachment of a coating to its substrate is a fundamental need that must be achieved in order to maintain the goal of the coating layer. Our main challenge to fulfil this need is the probable formation of aluminum-carbon bonds that are unstable in humid environment and the difference in the coating/substrate thermal expansion coefficients that may cause stress and a subsequent adhesive failure. For these reasons, we applied a titanium intermediate layer (0.5-1.5 μm) and performed a systematic study of the coating process parameters that affect the deposited film. We investigated the impact of the process parameters on the microstructure, morphology, composition and adhesion of the boron carbide coating onto the aluminum substrate. We observed a columnar coating structure that turned finer with increasing the bias voltage. Moreover, under the application of a bias voltage higher than ~ - 100 V, "craters" like morphology was detected on the surface as a consequence of the enhanced surface bombardment of argon atoms that caused re-sputtering. Coatings deposited under the application of a bias voltage higher than ~ - 150 V exhibited poor adherence to their substrate. Furthermore, we discovered that increasing the deposition power supplied (3.3-10 W/cm2) did not affect much, but the expected higher deposition rate, nevertheless, adhesion remained unaffected. With increasing the energy supplied during deposition oxidized and carbonaceous species were detected on the surface. Based on this study, we deduce that the optimal bias voltage is ~ -60 V together with a power of ~ 10 W/cm2. By employing 1.5 μm thick titanium layer, boron carbide coatings with thickness of at least 3.5 μm remained adhere for several months (until today), in an environment of 2 % RH. Based upon the current research, a strong and durable attachment of a dense boron carbide coating, with an amorphous structure and B_4C composition was successfully deposited onto an aluminum substrate.

A breakthrough technological solution in the nano-conformal coating world

Tal Kaufman
Simtal

Parylene Coating - How it all began:

In 1947 Michael Moses Schwartz left Eastern Europe and moved to Manchester, England. There Schwartz began studying chemistry and physics focusing his research on the chemical attraction between Aliphatic Carbon and Hydrogen.

After researching countless materials and elements he finally came across Para-Xylene, which left a residue much like the skin shed by a snake. At this stage he decided it is best to research the physical and chemical qualities of his discovery and find out if he was onto something.

Schwartz's 'snake skin' was the first experience of what was later to become known as Parylene.

In the initial stages of the research, Schwartz's discovery of the materials' exceptional thermal stability, encouraged researchers around the world to continue searching for more polymers of the same family. Among the curios were well known companies with established research labs, included: ICI, UNION - CARBIDE, DuPont and others .

Nearly two decades of research later, in 1965, Dr. William Franklin Gorham and the UNION - CARBIDE labs found a way to mass produce and commercialize the material we know today as Parylene.

NASA's best kept secret is finally out:

Initially Parylene was most commonly used in the aeronautic and space industries with NASA as Parylene's most prestigious fan. Over the last 40 years many patents have expired and what was once a military and commercial secret came to light, exposing many more industries to the wonders of Parylene.

In essence, Parylene is a polymer most commonly used as a world leading surface modifier (conformal coating), protecting and insulating vast and varied applications from harsh environments such as: chemicals, acids, aggressive gases, extreme temperatures and humidity. Other uses for Parylene include nano–packaging, friction reduction and more.

Parylene conformal coating offers several unparalleled advantages, not the least of which, is the fact that while trying to solve a single problem you always receive the complete package of advantages.

With a multitude of invaluable characteristics, Parylene is one of the world's most advanced polymer coatings.

Used in a wide variety of industries (including: industrial medical and bio-med, electronics and PCB, military, chemical aeronautic, automotive and space industries), a single polymer, Parylene combines the advantages of all other coating techniques including; silicone, polyurethane, epoxy, acrylic and others. While each technique comes with its

own set of advantages, only Parylene offers all of advantages, strengths and all of the qualities in a single synergistic solution.

Unlike conventional conformal coatings applied by spraying, brushing or dipping and even other vacuum based coatings such as sputtering, which is an eye sight coating process that leaves many areas in the shadows and non-coated. Parylene is a volumetric (CVD) process applied by evaporation in a vacuum; hence its unique penetrability into every space and hidden crevice.

Characterized by its multiple advantages, Parylene is most often the coating method of choice by leading global companies around the world, requiring the highest quality coating for their products.

Session 6
Materials for Energy II

Session chairs:
Lioz Etgar

Location: Teddy A

Metal-oxide photoelectrodes for solar water splitting

Daniel Grave
Ben-Gurion University of the Negev

Photoelectrochemical (PEC) water splitting is an attractive route for green hydrogen production. The key challenge in PEC water splitting lies in the design of the photoelectrode material responsible for absorption of light, photogeneration of charge carriers and their transport to the device terminals to drive the water oxidation and reduction reactions. Transition metal-oxides (TMOs) are widely viewed as the most promising photoelectrode materials for their exceptional stability in aqueous electrolytes. However, TMOs with with suitable band gaps for visible light absorption suffer from low photoconversion efficiency, generally attributed to charge carrier recombination arising from poor charge transport properties (low mobility and short minority carrier lifetimes). Using α-Fe_2O_3 as a case study, we show that while charge transport limitations can be mitigated by clever device design, a non-unity photogeneration yield of mobile charge carriers is an additional, yet overlooked loss mechanism that is more difficult to surmount. We develop several methods for spectral characterization of the mobile charge carrier photogeneration yield in thin film photoelectrodes and demonstrate that a non-unity photogeneration yield fundamentally limits the achievable performance of such materials.

Design of Aerogel-based Electrocatalysts for Oxygen Reduction Rection in Fuel Cells

Lior Elbaz
Bar Ilan University

In the past couple of decades great advancements have been made in the development of PGM-free catalysts based on earth-abundant elements, nitrogen, carbon and transition metals (usually Fe or Co), inspired by biological systems such as porphyrins and phthalocyanines. In order to overcome the poor stability and low catalytic activity of transition-metal complexes, a new class of high temperature-treated (HT-treated) catalysts, composed of the same elements, i.e., a transition metal, carbon and nitrogen, was developed. Although HT-treated PGM-free catalysts exhibit improved activity and stability, their performance remains inferior to PGM catalysts, calling for further improvements to make them a viable alternative to the state-of-the-art materials.

In this work, we designed, synthesized and characterized ORR catalysts based on iron, carbon and nitrogen in a well-defined, high surface-area covalent framework (COF) of aerogels. Aerogels are ultralight, porous materials, with ultra-low density and high void volume (> 97%), also known for their unique physicochemical properties such as high porosity, controllable pore size and surface area, low thermal conductivity, just to name a few. The variety of precursors used for aerogel synthesis makes them promising candidates for a wide range of applications in catalysts, capacitors, insulators, absorbents, and many more. In the context of electrocatalysis of fuel cell reactions, carbon-aerogels have been mostly used so far as catalyst supports for PGM and PGM-free catalysts.

In their inorganic form, aerogels can have ultra-high catalytic site density, high surface area, and tunable physical and chemical structures - all very important features for a heterogeneous catalyst. In this talk, we will discuss the synthesis and electrocatalytic properties of an iron-porphyrin aerogel. 5,10,15,20-(tetra-4-aminophenyl)porphyrin (H_2TAPP) and Fe(II) were used as the building blocks of the aerogel, which was later heat-treated at 600 °C to enhance electronic conductivity and catalytic activity while preserving its macro-structure. The resulting material has a very high concentration of atomically dispersed catalytic sites ($4.01 \cdot 10^{19}$ sites cm^{-3}), capable of catalyzing the oxygen reduction reaction in alkaline solution (E_{onset} = 0.93 V vs. RHE, TOF = 0.2 e- $site^{-1}$ s^{-1} at 0.8 V vs. RHE). At the end of the talk I will also show some of our recent results with other types of aerogels, some for different applications.

Graphite-GnP-salt composite: Thermal properties enhancement for energy storage applications

Adi Lavi
Ben-Gurion University

Thermal energy storage is required in the renewable energy field due to the increasing global demand for energy, alongside finite available resources of fossil fuels. Thermo-solar energy is stored during daytime and used at night. The storage principle of phase change materials (PCM) is based on the heat of fusion and solidification-melting transitions of PCM, e.g., salts, which demonstrate high thermal energy storage density. Salts are also completely green compared to fossil fuels, and are already integrated in existing industrial systems, such as thermo-solar power plants. However, the thermal conductivity of *salt* - crucial for the energy storage process - is rather low (<1 W/mK). We aim at enhancing its thermal conductivity by loading it with high thermal conductivity fillers, such as carbon-based materials, such as graphite, leading to the formation of a composite. We found that the molten salt treatment exfoliates the graphite to graphene nanoplatelets (GnP, <100 nm thick), hence enhancing the thermal conductivity of the salt-based composite.[1] The exfoliation of graphite in molten NaCl–KCl salt (@750 °C) yielded a homogeneous composite, from which salt-free GnP could be easily and completely separated. The produced GnP displayed relatively large-size particles (12 μm, TEM, SEM, laser diffraction) and low defect density (Raman, XPS), indicating the superiority of the molten salt approach over conventional liquid-phase exfoliation. Moreover, the large-size and low defect density GnP obtained in the molten salt are directly applicable in enhancing the thermal properties of the composite: in the GnP-salt composite, the thermal conductivity is enhanced by more than one order of magnitude (up to ~44 W/mK, Figure 1a, squares) compared to the neat salt matrix (~0.6 W/mK, Figure 1a, diamond). Our developed GnP-loaded molten salt could be used as a high thermal conductivity PCM for high-temperature thermal energy storage applications, where the filler is both produced and directly dispersed in the salt matrix (Figure 1b).

Methanol conversion to hydrogen on copper surfaces: A molecular level study

Roey Ben David
Weizmann Institute of Science

Methanol is a promising hydrogen carrier with a large gravimetric and volumetric hydrogen storage capacity. However, since methanol is a chemical (covalent) hydride, a catalyst is required for converting it into hydrogen at moderate temperatures. Cu-based materials show promise to be efficient catalysts; yet, the reaction mechanism and the evolution of surface intermediates at ambient conditions, including the effect of the Cu surface structure, remain unsolved. Here, the interaction of methanol vapor with different Cu single crystal surfaces, Cu(111), Cu(100) and Cu(110), was studied with surface-sensitive infrared (IR) and x-ray spectroscopy techniques under 1 mbar methanol pressure in the temperature range of 25-100 °C. The first step of methanol decomposition, i.e., breaking the O-H bond to form surface-bound methoxy (CH_3O^*), readily occurs at these conditions. The temporal evolution of the IR spectra indicates that a transient state of a high coverage methoxy layer is formed immediately after methanol exposure. This state and the evolution of methoxy coverage cannot be explained using standard adsorption models. We assign this nonequilibrium coverage to a precursor state of H-bonded methanol assembly. To achieve an equilibrium coverage, the methoxy excess is eliminated from the surface via further dehydrogenation to CO that desorbs to the gas phase. The kinetics of this process, which involves activation of C-H bonds, displays a significant structure sensitivity with considerably faster kinetics on Cu(110) surface compared to Cu(111) and Cu(100) surfaces. Our suggested mechanism implies that CO generation during dry methanol dehydrogenation on bare Cu surfaces cannot be avoided, as it is an inherent consequence of precursor-mediated dissociative adsorption.

Assembly of a MOF Membrane on Solid Electrocatalyst: Molecular-Level Control Over Heterogeneous CO_2 Reduction

Subhabrata Mukhopadhyay
Ben-Gurion University of the Negev

Catalytic enzymes have evolved chemical and structural mechanisms that modulate the surroundings of the active site and hence regulate the activity and selectivity of a desired catalytic reaction. For instance, membrane proteins have provided precise control over the rate of proton delivery towards the active site in order to regulate redox-based proton-coupled electron transfer (PCET) reactions. Moreover, an enzyme may modulate the secondary coordination sphere of the active site via the incorporation of pendant functional groups, such as proton relays or charge-bearing moieties. These groups play a crucial role during catalysis, as they may stabilize the intermediate species and enhance the reaction rate and selectivity. Inspired by this, we demonstrate that, when assembled on a solid Ag CO_2 reduction electrocatalyst, a non-catalytically active UiO-66 MOF acts as a porous membrane that systematically tunes the active sites immediate chemical environment, leading to a drastic enhancement of electrocatalytic activity and selectivity. Electrochemical analysis shows that the MOF membrane improves catalytic performance through physical and electrostatic regulation of reactants delivery towards the catalytic sites. The MOF also stabilizes catalytic intermediates via modulation of active sites secondary coordination sphere. This concept can be expanded to a wide range of proton-coupled electrochemical reactions, providing new means for precise, molecular level manipulation of heterogeneous solar fuel.

Carbon Nitride Layers as Light-Harvesting Semiconductors for Photoelectrochemical Cells.

Menny Shalom
Ben-Gurion University of the Negev

One of the most promising future sources of alternative energy involves water-splitting photoelectrochemical cells (PECs) – a technology that could potentially convert sunlight and water directly to a clean, environmentally friendly, and cheap hydrogen fuel. Practical PEC-mediated hydrogen production requires robust and highly efficient semiconductors, which should possess good light-harvesting properties, a suitable energy band position, stability in harsh conditions, and a low price. Despite significant progress in this field, new semiconductors that entail such stringent requirements are still sought after.

Over the past few years, graphitic carbon nitride (CN) has attracted widespread attention due to its outstanding electronic properties, which have been exploited in various applications, including photo- and electro-catalysis, heterogeneous catalysis, CO_2 reduction, water splitting, light-emitting diodes, and PV cells. CN comprises only carbon and nitrogen, and it can be synthesized by several routes. Its unique and tunable optical, chemical, and catalytic properties, alongside its low price and remarkably high stability to oxidation (up to 500 °C), make it a very attractive material for photoelectrochemical applications. However, only a few reports regarded CN utilization in PECs due to the difficulty in acquiring a homogenous CN layer on a conductive substrate and our lack of basic understanding of the intrinsic layer properties of CN.

In this talk, I will introduce new approaches to grow CN layers with altered properties on conductive substrates for photoelectrochemical application. The growth mechanism and their chemical, photophysical, electronic, and charge transfer properties will be discussed.

IR Nanospectroscopy Measurements Uncover Structure-Reactivity Correlations in Catalytic Nanostructures

Elad Gross
The Hebrew University of Jerusalem

The development of optimized (electro)catalysts that can address the energy challenges of the 21st century requires in-depth understanding of the basic elements that control the reactivity of catalytic nanoparticles. However, heterogeneities in the structure and composition of catalytic materials make it difficult to monitor the influence of local physicochemical parameters on the global reactivity. In this talk I will demonstrate that structure-reactivity correlations at the nanoscale can be identified by conducting IR nanospectroscopy measurements while using N-heterocyclic carbene molecules as probes for surface-induced reactivity. Using this approach, we identified the influence of different surface sites on the catalytic reactivity of Au and Pt nanoparticles and the ways by which site-dependent reactivity varies in response to reaction conditions. In addition, by conducting IR nanospectroscopy measurements we uncovered the ways by which communication between neighboring surface sites dictates the globular reactivity pattern of catalytic nanoparticles. These findings provide fundamental understating about the elements that direct the catalytic reactivity of metallic nanoparticles and deliver guidelines for the design of optimized catalysts.

Session 7

2D Materials II

Session chairs:

Doron Naveh, Ariel Ismach

Location: Teddy B

The influence of global and local magnetism on optical properties of two-dimensional semiconductors

Efrat Lifshitz
Technion

Magnetism is a topic of a wide interest since the discoveries of motors/generators, through magneto-resistance and up to modern times, where low dimensional materials offer a support for new magnetic phenomena. The talk will focus on the influence of magnetic moments and magnetism on the optical magneto-properties of semiconductors in an ultimate two-dimensional limit found in van der Waals transition metal tri-chalcogenides and perovskite nanoplatelets. A few types of magnetic properties will be discussed: The long-range magnetic order, ferromagnetism, anti-ferromagnetism or special spin textures; An interfacial developed Rashba spin-orbit effect; Nuclear spin Overhauser effect; Magnetic polaron, all gaining special stabilization by the size confinement and a shape anisotropy. The mentioned intrinsic fields lead to a lift of energy or momentum degeneracy at band-edge states with selective spin orientation in the ground or/and excited state, being of a special interest in emerging technologies of spin-electronics and quantum computation.

Long-range magnetic order in metal phosphor tri-chalcogenide compounds: Metal phosphor tri-chalcogenides with the general chemical formula MPX_3 (M=metal, X=chalcogenide) closely resembling the metal di-chalcogenides, but the metal being paramagnetic elements, while one-third of them are replaced by phosphor pairs. The metal ions within a single layer produce a ferromagnetic or anti-ferromagnetic arrangement, endowing those materials with unique magnetic and magneto-optical properties. Most recent magneto-optical measurements will be reported, exposing dual relation between magnetism and electronic properties.

Rashba and Overhauser effects in perovskite materials: Perovskite materials are composed of organic-inorganic or all inorganic constituents. They mostly contain octahedral units of metal-halides or metal-oxides, generating an inorganic network with voids that are filled by organic or inorganic counter ions. The studies to be reported are related to compounds with chemical formula $APbX_3$ (A = methylammonium or Cs; X= I, Br) grown in 2D and 3D forms. The magneto-optical properties of such compounds revealed selective exciton' circular polarization components following a non-linear energy split upon an increase of an applied external magnetic field, which was associated with the involvement of a Rashba effect. Furthermore, degree of circular polarization dependence on the applied magnetic field, exposed a trend related to the Overhauser effect

Overall, the observation designated a strong influence of intrinsic magnetic effect on spin and optical properties in two-dimensional semiconductors, with a large impact on their implementation in modern spin-electronics and spin-optical devices.

Effects of non-uniform strain in transition-metal dichalcogenides

Moshe Haratz
Ben-Gurion University of the Negev

2D materials are elastic materials that can sustain high strain. While the response of these materials to spatially uniform strain is well studied, the effects of spatially non-uniform strain are understood much less. In this talk I will show the response of transition metal dichalcogenides monolayers under non-uniform strain. It was predicted that non-uniform strain will allow transport or "funneling" of neutral charge excitons which can be useful as an efficient solar cell [1]. I show that while transport or "funneling" of excitons is relatively inefficient, a different process, a strain-related conversion of excitons to trions is dominant and is universal for any configuration of non-uniform strain [2-3]. Lastly, I will discuss different experimental directions that will allow high "funneling" efficiency by straining heterostructures [4].

[1] J. Feng, X. Qian, C.-W. Huang, and J. Li, Nature Photonics 6, (2012), 866–872.

[2] M. G. Harats, J. N. Kirchhof, M. Qiao, K. Greben, and K. I. Bolotin, Nature Photonics, 14 (5), (2020), 324-329

[3] S. Kovalchuk, M. G. Harats, G. López-Polín, J. N. Kirchhof, K. Höflich, K. I. Bolotin, 2D Materials 7 (3), (2020), 035024

[4] M. G. Harats, K. I. Bolotin, 2D Materials 8 (1), (2020), 015010

Asymmetric "misfit" nanotubes: Chemical affinity outwits the entropy at high-temperature solid-state reactions

M.B. Sreedhara
Weizmann Institute of Science

Asymmetric two-dimensional structures and nanotubes have tremendous scope in material chemistry due to a lack of inversion symmetry and time-reversal symmetry. But the synthesis of these structures is fundamentally difficult due to the entropy-driven randomized distribution of chalcogens. Serendipitously, a family of misfit superstructures such as LaX-TaX2 (where X= S/Se) were found to form asymmetric structures at high-temperature chemical vapor transport reaction. The Se exclusively bind to Ta atoms and La binds to S atoms, rather than the anticipated random distribution. With increasing Se concentration, the well-known (O-T) superstructure of LaS-TaX2 gradually transforms into (O-T-T) superstructure (LaS-TaSe2-TaSe2). Beyond xSe>0.8, the MLC became unstable due to sulfur starvation and decomposed into binary compounds. These counterintuitive results shed new light on the chemical selectivity and stability of MLC. The lack of inversion symmetry in these asymmetric compounds and time-reversal symmetry in the chiral nanotubes offers intriguing physical observations and applications as thermoelectric nanomaterials.

Reference

Sreedhara et al., Asymmetric misfit nanotubes: Chemical affinity outwits the entropy at high-temperature solid-state reactions. PNAS 2021, 118, (35), e2109945118

Molten Salt-Assisted Exfoliation of Graphite to Graphene: A Mechanistic Study

Efrat Ruse

Nuclear Research Center, Negev

The exfoliation of graphite to graphene nanoplatelets (GnP) in a molten salt medium was investigated in this study. It was shown that this mechanical force-free process yielded a large-sized GnP product (>15 microns) with a low defect density. Previous studies on liquid-phase exfoliation indicated that graphene is dispersed efficiently in liquids with matching surface tension values, but the liquids used to date are highly toxic. Molten salts, on the other hand, are an attractive environmentally green alternative liquid media for graphite exfoliation [1]. They offer a unique nonaqueous working environment characterized by a variety of salt types, providing a wide range of melting temperatures and surface tensions. In this study, the effect of molten salt surface tension on graphite exfoliation efficiency was investigated for a series of alkali chloride salts (CsCl, KCl, NaCl, and eutectic NaCl-KCl) at 850 °C. It was demonstrated that GnP was produced, and it could be completely and easily separated from the salt. Molten salt with the lowest value of surface tension (CsCl) displayed the highest wettability of the graphitic layers and hence enables total conversion of the graphite to GnP. The proposed exfoliation mechanism involves the impregnation of a hole-rich melt into the graphite interlayers, which facilitates gentle graphite exfoliation to GnP.

[1] E. Ruse, M. Larboni, A. Lavi, M. Pyrikov, Y. Leibovitch, A. Ohayon-Lavi, L. Vradman, O. Regev, Molten salt in-situ exfoliation of graphite to graphene nanoplatelets applied for energy storage, Carbon. 176 (2021) 168–177.

Study of 2D Alloys $Bi_2Se_{(3-x)}S_x$ Optical and Optoelectronic Properties

Michal Poplinger
Bar Ilan University

Topological insulators (TIs) are a state of quantum matter that differs from simple metals and insulators by having a bandgap in the bulk of the material but metallic states along their surface. The surface states are topologically protected by time reversal symmetry, making them indestructible by impurities. Bi_2Se_3 is one of the most studied TIs, as its topological effects are observed at room temperature owing to the relatively strong spin-orbit coupling effect occurring in heavy elements such as Bi.

Alloying is a key technique for tuning the structural, optical and electrical properties of a material. Here we report on $Bi_2Se_{(3-x)}S_x$ alloys that are formed by incorporating sulfur atoms to Bi_2Se_3, leading to widening of the bulk bandgap, relative to ~0.3 eV of pure Bi_2Se_3. With that, we study the structural and topological phase diagram of $Bi_2Se_{(3-x)}S_x$ alloys by means of structure, transport and optical properties and compare our results to computational predictions. In addition, device applications of hybrid photodetectors comprising topological alloys and graphene elucidate their potential in high performance photodetector at the visible-Mid IR spectral range.

Electrical Contact Resistance to Atomically Thin Semiconductors

Eilam Yalon
Technion

Achieving good electrical contacts is one of the major challenges in realizing devices based on atomically thin two-dimensional (2D) semiconductors. This talk will review strategies to achieve state-of-the-art contacts to 2D semiconductors as well as the underlying physics that governs their electrical resistance.

"Slide-Tronics"

Moshe Ben-Shalom
Tel Aviv University

A ferroelectric system, only two-atoms-thick is presented [1]. Stacking two layers of hexagonal boron nitride (hBN) atop each other, with a parallel crystal orientation, results in a permanent electric polarization pointing out of the plane. Furthermore, applying an opposite external electric field switches the vertical polarization by a horizontal sliding between the layers of a full atomic spacing distance.

I will describe our atomic force experiment, DFT calculations, and a simplistic cohesion model, allowing us to explore the interfacial-ferroelectricity and its unique Slide-Tronics switching mechanism.

If time allows, I will further discuss our efforts to induce intrinsic electric and magnetic gauge-fields in graphene by particular strain-engineering schemes [2].

[1] arxiv.org/abs/2010.05182
[2] arxiv.org/abs/1909.09991

Session 8
Oxides and Engineered Quantum Materials

Session chairs:
Yoram Dagan, Shmulik Hayun

Location: Teddy C

Surface state at $BaSnO_3$ evidenced by angle-resolved photoemission spectroscopy and ab initio calculations

Muntaser Naamneh
Ben-Gurion University of the Negev

Perovskite alkaline earth stannates, such as $BaSnO_3$ and $SrSnO_3$, showing light transparency and high electrical conductivity (when doped), have become promising candidates for novel optoelectronic devices. Such devices are mostly based on hetero-structures and understanding of their electronic structure, which usually deviate from the bulk, is mandatory for exploring a full application potential. Employing angle-resolved photoemission spectroscopy and ab initio calculations we reveal the existence of a 2-dimensional metallic state at the SnO_2-terminated surface of a 1% La-doped $BaSnO_3$ thin film. The observed surface state is characterized by distinct carrier density and a smaller effective mass in comparison with the corresponding bulk values. The small effective mass of the surface state of about $0.12m_e$ warrants that BSO can be an essential ingredient in transition metal oxide heterostructures with a significantly improved electrical conductivity.

Imaging the magnetic landscape in a superconductor-correlated insulator alternate stacking 4Hb-TaS2

Beena Kalisky
Bar Ilan University

Van der Waals heterostructures provide a unique opportunity to examine proximity effects between materials with vastly different ground states. 4Hb-TaS2 naturally realizes this opportunity as its structure is an alternate stacking of two lattice structures, 1T and 1H, a candidate chiral spin liquid and a superconductor. In my talk, I will show scanning superconducting quantum interference device (SQUID) data, mapping the magnetic landscape of this compound. The data reveal magnetic history that affects the superconducting state, and survives in the normal state. Our results indicate that the coupling between the two constituent layers generates a new unconventional ground state.

Strain glass properties in Sm doped ceria

Anna Lavie
Weizmann Institute of Science

Ferroelasticity is characterized by a hysteresis loop in the strain-stress dependence of the material. The hysteresis in strain upon application of external stress is enabled by mechanical switching between at least two orientation states of the crystal, i.e. non-cubic structure . In strain glass, the material contains small regions or domains that have lower symmetry in comparison to the average symmetry of the material. This means that in contrast to ferroelastic material, even materials with average cubic symmetry can be in a strain glass state. Similarly, to the ferroelastic case, the elastic domains in a strained glass can be orientated. Unlike the ferroelastic case, the process strongly depends on frequency, material history and does not change the average material symmetry.

In the last decade, oxygen ion conductors of the fluorite symmetry, such as reduced ceria $CeO_{2-\delta}$, doped ceria $RExCe_{1-x}O_{2-x/2}$ (RE= Rare Earth, e.g. Gd, Sm, Yb, etc.), were found to exhibit strong anelastic effects. These observed effects include room temperature creep and time dependence of elastic moduli. Moreover, these materials exhibit a very strong second order electro-mechanical response (electrostriction). It was suggested, that these effects are correlated with elastic domains, which form in high concentration (>1%) of oxygen vacancies. The preliminary results of the current study show that in Sm doped ceria, electrostrictive strain generated at sufficiently low frequencies, does not recover upon electric field removal. The recovery of this long-term strain is however, accelerated by moderate heating. This hysteresis strain behavior suggests that these materials may be classified as ‘strain glasses’.

Water adsorption and oxidation in the $Th_{1-x}U_xO_2$ system

Lee Shelly
Ben-Gurion University of the Negev / NCRN

Water adsorption and oxidation behavior of thorium and uranium oxides are highly valued due to their use in nuclear reactors. The measurement of water adsorption energy and amount of adsorption is rarely measured and almost always calculated using complex models. Both oxides form in the fluorite structure and form a solid solution throughout the rage. In contrast, the main difference between these oxides is the oxidation behavior, whereas thorium has a very stable valence of Th^{4+} while uranium can further oxidize to U^{5+} and U^{6+}. In the present work, A combination of a calorimeter and a dosing system is utilized in order to measure the adsorption energy and the amount of water adsorbed on a series of $Th_{1-x}U_xO_2$ samples. The results show that the addition of uranium increases adsorption energy but lowers the overall amount adsorbed. In addition, the effect of temperature and oxygen partial pressure on the lattice parameter, electronic configuration, and cation segregation to the surface was studied using HRXRD and X-ray photoelectron spectroscopy.

On the stability of MXene in aqueous colloidal suspensions

Maxim Sokol
Tel Aviv University

MXene is a recently discovered family of two-dimensional transition metal carbides, nitrides, and carbonitrides that have shown a lot of promise in the field of energy storage with applications ranging from high-capacity anodes for lithium, sodium, potassium, and aluminum ion batteries, supercapacitors, and catalysts for hydrogen evolution, among several others. However, MXene oxidation in aqueous colloidal suspensions when stored in water at ambient conditions remains a critical challenge toward scaling up MXene production and its commercialization.

In this work, we examine the effect of various processing parameters on the properties of $Ti_3C_2T_z$ MXene. We focused on analyzing the stability and aggregation mechanism of $Ti_3C_2T_z$ colloids that was studied using zeta potential measurements as a function of pH. Based on the obtained results, we managed by simply capping the edges of individual MXene flakes, by polyanions, to reduce quite significantly their propensity for oxidation even when held in aerated water for weeks.

Processing and properties of transparent ceramics by high-pressure spark plasma sintering

Barak Ratzker
Ben-Gurion University of the Negev

Producing dense bulk nanocrystalline ceramics is a challenge, making it difficult to study their mechanical behavior and distinctive deformation mechanisms. The mechanical properties (e.g., strength and hardness) of polycrystalline materials typically improve with reduction of grain size, following the Hall-Petch relationship. However, when reaching very fine nanoscale grains (<50 nm) the behavior changes and further reduction of the grain size will lower mechanical properties. The powder densification method of high-pressure spark plasma sintering (HPSPS) enables fabrication of fully dense nanostructured ceramics. Thus, allowing to study bulk nanocrystalline ceramics and investigate fundamental aspects of their unique mechanical behavior. In the present study, nanostructured $MgAl_2O_4$ with an average grain size of about 20-40 nm was fabricated by HPSPS and deformed in a controlled manner using a microhardness Vickers indenter. Samples of the deformed area under the indentation tip were prepared by focused ion beam (FIB) and examined by scanning transmission electron microscopy (STEM) and transmission electron microscopy (TEM). This analysis revealed many interesting deformation characteristics. Three different regions under the indentation were observed, a heavily strained region directly under the indentation, a virtually strain-free area far enough below the indentation and a transitional medium strained region in-between. Additionally, micro and nano-cracks were observed mostly outside the heavily strained region and nano-voids were present between grains in the medium-strained region. Furthermore, shear bands were also clearly observed throughout the deformed specimens. Finally, analysis of the strained regions by selected area electron diffraction (SAED) confirmed misorientation of the grains, suggesting a large magnitude of grain boundary sliding and rotation. The microstructural evidence uncovered in this study implies that a combination of grain boundary sliding and dislocations govern deformation in the nanostructured material. Apparently, as the grains become smaller the grain boundary mediated mechanisms become more dominant.

Oxide interfaces and device building blocks for oxide electronics

lior kornblum
Technion

Oxides with correlated electrons exhibit rich physics and they are often highlighted for their potential for application in novel devices. Interfaces of such oxides are particularly interesting as they herald emerging phenomena and allow additional degrees of freedom to control them. I will describe some of our efforts to understand the electronic behavior of oxide interfaces, focusing on their conductivity, band offsets and how they are affected by the interface's material properties. Using this knowledge, we designed basic device building blocks, including a metal oxide semiconductor (MOS) capacitor, memristor and a diode. I will show how using device-physics perspective can contribute to our understanding of the interface, and how this helped developing robust insulators for current and future devices. With these small building blocks we hope to mature oxide interfaces closer towards practical applications in new types of devices.

MeV Proton induced radiation damage in tungsten and tantalum

Inbal Segev Gavish
Technion

The effects of high-energy proton irradiation on the refractory metals tungsten and tantalum and their properties, were studied at the Soreq Applied Research Accelerator Facility (SARAF) using a high-flux 2.2 MeV proton beam. Samples were characterized by optical interferometry, nanoindentation and Time of Flight Secondary Ion Mass Spectrometry (ToF-SIMS), to study the effect of radiation damage. Tungsten exhibited well-developed blisters while similar doses in tantalum only produced swelling. The volume expansion in Ta was found to be correlated to the total proton fluence. No blistering was observed in Ta up to a total fluence of 1.9E+20 P/cm2 , extending the lower bound by almost an order of magnitude to more than three orders of magnitude higher than the critical fluence for blistering in tungsten. In Ta we observed extensive diffusion of the hydrogen into the material in contrast to tungsten. A reaction-diffusion model was employed to analyze the spatial distribution of the point defects, to assist in the interpretation of the results in comparison with tungsten, and to identify the role of the hydrogen diffusion. We conclude that tantalum is a promising structural material in proton radiation environments.

Session 9
Metallurgy and Processing

Session chairs:
Louisa Meshi, Nachum Frage

Location: Oren 2

Thermochemistry of High Entropy Alloys

Shmuel Hayun
Ben-Gurion University of the Negev

With the introduction of the high entropy alloy (HEA) concept about 16 years ago, new ideas have stimulated the exploration of the vast composition space offered by multi-principal element alloys (MPEA). Understanding the thermodynamics of such MPEA is crucial to addressing their synthesis, properties, stability, materials compatibility, and technological applications. While the thermodynamics of binary and ternary alloys are relatively well investigated both experimentally and theoretically in the last five decades, this is not the case for multi-component (> 4 elements) alloys. Unfortunately, the methods used for alloys have limitations for application to multicomponent alloys containing a variety of elements with different chemical properties. They are not general but must be tailored carefully to the specific system of interest, and sometimes are simply inadequate. A more flexible and general calorimetric approach is needed. In the present talk, a new methodology for measuring the enthalpy of formation and mixing of metals will be introduced. This new calorimetric technique is designed for a new and broad class of materials and to increased understanding of the thermodynamics of MPEA, especially to address questions of local ordering and phase transition which may influence their thermodynamic and physical properties, as well as the generation of data to constrain phase diagram calculations.

The role of grain and interphase boundaries in nucleation-controlled plasticity

Eugen Rabkin
Technion

We demonstrated that single crystalline Ag nanoparticles produced by solid state dewetting of thin Ag films deposited on sapphire substrate exhibit extraordinary size-independent compressive strength of 8.2±1.2 GPa [1]. Surprisingly, coating single crystalline Ag nanoparticles with a thin polycrystalline Au layer leaded to drastic weakening of the particles [2]. This is in strong contrast with the behavior of bulk polycrystalline metals, in which a reduction in the grain size leads to hardening, since the grain boundaries represent efficient barriers for slip transfer between the adjacent crystalline grains. Moreover, while the single crystalline Ag nanoparticles yielded in a single large displacement burst when loaded in compression, their Ag-Au core-shell counterparts demonstrated a more homogeneous deformation with signs of strain hardening. Our molecular dynamics simulations demonstrated that particle weakening at low strains is attributed to the plasticity confinement in the polycrystalline shell, in which the grain boundaries play a dual role of dislocations sources and sinks. At higher strains the plasticity within the Ag core is initiated by the dislocations nucleating at the Ag-Au interphase boundary. The results of this study show that adding imperfect material to super-strong single crystalline metal nanoparticles makes them weaker. At the same time, thin nanocrystalline coatings can be employed to improve the formability of metals at the nanoscale.

References

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Pseudoelasticity of metal nanoparticles is caused by their ultra-high strength Advanced Functional Materials 30 (2020) 1807554

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When more is less: plastic weakening of single crystalline Ag nanoparticles by the polycrystalline Au shell, ACS Nano 15 (2021) 14061-14070

Solid-state dewetting synthesis of Nickel-Platinum nanoparticles

Mor Levi
Technion

Nanoparticles of Ni-Pt alloys attract great attention because they can replace more expensive Pt in several catalysis-related applications. The shape, size, and distribution of such nanoparticles can influence application functionality.

This work studied the morphology and nanoparticles orientation of Ni-Pt nanoparticles synthesized by solid-state dewetting of the Ni-Pt bilayers deposited on a sapphire substrate. The nanoparticles of Ni-Pt alloys of several compositions were produced employing the solid-state dewetting of Ni-Pt bilayers at various temperatures and for different heat treatment durations and stacking orders of Ni and Pt sub-layers. We used multiple characterization methods such as atomic force microscopy, scanning electron microscopy, electron backscatter diffraction, and x-ray diffraction to investigate the attribute of the nanoparticles.

We found that the shape of the nanoparticles depends on composition: Increasing Pt content resulted in lower and wider nanoparticles, and the orientation of the nanoparticles varied. Surprisingly, the shape of the nanoparticles of the same composition depended on the stacking order of the Ni and Pt sub-layers from which they were formed. Nanoparticles fabricated by dewetting bilayers with Pt sublayer on the top exhibited greater area density than their counterparts fabricated from bilayers in which Ni was on the top. The shapes of the particles in the samples with two stacking orders were also different.

Comprehensive study of phase transitions in Al0.5CoCrFeNi high-entropy alloy at intermediate temperatures (400 ≤ T ≤ 900°C)

Einat Strumza

Ben-Gurion University of the Negev

High-entropy alloys (HEAs) have been extensively investigated largely because of their wide range of properties (mechanical, thermal, corrosion etc.) that enable their application in countless applications. One of the most promising families is the AlxCoCrFeNi based HEA, which tends to form simple phases and exhibit simple phase evolution with temperature. In this system, the complexity of the phase evolution tends to increase with decreasing temperatures, which complicates the collection and analysis of experimental thermodynamic data. Therefore, most of the work done in this system regarding phase transitions has been at high temperatures (T > 1000 °C). Al0.5CoCrFeNi has promising mechanical properties due to its duplex nature. At low temperatures, it has an FCC dendrite core (DC) region, which occupies about 90 vol%: the reminder is a B2/BCC mixture inter-dendritic (ID) region. Each region has different chemical composition, which leads to different phase evolution at intermediate temperatures (400 ≤ T ≤ 900 °C). In the present talk, the phase evolution using high-sensitive thermal analysis together with in-depth microstructural characterization will be presented. The DC region exhibits a simpler phase evolution with ordered FCC (L12) nano-precipitation at 508 °C that transitions to B2 precipitation at 778 °C. The L12 → B2 transition is associated with a large exothermic event caused by the release of 'symmetry-breaking' strain and large shrinkage. The ID region exhibits a more complicated phase evolution that starts with precipitation of a Cr-Fe rich HCP phase at 626 °C and continues with the precipitation of Cr-Fe rich sigma (σ) phase along the boundaries between the regions at 699 °C, followed by the transition of the BCC precipitation into FCC at 733 °C. All these transitions in the ID region are associated with non-linear expansion.

Emerging Opportunities in the Fields of Metallurgy and Processing

Itamar Gutman
Rafael

Rapid technological advances in robotics, software and computing power have prompted the 4th industrial revolution. New possibilities, taking advantage of the technological abilities to apply multiple degrees of freedom, make it possible to tailor unique products like never before. Nowadays, technological abilities allow these designs and products to be efficiently and rapidly optimized despite numerous design constraints.

Additive Manufacturing (AM) is just one example of such an emerging technology, making it possible for small and large businesses to construct vertically integrated R&D and production lines, implementing ideas into products. The path to turning innovative ideas into products is shorter than ever and relatively inexpensive. Taking this path demands engineers and scientists mastering both creative thinking and multidisciplinary science and engineering.

In this talk, I will discuss the challenges and opportunities in metallurgy and processing which come with the new technologies. These new technologies force a substantial change in both science and industry. Today, I will present some building blocks that need to gain substantial progress to meet the ongoing changes. Among them are premium metal alloy powders that could be transformed into high-end critical aerospace or medical components; More approachable atomic-level simulation methods essential for optimizing these alloys; Multi-material designs combining mechanical, physical, and unique functional properties that will allow real technological breakthroughs.

Phase diagrams under pressure: Experiments and thermodynamic modelling

Eyal Yahel
Kamag

Binary phase diagrams are of scientific and practical importance in materials science. The experimental construction of phase diagrams requires accurate and well equilibrated thermo-physical measurements to obtain the equilibrium thermodynamic conditions. Hence, it took decades to map the complex phase space of thousands of binary systems at ambient conditions. Pressure affects phase diagrams by altering the interactions, which control the nature of the diagram and by the emergence of new phases and phase boundaries. However, measuring accurately the thermophysical properties under pressure and high temperature is challenging. Therefore, combining experimental measurements and thermodynamic modelling is useful in order to achieve a full understanding of the pressure evolution of binary systems. The experimental study employed electrical resistivity and differential thermal analysis (DTA) at ambient and high pressures up to few GPa and temperatures in the range of ambient to several hundred degrees Celsius. To apply high pressures, we utilized a large volume press – a 'Paris-Edinburgh' press. In particular we developed a unique sample cells for resistivity and DTA measurements under pressure. In addition, we made use of accurate ambient pressure sound velocity measurements to estimate the pressure dependence of the interaction parameters. Within the framework of solution-type models, the variation is controlled by the pressure dependence of the elemental end members, which is relatively well known, and that of theexcess interaction, which is relatively unknown. By incorporating pressure into the model and validating the results against accurate measurements, we are able to predict the pressure dependence of binary phase diagrams, including changes in the nature of the diagram and the evolution of interaction parameters with pressure. Thermodynamic relationships for the pressure and temperature dependence of the interaction parameters in an alloy solution are developed and related to the composition dependence of the excess thermodynamic quantities measured at ambient conditions. The effects of pressure modification of selected phase diagrams, including transformation from isomorphous to eutectic forms and shifts of the eutectic point are explored. Model predictions are compared with experimental data, obtained by novel techniques at high pressure, measured in a 'Paris-Edinburgh' large volume cell. In the present contribution we shall review recent results obtained by experimental study and thermodynamic modelling of both elemental systems e.g., Bi, Ga, In and binary systems e.g., Ga-In, Bi-Ga and Bi-Sb at high pressures and temperatures.

Periodic Nanowire Arrays with Alternating Compositions and Structures Fabricated using a Simultaneous Nanowire Formation Step

Ofer Burg
The Hebrew University of Jerusalem

Patterned metallic nanostructures have many applications such as photonics and catalysis. Alternating structures composed of two or more metals can produce novel surfaces with hybrid properties. However, creating these structures requires complex fabrication schemes with multiple steps. In this work we demonstrate a simple approach for creating arrays of nanowires with alternating features using block copolymers as templates. These polymers microphase separate to form periodic arrays with typical periodicities of a few tens of nanometers. Selective adsorption of metal precursors and subsequent plasma etching affords metallic nanostructures that inherit the underlying pattern of the polymer film. Our approach relies on spatial distinction between chemically identical P2VP cylindrical domains inside a microphase separated PS-b-P2VP bilayer film. Employing different conditions for the adsorption of different metal precursors alloys to limit the penetration of the precursors. This in turn gives different metal compositions between the P2VP domains that are exposed at the surface and those that are buried inside the film. After plasma etching, metallic nanowires form in an alternating array with different compositions of platinum and palladium. Additionally, selective deposition of gold nanoparticles on the block copolymer film enables decorating one kind of nanowire with nanoparticles to create alternating bare and decorated nanowires.

Session 10
Additive Manufacturing II (metals)

Session chairs:
Amnon Shirizly

Location: Oren 3

Development of generic parameters for additive manufacturing (AM) of Ti-alloys and 316L SS by powder bed electron beam melting (EBM) method

Eitan Tiferet
NRCN, Rotem Ind, AEAI

As in any production process, the desired properties of additively manufactured components, particularly in powder bed Electron Beam Melting processes, are ultimately dependent on the manufacturing process parameters. The correlations between parameters of preheating stages, processes temperature and melting characteristics were studied. The conducted experiments explored the effect of beam current and velocity, focus offset, and line offset. The additively manufactured components from Ti-6Al-4V alloy and 316-L SS using the suggested recipe of printing display 99.7% relative density. Future work will further develop optimal printing parameters of complex shape parts.

Additive Manufacturing in Biomedical Applications

Galit Katarivas Levy
Ben-Gurion University of the Negev

Additive manufacturing (AM) processes create three-dimensional structures for additive layering of materials. Those materials are not limited and constantly developing and advancing, ranging from liquid resin to powders to filaments and pellets.[1] AM is also designed to create complex structures that would be extremely difficult or impossible to produce using conventional techniques.[2] Today, AM is becoming a standard manufacturing practice for various biomaterials and biomedical devices and it is expected to revolutionize healthcare.[3] The extensive use of AM in the biomedical field is due to many advantages, such as personalization of medical products, biocompatibility, cost-effectiveness, improved productivity, accessibility, short production time, and simple assembly.[1,3] The most widely used biomedical applications of AM include the design of patient-specific prosthetics and implants, surgical planning models and tools, local and strategically timed drug delivery, etc.[1,2] In this talk, I will present three of my group's projects aiming to develop advanced biomaterials for healthcare applications using different AM technologies. The first project focus on fabricating functional bone reconstruction implants with porous architecture using the bound metal deposition AM process in order to improve the implant integrates with the bone and tissue and to reduce the prevalence of aseptic loosening and stress shielding. The second project deals with additive manufacturing of clear dental aligners using stereolithography technology. We aimed to investigate the possibility of printing the aligners directly as opposed to the conventional thermoforming methods. The third project aimed to develop a new printable bioink, based on patient autologous blood, to fabricate vascularized bone tissue constructs using 3D bioprinter.

Compositionally graded SS316 to C300 Maraging steel using additive manufacturing

Adi Ben-Artzy
Ben-Gurion University of the Negev / Berekely

Joining of dissimilar metals is required for numerous applications in industries such as chemical, energy and automotive. It is challenging due to differences in melting point, density, and thermal expansion of the metals being joined. Common welding techniques involve limiting melting and solidification to a narrow area leading to high thermal stresses and potentially brittle intermetallic phases. Furthermore, the geometric complexity of these welded joints can be rather limited. Additive Manufacturing (AM) presents new techniques for joining of dissimilar metals. One of the emerging methods is the building of functionally graded parts using Directed Energy Deposition (DED) to spatially vary composition. In this paper, a SS316 L and C300 maraging steel couple were joined by DED and heat treated. 13 discrete composition layers were selected using metallurgical considerations, in order to ensure a smooth transition in properties and microstructure. The mechanical properties of the as-built joints were found to be similar to the SS part and no intermetallic phases were found in the interface.

Additive manufacturing of high entropy alloy WTaMoNbV produced by SLM process using elemental powder mixture

Tomer Ron
Ben-Gurion University of the Negev

High entropy alloys (HEAs) exhibit unique properties in terms of their excellent mechanical properties and corrosion resistance. The growing interest in these alloys provokes increased research activities related to their production by additive manufacturing (AM) technology. However, machining difficulties and the necessity to use pre-alloyed powder as row material made this process even more expansive than conventional production technologies. The aim of this research is to produce an innovative HEA alloy in the form of WTaMoNbV by SLM technology using elemental powder mixture and evaluate its corrosion behavior. For reference consideration a counterpart alloy was produced by a conventional technology using arc furnace facility. The microstructure of the tested alloys was examined by scanning electron microscopy (SEM), transmission electron microscopy (TEM) and X-ray diffraction (XRD) analysis while mechanical properties were assessed by compression test. The corrosion behavior was evaluated by potentiodynamic polarization analysis in 3.5% NaCl solution at room temperature.

The obtained results indicated that the crystal structure of the AM alloy and its counterpart alloy were BCC and their microstructure was composed from a single phase as expected from typical HEA with adequate syntheses conditions. However, the microstructure of the printed alloy was relatively finer with clear signs of preferred orientation that were attributed to the rapid solidification characteristics of AM technology. The electrochemical behavior of the two alloys revealed that both alloys exhibit active passive transition with relatively excellent corrosion resistance.

Additively manufactured Ti-6Al-4V lattice infiltrated with biodegradable Zn-base alloy as a hybrid structure for osseointegrated implants

Noa Gabay
Ben-Gurion University of the Negev

Osseointegrated implants aims at upgrading the bonding strength between a natural bone and a permanent implant as well as reducing the risk of stress shielding in orthopedic applications. Currently the bonding between the implant and a natural bone is mainly obtained by using biological cement that does not provide complete integration between the two objects. The objective of the present study is to evaluate the possibility of using a hybrid system made from additively manufactured Ti-base lattice and infiltrated biodegradable Zn-2%Fe alloy as an osseointegrated implant. The idea behind this study is that the open spaces created by the natural degradation of the infiltrated alloy will enable osteoblasts and connecting tissue to migrate into the Ti-base lattice during natural bone growth. This will dramatically increase the integration between the bone and the permanent implant and strengthen their bonding. In addition the use of additive manufacturing technology to produce the permanent implant enables the production of complex structures with a variety of geometries and controlled porosity. The current in-vitro examination included microstructure analysis by scanning electron microscopy (SEM) and X-ray diffraction, mechanical properties assessment in terms of compression strength, corrosion performance in simulated physiological environment, electrochemical analysis by potentiodynatic polarization and electrochemical impedance spectroscopy and cytotoxicity assessment in terms of indirect cell viability. The obtained results showed that the hybrid structure was non-cytotoxic and demonstrate adequate performance in terms of preserving its structural integrity and generating acceptable corrosion rate by the infiltrated biodegradable alloy. Further development work will be required in order to evaluate the osseointegration performance of the proposed hybrid structure in in-vivo conditions.

Pushing LPBF the the edge - the boundaries between design and manufacturing

Yuval Gale
IAI

The lecture will focus on the design-manufacturing-qualification cycle of a satellite component and the benefits that can be gained by designing products for Additive Manufacturing (AM) such as cost reduction and new application opportunities that can only be achieved by AM

Session 11
Soft matter and Bio materials I

Session chairs:
Jacob Klein, Alejandro Sosnik

Location: Teddy A

Peptides assemblies as a versatile platform for enhancing the functionality of biomaterials

Hanna Rapaport
Ben-Gurion University of the Negev

Peptides can be designed and formulated to generate beta-sheet structures that spontaneously organize into different molecular architectures. These assemblies can be incorporated with various biological cues and combined with natural biopolymers to generate bottom-up designed biomaterials. We have created the first family of anionic and amphiphilic beta-sheet peptide hydrogels that were demonstrated to form biocompatible and regenerative scaffolds. We also designed cationic and amphiphilic beta-sheet peptides. These were utilized along with various biopolymers to develop functional biomaterials such as broad-spectrum antimicrobial hydrogels, coatings, and drug-delivery nanoparticle vehicles. In my talk, I will describe the principles that guided the design of our peptides, their formulation into hydrogels and nanoparticles, and various studies we performed to demonstrate the advantages of these biomaterials.

Where plants meet material science: "bio-facturing" cellulose fibers with tailored properties

Filipe Natalio
Weizmann Institute of Science

The use of biological systems for future sustainable production of commercially valuable materials is gaining momentum spearheaded by synthetic biology, green synthesis of functional and adaptive materials. Material farming is a new and alternative concept. It harnesses "already in place" optimized biological strategies and mechanisms from higher organisms with chemically synthesized molecules carrying desired functionalities as biofactories to yield new materials with tailored properties.

As a proof-of-concept, we combined chemical synthesis of glucose derivatives and in vitro cotton growth cultures to demonstrate in situ biological fabrication of cotton cellulose fibers with build-in properties such as fluorescence, supermagnetism, or increased water-retaining capabilities. These results support the idea that higher organisms' complexity can be harnessed toward future "bio-facturing" strategies for new biological-based of commercially valuable materials.

TUNING THE SIZE AND COMPOSITION OF NANOHYDROGELS USING A "PHANTOM MONOMER" FOR BIOLOGICAL APPLICATIONS.

Gerardo Byk
Bar Ilan University

We have designed series of monodispersed nanohydrogels (NHGs) with sizes ranging from 20 to 400 nm, generated from mixtures of N-isopropylacrylamide, di-block (hydrophilic-hydrophobic), and tri-block (hydrophobic-hydrophilic-hydrophobic) co-polymer acrylamide macro-monomers. When the monomers are mixed at high temperature they collapse into well-defined self-assemblies, which can be further polymerized leading to cross-linked NHGs with sizes matching the intermediate self-assemblies. The size of the self-assemblies can be tuned/calibrated by combining different ratios of the starting monomeric mixtures at high temperature. Herein, we defined the concept of " phantom monomers" which are the closest structure that mimic a selected monomer but lacks the active function for polymerization. The phantom monomer co-formulated with other monomers will be present in the intermediate self-assemblies due to its similarity with one of the active monomers. However, upon polymerization, the phantom monomer, lacking of a polymerizable function, will be excluded and a new NHGs will be generated. The comparative analyses of our previously obtained standard

NHGs (G1) with those obtained here using phantom monomers (G2 and G3) not only put in evidence the self-assembly mediated mechanism but also prove the generation of new monodispersed NHG's with improved

drug-loading properties. As proof of concept, the NHGs were loaded with doxorubicin (DOX) and tested in cells.

Results indicate that the drug-loading of the NHGs increases from G1 to G3 and while using the same drug concentration, different size NHGs affect differently the treated cells and disclose a different activity and localization as compared to free DOX by confocal microscopy.

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Hierarchical Assembly Pathways of Spermine-Induced Tubulin Conical-Spiral Architectures

Yael Levi-Kalisman
The Hebrew University of Jerusalem

Tubulin, an essential cytoskeletal protein, assembles into various morphologies by interacting with an array of cellular factors. One of these factors is the endogenous polyamine spermine, which may promote and stabilize tubulin assemblies. Nevertheless, the assembled structures and their formation pathways are poorly known. Here we show that spermine induced the in vitro assembly of tubulin into several hierarchical architectures based on a tubulin conical-spiral subunit. Using solution X-ray scattering and cryo-TEM, we found that with the progressive increase of spermine concentration, tubulin dimers assembled into conical-frustum-spirals of increasing length, containing up to 3 helical turns. The subunits with three helical turns were then assembled into tubules through base-to-top packing and formed antiparallel bundles of tubulin conical-spiral tubules in a distorted hexagonal symmetry. Further increase of the spermine concentration led to inverted tubulin tubules assembled in hexagonal bundles. Time-resolved experiments revealed that tubulin assemblies formed at higher spermine concentrations assembled from intermediates, similar to those formed at low spermine concentrations. These results are distinct from the classical transition between twisted ribbons, helical, and tubular assemblies, and provide insight into the versatile morphologies that tubulin can form. Furthermore, they may contribute to our understanding of the interactions that control the composition and construction of protein-based biomaterials.

Mechanical Regulation of the Cytotoxic Activity of Natural Killer Cells

Lital Mordechay
BIU/BGU

Mechanosensing has been explored for T cells and B cells and is hypothesized to be a part of their activation mechanism. We explored the mechanosensing of the third type of lymphocytes – Natural Killer (NK) cells, by showing that they modulate their immune activity in response to changes in the stiffness of a stimulating surface. Interestingly, it was found that this immune response is bell-shaped, and peaks for the stiffness of a few hundreds of kPa. This bell-shaped behavior was observed for surfaces functionalized with the activating ligand MHC class I polypeptide-related sequence A (MICA), and in the control surfaces with only physical stimulation, but in a less pronouncing way. In addition, it was found that stiffness does not affect uniformly all the cells but increases the size of a little group of extra-active cells, which in turn contributes to the overall activation effect of the entire cell population. We further imaged the clustering of costimulatory adapter protein DAP10 on the NK cell membrane and found that it shows the same bell-shaped dependence to surface stiffness. These findings reveal what seems to be "the tip of the iceberg" of mechanosensation of NK cells, and provide an important insight into the mechanism of their immune signaling.

Dynamic and stimuli-responsive protein constructs via interfacial engineering

Eyal Golub
Bar Ilan University

Proteins are nature's favorite building block as they can support numerous biological processes while exhibiting variable levels of complexities. It is often observed that the assembly of long-range ordered protein materials by nature results in the emergence of synergistic properties, and as such gaining understanding and attaining control over similar assembly processes is an exciting target. However, designing elaborate structures from scratch is non-trivial as it requires meticulous engineering of the interacting interfaces of the individual protein subunits. The toolkit that is often exercised by nature includes various motifs where dynamicity is a crucial factor in the formation of appropriately ordered materials. Also, symmetry is often nature's preferable design strategy that facilitates the formation of macromolecular structures using only a handful of interacting interfaces. As a design strategy for tailoring protein-protein interactions (PPIs) we employed a hybrid strategy that combines both covalent and non-covalent assembly motifs. On the one hand, the metal-directed protein self-assembly (MDPSA) method was employed where metal-binding ligands are installed on the designated interfaces, resulting in a predesigned symmetry within the assembled construct. Additionally, reversible covalent disulfide bonds were introduced as well allowing control of the rigidity of protein constructs with greater precision. We present the implementation of these methods to construct elaborate and highly symmetric protein constructs that exhibit stimuli-responsive assembly and disassembly properties. The careful selection and cross-integration of different assembly motifs allow controlling the stability and orientations of the structures via various stimuli, orthogonal and cross-interacting alike. Accordingly, this strategy can serve as the basis for dynamic materials that can alter their properties based on the designer's choice.

Proteins as a Gamechanger in Biomaterials

Luai Khoury
Technion

Proteins are remarkable machines; they play many important roles in various processes in our body such as helping in digesting food and boosting our immune system. Proteins are built from a chain of building blocks called amino acids. In nature, we have from 20 to 22 amino acids, which provide proteins with a unique chemical and structural diversity. The chemical forces between amino acids units fold the protein molecule in a specific 3D structure which determines its fate.

Engineering a new class of materials that combine the advantages of biocompatibility, chemical/biological diversity, and (un)folding nanomechanics derived from the main building unit, folded proteins, place protein-based materials as the next generation materials. During my talk, I will introduce the challenges in the field, how using biological technologies assists in investigating protein-based materials, and how the folding code of a protein can be translated into engineering new "smart" responsive biomaterials.

Session 12
Polymers and Composites

Session chairs:
Roy Shenhar, Shmuel Kenig

Location: Teddy B

Compression-enhanced thermal conductivity of polymer composites

Oren Regev
Ben-Gurion University of the Negev

The miniaturization, integration and compatibilization of electronic devices dictate efficient thermal management to prevent heat accumulation, which may damage these devices in several ways. Addressing this challenge requires the development of novel polymer-based composite materials with enhanced thermal conductivity. Here, we report a compression-based (25-250 bars) approach for the preparation of polymer composites loaded with hybrid fillers, comprising graphene nanoplatelets and graphite flakes or boron nitride nanoparticles — the graphite flakes contributing significantly to the thermal conductivity of the composite and the boron nitride providing the desirable inhibition of electrical conductivity (to avoid short circuit). An optimal thermal conductivity of up to 27.5 W/mK may be obtained for epoxy polymer loaded with graphene nanoplatelets and graphite flakes, vs 0.2 W/mK for the non-modified thermoset polymer.

Ohayon-Lavi A. et al., Carbon 163 1-8 (2020).

Enhancing the mechanical properties of polymers via metal-ligand interactions

Yuval Vidavsky
Nuclear research center

Modulating metal-ligand interactions in metallopolymers allows tuning the mechanical response of metallopolymers and provides a platform for understanding the connection between the reversible nature of the crosslinks and the macroscale mechanical properties. We present nickel(II) carboxylate as a tunable, reversible crosslinking interaction in UV curable metallopolymers. Different numbers and types of neutral ligands that coordinate to the metal center are introduced as a straightforward approach to modulate the strength of the ionic interactions in the nickel carboxylate crosslinks and allow macroscale mechanical properties to be tuned. The ability of the reversible crosslinking interactions to break and reform enables the relief of the residual stress generated during the curing process, thus allowing the 3D printing of polymer structures that boast higher spatial accuracy and superior mechanical properties.

Polymer- metal oxide nanocomposites and nanostructures via vapor-phase based growth within polymers

Tamar Segal-Perets
Technion

Sequential infiltration synthesis (SIS) has emerged in the past decade as a powerful technique for growth of inorganic materials within polymers through atomic layer deposition (ALD) chemistry. In SIS, ALD precursors diffuse into the polymer, leading to nanoscale inorganic materials growth within the polymer volume. This unique approach allows for a step-by-step, highly controllable process, where polymer nanostructures (films, patterns, fivers) are directly converted to hybrid and inorganic nanostructures.

Here, I will present our recent research in the field of SIS. We shed light on the atomic growth of metal oxide clusters and particles within polymers using high-resolution transmission electron microscopy and x-ray absorption spectroscopy. We follow SIS growth from the nanoscale to the macroscale, expanding our understanding of SIS mechanism and the role of polymer chemistry and reversible polymer-precursor interactions on SIS growth. These insights are then applied to fabrication by design of homopolymer and block copolymer-templated 3D nanostructures, fibers, and membranes. We fabricate Al_2O_3-ZnO heterostructure nanorod arrays and core-shell nano-fibers, where simultaneous but spatially-controlled growth of the two metal oxides within the polymer templates is performed via control over the two precursors diffusion time. Block copolymer particles and films template porous metal oxide particles and membranes with uniporous pore size and controlled surface chemistry. These examples highlight the versatility and potential of SIS nanostructure fabrication by design capabilities.

Short Fibers Polymer Matrix Composites (PMCs) Micro-Thermo-Mechanical Material Parametric Optimization

Omri Yannay
Ansys

In the development process of new advanced materials, the effective mechanical and thermal properties can change rapidly depends on numerous variations. Starting from the initial properties assigned for each phase, to geometrical ratios and statistical distributions. This presentation will show a parametric study optimization to achieve the desired equivalent material properties and the recommended manufacturing recipe for an optimal result using Ansys solutions.

The work being done is based on short fiber composites but can easily implemented to other type of materials structures and industries such as adaptive manufacturing.

Surface functionalization of textile as a tool for fabrication of smart fabrics

Elizabeth Amir
Shenkar handesaim

This talk will describe new strategies for chemical surface modification of textile, specifically seeking processes which are modular, inexpensive, technically simple and would not damage the fabric, while providing durable functional coatings. One of the methods is based on a two-step process that includes chemical grafting of bifunctional small molecule to the surface of woven, knitted and non-woven fabrics and a subsequent attachment of functional materials via UV-mediated reactions. This approach allows preparation of textile with controlled hydrophobicity/hydrophilicity, oil-water separation ability and pH regulation for advanced applications. In addition, preparation of hybrid antibacterial, antiviral and electro-conductive fabrics via in situ polymerization of cationic conjugated polymer will be presented.

Infrared Irradiated Reversible Shape Memory Polymer Mechanisms

Ronen Verker
Nuclear research center

Remote propulsion of miniaturized mechanical devices forms a great challenge for the scientific community. Here we present a light-weight two-way shape memory polymer (2WSMP)-based motor and demonstrate the propulsion of a miniature vehicle via a unique IR irradiated 2WSMP actuator.

Most of the polymers that possess 2WSMP properties suffer from low mechanical properties and low durability to harsh environments. In this work we unveil a 2WSMP bilayer actuator based on Kapton and polyPOSS (PP) that as a bilayer possess superior 2WSMP and mechanical properties, high lifting abilities, and durability to harsh environments. Kapton is well known for its outstanding physical properties. PP, a polyhedral oligomeric silsesquioxane (POSS)-based epoxy-like thermoset, was developed uniquely for this project. Its ability to maintain mechanical properties over a range of temperatures while presenting a constant coefficient of thermal expansion is essential for its 2WSMP actuation properties.

A detailed study is given regarding the effect of the layers' thickness on the force and deflection generated by the 2WSMP actuators during heating. A theoretical model is used to predict the actuator's deflection, based on the layers' thickness. These unique actuators present outstanding force/weight ratio of 6500 and a lifting capacity 400 times of their own mass.

On the swelling of hydrogen-bond dominated polymer networks

Noy Cohen
Technion

The penetration of water molecules into polymer networks such as resilin, which is a protein-based polymer commonly found in insects, and spider silk can lead to changes in stiffness that range over several order of magnitudes and supercontraction (i.e. a shortening of up to ~60% in length). These behaviors cannot be explained by the volumetric changes associated with the pure swelling/deswelling theories that are used to describe the swelling of standard polymer networks such as rubber. Rather, these unique responses stem from the swelling-induced breaking of hydrogen cross-linking bonds that connect the chains in the network. In this talk, a microscopically motivated model for the swelling and the mechanical response of hydrogen-bond dominated biopolymer networks is presented. It is shown that the penetration of water molecules into the network leads to the breaking of non-covalent crosslinking sites. In turn, the network experiences a reduction in the effective chain-density and an increase in entropy (leading to a decrease in free energy), thus explaining the dramatic softening. Additionally, the breaking of bonds alters the micro-structure and changes the quantitative elastic behavior of the network. The proposed model is found to be in excellent agreement with several experimental findings. The merit of this work is two-fold: (1) it accounts for the number and the strength of non-covalent cross-linking bonds, thus explaining the drastic reduction in stiffness upon water uptake, and (2) it provides a method to characterize the microstructural evolution of hydrogen-bond dominated networks. Consequently, the model can be used as a microstructural design-guide to program the response of synthetic polymers.

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Collaborator: Claus D. Eisenbach, Materials Research Laboratory, University of California, Santa Barbara, CA 93106, USA

Session 13
Surfaces of Materials

Session chairs:
Ilan Goldfarb

Location: Teddy C

Tracking the microscopic pathways of molecule's accommodation on a metal surface

Igor Rahinov
The Open University

The most common mechanism of catalytic surface chemistry is that of Langmuir and Hinshelwood (LH). In the LH mechanism, reactants adsorb, thermalize with the surface and subsequently react. At the same time, molecular vibration is known to enhance the rates of gas-phase chemical reactions as the motion associated with bond stretching facilitates the reactant molecule approach to the transition state [1]. However, for reactions occurring on via LH mechanism on metal surfaces, relevant for heterogeneous catalysis reactions, the ability of vibrational excitation to promote reactivity is hampered by rapid dissipation of the vibrational energy of the reactant into electronic excitation of the metal within several picoseconds [2]. Our recent findings challenge this paradigm: we have demonstrated that excited vibrational states can survive longer than expected [3,4] – suggesting vibrational excitation might promote or modify heterogeneously catalyzed LH-chemistry on metals. In our experiments IR laser excitation was used to prepare short pulses of vibrationally excited CO(v=2) molecules that impinged and scattered from clean Au(111) surface. By quantum-state-resolved scattering studied in temporally and spatially resolved fashion we have unambiguously demonstrated that vibrationally excited molecules, prepared in the v=2 state retain significant vibrational excitation, even after residing ~ 100 ps on Au(111). Furthermore, we show that the vibrational relaxation time can serve as an internal clock to follow the microscopic pathways of adsorption and equilibration on the surface. On the basis of molecular beam experiments and theoretical modeling we reveal the intricate interplay between physisorption and chemisorption states for the prototypical CO/Au(111) system, relevant to many other heterogeneous systems.

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Bioinspired and Meta-Materials - the Nearest Future of the Materials Science and Engineering

Edward Bormashenko
Ariel University

Bioinspired materials are synthetic materials whose structure, properties or function mimic those of natural materials or living matter. Examples of bioinspired materials are lotus-like self-cleaning interfaces, materials inspired by the Gecko effect, the Salvinia effect, the shark-skin effect and the rose petal effect, light-harvesting photonic materials that mimic photosynthesis, structural composites that imitate the structure of nacre, and metal actuators inspired by the movements of jellyfish. Laboratory of the Interface Science of the Ariel University developed a broad diversity of biomimetic materials enabling water/oil separation and manufacturing of omniphobic and anti-icing interfaces. Composite materials based on the "liquid marbles" were developed and investigated. Contrastingly, metamaterials are recently developed artificial materials demonstrating properties that are not found in naturally occurring materials. The domain of metamaterials covers a broad diversity of fields in physics and engineering, including: electromagnetics, acoustics, mechanics and thermodynamics. Laboratory of the Interface Science of the Ariel University is developing metamaterials exploiting the effect of the negative mass and the effect of the negative Poisson ratio, and, in particular, polymer metamaterials based on the Tachi-Miura polyhedrons.

Capping layers for $SrVO_3$ films and their influence on the near-surface region

Shaked Caspi
Technion

Perovskite oxides with electron correlation can exhibit interesting and unusual properties which are desirable for various applications. Since the transition-metal cation in these materials often shows a number of metastable oxidation states, the composition and the electronic structure of the near-surface region (NSR) tend to differ from the bulk as a result of over-oxidation, when exposed to ambient air. For practical applications of correlated oxides, such as field effect devices, ultrathin films are required. In this case, the NSR becomes more dominant and can dominate the properties of the entire film. In an attempt to prevent this scenario, we perform in-situ deposition of an ultrathin capping layer on top of an epitaxial $SrVO_3$ film grown using oxide molecular beam epitaxy (MBE). A surface-sensitive analysis of both capped and uncapped $SrVO_3$ films using x-ray photoelectron spectroscopy (XPS) reveals the efficiency of a 4 nm amorphous titanium oxide cap in preventing the over-oxidation of the vanadium cation and the formation of Sr-rich surface phases.

Surface Pyroelectricity and Piezoelectricity of Centrosymmetric Crystals

David Ehre
Weizmann Institute of Science

Polarity, i.e., spontaneous surface charge, is usually associated with the 10, polar, out of 32 existing crystallographic classes. However, all surfaces, including those delineating centrosymmetric crystals, are inherently polar, i.e., the directions toward and outward the surface are never equivalent. This allows for a fundamental possibility for crystals, even for those belonging to the non-polar classes, to have a near surface polar layer (NSPL) arising from local symmetry reduction. Polarity gives rise to piezo- and pyroelectric effects. Piezoelectricity is the ability of dielectric materials to develop electric polarization when subjected to mechanical stress (direct effect) or change their dimensions as a result of application of an external electric stimulation (converse effect). As opposed to piezoelectricity that exist in non-centrosymmetric dielectrics, only polar materials can exhibit pyroelectricity, i. e., develop surface charge due to temperature change. Piezo- and pyroelectric materials are used in a wide range of electronic and mechanical applications. Cellular phones, watches, as harvest energy materials and medical applications for production of ultrasound waves rely on piezoelectricity, while pyroelectric materials are used for sensors and night vision devices. Ability to detect polar layers in non-polar materials is of great scientific importance since it provides a new surface characterization technique. This allows for deepening our understanding on various surface relaxations, presence of defects and dopants near the surface and provides information on various crystal growth mechanisms. Furthermore, the existence of pyroelectric and piezoelectric NSPL on non-polar substrates has numerous practical implications. Presence of surface charge during the growth of thin-films may strongly affect the growth process and therefore the physical properties of the deposited films. For example, it can dictate the polar direction of grown ferroelectric films and affect the conductivity of two-dimensional electron gas. The existence of such layers was only recently demonstrated, as the advances in pyroelectric[1-3] and piezoelectric[4] measurement techniques made them sensitive enough for the task. In this presentation, I show that pyroelectric measurement carried out with periodic temperature change protocol (modified Chynoweth) might be a primary tool to study NSPL. Two fundamentally different examples are considered. (i) NSPL in alpha-glycine crystals develops as a result of solvent incorporation, e.g., water. This layer is maybe tens or even hundreds of micrometers thick, sometimes, thick enough to allow piezoelectric measurements. (ii) NSPL in $SrTiO_3$ results from surface relaxation and it is only a few Angstroms to few nanometers thick. Nevertheless, NSPL in $SrTiO_3$ has a polarization comparable with strongly ferroelectric materials, tens of $\mu C/cm^2$.

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Stability of cubic tin sulphide nanocrystals: role of ammonium chloride surfactant headgroups

Ran Eitan Abutbul
Ben-Gurion University of the Negev

New semiconducting metastable cubic phases have been recently discovered in the tin monosulfide and monoselenide systems. Surface energy calculations and experimental studies indicate that this cubic π-phase is stabilized by specific ligand adsorption on the surface. In this work, it is shown experimentally that the synthesis carried out using mixtures of oleylamine and oleylammonium chloride (OACl) surfactants result in the cubic phase, transforming the growth from orthorhombic to cubic nanoparticles with increasing OACl concentration up to a limiting point. Complementary ab initio calculations find that adsorbed ligands lower surface energies for both the cubic and orthorhombic phases relative to the pristine surfaces. The decrease in the surface energy increases with ligand coverage. Stronger binding energies to the cubic phase suggest a higher coverage, and therefore preferential stabilization of this phase. Upon further increasing the coverage, the surface energy becomes negative, effectively destabilizing the particles according to experimental observations. Bonding analysis shows that Cl bonds to Sn and replaces missing Sn–S bonds at the surface of the cubic structure. In the competing orthorhombic layered phase, Cl also bonds to an Sn atom but at the expense of one of the Sn–S bonds of this Sn atom. This observation can explain the trends of the surface energies. This combined experimental and computational analysis sheds light on the stabilization processes of these nano-materials and indicates the path to improve synthetic routes.

The physical and cellular mechanism of nano-crystals based color change in zebrafish

Dvir Gur
Weizmann Institute of Science

Animals such as chameleons and certain species of fish exhibit remarkable colors that are produced by the constructive interference of light reflected from arrays of intracellular molecular crystals. These animals can also tune their crystal-based structural colors to regulate body temperature, create camouflage, and facilitate kin recognition and mate choice. While it is known that these changes in color are caused by changes in the angle of the crystal arrays relative to incident light, the cellular machinery that drives color change is not understood. Here, we used the zebrafish iridophore as a model system to investigate the molecular mechanism of structural color change. Using a combination of super-resolution fluorescence light microscopy, 3D focused ion beam scanning electron microscopy (FIB-SEM), pharmacological perturbations, and micro-focused X-ray diffraction, we characterized the dynamics and 3D cellular reorganization of crystal arrays within iridophores during norepinephrine (NE)-induced color change. We found that color change results from a coordinated 20° tilting of the intracellular crystals, which alters both crystal packing and the angle at which impinging light hits the crystals. Importantly, addition of the dynein inhibitor dynapyrazole completely blocked this NE-induced red shift. Using a novel guanine crystal-binding dye to image crystals in living iridophores, we showed that dynapyrazole also blocks the change in crystal dynamics seen upon NE addition. FIB-SEM and microtubule-organizing center (MTOC) mapping showed that microtubules arise from two MTOCs located near the poles of the iridophore and run parallel to, and in between, individual crystals. Based on these observations, we suggest that dynein drives crystal angle change in response to NE by binding to the limiting membrane surrounding individual crystals and walking towards microtubule minus ends. Finally, we found that intracellular cAMP regulates the color change process. Together, our results provide mechanistic insight into the cellular machinery that drives nano-crystals based color change.

Observing Electrochemical Reactions on Suspended Graphene: An Operando Kelvin Probe Force Microscopy Approach

Eren Baran
Weizmann Institute of Science

The ability to probe chemical and physical processes occurring in solution at small scales is developing rapidly. Whereas recent advances in 3D SPM provide molecular-structuring information, and scanning ion conductance microscopy can provide electrochemical information at tens of nm resolution, a greater suite of established techniques is available for measurements made in air or vacuum conditions. Therefore, a second approach is to enclose a solution system by a very thin upper membrane which is transparent to radiation and/or electrons, enabling high resolution surface measurements of processes occurring at the interfacial liquid region. Graphene is an excellent choice of such membrane, being very thin yet mechanically robust. This concept has been applied recently in several studies. Nonetheless, interpretation of such measurements must account for graphene doping, width of double layer in liquid, influence of the graphene electromechanical response, and artifacts due to graphene contamination during preparation of the cell. In this work we apply scanning kelvin probe microscopy to study miniature cells with 500 nm diameter capped by graphene. The contact potential difference (CPD) was measured for systems at 2 different pH values (9 and 10, i.e., 10^-3 and 10^-4 M NaOH), as a function of voltage applied between the single layer graphene membrane and a Pt counter electrode located remotely in the solution. We found that the changes in CPD can be explained by the electric double layer thickness and changes in the graphene doping due to the gating of the liquid cell. At higher voltages, CPD and topographical changes provided evidence of reversible graphene functionalization and electro-wetting, which will also be discussed. The graphene membrane is robust to scanning and allows direct measurement of phenomena occurring near the lower liquid/graphene interface. The insights gained here provide a sound basis for further studies on more complex systems.

Session 14
Additive Manufacturing (General)

Session chairs:
Noam Eliaz

Location: Oren 2

The perks of using fused filament fabrication in polymer matrix composites processing

Noa Lachamn
Tel Aviv University

Fused filament fabrication (FFF), also known as the patented Fused Deposition Modeling (FDM), is one of the oldest and most widely used additive manufacturing (AM) methods. Its versatility in thermoplastics processing has made it useful in a variety of fields, from the highly complex military and medicinal, to the most trivial house-hold consuming. This versatility is further increased by the ability to introduce thermoplastic-matrix nanocomposites, gaining properties as conductivity, mechanical strength, and more. However, the addition of nanomaterials to the thermoplastic matrix alters its processing-related properties, including stiffness, heat transfer, and melt viscosity, to name a few. In the other direction, the printing process affects the dispersion and orientation of the nanoparticles within the resultant product, thus influencing the final properties. To fully benefit from FFF versatility, all of these effects need to be accounted for in the design and optimization of the process. This talk will present a few concepts and applications of the FFF process regarding composites, highlighting the similarity between the result of filaments-printing method and that of continuous-fibers composites. We further show that FFF process improves the dispersion of nanoparticles, thus increasing homogeneity, but also induces orientation in 1D and 2D nanoparticles, increasing directionality and thus anisotropy in the printed composite. We demonstrate the use of these phenomena to control post print conductivity of conductive nanocomposites, up to and including induced electrical anisotropy in an isotropic pre-printed material. These results demonstrate both the versatility of AM, and FFF specifically, in fine-tuning the properties of polymer composites, as well as the unique problems of such techniques. The applications of such smart-materials tailoring capabilities can range from mechanical bio-mimicry, to corrosion resistance integrated electrical devices.

Towards Smart Flexible Batteries

Diana Golodnitsky
Tel Aviv University

The focus on shifting towards miniaturized products coupled with the booming demand for consumer electronics are some of the key-driving factors behind the flexible-battery market. In the development of innovative power sources, freeing from design limitation along with the synthesis of reliable electrochemical materials with well-tuned features, is considered to be the most important technical prerequisite. The novel approach for the fabrication of flexible free form-factor batteries, which utilizes printing techniques will be presented. These technologies are still at an early stage, and most currently-printed batteries exploit printed electrodes sandwiching self-standing commercial polymer membranes, produced by conventional extrusion or papermaking techniques, followed by soaking in non-aqueous liquid electrolytes. We suggest a novel flexible-battery design and report the initial results of development and characterization of novel 3D printed all-solid-state electrolytes prepared by fused-filament fabrication (FFF). The electrolytes are composed of LiTFSI, polyethylene oxide (PEO), which is a known lithium-ion conductor, and polylactide (PLA) for enhanced mechanical properties and high-temperature durability. The flexible all-solid LiTFSI-based electrolyte exhibited bulk ionic conductivity of 3×10^{-5} S/cm at 90oC and 156 ohm/cm2 resistance of the solid electrolyte interphase (SEI). The feasibility of a fully printed solid battery will be demonstrated. These results pave the way for free-form-factor flexible geometries.

The Gutenberg-Write future with the 3D composite printing into aerospace structures

Rotem Almany Magal
Elbit

3D printers are no longer a new technology. Additive Manufacturing (AM), synonymous with 3D printing, creates objects layer by layer, and has many advantages for expending design freedom, reducing time to market, creating complex structures in a one-shot process and improving industrial sustainability. 3D printing technology offers a competitive advantage for low-volume production and custom-made parts, to develop tooling, functional prototypes, medical devices and industrial parts. However, it still faces major hurdles to manufacture structures with high strength and rigidity. This is part of the reason 3D printing still not widely used in aerospace structures, and is not competitive with other automated manufacturing techniques such as AFT. This talk will present an innovative and revolutionary research and development work made by the material engineering group in the UAV division of Elbit Systems, using FDM (Filament Deposition Modeling) printing process. FDM is a layered thermal plastic extrusion process that is based on three-dimensional solid CAD model definitions. The process uses a combination of build material and support material to fabricate very complex geometries in a low time for value ratio. The FDM machine consists of the following parts: a build platform; filament feed devices; heated extrusion nozzles; and a nozzle control apparatus. The FDM process feeds filaments of build material and support material to heated nozzles. These nozzles are used to lay down molten filaments of build and support materials in the desired cross sectional geometries. Once the process is completed, the part can be taken out and any support structures can be removed. FDM produces parts that have anisotropic properties. Design can be optimized to take full advantage of these properties. The production process provides stable, durable, and accurate parts in a short period of time. It allows the parts to be used in harsh environments such as in aviation. The work focuses on developing a printing technique of lightweight parts with repeatable strength while breaking through the many challenges of this immature technology. In order to develop FDM designed parts for aviation uses, Elbit performs ground tests of standard mechanical test coupons, and a few functional tests on parts. In order to compere FDM designed parts to composite designed parts and for material qualification propose. Nowadays Elbit uses FDM printed parts assembled on platforms for land and air applications, and working forward to improve and qualify FDM process and products.

Long-term stabilized amorphous calcium carbonate (ACC) as an ink for bio-inspired 3D printing

Hadar Shaked
Technion

Biominerals formed by organisms often possess complex morphologies, superior mechanical properties and unique textures despite their single-crystalline nature and their formation under ambient conditions. A good example for such biomineral, formed by the course of biomineralization, is calcium carbonate ($CaCO_3$). $CaCO_3$ is a biomineral commonly used by various organisms to form skeletons, protective shells, teeth, clamps, and optical mediums. The enhanced characteristics of biogenic $CaCO_3$ are achieved due to crystallization through an amorphous, unstable precursor, amorphous calcium carbonate (ACC).

In this work, inspired by organisms' amorphous-to-crystalline route for enhanced $CaCO_3$, we used robocasting, a common additive manufacturing technique, to 3D print long-term Mg-stabilized ACC under ambient conditions with high solid-loadings and on-demand crystallization. We tested three non-hydrated organic binders; glycerol (GLY), ethylene glycol (EG) and triethylene glycol (TEG), and examined their affect on the stabilization and crystallization route of ACC. We found that GLY, a highly hygroscopic compound, promotes slow crystallization endorsed by heat, allowing the growth of calcite crystals while using ACC as a reservoir. GLY has also exhibited larger grain size and higher Mg content in comparison to EG and TEG. Both EG and TEG exhibited long-term stabilization of ACC with minor crystallization in un-favorable directions of calcite and aragonite. Moreover, EG and TEG demonstrated the ability to perform on-demand crystallization by exposure to humid conditions. We believe that utilizing this bio-inspired method may pave the way for a new bio-inspired route to low-temperature 3D printing of ceramic materials for a multitude of applications.

Additive Manufacturing of 3D Wooden Structures

Doron Kam
The Hebrew University of Jerusalem

The common way to process wood is by a top-down approach, based on cutting down trees to be used for the fabrication of wooden objects. This approach led to enormous investment in utilizing side streams to reuse and to create sustainable wood-based products. We present a bottom-up that builds up wood objects through two 3D printing processes, extrusion, and inkjet. Making a 3D printed object which is composed mainly of wooden material, requires the use of suitable binders (resins) that eventually result in a composite material with the desired shape. Among the currently known resins in the wood industry, such as in wood composite panels (not for 3D printing), urea-formaldehyde (UF), and phenol-formaldehyde (PF) are the most widely used. However, the emission of harmful formaldehyde during the production and utilization of wood composite has been a severe concern in recent years. An alternative synthetic resin aiming to avoid the use of formaldehyde is methylene diphenyl diisocyanate (MDI). Nevertheless, MDI is an allergen and sensitizer.

Our approach uses wood waste microparticles (wood flour), and plant-extracted natural binders cellulose nanocrystals, and Xyloglucan without the need for any additional synthetic resins, which results in 3D printed wooden objects. Depending on the printing technology, a wide range of material properties is obtained, from strong dense objects to light cellular structures. Results show that indeed each technique with its pros and cons mimic wood while gaining a wide range of wood properties and beyond. Furthermore, by proper design of the printing process parameters, we can control wood shrinkage distortion beyond natural wood.

Particle-Free inks for 3D printing Dense Ceramic Structures by DLP

Tamar Rosental

The Hebrew University of Jerusalem

Particle-free ceramic compositions for stereolithography-based printing technologies present a promising alternative to the commonly used ceramic slurries. So far, such compositions were mainly based on pre-ceramic polymers which limit their applications to silicon-containing materials. However, particle-free compositions for fabricating other ceramic materials, in particular dense polycrystalline ones, is very little explored.

We present a new general fabrication approach which is based on all-solution compositions, by combining sol-gel chemistry with photopolymerization, for obtaining dense 3D ceramic structures, by Digital Light Processing (DLP). The printing composition is obtained by simple dissolution of electrolytes, alkoxides and polymerizable acrylates. The process is demonstrated for the fabrication of barium titanate. The hybrid ink presents excellent UV-curing behaviour, as well as high compositional flexibility. After proper aging, debinding and sintering, the printed ceramic objects reach densities close to the theoretical value.

Session 15
Computational and Theory

Session chairs:
Leeor Kronik, Maytal Caspary Toroker

Location: Oren 3

Performance of modified MP2 methods for solids

Tamar Goldzak Mizrachi
Bar Ilan University

In this work, we investigate the performance of modified second order Møller-Plesset (MP2) perturbation theory for the prediction of structural and energetic properties of three dimensions solids. Our implementation, which uses Gaussian type orbitals, Brillouin zone sampling, and density fitting, enables us to reliably converge our results to the thermodynamic limit. Specifically, we compare three versions of modified MP2 theory: spin-component scaled (SCSMP2), scaled opposite spin (SOS-MP2), and kappa-regularized MP2. These methods, with empirically chosen parameters, have shown improved performance over conventional MP2 for molecules. The SOS-MP2 can be efficiently implemented with density fitting and Laplace transformation, leading to an attractive low-scaling approach for solids with complex unit cells. Regularized MP2, which removes potential divergences in the denominator of the MP2 energy expression, is attractive for future applications to metals. With these three methods, we calculate the lattice constant, bulk modulus, and cohesive energy of various solids. By comparing to experiment, we determine the optimal scaling and regularization parameters, which are compared to their values for molecules.

Approaches for controlling the mechanism of molecular catalysts towards ORR

Ilya Grinberg
Bar Ilan University

In the search for replacement of the platinum-based catalysts for fuel cells, MN4 molecular catalysts based on abundant transition metals play a crucial role in modeling and investigation of the influence of the environment near the active site in platinum-group metal-free (PGM-free) oxygen reduction reaction (ORR) catalysts. We followed various approaches to understand how the ORR activity of molecular catalysts can be controlled by the active site structure through 1) increasing coordination number of the metal center with excess ligand 2) Hangman type substituents which interact strongly with the intermediates of the ORR 3) by tuning the pH of the active site environment. Experiments revealed a switch between two different ORR mechanisms and a change from 2e- to 4e- pathway in the pH range of 3.5-6 for the three corroles. This phenomenon was explained by density functional theory (DFT) calculations to be related to the protonation of the nitrogen atoms and carboxylic acid groups on the corroles indicated by the pKa values of the protonation sites in the vicinity of the ORR active sites. Control of the electron-withdrawing nature of these groups characterized by the pKa values could switch the ORR from the H+ to e- rate-determining step mechanisms.

Materials Modelling of π-Phase Monochalcogenide semiconductors

Guy Makov
Ben-Gurion University of the Negev

π-phase monochalcogenides are a family of cubic semiconductors, recently discovered in SnS and SnSe. Remarkably, they consist of a low-symmetry, non-centrosymmetric 64 atom simple cubic unit-cell and present unusual physical properties, such as an infrared bandgap. Moreover, they have been obtained only in nanometric form, which raises questions concerning their thermodynamic stability. We unravel the nature and properties of this family of materials through ab-initio materials modeling. This talk will focus on our results and their interplay with experimental studies.

We explored the materials design space for this phase across groups IV–VI. The structure and properties, including phonon spectra, mechanical and thermodynamic stability, and electronic structure, were studied using density functional theory. In particular, we examined the driving forces for the low-symmetry structure, the origin of the infrared bandgap, and surface ligands' role in stabilizing this phase.

The structure of the new π-phase is found to be a distorted rocksalt structure, and the bonding between the 64 atoms of the unit cell was elucidated. An analogy to Peierls distortion of half-filled bands can be made by analyzing the forces driving the distortion and increasing the bandgap. The electronic bandgaps were found to range from 1.0–1.4 eV, which may be attractive for a variety of photovoltaic and photo-sensing applications.

The π-phase is dynamically stable in the sulfides and selenides of tin and germanium, but unstable in their telluride compounds. The phonon spectra were calculated in SnS, SnSe, GeS, and GeSe. All these systems exhibit phonon band gaps in the infrared with widths of 0.7–2 THz. Raman measurements support the existence and magnitude of the calculated phonon band gaps in π-SnS and π-SnSe.

The phonon band spectra were analyzed and the bandgaps are found to originate from the acoustic and optical modes of the symmetric parent rocksalt structure with different atomic dynamics above and below the bandgap.

The energy differences between the π-phase and the bulk orthorhombic phases are tiny, suggesting that the π-phase could be stabilized in ambient conditions. Surface energy calculations and experimental studies indicate that the π-phase is stabilized by ligand adsorption on the surface. Ab-initio calculations find that ligand adsorption lowers surface energies with increasing coverage for the cubic and stable orthorhombic phases. Stronger binding energies to the cubic phase suggest a higher coverage and, therefore, preferential stabilization. Upon further increasing the coverage, the surface energy becomes negative, effectively destabilizing the particles in agreement with experimental observations.

The Effect of Cluster Size on the Intra-Cluster Ionic Polymerization Process

Tamar Stein
Hebrew University

Polycyclic aromatic hydrocarbons (PAHs) are ubiquitous in the interstellar medium (ISM)1. The mechanism for their formation in the ISM's low-temperature environment is, as of yet, nonetheless a mystery. Understanding the growth mechanism of complex molecules such as PAHs and nitrogen-based PAHs (PAHN) is a long-standing challenge that has been drawing much attention for several decades. Formation of the building blocks of PAHs and PAHNs upon ionization of van der Waals clusters will be presented. Results on small (up to 6 acetylene/HCN units) van der Waals clusters indicate that, since the clusters possess a large amount of extra energy after ionization, rich chemistry can occur2,3. For example, after ionization, structures on the $C_6H_6^+$ potential energy surface (PES) are accessible without barriers. Moreover, the formation of the basic building block of PAHs, namely the benzene cation, has been demonstrated using ab-initio molecular dynamics. The presence of spectator molecules has been proven to change the PES and partake a catalytic role in forming complex molecules2,3. The results lead to the question of whether clusters larger than those studied thus far promote aggregation beyond three acetylene units and whether larger clusters can result in higher $C_6H_6^+$ production. In this study, we report results from AIMD simulations modelling the ionization of 10 and 20 acetylene clusters. The simulations show aggregation of up to four acetylene units producing bonded $C_8H_8^+$. Interestingly, $C_8H_8^+$ bicyclic species were identified, setting a precedent for their astrochemical identification. Comparable reactivity rates were shown with 10 and 20 acetylene clusters.4 1. Ehrenfreund, P.; Sephton, M. A., Farad. Discuss. 2006, 133 (0), 277-288. 2. Stein, T.; Bandyopadhyay, B.; Troy, T. P.; Fang, Y.; Kostko, O.; Ahmed, M.; Head-Gordon, M., Proc Natl Acad Sci USA 2017, 114 (21), E4125-E4133. 3. Stein* T., Bera* P., Lee T., Head-Gordon M., "Molecular Growth upon Ionization of Van der Waals Clusters Containing HCCH and HCN is a pathway to prebiotic molecules." PCCP, 22 (36), 20337, (2020). 4. Molina E. R. and Stein T. "The effect of cluster size on the intra-cluster ionic polymerization process", Molecules 26 (16), 4782, (2021).

Flexoelectricity and Ferroelectric Domain Walls: Landau Theory from Density-Functional Theory Calculations

Oswaldo Dieguez
Tel Aviv University

Domain walls between two ferroelectric regions of a perovskite oxide with antiparallel polarization vectors are, in many of these materials, atomically thin. Despite of this, simple continuum Landau models where a thermodynamic potential is expanded as a function of strain, polarization, and the gradient of polarization give good predictions of wall energy, wall thickness, and atomic displacements. In the work presented in this talk, we developed Landau models for six different perovskites and we computed the coefficients of those models, some of which are related to the flexoelectric properties of the oxide. In the process, we addressed the role of some arbitrary choices that one faces regarding the definition of local strain, polar distortion pattern, and flexoelectric tensor, which have an impact in the predictions of the model---and we describe criteria that ensure physically meaningful results. We finally show that the solutions produced in this way agree very well with our full density-functional theory calculations.

computational studies of structure, composition, and electrochemical behavior of Li-ion battery components

Dan Thomas Major
Bar Ilan University

Considerable efforts have been invested in recent decades to further the improvement of lithium-ion battery components – electrodes, solutions, and separators. In this presentation we will focus on recent computational work in our group on cathodes, anodes, and electrolyte solutions. We will show how computations are an essential part of the analytical toolbox, allowing deeper understanding of physical phenomenon related to battery materials. First, we will discuss studies on layered Ni-rich cathode materials (i.e., Li[Ni-Co-Mn]O_2, NCM, family) for lithium-ion batteries.[1] Specifically, we will discuss lattice doping and coating in NCM materials, which is one of the most promising approaches to improve electrochemical properties, cycle life, and thermal behavior. Second, we will study cation and anion intercalation phenomenon in MXene materials.[2] Finally, we will show some recent simulations on Water-in-Salt electrolyte solutions

Session 16

Soft matter and Bio materials II

Session chairs:

Jacob Klein, Alejandro Sosnik

Location: Teddy A

Self-assembly phenomenon in biomaterials science

Ulyana Shimanovich
Weizmann Institute of Science

Self-assembly is the autonomous organization of components into patterns or structures without human intervention. A number of different assemblies can be formed by proteins. A particularly interesting example of protein self-assembly is a formation of highly ordered, nearly one-dimensional fibrilar structures. This high-level, long-range ordering is relatively independent of the molecular identity of the protein monomers. Interestingly, in nature, such structures can perform either beneficial roles or appear as aberrant protein aggregation, which is in a latter case results in the development of neurological disorders. The main objective of our research is to understand the evolution of protein complexes in the context of both biological function and malfunction as well as to draw the links between structure and properties of self-assembling materials based on natural polypeptides.

A multiscale study of bacterial biofilms. From isolated components to multicellular organisms

Liraz Chai
The Hebrew University of Jerusalem

Biofilms are multicellular microbial communities that encase themselves in a secreted network of biopolymers and attach to surfaces and interfaces. From a soft matter perspective, biofilms are regarded as colloidal hydrogels, with the cells playing the role of colloids and the extracellular matrix (ECM) compared with a cross-linked hydrogel. However, from a biological perspective, biofilms are heterogeneous communities that organize in space and time into functionally distinct subgroups, in a process resembling differentiation in higher organisms. Biofilm heterogeneity has been demonstrated at the cellular level, but the molecular level has been neglected. In this talk we focus on the properties of water, ECM, and metal ions in biofilms. Using simultaneous X-ray diffraction/fluorescence (XRD/XRF), we portrayed the dominant structural features in Bacillus subtilis biofilms and mapped them in space and time. Particularly, we revealed molecular-level structural hierarchy in the biofilms, that followed biofilm macroscopic morphology. Mapping the XRD and XRF signatures of intact biofilms in space and time allowed us to suggest an inclusive view of biofilm development, linking the ECM and the spores via the transport of water and metal ions.

A study of the SARS CoV-2 Spike protein adsorption on to various surfaces

Daniela Dobrynin
Technion

The Coronavirus disease (COVID19) was firstly reported in Wuhan, China, in December 2019, and has already caused more than 5 million deaths worldwide. Aerosol transmission is a major possible route for spreading the virus and causing human infection, however, it has been shown that it is also possible through contact with solid surfaces. Fomite transmission can occur because the virus survives on various surfaces such as plastics, metals and glass, from minutes up to days. Moreover, a dependence on the environment, such as temperature and exposure to light has been shown.

The mechanisms of transmission is through Spike glycoprotein that localize on the viruses' outer membrane, and is responsible for viral attachment and entering into human host cells, via angiotensin-converting enzyme 2 (ACE2) receptors. The Spike protein is composed of 3 subunits, which two of them, S1 and S2, have the main role in the infection process. A further understanding of the interaction of Spike S1 and S2 subunits with different chemical modified surfaces can be essential for preventing further infection through contact with surfaces. In this study, we used a Quartz Crystal Microbalance (QCM) device, which is based on a thin quartz disk , to study the adsorption mechanism of Spike protein on surfaces . QCM measures the difference in resonant frequency of the quartz, that changes due to deposited mass on the crystal sensor. We used several self-assembly monolayers (SAMs) to change the chemistry of the gold coated sensors, and used QCM to evaluate the attachment kinetics of Spike S1, Spike S2 and ovalbumin (as a control) proteins on these surfaces. The mass was calculated with 2 models: Sauerbrey for rigid thin films, and Voigt for soft films. We found that each protein adheres stronger to different SAMs, and this binding depends mainly on the hydrophobicity or the hydrophilicity of the SAM. In addition, we studied the attachment of Spike S1 protein to 11-mercapto undecanoic acid SAM (carboxylic acid end group) in different pH buffers. We found that an acidic environment decreases the binding to this SAM, and on the other hand, after the attachment, it encourages the disengagement of the attached mass from the surface. This basic understanding might have a great value for developing antiviral surfaces to better control this pandemic and other viral outbakes that might develop in the future.

Dynamic Surface-Layer Coiled Coil Proteins Processing Analog-to-Digital Information

Guillaume Le Saux
Ben- Gurion Yniversity of the Negev

Surface layer proteins perform multiple functions in prokaryotic cells, including cellular defense, cell-shape maintenance, and regulation of import and export of materials. However, mimicking the complex and dynamic behavior of such two dimensional biochemical systems is challenging, and hence research has so far focused mainly on the design and manipulation of the structure and functionality of protein assemblies in solution. Motivated by the new opportunities that dynamic surface layer proteins may offer for modern technology, we herein demonstrate that immobilization of coiled coil proteins onto an inorganic surface facilitates complex behavior, manifested by reversible chemical reactions that can be rapidly monitored as digital surface readouts. Using multiple chemical triggers as inputs and several surface characteristics as outputs, we are able to realize reversible switching and logic gate operations that are read in parallel. Moreover, using the same coiled coil protein monolayers for derivatization of nanopores drilled into silicon-nitride membranes facilitates control over ion and mass transport through the pores, thereby expanding the applicability of the dynamic coiled coil system for contemporary stochastic biosensing applications.

The influence of flexible mechanical constraints on the swelling of gels

Michal Levin
Technion

The submersion of a lightly cross-linked polymer network in an appropriate solvent leads to swelling and the formation of a gel. The equilibrium swollen configuration can be controlled by prescribing appropriate mechanical constraints. In this talk, we present an experimental method to investigate the influence of flexible (non-rigid) mechanical constraints on the equilibrium configuration of swollen gels. As a model material, we use commercially available hydrophilic water beads. The design of the mechanical constraints is based on 3D printing technologies. We define three experimental protocols: first, we characterize the free swelling (i.e. swelling in the absence of constraints) of the water bead. The second experiment investigates the uniaxial swelling of a bead that is transversely constrained. Here, the beads swell in 3D printed boxes with two open ends and various sizes. Lastly, we 3D print boxes of different sizes with four rigid faces and two soft faces. A water bead is then placed in a box and swells until equilibrium is reached, resulting in the bending of the soft faces. To understand the influence of constraints with various mechanical properties on the swelling, we use soft faces with five different stiffnesses. Our experiments show that larger stretches are obtained in boxes with softer walls. To estimate the tractions that the gels exert, we measure the deflections of the soft faces and employ the theory of plates, which provides explicit relations between the deflection of the soft faces and the applied tractions. A well-established model is used to help interpret the non-linear trends observed in our experiments. The main findings of this work are: (1) the equilibrium swollen configuration can be tuned by the application of appropriate (rigid or flexible) mechanical constraints and (2) the magnitude of the tractions that gels are capable of exerting decreases as the gel nears its freely swollen state. The insights from this work can be used to enhance the performance of swelling-based systems in various field such as actuators, sensors, and soft robotics.

Designing New Bioinspired 3D Nanostructure for Biological Applications

Lihi Adler-Abramovich
Tel Aviv University

The emerging demand for tissue engineering scaffolds capable of inducing bone regeneration using minimally invasive techniques prompts the need for the development of new biomaterials. One promising route is molecular self-assembly, a key direction in current nanotechnology and material science. In this approach, the physical properties of the formed supramolecular assemblies are directed by the inherent characteristics of the specific building blocks. Molecular co-assembly at varied stoichiometry substantially increases the structural and functional diversity of the formed assemblies, thus allowing tuning of their architecture and physical properties.

Here, in line with polymer chemistry paradigms, we applied a co-assembly approach using hydrogel-forming peptides, resulting in a synergistic modulation of their mechanical properties to form extraordinarily rigid hydrogels which supported osteogenic differentiation based on cells-mechanosensing. Furthermore, we designed a multi-component scaffold composed of polysaccharides, short self-assembling peptide and bone minerals. We demonstrate the formation of a rigid, yet injectable and printable hydrogel without the addition of cross-linking agents. The formed composite hydrogel displays a nanofibrous structure, which mimics the extracellular matrix and exhibits thixotropic behaviour and a high storage modulus. This composite scaffold can induce osteogenic differentiation and facilitate calcium mineralization. This work provides a conceptual framework for the utilization of co-assembly strategies to push the limits of nanostructure physical properties obtained through self-assembly for the design of new biomaterials for tissue engineering and personalized medicine applications.

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Cell Mechanomics for Precision Nanomedicine in Cancer

Ofra Benny
The Hebrew University of Jerusalem

The intelligent design of nanoparticles for obtaining maximal cell specificity is a central challenge in precision nanomedicine. While molecular targeting approaches are widely used for designing active targeted drug delivery systems, the effect of biomechanical properties on tissue specificity and targeting is less studied. We show that cell deformability as well as nanoparticle stiffness may have a major role in the reciprocal interaction that affects particle uptake and cell specificity. In many cancers, it was found that cancer cells are more deformable compared to normal cells in their surroundings and that this deformability is associated with an elevated degree of cell malignancy. In our study, using experimental and theoretical approaches we demonstrated that the unique biomechanics of cancer cells can be utilized for cell targeting with nano and microparticles. A wide range of biological assays including and 3D printed organ on-chip technologies were used to provide mechanistic insights related to the Triangular Correlation between cancer cell aggressiveness, biomechanics and particle uptake. Furthermore, novel multifunctional nanomaterials designed to remotely actuate drug delivery systems will be presented.

Session 17

Magnetic and Electronic Materials

Session chairs:

Rakefet Ofek Almog, Alexander Strikovsky

Location: Teddy B

TUNING RESISTIVE SWITCHING IN ENGINEERED MOTT INSULATORS

Yoav Kalcheim
Technion

In Mott insulators electrical currents can change resistance by orders-of-magnitude due to an insulator-metal phase transition. The volatility of switching in Mott insulators can be tuned, enabling both memory devices and neuron-like functionalities. In this talk I will present our recent advances in defect- and strain- engineering of Mott insulators, with the aim of developing highly energy-efficient resistive switching devices and novel functionalities.

I will first discuss how defects induced by ion irradiation in V_2O_3 and VO_2 devices can dramatically reduce the electric field and energy required for switching. Our direct and indirect methods of measuring the temperature of devices during switching show that this ultra-low energy consumption is due to the induction of non-thermal insulator-metal transitions. I will then discuss strain engineering in V_2O_3 which allows to tune the trajectory of the phase transition, allowing access to hitherto inaccessible regions of the phase diagram. These unusual states of matter hold great promise for resistive switching applications, both in terms of energy efficiency and functionality.

Controlling the Helicity of Aromatic Materials

Ori Gidron
The Hebrew University of Jerusalem

The properties of conjugated oligomers and polymers are commonly controlled by side group engineering, main chain engineering, or conformational engineering. The last approach typically involves controlling the dihedral angle around the interring single bonds in the backbone to prevent loss of conjugation. Here we demonstrate a new approach to conformational engineering that involves controlling the twist of the aromatic units comprising the backbone by using a tether of varying lengths. We demonstrate this approach by introducing an inherently twisted building unit comprised of helically locked anthracenes. We apply using this unit, we introduce a series of nine helical oligomers, from the monomer to the trimer, characterized by different tunable twist angles, with the aim of studying the combined effects of increasing backbone twist and length on π-conjugated systems.

We find that the properties of conjugated systems may be determined by the additive, antagonistic, or independent effects of backbone length and twist angle. Properties such as absorption/emission maxima arise from the additive effects of backbone length and twist, the extinction coefficient is an outcome of their antagonistic effects, whereas quantum efficiency is primarily determined by the backbone twist angle. Finally, we observe chiral amplification which arises from the formation of secondary helical structures.

Nanostructure effects in piezoelectric semiconductors and related magneto-semiconductor composites

Yonatan Calahorra
Technion

Adding functionality to semiconductors opens up possibilities for new semiconductor device applications. For example, piezoelectric semiconductors allow introducing electromechanical functionality to devices based thereof. In addition, realizing ferromagnetic/semiconductor material composites is a route for magnetic/semiconducting property coupling, parallel to dilute magnetic semiconductors. Coupling ferromagnetic materials to piezoelectric semiconductors therefore opens-up a magneto-mechano-semiconducting property coupling triangle. Such coupling effects are attractive for spintronics, spinoptics, sensing and more. GaN and other III-Vs are piezoelectric semiconductors. Their dominant role in optics and electronics inspires added functionality research; their mature processing further suggests the possibility of a monolithic, integrated, multifunctional semiconductor technology.

I will start this talk by examining the manifestation of piezoelectricity in piezoelectric-semiconductor based devices. In particular, I will discuss the piezotronic effect (change of a semiconductor device barrier height with mechanical input) and its distinction from its origin, the piezoelectric effect. I will then focus on the piezotronic effect in a GaAs nanowire-ensemble Schottky diode, operated as a pressure sensor. In this case nanoscale effects resulted in the highest reported piezotronic sensitivity (measured in meV/MPa). This result stands out in comparison to ZnO devices – a material considerably more piezoelectric than GaAs. Next, I will discuss the effect of nanoscale porosity on the piezoelectricity of GaN. Piezoresponse force microscopy measurements revealed that 40% porosity in volume resulted in about 3-fold increase in the axial piezoelectric coefficient (d_{33}). Corresponding finite-element simulations corroborated this finding. Interestingly, further investigation of the simulation revealed that while the intrinsic electromechanical coupling efficiency did not change due to porosity, the stress-based conversion figure-of-merit increased 10-fold, making this material attractive for applications such as force sensing. This is in contrast to ceramic piezoelectric materials, which suffer from polarization hindering effects related to porosity, compensating possible benefits.

Finally, the piezoelectric property engineering inspired further work on the ability to couple porous GaN to magnetic materials. I will present the most recent results studying the effect of porosity on the deposition and magnetization of nickel in the fabrication of nickel/porous-GaN composites. Overall, these results demonstrate the role of nanostructures in introducing and improving new functional properties in semiconductors.

Non-classical electrostriction: current understanding and potential applications

Igor Lubomirsky
Weizmann Institute of Science

We have recently demonstrated anomalously large electrostriction, a nonlinear induction of strain by an electric field, in three well-studied ionic conductors: aliovalent-doped ceria, (Nb, Y)-stabilized cubic bismuth oxide and acceptor-doped hydrated barium zirconate. At room temperature, all three materials exhibit a strain electrostriction coefficient (M11) exceeding 10-17 m2/V2 and can generate stress of tens of MPa without apparent signs of saturation. According to the theory of classical electrostriction, presented two decades ago by Prof. R. Newnham (Penn State), the electrostriction polarization coefficient (Q) scales with the ratio of elastic compliance to dielectric constant. This theory successfully describes most classes of materials from polymers, generating large strain and small stress, to relaxor ferroelectrics that generate small strain and large stress. However, the three ionic conductors mentioned above have a large elastic modulus (> 80 GPa) and moderately low dielectric constant (<100), which places their Q coefficients at least two orders of magnitude above the values predicted by the classical theory. Of these three materials, aliovalent-doped ceria is the most studied. For 10mol% Sm- or Gd-doped ceria, the measured longitudinal electrostriction strain coefficient, |M|, reaches 〖10〗^(-16) m^2/V^2; however, relaxation to < 〖10〗^(-18) m^2/V^2 is observed at frequencies > 1 Hz , well below the technologically important frequency range 100Hz-100 kHz. The introduction of aliovalent lanthanide dopants with smaller radii than that of Gd, such as Lu or Yb, succeeds in increasing |M| at 100Hz to » 〖10〗^(-17) m^2/V^2. Nevertheless, aliovalent dopants with radii smaller than that of Lu do not continue the trend.

The influence of dopants, oxygen vacancies, and protons on electrostrictive properties of proton-conducting acceptor-doped BaZr1-xXxO3-x/2+δH2δ ceramics with X= Ga, Sc, In, Y and Eu, and 0.05 £ x £ 0.2. The Young's and the shear moduli decrease by up to ~20% due to the presence of dopants and oxygen vacancies that cause local lattice distortions. An unexpectedly large electrostriction coefficient (M33 ~10-15 m2/V2) was detected for all dopants indicating non-classical electrostriction effect. The largest electromechanical response (M33 and electrostrictive strain saturation) and Young`s modulus was found for the dopant with the smallest size mismatch with the host (Sc). This suggests that lattice distortions, responsible for the change in Young`s modulus, are responsible for the non-classical electrostrictive response as well. M33 of the hydrated ceramics exhibits a Debye-type relaxation with the relaxation frequency exponentially increasing with the ionic radius.

The current model for non-classical electrostriction poses that it emerges due to field-induced rearrangement of highly polarizable elastic dipoles, induced by point defects: oxygen vacancies or proton interstitials. In this model, elastic and dielectric properties are largely defined by the host, while the electrostrictive strain is defined by the strength of the elastic dipoles. Our results imply that by systematically adjusting the composition, the potential exists for development of a new class of technologically useful electrostrictors.

Characterization of ZnO Nanostructures Decorated with Noble Metal Nano Particles

Rakefet Ofek Almog
Azrieli College of Engineering

ZnO nanowalls (NWLs) is a non-toxic, high surface-to-volume ratio, wide bandgap semiconducting nanostructure which has already showed potential applications in biosensing applications.
The nanowalls can be deposited on both rigid and flexible substrates at low temperature using rather simple and low-cost processes. Recently, it was discovered that decorating the metal oxide nanostructures with noble metal nanoparticles (NP) opens the doors to fabricating biosensors to detect volatile organic compounds. The aim our work is to improve the knowledge and understanding of fabricating ZnO nanowalls decorated with metal nanoparticles.

ZnO nanowalls was deposited both on rigid (Silicon/ SiO_2) substrate and on flexible (Polyimide) substrates. We examined the formation process of ZnO nanowalls on Polyimide substrate and studied the new obtained structure at the nanoscale, at different conditions such as growth temperature, concentration and time were used. The morphology of the ZnO nanowalls obtained under each of these conditions was studied using High Resolution Scanning Electron Microscopy and RBS (Rutherford backscattering spectrometry). The crystal structure of the ZnO nanowalls at different growth temperatures was studied by X-ray diffraction. Next, NP decoration using methods such as electroless deposition of gold and platinum was conducted. The ZnO nanowalls surface has to be activated in order to deposit Metal NP, and different schemes of surface functionalization in order to achieve the best NP deposition, were tested. A study of the nucleation and growth of the ZnO nanowalls, and of the NP decoration at different schemes of surface functionalization, was conducted.
The first attempts for NP deposition achieved NP clusters with irregular morphology, however at well-kept conditions we succeeded in achieving a good dispersion of NP as can be seen in figure 1(b).

The metal nanoparticle surface functionalization poses some material-related questions regarding the behavior of that nano-structured material, especially when exposed to biological electrolytes or volatile organic compounds (e.g. Ethylene). This will allow us to develop a novel family of biosensors that enable sensitivity, rapidity, and selectivity for the detection of a wide range of target analytes, from pathogens to volatile organic gases, compared to existing bio-electrochemical sensors.

The final goal is a flexible all-in-one, highly sensitive and selective biosensors using relatively simple and low cost materials and processing. The sensors will use recent advances in functionalized Gold NP decorated ZnO electrodes based sensors.

Package Materials & Processes for High-Speed IO – A Review

Ran Manor
NVIDIA

As data volume over the internet/cloud/data centers continues increasing exponentially, the technological requirements for higher bandwidth microelectronic components to switch and route this huge amount of data becomes more and more challenging. Fueled by huge data centers deployment, the cloud network bandwidth demand double itself on a yearly basis. The bandwidth of an ethernet switch doubles itself about every two years and now reaches 51.2Tbps in a single switch device. The high bandwidth is achieved by running in parallel large amounts of lanes (512), each of 100Gbps. Enabling this cutting-edge data rate is achieved by the most advanced Si manufacturing technologies as well as packaging materials.

Insertion loss & skin effect are both strongly enhanced as data rate frequency increases. New materials & processes are required to minimize the effect of the latter two. The challenges and requirements from the packaging materials and processes will be introduced and discussed.

Exploiting compositional variations in epitaxial Permalloy-silicide nanostructures on silicon to affect their magnetic properties

Anjan Bhukta
Tel Aviv University

Composition, structure and morphology of self-assembled nanostructure (NS) undoubtedly affect their physical properties and potential applications, e.g. magnetic properties for exploitation in high-density data storage and spintronics. MexSi1-x silicide phases with $x < 0.5$ (where Me stands for Fe, Co, Ni) are mostly non-ferromagnetic in the bulk state, in spite of FM nature of the metallic constituent. The FM order often observed in silicide NSs is routinely attributed to under-coordinated atoms at the NS boundaries. We demonstrate the dependence of magnetic response of a Permalloy – based silicide NS array, formed by solid phase epitaxy of $Ni_{80}Fe_{20}$ Permalloy on a vicinal Si(111) substrate, on the compositional, structural and morphological evolution of the silicide NSs in the array. Metastable CaF_2-type γ-Fe(Ni)Si_2 NSs are the first to crystallize in the sequence of phase formation initiated by post-deposition annealing cycles up to 600 °C. These islands assume disk-like shapes, exhibit high structural and compositional uniformity, and sharp and coherent interfaces with the substrate forming $(11\bar{1})$ Si $\parallel (11\bar{1})$ γ and (110) Si ∥ (110) γ epitaxial relations [1]. Annealing at higher than 600 °C temperature drives phase transformation from metastable cubic γ disilicide into a stable orthorhombic β disilicide with $(1\bar{1}1\bar{})$ Si ∥ $(2\bar{2}0)$ β and (011) Si ∥ (001) β orientation relations, accompanied by disk to bar NS shape transition. While electron microscopy examination of the β NSs was evident of a uniform single-phase orthorhombic structure throughout their entire cross-section, compositional analysis revealed massive in-diffusion of Ni towards the interface with the substrate, leaving the top parts of the NSs practically devoid of Ni, with a dramatic effect on magnetic properties [2]. Magnetometry of the uniformly composed γ NS arrays exhibited typical in-plane superparamagnetic magnetization reversal loop and ZFC/FC curves pointing to a median blocking temperature around 30 K. Contrary to that, the peculiarly figured magnetization reversal loop shapes of the β NSs resembled those of exchange spring magnet, due to coupling between two entities with different degrees of magnetic softness, likely due to a sharp compositional difference between the top and bottom parts of the NS islands.

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Session 18
Mechanical and Structural Materials

Session chairs:
Mirit Sharabi, Dan Mordehai

Location: Teddy C

Hierarchical interfaces as fracture propagation traps in natural layered composites

Daniel Wagner
Weizmann Institute of Science

The issue considered in the present lecture, in a mostly observational and qualitative way, deals with selected sophisticated design solutions offered by specific natural architectures to the problem of blocking fracture propagation in layered composite structures. The interest in this problem, extensively examined over the last few decades in the literature, originated in the brittle nature of engineering ceramic materials under tension or bending but which otherwise offer excellent thermomechanical properties. Indeed, modern structural materials are often used in critical applications such as aircraft jet engines, where reliability is the key property and thus sudden, unstoppable fracture is unacceptable. For those structures, toughness is at least as important as strength (if not more important). It is only recently that physics- and materials-based research has concentrated on the quest for materials and/or structures possessing high simultaneous strength and toughness [1]. Perhaps surprisingly at first sight, such structures are frequently found in nature, which explains the recent fascination at studying them. Here, we present some less well-known design patterns produced by nature to generate crack bifurcation and arrest in complex layered structures [2, 3].

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Macro to micro in fracture – from macroscopic cleavage energy to atomistic bond breaking mechanisms

Dov Sherman
Tel Aviv University

We aimed at bridging the gap between continuum mechanics based Griffith theory of brittle fracture and atomistic based physics of fracture, theories and simulations. The unresolved issues are the fracture energy at initiation and the associated crack speed, and energy dissipation mechanisms in fracture. The fundamental energy gap was investigated by selective fracture experiments of silicon crystal, atomistic simulations, and topological reasoning. We considered here the special role played by the macroscopic driving force for cracking, the quasi-static energy release rate (ERR), G0(a), its initial value upon initiation, G0(a0), and gradient, Q=dG0(a0)/da. We show that the cleavage energy, G0, known as the Griffith barrier of 2gs, is correct for low values of G0(a0) and Q. When G0(a0) and Q increase (primarily by shorter initial crack length, a0), so is the cleavage energy. We also show that G0(a0) and Q govern the entire range of fracture events - from the lower bound Griffith barrier to the upper bound lattice trapping barrier.

We underlined the fundamental importance of crack front shape in controlling the energy dissipation; the lower and upper energy bounds are dictated by varying energy dissipation mechanisms in the form of atomistic planar kink-advance (or migration) and kink-formation (or nucleation) in various ratios along the crack front.

The macro to micro in fracture is manifested by the relationship between the macroscopic cleavage energy and the microscopic bond breaking mechanisms: as G0(a0) Q increase, the crack front curvature increases to dissipate the higher energy upon initiation prior to being dynamic.

Following the above, we defined four new atomistic scale material properties. These properties bridge the gap between continuum mechanics and physics of fracture, and set the relationship between the macroscale fracture related materials properties and the microscale bond breaking mechanisms.

A polarized micro-Raman study of necked epoxy fibers

XiaoMeng Sui
Weizmann Institute of Science

Fully cured epoxy resins are typically brittle materials but according to recent research, cured epoxy fibers exhibit a singular mechanical behavior, including yielding followed by large deformation, and very high strength, toughness, and modulus. These properties appear to intensify as the fiber diameter decreases. The microstructural origin of this unusual behavior has not been fully determined. Here we use confocal polarized Raman spectroscopy to monitor the apparent molecular reorientation induced by plastic deformation of epoxy fibers, both qualitatively and quantitatively. Based on these and previous X-ray diffraction measurements, a likely molecular explanation for the extreme mechanical behavior of micro-sized epoxy fibers is proposed.

Extracellular Matrix Mechanics and Disease States

Joshua M. Grolman
Technion

Mammalian cell morphology has been linked to the viscoelastic properties of the adhesion substrate, which is particularly relevant in biological processes such as wound repair and embryonic development where cell spreading and migration are critical. Plastic deformation, degradation, and relaxation of stress are typically coupled in biomaterial systems used to explore these effects, making it unclear which variable drives cell behavior. Here we present a nondegradable polymer architecture that specifically decouples irreversible creep from stress relaxation and modulus. We demonstrate that network plasticity independently controls mesenchymal stem cell spreading through a biphasic relationship dependent on cell-intrinsic forces, and this relationship can be shifted by inhibiting actomyosin contractility. Kinetic Monte Carlo simulations also show strong correlation with experimental cell spreading data as a function of the extracellular matrix (ECM) plasticity. Furthermore, plasticity regulates many ECM adhesion and remodeling genes. Altogether, these findings confirm a key role for matrix plasticity in stem cell biophysics, and we anticipate this will have ramifications in the design of biomaterials to enhance therapeutic applications of stem cells.

Tracking twin boundary jerky motion at nanometer and microsecond scales

Emil Bronstein
Technion

Twinning is an essential mode of plastic deformation occurring via nucleation and motion of twin boundaries. This process governs the mechanical behavior of a variety of solid materials, such as hexagonal close-packed (HCP) metals (e.g., Mg and Ti), nano-crystalline and nano-structures of face-centered cubic (FCC) metals (e.g., Cu and Ni), and nano-structures of ceramic materials (e.g., zirconia). Additionally, twinning reorientation in ferroelastic oxide crystals is the main mechanism responsible for seismic wave attenuation in Earth's lower mantle. Twinning reorientation in ferroelectric materials, shape memory alloys (SMA), and ferromagnetic shape memory alloys (FSMA) facilitates significant straining, thus providing the fundamental mechanisms for transformation between electric/magnetic/thermal energy and mechanical energy, which are used in a variety of advanced actuation, sensing, and energy harvesting applications.

In this work, the jerky motion of twin boundaries in the ferromagnetic shape memory alloy Ni-Mn-Ga is studied by simultaneous measurements of stress and magnetic emissions (ME). A careful design of the experimental conditions results in an approximately linear relationship between the measured ME voltage and the nm-scale volumes exhibiting twinning transformation during microsecond-scale abrupt 'avalanche' events. This work shows that the same distributions of ME avalanches, related to features of jerky twin boundary motion, are found both during and between stress drop events. Maximum likelihood analysis of statistical distributions of several variables reveals a good fit to power laws truncated by exponential functions. Interestingly, the characteristic cutoffs described by the exponential functions are in the middle of the distribution range. Further, the cutoff values can be related to the physical characteristics of the studied problem. Particularly, the cutoff of amplitudes of ME avalanches matches the value predicted by high rate magnetic pulse tests performed under much larger driving force values. This observation implies that avalanches during slow rate twin boundary motion and velocity changes observed by high rate tests represent the same behavior and can be described by the same theory.

Plant wings as biocomposites

Benny Bar on
Ben-Gurion University of the Negev

Autorotating winged seeds, such as tree samaras, incorporate self-generating aerodynamic lift forces that reduce their falling velocities upon detachment from the tress and enable their passive dispersal into distant places by occasional winds. Understanding the structural–mechanical principles of the samara wings may pave the way to designing high-performance, small-scale wing elements for advanced unmanned aerial vehicles. From a structural–mechanical viewpoint, plant wings are complex hierarchical biocomposite elements that are supposed to resist aerodynamic forces to prevent undesired structural deformations that possibly deter their flying capabilities. In this work, we analyzed the anisotropic structural characteristics and the mechanical properties of the Tipuana tipu (T. tipu) samara wing biocomposite by microscale and nanoscale analysis methods. We quantified the effective elastic properties of wing segment experimentally by micro-tensile testing and its underlying material properties by nanoindentation experiment. Then, we used electron microscopy and computer tomography methods to identify the structural characteristics of the wing material. Finally, we used analytical composite-mechanic models to analyze the structural–mechanical relationship of the T. tipu samara wing. We found that the wing material includes substantial mechanical anisotropy, which its orientation locally varies within the wing; this mechanical "design" plays a significant role in the overall bending and twisting stiffness of the T. tipu samara wing. These insights may lead to new engineering concepts of small-scale wing elements.

(†) Authors of equal contributions

Complex hierarchical biominerals are the result of differential facet growth of a simple habit

Emanuel Avrahami
Weizmann Institute of Science

Directing crystal growth into complex morphologies is highly desirable in a variety of scientific and technological realms. Yet it remains challenging, as crystals have an intrinsic tendency to adopt thermodynamically stable habits. Nevertheless, many organisms evolved the ability to tailor crystal morphologies into intricate shapes. An example for such are coccoliths - micrometer-sized calcite crystal-arrays produced by unicellular algae. Traditionally, the complex morphologies of the coccolith crystals were assumed to materialize from numerous crystallographic facets, stabilized by fine-tuned interactions between organic molecules and the growing crystals. Here, utilizing high-resolution electron tomography, we examined multiple stages of coccolith development in 3D. We found that the complex crystals are expressing only one set of symmetry related crystallographic facets, which grow differentially to yield highly anisotropic shapes. Additionally, the chirality of coccolith morphology is dictated by the initial positioning of the crystals along specific edges of these same facets. These findings challenge conventional views on control over complex crystalline morphologies, and demonstrate that such can be attained with straightforward principles.

Polymer beads as interfacial obstacles in fibre composites

Carol Rodricks
Weizmann Institute of Science

Natural composites such as bone, feathers and nacre have attained a superior balance of strength, toughness and material utilisation through hierarchical structural design. Internal interfaces appear to govern this balance through mechanisms such as physical interlocking and anchoring of elements that promote strength, and crack deflection and increased pullout resistance that promote toughness. Most strength and toughness tuning in synthetic fibre-reinforced composites is accomplished through surface chemical treatment alone, which results in the degradation of either strength or toughness of the composite as these two properties are usually mutually exclusive of each other. The incorporation of structural obstacles at the interface of synthetic composites could, instead, be a promising way forward to simultaneously stronger and tougher engineering materials with tuneable properties that depend on the topography of the interface [1–3].

Bearing this in mind, a novel structural design for interfaces is proposed – one comprising of an array of cured uniformly spaced and shaped polymer beads along the length of a fibre. The beads are proposed to act as intermittent topographical obstacles that simultaneously generate strength and toughness in fibre-reinforced composites through two main mechanisms – (1) better anchorage of fibres in the matrix resulting in an increased stress transfer from the matrix to the fibre through the bead and (2) improved resistance to crack propagation through increased pull-out resistance of the beaded fibre as compared to a fibre without such obstacles. Single fibre pull-out tests performed on a model glass fibre–epoxy bead system support this hypothesis. Higher interfacial shear strength values were recorded for beaded fibres and the pull-out of beaded fibres also appeared to dissipate more plastic deformation energy than regular fibres.

The system has the potential to be highly tuneable. The polymer beads are formed by the Plateau-Rayleigh instability, through which successful control of the bead parameters (size, angle, spacing) has been achieved. An investigation into optimisation and fine-tuning the system is currently being conducted.

Session 19
Materials for Optics

Session chairs:
Tal Ellenbogen, Rami Cohen

Location: Oren 2

Heralded spectroscopy reveals exciton-exciton correlations in single colloidal nanocrystals

Dan Oron
Weizmann Institute of Science

Multiply-excited states in semiconductor nanocrystals feature intriguing physics and play a crucial role in nanocrystal-based technologies. While photo-luminescence provides a natural probe to investigate these states, room temperature single-particle spectroscopy of their emission has so far proved elusive due to the temporal and spectral overlap with emission from the singly excited and charged states. In this work, we perform heralded spectroscopy of single quantum dots by incorporating the rapidly developing technology of single-photon avalanche diode arrays in a spectrometer setup. This allows us to directly observe the biexciton-exciton emission cascade and to measure the biexciton binding energy of single nanocrystals at room temperature, even though it is well below the scale of thermal broadening of the transitions due to finite temperature and that of spectral diffusion, the shift of the transition energy due to fluctuating electric fields. Single-particle heralded spectroscopy enables us to identify correlations of the biexciton binding energy with both charge-carrier confinement and fluctuations of the local electrostatic potential, which are masked in ensemble measurements, and to overcome artifacts due to inhomogeneous broadening. Time-resolved spectrometry, as demonstrated here, has the potential of greatly extending our understanding of charge carrier dynamics in multielectron systems and of parallelization of quantum optics protocols.

Polarization Origin of Photoconductivity in MAPbI3 Thin Films

Cecile Saguy
Technion

A major challenge in photovoltaic solar cells is finding materials that produce high photoelectric conversion. MAPbI3 is a metal-organic hybrid perovskite that provides the highest efficiency in solar power conversion devices today [1]. Therefore, the question: "what is the fundamental mechanism that governs photoconductivity in highly efficient metal-organic-hybrid-perovskite solar cells?" is a fundamental scientific and technological question. Semiconducting ion migration and intrinsic-polarization-based conduction that is associated with ferroelectricity have been proposed as the competing origin of enhanced photoelectric activity, but the exact origin of these superior device properties is still the source of lively debates [2]. We developed atomic force microscopy capabilities, including nanoscale photoconductivity, with in-situ temperature variation and illumination to show that the photocurrent in MAPbI3 is governed by intrinsic polarization. Specifically, we show that this current is orientational and does not follow simply the external-field orientation, as opposed to ion-migration-based conductivity. In addition, we observed that the photocurrent is suppressed at the tetragonal-to-cubic transformation. Both observations fit only the intrinsic-polarization hypothesis, thus providing a definitive answer to the debate [3]. The obtained microscale results are confirmed by macroscale device measurements as well as variable temperature macroscopic X-ray structural characterization [4]. Our findings not only help reveal the origin of photoelectric activity in hybrid halide perovskite, but they also allow us to design devices with enhanced functionality as well as to pave the way for photoelectric memristive devices.

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Correlated emission in self assembled $CsPbBr_3$ perovskite superlattices

Orr Be'er
Technion

We use time-resolved cathodoluminescence (TRCL) to measure extremely short light pulses from cesium lead halide perovskite superlattices. These fast light pulses are attributed to superfluorescence, a collective emission from closely packed emitters. Here we demonstrate for the first time superfluorescence triggered with non-photonic excitation. We theoretically predict and experimentally demonstrate that the interaction of free electrons with perovskites triggers a collective emission. Due to the high localization of the free-electron excitation, it is possible to excite even a single emitter, changing the area of the excitation by the spot size of the electron beam. Altogether, this work paves the way for new class of fast, bright, and phosphorescence-less detection of high energy radiation.

Cathodoluminescence Nanoscopy of Plasmonic Structures

Adi Salomon
Bar Ilan University

We used cathodoluminescence and second harmonic generation to map local electric fields of well-defined plasmonic structures as well as 3D disorder metallic networks for hybrid materials formation, photochemistry, and optical sensing applications.

I will present cathodoluminescence characterization alongside SHG responses and imaging of meta-surfaces made of aluminum gold and silver and will discuss their hot-pots formation, localization and delocalization of the electromagntic field and the importance of the metal intrinsic properties.

Finally, a complete characterization of disorder plasmonic networks will be presented and discussed. In brief, the network is characterized by mixed eigenmodes with fluctuating frequencies and intensities at subwavelength distances, reflecting its topological complexity. The network connectivity, its local density of states and energy propagation through the network will be presented as well.

Broadband Emission from Metal-Halide Perovskites – Towards Light Emitting Diodes

Ido Hadar
The Hebrew University of Jerusalem

Low dimensional metal-halide perovskites are a vast group of materials that derive from the rapidly growing family of organic-inorganic perovskites. These compounds are formed by adding a supplementary organic cation to the 3D perovskite, acting as a spacer, breaking the 3D structure to lower dimensionality, and offering an additional knob to tune the material's properties. Many of these compounds show significantly improved stability compared to the 3D perovskites and the colloidal nano-perovskites, making them appealing for various optoelectronic applications, such as photovoltaic devices and light-emitting diodes.

Specifically, for light-emitting diodes, the ability to tune the photoluminescence properties is of importance. Depending on the exact structure and composition, low dimensional perovskites may show narrow excitonic PL, tunable by quantum confinement effects, low energy emission related to 'edge' states, and for some specific structures a broadband 'white-light' emission. The latter case is specifically desired as it can exhibit high PL quantum yield and offers a clear path toward simple and efficient illumination devices. Yet, the exact physical origin for the broad emission and the materials' criteria for obtaining it are still not fully resolved. Experimentally, it was found that perovskite structures exhibiting complex connectivity and strong distortion are more prone to show broadband emission, but there is no clear model of why.

In order to better understand the underlying structural and physical mechanism for the broadband emission, we investigated the simple single-layer 2D Ruddlesden-Popper perovskite – $(CH_3(CH_2)_3NH_3)_2PbI_4$, that can show such transition from narrow PL at room temperature to broadband PL at low temperature. This transition relates to a phase transition from the undistorted room temperature structure to a distorted phase below 200 K. We further study additional single layer 2D R-P samples, with longer organic cations as the spacer groups and formulate a more general correlation between distortions and the narrow to broadband PL transition. This study enables us to gain a better understanding of how the octahedra distortion in perovskites activates the low energy emissive states and leads to broadband emission, and give some simple design rules to approach the synthesis of such materials rationally.

Challenges in the design of Electro-Optics parts, using AM (additive manufacturing) of aluminum

Yoav Dias
Elbit

Additive manufacturing enable to produce 3D parts with complex geometries. Along with the advanced ability to create low weight and volume geometries, there is a need of designing and analyzing software for optimization of the complex structures. For example, topological optimization as well as lattice structures. In order to make optimal use of these design software one has to find the allowable properties of the printed material, consider printer parameters, part geometry and post process treatments. In this presentation I will review design tools developed at Elbit for the optimization of non-homogeneous lattice structures, as well as the challenges in finding the allowable properties of 3D printed aluminum (AlSi10Mg) in L-PBF manufacturing process.

Plasmonic cavities and individual quantum emitters in the strong coupling limit

Ora Bitton
Weizmann Institute of Science

The interaction of emitters with plasmonic cavities (PC) has been studied extensively during the last decade (1). Much of the experimental work has focused on the weak coupling regime, manifested most importantly by the celebrated Purcell effect. Recently there is a growing interest in studying the hybrid emitter-PC systems in the strong-coupling (SC) regime. In this regime, the excited state of an emitter hybridizes with that of the PC to generate new states termed polaritons. This phenomenon is termed vaccum Rabi splitting (VRS) and is manifested in the spectrum through splitting into two bands.

We study the SC of quantum dots (QDs) to plasmonic silver bowtie cavities. As bowtie structures demonstrate strong electric field enhancement in the gap between their two parts, they facilitate approaching the SC regime and even reaching it with just one to a few emitters within the bowtie gap. VRS was observed in our lab by optical dark-field microspectroscopy even in the limit of single QDs (2). We further used and electron energy loss spectroscopy (EELS), a near-field spectroscopic technique, to facilitate measuring SC not only to bright modes but also to subradiant, dark plasmonic modes (3).

Photoluminescence (PL) is another useful observable for probing the SC regime at the single-emitter limit. We recently used Hanbury Brown and Twiss interferometry to demonstrate the quantum nature of PL from QDs within plasmonic antennas, verifying that the measurements are indeed from one to three QDs. Further spectroscopic studies of QD-PC systems in fact manifested several surprising features, indicating discrepancies between scattering and PL spectra. These observations pointed to the contribution of multiple excited states with complex relaxation pathways.

I will explain how intelligently choosing the materials properties is critical for increasing the QD-PC coupling well into the SC regime. This will pave the way to exciting applications including generation of single-photon sources and studies of cavity-induced coherent interactions between emitters.

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Session 20
Materials for Defense and Security

Session chairs:
Orna Bruer, Michael Gozin

Location: Oren 3

Materials for Defense

Ehud Galun

Head of Materials Division, Directorate of Defense Research & Development, MAFAT, Israel

Materials for defence uses and applications are historically, "pre-historically", from the very early ages, are leading the humanity in its technological developments and revolution, today some time we call it duel use. Who was/is the first one? What is more important? A taste from the past, the story of today and a look in to the further will be presented. New materials, new Composites, new Meta-Martials and new manufacturing methods, dual uses as well as bio mimicking will be discussed.

Combustion of Boron-Water-AN Solid Propellants

Yinon Yavor
Afeka College of Engineering

Boron powder is considered as a promising energetic additive to solid propellants, due to its very high heat of combustion, which exceeds the heat of combustion of any metallic element (except of the toxic beryllium), and even surpasses the heat of combustion of hydrocarbons [1]. Therefore, the use of new, energetic, carbon-free propellant, containing boron powder was investigated. A propellant based on boron powder and water, with the addition of a carbon-free oxidizer, such as AN (ammonium nitrate, NH_4NO_3), has been proven to produce high theoretical energetic performance, and showed promising and adjustable mechanical properties. Until now, our studies conducted on metal-water propellants were focused on aluminum powder rather than boron, in the areas of hydrogen generation [2] and green rocket propulsion [3]. It was calculated that propellants containing boron, which possesses higher energetic potential than aluminum, will provide better propulsive properties.

In this work, green carbon-free solid propellants were prepared, poured into plastic tubes (7 mm diameter × 8-10 cm length), ignited from the top and burned vertically. These solid mixtures contained micron-size boron powder, water, and AN oxidizer, in mass fractions of 20:20:60, respectively. Combustion experiments were conducted in inert environment at pressures up to 45 bar, and the burning rates were obtained using three thin metallic wires, positioned horizontally through the propellant, 30 mm apart, as could be seen in Figure 1a. The solid propellant strand combustion is demonstrated in Figure 1b.

The results obtained from numerous combustion experiments are presented in Fig. 2. It can be observed that burning rate data follows well the conventional power-law behavior with pressure, as seen for most solid propellants. Although burning rate values are similar to the ones observed in composite solid propellants, the pressure exponent for the studied compound ($n = 0.84$) is somewhat high, and may require modifications in order to be further considered for operational use.

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The Plant Age; Materials for the future

Oded Shoseyov
The Hebrew University of Jerusalem

Bringing together the toughness of cellulose nano-fibers from the plant kingdom, the remarkable elasticity and resilience of resilin that enables flees to jump as high as 100 times their height from the insect kingdom combined with Human Recombinant Type I collagen produced in tobacco plants; These are the materials of the future; Nature's Gift. Resilin is a polymeric rubber-like protein secreted by insects to specialized cuticle regions, in areas where high resilience and low stiffness are required. Plant cell walls also present durable composite structures made of cellulose, other polysaccharides, and structural proteins. Plant cell wall composite exhibit extraordinary strength exemplified by their ability to carry the huge mass of some forest trees. Inspired by the remarkable mechanical properties of insect cuticle and plant cell walls we have developed novel composite materials of resilin and Crystalline Nano-Cellulose (resiline-CNC) that display remarkable mechanical properties combining strength and elasticity. As a central element of the extracellular matrix, collagen is intimately involved in tissue development, remodeling, and repair and confers high tensile strength to tissues. Numerous medical applications, particularly, wound healing, cell therapy, and bone reconstruction, rely on its supportive and healing qualities. Its synthesis and assembly require a multitude of genes and post-translational modifications. Historically, collagen was always extracted from animal and human cadaver sources, but bare risk of contamination and allergenicity and was subjected to harsh purification conditions resulting in irreversible modifications impeding its biofunctionality. A tobacco plant expression platform has been recruited to effectively express human collagen, along with three modifying enzymes, critical to collagen maturation. The plant extracted recombinant human collagen type I forms thermally stable helical structures, fibrillates, and demonstrates bioactivity resembling that of native collagen. Today in greenhouses all over Israel farmers grow transgenic tobacco plants producing human recombinant collagen that is used for the production of medical implants that have already been in clinical use. Combining collagen at the nano-scale with resilin to produce fibers resulted in super-performing fibers with mechanical properties which exceed that of natural fibers. We will demonstrate the utility of hrCollagen, Cellulose Nano Crystals, and resilin using Additive Manufacturing technologies ranging from micron to submicron resolution using 2-photon printing technology.

IMPACT RESPONSE OF THERMOREVERSIBLE METHYLCELLULOSE HYDROGELS

Daniel Rittel
Technion

Thermoreversible hydrogels, among which methylcellulose (MC), are a special class of materials that solidify (reversibly) upon heating, contrary to most materials in use today. While such materials can mimic to some extent biological tissues in terms of mechanical properties, their yet unexplored behavior under shock loading has led to several new and intriguing findings, such as shock-induced gelation along with a remarkable propensity to mitigate the shock energy, which makes those gels suitable for shock protection. The work reported here was performed at Technion, as a collaboration between the Chemistry (Prof. Yoav Eichen and Dr. Galit Parvari) and Mechanical Engineering Faculties (Dr. Yonathan Rotbaum, O. Guetta and BatHen Varfman).

Design Considerations in Energetic Materials Compatibility: Imbuing Service-Long Robustness of Weapon System Attributes

Eran Tuval
IDF/Aegisium

The increased complexity of weapon systems and the conflicting attributes ranging from effectiveness through safety to life-cycle cost concerns pose a serious design challenge. The most influencing, yet often overlooked design parameter is the compatibility of the energetic materials with other constituents of the weapon system.

The most common compatibility issue is that of bulk energetic materials packaged to be deployed as munition, e.g., propellant in artillery shells, solid rocket engine with its casing. This compatibility issue is governed by MIL-EX standard that sets vacuum stability test (VST) criteria. The service life of munition is greatly affected by the chemical interactions at the interface with coatings, rubber compounds and various maintenance chemicals. In order to support the designers in selecting proper materials, processes and maintenance procedures, a compatibility database was built, to optimize shelf life, performance, safety and life-cycle cost. The information gathered is part of an expert system that will be described herein. More elusive is the compatibility challenge posed by ion exchange between metal lattice and energetic materials. This phenomenon creates a new explosive substance from available precursors leeched from the materials in the presence of electrolyte. To illustrate the phenomenon a case study of spontaneous copper azide formation due to a solid-state migration of copper from the stainless steel torpedo's fuse cup in the presence of sea water (due to a faulty gasket) is presented. The copper azide is an unpredictable explosive that can spontaneously detonate, creating a serious safety issue.

The third issue is the compatibility trap of inadequate production technologies. These are usually manifested in the production of solid rocket engines. Modern rocket engines require superior mechanical properties and robust case bonding adhesion strength designed to withstand thermal, pressure and acceleration loads. The design of such engines must ensure structural soundness (no cracks) for the entire life-span of the rocket engine within the environmental storage envelope. Compatibility issue dealt with, in this case, involves the constituents of the solid rocket engine itself, the manufacturing process and its time-dependent characteristics (e.g., pot-life vs. mechanized production repetitiveness, rheological homogeneity). A case study to demonstrate the manifestation of said production-induced internal incompatibility is brought forward

Compounding and 3D Printing of a Tailored Electromagnetic Radiation Absorber

Matan Levin
Technion/Rafael

Electromagnetic radiation generated by electrical devices is a common by-product that may interfere with other electrical equipment and cause harm to animals and humans. With the increasing popularity of electronic devices and wireless communications, this radiation pollution has gone up. Therefore, there is a growing need for electromagnetic interference (EMI) shielding materials.

A common method of EMI shielding is the use of radiation absorbing materials (RAM). RAM can be challenging to integrate into radiation-emitting electronics while minimizing the weight and volume, and maintaining a broad spectrum of absorption. Common RAMs are based on composites of carbon allotropes fillers in a thermoplastic matrix. Traditional manufacturing methods of these materials are inherently limited in geometry and morphology, thus hindering their full absorption potential.

This study aimed to design and manufacture devices that effectively absorb electromagnetic radiation in the X band (8-12 GHz). For this purpose, we selected Polyamide 12 as a matrix and studied three carbon-based fillers: Graphite, Carbon black, and Carbon nanotubes. These were compounded, extruded into filaments, and printed using FDM (fused filament modeling) into periodic geometries. The complex dielectric coefficients of the compounds were characterized using rectangular waveguides. The optimal geometry of the device was selected using finite element analysis (CST Studio Suite™) to maximize the radiation absorption and minimize its reflection. The printed geometry of the radiation absorbing devices was a lattice structure with a triangle, square, or star of David's unit cell. The analyses were verified by comparison to reflectometry measurements of the printed models. It is shown that the device can be characterized by using a sufficiently small unit cell since the effective properties derived from the volume fraction of the printed material are not reliant upon the unit cell shape. Finally, we printed a "dynamic" RAM device with controllable magnitude and frequency of the absorbed radiation at different polarizations. This property was accomplished by the integration of thermoplastic urethane flexible joints in the RAM skeleton of the device. By compressing this device vertically, the maximum absorption in the vertical polarization increased by 60-fold, and the horizontal polarization decreased by 70-fold. The device compression enabled us to control the frequency and polarization at which maximum absorption occurred.

The developed methodology may be combined with topological analysis to achieve an intertwining of structural and absorbing properties.

Posters

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Dana Asaf
Unraveling the rate of the reverse martensitic transformation: A microsecond-scale time-resolved X-ray diffraction study

Biran Idan
Real space crystallography and polymorph-identification of small organic crystals using low dose focal series reconstruction for TEM images

Gavriely Shira
One-pot Bio-assisted synthesis of stable Ag-AgCl system using Jellyfish-Based Scaffold for Plasmonic Photocatalysis Applications

Khenkin Michal
Interactions of Langmuir Blodgett films with 2D materials

Shockner Rotem
Study of irradiation properties of quaternary FeCoCrNi, AlFeCoNi, AlCrFeNi and AlCoCrNi multicomponent alloys

Shockner Rotem
The effects of Cr alloying in the AlCoFeNiCrx high entropy alloy system

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X-Ray Photoelectron Spectroscopy System as a powerful platform for Surface Analysis

Unigovski Yaakov
Electrochemical Cold Drawing: A New Solution for Low-Ductility Alloys

Cherf Shiraz
Development of 3D Metal-Silicide Anodes for Lithium-Ion Batteries

Markman Emanuel
Effects of Additives on Hydrogen Release Reactivity of Magnesium Hydride Composites

Madar Naor
Development of thermoelectric material based on the $(GeTe)_{96.2}(Bi_2Te_3)_{3.8}$ alloy

Hayun Hagay
Towards thermal expansion tailoring in functional ceramics

Levy Davide
Crystal structure determination by laboratory X-ray Powder Diffractometer: the structure of Carbidopa

Sadia Yatir
Thermoelectric properties of $CuInX_2$ (x=S,Se,Te) doped with Ni and Cd

Moskovich Shachar
Radiation Damage in Electroless Deposited Silver Thin Films

Bassos Maxim
Stress corrosion performance of austenitic stainless steel produced by wire laser additive manufacturing (WLAM) process

Bendikov Tatyana
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Caspi Shaked
Capping layers for $SrVO_3$ films and their influence on the near-surface region

Varenik Maxim
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BASHA ADHAM
Measurements of elastic and inelastic mean free paths for scattering of fast electrons in amorphous SiO_2 and Ta_2O_5

Rabin Daniel
High entropy alloy on single sub-lattice in MNiSn Half-Heusler compound

Cahana Meital
Bismuth doping of induction furnace synthesized Mg_2Si, Mg_2Sn and Mg_2Ge thermoelectric compounds

Shmulevitsh Mati
The effect of the elastic energy on the shape and ordering of h-Ni_3Ti precipitates in lath martensite

Shmulevitsh Mati
Diffusion and trapping of hydrogen due to elastic interaction with η-Ni_3Ti precipitates in Custom 465® stainless steel

Warshavski Ori
Additive manufacturing of reaction bonded boron carbide from an optimal B_4C powder mixture

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The Effect of Composition and Temperature on the Raman Scattering in Cerium Hydrides

Sclar Hadar
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Dahan Moran
Influence of synthesis method on Ni exsolution and performance of $La_{0.2}Sr_{0.7}Ti_{0.95}Ni_{0.05}O_3$ SOFC anode materials

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Design Considerations in Energetic Materials Compatibility: Imbuing Service-Long Robustness of Weapon System attributes

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The Influence of Cr on the Grain Boundary Mobility of Alumina

Tzadikov Jonathan
Heteroatom Incorporated Carbon Materials

Fabri Noy
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UV Sensitization of Nitrate: A Powerful Tool for Groundwater Remediation

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Study of 2D Alloys $Bi_2Se_{(3-x)}Sx$ Optical and Optoelectronic Properties

Moreno Daniel
Side Effects in the In939 Superalloy AM Productions

Miyar Rebeca
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Grinberg Itzhak
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Rudelson Gregory
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MOHAPATRA PRANAB KISHORE
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Zadkani Nahum Elinor
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Byk Gerardo
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Segal Yuval
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Auslender Avi
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Shneider Mark
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Gabay Noa
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Perets Tohar
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Beitner Daniel
Coupled Molecular Emitters in Superstructures Interact with Plasmonic Nanoparticles

Elizur Hagar
Jellyfish-based smart wound dressing containing porous silicon nanoparticles loaded with antibiotics for drug release applications

Lang Arad
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Portal Lotan
Self-Catalytic Growth of 1D Materials Within Dislocations in Gold

Shaek Saar
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Hillel Guy
On the formation of anti phase boundaries in binary and ternary B2 phases

Bishara Hanna
The relationship between grain boundary structure and local electrical resistivity in a pure metal

Dishon Ben Ami Shiri
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Dror Shaked
Assembly and attachment of elpasolite monolayers and formation of colloidal nanoplatelets

Bram Avraham
The Effect of POSS Type on the Shape Memory Properties and Space Environment Durability of Epoxy-Based Nanocomposites

Ohad Guy
Band gaps of crystalline solids from Wannier-localization–based optimal tuning of a screened range-separated hybrid functional

Shepelenko Margarita
Polymorphism, Structure, and Nucleation of Cholesterol.H2O at Aqueous Interfaces and in Pathological Media: Revisited from a Computational Perspective

Chen Yu
Guest molecule-mediated energy harvesting in a dynamic peptide-metal organic framework

Shashar Eden
Zinc Oxide Nanowalls Decorated with Gold Nano Particles for Bio-Sensing Applications

Sela Sivan
Zirconium surface treatment using plasma electrolytic oxidation for biomedical applications

Keren Shachar
Mechanical behavior of hybrid organic-inorganic nanostructures fabricated by vapor precursors growth within polymers

Arad Elad
Hydrogels as a Matter of Charge: Electrostatically tuned co-assembly of amphiphilic peptides

Mordechay Lital
Mechanical Regulation of the Cytotoxic Activity of Natural Killer Cells

Saguy Cecile
Polarization Origin of Photoconductivity in $MAPbI_3$ Thin Films

Ifraimov Sabina
Advanced materials using a metallization process of polymers

Tzadka Sivan
Direct Nanoimprint on Chalcogenide Glasses substrate for Optical Applications

Perez Maayan
The Effect of Deposition Mechanism on the Properties of Epitaxial PbS Films Grown from Acidic Bath

Metzger Tzuriel
Utilizing Chiral Induced Spin Selectivity Effect to A-Symmetrical Surface Interactions

Brookstein Ori
Silky Graphite

Sobolev Alexande
Aluminum surface treatment by Plasma Electrolytic Oxidation in molten salt

Rulf Omri
3D printing utilizing plasmon effect of gold nanorods

Lieberman Rama
3D Printing Hydrogels by Photo-induced Thermal Polymerization with Carbon Nanotubes (CNTs)

Ayieko Vincent
Characterization of Siliplant 1 (Slp1) interactions with silicic acid to produce silica

Raveh-Amit Hadas
Containment of radioactively-contaminated soil: from differences in matrix composition to the performance of a remediation technique

Ginsbury Eran
BIOMIMETIC 3D PRINTED GRADED JOINT

Zimmerman Jonathan
Deformation-induced Surface Phenomena in Platinum Nanoparticles

Peled Hadar
The Effect of Peptide Folding on the Electrical Properties of Functionalized ZnO Surface

Bhattacharjee Yudhajit
Robust Core-shell Nanostructure Composites for EMI Shielding and other Associated Applications

Priel Elad
Cold compaction of Al-TiB_2 powders investigated using micromechanical multi-scale finite element modeling

Le Saux Guillaume
Dynamic Surface-Layer Coiled Coil Proteins Processing Analog-to-Digital Information

Shtuckmeyster Daniel
The dependence of sputtering and surface erosion on grain crystallographic orientation due to Helium implantation

Borenstein Arie
Laser processing of carbon nanomaterials

Ben Shalom Shir
Ga-In system under pressure: the anomalous pressure dependence of the eutectic point

Ben Shalom Shir
Bi-Sb system under pressure: the effect of the incommensurate Bi-III phase

Arad Elad
Beta-amyloid fibrils catalyze neurotransmitter degradation

Zakay Noy
Combinatorial Liquid Flow Deposition of PbS Semiconductor Thin Films

Barazani Eti
Navigating through the phase diagram of a Mott insulator by substrate-induced strain

Nguyen Long
High-pressure phase transition of SnO and PbO exploration by DFT and evolutionary algorithm

Bisht Anuj
Deformation behavior of bicrystalline Ni-Co nanoparticles with coherent twin boundary

Atar Nurit
Polyimide-Metal Hybrid Additive Manufacturing of Electronics

Elias Ester
The effect of nitrogen doping on the helium migration in plasma- facing materials

Finkelstein Gal
Piezoelectricity in Self-Assembled Biomaterials

Nudelman Roman
Bio-assisted synthesis of bimetallic nanoparticles featuring antibacterial and photothermal properties for the removal of biofilms

Banik Meneka
Coupling the chemistry and topography of block copolymer films patterned by soft lithography for nanoparticle organization

Appel Oshrat
Hydrogen-uranium interaction during in-situ 3-point bending test

Biran Ido
Determination of Thermal Expansion Coefficients of Sucrose Single Crystal Using X-Ray Diffraction

Yehuda Nofar
Antimicrobial Activity of Red Microalgal Polysaccharide Complex with Cu_2O

Simon Assaf
Hybrid Organic-Inorganic Isoporous Membranes with Tunable Pore Sizes and Functionalities for Molecular Separation

Ophek Nir
Phase diagrams of BiSb and SiGe binary systems under pressure from first principles

Cohen shai
Surface Oxidation of MNiSn (M=Ti, Zr, Hf) Half-Heusler Alloys

Dotan Tali
Microelectrodes patterning by supersonic cluster beam deposition (SCBD) and FS laser processing

Liberman Itamar
LOCALIZED SYNTHESIS AND IN-SITU CATALYTIC CHARACTERIZATION OF MOF-BASED MATERIALS USING SECM

Shachar Michaely Gal
Disperse-and-mix: oil as an 'entrance door' of carbon-based fillers to rubber composites

Shkury Ohad
Influence of mechanical stresses on thermal properties of ceramic blankets

Murali Mohan Reddy Samala
Enhancement of proton conductivity of bioinspired materials by counterion additives

Shikler Rafi
Phase Separation Dynamics in an Annealed Polymer: Fullerene Blend Analyzed using the Critical Point Model of the Permittivity

Toledo Esti
Molecular Scale Spatio-Chemical Control of the Activating-Inhibitory Signal Integration in NK Cells

Zilberberg Rotem
Single Crystal Substrates as Template for Eutectic Gold-Silicon Thin Films

Sharipova Aliya
Solid-state dewetting of thin Au films on oxidized surface of biomedical TiAlV alloy

Kadamannil Nila Nandha
Cryo-electron microscopy structure of hollow photocatalytic macrocyclic polydiacetylene nanotubes

Kirson zvi
Role of electromagnetic signalling in interactions between biological objects in aquoees environment

Wagner Avital
Enhancing photoluminescence of Ce: YAG transparent ceramic phosphors

Kirshon Yuri
High pressure-high temperature electrical resistance and differential thermal analysis measurements in a “Paris-Edinburgh” large volume press

Stein Eyal
Ambipolar Organic Electrochemical Transistors and Inverters based on organic semiconducting blends

Lazovski Guy
Advantages of automation and online monitoring of physical conditions during hot super-critical drying of aerogels

Muzaffar Kawasma Riham
Micelle-directed Assembly: Circular arrangement of Semiconductor Nanorods Around Block Copolymer Domains

Gorfman Semën
Identification of coherent twin relationship from high-resolution reciprocal space maps

Aviv Moran
Modification of a Single Atom Affects the Physical Properties of Double Fluorinated Fmoc-Phe Derivatives

PANDEY ASHISH
Fabrication of nanodevices with varying rigidity to understand various T cell interaction mechanisms

Kadan-Jamal Kian
“In cell” Electrical and Electrochemical Functional Biosensing.

Aibinder Polina
Polypeptide-Peptide Nanoparticles as a Drug Delivery Platform

Ranganathan Kamala Kannan
Transfer free WS_2/graphene Van der Waals heterostructure for photodector

Dahan Shahar
Antimicrobial FKF hydrogels

Sankhala Kirti
Understanding structure formation in the isoporous hollow fiber membranes

Dvorkin Dor
spherical membranes of hierarchically self-assembled bio-polymers and peptides for cell culture

Grishchenko Yana
Engineering the Piezoelectric Properties of Bacterial Cellulose Films

Be′er Orr
Data Science methods for analyzing materials: A case study on $CsPbBr_3$ colloidal synthesis

Petukhin Daniel
Nonmagnetic Atomic-Size Spintronics

Nagel Alina
New materials and methods for single photon emitters

Strokin Evgeny
Additive manufacturing of nano-composites using Powder Bed Fusion

Oohad Greenbaum
Mass contribution to dislocation motion: A molecular dynamics study.

Gadi Golan Novel Lateral Doped PV Cell

Undergraduate poster presentations

Aya Mrar	Azrieli	Electro polymerization of Conductive Polymers in Microelectronic Devices for Integration in Biosensors
Nazmi Abu Git	Azrieli	Engineering of solid reverse thermo-responsive displaying polymeric systems
Shoam Shamul	Azrieli	Electroless deposition of copper on PDMS polymer
Tal Livne	Tel-Aviv University	Platform Selection of Molybdenum Disulfide for Precious Metal Recovery Applications
Adva Raz	Tel-Aviv University	Microneedle Embedded Nanosensors Array for Minimally Invasive Biomarkers Detection by Blood Extraction-free Method.
Yifaa Nudel	Tel-Aviv University	Correlation between Printing Process Parameters and the Defects Created in AlSi10Mg Alloy Parts
Aviv Briger	Technion	Solubility Limit of Iron in α-Alumina
Nir Manasherov	Technion	Hydrothermal Deposition of Nickel Hydroxide upon Carbon Cloth Electrode: Morphology and Volumetric Capacity.
Jehan Abu Naji	Technion	Synthesizing and Characterizing Protein-Based Microparticles