# THE WORLD COMES HERE. TMS 2025 154th Annual Meeting & Exhibition



March 23–27, 2025 MGM Grand Las Vegas Hotel & Casino Las Vegas, Nevada, USA #TMSAnnualMeeting



### SUBMIT AN ABSTRACT FOR THE FOLLOWING TMS2025 SYMPOSIUM:

### **ELECTRONIC, MAGNETIC, AND ENERGY MATERIALS**

## Innovations in Energy Materials: Unveiling Future Possibilities of Computational Modelling and Atomically Controlled Experiments

This symposium will focus on recent developments at the intersection of materials science and computational methods, with a particular emphasis on sustainable energy materials. The urgency for renewable energy solutions is growing, and the search for innovative materials for energy generation, storage, and transportation is vital. This event aims to be a collaborative space for experts to discuss and advance these materials.

The symposium will explore computational predictions and experimental validations, seeking to hasten the practical application of new materials. Contributions are invited across a range of topics, including the discovery of new materials for various energy applications, advanced computational techniques for material behavior and property prediction, and the integration of machine learning and AI for materials discovery. This platform aims to foster innovation and bridge the gap between theoretical research and practical applications in sustainable energy materials.

Suggested topics include, but are not limited to:

- Novel Material Discovery: Computational predictions of new materials with tailored properties for energy applications, spanning photovoltaics, catalysts, batteries, fuel cells, materials for H2 and O2 storage, thermoelectrics, superconductors, and more
- Simulation and Modeling: Advanced computational techniques (e.g., density functional theory and beyond, interatomic potentials, molecular dynamics) and novel exascale-ready methodologies and computational workflows to simulate and predict the behavior, structure, and properties of energy materials at different scales
- Experimental-Computational Synergy: Studies showcasing the synergy between computational predictions and experimental validations, highlighting successful transitions from theoretical discoveries to practical applications
- Materials Design and Optimization: Computational strategies for material design, optimization, and characterization to enhance energy efficiency, durability, and performance
- Machine Learning in Materials Science: Applications of machine learning and AI in accelerating the discovery and design of energy materials, including data-driven approaches and predictive modeling

### **ORGANIZERS**

Paolo Mele, Shibaura Institute of Technology; Julio Gutierrez Moreno, Barcelona Supercomputing Center; Hussein Assadi, RIKEN (The Institute of Physical and Chemical Research); Esmail Doustkhah, Istinye University; Marco Fronzi, The University of Sydney; Donna P. Guillen, Idaho National Laboratory; Srujan Rokkam, Advanced Cooling Technologies, Inc.; Tuan A.H. Nguyen, University of Queensland

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