European Materials Research Society

2025 Spring Meeting

May 26 - 30 | Strasbourg Convention Centre

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SYMPOSIUM S

Computations for materials – discovery, design and the role of data

Oral sessions : ROME - GROUND FLOOR
Poster sessions : ETOILE - FIRST FLOOR

Symposium Organizers:

Elif ERTEKIN (Main organizer), University of Illinois at Urbana-Champaign, USA

Ivano CASTELLI, Technical University of Denmark, Department of Energy Conversion and Storage, Denmark

Vladan STEVANOVIC, Colorado School of Mines, USA

Monday May 26

S03 ML/AI-Assisted Materials Screening and Simulation I

View session abstracts

13:15	1465	Towards an autonomous robotic battery materials research platform powered by automated workflow and ontologized FAIR data management **BATTAGLIA Corsin (Invited)**
13:45	1239	Closing the theory-experiment loop in the search for optimal metal-organic frameworks **SIEGEL Donald (Invited)**
14:15	1683	Electronic and Photocatalytic Properties of Sn1-xTixO2 Alloys and (SnO2)n/(TiO2) m Superlattices under Biaxial Strain : A First-Principles and Evolutionary Algo-rithm Study. **HARRATI Najwa**
14:30	1102	High-Entropy Lead-free Halide Double Perovskites: Accelerating Discovery with ML-Driven Screening and DFT **GÜNTHERT Marina**
14:45	253	Rational Computational Design of Next-Generation Semiconductors **MANNODI-KANAKKITHODI Arun**
15:00	537	Computational workflows to explore halide perovskites material properties **KORTSTEE Lotte**
15:30	348	Structure prediction for surface reconstruction and band alignment of non-metal-lic spinel oxides **WANG Tianwei**
15:45	416	A machine learning approach to predict solute segregation energy in Ni grain boundaries **JHA Roshan Kumar**

Monday May 26

S04 ML/AI-Assisted Materials Screening and Simulation II

View session abstracts

16:30	2642	Accelerating and Autonomizing Materials Design: From Electrons to Devices **BHOWMIK Arghya (Invited)**
17:00	3094	Predictive Modeling of Bone Regeneration: Machine Learning Approach to Mecha-noregulation in Custom Implant Design **RAZZAQ Muhammad Hassan**
17:15	227	Integrated Data-Science and Density Functional Theory to Tackle Challenges of Complex Materials **AIDHY Dilpuneet**

17:30	203	Unsupervised Learning Framework for Understanding the Link Between Structure and Performance in Solid-State Electrolytes **Cortes Paez Henry Andres**
17:45	1592	Study of the Medium-Range Order in Silica using Locally Averaged Descriptors and Unsupervised Learning **LU Anh Khoa Augustin**
18:00	1222	Topology augmented with geometry in the assembly of structural databases: kagome intermetallics **HULAI Nataliia**
18:15	830	Ensemble machine learning for the prediction and understanding of the refractive index in Chalcogenide Glasses **Belciu Miruna-Ioana**

Tuesday May 27

S05 Surfaces, Interfaces, and Extended Defects

View session abstracts

08:30	2445	Ab initio study of high-and low mobility metal growth on silicon (100) substrate **MASTAIL Cedric**
08:45	963	A defect-chemistry-informed phase-field model of grain growth in oxide ceramics: application to Fe-doped $SrTiO_3$ **WANG Kai**
09:00	68	A computational investigation of metal-organofluorine interactions and their role in selective metal deposition for next-gen photovoltaics **FITKIN Arielle**
09:15	542	Modeling of interfaces stability in the Cu-Mo nanometric metallic multilayers using Molecular Dynamics **Akarou Abdelhafid**
09:45	37	Multiscale simulation on the fracture properties of polymer nanocomposite **GAO Yangyang**

Tuesday May 27

S06 Databases and Data Infrastructures for Materials

View session abstracts

10:30	954	NOMAD: A Federated Research Data Infrastructure Transforming Materials Science Laboratories **MARQUEZ PRIETO José A. (Invited)**

11:00	2144	A standardized database for data-driven design of nanoscale block copolymer self-assembling **MAGOSSO Chiara**
11:15	2105	Building Bridges Between Experimental and Computational Databases with an open-source experimental data infrastructure **MITTMANN Lena Angelika**
11:30	1889	Optimised Digital Workflow for multi-scale and bi-modal Fast Sparse Tomography to generate realistic AI Training database for fast Online defect analysis of Fibre reinforced composite materials **HASSANEEH Atefeh**
11:45	2582	Time Series Machine Learning Models for Organic Electrode Materials **Borislavov Lyuben**

Tuesday May 27

S07 Machine-Learning Interatomic Potentials

View session abstracts

13:45	1082	Unlocking the Potential of Lithium Thiophosphate: Atomistic Insights on its Surface Reactivity **TÜRK Hanna (Invited)**
14:15	1815	Machine Learning-Driven Compositional Engineering of Intrinsically Stable Mixed Halide Perovskites for Photovoltaic and Optoelectronic Applications **PANDEY Ayush Kumar**
14:30	2763	Phase transitions in 2D halide perovskites using machine learned potentials **FRANSSON Erik**
14:45	2772	Phase behaviour and dynamics of organic cations in Formamidinium Lead Iodide (FAPI) using machine-learned potentials **DUTTA Sangita**
15:00	2693	Hybrid QM/MM and Machine Learning for Zeolite Catalysts and Silica Polymorphism **ABDUL NASIR Jamal**
15:15	2492	Simulating the Oxygen Evolution Reaction at Perovskite/Water Interfaces: Insights into the Role of Dopants **SEHRAWAT Amit**
15:30	223	Developing solid-state electrolyte using machine-learned potential **LEE Byungju**
15:45	764	Distilling Lightweight Machine Learning Potentials from a Universal Potential: Application to Micelle Formation **JUNICHI Ishida**

Tuesday May 27

S08 Simulations of Electrochemistry and Photocatalysis

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16:30	3116	Fast dynamics of Lithium ion in Acetonitrile based electrolytes for fast charging batteries: A classical and ab-initio MD combined study **RANA Reman**
16:45	3115	Kinetics of Electrochemical Dendritic Evolution in Circular Domains **ARYANFAR Asghar**
17:00	2871	Benchmarking Graph Neural Networks for Heterogeneous Catalytic Applications on Intermetallic Alloy surfaces **AHMAD Rafia**
17:15	1195	Balancing impurity and interlayer effects in DFT simulation of La-loaded ZrS2/CoxNiyO(OH)z for photocatalytic water splitting **CELIS Joran**
17:30	880	Insight on the aqueous Zn deposition and electrode interface mechanism by reactive dynamics simulations **LI Yuyin**
17:45	983	Doped RuO2 Enhances Durability and Breaks Scaling for Acidic Oxygen Evolution **Musgrave Charles**
18:00	734	Computational Discovery of Materials for Selective Electrosynthesis of H2O2 **SIAHROSTAMI Samira**
18:15	454	Mechanical modification of honeycomb carbon membranes for reverse osmosis water desalination **VORONIN Aleksandr S.**

Wednesday May 28

S09 Finite Temperature and Transport from First Principles

View session abstracts

08:30	146	First-principles calculations of carrier transport in semiconductors: Benchmarks, Automation, and Cyberinfrastructure **GIUSTINO Feliciano (Invited)**
09:00	599	High-Throughput Unified Framework for Local Disorder, Anharmonicity, and Electron-Phonon Coupling **ZACHARIAS Marios**
09:15	1124	Anisotropic superconductivity in a ternary boride under pressure: A Migdal-Eliashberg approach **PRAMANICK Subhajit**
09:30	2610	High-performance predictions of electron and phonon transport from first-principles **COULTER Jennifer (Invited)**

Wednesday May 28

S10 Advanced First Principles Approaches

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10:30	1112	Accelerating Materials Discovery with the Amsterdam Modeling Suite: Integrating Atomistic Simulations, Machine Learning, and Data-Driven Workflows **ONOFRIO Nicolas**
10:45	669	Atomistic modelling of pyroelectricity for materials design and discovery **EKLUND Kim**
11:00	2172	High-Performance and Energy-Efficient Sub-5nm 2D Double-Gate MOSFETs Based on SiAs Monolayers **OZBEY Dogukan Hazar**
11:15	1065	DFTB Parametrization for Iodide and Bromide Perovskites and Heterostructures **JIANG Junke**
11:30	2150	Ab-initio-guided stabilization and optimization of inorganic halide perovskites for photovoltaic applications **GISSLER Antoine**
11:45	2821	Probing Ultrafast Dynamics in Battery Cathodes **CASTILLO ROBLES José María**

Wednesday May 28

SP03 Poster Session 1

View session abstracts

13:45	01_1028	Theoretical Understanding on the Interfacial Engineering of Electro- And Photo-catalysts with Support Materials for Enhanced Hydroxide-Mediated Oxidation of Water and Benzene **KWEON Youngha**
13:45	02_1034	Theoretical study on the crucial role of metal coordination number in optimizing electrocatalyst activity of defective 2D Ru nanosheets. **KWON Sungjae**
13:45	03_1061	First-principles studies on the magnetic properties, exchange interactions, and spin Hall conductivity of the half-Heusler alloy MgMnGe **ISLAM Safikul**
13:45	04_1136	Computational Investigation of Pd-based Alloy Systems for Hydrogen Separation Membranes Using A Universal Neural Network Potential **WATANABE Taku**
13:45	05_1220	Persistent homology analysis of lithium ion diffusion in partially crystallized lithium thiophosphate **XU Yang**

13:45	06_1223	Explainable Inverse Lithography: A Data-Driven Framework for Transparent Mask Fabrication **Kang Bosuk**
13:45	07_1425	Modeling and predicting the piezoelectric properties of (Ba,Ca)(Zr,Ti)O_3 (BCTZ) combinatorial PLD sample doped with cerium using machine learning **KUENTZ Hugo**
13:45	08_1456	Metastable solid solutions of group IV transition metal diborides: An ab initio perspective **GUTSCHKA Christian**
13:45	09_1496	Molecular dynamics simulations of grain boundary behavior in the presence of particles **KLI Amine**
13:45	10_1633	Tuning oxygen reduction selectivity and activity of covalent organic framework based single atom catalyst **PARK Yonghak**
13:45	11_1647	Learning Pairwise Interaction for Extrapolative and Interpretable Machine Learning Interatomic Potentials with Physics-informed Neural Network **HONG Minjoon**
13:45	12_1670	Molecular dynamic simulation and experimental study of ternary CuxZrxW100-2x thin films **ATAALITE Hassan**
13:45	13_1674	Electronic structure of copper-substituted lead apatites: a first-principles survey **KARBIVSKYY Volodymyr**
13:45	14_1813	DFT Study of WO_3 Catalysts on Alumina Substrates for the Reverse Water-Gas Shift Reaction **ORIQAT Nada**
13:45	15_1845	Design and performance analysis of ACIGS thin-film solar cells including silver concentration and temperature effects **DJEFFAL Faycal**
13:45	16_1848	Text-to-Battery Recipe: A language modeling-based protocol for automatic battery recipe extraction and retrieval **LEE Daeun**
13:45	17_1884	Wurtzite (AlN)(ScN)(SiC) alloys, thermochemistry and electro-mechanical properties from first-principles **WOLF Laszlo**
13:45	18_1898	Microscopic mechanism of the effect of Nb and Cr co-doping on the strength and ductility of Ti2AlC/Ti3Al coherent interface **JIANG Liwu**
13:45	19_19	Metal-organic frameworks meet Uni-MOF: a transformer-based gas adsorption detector **Liu Jiapeng**

13:45 20_191 Intelligent Design of Electron-Rich Materials: Advancing Catalysis and Energy Innovations
WANG Junjie

13:45 21_1922 Exploring the Impact of Carbazole Position on Thermally Activated Delayed Fluorescence and Room-Temperature Phosphorescence Properties in Phthalimide–Carbazole Conjugates: A Density-Functional Theory Study
PANAHA Panaha

13:45 22_3233 Multi-scale study of metallic thin films growth: impact of process parameters on early- stage growth
Muriel Adrian

13:45 23_2175 Structural models of amorphous C-based materials from machine learning interatomic potentials
FISICARO Giuseppe

13:45 24_2261 Advanced Anode Design: DFT-Driven Exploration of Pre-Sodiated Sn_2S_3 and Sb_2S_3 Composites Integrated with Biphenylene Network for High Performance Sodium-Ion Batteries
GANAIE Zubair

13:45 25_2271 The impact of interphase zone on effective mechanical properties of metal matrix composites
NOSEWICZ Szymon

13:45 26_2301 Prediction of MXenes photocatalysts for CO2 conversion by means of DFT supported machine learning algorithms
PISKUNOV Sergei

13:45 27_2343 electroreduction reaction mechanism of metal-nitrogen-carbon catalysts through numerical simulations
LI Shuzhou

13:45 28_2418 Cobalt-Based Heusler Alloy: Investigating Co_2NbMn for Sustainable Energy Technologies
ROONDHE Vaishali

13:45 29_2452 Exploring Penta $PdTe_2$ as a Promising Anode Material for Calcium-Ion Batteries
ROONDHE Basant

13:45 30_2525 Unveiling the Role of Sulfur-Metal Interactions in Al-S Batteries via Single-Atom Catalyst Screening
ALI Muhammad

13:45 31_2721 Machine-Aided Analysis of Photovoltaic Devices: Savitzky-Golay Filtering for Enhanced Data Accuracy
Son Dae-Ho

13:45 32_2899 Computational study and synthesis of microbial-carboxyl cellulose hydrogel for antimicrobial water treatment
AHMADI Shabnam

13:45 33_2921 Phonon structure of exciton emission band in CdTe
VARZARI Alexandru

13:45 34_294 De Novo Design of Molecules with Low Hole Reorganization Energy based on Quantum Enhanced Machine Learning Algorithms
MAESHIMA Hiroyuki

13:45 35_2969 A Data – Driven Approach for Optimization of Silver Nanowire Synthesis
BAYRAM Barkın

13:45 36_3011 DFT calculation of the less-common CdSe magic-size clusters with the $Cd_{13}Se_{16}$ and Cd_8Se_{13} cores
GURIN Valerij

13:45 37_3044 Computational Thermodynamic Optimization of Ti-6Al-4V Alloy for Additive Manufacturing
DEMIRAŘÜnver OŘulcan

13:45 38_3086 Leaching Behavior Analysis and Efficiency Optimization of Critical Metals from Secondary Sources: A Data-Driven Approach
Hasil Dilara

13:45 39_3122 Experimental and computational studies of the Bi-containing phosphate glasses and glass-ceramics
CHORNII Vitalii

13:45 40_3123 Molecular dynamics simulations of homo epitaxial growth of Cu with $_2$5 [210] grain boundary
MASTAIL Cedric

13:45 42_500 A DFT Study of Nitrogen Doping and Stacking Sequence Effects on Electronic Structure Modulation in Imine-Based COFs
SRIVASTAVA Diksha

13:45 43_529 Polymeric stabilization at the gas-liquid interface enables high-performance durable heterogeneous photocatalysis.
BANG Seong-Uk

13:45 44_538 Porphyrin derivatives as additives for lithium metal batteries - Adsorption study
RODRIGUEZ Sergio

13:45 45_580 First-principles design of a superior electrocatalyst to Pt for hydrogen production in alkaline media
LEE Haeshik

13:45 46_595 Density functional study on iridium-based electrocatalyst for an active and stable oxygen evolution reaction in acidic media
KWON Hee Jung

13:45 47_83 Spin polarized dichalcogenide alloy for selective adsorption of gases
AYESH Ahmad

13:45 48_850 Thermomechanical fatigue performance of Timetal 834 alloy: Experimental investigation and prediction of fatigue life using machine learning approach
KUMAR Ranjeet

13:45 49_907 Thermodynamic prediction of relative stability of rough silica surfaces using machine learned potential
RAGHAVENDRAN Sudeendra

Thursday May 29

S12 Materials Acceleration Platforms I

View session abstracts

08:30	362	A distributed scale-bridging Materials Acceleration Platform for Battery Research **VOGLER Monika (Invited)**
09:00	1299	Optimizing Hexagonal Boron Nitride (h-BN) Production via Compressible Flow Exfoliation (CFE) **ARABHA Saeed**
09:15	1697	In Silico Adaptive Framework for Molecular Engineering of Biomimetic Polymers **RAJPAL Soumya**
09:30	2091	Acceleration of the advanced characterization of thin films photovoltaic materials by multimodal, versatile, and automate platform based on artificial intelligence **FONOLL-RUBIO Robert**
09:45	2100	Explainable Artificial Intelligence driven methodology for accelerated research of complex technologies: Case study of thin films PV kesterite-based technology **GARÍ-GALÍNDEZ Jon**

Thursday May 29

S13 Materials Acceleration Platforms II

View session abstracts

11:00	1472	New applications of Bayesian optimization based on element mapping to design high-capacity $Na_3V_2(PO_4)_2F_3$ cathode of sodium-ion batteries **Park Sanghyeon**
11:15	842	Supervised Convolutional Neural Network for the Phase Retrieval of highly strained BCDI patterns **MASTO Matteo**
11:30	1440	Balancing the Activity and Stability of Ternary Catalysts for Oxygen Evolution Reaction by Autonomous Laboratory **HAN Sang Soo**
11:45	67	Leveraging machine learning to innovate flexible TiNiSn green-energy devices **MUSIC Denis**

Thursday May 29

S14 Materials Acceleration Platforms III

View session abstracts

13:45	3207	Object-Oriented Linked Data (OO-LD) and OpenSemanticLab (OSL): Integrating Ontologies, Digital Workflows, Large Language Models (LLMs) and FAIR Data Principles **Stier Simon (Invited)**
14:15	504	Accelerated Discovery of Perovskite Solid Solutions through Automated Materials Synthesis and Characterization **OMIDVAR Mojan**
14:45	3208	Applications of Machine Learning and Materials Acceleration Platforms for the Development of Novel Materials for Emerging PV Technologies **Hauch Jens (Invited)**
15:30	1203	Automated Computer Vision in High-Throughput Characterisation of Nanowires **TIRANDAZ Zeinab**
15:45	1900	MCIDN: Deblurring Network for Metal Corrosion Images **SHI Peng**

Thursday May 29

S15 Simulations of Structural or Configurational Disorder

View session abstracts

16:30	2594	Unraveling the Plastic Deformation Mechanism in Oxide Glasses via Atomistic Simulation and Coarse-Grained Analysis **ZHANG Jiahui**
16:45	611	Towards accurate thermodynamics from random energy sampling **SCHULER Thomas**
17:00	3193	Defects Act in an 'Introverted' Manner in FeNiCrCoCu High-Entropy Alloy under Primary Damage **ZHANG Weiwei**
17:15	1547	Computational investigation and generation of disordered materials **PETERSEN Martin Hoffmann**
17:30	3194	Self-supervised probabilistic models for exploring shape memory alloys **Ding Xiangdong**
17:45	1399	Microstructural Evolution of Irradiation-Induced Defects in Tungsten: cluster dynamics study **MOHAMED KUNJU Salahudeen**
18:00	1901	The mechanisms of hydrogen permeation in defective spinel γ-Al_2O_3: A first-principles study **ZHANG Chuan-Hui**
18:15	1260	Computational Simulations of Carbon-Based Nanoparticles for their Applications in Nanomedicine **ALISARAIE Laleh**