MSE 2024

24 - 26 Sep 2024 (Darmstadt)

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Topic M: Modelling and Simulation

M06: Energy Materials Research Driven by Modelling and Simulation

Development of energy storage and conversion materials is regarded as an urgent subject for human being's sustainability therefore receiving intensive public interests. However, while there has been significant progress in the development of materials for renewable energy, the current state of affairs still falls short of meeting the demands of our society to completely replace fossil fuels in our daily lives. Since new energy materials discovery and processing optimization require huge amounts of time and are costly, innovative breakthroughs have become a necessity. Recently, quite a good number of research groups combine computer simulation and modelling methods with experimental energy materials research, to sensationally accelerate the materials discovery and developments. For accelerated discovery of new energy materials and advanced understanding, first-principles calculations, molecular dynamics, and finite element methods have been successfully used. Now, it seems to be a good time for researchers working on energy materials research using simulation methods to assemble to share their achievements.

This symposium is focused on:

- Theoretical methodology for energy materials research
- High-throughput screening of new energy materials
- Mechanism of energy conversion and storage in nanomaterials
- Experiments-computation interface
- In silico methods for both designing materials and predicting their properties

Symposium Organizer


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