

# SCIENTIFIC PROGRAMME

## Materials in an Explosively Growing Informatics World

### OPENING SESSION

#### WELCOME ADDRESSES

#### Plenary Lectures

**PL1 The second decade of the Material Genome Initiative**

**J.A. WARREN**, Material Measurement Laboratory, National Institute of Standards and Technology, Gaithersburg, MD, USA

**PL2 Quantum Computing with Semiconductors: On and Off the Beaten Path**

**G. SCAPPUCCI**, QuTech, TU Delft, Delft, The Netherlands

**PL3 Quantum Technologies based on Si/SiGe and SiCOI**

**T. LADD**, HRL Laboratories, LLC, Malibu, CA, USA

### TRACK A

#### ADVANCES IN FUNDAMENTALS OF THEORY, COMPUTATION AND SIMULATION OF MATERIALS SYSTEMS: CLASSICAL TO QUANTUM

#### Session A-1

Ab-initio methods for bulk and reduced-dimensional materials

**A-1:IL01 Twisted Bilayer Graphene: Where is the “Magic”?**

**E. KAXIRAS**, D. BENNETT, D. LARSON, L. SHARMA, S. CARR, Department of Physics and School of Engineering and Applied Sciences, Harvard University, Cambridge, MA, USA

**A-1:IL02 Ab initio Extended Hubbard Interactions and their Applications**

**YOUNG-WOO SON**, Korea institute for Advanced Study, Seoul, South Korea

**A-1:IL03 New Algorithms for Real-space Solutions to the Electronic Structure Problem for Confined Systems: Quantum Dots with Nearly a Million Electrons**

**J.R. CHELIKOWSKY**, University of Texas at Austin, Austin, TX, USA

**A-1:IL04 Quantum Monte Carlo Study of Straintronic Response of 2D Materials: Monolayer Phosphorene and MoS<sub>2</sub>**

**Y. HUANG**, J. BRNDIAR, **I. STICH**, Institute of Informatics, Slovak Academy of Sciences, Bratislava, Slovakia

**A-1:IL05 First-principles Computations of Light and Matters in the Window of Condensed Matter Physics**

**N. PARK**, Department of Physics, Ulsan National Institute of Science and Technology, Ulsan, South Korea

**A-1:IL06 Engineering the Properties of 2D Materials by Defect Creation, Strain and Intercalation**

**A. KRASHENINNIKOV**, Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

**A-1:IL07 Are Simulations and Experiments Accurate for the Lattice Energies of Molecular Crystals?**

**F. DELLA PIA**, **A. ZEN**, **D. ALFÈ**, **A. MICHAELIDES**, Department of Earth Sciences, University College London, London, UK

**A-1:IL08 Many-body Effects on the Photophysics of 2D Materials**

**D.Y. QIU**, Yale University, New Haven, CT, USA

**A-1:IL09 Accelerate the Discovery of Rare-earth-free Magnetic Materials using Deep Machine Learning**

**CAI-ZHUANG WANG**, Ames National Laboratory - USDOE and Department of Physics, Iowa State University, Ames, Iowa, USA

**A-1:IL10 Auxiliary-field Quantum Monte Carlo Beyond Hartree-Fock Trial Wavefunctions**

**JONHO LEE**, Harvard University, Cambridge, MA, USA

**A-1:IL11 Point-defects Formation and Atomic Diffusion in Cementite: An Ab-initio based Study**

**A. LEMERCIER**, C.-C. FU, F. SOISSON, J.-L. BECHADE, Université Paris-Saclay, CEA, Section de recherche en Corrosion et Comportement des Matériaux, SRMP, France

**A-1:IL12 Atom System: The Structuring Mechanisms of Atomic Shells**

**J. NIEWIADOMSKA-KAPLAR**, Tab Edizioni, Rome, Italy

#### Session A-2

Quantum many-body methods for study of electron-electron and electron-phonon interactions

**A-2:IL01 Correlation-enhanced Electron-phonon Interaction in Oxide Superconductors from GW Perturbation Theory**

**ZHENGLU LI**, Mork Family Department of Chemical Engineering and Materials Science, University of Southern California, Los Angeles, CA, USA

**A-2:IL02 Fundamental Theory of Geometric Phase and Non-adiabatic Phenomena**

**R. REQUIST**, Fritz Haber Center for Molecular Dynamics, Hebrew University of Jerusalem, Jerusalem, Israel

#### Session A-3

Molecular dynamics, Langevin dynamics, stochastic and finite element methods

**A-3:IL01 Universal First Principles Force-fields for Materials Simulations based on Sparse Gaussian Process Regression**

**KWANG S. KIM**, Department of Chemistry, Ulsan National Institute of Science and Technology (UNIST), 50 UNIST-gil, Ulsan, South Korea

**A-3:IL02 Rigorous Non-equilibrium Molecular Dynamics of an Open System based on Generalised Langevin Dynamics Formalism**

**L. KANTOROVICH**<sup>1</sup>, H. NESS<sup>1</sup>, L. STELLA<sup>2</sup>, C.D. LORENZ<sup>1</sup>,  
<sup>1</sup>Department of Physics, Faculty of Natural and Mathematical Sciences, King's College London, Strand, London, UK;  
<sup>2</sup>Atomistic Simulation Centre, School of Mathematics and Physics, Queen's University Belfast, Northern Ireland, UK

**A-3:IL03 Prediction of a Supersolid Phase in High-pressure Deuterium**

**CHANG WOO MYUNG**, Department of Energy Science, Sungkyunkwan University, Suwon, South Korea

**A-3:IL04 Graph Theory Ideas Reveal Long Range Conduction Pathways**

**M.A. GOMEZ**, Department of Chemistry, Mount Holyoke College, South Hadley, MA, USA

Session A-4

Advances in multiscale computation methods, from the atomistic to the mesoscopic and continuum levels

**A-4:IL01 Microstructure Prediction of High Temperature Alloys by a First-principles Phase Field Method**

**RYOJI SAHARA**<sup>1</sup>, T.N. PHAM<sup>2</sup>, S. BHATTACHARYYA<sup>2, 3</sup>, R. KUWAHARA<sup>4</sup>, K. OHNO<sup>1, 2</sup>, <sup>1</sup>National Institute for Materials Science, Japan; <sup>2</sup>Yokohama National University, Japan; <sup>3</sup>Birla Institute of Technology and Science Pilani, India; <sup>4</sup>Dassault Systèmes K.K., Japan

**A-4:IL02 Ab Initio Informed Microstructure and Process Modelling of Metals**

**D. SCHEIBER**, Materials Center Leoben Forschung GmbH, Leoben, Austria

**A-4:IL03 Topological Reconstruction of Elasticity Theory**

**V. RYABOV**, National Research Centre RF "Kurchatov Institute", Moscow, Russia

Session A-5

Ultrafast excitation and decay processes in materials

**A-5:IL01 Quantum Dynamics of Charge Carriers in Optoelectronic Materials**

**O. PREZHDO**, University of Southern California, Los Angeles, CA, USA

**A-5:IL02 Correlated Electron-nuclear Dynamics of Extended Systems Based on Exact Factorization**

**SEUNG KYU MIN**, Ulsan National Institute of Science and Technology, Ulsan, South Korea

**A-5:IL03 Ab initio Studies of Field-driven Ultrafast Excitations and Time-dependent Phenomena**

**YANG-HAO CHAN**, D.Y. QIU, F.H. DA JORNADA, S.G. LOUIE, Institute of Atomic and Molecular Sciences, Academia Sinica and Physics Division, National Center for Theoretical Sciences, Taipei, Taiwan; Department of Physics, University of California at Berkeley, CA, USA and Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA, USA

**A-5:IL04 Rapid Solidification as a Method of Obtaining Unusual Properties of Materials: Modeling and Experimental Data**

**P.K. GALENKO**, Friedrich Schiller University Jena, Jena, Germany

**A-5:IL05 Excitons in Complex Materials from First Principles**

**J.B. NEATON**, Department of Physics, University of California, Berkeley Materials Sciences Division, Lawrence Berkeley National Laboratory Kavli Energy Nanosciences Institute at Berkeley, Berkeley, CA, USA

**A-5:IL06 Light Control of Charge Transport and Phase Transitions**

**SHENG MENG**, Institute of Physics, Chinese Academy of Sciences, Beijing, China

**A-5:IL07 Atomistic Modeling of Laser-induced Melting and Ablation of Thin Films and Nanoparticles**

**L.V. ZHIGILEI**, C. CHEN, M.I. AREFEV, H. HUANG, A.S. VALAVANIS, Department of Materials Science and Engineering, University of Virginia, Charlottesville, VA, USA

TRACK B

**COMPUTATIONAL MESOSCALE  
STRUCTURE AND PHYSICO-CHEMICAL  
PROPERTY EVOLUTION OF SOLID  
MATERIALS**

Session B-1

Databases of physico-chemical properties of materials

**B-1:IL01 Diffusion in High-entropy Alloys: "Sluggish" or "Anti-sluggish"? Lattice Structure vs. Chemical Complexity**

**S. DIVINSKI**, Institute of Materials Physics, University of Münster, Münster, Germany

**B-1:IL02 Ab-initio Accurate Simulation of Plasticity and Thermodynamics**

P. GRIGOREV, **T.D. SWINBURNE**, CNRS / Aix-Marseille University, Marseille, France; M.C. MARINICA, CEA Saclay, France; J.R. KERMODE, University of Warwick, UK; R. DSOUZA, J. NEUGEBAUER, Max-Planck-Institut für Eisenforschung GmbH, Germany

**B-1:IL03 Thermodynamic Databases for Multicomponent Materials - CALPHAD, ab initio and ML**

**M. TO BABEN**, C. FRÜH, GTT-Technologies, Herzogenrath, Germany

**B-1:IL04 Atomic Cluster Expansion for a Unified Approach to Machine Learning Potentials**

**R. DRAUTZ**, Ruhr-University Bochum, Bochum, Germany

**B-1:IL05 Creating an Efficient Alloy Database Infrastructure and Detecting Abnormal Data**

**A.M. KRAJEWSKI**, A. DEBNATH, S. LIN, M. AHN, H. SUN, W. REINHART, A. BEESE, Z.-K. LIU, Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA, USA

**B-1:IL06 Reactive Sintering of Boron Carbides: Dependence on Elemental Precursors**

**D. OLEVANO**, S. LIONETTI, U. MARTINI, Rina Consulting Centro Sviluppo Materiali S.p.A., Rome, Italy; S. LEMONNIER, F. MOITRIER, ISL, Institut Franco-Allemand de recherches de Saint-Louis, Saint-Louis, France

## Session B-2

## Theory of phase transitions

**B-2:IL01 Quantitative Predictive Theories for Physico-chemical Property of Solid Phases**

**ZI-KUI LIU**, Pennsylvania State University, University Park, PA, USA

**B-2:IL02 Phase-field Modelling of Nonequilibrium Interface Dynamics in Diffusion-controlled Phase Transition of Alloys**

**MUNEKAZU OHNO**, Hokkaido University, Sapporo, Hokkaido, Japan

**B-2:IL03 Moire Patterns and Inversion Boundaries in Graphene/Hexagonal Boron Nitride Bilayers**

**K.R. ELDER**, Oakland University, Rochester, MI, USA; **Z.-F. HUANG**, Wayne State University, Detroit, MI, USA; **T. ALANISSILA**, Aalto University, Espoo, Finland

**B-2:IL04 Advancing MOCVD Synthesis of Wafer-scale 2D Materials: A Computational Framework**

**K. MOMENI**, Department of Mechanical Engineering, University of Alabama, Tuscaloosa, AL, USA; Materials Research Institute, Pennsylvania State University, University Park, PA, USA

## Session B-3

## Strain and size effects on phase equilibria, phase transitions, and mesoscale domain states

**B-3:IL01 Hydride Formation in Superconducting Q-Bits**

**T. LEIBENGOOD**, **P. VOORHEES**, Department of Materials Science and Engineering, Northwestern University, Evanston, IL, USA; **P.-C. SIMON**, Idaho National Laboratory, USA

**B-3:IL02 Explaining Anomalous Low-temperature Irradiation Creep with Predictive Atomistic Simulations: A Case Study of Developing a Quantitative Virtual Experiment**

**M. BOLEININGER**, S.L. DUDAREV, D.R. MASON, L. REALI, UK Atomic Energy Authority, Oxfordshire, UK; **A. FEICHTMAYER**, **J. RIESCH**, **T. HÖSCHEN**, **M. FUHR**, **R. NEU**, **T. SCHWARZSELINGER**, Max Planck Institute for Plasma Physics, Garching, Germany

**B-3:L03 Mechanisms of Nanostructure Formation During Dealloying**

**G. HENKELMANN**, **J. WEISSMÜLLER**, Hamburg University of Technology, Institute of Materials Physics and Technology, Hamburg, Germany

**B-3:IL04 Strain Phase Thermodynamics and Phase-field Modeling of Strain Phase Equilibria and Mesoscale Transformations in Ferroelectric Heterostructure**

**B. WANG**, **T.N. YANG**, **C. DAI**, **M.H. ZHANG**, **LONG-QING CHEN**, Materials Research Institute and Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA, USA

**B-3:IL05 Coherent Phase Change in Interstitial Solutions – a Hierarchy of Instabilities**

**J. WEISSMÜLLER**, Hamburg University of Technology, Hamburg, Germany and Helmholtz-Center Hereon, Geesthacht, Germany

**B-3:IL06 Modeling of Microstructure Formation in FePt High-density Magnetic Recording Media Based on a Phase-field Method Enhanced by Machine Learning Techniques**

**TOSHIYUKI KOYAMA**, Nagoya University, Nagoya, Japan

**B-3:IL07 Computational Microstructural Design for Multi-phase Multi-principal Element Alloys**

**S.R. KONERU**, **K. KADIRVEL**, **Z. KLOENNE**, **H. FRASER**, **YUNZHI WANG**, Department of Materials Science and Engineering, The Ohio State University, Columbus, OH, USA

**B-3:IL08 Microstructure Evolution with Elastic Strains: Recent Phase Field Results**

**Y. LE BOUAR**, **A. FINEL**, Université Paris-Saclay, ONERA, CNRS, LEM, Châtillon, France; **M. COTTURA**, **B. APPOLAIRE**, Institut Jean Lamour, Université de Lorraine - CNRS, Nancy, France

**B-3:IL09 First-principles Study on Alloy Phase Equilibria with Lattice Strain Relaxation**

**YING CHEN**, Tohoku University, Sendai, Japan; **T. HORIUCHI**, **T. MOHRI**, Hokkaido University of Science, Sapporo, Japan

## Session B-4

## Structural, electric, and magnetic domain structures and their evolution under external stimuli

**B-4:IL01 Understanding and Design of metallic Alloys Guided by Integrated Phase-field Simulation**

**YUHONG ZHAO**, North University of China, University of Science and Technology Beijing, Taiyuan, China

**B-4:L02 Ferroelectric Domain Structures in Twistronic 2D Crystals**

**V. FALKO**, University of Manchester, Manchester, UK

**B-4:L03 Charged Dislocations in Ionic Ceramics: Equilibrium and Kinetics**

**E. GARCIA**, Purdue University, West Lafayette, IN, USA

**B-4:L04 Magnetic Structures Stimulated by External Mechanical Stress and Temperature Distribution in Amorphous Microwires used in Magnetic Sensors**

**A. CHIZHIK**<sup>1</sup>, **V. ZHUKOVA**<sup>1</sup>, **P. CORTE-LEON**<sup>1</sup>, **A. ZHUKOV**<sup>1,2</sup>, <sup>1</sup>Universidad del País Vasco, UPV/EHU, San Sebastián, Spain; <sup>2</sup>KERBASQUE, Basque Foundation for Science, Bilbao, Spain

**B-4:IL05 Giant Negative Compressibility of Flexible Nanoporous Materials under High-pressure Intrusion-extrusion Process: From Energy Applications to Biological Channels**

**D. CAPRINI**<sup>1</sup>, **F. BATTISTA**<sup>2</sup>, **P. ZAJDEL**<sup>3</sup>, **G. DI MUCCIO**<sup>2</sup>, **C. GUARDIANI**<sup>2</sup>, **B. TRUMP**<sup>4</sup>, **M. CARTER**<sup>4</sup>, **A.A. YAKOVENKO**<sup>5</sup>, **E. AMAYUELAS**<sup>6</sup>, **L. BARTOLOME**<sup>6</sup>, **S. MELONI**<sup>7</sup>, **Y. GROSU**<sup>6,8</sup>, **C.M. CASCIOLA**<sup>2</sup>, **A. GIACOMELLO**<sup>2</sup>, <sup>1</sup>Center for Life Nano- & Neuro-Science, Istituto Italiano di Tecnologia, Rome, Italy; <sup>2</sup>Dipartimento di Ingegneria Meccanica e Aerospaziale, Sapienza Università di Roma, Rome, Italy; <sup>3</sup>A. Chełkowski Institute of Physics, University of Silesia, Chorzow, Poland; <sup>4</sup>Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, MD, USA; <sup>5</sup>X-Ray Science Division, Advanced Photon Source, Argonne National Laboratory, Argonne, IL, USA; <sup>6</sup>Centre for Cooperative Research on Alternative Energies (CIC energiGUNE), Basque Research and Technology Alliance (BRTA), Alava Technology Park, Vitoria-Gasteiz, Spain; <sup>7</sup>Dipartimento di Scienze Chimiche e Farmaceutiche, Università degli Studi di Ferrara, Ferrara, Italy; <sup>8</sup>Institute of Chemistry, University of Silesia, Katowice, Poland

**B-4:IL06 Computational Modeling for Prediction of Material Topology by Quantum Annealing**

**K. ENDO**, **MAYU MURAMATSU**, Keio University, Yokohama, Kanagawa, Japan

## Session B-5

## Thermodynamics of mesoscale states and phase transitions

**B-5:IL01 Grain Boundaries are Natural Brownian Ratchets: Directional GB Anisotropy**

C. QIU<sup>1</sup>, M. PUNKE<sup>2,3</sup>, S. WANG<sup>1</sup>, Y. SU<sup>4</sup>, Y. TIAN<sup>5</sup>, X. PAN<sup>6</sup>, M. SALVALAGLIO<sup>2,3</sup>, J. HAN<sup>1</sup>, **D.J. SROLOVITZ**<sup>6</sup>, <sup>1</sup>Department of Materials Science and Engineering, City University of Hong Kong, Hong Kong SAR, China; <sup>2</sup>Institute of Scientific Computing, TU Dresden, Dresden, Germany; <sup>3</sup>Dresden Center for Computational Materials Science, TU Dresden, Dresden, Germany; <sup>4</sup>School of Materials Science and Engineering, Shanghai Jiao Tong University, Shanghai, China; <sup>5</sup>Department of Physics and Astronomy, University of California, Irvine, CA, USA; <sup>6</sup>Department of Mechanical Engineering, The University of Hong Kong, Hong Kong SAR, China

**B-5:IL02 Grain Boundary Segregation and Solute Drag in Multicomponent Alloys**

**F. ABDELJAWAD**, M. TAGHIZADEH, Lehigh University, Bethlehem, PA, USA

**B-5:IL03 Mesocanonical Ensemble as a Rationale for Studying Metastability and Hysteretic Transitions in Confined Nanophases**

**A.V. NEIMARK**, Department of Chemical and Biochemical Engineering, Rutgers, The State University of New Jersey, Piscataway, NJ, USA

**B-5:IL04 Adsorption Induced Structural Transformations in Nanopores**

**B. KUCHTA**<sup>1,2</sup>, L. FIRLEJ<sup>1,3</sup>, B. MAZUR<sup>1</sup>, <sup>1</sup>Department of Micro, Nano, and Bioprocess Engineering, Faculty of Chemistry, Wrocław University of Science and Technology, Wrocław, Poland; <sup>2</sup>MADIREL, CNRS, Aix-Marseille University, Marseille, France; <sup>3</sup>Laboratoire Charles Coulomb, University of Montpellier-CNRS, Montpellier, France

**B-5:IL05 Liquid Metal Embrittlement in Zn Coated Steels: Computational Revelation of the Origin and Potential Solution**

**R. DARVISHI KAMACHALI**, Federal Institute for Materials Research and Testing (BAM), Berlin, Germany

## Session B-6

## Thermal, mechanical, electric, magnetic, and multifunctional properties of mesoscale structures

**B-6:IL01 Multiphysics-multiscale Simulations of Additive Manufactured Fe-Ni Permalloy**

**BAI-XIANG XU**, Y. YANG, Division Mechanics of Functional Materials, Institute of Materials Science, Technische Universität Darmstadt, Darmstadt, Germany

**B-6:IL02 Thermomechanical Properties of Highly Defective Metals for Fusion Power**

**F. HOFMANN**, A. REZA, K. SONG, I. TOLKACHEV, G. HE, Department of Engineering Science, University of Oxford, Oxford, UK; D.R. MASON, S.L. DUDAREV, P.W. MA, UK Atomic Energy Authority, Culham Science Centre, UK; S. DAS, Department of Mechanical Engineering, University of Bristol, Bristol, UK; H. YU, Canadian Nuclear Laboratories, Chalk River, Canada

**B-6:IL03 Physics-based Data-driven Modeling to Accelerate Materials Design**

**I. ROSLYAKOVA**, Materials Discovery and Interfaces (MDI), Institute for Materials, Ruhr-Universität Bochum, Bochum, Germany

**B-6:IL04 Phase-field Simulation of Elastocaloric and Magneto-elastocaloric Effect**

**MIN YI**, Nanjing University of Aeronautics and Astronautics, Nanjing, China

## TRACK C

## COMPUTATIONAL TOOLS IN MATERIALS SYNTHESIS AND PROCESSING SCIENCE

## Session C-1

## 0D, 1D and 2D nanomaterials and nanostructures

**C-1:IL01 Understanding Defect Dynamics in Two-dimensional Materials using Atomistic Simulations and Machine Learning**

**B. NARAYANAN**, Mechanical Engineering, University of Louisville, Louisville, KY, USA

**C-1:IL02 Theoretical Design and Modeling of 2D Conjugated Polymer for Overall Water Splitting under Visible Light**

**XIAOJUN WU**, University of Science and Technology of China, Hefei, China

**C-1:IL03 Determination of Stable Atomic Structures for 2D Materials by Numerical Simulations**

**T. BURCZYNSKI**<sup>1</sup>, W. KUS<sup>2</sup>, M. MAZDZIARZ<sup>1</sup>, A. MROZEK<sup>3</sup>, <sup>1</sup>Institute of Fundamental Technological Research of Polish Academy of Sciences, Warsaw, Poland; <sup>2</sup>Silesian University of Technology, Gliwice, Poland; <sup>3</sup>AGH University of Science and Technology, Kraków, Poland

**C-1:IL04 3D Printed Functional MXene-based Ceramics**

**S. BARG**, University of Augsburg, Institute of Materials Resource Management, Augsburg, Germany

**C-1:IL05 Molecular Dynamics Investigation of Nanoparticle Coalescence under Realistic Gas-phase Synthesis Conditions**

**P. GRAMMATIKOPOULOS**<sup>1,2</sup>, S.E. PRATSINIS<sup>2</sup>, <sup>1</sup>Department of Materials Sciences and Engineering, Guangdong Technion Israel Institute of Technology, Shantou, Guangdong, China; <sup>2</sup>Particle Technology Laboratory, Institute of Process Engineering, Department of Mechanical and Process Engineering, ETH Zürich, Zürich, Switzerland

**C-1:IL06 Computational Theoretical Study of the Interaction of a Molecule of Water with Two-dimensional Hexagonal Boron Nitride and with Titanium in Two-dimensional Hexagonal Boron Nitride**

**G. RUIZ-CHAVARRIA**, Universidad Autonoma Chapingo, Texcoco, Mexico

## Session C-2

## Soft condensed matter systems

**C-2:IL01 A Molecular Dynamics Simulation Interpreter for Polymers**

**YOU-LIANG ZHU**, State Key Laboratory of Supramolecular Structure and Materials, College of Chemistry, Jilin University, Changchun, China

**C-2:IL02 Molecular Dynamics Simulations of the Ordered Structures Induced by External Fields**

**ZHAO-YAN SUN**, State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun, China

**C-2:L03 Study of Colloidal Aggregate Morphology in a Confined Environment using SRD-MD**

**H. SEMAAN**<sup>1,2</sup>, M. CERBELAUD<sup>1</sup>, J. GERHARDS<sup>1</sup>, B. CRESPIN<sup>2</sup>, R. FERRANDO<sup>3</sup>, A. VIDECOQ<sup>1</sup>, <sup>1</sup>Univ. Limoges, CNRS, IRCER, UMR 7315, Limoges, France; <sup>2</sup>Univ. Limoges, CNRS, XLIM, UMR 7252, Limoges, France; <sup>3</sup>Physics Department, University of Genoa, Genoa, Italy

**Session C-3**

Powders, granular materials, single crystal growth

**C-3:IL01 Multi-scale Modelling of Single-crystal Diamond Growth via the HPHT Process**

**J.J. DERBY**, S.S. DOSSA, University of Minnesota, Minneapolis, MN, USA; I. PONOMAREV, Euclid Beamlabs, Beltsville, MD, USA; B. FEIGELSON, US Naval Research Laboratory, Washington, DC, USA; M. HAINKE, C. KRANERT, J. FRIEDRICH, Fraunhofer IISB, Erlangen, Germany

**C-3:IL02 Theoretical Modeling of Nucleation and Growth of Particulate Matter**

**ZHENYHU LI**, Key Lab. of Precision and Intelligent Chemistry, University of Science and Technology of China, Hefei, China

**C-3:IL03 Reassessment of the Criterion for Layer-by-layer Metal Growth: What Determines the Ehrlich-Schwoebel Barrier?**

**H. JONSSON**, Science Institute and Faculty of Physical Sciences, University of Iceland, Reykjavík, Iceland

**C-3:L04 Aerosol Processing of Materials: Inelastic Collisions and the Gas Mean Free Path**

D. TSALIKIS, V. MAVRANTZAS, **S.E. PRATSINIS**, Particle Technology Laboratory, Institute of Process Engineering, Department of Mechanical & Process Engineering, ETH Zurich, Switzerland and Department of Chemical Engineering, University of Patras, Greece

**C-3:IL05 Impact of Configurational Entropy on Point Defect Thermodynamics in Crystalline Silicon**

**T. SINNO**, Dept of Chemical and Biomolecular Engineering, University of Pennsylvania, Philadelphia, PA, USA; J. LUO, L. LIU, School of Energy and Power Engineering, Xi'an Jiaotong University, Xi'an, Shaanxi, China; J.F. DOUGLAS, Material Measurement Lab., Material Science and Eng. Division, National Institute of Standards and Technology, Gaithersburg, MD, USA

**C-3:IL06 Modeling of Solidification Processes under Consideration of Particle Transport in the Melt for Terrestrial and Microgravity Conditions**

H. KOCH<sup>1</sup>, P. OTT<sup>2</sup>, T. JAUSS<sup>2</sup>, T. SORGENFREI<sup>2</sup>, M. HAINKE<sup>1,3</sup>, C. KRANERT<sup>1</sup>, **J. FRIEDRICH**<sup>1</sup>, <sup>1</sup>Fraunhofer IISB, Erlangen, Germany; <sup>2</sup>University of Freiburg, Crystallography, Freiburg, Germany; <sup>3</sup>Ostbayerische Technische Hochschule (OTH), Amberg-Weiden, Germany

**Session C-4**

3D-bulks, composites and porous materials

**C-4:IL01 Valence Stability of Cerium Ions in Various Oxide Lattices: Revisiting of Madelung Lattice Site Potential Calculation**

**MASAHIRO YOSHIMURA**<sup>1,2</sup>, K. SARDAR<sup>1</sup>, <sup>1</sup>National Cheng Kung University, Tainan, Taiwan; <sup>2</sup>Tokyo Institute of Technology Japan

**C-4:IL02 A Framework for a High Throughput Screening Method for Polymeric Systems using Molecular Dynamics**

L. SMITH, H.A. KARIMI-VARZANEH, S. FINGER, G. GIUNTA, A. TROISI, **P. CARBONE**, Department of Chemical Engineering, School of Engineering, The University of Manchester, Manchester, UK; Continental Reifen Deutschland GmbH, Hanover, Germany; BASF, Ludwigshafen, Germany; Department of Chemistry, Liverpool, UK

**C-4:L03 Reaction-diffusion Synthesis of Inorganic 3D Material with Regular Microstructure: Diamond - Silicon Carbide Composite "Ideal"**

V.YA SHEVCHENKO, **S.N. PEREVSLOV**, S.V. BALABANOV, M.M. SYCHOV, NRC "Kurchatov Institute" – CRISM "Prometey", St. Petersburg, Russia

**Session C-5**

Thin/thick films, layered structures and surface processing

**C-5:IL01 Contribution of Molecular Dynamics to the Study of Metallic Nanometric Multilayers**

**O. POLITANO**<sup>1</sup>, Y. LI<sup>1</sup>, V. TURLO<sup>2</sup>, F. BARAS<sup>1</sup>, <sup>1</sup>Lab. Interdisciplinaire Carnot de Bourgogne, UMR 6303, CNRS-Université de Bourgogne, Dijon, France; <sup>2</sup>Lab. for Advanced Materials Processing, Empa - Swiss Federal Labs for Materials Science and Technology, Thun, Switzerland

**C-5:IL02 Experimentally Validated Discrete Element Method Framework for Modeling Laser-material Interactions with Multiple Reflections applied to Nanoparticle-assisted Microwelding of Copper**

**V. TURLO**, Empa - Swiss Federal Laboratories for Materials Science and Technology, Thun, Switzerland

**C-5:IL03 Formation of Lattice-aligned Gallium Oxynitride Nanolayer on Gallium Nitride**

**JUNLEI ZHAO**, J. CHEN, M. HUA, Southern University of Science and Technology, Shenzhen, China

**C-5:L04 Tunable Fano-resonant Thin-film Optical Filters**

**YI-SIOU HUANG**, C.Y. LEE, I. TAKEUCHI, C.A. RÍOS OCAMPO, Department of Materials Science and Engineering, University of Maryland, College Park, MD, USA

**C-5:L05 Prediction of Thermal Stresses in NiTi Coating Layer on Substrate Stainless Steel using Simulation Method by Comsol Multiphysics**

**S. SAMAL**, FZU-Institute of Physics of Czech Academy of Science, Prague, Czech Republic

## Session C-6

## Additive manufacturing of multiscale and multi-material structures

**C-6:IL01 Additive Manufacturing of Hierarchically Structured Ceramics for CO<sub>2</sub> Capture**

M. D'AGOSTINI<sup>1</sup>, M. CAVALLO<sup>2</sup>, N.G. PORCARO<sup>2</sup>, F. BONINO<sup>2</sup>, V. CROCELLÀ<sup>2</sup>, P. COLOMBO<sup>1,3</sup>, **G. FRANCHIN**<sup>1</sup>, <sup>1</sup>Department of Industrial Engineering, University of Padova, Padova, Italy; <sup>2</sup>Department of Chemistry, NIS and INSTM Centres, University of Torino, Torino, Italy; <sup>3</sup>The Pennsylvania State University, Department of Materials Science and Engineering, University Park, PA, USA

**C-6:L02 Optimizing 3D and 4D Printing for Numerous Applications: The Impact of Computational Models**

**T.J. WEBSTER**, Hebei University of Technology, Tianjin, China and Interstellar Therapeutics, Mansfield, MA, USA

**C-6:IL03 Optimizing the Design and Manufacturing of Bioceramic Scaffolds towards Bone-like Architectures**

**F. BAINO**<sup>1</sup>, R. GABRIELI<sup>1</sup>, A. SCHIAVI<sup>2</sup>, G. ORLYGSSON<sup>3</sup>, M. SCHWENTENWEIN<sup>4</sup>, L. D'ANDREA<sup>5</sup>, P. VENA<sup>5</sup>, E. VERNÉ<sup>1</sup>, <sup>1</sup>Institute of Materials Physics and Engineering, Department of Applied Science and Technology, Politecnico di Torino, Turin, Italy; <sup>2</sup>National Institute of Metrological Research (INRiM), Applied Metrology and Engineering Division, Turin, Italy; <sup>3</sup>Ice Tec, Reykjavik, Iceland; <sup>4</sup>Lithoz GmbH, Vienna, Austria, <sup>5</sup>Department of Chemistry, Materials and Chemical Engineering "Giulio Natta", Laboratory of Biological Structure Mechanics (LaBS), Politecnico di Milano, Milano, Italy

**C-6:L04 Smart Materials and Structures: From 3D to 4D Printing**

**DAINING FANG**, Institute of Advanced Structure Technology, Beijing Institute of Technology, Beijing, China

**C-6:L05 New Generation of Cellular Structures based on Crystallomorphic Design and Additive Technologies**

V.YA SHEVCHENKO, **M.M. SYCHOV**, M.Y. ARSENTIEV, E.I. SYSOEV, A.I. MAKOGON, S.N. PEREVISLOV, NRC "Kurchatov Institute" – CRISM "Prometey", St. Petersburg, Russia

## Session C-7

## Data driven, machine learning to accelerate and optimize materials processing

**C-7:IL01 Machine Learning for Prediction of Combustion Synthesis Kinetics and Properties of Combustion-derived Solid Solutions**

**S. VOROTILO**, King Abdullah University of Science and Technology (KAUST), Saudi Arabia; K. SIDNOV, V. KURBATKINA, D.O. MOSKOVSKIKH, National University of Science and Technology MISiS, Moscow, Russia

**C-7:L02 Multi-objective Optimization of Silver-nanowire Deposition for Flexible Transparent Conducting Electrodes**

**J.W.P. HSU**, M. LEE, R. PIPER, B. BHANDARI, University of Texas at Dallas, Richardson, TX, USA

**C-7:L03 AI-based Autonomous Microfluidic Platform for Fast Optimization in the Manufacturing of Drug-loaded Nanoparticles**

A. MOTTAFEGH, **DONG-PYO KIM**, Center for Intelligent Microprocess of Pharmaceutical Synthesis, Department of Chemical Engineering, Pohang University of Science and Technology (POSTECH), Pohang, South Korea

## Special Session C-8

**EXPLOITING COMPUTATIONAL TOOLS IN MATERIALS MANUFACTURING AND IN THE USER INDUSTRY**

## Session C-8.1

## Metal and metal alloys

**C-8.1:L01 Phase Selection in 316L Processed by Laser-powder Bed Fusion**

**C.-A. GANDIN**, G. GUILLEMOT, P. MARTIN, MINES Paris, PSL University, CEMEF UMR CNRS 7635, CS10207, Sophia Antipolis, France; P.W. VOORHEES, C.A. HARELAND, Department of Materials Science and Engineering, Northwestern University, Evanston, IL, USA

**C-8.1:L02 Ab-initio Investigation of the Role of Vacancies in Hydrogen Trapping at Transition Metal Carbonitrides in Steel**

**P. HAMMER**<sup>1</sup>, W. ECKER<sup>1</sup>, M. GALLER<sup>2</sup>, L. ROMANER<sup>3</sup>, V. RAZUMOVSKIY<sup>1</sup>, <sup>1</sup>Materials Center Leoben Forschung GmbH, Leoben, Austria; <sup>2</sup>voestalpine Wire Rod Austria GmbH, St. Peter-Freienstein, Austria; <sup>3</sup>Department of Materials Science, Montanuniversität Leoben, Leoben, Austria

**C-8.1:L03 First Principles-based Analysis of Hydrogen Embrittlement Susceptibility in Precipitation Hardened fcc Alloys**

**N. DAMM**<sup>1</sup>, F. MOITZI<sup>1</sup>, J. PLATL<sup>2</sup>, L. ROMANER<sup>3</sup>, V. RAZUMOVSKIY<sup>1</sup>, <sup>1</sup>Materials Center Leoben Forschung GmbH, Leoben, Styria, Austria; <sup>2</sup>voestalpine BÖHLER Edelstahl GmbH & Co KG, Kapfenberg, Styria, Austria; <sup>3</sup>Montanuniversität Leoben, Styria, Austria

**C-8.1:L04 Computational Thermodynamics for Multi-component System**

**B. SUNDMAN**, OpenCalphad, Gif-sur-Yvette, France

## Session C-8.2

## Ceramics, glass and cement

**C-8.2:IL01 Machine Learning of Phase Diagrams**

J. LUND, H. WANG, R. BRAATZ, **R.E. GARCÍA**, Purdue University, West Lafayette, IN, USA

**C-8.2:IL02 Chemical-Reaction-Induced Wear Process Simulations of Carbon- and Silicon-based Solid Materials**

**YANG WANG**, Research Institute of Frontier Science, Southwest Jiaotong University, Chengdu, China

**C-8.2:L03 Multi-scale Simulation Approach for Exploring Optimized Electrode Structure of Dye-sensitized Solar Cell Devices**

**M. ONODERA**<sup>1</sup>, M. KUBO<sup>1,2</sup>, <sup>1</sup>Institute for Materials Research, Tohoku University, Sendai, Japan; <sup>2</sup>New Industry Creation Hatchery Center, Tohoku University, Aramaki, Aoba-ku, Sendai, Japan

## Session C-8.3

## Polymers and related materials

**C-8.3:IL01 Tailoring Molecular Topology to Control the Mechanical Properties of Polymeric and Nanoparticle Networks**

**S. KETEN**, Dept. of Mechanical Engineering, Dept. Civil and Environmental Engineering, Northwestern University, Evanston, IL, USA

**C-8.3:IL02 Alternative Low Carbon Fuel: a Molecular Modeling Investigation on Corrosion Inhibition**

**S. LOEHLE**, TotalEnergies OneTech, Solaize, France; **A. SALCEDO**, **S. STEINMANN**, **C. MICHEL**, ENS, Lyon, France

**C-8.3:IL03 Meso-scale Proton and Oxygen Diffusivity Analysis in Cathode Catalyst Layer towards Boosting Polymer Electrolyte Fuel Cell Performance: Large-scale Reactive Molecular Dynamics Simulations**

**TETSUYA NAKAMURA**, **K. MORI**, **S. SHOGO**, **Y. SU**, **Y. ASANO**, **Y. OOTANI**, **N. OZAWA**, **M. KUBO**, Institute for Materials Research, Tohoku University, Sendai, Miyagi, Japan

**C-8.3:IL04 Coarse-grained Modeling of Thermosets: A General Machine Learning Approach to Tunable Force-Fields**

**A. GIUNTOLI**, University of Groningen, Groningen, Netherlands; **A. VAN BEEK**, University College Dublin, Dublin, Ireland; **Nitin Hansoge**, 3M, Minneapolis, USA; **T. W. SIRK**, Army Research Lab, USA; **S. PAL**, **K. DANSUK**, **W. CHEN**, **S. KETEN**, Northwestern University, IL, USA

**C-8.3:IL05 Drilling of CFRPs Using Single Layer Diamond Tools**

**ZHONGDE SHI**, **M.H. ATTIA**, National Research Council Canada, Montreal, Quebec, Canada

**C-8.3:IL06 Large-scale Molecular Dynamics Simulations for Deformation and Fracture Processes of Crystalline Polyethylene**

**YUJI HIGUCHI**, Research Institute for Information Technology, Kyushu University, Fukuoka, Japan

## TRACK D

## COMPUTER MODELLING AND SIMULATION OF MATERIALS PROPERTIES

## Session D-1

## Materials for electronics, opto-electronics and photonics

**D-1:IL01 Role of the Trap-assisted Auger-Meitner Effect in Nonradiative Recombination**

**F. ZHAO**, **M. TURIANSKY**, **C.G. VAN DE WALLE**, Materials Department, University of California, Santa Barbara, CA, USA

**D-1:IL02 Van der Waals Interactions in Materials Modelling**

**A. TKATCHENKO**, Department of Physics and Materials Science, University of Luxembourg, Luxembourg

**D-1:IL03 Controlling Spin by Materials Design in Light-emitting Applications: A Computational Perspective**

**Y. OLIVIER**, University of Namur, Namur Institute of Structured Matter, Namur, Belgium

**D-1:IL04 MOMAP: A Computational Software for Molecular Materials for Optoelectronic Property**

**ZHIGANG SHUAI**, School of Science and Engineering, The Chinese University of Hong Kong, Shenzhen, China

**D-1:IL05 On the Nature of Oxygen Vacancies in Amorphous Alumina**

**A. SHLUGER**<sup>1,2</sup>, **J. STRAND**<sup>1,3</sup>, <sup>1</sup>Department of Physics and Astronomy, University College London, London, UK; <sup>2</sup>WPI-Advanced Institute for Materials Research (WPI-AIMR), Tohoku University, Sendai, Japan; <sup>3</sup>Nanolayers Research Computing Ltd., London, UK

**D-1:IL06 Theoretical Investigations of Purely Organic Thermally Activated Delayed Fluorescence (TADF) Materials for Organic Light-emitting Diodes (OLED) Applications**

**XIAN-KAI CHEN**, Institute of Functional Nano and Soft Materials, Soochow University, Suzhou, China

**D-1:IL07 Novel Electronic, Excitonic, and Optical Features in 2D and 1D Lead-halide Hybrid Perovskites via Tuning of the Electronic Couplings between Organic Spacers and Inorganic Layers**

**HONG LI**, The University of Arizona, Tucson, AZ, USA

**D-1:IL08 Unveiling the Optical and Electronic Properties of Dimensionally Confined Halide Perovskites with Ab-initio Simulations**

**C. QUARTI**, University of Mons, Mons, Belgium

**D-1:IL09 A Feedback Model for Relaxor Ferroelectrics**

**H. KLIEM**, **A. LESCHHORN**, Saarland University, Saarbruecken, Germany

**D-1:IL10 The Topological Design of Exceptional Points for Multi-optical-parameter Control based on Deep Learning**

**CHANGZHI GU**, **PENG FU**, Institute of Physics, Chinese Academy of Sciences, Beijing, China

**D-1:IL11 Large-scale Nonadiabatic Dynamics Methods and Applications to Quantum Dots**

**LINJUN WANG**, Department of Chemistry, Zhejiang University, Hangzhou, China

**D-1:IL12 Electronic Structure of Pristine and Defective Layered Materials**

**S.M. GALI**, Laboratory for Chemistry of Novel Materials, Materials Research Institute, University of Mons, Mons, Belgium

**D-1:IL13 Progress in Multiphysics Modelling of Nanophotonics Components based on Phase Change Materials**

**D.N. CHIGRIN**, DWI Leibniz Institute for Interactive Materials, Aachen, Germany, I. Physikalisches Institut (1A), RWTH Aachen University, Aachen, Germany

**D-1:IL14 Charge and Exciton Dynamics in the Transient Delocalization Regime**

**S. GIANNINI**, **G. PRAMPOLINI**, **F. SANTORO**, Institute of Chemistry of OrganoMetallic Compounds, National Research Council (ICCOM-CNR), Pisa, Italy; **J. BLUMBERGER**, University College London, Department of Physics and Astronomy, Gower Street, London, UK; **D. BELJONNE**, Laboratory for Chemistry of Novel Materials, University of Mons, Mons, Belgium

**D-1:IL15 Molecular Engineering of D- $\pi$ -A-Type Structures Based on Nitrobenzofurazan (NBD) Derivatives for Both Organic Solar Cells and Nonlinear Optical Response**

**B. ABDELAZIZ**<sup>1,2</sup>, **S. PATANÉ**<sup>2</sup>, **S. AYACHI**<sup>1</sup>, <sup>1</sup>Laboratory of Physico-Chemistry of Materials (LR01ES19), Faculty of Sciences, University of Monastir, Monastir, Tunisia; <sup>2</sup>Department of Mathematical and Computer Sciences, Physical Sciences and Earth Sciences, University of Messina, Messina, Italy

## Session D-2

## Materials for energy generation and storage

**D-2:IL01 Interfacing Doped Graphene with Metal Surfaces or Molecular Layers**

**C. DI VALENTIN**, D. PERILLI, Dipartimento di Scienza dei Materiali, Università di Milano Bicocca, Milano, Italy

**D-2:IL02 Property Analysis and Simulation Package for Materials (PASP) and its Applications to Ferroic Materials**

**HONGJUN XIANG**, Department of Physics, Fudan university, Shanghai, China

**D-2:IL03 Predicting Solar Cell Efficiency from First Principles**  
**XINWEI WANG**<sup>1</sup>, S.R. KAVANAGH<sup>1</sup>, A. WALSH<sup>1,2</sup>, <sup>1</sup>Thomas Young Centre and Department of Materials, Imperial College London, London, UK; <sup>2</sup>Department of Physics, Ewha Womans University, Seoul, South Korea

**D-2:IL04 Capturing the Lone Pair Interactions in BaSnF<sub>4</sub> using Machine Learning Potential**

**XILIANG LIAN**<sup>1</sup>, M. SALANNE<sup>1,2,3</sup>, <sup>1</sup>Sorbonne Université, CNRS, Physicochimie des Électrolytes et Nanosystèmes Interfaciaux, France; <sup>2</sup>Réseau sur le Stockage Electrochimique de l'Energie (RS2E), FR CNRS 3459, Amiens Cedex, France; <sup>3</sup>Institut Universitaire de France (IUF), Paris, France

**D-2:IL05 Prediction of High-strain Polar Phases in Antiferroelectric PbZrO<sub>3</sub> from a Multiscale Approach**

**S. LISENKOV**, I. PONOMAREVA, University of South Florida, Tampa, FL, USA

**D-2:IL06 Design of Energy Conversion Materials by Computation and AI**

**WAN-JIAN YIN**, College of Energy, Soochow University, Suzhou, Jiangsu, China

**D-2:IL07 Modeling Organic Semiconductors from Low Doping to Ultra-high Charge Densities**

**G. D'AVINO**, Institut Néel, CNRS, Grenoble, France

**D-2:IL08 Modelling of Energy Storage and Optoelectronic Properties in Organic Molecular Materials**

**F. NEGRI**, Department of Chemistry "Giacomo Ciamician", University of Bologna, Italy and INSTM, UdR Bologna, Italy

**D-2:IL09 Electrochemical Energy Storage Material Design through Regulating Local Structure Properties**

**JIANJUN LIU**, Integrated Computational Materials Scientific Research Center, Shanghai institute of Ceramics, Chinese Academy of Sciences, Shanghai, China

**D-2:L10 Artificial Swimmers that Follow Traffic Signs, Move Against Flow and Climb Cliffs**

Q. BROSSEAU, F. BALBOA USABIAGA, E. LUSHI, Y. WU, L. RISTROPH, M.D. WARD, M.J. SHELLEY, **JUN ZHANG**, New York University, New York, and NJIT, USA

## Session D-3

## Materials for quantum information science

**D-3:IL01 Modelling Adatom Defects in Van der Waals Material Flakes: Interfacing Quantum Optics with Material Science**

D. DAMS, C. ROCKSTUHL, Karlsruhe Institute of Technology, Karlsruhe, Germany; G.W. BRYANT, Joint Quantum Institute, University of Maryland and National Institute of Standards and Technology, Gaithersburg, MD, USA; A. AYUELA, Centro de Física de Materiales and Donostia International Physics Center, San Sebastian, Spain; A. GHOSH, J. SZCZUCZKO, M. PELC, **K. SLOWIK**, Nicolaus Copernicus University in Torun, Torun, Poland

**D-3:L02 Cluster Dynamics Modeling Study of Irradiation-induced Microstructural Evolution in Tungsten**

**S. MOHAMED**, Q. YUAN, E. GAGANIDZE, J. AKTAA, Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany; J. GAO, Fudan University, Yangpu District, Shanghai, China

**D-3:L03 Gibbs Sampling via Cluster Expansions**

**N.M. EASSA**, M.M. MOUSTAFA, A. BANERJEE, Purdue University, West Lafayette, IN, USA; J.Y COHN, IBM

**D-3:IL04 Ab Initio Theory of Solid State Defect Qubits**

**A. GALI**, HUN-REN Wigner Research Centre for Physics & Budapest University of Technology and Economics, Budapest, Hungary

**D-3:IL05 Theoretical Design Ge/Si Quantum Wells towards Si-based Spin Qubits**

**JUN-WEI LUO**, State Key Laboratory of Superlattices and Microstructures, Institute of Semiconductors, Chinese Academy of Sciences, Beijing, China

**D-3:IL06 Theoretical Description of Topological Phases in Purely Organic 2D Materials**

**XIAOJUAN NI**, J.-L. BREDAS, Department of Chemistry and Biochemistry, The University of Arizona, Tucson, AZ, USA

## TRACK E

## COMPUTATIONAL MECHANICS OF MATERIALS ACROSS THE SCALES

## Session E-1

## Computational mechanics of nanoscale materials

**E-1:IL01 Mechanics of Additively Manufactured Materials**  
**L. VALDEVIT**, University of California, Irvine, CA, USA

**E-1:IL02 Simulations of Structural Phase Transitions in Crystals Using Metadynamics**

**R. MARTONAK**, Faculty of Mathematics, Physics and Informatics, Comenius University in Bratislava, Bratislava, Slovakia

**E-1:IL03 Lubricity in Hard and Soft Matter Contacts**

**A. VANOSSI**, CNR-IOM & SISSA, Trieste, Italy, in collaboration with: C. BECHINGER, A. BENASSI, T. BRAZDA, X. CAO, L. GIGLI, R. GUERRA, S. KAWAI, A. KHOSRAVI, D. MANDELLI, N. MANINI, E. MEYER, E. PANIZON, A. SILVA, E. TOSATTI, M. URBACH, J. WANG

**E-1:IL04 Transformation-induced Plasticity in Ceramics: Leveraging Machine-learning Potentials**

**D. RODNEY**, G. HUYNH, JUN-YU ZHANG, T. ALBARET, University of Lyon, Villeurbanne, France

**E-1:IL05 Stretching and Breaking of Polymeric Nanofibres**

E. BERING<sup>1</sup>, **A.S. DE WIJN**<sup>2</sup>, <sup>1</sup>Department of Physics and PoreLab, NTNU, Trondheim, Norway; <sup>2</sup>Department of Mechanical and Industrial Engineering and PoreLab, NTNU, Trondheim, Norway

**E-1:IL06 How Temperature- and Electric-field-driven Chain Reorientation affects Friction**

**M.M. GIANETTI**, Dept of Mechanical and Industrial Engineering (MTP), Norwegian University of Science and Technology (NTNU), Trondheim, Norway; R. GUERRA, Center for Complexity and Biosystems, Dept of Physics, University of Milan, Milan, Italy; A. VANOSSI, CNR-IOM, Consiglio Nazionale delle Ricerche - Istituto Officina dei Materiali and International School for Advanced



Studies (SISSA), Trieste, Italy; M. URBAKH, Dept of Physical Chemistry, School of Chemistry, The Raymond and Beverly Sackler Faculty of Exact Sciences and The Sackler Center for Computational Molecular and Materials Science, Tel Aviv University, Tel Aviv, Israel; N. MANINI, Dipartimento di Fisica, Università degli Studi di Milano, Milan, Italy

**E-1:IL07 In situ Formation of Superlubricious Surfaces by Mechano-chemical Decomposition of Organic Friction Modifiers**

**TAKUYA KUWAHARA**, Osaka Metropolitan University, Sakai, Osaka, Japan

**E-1:IL08 Atomistic Simulation for Hetero-deformation in Gradient Nanograined Structure**

LIKE XU, DAQIAN XU, FEI CHEN, **ZHIFENG HUANG**, International School of Materials Science and Engineering, Wuhan University of Technology, Wuhan, China State Key Laboratory of Advanced Technology for Materials Synthesis and Processing, Wuhan University of Technology, Wuhan, China

**E-1:IL09 The Mechanism of Strong Reinforcement of Si Nano-powders by thin Continuous SiC Coatings**

K. KAYANG, **A.N. VOLKOV**, Department of Mechanical Engineering, University of Alabama, Tuscaloosa, AL, USA

**E-1:IL10 SEM2: A Coarse-grained Particle Framework for Multiscale Cell Mechanics**

S. CHATTARAJ, **F. PASQUALINI**, University of Pavia, Pavia, Italy

**E-1:IL11 Tribologically Induced Nanoscale Materials Transformations**

**G. MORAS**, T. REICHENBACH, M. MOSELER, Fraunhofer IWM and MikroTribologie Centrum  $\mu$ TC, Freiburg, Germany; L. PASTEWKA, University of Freiburg, Germany

**E-1:IL12 Probing the Solute Effect on Twin Embryo Growth in Mg Alloys**

**YANG HU**, D.M. KOCHMANN, Mechanics & Materials Lab, ETH Zurich, Zurich, Switzerland

### Session E-2

Computational mechanics in nanodevice applications

**E-2:IL01 Design and Simulation of Micro- and Nanotechnology Tools for Biomedical Applications**

**E. CIMETTA**, Università degli Studi di Padova, Padova, Italy

**E-2:IL02 Molecular Dynamics Investigation of Cross-linked Gold Nanoparticle Thin Film**

KAI-CHIH YEH, YA-YUN TSAI, **SHU-WEI CHANG**, Department of Civil Engineering, National Taiwan University, Taipei, Taiwan

### Session E-3

Computational mechanics at mesoscopic / macroscopic scale

**E-3:IL01 A Mapping between the Non-linear Micromechanics of Glasses and Elasto-plastic Models**

**D. RICHARD**, Laboratoire Navier, Champs-sur-Marne, France

**E-3:IL02 Extreme Events on Structures. The Key Role of Multiphysics Simulation**

**A. LARESE**<sup>1,2</sup>, L. MORENO<sup>4</sup>, V. SINGER<sup>3</sup>, N. CRESCENZIO<sup>1</sup>, R. WUECHNER<sup>4</sup>, <sup>1</sup>Dept. of Mathematics, Università di Padova, Padova, Italy; <sup>2</sup>Institute for Advanced Studies of the Technical University of Munich TUM-IAS, Germany; <sup>3</sup>Chair for Structural Analysis, Technical University of Munich, Germany; <sup>4</sup>Institute of Structural Analysis, Technical University of Braunschweig, Germany

**E-3:IL03 Multifractal Mechanics and Thermal Transport of Solids: Theory, Experiments, and Uncertainty Analysis Across Scales**

**W.S. OATES**, B. PAHARI, M. CARVAJAL, Florida State University, Department of Mechanical Engineering, Tallahassee, FL, USA

**E-3:IL04 Unveiling Microstructure Effects on Fracture: Atomistic Simulations, Mesoscale Models and Micro-mechanical Tests**

**E. BITZEK**, Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

**E-3:IL05 Multiscale Modeling of Nanomechanical Deformation in High Entropy Alloys**

**S. PAPANIKOLAOU**, National Centre of Nuclear Research, Otwock, Poland

**E-3:IL06 Modeling the Deformation and Ductile Damage of Irradiated EUROFER97**

**R. RAJAKRISHNAN**, E. GAGANIDZE, J. AKTAA, Karlsruhe Institute of Technology (KIT), Institute for Applied Materials, Eggenstein-Leopoldshafen, Germany

**E-3:IL07 Nonlocal Fracture in Elastomers: Experiments and Continuum Modeling**

**HANSOHL CHO**, JAEHEE LEE, JEONGUN LEE, Korea Advanced Institute of Science and Technology, Yuseong Gu, Daejeon, South Korea

**E-3:IL08 Multiscale Modelling of Ceramic Matrix Composites**

**E. BARANGER**, Université Paris-Saclay, CentraleSupélec, ENS Paris-Saclay, CNRS, LMPS - Laboratoire de Mécanique Paris-Saclay, France

**E-3:IL09 Modelling the Data of Nonlinear Mechanical Properties of Fabrics by Decomposing Friction**

**G. STYLIOS**, L. LUO, Heriot Watt University, Scotland

**E-3:IL10 Novel Tool to Perform Thermomechanical Characterisation on Refractory Microstructure Design using Discrete Element Method (DEM)**

**H. RANGANATHAN**<sup>1,2</sup>, D. ANDRE<sup>2</sup>, M. HUGER<sup>2</sup>, R. SOTH<sup>1</sup>, C. WÖHRMEYER<sup>1</sup>, <sup>1</sup>Imerys Technology Center, Vaulx-Milieu, France; <sup>2</sup>University of Limoges, IRCER, UMR CNRS 7315, Limoges, France

**E-3:IL11 Numerical Simulation of Seismic Wave Field in the Two-phase Viscoelastic EDA Media**

**ANG-YANG YU**, Harbin Engineering University, Harbin, China

### Session E-4

Computational mechanics in simulated operating conditions

**E-4:IL01 Cluster Dynamics Modelling of Irradiation Induced Defects and their Evolution**

**JIE GAO**, Applied Ion Beam Physics Laboratory, Institute of Modern Physics, Fudan University, Shanghai, China

**E-4:IL02 Novel Approaches to Computational Additive Manufacturing**

D. SOLDNER, **J. MERGHEIM**, Institute of Applied Mechanics FAU Erlangen-Nürnberg, Erlangen, Germany

**E-4:IL03 Computational Mechanobiology Towards Applications in Tissue Engineering**

**J.H. HENDERSON**, Syracuse University, Syracuse, NY, USA

## Session E-5

## Advances in theory and computational methods

**E-5:IL01 Recent Advances in Tribological Modelling and Simulations Across the Scales**

**D. DINI**, Department of Mechanical Engineering, Imperial College London, South Kensington Campus, London, UK

**E-5:IL02 Novel Approaches to Computational Continuum-atomistic Coupling for Polymers**

**S. PFALLER**, L. LAUBERT, M. RIES, F. WEBER, W. ZHAO, Institute of Applied Mechanics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

**E-5:IL03 Concurrent Multiscale Modeling of Boundary Lubrication, Enabled by Machine Learning**

**H. HOLEY**<sup>1, 2, 3</sup>, P. GUMBSCH<sup>1, 3</sup>, L. PASTEWKA<sup>2</sup>, <sup>1</sup>Karlsruhe Institute of Technology, Karlsruhe, Germany; <sup>2</sup>University of Freiburg, Freiburg, Germany; <sup>3</sup>Fraunhofer IWM Freiburg, Freiburg, Germany

**E-5:IL04 Eigenstrain Representation of Defects, Dislocations, and Dislocation Networks**

**S.L. DUDAREV**, P.-W. MA, A.R. WARWICK, M. BOLEININGER, L. REALI, UKAEA, Culham Science Centre, Oxfordshire, UK

**E-5:IL05 Some Recent Advances and Applications in Isogeometric Analysis**

**A. REALI**, Department of Civil Engineering and Architecture, University of Pavia, Pavia, Italy

**E-5:IL06 Adaptive (Iso-)geometric Modeling for CAD/CAE Applications**

**C. GIANNELLI**, University of Florence, Florence, Italy

**E-5:IL07 Mechanics of Bioinspired, Bionic, Nano and Meta Materials**

**N. PUGNO**, University of Trento, Italy

**E-5:IL08 The Forming, Function and Optimization of Bio-inspired Composites by Multiphysics Simulations and Generative Model**

**ZHAO QIN**, Syracuse University, Syracuse, NY, USA

**F-1:L03 Microstructure Design of Polycrystalline Ceramics for Energy Applications**

**E. GARCIA**, Purdue University, West Lafayette, IN, USA

**F-1:IL04 Accelerated Autonomous Exploration of Oxide Electrode Materials for High-temperature Electrolyzers and Fuel Cells**

**JAKE HUANG**<sup>1</sup>, M. PAPAC<sup>2</sup>, D. FEBBA<sup>1</sup>, R. O'HAYRE<sup>3</sup>, A. ZAKUTAYEV<sup>3</sup>, <sup>1</sup>National Renewable Energy Laboratory, Golden, CO, USA; <sup>2</sup>National Institute of Standards and Technology, Gaithersburg, MD, USA; <sup>3</sup>Colorado School of Mines, Golden, CO, USA

**F-1:L05 Relation between Double Layer Structure, Capacitance and Surface Tension in Electrowetting of Graphene and Aqueous Electrolytes**

**Z. WEI**, J.D. ELLIOTT, A.A. PAPADERAKIS, R.A.W. DRYFE, **P. CARBONE**, Dept of Chemical Engineering, The University of Manchester, Manchester, UK; Diamond Light Source, Diamond House, Harwell Science and Innovation Park, Didcot, Oxfordshire, UK; Dept of Chemistry and Henry Royce Institute, The University of Manchester, Manchester, UK

**F-1:L06 Battery Simulations with Ab Initio Molecular Dynamics**

**M. SMEU**, Department of Physics, Binghamton University - SUNY, Binghamton, NY, USA

**F-1:L07 Solar Fuel from Photoelectrochemical Water Splitting: A Case Study of ZnO (Wurtzite) Single Crystals and Dense Thin Films**

**L. KAVAN**<sup>1</sup>, H. KRYSOVA<sup>1, 2</sup>, V. MANSFELDOVA<sup>1</sup>, H. TARABKOVA<sup>1</sup>, A. PISARIKOVA<sup>2</sup>, Z. HUBICKA<sup>2</sup>, <sup>1</sup>J. Heyrovsky Institute of Physical Chemistry, Czech Academy of Sciences, Prague, Czech Republic; <sup>2</sup>Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic

## Session F-2

## Photovoltaics

**F-2:IL01 First-principles Study of Defect Control in Thin Film Solar Cell**

**SU-HUAI WEI**, Beijing Computational Science Research Center, Beijing, China

**F-2:IL02 Understanding and Design of Photovoltaic and Energy Storage Materials**

**M. CHAN**, Center for Nanoscale Materials, Argonne National Laboratory, Lemont, IL, USA

**F-2:L03 Accelerated Screening of Ternary Chalcogenides for Potential Photovoltaic Applications**

**TIANSHU LI**, Department of Materials, Imperial College London, London, UK

**F-2:L04 Solar Cells Efficiency Enhancement via the Plasmonic Effect**

**A. AXELEVITCH**, Holon Institute of Technology (HIT), Holon, Israel

**F-2:L05 Photovoltaic and Thermoelectric Properties of Ag<sub>2</sub>MnGeS<sub>4</sub> Kesterite: First-principal Investigations**

**N.F. ZAHRA**, **H. JEBARI**, N. BEKKIOUI, H. EZ-ZAHRAOUI, Laboratory of Condensed Matter and Interdisciplinary Sciences, Unitei de Recherche Labelliseie CNRST, URL-CNRST-17, Faculty of Sciences, Mohammed V University of Rabat, Morocco

**F-2:IL06 Spin and Transient Delocalization Effects in Organic Semiconductors**

**D. BELJONNE**, University of Mons, Mons, Belgium

## TRACK F

## DESIGNING MATERIALS FOR SUSTAINABLE ENERGY APPLICATIONS

## Session F-1

## Electrochemical energy systems

**F-1:IL01 Computer Modeling of Solid-state Batteries**

**V.I. YAMAKOV**<sup>1, 2</sup>, Y. LIN<sup>2</sup>, A.A. RAINS<sup>3, 4</sup>, J. SU<sup>2</sup>, J.H. KANG<sup>2</sup>, D.A. DORNBUSCH<sup>5</sup>, R.P. VIGGIANO<sup>5</sup>, <sup>1</sup>Analytical Mechanics Associates, Hampton, VA, USA; <sup>2</sup>NASA Langley Research Center, Hampton, VA, USA; <sup>3</sup>NASA Interns, Fellows, and Scholars (NIFS) Program, NASA Langley Research Center, Hampton, VA, USA; <sup>4</sup>University of Georgia, Athens, GA, USA; <sup>5</sup>NASA Glenn Research Center, Cleveland, OH, USA

**F-1:IL02 Recent Advance in Computational Approaches to Electrochemical Interfaces**

**M.-L. DOUBLET**, ICGM, Univ Montpellier, CNRS, Montpellier, France

**F-2:IL07 Shift and Ballistic Currents from First Principles**  
Z. DAI, University of Texas, Austin, TX, USA; A.M. SCHANKLER, A.M. RAPPE, University of Pennsylvania, USA

**F-2:IL08 Selenium as a Top-cell Absorber for Tandem Photovoltaic- and PEC-cells**

R. NIELSEN, T. YOUNGMAN, A. AZZAR, A. CROVETTO, B. SEGER, H. MOUSTAFA, S. LEVCENCO, H. HEMPEL, T. OLSEN, O. HANSEN, I. CHORKENDORFF, T. UNOLD, P.C.K. VESBORG, Technical University of Denmark, Kgs. Lyngby, Denmark

**F-2:IL09 Manipulation of Bulk Photovoltaic Effect in Low-dimensional Semiconductors: A First-principles Study**  
BING HUANG, Beijing Computational Science Research Center, Beijing, China

**F-2:L10 Engineering of the Electronic Structure of Semiconducting Oxides for Application in Li-ion and Li-sulfur Batteries**

M. ZUKALOVA, M. VINARCIKOVA, B. PITNA LASKOVA, L. KAVAN, J. Heyrovsky Institute of Physical Chemistry, Czech Acad. Sci, Prague, Czech Rep.; O. PORODKO, M. FABIAN, Institute of Geotechnics, Slovak Acad. Sci, Kosice, Slovak Rep.

### Session F-3

#### Thermoelectrics

**F-3:IL01 Accelerated Discovery of Thermoelectric Materials using Machine Learning**

A.K. SINGH, Indian Institute of Science, Bangalore, India

**F-3:IL02 Manipulation of Interatomic Bonding to Effectively Suppress Phonon Thermal Conduction in Materials**

MASATO YOSHIYA, W. SEKIMOTO, T. HARA, R. NISHIOKA, T. CONG TRAN, Susumu Fujii Div. of Mats and Manufacturing Sci., Graduate School of Eng., Osaka University, Suita, Osaka, Japan

**F-3:L03 Accelerated Discovery of Efficient Thermoelectric Materials Using a Novel Machine Learning Approach**

S. ATHAR, N. RAMSAHYE, P. JUND, ICGM, Université de Montpellier, CNRS, Montpellier, France

**F-3:L04 Silicon Thermoelectrics for Energy Autonomous Integrated Circuits**

M. LEE, The University of Texas at Dallas, Richardson, TX, USA

### Session F-4

#### Catalysts and catalytic processes for energy applications

**F-4:IL01 Targeted Design of Organic Photocatalysts for Energy and Materials Conversion**

J. GIERSCHNER, Madrid Institute for Advanced Studies, IMDEA Nanoscience, Madrid, Spain

**F-4:IL02 DFT-CES: Eyes to See the Unseen, Buried Electric Double Layer**

HYUNGJUN KIM, Department of Chemistry, KAIST, Daejeon, South Korea

**F-4:IL03 MOFs as Potential Heterogeneous Catalysts for Alkene Hydroformylation**

YIFEI CHEN, L.T. WANG, H. GONG, M.H. ZHANG, R & D Center for Petrochemical Technology, Tianjin University, China

**F-4:IL04 Exploring Catalytic Reaction Networks with Machine Learning**

K. REUTER, Fritz Haber Institute of the Max Planck Society Berlin, Germany

**F-4:IL05 Accelerating Catalysis Simulations with Robust Gaussian Processes**

T. BLIGAARD, A.L. VISHART, Catalysis Theory Center, Technical University of Denmark, Lyngby, Denmark

### TRACK G

## BIG DATA, ARTIFICIAL INTELLIGENCE AND MACHINE LEARNING METHODS FOR ACCELERATED MATERIALS DISCOVERY AND ADVANCEMENT

### Session G-1

Advances in machine learning principles, algorithms, descriptors and databases, machine learning approaches, their interpretability and potential pitfalls

**G-COST The EuMINE COST Action: Advancing Materials Informatics for Coordinated Innovation in European Research**

F. MERCURI, CNR, Bologna, Italy

**G-1:IL01 Enabling the 4th Paradigm for Accelerated Materials Innovation**

K.A. PERSSON, University of California at Berkeley, Berkeley, CA, USA

**G-1:IL02 Construct Exchange-correlation Functional via Machine Learning and Delta-learning Method**

GUANHUA CHEN, The University of Hong Kong, Shatin, Hong Kong

**G-1:IL03 New Approaches to Predicting and Understanding the Electrochemical Stability of Inorganic Materials**

J. MONTOYA, Toyota Research Institute, Los Altos, CA, USA

**G-1:IL04 Materials Discovery using Simulations and Deep Learning**

A. MERCHANT, S. BATZNER, M. AYKOL, E.D. CUBUK, Google DeepMind, Mountain View, CA, USA

**G-1:IL05 Vibrational Properties of Inorganic Materials from High-throughput Density-functional Perturbation Theory and Machine-learning**

G.-M. RIGNANESE, Institute of Condensed Matter and Nanosciences (IMCN), UCLouvain, Louvain-la-Neuve, Belgium

**G-1:L06 Equivariant Tensor Network Potentials**

M. HODAPP, Materials Center Leoben, Leoben, Austria; A. SHAPEEV, Skoltech, Moscow, Russia

**G-1:L07 Utility of Transfer Learning in Computational Materials Science**

S.G. GOPALAKRISHNAN<sup>1</sup>, R. DEVI<sup>1</sup>, K.T. BUTLER<sup>2</sup>, <sup>1</sup>Dept of Materials Eng., Indian Institute of Science, Bengaluru, India; <sup>2</sup>Dept of Chemistry, University College London, London, UK

**G-1:L08 Physical Insights from Materials Informatics: A Generalized Analysis Framework**

D. BENIWAL, P.K. RAY, IDEAs Laboratory, Metallurgical and Materials Engineering, IIT Ropar, Rupnagar, India

**G-1:L09 Multiscale Study of the Electronic Structure of Halide Perovskites Slabs**

A. CHARKIN-GORBULIN, D. BELJONNE, C. QUARTI, University of Mons, Mons, Belgium; I. POLTAVSKY, A. TKATCHENKO, University of Luxembourg, Luxembourg

**G-1:L10 Performance and Trustworthiness of Different AI models for Predicting Mechanical Properties of Steel Sheets**

G. MILLNER<sup>1</sup>, L. ROMANER<sup>2</sup>, D. SCHEIBER<sup>1</sup>, M. MÜCKE<sup>1</sup>, <sup>1</sup>Materials Center Leoben Forschungs GmbH, Leoben, Austria; <sup>2</sup>Montanuniversität Leoben, Leoben, Austria

**G-1:IL11 Symmetry Constraints in Machine Learning Models of Electronic and Atomic Interactions**

B. KOZINSKY, Harvard University, USA

## Session G-2

## Virtual materials design and evaluation

**G-2:IL01 Navigating Materials Space at Warp Speed**

**A. WALSH**, Department of Materials, Imperial College London, London, UK

**G-2:IL02 Tackling Ion Transport and Interfacial Evolutions in Solid-state Batteries Machine-learning and Cluster Expansion Strategies**

Z. DENG<sup>1</sup>, A.A. PANCHAL<sup>2,3</sup>, W. XIE<sup>1</sup>, G.S. GAUTAM<sup>4</sup>, **P. CANEPA**<sup>1,2,3</sup>, <sup>1</sup>Department of Materials Science and Engineering, National University of Singapore, Singapore; <sup>2</sup>Department of Electrical and Computer Engineering, University of Houston, Houston, TX, USA; <sup>3</sup>Texas Center for Superconductivity, University of Houston, Houston, TX, USA; <sup>4</sup>Department of Materials Engineering, Indian Institute of Science, Bengaluru, Karnataka, India

**G-2:L03 A Physics-informed Deep Learning Framework for Closed-loop Material Discovery**

**M. SHARMA PRIYADARSHINI**, O. ROMILUYI, G. WANG, Department of Chemical and Biomolecular Engineering at The Johns Hopkins University, Baltimore, MD, USA; K. MISKIN, Department of Materials Science & Engineering at The Johns Hopkins University, Baltimore, MD, USA; P. CLANCY, Department of Chemical and Biomolecular Engineering at The Johns Hopkins University, Baltimore, MD, USA

**G-2:L04 Inverse Design of Metal-organic Frameworks for Direct Air Capture of CO<sub>2</sub> via Deep Reinforcement Learning**

**HYUNSOO PARK**, S. MAJUMDAR, X. ZHANG, J. KIM, B. SMIT, Imperial College London, London, UK

**G-2:IL05 Self-driving Fluidic Labs: Accelerated Materials Discovery, Optimization, and Manufacturing**

**M. ABOLHASANI**, Department of Chemical & Biomolecular Engineering, North Carolina State University, Raleigh, NC, USA

**G-2:IL06 Machine Learning Discovery of Materials**

**J. SCHMIDT**, Materials Theory ETH Zurich, Zurich, Switzerland; P. BORLIDO, Department of Physics, University of Coimbra, Portugal; A. ROMERO, Department of Physics and Astronomy West Virginia University, USA; T. CERQUEIRA, Department of Physics, University of Coimbra, Portugal; S. BOTTI, RC-FEMS and Faculty of Physics, Ruhr University Bochum, Germany; M. MARQUES, RC-FEMS and Faculty of Mechanical Engineering Ruhr University Bochum, Germany

**G-2:L07 Accelerated Alloy Discovery and Optimization through the Batch-wise Improvement in Reduced Design Space using a Holistic Optimization Technique (BIRDSHOT)**

**R. ARROYAVE**, Texas A&M University, College Station, TX, USA

## Session G-3

## Integrating machine learning and simulations for materials design and manufacturing

**G-3:IL01 Machine Learning Guided High-throughput Combinatorial Printing and Characterization towards Autonomous Materials Discovery and Manufacturing**

**YANLIANG ZHANG**, University of Notre Dame, Notre Dame, IN, USA

**G-3:IL02 Material Discovery and Simulation using Machine Learning Potentials**

**SEUNGWU HAN**, Department of Materials Science and Engineering, Seoul National University, Seoul, South Korea

**G-3:L03 Structure Complements: A New Materials Taxonomy for ML-guided Materials Discovery**

**J.M. RONDINELLI**, K.D. MILLER, Northwestern University, Evanston, IL, USA

**G-3:L04 Bayesian Optimization of Carbide Free Bainitic Steels**

**B. SCHUSCHA**<sup>1</sup>, D. SCHEIBER<sup>1</sup>, D. BRANDL<sup>1</sup>, M. MÜCKE<sup>1</sup>, L. ROMANER<sup>2</sup>, <sup>1</sup>Materials Center Leoben Forschung GmbH, Leoben, Austria; <sup>2</sup>Dept of Materials Science, Montanuniversität Leoben, Leoben, Austria

**G-3:L05 An AI Method for Phase Diagram Construction from First Principles**

T. MIRYASHKIN<sup>1</sup>, O. KLIMANOVA<sup>1</sup>, V. LADYGIN<sup>2</sup>, **A. SHAPEEV**<sup>1</sup>, <sup>1</sup>Skolkovo Institute of Science and Technology, Moscow, Russia; <sup>2</sup>California Institute of Technology, USA

**G-3:IL06 Materials and Molecular Modelling, Imaging, Informatics and Integration (M3I3)**

**SEUNGBUM HONG**, KAIST, Daejeon, South Korea

**G-3:IL07 Design Metastability in High-entropy Alloys by Tailoring Unstable Fault Energies**

**WEI CHEN**, Dept of Materials Design and Innovation, University at Buffalo, State University of New York, Buffalo, NY, USA

**G-3:L08 The MCL-MAP: A Platform for Accelerated Materials Design Based on Active Learning**

**J. SPITALER**, D. SCHEIBER, N. BEDOYA, Materials Center Leoben Forschung GmbH, Leoben, Austria; H. TRAN, H. GURSCH, Know Center GmbH, Graz, Austria; L. ROMANER, Montanuniversität Leoben, Leoben, Austria

**G-3:L09 Metastable Transition Metal Dichalcogenides from Machine Learning Force Fields**

**ZHENZHU LI**, A. WALSH, Department of Materials, Imperial College London, UK

**G-3:IL10 Accelerated Development of Materials using High-throughput Strategies and AI/ML**

**S.R. KALIDINDI**, Georgia Tech, Atlanta, GA, USA

**G-3:IL11 Machine Learning-driven Optimization of 3D Printing Composite Structures and Processes**

**SEUNGHWA RYU**, Mechanical Engineering, Korea Advanced Institute of Science and Technology, Daejeon, South Korea

**G-3:L12 Composition and Property Prediction of Polymer-derived Silicon Oxycarbides**

**KATHY LU**, University of Alabama at Birmingham, Birmingham, AL, USA; YI JE CHO, Sunchon National University, South Korea

**G-3:L13 Machine Learning Point Defect Reconstructions**

**I. MOSQUERA-LOIS**<sup>1</sup>, S.R. KAVANAGH<sup>1,2</sup>, D.O. SCANLON<sup>3</sup>, A. GANOSE<sup>4</sup>, A. WALSH<sup>1,5</sup>, <sup>1</sup>Thomas Young Centre & Dept of Materials, Imperial College London, London, UK; <sup>2</sup>Thomas Young Centre & Dept of Chemistry, University College London, London, UK; <sup>3</sup>School of Chemistry, University of Birmingham, Edgbaston, Birmingham, UK; <sup>4</sup>Thomas Young Centre & Dept of Chemistry, Imperial College London, London, UK; <sup>5</sup>Dept of Physics, Ewha Womans University, Seoul, South Korea

## Session G-4

## High throughput materials characterization and testing

**G-4:IL01 A-lab: An Autonomous Laboratory for the Accelerated Synthesis of Novel Inorganic Materials**

**G. CEDER**, University of California at Berkeley and Lawrence Berkeley National Laboratory, Berkeley, CA, USA

**G-4:IL02 Autonomous Combinatorial Experimentation for Atomic Layer Synthesis**

**ICHIRO TAKEUCHI**, University of Maryland, College Park, MD, USA

**G-4:L03 Data-driven Material Exploration of Multi-element Substituted Fluorides toward high Conductivity**

**TETSUYA YAMADA**<sup>1,2</sup>, Y. TAKETOMI<sup>3</sup>, F. HAYASHI<sup>1</sup>, K. TESHIMA<sup>1,2</sup>, <sup>1</sup>Faculty of Engineering, Shinshu University, Nagano, Japan; <sup>2</sup>Research Initiative for Supra-Materials, Shinshu University, Japan; <sup>3</sup>Graduate School of Science and Technology, Shinshu University, Japan

**G-4:L04 Machine Learning Aids High Throughput Material Characterization**

**Q. ALI**, A. KOVACS, J. FISCHBACHER, H. OEZELT, M. GUSENBAUER, D. BOEHM, H. MOUSTAFA, T. SCHREFL, Christian Doppler Laboratory for magnet design through physics informed machine learning, Department for Integrated Sensor Systems, University for Continuing Education Krems, Wiener Neustadt, Austria; M. YANO, N. SAKUMA, A. KINOSHITA, T. SHOJI, Advanced Materials Engineering Division, Toyota Motor Corporation, Susono, Japan; Y. HONG, T. DEVILLERS, N.M. DEMPSEY, Institute Néel, Université Grenoble Alpes, CNRS, Grenoble INP, Grenoble, France

**G-4:IL05 Automated and Autonomous Materials Synthesis Characterization of Inorganic Film Materials**

D. FEBBA, **A. ZAKUTAYEV**, National Renewable Energy Laboratory, Golden, CO, USA

**G-4:L06 Systematic Data Enabled Element-wise Machine Learning Strategy for Predicting Metallic Glass-forming Ability in Ternary Systems**

Z. LIU, C. CHEN, Y. ZHOU, **LANTING ZHANG**, H. WANG, Shanghai Jiao Tong University, Shanghai, China

**G-4:L07 Passive Ultrasonic Beamforming for Fast and Efficient Imaging of Solids**

**F. LANZA DI SCALEA**, C. HUANG, A.Z. HOSSEINZADEH, Experimental Mechanics & NDE Laboratory, Department of Structural Engineering, University of California San Diego, La Jolla, CA, USA

Session G-5

Big data, machine learning and artificial intelligence moving towards next generation smart manufacturing and sustainable development

**G-5:IL01 Collaborative Intelligence for Accelerated Development of Clean Energy Technologies**

**SHIJING SUN**, University of Washington, Seattle, WA, USA

**G-5:L02 Prediction of Performance and Assessment of Reusability and Recycling of Refractory Materials using Non-destructive Online Evaluation and Machine Learning Algorithms**

**A.K. GOPE**<sup>1,2</sup>, A. BOULLE<sup>2</sup>, M. PICICCOA<sup>1</sup>, F. BIRKELBACH<sup>3</sup>, L. REBOUILLAT<sup>4</sup>, S. ROMERO BAIVIER<sup>1</sup>, M. HUGER<sup>2</sup>, <sup>1</sup>Vesuvius group plc, Dept of Advanced Refractories, Ghlin, Belgium; <sup>2</sup>University of Limoges, IRCER, UMR CNRS 7315, Limoges, France; <sup>3</sup>TU Wien, Institute for Energy Systems and Thermodynamics, Vienna, Austria; <sup>4</sup>Pyrotek Inc, Mineral Processing, Iron & Steel Dept, Drummondville, QC, Canada

**G-5:IL03 Utilizing Latent Space for Material Research and Development and Toward Digital Transformation**

**TETSUYA SHOJI**, Toyota Motor Corporation, Advanced R&D and Engineering Company, Advanced Data Science Management Div. WAVEBASE project, Susono, Shizuoka, Japan

**G-5:IL04 FAIR Data for Accelerated Materials Discovery: The NOMAD Project**

**C. DRAXL**, Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

**G-5:IL05 Accelerating Development of Materials with Artificial Intelligence and Machine Learning**

J. SAAL, **M. MUSTO**, Citrine Informatics, Bad Wiessee, Germany

**G-5:IL06 A Field Polarized by AI: How to Navigate the Conclusions and Delusions?**

**J.C. AGAR**, Department of Mechanical Engineering and Mechanics, Drexel University, Philadelphia, PA, USA

TRACK H

**ADVANCES IN MATERIALS AND DEVICES RESEARCH FOR DIGITAL, NEUROMORPHIC AND UNCONVENTIONAL COMPUTING**

Session H-1.1

Memristive materials and devices for brain inspired computing

**H-1.1:IL01 Memristive Devices for Bio-inspired Information Pathways**

A. LINKENHEIL<sup>1</sup>, Z. GENG<sup>1</sup>, K. NIKIRUY<sup>1</sup>, B. SPETZLER<sup>1</sup>, J. SCHNEEGASS<sup>2</sup>, T. IVANOV<sup>1,2</sup>, F. SCHWIERZ<sup>1</sup>, **M. ZIEGLER**<sup>1,2</sup>, <sup>1</sup>Micro- and Nanoelectronic Systems, Dept of Electrical Eng. and Information Technology, TU Ilmenau, Germany; <sup>2</sup>Institute of Micro- and Nanotechnologies MacroNano®, TU Ilmenau, Germany

**H-1.1:IL02 Oxide Materials for Artificial Neurons**

M. SALVERDA, M. VAN DEN BROEK, R. HAMMING-GREEN, P. NUKALA, **B. NOHEDA**, University of Groningen, Zernike Institute for Advanced Materials, Groningen, Netherlands

**H-1.1:IL03 Leveraging Ferroelectric Technologies for Neuromorphic Computing**

**E. COVI**, NaMLab gGmbH, Dresden, Germany

**H-1.1:IL04 Materials Design and Defect Engineering towards Quantum Conductance and Neuromorphics in Memristive Devices**

**L. ALFF**, Materials Science, Technische Universität Darmstadt, Darmstadt, Germany

**H-1.1:L05 Effect of the La<sub>2</sub>NiO<sub>4</sub>+ $\sigma$  Deposition Temperature on the Memristive Properties of the TiN/La<sub>2</sub>NiO<sub>4</sub>+ $\sigma$ /Pt Devices**

**A. KOROLEVA**<sup>1,2</sup>, N.A. NGUYEN<sup>1,2</sup>, C. TERNON<sup>2</sup>, M.A. BURRIEL<sup>2</sup>, E.-I. VATAJELU<sup>1</sup>, <sup>1</sup>Université Grenoble Alpes, CNRS, Grenoble INP, TIMA, Grenoble, France; <sup>2</sup>Université Grenoble Alpes, CNRS, Grenoble INP, LMGP, Grenoble, France

**H-1.1:L06 Reduction of Energy Requirements in Halide Memristors by using Oxidized Metallic Buffer Layers**

**A. GUERRERO**, Institute of Advanced Materials (INAM), Universitat Jaume I, Castelló, Spain

**H-1.1:L07 Ferroelectric Memristors: From Biorealistic Synapses to Spiking Neurons**

**A. KHANAS**, N. SIZYKH, N. ZHIDKOV, A. ZENKEVICH, Moscow Institute of Physics and Technology (National Research University), Dolgoprudny, Moscow region, Russian Federation; C. HEBERT, L. BECERRA, N. JEDRECY, Institut des Nano Sciences de Paris (INSP), CNRS UMR 7588, Sorbonne Université, Paris Cedex, France

## Session H-1.2

## Phase change materials and applications

**H-1.2:IL01 Phase Change Materials for Reliable Flexible Memories**

**S. CALVI**<sup>1</sup>, M. BERTELLI<sup>2</sup>, S. DE SIMONE<sup>2</sup>, F. MAITA<sup>2</sup>, F. DE MATTEIS<sup>3</sup>, S. PRILI<sup>1, 2</sup>, F. RIGHI RIVA<sup>1</sup>, V. MUSSI<sup>2</sup>, A. DIAZ FATTORINI<sup>1</sup>, F. ARCIPRETE<sup>1, 2</sup>, M. LONGO<sup>2, 4</sup>, R. CALARCO<sup>2</sup>, <sup>1</sup>Department of Physics University of Rome Tor Vergata, Rome, Italy; <sup>2</sup>Institute for Microelectronics and Microsystems (CNR-IMM), Rome, Italy; <sup>3</sup>Department of Industrial Engineering University of Rome Tor Vergata, Rome, Italy; <sup>4</sup>Department of Chemistry University of Rome Tor Vergata, Rome, Italy

**H-1.2:L02 Sb-Te Based Thin Films Containing Gallium: Deposition and Properties**

M. KOTRLA, P. JANICEK, J. GUTWIRTH, J. PRIKRYL, T. HALENKOVIC, **P. NEMEC**, Faculty of Chemical Technology, University of Pardubice, Pardubice, Czech Republic; F. CHEVIRE, V. NAZABAL, Institut des Sciences Chimiques de Rennes, UMR CNRS 6226, Université de Rennes, Rennes, France

**H-1.2:L03 The Influence of Sb/Te Ratio on the Crystallization Kinetics of GeSbTe Alloys**

**O. DAOUDI**<sup>1</sup>, E. NOLOT<sup>1</sup>, F. FILLOT<sup>1</sup>, J. LI<sup>1</sup>, M. BERNARD<sup>1</sup>, N. BERNIER<sup>1</sup>, V.-H. LE<sup>1</sup>, H. RENEVIER<sup>2</sup>, G. NAVARRO<sup>1</sup>, <sup>1</sup>Univ. Grenoble Alpes, CEA, Leti, Grenoble, France; <sup>2</sup>Univ. Grenoble Alpes, Grenoble-INP, LMGP, Grenoble, France

**H-1.2:L04 Valence Transition in SmTe Films Enabling Non-volatile Resistive Change without Structural Transition**

**SHOGO HATAYAMA**<sup>1</sup>, S. MORI<sup>2</sup>, Y. SAITO<sup>1</sup>, P. FONS<sup>3</sup>, Y. SHUANG<sup>2</sup>, Y. SUTOU<sup>2</sup>, <sup>1</sup>National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan; <sup>2</sup>Tohoku University, Japan; <sup>3</sup>Keio University, Japan

**H-1.2:L05 Novel Broadband Transparent Optical Phase Change Materials for Nonvolatile Photonics Employing High-throughput Combinatorial Study**

**CHIH-YU LEE**<sup>1</sup>, Y.-S. HUANG<sup>1, 2</sup>, H. SUN<sup>1, 2</sup>, C. LIAN<sup>1, 2</sup>, C.A. RÍOS OCAMPO<sup>1, 2</sup>, I. TAKEUCHI<sup>1, 3</sup>, <sup>1</sup>Department of Materials Science and Engineering, University of Maryland, College Park, MD, USA; <sup>2</sup>Institute for Research in Electronics and Applied Physics, University of Maryland, College Park, MD, USA; <sup>3</sup>Quantum Materials Center, Department of Physics, University of Maryland, College Park, MD, USA

## Session H-2

Advances in memory and memristive devices: devices, mechanisms, and applications for computing

**H-2:IL01 Architectures and Materials for Storage Class Memories**

**P. FANTINI**, Micron Semiconductor, Vimercate, Italy

**H-2:IL02 Integration Aspects of Hafnium Oxide-based Memristive Devices**

E. PEREZ-BOSCH QUESADA, A. BARONI, E. PEREZ, K. DORAI SWAMY REDDY, **CH. WENGER**, IHP - Leibniz Institute for High Performance Microelectronics

**H-2:IL03 CMOS Compatible Materials and Devices for beyond von Neumann**

**V. BRAGAGLIA**, IBM Research Europe, Zurich, Switzerland

**H-2:L04 Resistive Memory Window Enhanced through Bandgap Tuning in V-substituted Cr2O3 Thin Films**

**J. TRANCHANT**, M. RODRIGUEZ FANO, M. HAYDOURA, B. CORRAZE, E. JANOD, M.-P. BESLAND, L. CARIO, CNRS, Institut des Matériaux de Nantes Jean Rouxel, (IMN), Nantes, France

**H-2:L05 Exploring, Tailoring, and Harnessing Electrical Noise in Resistive Switching Memories**

**Z. BALOGH**, A. NYÁRY, B. SÁNTA, J.G. FEHÉRVÁRI, S.W. SCHMID, L. PÓSA, A. HALBRITTER, Department of Physics, Institute of Physics, Budapest University of Technology and Economics, Budapest, Hungary

**H-2:L06 Pulse Frequency-dependent Capacitive and Inductive Halide Perovskite Memristor for Low-energy Neuromorphic Computing**

**P.N. KUMAR**, A. GUERRERO, J. BISQUERT, Applied Physics, Institute of Advanced Materials (INAM), Universitat Jaume I, Castelló, Spain

**H-2:IL07 Brain-inspired Computing with Nonlinear Dynamical Materials**

**R.S. WILLIAMS**, Department of Electrical and Computer Engineering, Texas A&M University, College Station, TX, USA

**H-2:L08 Noise Diagnostics of Nanoscale Memristor Devices**

**S. SCHMID**<sup>1</sup>, Z. BALOGH<sup>1, 2</sup>, B. SÁNTA<sup>1, 2</sup>, L. PÓSA<sup>1, 3</sup>, A. HALBRITTER<sup>1, 2</sup>, <sup>1</sup>Department of Physics, Institute of Physics, Budapest University of Technology and Economics, Budapest, Hungary; <sup>2</sup>ELKH-BME Condensed Matter Research Group, Budapest, Hungary; <sup>3</sup>Institute of Technical Physics and Materials Science, Centre for Energy Research, Budapest, Hungary

**H-2:IL09 Development of Ferroelectric Tunnel Junctions and Field-effect Transistors Compatible with Back-end-of-line Integration for Neuromorphic Computing**

T.L. PHAN<sup>1</sup>, K.S. NAIR<sup>1, 2</sup>, M.H. RAZA<sup>1</sup>, V. DESHPANDE<sup>1</sup>, W. HAMOUDA<sup>1</sup>, **C. DUBOURDIEU**<sup>1, 2</sup>, <sup>1</sup>Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany; <sup>2</sup>Freie Universität Berlin, Physical Chemistry, Berlin, Germany

**H-2:IL10 Domain Switching Dynamics in the Ferroelectric AIsCN Thin Film Capacitors**

**A. GRUVERMAN**, Department of Physics and Astronomy, University of Nebraska, Lincoln, NE, USA

**H-2:IL11 Tuning the Switching Speed of Valence Change-based Memristive Devices by Thermal Enhancement Layers**

A. SARANTOPOULOS, S. MENZEL, **R. DITTMANN**, Forschungszentrum Jülich GmbH, Germany; K. LANGE, IWE II, RWTH Aachen University, Germany, F. RIVADULLA, CIQUS, Universidad de Santiago de Compostela, Spain

**H-2:L12 Correlation between Electronic Structure and Microstructure of Al2O3/TiOx-based Memristive Cells Switched in Filamentary- and Area-mode**

**S. HOFFMANN-EIFERT**, S. AUSSEN, F. CÜPPERS, C. FUNCK, S. MENZEL, R. DITTMANN, R. WASER, Peter Grünberg Institut (PGI 7 and 10) and JARA-FIT, Forschungszentrum Jülich GmbH, Jülich, Germany; S. WERNER, C. PRATSCH, Helmholtz-Zentrum für Materialien und Energie GmbH, Department X-ray Microscopy, Berlin, Germany; J. JO, R. DUNIN-BORKOWSKI, Ernst Ruska-Center (ERC-1 / PGI-5) and JARA-FIT, Forschungszentrum Jülich GmbH, Jülich, Germany

**H-2:L13 Resolving the Dynamics of Picosecond Time-scale Resistive Switching**

**M. CSONTOS**<sup>1</sup>, S.W. SCHMID<sup>2</sup>, L. PÓSA<sup>2, 3</sup>, T.N. TÖRÖK<sup>2, 3</sup>, Y. HORST<sup>1</sup>, N.J. OLALLA<sup>1</sup>, U. KOCH<sup>1</sup>, I. SHORUBALKO<sup>4</sup>, J. LEUTHOLD<sup>1</sup>, J. VOLK<sup>3</sup>, A. HALBRITTER<sup>2, 5</sup>, <sup>1</sup>Institute of Electromagnetic Fields, ETH Zurich, Switzerland; <sup>2</sup>Department of Physics, Budapest University of Technology and Economics, Hungary; <sup>3</sup>Institute of Technical Physics and Materials Science, Centre for Energy Research, Budapest, Hungary; <sup>4</sup>Transport at Nanoscale Interfaces Laboratory, Empa, Switzerland; <sup>5</sup>ELKH-BME Condensed Matter Research Group, Hungary

**H-2:IL14 Solution Processing of Metal Oxide Memristors: from Coating to Printing**

**E. CARLOS**, R.A. MARTINS, M. FRANCO, J. DEUERMEIER, R. MARTINS, A. KIAZADEH, i3N/CENIMAT, Department of Materials Science, NOVA School of Science and Technology, Universidade NOVA de Lisboa and CEMOP/UNINOVA, Caparica, Portugal

**Session H-3**

Neuromorphic and unconventional computing: devices, algorithms, circuits, theory

**H-3:IL01 Silicon Oxide Memristors: Low-cost, CMOS Compatible, High-density Emerging Memory Technology**

**F. AGUIRRE**<sup>1</sup>, W.H. NG<sup>1,2</sup>, M. SCHORMANS<sup>1</sup>, M. DICKINSON<sup>1</sup>, A.J. KENYON<sup>1,2</sup>, B. JONES<sup>1</sup>, A. MEHONIC<sup>1,2</sup>, <sup>1</sup>Intrinsic Semiconductor Technologies Ltd., Madrid, Spain; <sup>2</sup>University College London, UK

**H-3:IL02 Multi-input Logic-in-Memory and Neural Inference Accelerators with RRAM Devices**

**T. ZANOTTI**, P. PAVAN, F.M. PUGLISI, Università degli studi di Modena e Reggio Emilia, Modena, Italy

**H-3:IL03 Memristor Prototyping Platforms for Material, Device and Neural Network-level Integration and Benchmarking**

**G.C. ADAM**, Electrical and Computer Engineering Department, George Washington University, Washington, DC, USA

**H-3:L04 An Optical Neuromorphic Device for Classification and Pattern Recognition**

**P. MILANI**, B. PAROLI, M.A.C. POTENZA, CIMAINA and Dipartimento di Fisica, Università di Milano, Milano, Italy

**H-3:L05 Applying Neurodynamic Behavior of Mott Insulators for Auditory Sensing**

**T.N. TÖRÖK**, R. KÖVECS, D. MOLNÁR, A. HALBRITTER, Dept of Physics, Budapest University of Technology and Economics, Budapest, Hungary; L. PÓSA, GY. MOLNÁR, N.Q. KHÁNH, F. BRAUN, J. VOLK, Institute of Technical Physics and Materials Science, Centre for Energy Research, Budapest, Hungary

**H-3:L06 Harnessing the Frequency Response of Silicon Oxide Memristors**

**H.R.J. COX**<sup>1</sup>, W.H. NG<sup>1</sup>, T. BENKOHEN<sup>1</sup>, D. DAS<sup>1</sup>, A. MEHONIC<sup>1</sup>, C. HENDERSON<sup>1</sup>, A. XHAMENI<sup>2</sup>, E. ZANGANEH<sup>2</sup>, A. JAMAN<sup>3</sup>, R. JACKMAN<sup>1</sup>, T. BANERJEE<sup>3</sup>, A. LOMBARDO<sup>2</sup>, A.J. KENYON<sup>1</sup>, <sup>1</sup>Dept. of Electronic and Electrical Engineering, University College London, London, UK; <sup>2</sup>London Centre for Nanotechnology, University College London, London, UK; <sup>3</sup>Faculty of Science and Eng., University of Groningen, Groningen AG, Netherlands

**H-3:L07 Tunable Photoresponsivity Associated with Synaptic Functions in Zinc-Tin Oxide Phototransistor for In-Sensor and Neuromorphic Computing**

**LI-CHUNG SHIH**, CHUN-TAO CHEN, YA-CHI HUANG, SHUAI-MING CHEN, YU-CHIEH CHEN, JEN-SUE CHEN, Department of Materials Science and Engineering, National Cheng Kung University, Tainan, Taiwan

**H-3:IL08 Bayesian Inference Leveraging Nanoscale Device Stochasticity**

**B. RAJENDRAN**, King's College London, London, UK

**H-3:IL09 Deep Neural Network Inference with a 64-core in-Memory Compute Chip based on Phase-change Memory**

**M. LE GALLO**, IBM Research Europe, Rüschlikon, Switzerland

**H-3:IL10 Computing with Physical Systems based Oscillatory Neural Networks**

**A. TODRI-SANIAL**, NanoComputing Research Lab, Electrical Engineering Department, Eindhoven University of Technology, Eindhoven, Netherlands

**H-3:L11 Single-node Reservoir Computing through a Memristive Circuit with Complex Dynamics**

**S. BRIVIO**, M. ESCUDERO, S. SPIGA, CNR – IMM, Unit of Agrate Brianza, Italy

**H-3:L12 Autonomous Neural Information Processing by a Dynamical Memristor Circuit**

D. MOLNAR<sup>1,2</sup>, T.N. TÖRÖK<sup>1,3</sup>, R. KÖVECS<sup>1</sup>, L. PÓSA<sup>1,3</sup>, P. BALÁZS<sup>1</sup>, GY. MOLNÁR<sup>3</sup>, N.J. OLALLA<sup>4</sup>, J. LEUTHOLD<sup>4</sup>, J. VOLK<sup>3</sup>, M. CSONTOS<sup>4</sup>, **A. HALBRITTER**<sup>1,2</sup>, <sup>1</sup>Department of Physics, Institute of Physics, Budapest University of Technology and Economics, Budapest, Hungary; <sup>2</sup>HUN-REN-BME Condensed Matter Physics Research Group, Budapest, Hungary; <sup>3</sup>Institute of Technical Physics and Materials Science, Centre for Energy Research, Budapest, Hungary; <sup>4</sup>Institute of Electromagnetic Fields, ETH Zurich, Zurich, Switzerland

**H-3:L13 Nonlinear Dynamics and Local Activity in Bio-inspired Memristor Networks**

A. ASCOLI<sup>1</sup>, **F. CORINTO**<sup>1</sup>, M. GILLI<sup>1</sup>, R. TETZLAFF<sup>2</sup>, <sup>1</sup>Dept of Electronics and Telecommunications, Politecnico di Torino, Turin, Italy; <sup>2</sup>Institute of Circuits and Systems, Faculty of Electrical and Computer Engineering, TU Dresden, Dresden, Germany

**H-3:IL14 Edge of Chaos Theory for Unconventional Computing**

**R. TETZLAFF**<sup>1</sup>, A. DEMIRKOL<sup>1</sup>, A. ASCOLI<sup>1</sup>, L.O. CHUA<sup>2</sup>, <sup>1</sup>Institute of Circuits and Systems, TU Dresden, Dresden, Germany; <sup>2</sup>Department of Electrical Engineering and Computer Sciences, University of California Berkeley, Berkeley, CA, USA

**Session H-4**

Theory, modelling and simulation of materials and devices for future computing

**H-4:IL01 Latest Advances in Modelling of Valence Change and Electrochemical Resistive Switching Devices**

**S. MENZEL**, Forschungszentrum Jülich, Peter Grünberg Institut (PGI-7), Jülich, Germany

**H-4:IL02 Density Functional Simulations of Ag Migration in a Conductive Bridging Random Access Memory Cell**

**J. AKOLA**, Department of Physics, Norwegian University of Science and Technology (NTNU), Trondheim, Norway

**H-4:IL03 Multi-scale Modelling of Valence Change Memory Cells**

**M. LUISIER**, M. KANISELVAN, M. MLADENOVIC, Integrated Systems Laboratory, ETH Zurich, Zurich, Switzerland

**H-4:L04 Interplay of Thermal and Electronic Effects in the Mott Transition of Nanosized VO<sub>2</sub> Phase Change Memory Devices**

**L. POSA**<sup>1,2</sup>, P. HORNUNG<sup>2</sup>, T. TÖRÖK<sup>1,2</sup>, A. HALBRITTER<sup>1,3</sup>, J. VOLK<sup>2</sup>, <sup>1</sup>Institute of Technical Physics and Materials Science, HUN-REN Hungarian Research Network, Budapest, Hungary; <sup>2</sup>Department of Physics, Institute of Physics, Budapest University of Technology and Economics; <sup>3</sup>HUN-REN-BME Condensed Matter Research Group, Budapest University of Technology and Economics, Hungary

**H-4:L05 A Machine-learning Interatomic Potential for GeSbTe Phase Change Alloys**

O. ABOU EL KHEIR, D. BARATELLA, Department of Materials Science, University of Milano-Bicocca, Milano, Italy; L. BONATI, M. PARRINELLO, Italian Institute of Technologies (IIT), Genova, Italy; **M. BERNASCONI**, Department of Materials Science, University of Milano-Bicocca, Milano, Italy

#### H-4:L06 Are Machine Learning Interatomic Potentials Always Better for Modeling Amorphous Metal Oxides?

**S. GRAMATTE**<sup>1,2,3</sup>, V. TURLO<sup>1</sup>, O. POLITANO<sup>2</sup>, <sup>1</sup>Lab. for Advanced Materials Processing, Empa - Swiss Federal Labs for Materials Science and Technology, Thun, Switzerland; <sup>2</sup>Lab. Interdisciplinaire Carnot de Bourgogne, UMR 6303 CNRS-Université de Bourgogne, Dijon Cedex, France; <sup>3</sup>Lab. for Joining Technologies and Corrosion, Empa - Swiss Federal Labs for Materials Science and Technology, Dübendorf, Switzerland

#### H-4:L07 Modelling of Stochastic Switching in Monolayer MoS<sub>2</sub> RRAMs with Kinetic Monte Carlo

L. PEDDABOINA, G. HEGDE, J.S.A. NANDAN KARALAPATI, O. BADAMI, **S. BHATTACHARJEE**, IIT Hyderabad, Kandi, Sangareddy, India

### Session H-5

#### 2D materials- and soft materials-based devices

#### H-5:IL01 Devices for Neuromorphic Computing with 2D MoS<sub>2</sub>

**T. ROY**, Duke University, Durham, NC, USA

#### H-5:L02 Resistive Switching in CVD-grown Transition Metal Dichalcogenide Memristive Devices

**A. LINKENHEIL**<sup>1</sup>, J.-P. GLAUBER, M. WILKEN<sup>2</sup>, J. SCHNEEGASS<sup>1</sup>, S. THIELE<sup>3</sup>, B. SPETZLER<sup>4</sup>, J. PEZOLDT<sup>3</sup>, A. DEVI<sup>5</sup>, M. ZIEGLER<sup>1</sup>, <sup>1</sup>Micro- and Nanoelectronic Systems, Dept of Electrical Eng and Information Technology / Institute of Micro- and Nanotechnologies MacroNano®, TU Ilmenau, Ilmenau, Germany; <sup>2</sup>Inorganic Materials Chemistry, Faculty of Chemistry and Biochemistry, Ruhr-Universität Bochum, Bochum, Germany; B. HÄHNLEIN, Micro- and Nanoelectronic Systems, Dept of Electrical Eng and Information Technology / Technical Physics I, Dept of Mathematics and Natural Sciences / Institute of Micro- and Nanotechnologies MacroNano®, TU Ilmenau, Ilmenau, Germany; <sup>3</sup>Nanotechnology, Dept of Electrical Eng and Information Technology / Institute of Micro- and Nanotechnologies MacroNano®, TU Ilmenau, Ilmenau, Germany; <sup>4</sup>Micro- and Nanoelectronic Systems, Dept of Electrical Eng and Information Technology, TU Ilmenau, Ilmenau, Germany; <sup>5</sup>Inorganic Materials Chemistry, Faculty of Chemistry and Biochemistry, Ruhr-Universität Bochum, BOCHUM / Fraunhofer Institute for Microelectronics Circuits and Systems (IMS), Duisburg, Germany

#### H-5:L03 Visual Memory in a 2D Memmitter Based on WS<sub>2</sub>

**F. FERRARESE LUPI**, G. MILANO, A. ANGELINI, Advanced Materials Metrology and Life Science Division, INRiM (Istituto Nazionale di Ricerca Metrologica), Torino, Italy; M. ROSERO REALPE, B. TORRE, Department of Applied Science and Technology (DISAT), Politecnico di Torino, Torino, Italy; E. KOZMA, CNR-SCITEC, Milano, Italy; C. MARTELLA, C. GRAZIANETTI, CNR-IMM, Unit of Agrate Brianza, Agrate Brianza Italy

#### H-5:L04 2D Van der Waals NbTe<sub>4</sub> Phase Change Material: Enabling Ultralow Thermal Consumption

**YI SHUANG**<sup>1</sup>, Q. CHEN<sup>2,3</sup>, M. KIM<sup>4</sup>, Y. WANG<sup>4</sup>, Y. SAITO<sup>5</sup>, S. HATAYAMA<sup>5</sup>, P. FONS<sup>6</sup>, D. ANDO<sup>4</sup>, M. KUBO<sup>2,3</sup>, Y. SUTOU<sup>1,4</sup>, <sup>1</sup>WPI Advanced Institute for Materials Research, Tohoku University, Aoba, Sendai, Japan; <sup>2</sup>New Industry Creation Hatchery Center, Tohoku University, Aramaki, Aoba-ku, Sendai, Japan; <sup>3</sup>Institute for Materials Research, Tohoku University, Aoba-ku, Sendai, Japan; <sup>4</sup>Department of Materials Science, Graduate School of Engineering, Tohoku University, Sendai, Japan; <sup>5</sup>Device Technology Research Institute, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba Central 2, Tsukuba, Japan; <sup>6</sup>Department of Electronics and Electrical Engineering, Faculty of Science and Technology, Keio University, Yokohama, Kanagawa, Japan

#### H-5:L05 Band Gap Effect on Terahertz Photodetection in Bilayer Graphene

**E.I. TITOVA**<sup>1,2</sup>, D. MYLNIKOV<sup>2</sup>, M. KASHCHENKO<sup>1,2</sup>, I. SAFONOV<sup>1,2</sup>, S. ZHUKOV<sup>2</sup>, K. NOVOSELOV<sup>3,1</sup>, D. BANDURIN<sup>4</sup>, G. ALYMOV<sup>2</sup>, D. SVINTSOV<sup>2</sup>, <sup>1</sup>Programmable Functional Materials Lab, Center for Neurophysics and Neuromorphic Technologies, Moscow, Russia; <sup>2</sup>Center for Photonics and 2D Materials, MIPT, Moscow, Russia; <sup>3</sup>Institute for Functional Intelligent Materials, National University of Singapore, Singapore; <sup>4</sup>Department of Materials Science and Engineering, National University of Singapore, Singapore

#### H-5:L06 3D Printable High-performance Soft Material for Neural Interface Applications

**TAO ZHOU**, Dept of Engineering Science and Mechanics, Pennsylvania State University, PA, USA; Center for Neural Engineering, Pennsylvania State University, PA, USA; Huck Institutes of The Life Sciences, Pennsylvania State University, PA, USA; Materials Research Institute, Pennsylvania State University, PA, USA

#### H-5:L07 Resistive Switching Memory Behaviours in Biodegradable Composites

**V.S. VALLABHAPURAPU**<sup>1</sup>, Z.W. DLAMINI<sup>2</sup>, S. VALLABHAPURAPU<sup>3</sup>, <sup>1</sup>Department of Physics, University of South Africa, Johannesburg, South Africa; <sup>2</sup>Central University of Technology, South Africa; <sup>3</sup>School of Computing, University of South Africa, Johannesburg, South Africa

### Session H-6

#### Nanomaterials and unconventional substrates for computing

#### H-6:IL01 Reservoir Computing with Nanowire Networks

**G. MILANO**<sup>1</sup>, C. RICCIARDI<sup>2</sup>, <sup>1</sup>Advanced Materials Metrology and Life Science Division, INRiM (Istituto Nazionale di Ricerca Metrologica), Italy; <sup>2</sup>Department of Applied Science and Technology, Politecnico di Torino, Italy

#### H-6:IL02 Materializing Cognition – Information Processing in Cognitive Matter

**W.G. VAN DER WIEL**, Center for Brain-Inspired Nano Systems (BRAINS), University of Twente, Enschede, The Netherlands and Institute of Physics, University of Münster, Münster, Germany

#### H-6:IL03 Emergent Brain-like Dynamics from Memristive Networks

**Z. KUNCIC**, School of Physics, University of Sydney, NSW, Australia; F. CARAVELLI, Theoretical Division (T4), Los Alamos National Laboratory, Los Alamos, NM, USA

#### H-6:L04 Composite Nanogranular Networks: Brain-like Resistive Switching Patterns and In Situ Current Path Imaging

B. ADEJUBE<sup>1</sup>, O. GRONENBERG<sup>2</sup>, T. HEMKE<sup>3</sup>, N. CARSTENS<sup>1</sup>, R. GUPTA<sup>1</sup>, O.-H. ASNAZ<sup>4</sup>, T. STRUNSKUS<sup>1,5</sup>, F. FAUPEL<sup>1,5</sup>, T. MUSSENBROCK<sup>3</sup>, J. BENEDIKT<sup>4,5</sup>, L. KIENLE<sup>2,5</sup>, **A. VAHL**<sup>1,5</sup>, <sup>1</sup>Dept of Materials Science - Chair for Multicomponent Materials, Faculty of Engineering, Kiel University, Kiel, Germany; <sup>2</sup>Dept of Materials Science - Synthesis and Real Structure, Faculty of Engineering, Kiel University, Kiel, Germany; <sup>3</sup>Chair of Applied Electrodynamics and Plasma Technology (AEPT), Ruhr University Bochum, Bochum, Germany; <sup>4</sup>Experimental Plasma Physics, Institute of Experimental and Applied Physics, Kiel University, Kiel, Germany; <sup>5</sup>Kiel Nano Surface and Interface Science KiNSIS, Kiel University, Kiel, Germany

#### H-6:L05 In-materia Adaptive Computing Devices based on Random-assembled Clusters Network

**F. BORGHI**, G. NADALINI, S. BRESSAN, P. MILANI, CIMAINA and Dipartimento di Fisica, Università di Milano, Italy



## Session H-7

New developments in characterization methods for materials and devices

**H-7:IL01 A New Era of Materials Characterization: Can we Achieve Atomic Sensitivity using Visible Light?**

**G. DI MARTINO**, Dept. of Material Science and Metallurgy, University of Cambridge, Cambridge, UK

**H-7:IL02 Photoelectron Spectroscopy of Functional Oxides for Novel Electronic Device Concepts**

**M. MÜLLER**, University of Konstanz, Germany Complex Materials Group, Konstanz, Germany

**H-7:IL03 Advanced Nanoscale Spectroscopic Investigation of Nanostructures for Single Photon Source**

**P. PRETE**, IMM-CNR, Lecce, Italy

**H-7:IL04 Progress on Tomographic Filaments Observation with Adaptive Scalpel Scanning Probe Microscopy**

**U. CELANO**, School of Electrical, Computer & Energy Engineering, Arizona State University, Scottsdale, AZ, USA

**H-7:IL05 Infrared Nanoimaging of Hydrogenated Perovskite Nickelate Memristive Devices**

S. GAMAGE<sup>1</sup>, S. MANNA<sup>2,3</sup>, M. ZAJAC<sup>4</sup>, S. SLAC HANCOCK<sup>4</sup>, Q. WANG<sup>5</sup>, S. SINGH<sup>1</sup>, M. GHAFARIASL<sup>1</sup>, K. YAO<sup>4</sup>, T. TIWALD<sup>6</sup>, T.J. PARK<sup>5</sup>, D. LANDAU<sup>4</sup>, H. WEN<sup>2</sup>, S. SANKARANARAYANAN<sup>2,3</sup>, P. DARANCET<sup>2,7</sup>, S. RAMANATHAN<sup>5,8</sup>, **Y. ABATE**<sup>1</sup>, <sup>1</sup>University of Georgia, Department of Physics and Astronomy, Athens, GA, USA; <sup>2</sup>Argonne National Laboratory; <sup>3</sup>University of Illinois Chicago; <sup>4</sup>University of Georgia; <sup>5</sup>Purdue University; <sup>6</sup>J A Woollam Co Inc; <sup>7</sup>Northwestern Argonne Institute of Science and Engineering; <sup>8</sup>Rutgers The State University of New Jersey, USA

**H-7:IL06 Metrology of Ferroelectric HZO with STEM EBIC Imaging**

**B.C. REGAN**, H.L. CHAN, T. O'NEILL, Y. CHEN, UCLA, Los Angeles, CA, USA; S.S. FIELDS, J.F. IHLEFELD, University of Virginia, Charlottesville, VA, USA; W.A. HUBBARD, NanoElectronic Imaging Inc., Los Angeles, CA, USA

**H-7:IL07 Dead Samples Tell No Tales: STEM EBIC of PFIB-prepared Devices**

**W.A. HUBBARD**, NanoElectronic Imaging, Los Angeles, CA, USA

Special AFOSR Session H-8

**FROM BRAIN-INSPIRED NETWORKS FOR MULTIFUNCTIONAL SYSTEMS TO NEUROMORPHIC COMPUTING AT THE EDGE OF BIOLOGY**

**H-8:IL01 Brain-inspired Synaptic Resistor Circuits for Multifunctional Intelligent Systems with Real-time Learning**  
**YONG CHEN**, University of California, Los Angeles, CA, USA

**H-8:IL02 Synstor-based Device Simulations and Learning Algorithms for Self-programming Neuromorphic Integrated Circuit**

H.-T. CHIEN, **SUIN YI**, Texas A&M University, College Station, TX, USA

**H-8:IL03 Multimodal Actuators and Multifunctional Skins for Integrated Autonomous Systems**

**J.W. BOLEY**, Boston University, Boston, MA, USA

**H-8:L04 Mechanical Neural Networks that Learn to Design other Passive Metamaterials**

**J.B. HOPKINS**, University of California, Los Angeles, CA, USA

**H-8:L05 Grayscale Digital Light Processing 3D Printing for Multimaterial Additive Manufacturing**

**H. JERRY QI**, The George W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA, USA

**H-8:IL06 Hybrid Biomolecular Synapses for Sensing and Neuromorphic Computing at the Edge of Biology**

**S.A. SARLES**, J. MARAJ, M. MANSOUR, University of Tennessee, Knoxville, TN, USA; E. SCHAFER, V. HU, N. KAMAT, J. RIVNAY, Northwestern University, USA

**H-8:L07 Drawing Inspiration from the Hippocampus for Next-generation Neuromorphic Computing**

**G.C. ADAM**, Electrical and Computer Engineering Department, George Washington University, Washington, DC, USA

**H-8:L08 Autonomous Fly-by-feel Camber Morphing Gust Rejection**

**K.PT HAUGHN**, Army Research Laboratory, Baltimore, MD, USA; C. HARVEY, University of California at Davis, USA; D. INMAN, University of Michigan, USA

**H-8:L09 Biomolecular Materials and Networks Enabling Neuromorphic Computing at the Edge of Biology**

**J.S. NAJEM**, N.X. ARMENDAREZ, A. MOHAMED, The Pennsylvania State University, University Park, PA, USA; M.S. HASAN, University of Mississippi, Oxford, MS, USA

**H-8:L10 Geopolymer Memristors Mimic Synaptic Plasticity**

**M.A. SHAKIB**, Z. GAO, C. LAMUTA, Department of Mechanical Engineering, University of Iowa, Iowa City, IA, USA

**H-8:IL11 High-precision Analog Computing with Memristors**

**J. JOSHUA YANG**, University of Southern California, Los Angeles, CA, USA

**H-8:L12 Effect of Oxygen Vacancy and Si Doping on the Memristive Electrical Properties of Ta2O5**

S. ISLAM, Spectral Energies; J. LEE, ARCTOS Technology Solutions; S. GANGULI, **A.K. ROY**, Air Force Research Laboratory, Wright-Patterson AFB, OH, USA

**H-8:L13 Ferroelectrics for Emergent Silicon-integrated Optical Computing**

**A. DEMKOV**, The University of Texas at Austin, Austin, TX, USA and La Luce Cristallina, Inc. Austin, TX, USA

**H-8:L14 SWaP-Efficient System-on-a-Chip for Neuromorphic Computing**

E. YESIL, C.-J. TIEN, R. HADI, H. YONG, D. HUANG, Y. CHEN, **MAU-CHUNG FRANK CHANG**, UCLA, Los Angeles, CA, USA

TRACK I

**TOWARDS SCALABLE QUANTUM COMPUTING: THEORY, MATERIALS AND TECHNOLOGY CHALLENGES**

Session I-1

Superconducting qubits

**I-1:IL01 New Material Platforms for Quantum Computing**

**N. DE LEON**, Department of Electrical and Computer Engineering, Princeton University, Princeton, NJ, USA

**I-1:IL02 Integer Fluxonium Qubit**

**V. MANUCHARYAN**, EPFL, Lausanne, Switzerland

**I-1:IL03 Manufacturing High-coherence Superconducting Qubits in an Advanced 300 mm Fabrication Environment**  
**K. DE GREVE**, Y. CANVEL, T.IVANOV, J. JUSSOT, S. KUBICEK, R. LEUNG, S. MASSAR, M. MONGILLO, D. PEREZ-LOZANO, A. PACCO, A. POTOCHNIK, A.M. VADIRAJ, J. VANDAMME, D. WAN, imec and KU Leuven, Department of Electrical Engineering, Leuven, Belgium

**I-1:IL04 Outstanding Materials Challenges & Opportunities for Developing Superconducting Quantum Information Systems**

**R.W. SIMMONDS**, National Institute of Standards & Technology, Boulder, CO, USA

**I-1:IL05 Giant Atoms with Superconducting Qubits**

**A. FRISK KOCKUM**, Chalmers University of Technology, Gothenburg, Sweden

**I-1:IL06 Quantum Error Correction Beyond Break-even**

**V.V. SIVAK**, A. EICKBUSCH, B. ROYER, S. SINGH, I. TSIOUTSIOS, S. GANJAM, A. MIANO, B.L. BROCK, A.Z. DING, L. FRUNZIO, S.M. GIRVIN, R.J. SCHOELKOPF, M.H. DEVORET, Departments of Physics and Applied Physics and Yale Quantum Institute, Yale University, New Haven, CT, USA

**I-1:IL07 Two-level Defects in Superconducting Quantum Computing Chips**

**A. USTINOV**, Physics Institute, Karlsruhe Institute of Technology, Karlsruhe, Germany

### Session I-2

#### Defects and color centers in semiconductors

**I-2:IL01 Quantum Embedding for Point Defects: Benchmarking and Applications**

**M. ROESNER**, Theory of Condensed Matter Department (TCM), Institute for Molecules and Materials (IMM), Radboud University, Nijmegen, Netherlands

**I-2:IL02 Radiative/Non-radiative Transitions and Charge-state Dynamics in Color Centers from First-principles**

**YU-NING WU**, R. BAI, East China Normal University, Shanghai, China; S. CHEN, Fudan University, Shanghai, China

**I-2:IL03 Recombination Mechanisms in Quantum Defects**

**M.E. TURIANSKY**, Materials Department, University of California, Santa Barbara, CA, USA; A. ALKAUSKAS, Center for Physical Sciences and Technology (FTMC), Vilnius, Lithuania; F. ZHAO, C.G. VAN DE WALLE, Materials Department, University of California, Santa Barbara, CA, USA

**I-2:IL04 Quantum Networks based on Color-center Spin Qubits**

**T.H. TAMINIAU**, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, Delft, Netherlands

### Session I-3

#### Trapped-ion, photonic and topological insulators-based qubits

**I-3:IL01 Molecular Dynamics Simulations of Adsorbate-related Electric Field Noise in Surface Ion Traps**

**V. LORDI**, Lawrence Livermore National Laboratory, Livermore, CA, USA

**I-3:IL02 State of the Art and Challenges of Scaling Ion-trap Quantum Computer**

**C. OSPELKAUS**, for the QVLS-Q1 and ATIQ projects Leibniz Universität Hannover and PTB Braunschweig, Hannover, Germany

**I-3:IL03 Superconducting Diode Effect due to Magnetochiral Anisotropy in Topological Insulator and Rashba Nanowires**  
**J. KLINOVAJA**, H. LEGG, K. LAUBSCHER, D. LOSS, University of Basel, Basel, Switzerland

**I-3:IL04 Topological States in Iron-based Superconductors for Quantum Computing**

**QIANG LI**, Stony Brook University and Brookhaven National Laboratory, Stony Brook, NY, USA

**I-3:IL05 Quantum Photonic State Engineering with Compound Semiconductor-on-Insulator**

**G. MOODY**, University of California Santa Barbara, Santa Barbara, CA, USA

**I-3:IL06 III-V Nanowire Heterostructures for Quantum Photonics**

**N. LOVERGINE**, Università del Salento, Lecce, Italy

### Session I-4

#### Semiconductor quantum dot and dopant-based qubits

**I-4:IL01 Detecting Electric, Magnetic and Strain Fields with a Single High-spin Nucleus in Silicon**

**A. MORELLO**, UNSW Sydney, Sydney, Australia

**I-4:IL02 Towards Quantum Computing with Hole Spin Qubits**

**A. FUHRER**, IBM Research Europe - Zurich, Rüschlikon, Switzerland

**I-4:IL03 Circuit Quantum Electrodynamics Experiments in Planar Germanium**

**G. KATSAROS**, Institute of Science and Technology Austria, Klosterneuburg, Austria

**I-4:IL04 Role of Material Disorder on the Metrics of Silicon Spin Qubits**

**R. RAHMAN**, School of Physics, University of New South Wales, Sydney, Australia

**I-4:IL05 Quantum Computation with Spins in Silicon - Coherence, Integration, and Scaling**

**XIAO XUE**, L.M.K. VANDERSYPEN, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, Delft, Netherlands

**I-4:IL06 Local Variation and Tunability of Spin-orbit Interaction in Planar Germanium**

**K.L. HUDSON**, D. COSTA, L.E.A. STEHOUWER, G. SCAPPUCCI, QuTech - TU Delft, Delft, Netherlands

**I-4:IL07 Investigating Frequency Shifts in Silicon Spin Qubits influenced by Environmental Coupling**

**I. HEINZ**, G. BURKARD, Department of Physics, University of Konstanz, Konstanz, Germany

**I-4:IL08 Hole Spin Qubits for Quantum Computing in Si and Ge Quantum Dots**

**D. LOSS**, University of Basel, Basel, Switzerland

**I-4:IL09 Two-qubit Operations in Silicon Quantum Dots made on a 300mm Process measured using a Radiofrequency Electron Cascade**

J.F. CHITTOCK-WOOD<sup>1,2</sup>, R.C.C. LEON<sup>2</sup>, M.A. FOGARTY<sup>2</sup>, S. PATOMÄKI<sup>1,2</sup>, F. EKKEHARD VON HORSTIG<sup>2,3</sup>, N. JOHNSON<sup>1</sup>, A. SEIGEL<sup>2,4</sup>, H. JNANE<sup>2,4</sup>, J. JUSSOT<sup>5</sup>, S. KUBICEK<sup>5</sup>, B. GOVOREANU<sup>5</sup>, S.C. BENJAMIN<sup>2,4</sup>, **M.F. GONZALEZ-ZALBA**<sup>2</sup>, J.J.L. MORTON<sup>1,2</sup>, <sup>1</sup>University College London, UK; <sup>2</sup>Quantum Motion, London, UK; <sup>3</sup>University of Cambridge, UK; <sup>4</sup>University of Oxford, UK; <sup>5</sup>IMEC, Belgium

**I-4:IL10 Tuning Quantum Dot Arrays with Rays**

**J.P. ZWOLAK**, National Institute of Standards and Technology, Gaithersburg, MD, USA

**I-4:IL11 High-throughput Spectroscopic Characterization of Nanowire-based Quantum Structures for Quantum Information Technologies**

**P. PARKINSON**, N. PATEL, S. CHURCH, University of Manchester, Manchester, UK; **A. SANCHEZ**, University of Warwick, UK; **H. LIU**, University College London, UK

## Poster Presentations

**P01 Modeling of Diffusion Mechanisms in Ordered Structures**

**A.V. NAZAROV**, D.A. BELOBRAGA, National Research Nuclear University MEPhI, Moscow, Russia

**P02 Influence of Crystal Size and Crystalline Fraction on Toughness of Stoichiometric Lithium Disilicate Glass-ceramics**

**D.C. NIERO FABRIS**<sup>1</sup>, K. HURLE<sup>2</sup>, F. GÖTZ-NEUNHOEFFER<sup>2</sup>, R. BELLI<sup>1</sup>, U. LOHBAUER<sup>1</sup>, <sup>1</sup>Friedrich-Alexander Universität Erlangen-Nürnberg (FAU), Zahnklinik 1 - Zahnerhaltung und Parodontologie, Forschungslabor für dentale Biomaterialien Erlangen, Germany; <sup>2</sup>Friedrich-Alexander-Universität Erlangen-Nürnberg, GeoZentrum Nordbayern, Mineralogy, Germany

**P03 Change in Potential Energy as Descriptor for Nanoparticle Coalescence**

**A. DAMIANIDIS**<sup>1</sup>, Y. WANG<sup>1</sup>, P. GRAMMATIKOPOULOS<sup>1,2</sup>, <sup>1</sup>Department of Materials Sciences and Engineering, Guangdong Technion - Israel Institute of Technology, Shantou, Guangdong, China; <sup>2</sup>Particle Technology Laboratory, Institute of Process Engineering, Department of Mechanical and Process Engineering, ETH Zürich, Zürich, Switzerland

**P04 Predicting Surfactant pKa Shifts using Molecular Dynamics**

**A.J. HODALA**, P. CARBONE, University of Manchester, Manchester, UK

**P05 Synthesis of Nano and Meso-porous Materials: Understanding the Kinetics and Porosity Development**

I. SHERE, **A. MALANI**, Department of Chemical Engineering, IIT Bombay, Mumbai, India

**P06 Inkjet Printing of Ceramic Coatings from Polysilazane and SiC Nanoparticles for High-temperature MEMS Applications**

**A. QAZZAZIE-HAUSER**<sup>1</sup>, K. HONNEF<sup>1</sup>, T. HANEMANN<sup>1,2</sup>, <sup>1</sup>Department of Microsystems Engineering, University of Freiburg, Freiburg, Germany; <sup>2</sup>Institute for Applied Materials IAM-WK, Karlsruhe Institute of Technology KIT, Eggenstein-Leopoldshafen, Germany

**P07 The Effect Local Residual Stress States on the Internal Pore Growth in Laser-welded Ti6Al4V**

**WEI SUN**, X. JIANG, M. CHEN, Xi'an Jiaotong-Liverpool University, Suzhou, China; **G. FAN**, Nanjing Tech University, Nanjing, China

**P08 Self-propagating High-temperature Synthesis of the Ternary Boride Cr<sub>3</sub>AlB<sub>4</sub> MAB Phase**

**J. SLOMINSKI**, S. KOMAREK, D. ZIENTARA, A. GUBERNAT, AGH University of Krakow, Faculty of Material Science and Ceramics, Department of Ceramics and Refractories, Krakow, Poland

**P09 Microstructural and Oxidation Studies of Borosilicate Forming Materials**

**J. JHALAK**, Indian Institute of Technology Ropar, Rupnagar, Punjab, India; **P.K. RAY**, Indian Institute of Technology Ropar, Rupnagar, Punjab, India; **G. BALASUBRAMANIAN**, Institute of Functional Materials & Devices, Lehigh University, Bethlehem, PA, USA

**P10 Coarse-grained Molecular Dynamics Simulations on Aggregation and Dispersion Mechanisms of Organically Modified Nanoparticles**

**M. NAKAMURA**<sup>1</sup>, K. JOJIMA<sup>1</sup>, R. TANIAI<sup>1</sup>, Y. OOTANI<sup>1</sup>, N. OZAWA<sup>2,1</sup>, M. KUBO<sup>1,2</sup>, <sup>1</sup>Institute for Materials Research, Tohoku University, Aoba-ku, Sendai, Japan; <sup>2</sup>New Industry Creation Hatchery Center, Tohoku University, Aoba-ku, Sendai, Japan

**P11 Preparation of Fe<sub>3</sub>O<sub>4</sub>@Ag Nanoparticle via Self-assembly Method and Amino Functionalization**

**GYE SEOK AN**, JI HUN JUNG, JONG HUN KIM, SU YOUNG KANG, YOUNG SEO KIM, Department of Advanced Material Engineering, Kyonggi University, Suwon-si, South Korea

**P12 Soft Sensors for Predicting Product Quality Data in Process Manufacturing: A Systematic Review**

J.G. GALLARETA, **P. MUNOZ**, C. GONZÁLEZ, INeS research group, Universidad Internacional de La Rioja, Logrono, Spain

**P13 Multiscale Modeling of Nanoparticle Synthesis by Pulsed Laser Ablation in Liquid**

**CHAOBO CHEN**, L.V. ZHIGILEI, Materials Science and Engineering, University of Virginia, Charlottesville, VA, USA

**P14 Computational Studies on Optoelectronic and Nonlinear Optical Properties of Para-substituted Nitrobenzofurazan Compound**

**I. CHÉRIF**<sup>1</sup>, H. RAISS<sup>2</sup>, K. ABIEDH<sup>3</sup>, B. GASSOUMI<sup>4</sup>, M.T. CACCAMO<sup>5</sup>, S. MAGAZU<sup>5</sup>, A.H. SAID<sup>4,6</sup>, F. HASSEN<sup>3</sup>, T. BOUBAKER<sup>2</sup>, S. AYACHI<sup>1</sup>, <sup>1</sup>Laboratory of Physico-Chemistry of Materials (LR01ES19), Faculty of Sciences, University of Monastir, Monastir, Tunisia; <sup>2</sup>Laboratoire de Chimie Heterocyclique, Produits Naturels et Reactivite (LR11ES39), Faculte des Sciences, Universite de Monastir, Monastir, Tunisia; <sup>3</sup>Laboratoire de Micro-Optoelectronique et Nanostructures (LR99/ES29), Faculte des Sciences, Universite de Monastir, Monastir, Tunisia; <sup>4</sup>Laboratoire Interfaces et Materiaux Avances (LIMA), Faculte des Sciences, Universite de Monastir, Monastir, Tunisia; <sup>5</sup>Dipartimento di Scienze Matematiche e Informatiche, Scienze Fisiche e Scienze della Terra Università di Messina, S. Agata, Messina, Italy; <sup>6</sup>Centre de Recherche en Microelectronique et Nanotechnologie, Technopole de Sousse, Sahloul, Sousse, Tunisia

**P15 Structural Differences of Hf<sub>0.5</sub>Zr<sub>0.5</sub>O<sub>2</sub> in Two Polarization States and their Evolution during Wake-up**

**I.G. MARGOLIN**, E.V. KOROSTYLEV, E.B. KALIKA, D.V. NEGROV, A.A. CHOUPRIK, Moscow Institute of Physics and Technology, Dolgoprudny, Moscow Region, Russia

**P16 Effect of Mechanical Stress in Thin Hafnium Oxide Films**

**E.B. KALIKA**, V.V. MIKHEEV, I.G. MARGOLIN, A.A. CHOUPRIK, Moscow Institute of Physics and Technology, Dolgoprudny, Russia

**P17 Hybrid Improper Ferroelectricity in Ba<sub>3</sub>Ce<sub>2</sub>O<sub>7</sub> Predicted by First-principles Calculation**

**XIANG MING CHEN**, B.H. CHEN, X.Q. LIU, School of Materials Science and Engineering, Zhejiang University, Hangzhou, China

**P18 Computational Modeling of Semimetallic, Half-metallic and Other States in the Gd-Sb Compounds with Strong Electron Correlations**

**A.V. LUKOYANOV**, R.D. MUKHACHEV, S.T. Baidak Institute of metal physics Mikheev UB RAS, Ekaterinburg, Russia

**P19 Stability and Structure of the Aqueous LiTFSI/LiCl Interface**

H. WOOD, H. BURNETT, R. DRYFE, P. CARBONE, University of Manchester, Manchester, UK

**P20 Enhancing the Electrolyte Wetting in Electrodes of Lithium-ion Batteries**

DONG HYUP JEON, Dongguk University, Gyeongju, South Korea

**P21 A Deep Learning Model for Driving the Interaction of Data-variability Features in Dynamic-stress Time Series' Information**

B. HAN, J. HO, J. AHN, Y. KIM, DAEWON CHUNG, J. JEON, Department of Advanced Battery Convergence Engineering, Dongguk University-Seoul, South Korea

**P22 Computational Modeling of Mechanical Properties and Mechanism of Keratin-based Polymer Materials**

CHIA-HUNG WU, CHIA-CHING CHOU, Institute of Applied Mechanics, National Taiwan University, Taipei, Taiwan

**P23 Understanding Fundamental Binding Mechanisms of Ion Selectors by DFT Calculations for Applications in Ion Sensors**

S-H. CHOI, J-S. LEE, SEON-JIN CHOI, Division of Materials of Science and Engineering, Hanyang University, Seongdong-gu, Seoul, South Korea

**P24 Structural Superlubricity of Macroscale Patterned Contact Network: A Simulation Study**

VIET HUNG HO, M. GIANETTI, B. HAUGEN, A.S. DE WIJN, Department of Mechanical and Industrial Engineering, Norwegian University of Science and Technology (NTNU), Trondheim, Norway

**P25 Multiscale Computational Study of Surface Modification by Nonlinear Laser-induced Surface Acoustic Waves**

YUAN XU, L.V. ZHIGILEI, University of Virginia, Charlottesville, VA, USA

**P26 Computational Fluid Dynamics (CFD) Simulations on Optimal Designs and Performances of Various Operating Conditions in a 20kWe Class Solid Oxide Electrolysis Cell (SOEC) Stack**

SANG SHIN PARK, SUN-DONG KIM, Korea Institute of Energy Research (KIER), Daejeon, South Korea

**P28 LaFeO<sub>3</sub> Doped Material La<sub>0.5</sub>Sr<sub>0.5</sub>Fe<sub>0.5</sub>Ti<sub>0.5</sub>O<sub>3</sub> as an Air Electrode and the Bifunctional Catalyst for Fuel Cell**

U. SHARMA, P.A. JHA, P.K. JHA, P. SINGH, Department of Physics, Indian Institute of Technology, Banaras Hindu University, Varanasi, India

**P29 Molecular Dynamics Simulation of the Effect of Dopant Distribution Homogeneity on the Oxide Ion Conductivity of Perovskite-type LaInO<sub>3</sub>**

M.-Y. YOON<sup>1</sup>, K. KIM<sup>1</sup>, S.-M. JEONG<sup>2</sup>, HAE-JIN HWANG<sup>1</sup>, <sup>1</sup>Inha University, Incheon, South Korea; <sup>2</sup>Korea Institute of Ceramic Engineering and Technology, South Korea

**P30 Designing the Nano-scale Architecture of the Air Electrode for High-performance and Robust Reversible Solid Oxide Cells**

SEUNG-BOK LEE, Fuel Cell Laboratory, Korea Institute of Energy Research, Daejeon, South Korea

**P31 Development of Solid Oxide Cells and Stacks for Green Hydrogen Manufacturing**

SUN-DONG KIM, Korea Institute of Energy Research (KIER), Daejeon, South Korea

**P32 Synthesis and Characterization of Mg-doped Li<sub>3</sub>V<sub>2</sub>(PO<sub>4</sub>)<sub>3</sub> Cathode for Li-ion Batteries**

D. MOHANTY, Z.-L. LU, I-MING HUNG, Yuan Ze University, Chung-Li, Taiwan

**P33 Improvement of the Electrochemical Activity of WO<sub>3</sub> Nanostructures Incorporating Sulfur for Energy Storage Application**

G. ROSELLÓ-MÁRQUEZ, D.M. GARCÍA-GARCÍA, M. CIFRE-HERRANDO, J. GARCÍA-ANTÓN, Ingeniería Electroquímica y Corrosión (IEC), Instituto Universitario de Seguridad Industrial, Radiofísica y Medioambiental (ISIRYM), Universitat Politècnica de València, Valencia, Spain

**P34 The Study of Indium-ion Diffusion for Multilayer Indium Tin Oxide Thin Films via Optoelectronic Characterization and Neutron Reflectometry**

N. XIA<sup>1</sup>, J. KEUM<sup>2,3</sup>, A. IEVLEV<sup>3</sup>, I. IVANOV<sup>3</sup>, V. LAUTER<sup>2</sup>, R.A. GERHARDT<sup>1</sup>, M. MAYS<sup>1</sup>, <sup>1</sup>School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA, USA; <sup>2</sup>Neutron Scattering Division, Oak Ridge National Laboratory, USA; <sup>3</sup>Center for Nanophase Materials Science, Oak Ridge National Laboratory, USA

**P35 Robust Closed-loop Linear Control of NiTiIn Wires**

B. TONDU, Institut National de Sciences Appliquées, Campus de Rangueil, Toulouse, and LAAS/CNRS, Toulouse, France

**P36 A High Efficiency Bromine-complexing Agent for Zinc-bromine Flow Batteries: 1,2-dimethyl-3-ethylimidazolium Bromide Compound**

C. KIM, B. HAN, S. LEE, D. YUN, D. CHUNG, JOONHYEON JEON, Department of Advanced Battery Convergence Engineering, Dongguk University-Seoul, Seoul, South Korea

**P37 Composition-property Maps and Multi-objective Design of Compositionally Complex Alloys using Machine Learning Models**

D. BENIWAL, P.K. RAY, Metallurgical and Materials Engineering, Indian Institute of Technology Ropar, Rupnagar, Punjab, India

**P38 A Framework for a High Throughput Screening Method to Assess Polymer/Plasticizer Miscibility**

L. SMITH<sup>1</sup>, A. KARIMI-VARZANEH<sup>2</sup>, S. FINGER<sup>2</sup>, G. GIUNTA<sup>3</sup>, A. TROISI<sup>4</sup>, P. CARBONE<sup>1</sup>, <sup>1</sup>University of Manchester, Salford, UK; <sup>2</sup>Continental Reifen Deutschland GmbH, Germany; <sup>3</sup>BASF, Germany; <sup>4</sup>University of Liverpool, Department of Chemistry, UK

**P39 High-throughput Investigation of Composition-dependent Lattice Constants of Multicomponent Metallic Solid Solutions Coupled with Machine Learning**

Y. ZHOU, B. WU, J. WANG, HUI XING, L. ZHANG, H. WANG, Shanghai Jiao Tong University, Shanghai, China

**P40 Building Information Modeling BIM and Mechanical, Thermal and Fire Protection Properties for Product Data Passport PDP**

A. GLEMA, W. SZYMKUĆ, Ł. MALEWSKI, Poznan University of Technology, Poznan, Poland

**P41 Transfer Learning based Prediction of Material Properties of Bulk-metallic Glasses**

CHUNGHEE NAM, Department of Electrical and Electronic Engineering, Hannam University, Daejeon, South Korea

**P42 Improvement of Strained Quantum Well based on New Material ZnSnN<sub>2</sub>/InyGa<sub>1-y</sub>N for Optical Components Applications**

A. AISSAT<sup>1,2</sup>, L. CHENINI<sup>1</sup>, S. NACER<sup>1</sup>, J.P. VILCOT<sup>2</sup>, LATS Laboratory, Faculty of Technology, University of Blida, Blida, Algeria; <sup>2</sup>Institute of Electronics, Microelectronics and Nanotechnology (IEMN), UMR CNRS 8520, University of Sciences and Technologies of Lille, Villeneuve of Ascq, France

**P43 Structural, Magnetic and Dielectric Study of Yb-ion Substituted Spinel Ferrites**

Q. KHAN, R. AHMAD, Department of Chemistry, University of Malakand, Malakand, Pakistan

**P44 Tunable Synaptic Plasticity in a Double Gated MoS<sub>2</sub> FET**

J.S.A. NANDAN KARALAPATI, **O. BADAMI**, S. BHATTACHARJEE, Electrical Engineering, IIT Hyderabad, Kandi, Sangareddy, India

**P45 Square SnO<sub>2</sub> Nanotubes: Neuromorphic Device Properties**

**M.W. ALLEN**, Dept. Electrical and Computer Engineering, University of Canterbury, Christchurch, New Zealand and MacDiarmid Institute for Advanced Materials and Nanotechnology, New Zealand

**P46 Synthesis and Analysis of Thin Ferroelectric Hafnium Oxide Film**

**YUJIN JEONG**, Department of Materials Science and Engineering, KAIST, South Korea

**P47 The Connection Between Power Dissipation and Energy Consumption in Memristive Devices during the Programming Phase**

**E. MIRANDA**, F.L. AGUIRRE, J. SUÑÉ, Universitat Autònoma de Barcelona, Cerdanyola del Valles, Spain; E. PIROS, T. KIM, P. SCHREYER, J. GEHRUNGER, T. OSTER, K. HOFMANN, C. HOCHBERGER, L. ALFF, Technische Universität Darmstadt, Darmstadt, Germany

**P48 Production of Free-standing, Thin and Lead-free Barium Titanate Piezoceramics by Inkjet Printing**

**I. KETTERER**<sup>1</sup>, C.-K. YANG<sup>1</sup>, E. CIMEN<sup>1</sup>, M. WAPLER<sup>2</sup>, T. HANEMANN<sup>1,3</sup>, <sup>1</sup>Laboratory for Materials Processing, Department of Microsystems Engineering (IMTEK), University of Freiburg, Germany; <sup>2</sup>Chair of Microsystems Engineering, Institute of Medical Engineering, Otto-von-Guericke University Magdeburg, Germany; <sup>3</sup>Institute for Applied Materials - Materials Sciences and Engineering (IAM-WK), Karlsruhe Institute of Technology, Germany

**P49 Tailoring Over-percolated Ag Nanowires for Unveiling Critical Properties**

J.I. DIAZ SCHNEIDER, E. MARTÍNEZ, DyS - GF - GAIDI - CAB - Comisión Nacional de Energía Atómica (CNEA) and INN-nodo Bariloche, Bariloche, Río Negro, Argentina; C. QUINTEROS, UNSAM, San Martín (B1650), Buenos Aires, Argentina; L. GRANJA, **P. LEVY**, FMC - GlyA - GAIDI - CAC - Comisión Nacional de Energía Atómica (CNEA) and INN-nodo Constituyentes, San Martín, Buenos Aires, Argentina; + all authors are members of CONICET - Argentina

**P50 Halide Perovskite Dynamical Memristors Controlled by Hybrid Electrical and Optical Stimuli**

**I. MATCHENYA**, R. PODGORNİY, D. SHIRKIN, A. PUSHKAREV, A. MARUNCHENKO, ITMO University, School of Physics and Engineering, St. Petersburg, Russian Federation; A. KHANAS, N. SIZYKH, A. ZENKEVICH, Moscow Institute of Physics and Technology (National research university), Dolgoprudny, Moscow Region, Russian Federation; A. NASIBULIN, Skolkovo Institute of Science and Technology, Moscow, Russian Federation; I. SCHEBLYKIN, A. MARUNCHENKO, Chemical Physics and NanoLund, Lund University, Lund, Sweden

**P51 Resistive Switching Property of Cow Milk Dispersed with Selenium Particles**

**Z.W. DLAMINI**<sup>1</sup>, S. VALLABHAPURAPU<sup>2</sup>, V.S. VALLABHAPURAPU<sup>2</sup>, <sup>1</sup>Central University of Technology, Bloemfontein, Free State, South Africa; <sup>2</sup>University of South Africa, Florida Park, Gauteng, South Africa

**P52 Structural Changes and Resistive Switching Behaviors of CoOx and CuxO Films by Post-thermal Annealing**

J. SEO, J. AHN, T. KIM, Y. KIM, **EUN KYU KIM**, Department of Physics, Hanyang University, Seoul, South Korea

**P53 Electric Field Engineering of Switching Mechanisms in CB-RAM Devices**

**TAEWOOK KIM**, T. VOGEL, E. PIROS, N. KAISER, P. SCHREYER, A. ARZUMANOV, S. PETZOLD, L. ALFF, Advanced Thin Film Technology Division, Technische Universität Darmstadt, Darmstadt, Germany; D. NASIOU, R. WINKLER, A. ZINTLER, L. MOLINA-LUNA, Advanced Electron Microscopy Division, Materials, Technische Universität Darmstadt, Darmstadt, Germany

**P54 A Possible bio-ReRAM using Aloe Vera for Green Computing**

**S. VALLABHAPURAPU**, School of Computing, University of South Africa, Florida Park, South Africa; Z. WISEMAN DLAMINI, Maths, Science and Technology Education, Central University of Technology, Bloemfontein, South Africa

**P55 In Situ Thermal Measurement and Modeling of the Operation of Ovonic Threshold Switch**

J.H. PARK, M.J. JUNG, H. KIM, S.Y. LEE, J.H. JANG, G.H. KIM, M.K. YANG, **BYUNG JOON CHOI**, Seoul National University of Science and Technology, Seoul, South Korea

**P56 Study on the Strain Compensated 4.8 Micrometer InGaAs/InAlAs Quantum Cascade Lasers**

W.J. LEE, J.W. SEO, J.H. KANG, **IL KI HAN**, Nanophotonics Research Center, KIST, South Korea; S. KIM, J. KIM, Department of Information Display, Kyung Hee University, South Korea; J.C. SHIN, Div. Electronics and Electrical Engineering, Dongguk University, South Korea; T.G. KIM, School of Electrical Engineering, Korea University, South Korea