European Materials Research Society

2023 Spring Meeting May 29 | June 2

40th Anniversary

Congress & Exhibition Centre, Strasbourg, France

SYMPOSIUM P

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

Symposium Organizers:

Ivano CASTELLI, Technical University of Denmark, Lyngby, Denmark

Elif ERTEKIN, University of Illinois at Urbana-Champaign, USA

Vladan STEVANOVIC, Colorado School of Mines, Golden, USA

Monday May 29

P01
Materials Discovery

Chairperson(s) : ERTEKIN Elif - STEVANOVIC Vladan

Londres 2 (Ground floor)

08:45	2323	INV	Employing Chemical Heuristics in Computational Materials Design of Functional Materials	**SCANLON David**
09:15	1233		Molecular Dynamics Simulations of the Structure and Dynamics at Catalyst-Ionomer Interfaces	**A. DAVIS Binny**
09:30	708		Influence of Exchange-Correlation Functional on Descriptors for High-Entropy Protonic Ceramic Fuel Cells	**HECKSCHER SJØLIN Benjamin**

Monday May 29

P02
Batteries

Chairperson(s) : SCANLON David

Londres 2 (Ground floor)

10:30	390	INV	Identification of descriptors in battery research	**GROSS Axel**
11:00	1258		Towards accurate computation of charged electrochemical interfaces at realistic reaction conditions	**TESCH Rebekka**
11:15	470		Pre-Pilot line upscaling of Na-ion batteries using robotic assembly	**NUSS Leah**
11:30	190		Catalysing the Performance of Li-Sulfur Batteries with Two-Dimensional Conductive Metal Organic Frameworks	**BHAURIYAL Preeti**
11:45	752		Autonomous millimeter scale high throughput battery research system (Auto-MISCHBARES)	**RAHMANIAN Fuzhan**

Monday May 29

P03
Electrochemistry

Chairperson(s) : ERTEKIN Elif

Londres 2 (Ground floor)

13:30	396	INV	Steps towards the understanding of the oxygen evolution reaction enigma by operando techniques supported by computational studies	**FABBRI Emiliana**
14:00	644		Accelerating the Discovery of 2D MXenes for Hydrogen Evolution Reaction through Machine Learning Strategy	**BOKINALA Moses Abraham**
14:15	1534		Atomistic Study of the Impact of Oxygen Vacancy Defect on Catalytic Activity of Monoclinic Zirconia	**FAZELI Sara**
14:30	328		Machine Learning Prediction of Surface Pourbaix Diagrams for the Electrochemical Stability of Metallic Nanoparticles	**HAN Sang Soo**
14:45	1479		Sustainable Hydrogen Production A Computational Study	**LIU Xinyue**
15:00	1110		Autonomous Discovery of Near Room Temperature Oxide Ion Conductors.	**MORIN MARTINEZ Armando**
15:15	2332		A multiphysics model of a proton exchange membrane acid-alkaline electrolyzer: Implications on novel materials for improved performance	**OCON Joey**

Monday May 29

P04
2D Materials

Chairperson(s) : GROSS Axel

Londres 2 (Ground floor)

16:30	324	INV	Topological Phases of MoS2 Diperiodic Crystal Phases	**MILOSEVIC Ivanka**
17:00	1900		From Enhanced Sampling to Design – Exploring the Combined Powers of Classification and Molecular Dynamics Simulations	**MENDELS Dan**
17:15	911		First-principles Perspectives on Selected Functional 2d Materials	**DE SARKAR Abir**

17:30	**650**	Exploration of 2D ferromagnetic materials induced by hole doping	**MENG Ruishen**
17:45	**919**	DFTB study on mixed functionalized MXene	**SAKHRAOUI Taoufik**
18:00	**1388**	Transitions in Xenes between excitonic, topological and trivial insulator phases: influence of screening, band dispersion and external electric field	**PULCI Olivia**
18:15	**1908**	Electronic Consequences of 2D Tilt Layer Formation in Halide Perovskites	**JUNG Young-Kwang**

Tuesday May 30

P05
AI-Accelerated Materials Discovery I

Chairperson(s) : TKATCHENKO Aexandre

Londres 2 (Ground floor)

10:00	1053	INV	Active materials exploration and characterization with Bayesian optimization	**RINKE Patrick**
10:30	24		Overlooked design parameters for efficient thermoelectric devices	**MUSIC Denis**
10:45	2517		Concepts for Predicting Phase Transition	**GRAML Mario**
11:00	1098		How quantum crystallography can aid materials design	**GRABOWSKY Simon**
11:15	1317		Lessons learned from an international Materials Acceleration Platform	**VOGLER Monika**
11:30	2527		Accurate estimation of diffusion coefficients and their uncertainties from computer simulation	**MORGAN Benjamin**
11:45	92		Machine Learning small datasets: The good, the bad and the average	**VANPOUCKE Danny**

Tuesday May 30

P06
High-entropy and Disordered Materials

Chairperson(s) : STEIN Helge

Londres 2 (Ground floor)

13:30	2359	INV	Alchemical machine learning for high-entropy alloys	**CERIOTTI Michele**
14:15	549		Effects of disorder in the electronic properties of monolayers and nanoribbons MoS2	**CASTENETTO Pauline**
14:30	961	INV	High-Entropy Alloys for Catalyst Discovery	**CLAUSEN Christian Møgelberg**
15:00	2703		ULtrahigh TEmperature Refractory Alloys (ULTERA) Database and Data Quality Assurance	**KRAJEWSKI Adam**
15:15	1898		Materials for quantum computing : Magnetic impurities embedded in superconductors from first principles	**ANTOGNINI SILVA David**

15:30	2247	Ab-initio simulations in HfNbTiVZr high-entropy alloy: electronic structure and defects	**CASILLAS TRUJILLO Luis**
15:45	2349	Vacancy-ordered double perovskites Cs2BI6 (B = Pt, Pd, Te, Sn): an emerging class of thermoelectric materials	**BHUMLA Preeti**

Tuesday May 30

P07
PV materials

Chairperson(s) : GIORGI Giacomo

Londres 2 (Ground floor)

16:30	983	Computational insights into emerging chalcogenide perovskite photovoltaics	**WANG Shirui**
16:45	2616	Computational screening for n-type doped ultrawide band gap oxides for power electronics	**GARRITY Emily**
17:15	1843	Designing novel semiconductor-ferroelectric photovoltaic devices using a new scheme to model semiconductor interfaces from first principles	**ONTANEDA Jorge**
17:30	35	First-principles Calculations combined with Machine Learning Design Approach toward Electrochemical Energy Storage and Conversion Materials	**HAN Byungchan**

Wednesday May 31

P08
Biomaterials Design

Chairperson(s) : ERTEKIN Elif

Londres 2 (Ground floor)

10:00	892		Nucleation of dislocation loop in TWIP steel: Assessing the meta-atom framework	**KUMARI Sweta**
10:15	1177		First principles electron transport in magnetoelectric SrRuO3/BaTiO3/SrTiO3 interfaces	**PLUGARU Neculai**
10:30	2599		First-principles modeling of glasses as ensembles of crystalline microstates	**WOLF Laszlo**
10:45	2250		Symmetry-Induced Singlet-Triplet Inversions Beyond Azaphenalenes: New Molecular Emitters from Known Chemistry	**BLASKOVITS J. Terence**
11:00	1174		Prediction of Biomaterials Properties via Machine Learning	**GRIBOVA Varvara**
11:15	1032		Knowledge acquisition of superconductivity information in literature and applications to materials science	**ASAHI Ryoji**
11:30	651		Modulating the Electromechanical Response of Bio-Inspired Amino Acid-Based Architectures through Supramolecular Co-Assembly	**THOMPSON Damien**
11:45	1218		Change point detection and econometrics in nanoscience data analysis	**HAMILL Joseph**

Wednesday May 31

P09
AI-Accelerated Materials Discovery II

Chairperson(s) : ZAKUTAYEV Andriy

Londres 2 (Ground floor)

13:30	1611	INV	How deep learning can help with materials design.	**KADKHODAEI Sara**
14:00	2511		Machine Learning-Assisted Discovery of Lead-Free Perovskites for Solar Cell Applications	**SEUNG HWAN Jung**

14:15	2369		Fundamentals of photoactive chiral materials from simulation workflows	**PIETROPAOLO Adriana**
14:30	2364		Computational approaches for the design of materials with desired physicochemical properties	**KOTSIS Konstantinos**
14:45	2251		Computational Design of Photocathodes for Next Generation Light Sources	**MILDNER Felix**

Wednesday May 31

P10
Optical and Magnetic Properties

Chairperson(s) : CHAN Maria

Londres 2 (Ground floor)

15:00	776	INV	Optoelectronic Features of 3D, mixed 2D/3D, and 2D Hybrid and Full Inorganic Perovskites from first principles	**GIORGI Giacomo**
15:30	135		Ferromagnetism and Ferroelectricity in a Superlattice of Antiferromagnetic Perovskite Oxides Without Ferroelectric Polarization	**RAY Avijeet**
15:45	1148		Tuning octahedral rotation and magnetism in perovskites	**JIA Jiahui**

Wednesday May 31

P_P
Poster session

Etoile (1st floor) - 4.30 p.m to 6.30 p.m

01_1589		Quantitative analysis of CNT network morphology of R2R-printed CNT-TFTs via machine learning AFM image processing	**NA Soyoung**
02_1670		Electronic Structure and magnetic properties of Eu doped GaN nanowires: An Ab-initio study for spin-optoelectronic applications	**GUDELLI Vijay Kumar**
03_1704		Locating the solvated electrons in alkali metal doped zeolites	**SARKER Debalaya**
05_2182		Prediction of icephobic performance on textured surfaces using experimental techniques combined with data-driven approach	**MARZOOK Mariam**

06_134	YSrFeCrO6 as a Robust Ferromagnetic Semiconductor with Large Photovoltaic Efficiency	**RAY Avijeet**
07_2440	Hydrogen impurity in the bulk and proper/ imporper ferroelectric domain walls	**KHALID Muhammad Muhammad**
08_2396	Modelling crack initiation processes in boron-based ceramics	**KOUTNA Nikola**
09_2452	Cellular Automata Simulation of Crystal Growth	**TIRKEY Daya Kishor**
10_1295	Physical Unclonable Functions with Unpredictably Disordered Resistance of HGO and PGO According to Concentration Control of Differently Synthesized Graphene Oxide Flakes	**LEE Subin**
11_1448	A neural network interatomic potential for nanoindentation: The case of pure molybdenum	**NAGHDI DORABATI Amirhossein**
12_74	Systematic Modification of Functionality Through Free Energy Surface Tailoring	**MENDELS Dan**
13_306	Calcium Silicate Hydrate Surface - Ca or Si Termination?	**CASAR Ziga**
14_474	Ab Initio Calculations of the Raman Spectra of Thin Strontium Titanate Films with and without Adsorbates	**KRASNENKO Veera**
15_584	Protamine-Controlled Reversible DNA Packaging: A Molecular Glue	**LANSAC Yves**
16_585	Molecular Modeling of Flexible Electronics: Enhancement of Conductivity and Stretchability of PEDOT:PSS by Hard-Cation-Soft-Anion Ionic Liquids	**JANG Yun Hee**
17_645	Interaction of graphene with 3d Cu(n) & 5d Au(n) atomic clusters (n =1-5): ab initio study to probe the structural, electronic, and spin-based properties	**MURUGESAN Ramasamy**
18_895	Core structure analysis of dislocations in TWIP steel under the Meta-atom framework: An assessment	**PULAGAM Sri Sadgun Reddy**
19_120	Fermi Level Instability as the Way to Tailor Properties of La3Te4	**KHAN Muhammad Rizwan**
21_244	Molecular Dynamics Studies of Organic Photovoltaics	**HONG Janghee**
22_275	Deciphering the electrochemical window potentials of ionic liquid electrolytes for Dual Ion Batteries: A Machine Learning Based Approach	**MANNA Surya Sekhar**

23_286	Role of Electrolyte Components in Solid Electrolyte Interphase formation in Al Anode Dual-Ion Batteries	**DAS Sandeep**
24_310	Dynamical thermal activated effects of metal atoms doped molecular and atomic gas adsorption in graphene: A multiscale computational study by SCC-DFTB	**ALIGAYEV Amil**
25_336	Giant anomalous thermal Hall effect in tilted type-I magnetic Weyl semimetal Co3Sn2S2	**ROY KARMAKAR Abhirup**
26_414	Effects of exchange-correlation functionals on predicted bulk properties of hexagonal hydroxyapatite	**WANG Xian**
27_422	Machining mechanism and deformation behavior of NiAlTiCuZr alloy under conventional and multi-dimensional vibration cutting	**FANG Te-Hua**
28_455	Effect of magnetic ordering on optoelectronic properties of 2D materials	**YADAV Asha**
29_462	Noble gas defects promoting formation of acceptor defects in ZnO	**LOVELESH Lovelesh**
30_523	Role of band filling correction in accurate calculations of defect formation energy in gapped metals	**GOPIDI Harshan Reddy**
31_555	Martensitic Transformation and Electronic Properties in Zr and Cu-doped NiTi Alloys: A First-Principles Investigation	**ADHIKARY Tapasendra**
34_1121	High Pressure Chemistry of Some Iron Complexes	**GAIN Pranab**
32_602	Nonlocal correlation effects due to virtual spin-flip processes	**BUCZEK Pawel**
33_877	Thermodynamic computations for the refractory compounds high temperature electrochemical synthesis possibility substantiation	**STESYUK Tatyana**
35_1045	Data-Driven Design of Transition Metal-Substituted NASICON-Type Electrodes for Sodium Ion Battery Utilizing Graph-Based Neural Network	**YOONSU Shim**
36_1106	High Pressure Chemistry of Some Iron Complexes	**GAIN Pranab**
37_1143	Investigation of structural and magnetic properties for magnetic materials	**OKOS Alexandru**
38_1260	A multi-scale study of Co-Free Cantor alloy: Thermodynamic stability and mechanical properties	**ALVAREZ-DONADO Rene**

39_1315	AI-based spreadability analysis of cosmetics and topical medications for improving sensory evaluation	**YANG Yong Suk**
40_1347	Giant Flexoelectricity in Janus IV–VI Nanotubes	**ZHENG Kai**
41_1505	Calculation of the Judd-Ofelt parameters for neodymium-activated new oxochloride lead-borate glasses	**AVETISOV Igor**
42_1608	A novel kinetic Monte Carlo model for magnesium phosphate conversion coatings film growth on a Mg AZ31 alloy substrate for car body applications	**KEKARJAWLEKAR Prathamesh**
43_1529	Effects of Crystallographic Orientation on Deformation Behavior of Monoclinic Zirconia Subjected to Nanoindentation: Molecular Dynamics Simulations	**FAZELI Sara**
44_1613	First-Principles Calculations of Energy Loss Near Edge Structure (ELNES) spectra of High-k Dielectric Thin Films	**PARK Jucheol**
45_1723	Synthetic Image Generation for Improving Surface Defect Classification in Solid Oxide Fuel Cells using Generative Adversarial Networks	**LEE Won Jun**
46_1631	Computational study of lipid-modified DNA: self-assembly and interaction with a bilayer membrane	**JEON Eunryul**
47_1859	Kinetic Monte Carlo (KMC) Simulation of Single-layer MoS2 Compared to Actual Growth	**KANG Yoonbeen**
48_1886	Enhancing Materials Science Research through Machine Learning: A Study of Meta-Learning Techniques for Improving Predictions with Limited Data	**BONG Seon Jong**
49_1973	Computational Characterization for Electrical Conductivity of Hybrid Nanocomposite under mechanical deformation	**AN Hyeontae**
50_1978	First-principles study on phase stability of Ce1-xNixO2-d solid solution	**KIM Hyun-Kyu**
51_1991	Data-driven Fatigue Strength Prediction of Aluminum Alloys	**QURAISHY Md. Shahbaz**
52_2008	A high-throughput search of 2d materials for Li-ion batteries	**ALIPOUR Hassan**
53_2016	Ab initio study of ScAlO3 under high pressure	**MUÑOZ Alfonso**

54_2141	Time dependent density functional theory calculations of semiconducting materials for efficient visible light driven photocatalytical water splitting and photovoltaics	**PISKUNOV Sergei**
55_2327	Topology Optimization of Cantilevered Energy Harvesting Piezoelectric Structures	**MERCADO Candy**
56_2330	A Machine Learning-accelerated Density Functional Theory (ML-DFT) Screening of Bimetallic Transition Metal Surfaces based on Single-Atom Adsorption Energy Predictions	**OCON Joey**
57_2581	A DFT study of oxygen vacancy formation in pure and transition metal doped titanates	**BORKOVSKA Lyudmyla**

Thursday June 1

P11

Methods for Materials Discovery I

Chairperson(s) : ERTEKIN Elif

Londres 2 (Ground floor)

10:00	224	INV	Fully Quantum (Bio)Molecular Simulations: Dream or Reality?	**TKATCHENKO Alexandre**
10:30	1204		Thermodynamic Origin of nuclei formation, unimodal size distribution, and its temperature-dependent shape transition	**SUNG Jaeyoung**
10:45	1780		3d kMC modelling of Cu on Cu(001) homoepitaxy under GLAD growth conditions: ripple's formation and their orientation transition	**NITA Florin**
11:00	1953		Ab-initio high-throughput screening for magnetic MAX phases	**MALIK Ali Muhammad**
11:15	2627		Strutural and energetic studies of boronic-acid-functionalized polyaniline (B@Pani) monomers and dimers using Density Functional Theory approach	**SALVADOR Michele A.**
11:30	2056		Combining Theoretical Approaches in Understanding Defect Chemistry and Ionisation Potential of CeO2	**ZHANG Xingfan**
11:45	2734		Off-stoichiometry and ordered defect compounds in Cu-(In,Ga)-Se system	**SOPIHA Kostiantyn**

Thursday June 1

P12

Materials Acceleration Platforms

Chairperson(s) : KADKHODAEI Sara

Londres 2 (Ground floor)

13:30	368	INV	The engineering of research - from screening to acceleration and beyond	**STEIN Helge**
14:00	1310		Improving Lithium metal battery performance by pulsed current charging and discharging	**CICVARIC Katarina**
14:30	2702	INV	Accelerated experimental synthesis of theoretically predicted semiconductors	**ZAKUTAYEV Andriy**

15:00	2276	INV	Integrating theory and AI/ML for materials characterization	**CHAN Maria**
15:45	1869		Atomistic simulation of strain ageing in low carbon steel	**EKTA Ekta**

Thursday June 1

P13

Methods for Materials Discovery II

Chairperson(s) : STEVANOVIC Vladan

Londres 2 (Ground floor)

16:30	2228	INV	Generative adversarial networks for microstrucute generation: A primer to Process-Structure linkage.	**NIMMAL HARIBABU Gowtham**
17:00	1057		Multiscale modelling to study the evolution of texture and associated deformation mechanism during single point incremental forming	**RAKSHIT Rahul**
17:15	451		A computational approach for the exciton diffusion in organic solar cells based on first-principles molecular dynamics	**DIARRA Cheick Oumar**
17:30	761		Efficient and reliable first-principles calculation method for evaluating electronic transport in complex materials	**LI Zhen**
17:45	191		A Combined DFT and Machine Learning-Driven Discovery of g-C3N4 based Single Atom Catalysts for Efficient Hydrogen Generation	**V JYOTHIRMAI Mullapudi**
18:00	250		Predicting PV-PEC promising materials based on chemical composition: data-driven accelerated machine learning study	**KIM Chihun**
18:15	394		Accelerated design for magnetocaloric performance in Mn-Fe-P-Si compounds using machine learning	**TU Defang**