

# SESSIONS BY DAY

International Conference

# materials

in an explosively  
growing  
informatics  
world

Montecatini Terme, Italy

June 20-24, 2024



**CIMTEC**2024  
JUNIOR EDITION

# CIMTEC

## JUNIOR EDITION 2024

| <i>Flowsheet</i>                                      |                         | JUNE 20<br>P.M. | JUNE 21<br>A.M. P.M. | JUNE 22<br>A.M. P.M. | JUNE 23<br>A.M. P.M. | JUNE 24<br>A.M. P.M. |
|---|-------------------------|-----------------|----------------------|----------------------|----------------------|----------------------|
| MATERIALS IN AN EXPLOSIVELY GROWING INFORMATICS WORLD | REGISTRATION            |                 |                      |                      |                      |                      |
|   | TRACK A                 |                 |                      |                      |                      |                      |
|   | TRACK B                 |                 |                      |                      |                      |                      |
|   | TRACK C                 |                 |                      |                      |                      |                      |
|   | TRACK D                 |                 |                      |                      |                      |                      |
|   | TRACK E                 |                 |                      |                      |                      |                      |
|   | TRACK F                 |                 |                      |                      |                      |                      |
|   | TRACK G                 |                 |                      |                      |                      |                      |
|   | TRACK H                 |                 |                      |                      |                      |                      |
|   | TRACK I                 |                 |                      |                      |                      |                      |
|   | AFOSR (Private Session) |                 |                      |                      |                      |                      |
|   | POSTER MOUNTING         |                 |                      |                      |                      |                      |
|   | POSTER DISCUSSION       |                 |                      |                      |                      |                      |
|   | SOCIALS                 |                 |                      |                      |                      |                      |

WELCOME RECEPTION



CONCERT



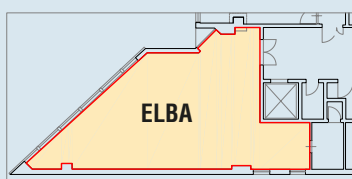
FAREWELL PARTY



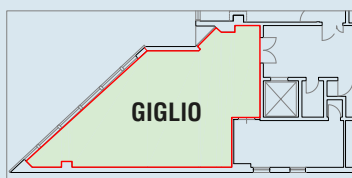
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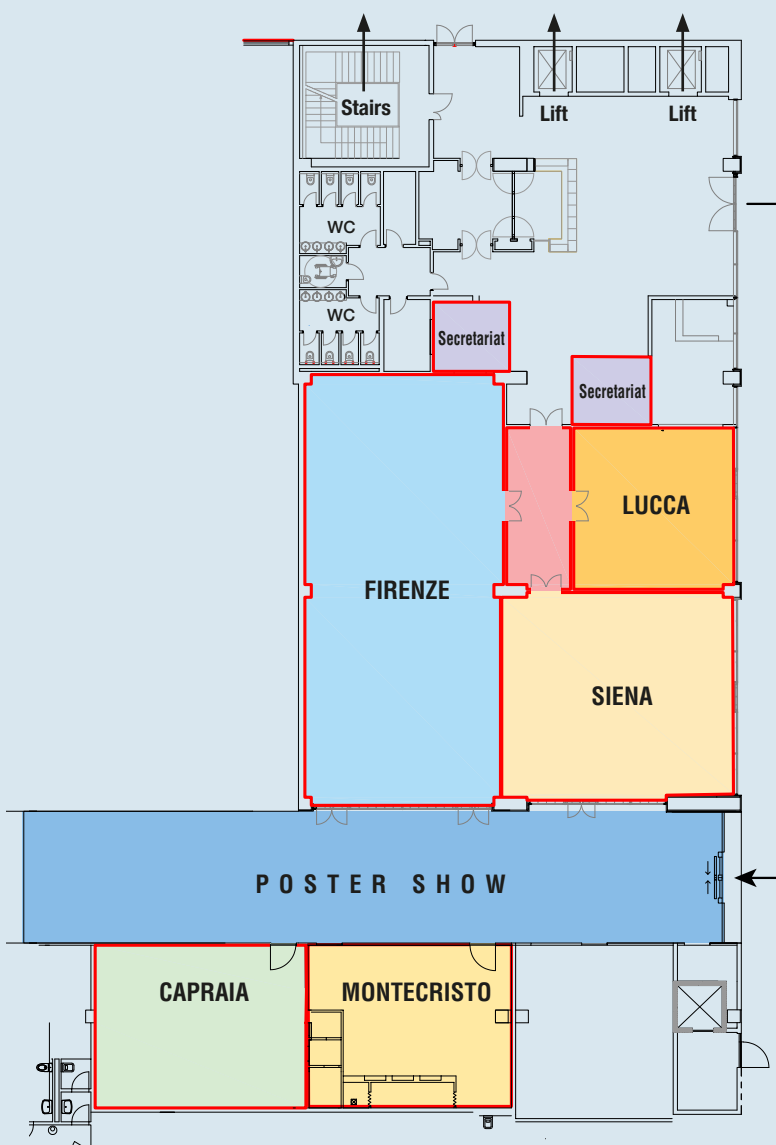
# MEETING ROOMS



**FOURTH FLOOR**

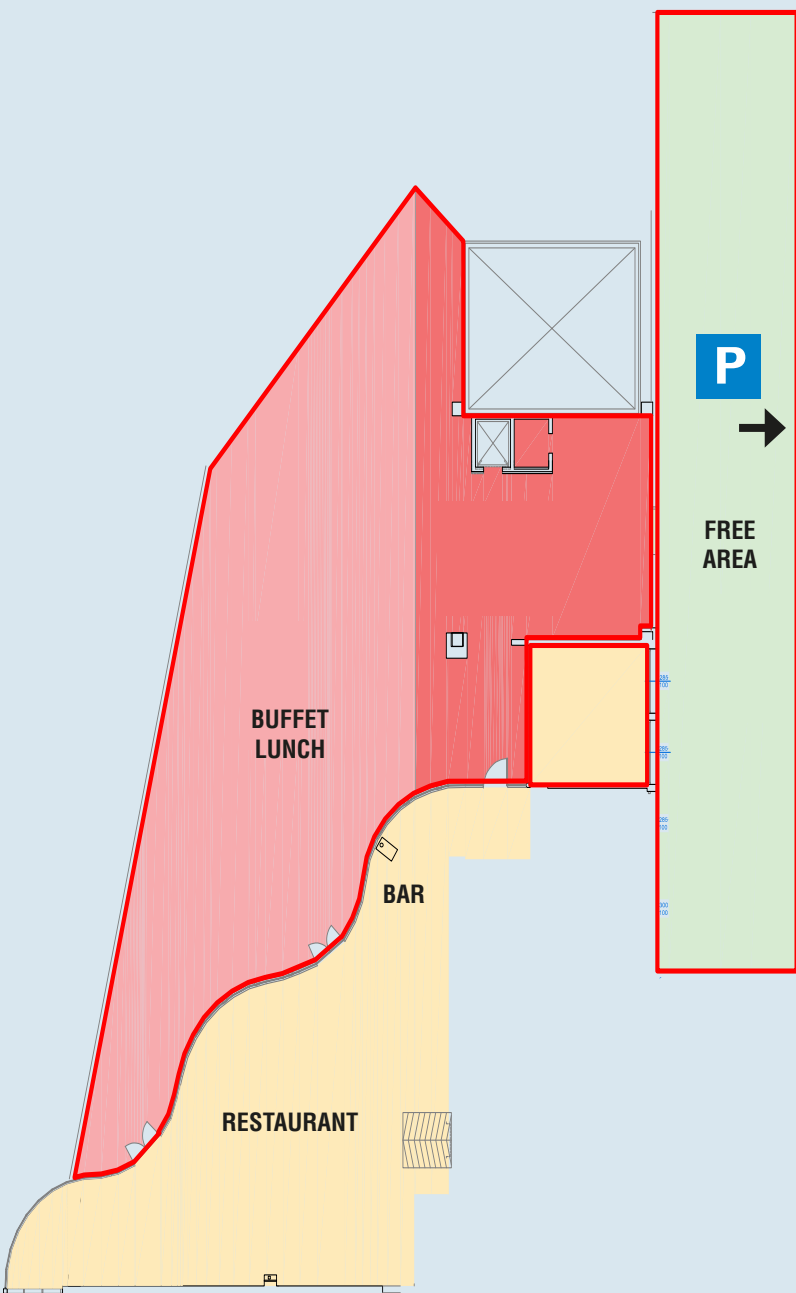


**THIRD FLOOR**



**GROUND FLOOR**





**FIRST FLOOR**

# CONFERENCE OUTLINE

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## TRACK **A**

Advances in Fundamentals of Theory,  
Computation and Simulation of Materials  
Systems: Classical to Quantum

## TRACK **B**

Computational Mesoscale Structure and Physico-  
chemical Property Evolution of Solid Materials

## TRACK **C**

Computational Tools in Materials Synthesis and  
Processing Science

### *Special Session **C-8***

*Exploiting Computational Tools in Materials Manufacturing  
and in the User Industry*

## TRACK **D**

Computer Modelling and Simulation of Materials  
Properties

## TRACK **E**

Computational Mechanics of Materials Across the  
Scales

## TRACK **F**

Designing Materials for Sustainable Energy  
Applications

## TRACK **G**

Big Data, Artificial Intelligence and Machine  
Learning Methods for Accelerated Materials  
Discovery and Advancement

## TRACK **H**

Advances in Materials and Devices Research  
for Digital, Neuromorphic and Unconventional  
Computing

### *Special AFOSR Session **H-8***

*From Brain-Inspired Networks for Multifunctional Systems  
to Neuromorphic Computing at the Edge of Biology*

## TRACK **I**

Towards Scalable Quantum Computing: Theory,  
Materials and Technology Challenges

# *Meeting Rooms by Tracks*

OPENING SESSION .....AUDITORIUM

Track A ..... LUCCA

Track B ..... GIGLIO

Track C ..... ELBA

Track D ..... SIENA

Track E ..... MONTECRISTO

Track F ..... SIENA

Track G ..... CAPRAIA

Track H ..... FIRENZE

Track I ..... LUCCA

## ***Private Session of AFOSR Members***

Monday June 24 16.00-18.30 ..... GIGLIO

# *Events by Day*

## **Thursday June 20**

15.00-19.00

REGISTRATION  
Hotel Tuscany Inn  
Via Cividale, 86/E  
Montecatini Terme, Pistoia, Italy

## **Friday June 21**

**Morning:** 10.00-13.00

### **Opening Session**

Plenary Lectures (PL1-PL3)

**Afternoon:** 14.25-19.00

|         |  |
|---------|--|
| Track A | (A-1:IL02 to IL06)   |
| Track B | (B-1:IL02 to IL04)<br>(B-1:IL05 to L06)                      |
| Track C | (C-1:IL02 to L05)<br>(C-2:L03)                               |
| Track D | (D-1:IL01 to L05)  |
| Track E | (E-1:IL02 to IL06)   |
| Track F | (F-1:IL01 to L03)  |
| Track G | (G-1:IL01 to IL03)<br>(G-1:IL04 to L07)                      |
| Track H | (H-2:IL01 to L04)<br>(H-2:IL07 + L05)<br>(H-1.2:IL01 to L04) |
| Track I | (I-1:IL01 to IL04)   |

9.30-18.00

*POSTER MOUNTING*

20.30-22.00

*Welcome Reception*

## Saturday June 22

### Morning: 9.00-13.00

|         |   |
|---------|---|
| Track A | (A-1:IL07 to IL10)                        |
| Track B | (B-2:IL01 to IL04)<br>(B-3:IL01 to IL02)  |
| Track C | (C-3:IL01 to L04)                         |
| Track D | (D-1:IL07 to L10)<br>(D-1:IL11 to L14)    |
| Track E | (E-1:IL07 to L09)<br>(E-1:IL10 to L12)    |
| Track G | (G-1:L09 to L10)<br>(G-2:IL01 to L04)     |
| Track H | (H-2:IL09 to IL14)<br>(H-1.1:IL01 to L05) |

### Afternoon: 14.30-19.00

|         |  |
|---------|--|
| Track B | (B-3:L03 to IL05)<br>(B-3:IL06 to IL09)  |
| Track C | (C-3:IL05 to IL06)<br>(C-6:IL01 to IL03) |
| Track E | (E-2:IL01 to IL02)<br>(E-3:IL01 to L03)  |
| Track F | (F-1:IL04 to L07)<br>(F-2:IL01 to L03)   |
| Track G | (G-2:IL05 to L07)<br>(G-3:IL01 to L04)   |
| Track H | (H-4:IL01 to L07)<br>(H-5:L03 to L07)    |
| Track I | (I-2:IL01 to IL04)<br>(I-3:IL02 to IL07) |

## Sunday June 23

### Morning: 9.00-13.00

|         |  |
|---------|--|
| Track A | (A-2:IL01 to IL02)<br>(A-3:IL01 to L04)<br>(A-4:IL01 to L02) |
| Track B | (B-4:IL01 to L04)<br>(B-4:IL05 to IL06)<br>(B-5:IL01)        |
| Track C | (C-4:IL01 to IL02)<br>(C-5:IL01 to L05)                      |
| Track D | (D-2:IL01 to L04)<br>(D-2:IL06 to IL09)                      |
| Track E | (E-3:IL04 to IL07)<br>(E-3:IL08 to L10)                      |
| Track G | (G-3:IL06 to L09)<br>(G-3:IL11 to L13)                       |
| Track H | (H-7:IL02 to L07)<br>(H-6:IL01 to L05)                       |

### Afternoon: 14.30-19.00

|         |  |
|---------|--|
| Track B | (B-6:IL01 to IL04)                       |
| Track C | (C-7:IL01 to L02)                        |
| Track E | (E-4:IL02 to IL03)<br>(E-5:IL01 to IL02) |
| Track F | (F-2:IL06 to L10)<br>(F-3:L03 to L04)    |
| Track G | (G-4:IL01 to L03)<br>(G-4:L04 to L07)    |
| Track H | (H-3:IL01 to L07)<br>(H-8:IL01 to L05)   |
| Track I | (I-1:IL05 to L07)<br>(I-4:IL01 to IL03)  |

21.00-23.00  
*Concert*

# Monday June 24

## Morning: 9.00-13.00

|         |   |
|---------|---|
| Track B | (B-5:IL02 to IL03)  |
| Track C | (C-8.1:L01)<br>(C-8.2:IL01 to L03)<br>(C-8.3:IL01 to L03) |
| Track E | (E-5:L04 to L05)<br>(E-5:IL06 to IL08)                    |
| Track F | (F-4:IL02 to IL04)  |
| Track G | (G-1:IL11)<br>(G-5:IL01 to IL03)<br>(G-5:IL04 to IL06)    |
| Track H | (H-3:IL08 to IL14)<br>(H-8:IL06 to L09)                   |
| Track I | (I-4:IL11+IL05+L07)<br>(I-4:IL08 to IL10)                 |

## Afternoon: 14.30-19.00

|         |  |
|---------|--|
| Track A | (A-5:IL01 to IL03)<br>(A-5:IL05 to IL07) |
| Track C | (C-8.3:IL04 to IL06)                     |
| Track D | (D-3:IL01 to IL05)                       |
| Track H | (H-8:IL11 to L14)                        |

16.00-18.30

Private Session of AFOSR Members

16.00-18.30

**POSTER DISCUSSION**

20.30-22.30

*Farewell Party*

# SESSIONS FLOWSHEET

## June 21-24

### Chair

**Pietro Vincenzini**

World Academy of Ceramics  
National Research Council, Italy

### *Conveners*

#### Track A

**Steven Louie**, USA

#### Track B

**Long-Qing Chen**, USA

#### Track C

**Yury Gogotsi**, USA

#### Track D

**David Beljonne**, Belgium

#### Track E

**Nicola Manini**, Italy

#### Track F

**Su-Huai Wei**, China

#### Track G

**Christopher M. Wolverton**, USA

#### Track H

**Sabina Spiga**, Italy

#### Track I

**David Awschalom**, USA  
**Andrea Morello**, Australia



**OPENING SESSION  
AUDITORIUM**

*Chair:*

Andrea MORELLO,  
University of New South Wales, Sydney, Australia

*Plenary Lectures*

10.00 - 10.50

*PL1*

**The Second Decade of the Material Genome Initiative**

James A. WARREN

Material Measurement Laboratory, National Institute of  
Standards and Technology, Gaithersburg, MD, USA

11.00 - 11.50

*PL2*

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

Giordano SCAPPUCCI

QuTech, TU Delft, Delft, The Netherlands

12.00 - 12.50

*PL3*

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

Thaddeus D. LADD

HRL Laboratories, LLC, Malibu, CA, USA

**TRACK A**  
**ADVANCES IN FUNDAMENTALS**  
**OF THEORY, COMPUTATION AND**  
**SIMULATION OF MATERIALS SYSTEMS:**  
**CLASSICAL TO QUANTUM**

*Room:* **LUCCA**

*Chair:* Steven G. LOUIE, USA (*Convener*)

14.25 *Welcome*

**Session A-1**

**Ab-initio methods for bulk and reduced-dimensional materials**

14.30 *A-1:IL02* **Ab initio Extended Hubbard Interactions and their Applications**  
**YOUNG-WOO SON**, Korea Institute for Advanced Study, Seoul, South Korea

15.00 *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

15.30 *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

16.00 *Break*

16.25 *Session I-1 (see page 21)*

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

Room: **GIGLIO**

Chair: Long-Qing CHEN, USA (*Convener*)

14.25 *Welcome*

Session B-1

Databases of physico-chemical properties of materials

14.30 *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

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

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

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

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

16.15 *Break*

Chair: Thomas D. SWINBURNE, France

16.45 *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, Dept of Materials Science and Engineering, The Pennsylvania State University, University Park, PA, USA

17.20 *B-1:L06* **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

TRACK C  
**COMPUTATIONAL TOOLS IN MATERIALS  
SYNTHESIS AND PROCESSING SCIENCE**

Room: **ELBA**

Chair: Yury GOGOTSI, USA (*Convener*)

14.25 *Welcome*

Session C-1/2

0D, 1D and 2D nanomaterials and nanostructures  
and soft-condensed matter

14.30 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

15.05 C-1:IL04 **3D Printed Functional MXene-based Ceramics**  
**S. BARG**, University of Augsburg, Institute of Materials Resource Management, Augsburg, Germany

15.40 *Break*

16.10 C-1:L05 **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>Dept of Materials Sciences and Engineering, Guangdong Technion Israel Institute of Technology, Shantou, Guangdong, China; <sup>2</sup>Particle Technology Laboratory, Institute of Process Engineering, Dept of Mechanical and Process Engineering, ETH Zürich, Zürich, Switzerland

16.35 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. CRESPI<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

**TRACK D**  
**COMPUTER MODELLING AND**  
**SIMULATION OF MATERIALS**  
**PROPERTIES**

*Room:* **SIENA**

*Chair:* David BELJONNE, Belgium (*Convener*)

14.25 *Welcome*

**Session D-1**

**Materials for electronics, opto-electronics and photonics**

- 14.30 *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
- 15.00 *D-1:IL02* **Van der Waals Interactions in Materials Modelling**  
**A. TKATCHENKO**, Department of Physics and Materials Science, University of Luxembourg, Luxembourg
- 15.30 *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
- 16.00 *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
- 16.30 *D-1:L05* **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
- 16.50 *Break*
- 17.20 *Session F-1 (see page 17)*

TRACK E  
**COMPUTATIONAL MECHANICS OF  
MATERIALS ACROSS THE SCALES**

Room: **MONTECRISTO**

Chair: Nicola MANINI, Italy (*Convenor*)

14.25 *Welcome*

Session E-1

Computational mechanics of nanoscale materials

14.30 *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

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

**A. SILVA**, CNR - Istituto Officina dei Materiali (IOM) & International School for Advanced Studies (SISSA), Trieste, Italy. In collaboration with: A. VANOSSI, C. BECHINGER, A. BENASSI, T. BRAZDA, X. CAO, L. GIGLI, R. GUERRA, S. KAWAI, A. KHOSRAVI, D. MANDELLI, N. MANINI, E. MEYER, E. PANIZON, E. TOSATTI, M. URBACH, J. WANG

15.40 *Break*

16.10 *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

16.45 *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. URBACH, 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

**TRACK F**  
**DESIGNING MATERIALS FOR**  
**SUSTAINABLE ENERGY APPLICATIONS**

*Room:* **SIENA**

*Chair:* Su-Huai WEI, China (*Convener*)

17.20 *Welcome*

**Session F-1**  
**Electrochemical energy systems**

- 17.25 *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
- 17.55 *F-1:L03* **Microstructure Design of Polycrystalline Ceramics for Energy Applications**  
**E. GARCIA**, Purdue University, West Lafayette, IN, USA

TRACK G

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

Room: **CAPRAIA**

Chair: Christopher M. WOLVERTON, USA (*Convener*)

14.25 *Welcome*

Session G-1

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

14.30 *G-1:IL01* **Enabling the 4th Paradigm for Accelerated Materials Innovation**  
**K.A. PERSSON**, University of California at Berkeley, Berkeley, CA, USA

15.05 *G-1:IL02* **Construct Exchange-correlation Functional via Machine Learning and Delta-learning Method**  
**GUANHUA CHEN**, The University of Hong Kong, Shatin, Hong Kong

15.40 *G-1:IL03* **New Approaches to Predicting and Understanding the Electrochemical Stability of Inorganic Materials**  
**J. MONTOYA**, Toyota Research Institute, Los Altos, CA, USA

16.15 *Break*

Chair: Kristin PERSSON, USA

16.45 *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

17.20 *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

17.55 *G-1:L06* **Equivariant Tensor Network Potentials**  
**M. HODAPP**, Materials Center Leoben, Leoben, Austria; A. SHAPEEV, Skoltech, Moscow, Russia

18.20 *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



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

*Room:* **FIRENZE**

*Chair:* Sabina SPIGA, Italy (*Convener*)

14.25 *Welcome*

**Session H-2**

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

14.30 *H-2:IL01* **Architectures and Materials for Storage Class Memories**  
**P. FANTINI**, Micron Semiconductor, Vimercate, Italy

14.55 *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

15.20 *H-2:IL03* **CMOS Compatible Materials and Devices for *beyond von Neumann***  
**V. BRAGAGLIA**, IBM Research Europe, Zurich, Switzerland

15.45 *H-2:L04* **Resistive Memory Window Enhanced through Bandgap Tuning in V-substituted Cr<sub>2</sub>O<sub>3</sub> 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

16.00 *Break*

*Continued on next page*

*Continued from preceding page*

*Chair:* Valeria BRAGAGLIA, Switzerland

- 16.30 *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
- 16.55 *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

*Chair:* Paolo FANTINI, Italy

## Session H-1.2

### Phase change materials and applications

- 17.10 *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
- 17.35 *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
- 17.50 *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

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

*Room:* **LUCCA**

*Chair:* Andrea MORELLO, Australia (*Convener*)

16.25 *Welcome*

**Session I-1**  
**Superconducting qubits**

- 16.30 *I-1:IL01* **New Material Platforms for Quantum Computing**  
**N. DE LEON**, Department of Electrical and Computer Engineering,  
Princeton University, Princeton, NJ, USA
- 17.00 *I-1:IL02* **Integer Fluxonium Qubit**  
**V. MANUCHARYAN**, R. MENCIA, EPFL, Lausanne, Switzerland
- 17.30 *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
- 18.00 *I-1:IL04* **Outstanding Materials Challenges & Opportunities for Developing Superconducting Quantum Information Systems**  
**R.W. SIMMONDS**, National Institute of Standards & Technology,  
Boulder, CO, USA

**TRACK A**  
**ADVANCES IN FUNDAMENTALS**  
**OF THEORY, COMPUTATION AND**  
**SIMULATION OF MATERIALS SYSTEMS:**  
**CLASSICAL TO QUANTUM**

*Room:* **LUCCA**

**Session A-1**

**Ab-initio methods for bulk and reduced-dimensional materials**

*Chair:* Young-Woo SON, South Korea

- 9.00 *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
- 9.30 *A-1:IL08* **Many-body Effects on the Photophysics of 2D Materials**  
**D.Y. QIU**, Yale University, New Haven, CT, USA
- 10.00 *A-1:IL10* **Auxiliary-field Quantum Monte Carlo Beyond Hartree-Fock Trial Wavefunctions**  
**JOONHO LEE**, Harvard University, Cambridge, MA, USA

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

*Room:* **GIGLIO**

**Session B-2**  
**Theory of phase transitions**

*Chair:* Ralf DRAUTZ, Germany

- 9.00 *B-2:IL01* **Quantitative Predictive Theories for Physico-chemical Property of Solid Phases**  
**ZI-KUI LIU**, Pennsylvania State University, University Park, PA, USA
- 9.35 *B-2:IL02* **Phase-field Modelling of Nonequilibrium Interface Dynamics in Diffusion-controlled Phase Transition of Alloys**  
**MUNEKAZU OHNO**, Hokkaido University, Sapporo, Hokkaido, Japan
- 10.10 *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. ALA-NISSILA**, Aalto University, Espoo, Finland
- 10.45 *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
- 11.20 *Break*

**Session B-3**  
**Strain and size effects on phase equilibria, phase transitions, and mesoscale domain states**

*Chair:* Munekazu OHNO, Japan

- 11.50 *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
- 12.25 *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. SCHWARZ-SELINGER**, Max Planck Institute for Plasma Physics, Garching, Germany

**TRACK C**  
**COMPUTATIONAL TOOLS IN MATERIALS  
SYNTHESIS AND PROCESSING SCIENCE**

*Room:* **ELBA**

**Session C-3**

**Powders, granular materials, single crystal growth**

*Chair:* Jochen FRIEDRICH, Germany

- 9.00 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
- 9.35 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
- 10.10 *Break*
- 10.40 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
- 11.15 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, Dept of Mechanical & Process Engineering, ETH Zurich, Switzerland and Dept of Chemical Engineering, University of Patras, Greece

**TRACK D**  
**COMPUTER MODELLING AND**  
**SIMULATION OF MATERIALS**  
**PROPERTIES**

*Room:* **SIENA**

**Session D-1**

**Materials for electronics, opto-electronics and photonics**

*Chair:* **Chris G. VAN DE WALLE, USA**

9.00 *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

9.30 *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

10.00 *D-1:L09* **A Feedback Model for Relaxor Ferroelectrics**  
**H. KLIEM**, A. LESCHHORN, Saarland University, Saarbruecken, Germany

10.20 *D-1:L10* **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

10.40 *Break*

*Chair:* **Alexander SHLUGER, UK**

11.10 *D-1:IL11* **Large-scale Nonadiabatic Dynamics Methods and Applications to Quantum Dots**  
**LINJUN WANG**, Department of Chemistry, Zhejiang University, Hangzhou, China

11.40 *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

12.10 *D-1:L14* **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

**TRACK E**  
**COMPUTATIONAL MECHANICS OF**  
**MATERIALS ACROSS THE SCALES**

*Room:* **MONTECRISTO**

**Session E-1**

**Computational mechanics of nanoscale materials**

*Chair:* **Andrea SILVA**, Italy

**9.00 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

**9.35 E-1:L09 The Mechanism of Strong Reinforcement of Si Nanopowders by thin Continuous SiC Coatings**

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

**10.00 Break**

*Chair:* **Takuya KUWAHARA**, Japan

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

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

**11.05 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

**11.40 E-1:L12 Probing the Solute Effect on Twin Embryo Growth in Mg Alloys**

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



**TRACK G**

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

*Room:* **CAPRAIA**

**Session G-1**

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

*Chair:* Aron WALSH, UK

**9.00 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

**9.25 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

**9.50 Break**

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**Session G-2**  
**Virtual materials design and evaluation**

*Chair:* Gian-Marco RIGNANESE, Belgium

- 10.20 *G-2:IL01* **Navigating Materials Space at Warp Speed**  
**A. WALSH**, Department of Materials, Imperial College London, London, UK
- 10.55 *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
- 11.30 *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
- 11.55 *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

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

Room: **FIRENZE**

**Session H-2**

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

*Chairs:* Erika COVI & Martin ZIEGLER, Germany

- 9.00 *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
- 9.25 *H-2:IL10* **Domain Switching Dynamics in the Ferroelectric AlScN Thin Film Capacitors**  
**A. GRUVERMAN**, Department of Physics and Astronomy, University of Nebraska, Lincoln, NE, USA
- 9.50 *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
- 10.15 *H-2:L12* **Correlation between Electronic Structure and Microstructure of Al<sub>2</sub>O<sub>3</sub>/TiO<sub>x</sub>-based Memristive Cells Switched in Filamentary- and Area-mode**  
**S. HOFFMANN-EIFERT**, S. AUSSSEN, 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, Dept 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
- 10.30 *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>Dept 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 Lab., Empa, Switzerland; <sup>5</sup>ELKH-BME Condensed Matter Research Group, Hungary
- 10.45 *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, Dept of Materials Science, NOVA School of Science and Technology, Universidade NOVA de Lisboa and CEMOP/UNINOVA, Caparica, Portugal
- 11.10 *Break*

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**Session H-1.1**

**Memristive materials and devices for brain inspired computing**

*Chairs:* Catherine DUBORDIEU & Regina DITTMAN, Germany

- 11.30 *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, Department of Electrical Engineering and Information Technology, TU Ilmenau, Germany;  
<sup>2</sup>Institute of Micro- and Nanotechnologies MacroNano®, TU Ilmenau, Germany
- 11.55 *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
- 12.20 *H-1.1:IL03* **Leveraging Ferroelectric Technologies for Neuromorphic Computing**  
**E. COVI**, University of Groningen, Zernike institute for Advanced Materials and Groningen Cognitive Systems and Materials Center (CogniGron), Groningen, Netherlands
- 12.45 *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
- 13.10 *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

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

*Room:* **GIGLIO**

**Session B-3**

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

*Chair:* **Peter W. VOORHEES, USA**

**14.30 B-3:LO3 Mechanisms of Nanostructure Formation During Dealloying**  
**G. HENKELMANN**, J. WEISSMÜLLER, Hamburg University of Technology, Institute of Materials Physics and Technology, Hamburg, Germany

**14.55 B-3:LO4 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

**15.30 B-3:LO5 Coherent Phase Change in Interstitial Solutions – A Hierarchy of Instabilities**  
**J. WEISSMÜLLER**, Hamburg University of Technology, Hamburg, Germany and Helmholtz-Center Hereon, Geesthacht, Germany

**16.05 Break**

*Chair:* **Joerg WEISSMUELLER, Germany**

**16.35 B-3:LO6 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

**17.10 B-3:LO8 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

**17.45 B-3:LO9 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

**TRACK C**  
**COMPUTATIONAL TOOLS IN MATERIALS**  
**SYNTHESIS AND PROCESSING SCIENCE**

*Room:* **ELBA**

**Session C-3**

**Powders, granular materials, single crystal growth**

*Chair:* Hannes JONSSON, Ireland

**14.30 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

**15.05 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

**15.40 Break**

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**Session C-6**

**Additive manufacturing of multiscale and  
multi-material structures**

*Chair:* Jeff DERBY, USA

- 16.10 **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
- 16.45 **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
- 17.10 **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

**TRACK E**  
**COMPUTATIONAL MECHANICS OF**  
**MATERIALS ACROSS THE SCALES**

*Room:* **MONTECRISTO**

**Session E-2**

**Computational mechanics in nanodevice applications**

*Chair:* David RICHARD, France

- 14.30 *E-2:IL01* **Design and Simulation of Micro- and Nano-technology Tools for Biomedical Applications**  
**E. CIMETTA**, Università degli Studi di Padova, Padova, Italy
- 15.05 *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
- 15.40 *Break*

**Session E-3**

**Computational mechanics at  
mesoscopic / macroscopic scale**

*Chair:* Shu-Wei CHANG, Taiwan

- 16.10 *E-3:IL01* **A Mapping between the Non-linear Micromechanics of Glasses and Elasto-plastic Models**  
**D. RICHARD**, Laboratoire Navier, Champs-sur-Marne, France
- 16.45 *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
- 17.20 *E-3:L03* **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



**TRACK F**  
**DESIGNING MATERIALS FOR**  
**SUSTAINABLE ENERGY APPLICATIONS**

*Room:* **SIENA**

**Session F-1**  
**Electrochemical energy systems**

*Chair:* Vesselin YAMAKOV, USA

- 14.30 *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
- 15.00 *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
- 15.20 *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

15.40 *Break*

**Session F-2**  
**Photovoltaics**

*Chair:* Andrew M. RAPPE, USA

- 16.10 *F-2:IL01* **First-principles Study of Defect Control in Thin Film Solar Cell**  
**SU-HUAI WEI**, Beijing Computational Science Research Center, Beijing, China
- 16.40 *F-2:IL02* **Understanding and Design of Photovoltaic and Energy Storage Materials**  
**M. CHAN**, Center for Nanoscale Materials, Argonne National Laboratory, Lemont, IL, USA
- 17.10 *F-2:L03* **Accelerated Screening of Ternary Chalcogenides for Potential Photovoltaic Applications**  
**TIANSHU LI**, Department of Materials, Imperial College London, London, UK

**TRACK G**

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

*Room:* **CAPRAIA**

**Session G-2**

**Virtual materials design and evaluation**

*Chair:* Pieremanuele CANEPA, USA

- 14.30 *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
- 15.05 *G-2:IL06* **Machine Learning Discovery of Materials**  
**J. SCHMIDT**, Materials Theory ETH Zurich, Zurich, Switzerland; P. BORLIDO, Dept of Physics, University of Coimbra, Portugal; A. ROMERO, Dept of Physics and Astronomy West Virginia University, USA; T. CERQUEIRA, Dept 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
- 15.40 *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
- 16.05 *Break*

**Session G-3**

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

*Chair:* Milad ABOLHASANI, USA

- 16.35 *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
- 17.10 *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
- 17.45 *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
- 18.10 *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

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

*Room:* **FIRENZE**

**Session H-4**

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

*Chairs:* **Stefano BRIVIO & Gianluca MILANO, Italy**

- 14.30 *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
- 14.55 *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
- 15.20 *H-4:IL03* **Multi-scale Modelling of Valence Change Memory Cells**  
**M. LUISIER**, M. KANISELVAN, M. MLADENOVIC, Integrated Systems Laboratory, ETH Zurich, Zurich, Switzerland
- 15.45 *H-4:L05* **A Machine-learning Interatomic Potential for GeSbTe Phase Change Alloys**  
O. ABOU EL KHEIR, D. BARATELLA, Dept of Materials Science, University of Milano-Bicocca, Milano, Italy; L. BONATI, M. PARRINELLO, Italian Institute of Technologies (IIT), Genova, Italy; **M. BERNASCONI**, Dept of Materials Science, University of Milano-Bicocca, Milano, Italy
- 16.00 *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
- 16.15 *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
- 16.30 *Break*

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**Session H-5**

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

*Chairs:* Martina MUELLER, Germany & Emanuel CARLOS, Portugal

- 17.00 *H-5:L03* **Visual Memory in a 2D Memitter Based on WS2**  
**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
- 17.15 *H-5:L04* **2D Van der Waals NbTe4 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>6</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
- 17.30 *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
- 17.45 *H-5:L07* **Resistive Switching Memory Behaviours in Bio-degradable 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

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

Room: **LUCCA**

Session I-2

Defects and color centers in semiconductors

Chair: Nicola LOVERGINE, Italy

- 14.30 *I-2:IL01* **Quantum Embedding for Point Defects: Bench-marking and Applications**  
**M. ROESNER**, Theory of Condensed Matter Dept (TCM), Institute for Molecules and Materials (IMM), Radboud University, Nijmegen, Netherlands
- 15.00 *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
- 15.30 *I-2:IL03* **Recombination Mechanisms in Quantum Defects**  
**M.E. TURIANSKY**, Materials Dept, 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 Dept, University of California, Santa Barbara, CA, USA
- 16.00 *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
- 16.30 *Break*

Session I-3

Trapped-ion, photonic and topological insulators-based qubits

Chair: Tim Hugo TAMINIAU, Netherlands

- 16.45 *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
- 17.15 *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
- 17.45 *I-3:IL06* **III-V Nanowire Heterostructures for Quantum Photonics**  
**N. LOVERGINE**, Università del Salento, Lecce, Italy
- 18.15 *I-3:IL07* **Visualizing Topological Phases of Matter – Towards Future Anyonic Braiding**  
**ZHI-XUN SHEN**, Dept of Physics and Applied Physics, Stanford University, Stanford, CA, USA

**TRACK A**  
**ADVANCES IN FUNDAMENTALS**  
**OF THEORY, COMPUTATION AND**  
**SIMULATION OF MATERIALS SYSTEMS:**  
**CLASSICAL TO QUANTUM**

*Room:* **LUCCA**

**Session A-2**

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

*Chair:* **James R. CHELIKOWSKY, USA**

- 9.00 *A-2:IL01* **Correlation-enhanced Electron-phonon Interaction in Oxide Superconductors from GW Perturbation Theory**  
**ZHENGLU LI**, Mork Family Dept of Chemical Engineering and Materials Science, University of Southern California, Los Angeles, CA, USA
- 9.30 *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

10.00 *Break*

**Session A-3**

**Molecular dynamics, Langevin dynamics, stochastic and  
finite element methods**

*Chair:* **Ryan REQUIST, Israel**

- 10.30 *A-3:IL01* **Universal First Principles Force-fields for Materials Simulations based on Sparse Gaussian Process Regression**  
**KWANG S. KIM**, Dept of Chemistry, Ulsan National Institute of Science and Technology (UNIST), 50 UNIST-gil, Ulsan, South Korea
- 11.00 *A-3:IL03* **Prediction of a Supersolid Phase in High-pressure Deuterium**  
**CHANG WOO MYUNG**, Dept of Energy Science, Sungkyunkwan University, Suwon, South Korea
- 11.30 *A-3:L04* **Graph Theory Ideas Reveal Long Range Conduction Pathways**  
**M.A. GOMEZ**, Dept of Chemistry, Mount Holyoke College, South Hadley, MA, USA

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**Session A-4**

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

*Chair:* Arcady KRASHENINNIKOV, Germany

- 11.50 *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
- 12.20 *A-4:L02* **Ab Initio Informed Microstructure and Process Modelling of Metals**  
**D. SCHEIBER**, Materials Center Leoben Forschung GmbH, Leoben, Austria

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

*Room:* **GIGLIO**

**Session B-4**

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

*Chair:* Yaroslav GROSU, Spain

- 9.00 *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
- 9.35 *B-4:L03* **Charged Dislocations in Ionic Ceramics: Equilibrium and Kinetics**  
**E. GARCIA**, Purdue University, West Lafayette, IN, USA
- 10.00 *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>IKERBASQUE, Basque Foundation for Science, Bilbao, Spain
- 10.25 *Break*

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**Chair:** Edwin GARCIA, USA

**10.55 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. Chelkowski 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

**11.30 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**

**12.05 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>5</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

*(rescheduled upon request of the Speaker)*

**TRACK C**  
**COMPUTATIONAL TOOLS IN MATERIALS**  
**SYNTHESIS AND PROCESSING SCIENCE**

*Room:* **ELBA**

**Session C-4**

**3D-bulks, composites and porous materials**

*Chair:* **Francesco BAINO**, Italy

**9.00 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

**9.35 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**, Dept of Chemical Engineering, School of Engineering, The University of Manchester, Manchester, UK; Continental Reifen Deutschland GmbH, Hanover, Germany; BASF, Ludwigshafen, Germany; Dept of Chemistry, Liverpool, UK

**10.10 Break**

**Session C-5**

**Thin/thick films, layered structures and surface processing**

*Chair:* **Masahiro YOSHIMURA**, Taiwan

**10.30 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

**11.05 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

**11.40 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

**12.15 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

**12.40 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

**TRACK D**  
**COMPUTER MODELLING AND**  
**SIMULATION OF MATERIALS PROPERTIES**

*Room:* **SIENA**

**Session D-2**

**Materials for energy generation and storage**

*Chair:* **Fabrizia NEGRI, Italy**

- 9.00 *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
- 9.30 *D-2:IL02* **Property Analysis and Simulation Package for Materials (PASP) and its Applications to Ferroic Materials**  
**HONGJUN XIANG**, Dept of Physics, Fudan university, Shanghai, China
- 10.00 *D-2:L03* **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 Dept of Materials, Imperial College London, London, UK; <sup>2</sup>Dept of Physics, Ewha Womans University, Seoul, South Korea
- 10.20 *D-2:L04* **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
- 10.40 *Break*
- Chair:* **Cristiana DI VALENTIN, Italy**
- 11.10 *D-2:IL06* **Design of Energy Conversion Materials by Computation and AI**  
**WAN-JIAN YIN**, College of Energy, Soochow University, Suzhou, Jiangsu, China
- 11.40 *D-2:IL07* **Modeling Organic Semiconductors from Low Doping to Ultra-high Charge Densities**  
**G. D'AVINO**, Institut Néel, CNRS, Grenoble, France
- 12.10 *D-2:IL08* **Modelling of Energy Storage and Optoelectronic Properties in Organic Molecular Materials**  
**F. NEGRI**, Dept of Chemistry "Giacomo Ciamician", University of Bologna, Italy and INSTM, UdR Bologna, Italy
- 12.40 *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

**TRACK E**  
**COMPUTATIONAL MECHANICS OF**  
**MATERIALS ACROSS THE SCALES**

*Room:* **MONTECRISTO**

**Session E-3**

**Computational mechanics at  
mesoscopic / macroscopic scale**

*Chair:* **George STYLIOU, Scotland**

- 9.00 *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
- 9.35 *E-3:IL05* **Multiscale Modeling of Nanomechanical Deformation in High Entropy Alloys**  
**S. PAPANIKOLAOU**, National Centre of Nuclear Research, Otwock, Poland
- 10.10 *E-3:L06* **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
- 10.35 *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
- 11.10 *Break*

*Chair:* **Erik BITZEK, Germany**

- 11.40 *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
- 12.15 *E-3:IL09* **Modelling the Data of Nonlinear Mechanical Properties of Fabrics by Decomposing Friction**  
**G. STYLIOU**, L. LUO, Heriot Watt University, Scotland
- 12.50 *E-3:L10* **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

**TRACK G**

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

*Room:* **CAPRAIA**

**Session G-3**

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

*Chair:* **Seunghwa RYU**, South Korea

- 9.00 *G-3:IL06* **Materials and Molecular Modelling, Imaging, Informatics and Integration (M3I3)**  
**SEUNGBUM HONG**, KAIST, Daejeon, South Korea
- 9.35 *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
- 10.10 *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
- 10.35 *G-3:L09* **Metastable Transition Metal Dichalcogenides from Machine Learning Force Fields**  
**ZHENZHU LI**, A. WALSH, Department of Materials, Imperial College London, UK
- 11.00 *Break*

*Chair:* **Wei CHEN**, USA

- 11.30 *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
- 12.05 *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
- 12.30 *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

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

*Room:* **FIRENZE**

**Session H-7**

**New developments in characterization methods for  
materials and devices**

*Chairs:* **Lambert ALFF**, Germany & **Sabina SPIGA**, Italy

- 9.00 *H-7:IL02* **Photoelectron Spectroscopy of Functional Oxides for Novel Electronic Device Concepts**  
**M. MÜLLER**, University of Konstanz, Germany Complex Materials Group, Konstanz, Germany
- 9.25 *H-7:IL03* **Advanced Nanoscale Spectroscopic Investigation of Nanostructures for Single Photon Source**  
**P. PRETE**, IMM-CNR, Lecce, Italy
- 9.50 *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
- 10.15 *H-7:L05* **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, Dept 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
- 10.30 *H-7:L06* **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
- 10.45 *H-7:L07* **Dead Samples Tell No Tales: STEM EBIC of PFIB-prepared Devices**  
**W.A. HUBBARD**, NanoElectronic Imaging, Los Angeles, CA, USA
- 11.00 *Break*

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**Session H-6**

**Nanomaterials and unconventional substrates for computing**

*Chairs:* **Fernando AGUIRRE**, Spain & **Beatriz NOHEDA**, Netherlands

- 11.30 *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
- 11.55 *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
- 12.20 *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
- 12.45 *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. MUSSENBRÖCK**<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
- 13.00 *H-6:L05* **In-material Adaptive Computing Devices based on Random-assembled Clusters Network**  
**F. BORGHI**, **G. NADALINI**, **S. BRESSAN**, **P. MILANI**, CIMAINE and Dipartimento di Fisica, Università di Milano, Italy

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

*Room:* **GIGLIO**

**Session B-6**

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

*Chair:* **David J. SROLOVITZ, Hong Kong**

**14.30 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

**15.05 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

**15.40 Break**

**16.10 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

**16.45 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**

*Room:* **ELBA**

**Session C-7**

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

*Chair:* Paola CARBONE, UK

- 14.30 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
- 15.05 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

**TRACK E**  
**COMPUTATIONAL MECHANICS OF**  
**MATERIALS ACROSS THE SCALES**

*Room:* **MONTECRISTO**

**Session E-4**  
**Computational mechanics in simulated operating**  
**conditions**

*Chair:* **Sergei DUDAREV, UK**

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

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

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

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

**15.40 Break**

**Session E-5**  
**Advances in theory and computational methods**

*Chair:* **Nicola M. PUGNO, Italy**

**16.10 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

**16.45 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

**TRACK F**  
**DESIGNING MATERIALS FOR**  
**SUSTAINABLE ENERGY APPLICATIONS**

*Room:* **SIENA**

**Session F-2**  
**Photovoltaics**

*Chair:* Maria K.Y. CHAN, USA

- 14.30 *F-2:IL06* **Spin and Transient Delocalization Effects in Organic Semiconductors**  
**D. BELJONNE**, University of Mons, Mons, Belgium
- 15.00 *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
- 15.30 *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
- 16.00 *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
- 16.30 *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.
- 16.50 *Break*

**Session F-3**  
**Thermoelectrics**

*Chair:* Peter C.K. VESBORG, Denmark

- 17.20 *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
- 17.40 *F-3:L04* **Silicon Thermoelectrics for Energy Autonomous Integrated Circuits**  
**M. LEE**, The University of Texas at Dallas, Richardson, TX, USA

**TRACK G**

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

*Room:* **CAPRAIA**

**Session G-4**

**High throughput materials characterization and testing**

*Chair:* **Tetsuya SHOJI**, Japan

- 14.30 *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
- 15.05 *G-4:IL02* **Autonomous Combinatorial Experimentation for Atomic Layer Synthesis**  
**ICHIRO TAKEUCHI**, University of Maryland, College Park, MD, USA
- 15.40 *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
- 16.05 *Break*

*Chair:* **Gerbrand CEDER**, USA

- 16.35 *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 Lab. for magnet design through physics informed machine learning, Dept 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 Corp., Susono, Japan; Y. HONG, T. DEVILLERS, N.M. DEMPSEY, Institut Néel, Université Grenoble Alpes, CNRS, Grenoble INP, Grenoble, France
- 17.00 *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, Dept of Structural Engineering, University of California San Diego, La Jolla, CA, USA

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

*Room:* **FIRENZE**

**Session H-3**

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

*Chairs:* **Stephan MENZEL**, Germany & **Sabina SPIGA**, Italy

- 14.30 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
- 14.55 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
- 15.20 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
- 15.45 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
- 16.00 H-3:L05b The Simplest Ever-Reported Three-Circuit-Element Hodgkin-Huxley Neuristor**  
**A. ASCOLI**<sup>1</sup>, A.S. DEMIRKOL<sup>2</sup>, S. SLESAZECK<sup>3</sup>, F. CORINTO<sup>1</sup>, M. GILLI<sup>1</sup>, T. MIKOLAJICK<sup>3,4</sup>, R. TETZLAFF<sup>2</sup>, L.O. CHUA<sup>5</sup>, <sup>1</sup>Dept of Electronics and Telecommunications, Politecnico di Torino, Turin, Italy; <sup>2</sup>Institut für Grundlagen der Elektrotechnik und Elektronik, Technische Universität Dresden, Dresden, Germany; <sup>3</sup>Institut für Halbleiter- und Mikrosystemtechnik, Technische Universität Dresden, Dresden, Germany; <sup>4</sup>NaMLab gGmbH, Dresden, Germany; <sup>5</sup>Dept of Electrical Engineering and Computer Sciences, University of California at Berkeley, Berkeley, CA, USA
- 16.15 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

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- 16.30 *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

- 16.45 *Break*

**Special AFOSR Session H-8**  
**FROM BRAIN-INSPIRED NETWORKS FOR**  
**MULTIFUNCTIONAL SYSTEMS TO NEUROMORPHIC**  
**COMPUTING AT THE EDGE OF BIOLOGY**

*Chair:* Yong CHEN, USA

- 17.15 *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
- 17.45 *H-8:L02* **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
- 18.05 *H-8:L03* **Multimodal Actuators and Multifunctional Skins for Integrated Autonomous Systems**  
**J.W. BOLEY**, Boston University, Boston, MA, USA
- 18.25 *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

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

*Room:* **LUCCA**

**Session I-1**  
**Superconducting qubits**

*Chair:* Pasquale SCARLINO, Switzerland

- 14.30 *I-1:IL05* **Giant Atoms with Superconducting Qubits**  
**A. FRISK KOCKUM**, Chalmers University of Technology,  
Gothenburg, Sweden
- 15.00 *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
- 15.30 *I-1:L07* **Two-level Defects in Superconducting Quantum  
Computing Chips**  
**A. USTINOV**, Physics Institute, Karlsruhe Institute of Technology,  
Karlsruhe, Germany
- 15.50 *Break*

**Session I-4**  
**Semiconductor quantum dot and dopant-based qubits**

*Chair:* Anton FRISK KOCKUM, Sweden

- 16.20 *I-4:IL01* **Detecting Electric, Magnetic and Strain Fields with a  
Single High-spin Nucleus in Silicon**  
**A. MORELLO**, UNSW Sydney, Sydney, Australia
- 16.50 *I-4:IL02* **Hybrid Circuit Quantum Electrodynamics with Semi-  
conductor QDs**  
**P. SCARLINO**, EPFL, Switzerland
- 17.20 *I-4:IL03* **Circuit Quantum Electrodynamics Experiments in  
Planar Germanium**  
**G. KATSAROS**, Institute of Science and Technology Austria,  
Klosterneuburg, Austria

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

*Room:* **GIGLIO**

Session B-5

Thermodynamics of mesoscale states and phase  
transitions

*Chair:* Long-Qing CHEN, USA

- 9.00 *B-5:IL02* **Grain Boundary Segregation and Solute Drag in Multicomponent Alloys**  
**F. ABDELJAWAD**, M. TAGHIZADEH, Lehigh University, Bethlehem, PA, USA
- 9.35 *B-5:IL03* **Mesocanonical Ensemble as a Rationale for Studying Metastability and Hysteretic Transitions in Confined Nanophases**  
**A.V. NEIMARK**, Dept of Chemical and Biochemical Engineering, Rutgers, The State University of New Jersey, Piscataway, NJ, USA



**Special Session C-8**  
**EXPLOITING COMPUTATIONAL TOOLS IN**  
**MATERIALS MANUFACTURING AND IN THE USER**  
**INDUSTRY**

*Room:* **ELBA**

**Session C-8.1/2**  
**Metals, ceramics, glass and cement**

*Chair:* Momoji KUBO, Japan

- 9.00 C-8.1:IL01 **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, Dept of Materials Science and Engineering, Northwestern University, Evanston, IL, USA
- 9.25 C-8.2:IL01 **Machine Learning of Phase Diagrams**  
J. LUND, H. WANG, R. BRAATZ, **R.E. GARCÍA**, Purdue University, West Lafayette, IN, USA
- 10.00 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
- 10.35 C-8.2:IL03 **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
- 11.00 *Break*

**Session C-8.3**  
**Polymers and related materials**

*Chair:* Zhongde SHI, Canada

- 11.30 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
- 12.05 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
- 12.40 C-8.3:L03 **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

**TRACK E**  
**COMPUTATIONAL MECHANICS OF**  
**MATERIALS ACROSS THE SCALES**

*Room:* **MONTECRISTO**

**Session E-5**

**Advances in theory and computational methods**

*Chair:* Zhao QIN, USA

9.00 *E-5:L04* **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

9.25 *E-5:L05* **Some Recent Advances and Applications in Isogeometric Analysis**  
**A. REALI**, Department of Civil Engineering and Architecture, University of Pavia, Pavia, Italy

9.50 *Break*

*Chair:* Nicola MANINI, Italy

10.20 *E-5:IL06* **Adaptive (Iso-)geometric Modeling for CAD/CAE Applications**  
**C. GIANNELLI**, University of Florence, Florence, Italy

10.55 *E-5:IL07* **Mechanics of Bioinspired, Bionic, Nano and Meta Materials**  
**N. PUGNO**, University of Trento, Italy

11.30 *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

**TRACK F**  
**DESIGNING MATERIALS FOR**  
**SUSTAINABLE ENERGY APPLICATIONS**

*Room:* **SIENA**

**Session F-4**

**Catalysts and catalytic processes for energy applications**

*Chair:* Su-Huai WEI, China

- 9.00 *F-4:IL02* **DFT-CES: Eyes to See the Unseen, Buried Electric Double Layer**  
**HYUNGJUN KIM**, Department of Chemistry, KAIST, Daejeon, South Korea
- 9.30 *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
- 10.00 *F-4:IL04* **Exploring Catalytic Reaction Networks with Machine Learning**  
**K. REUTER**, Fritz Haber Institute of the Max Planck Society Berlin, Germany

TRACK G

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

*Room:* **CAPRAIA**

Session G-5

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

*Chair:* Claudia DRAXL, Germany

- 9.00 *G-1:IL11* **Symmetry Constraints in Machine Learning Models of Electronic and Atomic Interactions**  
**B. KOZINSKY**, Harvard University, USA
- 9.35 *G-5:IL01* **Collaborative Intelligence for Accelerated Development of Clean Energy Technologies**  
**SHIJING SUN**, University of Washington, Seattle, WA, USA
- 10.10 *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
- 10.45 *Break*

*Chair:* Christopher M. WOLVERTON, USA

- 11.15 *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
- 11.50 *G-5:IL05* **Accelerating Development of Materials with Artificial Intelligence and Machine Learning**  
J. SAAL, **M. MUSTO**, Citrine Informatics, Bad Wiessee, Germany
- 12.25 *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**

Room: **FIRENZE**

Session H-3

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

Chair: Tommaso ZANOTTI, Italy & Wilfred VAN DER WIEL,  
Netherlands

- 9.00 *H-3:IL08* **Bayesian Inference Leveraging Nanoscale Device Stochasticity**  
**B. RAJENDRAN**, King's College London, London, UK
- 9.25 *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
- 9.50 *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
- 10.05 *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>Dept 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
- 10.20 *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
- 10.35 *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
- 11.00 *Break*

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**Special AFOSR Session H-8  
FROM BRAIN-INSPIRED NETWORKS FOR  
MULTIFUNCTIONAL SYSTEMS TO NEUROMORPHIC  
COMPUTING AT THE EDGE OF BIOLOGY**

*Chair:* Andy SARLES, USA

- 11.30 *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
- 12.00 *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
- 12.20 *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

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

Room: **LUCCA**

Session I-4

Semiconductor quantum dot and dopant-based qubits

Chair: Andrea MORELLO, Australia

- 9.00 *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
- 9.30 *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
- 10.00 *I-4:L07* **Investigating Frequency Shifts in Silicon Spin Qubits influenced by Environmental Coupling**  
**I. HEINZ**, G. BURKARD, Department of Physics, University of Konstanz, Konstanz, Germany
- 10.20 *Break*
- 10.50 *I-4:IL08* **Hole Spin Qubits for Quantum Computing in Si and Ge Quantum Dots**  
**D. LOSS**, University of Basel, Basel, Switzerland
- 11.20 *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
- 11.50 *I-4:IL10* **Tuning Quantum Dot Arrays with Rays**  
**J.P. ZWOLAK**, National Institute of Standards and Technology, Gaithersburg, MD, USA

TRACK A  
**ADVANCES IN FUNDAMENTALS  
OF THEORY, COMPUTATION AND  
SIMULATION OF MATERIALS SYSTEMS:  
CLASSICAL TO QUANTUM**

Room: **LUCCA**

Session A-5

Ultrafast excitation and decay processes in materials

Chair: Kwang Soo KIM, South Korea

14.30 A-5:IL01 **Quantum Dynamics of Charge Carriers in Opto-electronic Materials**  
**O. PREZHDO**, University of Southern California, Los Angeles, CA, USA

15.00 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

15.30 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

16.00 Break

Chair: Steven G. LOUIE, USA

16.30 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

17.00 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



**Special Session C-8**  
**EXPLOITING COMPUTATIONAL TOOLS IN**  
**MATERIALS MANUFACTURING AND IN THE USER**  
**INDUSTRY**

*Room:* **ELBA**

**Session C-8.3**  
**Polymers and related materials**

*Chair:* Marc HUGER, France

- 14.30 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
- 15.05 C-8.3:IL05 **Drilling of CFRPs Using Single Layer Diamond Tools**  
**ZHONGDE SHI**, M.H. ATTIA, National Research Council Canada, Montreal, Quebec, Canada
- 15.40 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**

*Room:* **SIENA**

**Session D-3**

**Materials for quantum information science**

*Chair:* Linjun WANG, China

**14.30 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

**15.00 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

**15.20 Break**

**15.50 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

**16.20 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

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## MONDAY JUNE 24 AFTERNOON

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Special AFOSR Session H-8  
**FROM BRAIN-INSPIRED NETWORKS FOR  
MULTIFUNCTIONAL SYSTEMS TO NEUROMORPHIC  
COMPUTING AT THE EDGE OF BIOLOGY**

*Room:* **FIRENZE**

*Chair:* Joshua YANG, USA

- 14.30 *H-8:IL11* **High-precision Analog Computing with Memristors**  
**J. JOSHUA YANG**, University of Southern California, Los Angeles, CA, USA
- 15.00 *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
- 15.20 *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
- 15.40 *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

16.00-18.30

*Room:* **GIGLIO**

*Chair:* R. Stanley Williams, Univ. of Southern California, USA

Private Session of AFOSR Members

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## POSTER PRESENTATIONS

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# POSTER DISCUSSION

MONDAY JUNE 24 16.00 - 18.30

### Posters desmounting:

(Soon after the poster discussion)

**P01 Evaluation of Effect of Microstructures on Mechanical Properties of Dual-phase Steel**

**MISATO SUZUKI**, K. SHIZAWA, M. MURAMATSU, Keio University, Yokohama, Japan

**P02 Strain Phase Equilibria and Diagrams of Functional Materials**

**BO WANG**, Lawrence Livermore National Laboratory, Livermore, USA; LONG-QING CHEN, Penn State University, USA

**P03 3D Printing of Clay Components for Improving Passive Indoor Moisture Buffering**

V. GENTILE<sup>1</sup>, J.D. VARGAS VELASQUEZ<sup>1</sup>, S. FANTUCCI<sup>1</sup>, G. AUTRETTO<sup>1</sup>, R. GABRIELI<sup>2</sup>, P. KUMAR GIANCHANDANI<sup>2, 3</sup>, M. ARMANDI<sup>2</sup>, **F. BAINO**<sup>2</sup>, <sup>1</sup>Department of Energy (DENERG), Politecnico di Torino, Turin, Italy; <sup>2</sup>Department of Applied Science and Technology (DISAT), Politecnico di Torino, Turin, Italy; <sup>3</sup>Department of Textile Engineering, Mehran University of Engineering & Technology, Jamshoro, Sindh, Pakistan

**P04 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

**P05 Ionomer Cements Containing Bioglass and Glass-ceramic Reinforcements**

A. ZANDI KARIMI, E. REZABEIGI, **R.A.L. DREW**, Mechanical, Industrial and Aerospace Engineering, Concordia University, Montreal, Canada

**P06 Predicting Surfactant pKa Shifts using Molecular Dynamics**

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

**P07 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

**P08 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

**P09 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

**P10 Model and Analysis of the Solid-state Crystal-clad Growth from the Ti:sapphire Core**

**SHENG-LUNG HUANG**, National Taiwan University, Taipei, Taiwan

**P11 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

**P12 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

**P13 A Highly Effective Data Modeling Approach for Transformers based on 1D CNN Methods for Improving SOC Estimation Accuracy**

**JUNGWOO HO**, B. HAN, C.S. KIM, Y. KIM, S. LEE, D. YUN, D. CHUNG, J. JEON, Department of Advanced Battery Convergence Engineering, Dongguk University, Seoul, South Korea

**P14 Stability and Structure of the Aqueous LiTFSI/LiCl Interface**

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

**P15 Enhancing the Electrolyte Wetting in Electrodes of Lithium-ion Batteries**

**DONG HYUP JEON**, Dongguk University, Gyeongju, South Korea

**P16 A Deep Learning Model for Driving the Interaction of Data-variability Features in Dynamic-stress Time Series' Information**

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

**P17 A Comparison of LSTM and GRU Networks using many to many method for State of Charge estimation on EV**

**YUNSUN KIM**, B. HAN, C.S. KIM, J. HO, J. AHN, S. LEE, D. CHUNG, J. JEON, Dongguk University, Seoul, South Korea

**P18 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

**P19 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

**P20 Multiscale Computational Study of Surface Modification by Nonlinear Laser-induced Surface Acoustic Waves**

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

**P21 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

**P22 Molecular Dynamics Simulations of Illite Clay Surface and Particle**

**GE LI**, A.S. DE WIJN, Norwegian University of Science and Technology (NTNU), Trondheim, Norway

**P23 Molecular Dynamics Simulation of the Effect of Dopant Distribution Homogeneity on the Oxide Ion Conductivity of Perovskite-type  $\text{LaInO}_3$**

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

**P24 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

**P25 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

**P26 Robust Closed-loop Linear Control of NiTiNol Wires**

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

**P27 A High Efficiency Bromine-complexing Agent for Zinc-bromine Flow Batteries: 1,2-dimethyl-3-ethylimidazolium Bromide Compound**

**CHANGSEONG KIM**, BYEONGJIK HAN, SOHYEON LEE, DEOKHEE YUN, DAEWON CHUNG, JOONHYEON JEON, Department of Advanced Battery Convergence Engineering, Dongguk University-Seoul, Seoul, South Korea

**P28 Descriptors of the Surface Energy Based on the Crystal Structure**

**YOYO HINUMA<sup>1</sup>**, S. YASUMURA<sup>2</sup>, T. TOYAO<sup>3</sup>, T. KAMACHI<sup>4</sup>, KEN-ICHI SHIMIZU<sup>3</sup>, <sup>1</sup>AIST, Japan; <sup>2</sup>University of Tokyo, Japan; <sup>3</sup>Hokkaido University, Japan; <sup>4</sup>Fukuoka Institute of Technology, Japan

**P29 Unveiling New Ferroaxial Material via High-throughput Virtual Screening and Experimental Verification**

**RYUSUKE MISAWA<sup>1</sup>**, S. YAMAGISHI<sup>2</sup>, T. HAYASHIDA<sup>3</sup>, T. MURATA<sup>1</sup>, S. HIROSE<sup>1</sup>, T. KIMURA<sup>3</sup>, <sup>1</sup>Murata Manufacturing Co., Ltd., Japan; <sup>2</sup>Department of Advanced Materials Science, University of Tokyo, Japan; <sup>3</sup>Department of Applied Physics, Graduate School of Engineering/Faculty of Engineering, The University of Tokyo, Japan

**P30 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

**P31 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

**P32 Photothermal Crosslinking of Zirconium-Oxo Clusters for High Performance Dielectric and Memristor Applications**

**MYUNG-GIL KIM**, Sungkyunkwan University, Suwon, South Korea

**P33 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>, **J. SCHÖNFELDER<sup>1</sup>**, <sup>1</sup>Lab. for Materials Processing, Dept 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

**P34 Versatile Solution-processed Reductive Interface Layers for Flexible Electronic Devices**

**KANG-JUN BAEG**, Pukyong National University, Busan, South Korea

**P35 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

**P36 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

**P37 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

**P38 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

# *Publication Policy*

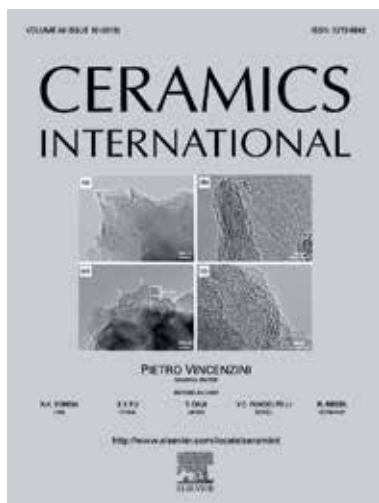
Authors at CIMTEC 2024 may submit their contributions to a purportedly planned special issue of Elsevier/Techna Group journal *Ceramics International*

<https://www.sciencedirect.com/journal/ceramics-international>

A window for papers submission will be opened at journal website as from June 25 to September 15. We regret that late submissions will not be considered.

## **SUBMISSION INFORMATION**

- 1- Only papers presented at CIMTEC 2024 by Authors who attended the conference may be submitted.
- 2- The Corresponding Author for the submitted paper shall be the one registered at the Conference as Presenting Author for the paper.
- 3- The Code Number assigned to the paper shall be mandatorily reported at the end of the title of the submitted paper.  
*Example: Machine Learning Discovery of Materials (G-2:IL06).*
- 4- All papers will be subjected to a single blind peer review process.



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# ***Social Programme***

## ***Welcome Reception Hotel Tuscany Inn***

*Friday June 21  
20.30 - 22.00*

## **“Spumante Party”**

Revive old friendships and establish new ones while enjoying a selection of Italian sparkling wines and a light buffet dinner



*Entrance fee for companions not registered: 35.00 EUR*

## *Gala Concert*

### *Nuovo Teatro Verdi*

*Sunday June 23*  
*21.00 - 23.00*

The “Ensemble Le Muse” is an orchestra entirely composed of women coming from the most important conservatories in Italy. The concert activity has led the Ensemble to perform in main concert halls around the world (Morocco, USA, Canada, Turkey, Russia, Thailand, India and several others). The “Ensemble Le Muse” under the direction of Maestro Andrea Albertini will perform the concert “Tribute to Ennio Morricone” that has been awarded with the High Patronage of President of the Italian Republic. The concert will include several of the most famous films soundtracks created by Ennio Morricone.



*Entrance fee for companions not registered: 35.00 EUR*

Maestro Ennio Morricone was an extraordinary talent composer and arranger, beloved by all for his rare ability to reach and move people with very different musical tastes. He embraced a huge amount of musical genres that made him one of the most important and influential film composers worldwide. International fame was at first gained from soundtracks of the so-called “Italian Westerns” (also known as “Spaghetti Westerns”). As from the 1970’s Morricone entered the Hollywood world composing soundtracks for films directed by John Carpenter, Brian De Palma, Barry Levinson, Mike Nichols, Terrence Malick, Oliver Stone, Roman Polanski and Quentin Tarantino.



*Ennio Morricone*  
*1928-2020*

Morricone recognitions include: two “Oscar Prizes” (2007 and 2016), three “Grammy Awards”, three “Golden Globe”, six “BAFTA”, ten “David di Donatello”, eleven “Silver Ribbons”, two “European Film Awards”, one “Leone d’Oro” and one “Polar Music Prize”. Over 70 million disks of Morricone’s soundtracks have been sold worldwide.

## ***Farewell Party Terme Tettuccio***

*Monday June 24  
20.30 - 22.30*

The Farewell Party will be held on June 24 evening at the magnificent “Tettuccio” (“Small Roof”) establishment, the most important and renowned Spa in Montecatini.

The Tettuccio establishment, known as the “bagno nuovo” (new baths) from as early as the 14th century, derived its name from the canopy (or tettoia) that covered the spring. The building, designed by architect Gaspero Maria Paoletti, between 1779 and 1781, had a particularly striking rusticated door. In 1916, Florentine architect Ugo Giovannozzi drew up plans to renovate the entire complex. This project, based on the concept of the Roman baths, was for a Spa establishment set in leafy grounds planted with Lebanon cedars, palms, sequoias, acacias, laurel trees, wisteria, pines and lime trees, and adorned with impressive colonnades,



rostra, fountains and large flower-beds bordered by box hedges. The building’s main focus was to be a conch-shaped granite fountain, held up by a group of bronze statues of marine figures, whose waters would be collected in a pool with a parapet decorated with seahorses. At the Farewell Party delegates will enjoy a taste of a large variety of the renowned Tuscania traditional dishes and drinks in an elegant and friendly environment.



*Entrance fee for companions not registered: 55.00 EUR*

# *Optional Tours*

## *LUCCA*

*Saturday June 22, full day*

*9.00 - 19.00*

A monumental city still wound by intact walls containing unique art treasures. Lucca is the only among the Tuscany district cities to have maintained its independence until 1847. This allowed full preservation of the over 4 km perimetral walls (XVI-XVII Century) surrounding the city centre inclusive of 10 bastions, one gun platform and well conserved or restored battlements. The tour in the medieval city includes views of art monuments belonging to the different periods such as the Roman Theatre, the Basilica of San Frediano,



the San Michele church and square, the Duomo of San Martino with sculptures of Jacopo della Quercia, the Guinigi tower, Fillungo street, and the Palazzo Ducale in Napoleone Square, the last to bear witness of Lucca Princedom.



*Meeting point: "Hotel Tuscany Inn" at 9.00. Return to Montecatini Terme at about 19.00. The participation fee (75 EUR) includes: transportation, city entrance tax, English speaking hostess, local guides and served lunch.*



## FLORENCE

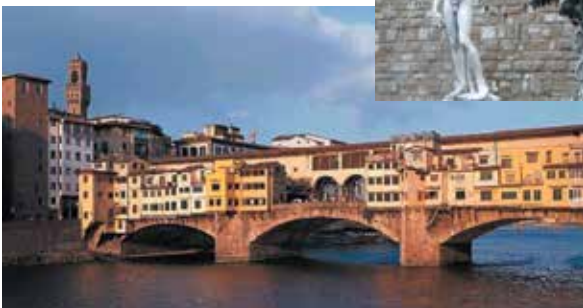
*Sunday June 23, full day  
9.00 - 19.00*

In the morning visit to the City Center. An unrivalled itinerary of art and culture in the heart of Florence, Cathedral (Santa Maria del Fiore), with its Cupola by Brunelleschi, the Campanile (Bell Tower) by Giotto, and the Baptistery with the famous Gates of Paradise by Ghiberti and Andrea Pisano, Piazza della Signoria dominated by imposing Palazzo



della Signoria flanked by the Loggia of Lanzi and the beautiful Neptune Fountain, Ponte Vecchio, the Uffizi Gallery, etc.

In the afternoon, after lunch, visit to Poggio Imperiale, Piazzale Michelangelo and San Miniato Church.



*Meeting point: "Hotel Tuscany Inn" at 9.00. Return to Montecatini Terme at about 19.00.*

*The participation fee (80 EUR) includes transportation, city entrance tax, English speaking hostess, local guide, entrance ticket in the Cathedral and served lunch.*

## ***PISA***

*Monday June 24, morning  
9.00 - 13.00*

Shown is one of the loveliest architectural complexes in the world. On a large smooth lawn stands the Cathedral, the Baptistery and the famous Leaning Tower, a unique group of buildings in an unrivaled setting, the legacy of a past age which now belongs to all mankind. Along the southern side of the piazza lie the buildings of the old University, center of research and thought and famous for scientific disciplines.



*Meeting point: "Hotel Tuscany Inn" at 9.00. Return to Montecatini Terme at about 13.00. The participation fee (55 EUR) includes transportation, city entrance tax, English speaking hostess and local guide.*





