Convegno sulla modellazione molecolare per l'energia e l'ambiente

Conference on Molecular Modeling for Energy and the Environment

SUPSI

08.10.2025

13:30-13:40 **Registration and welcoming**

13:40-14:00 Opening: Maurizio Barbato & Daniela Polino, Milena Properzi & Federico Bosi

Session 1: In operando modeling of catalytic systems

Chair: GiovanniMaria Piccini (UniMoRe)

14:00-14:30 Michele Parrinello: The weird and wonderful World of Catalysis

14:30-15:00 Umberto Raucci: Dynamic Transformations of Heterogeneous Catalysts in Operando Conditions

15:00-15:30 Luigi Bonati: Unveiling catalytic dynamics via machine learning and enhanced sampling

15:30-16:00 **Coffee break**

Session 2: Molecular modeling for catalyst design

Chair: Carlo Cavallotti (Politecnico di Milano)

16:00-16:30 Christophe Copéret: Bridging Gaps between Experimental and Computational Catalysis

16:30-17:00 Matteo Maestri: Structure Sensitivity in Heterogeneous Catalysis: Active Sites, Shape, and Size

17:00-17:15 Raffaele Cheula: Modeling and design of catalyst materials with graph models and machine learning potentials

17:15-17:30 Giovanni di Liberto: Modelling Single Atom Catalysts

17:30-19:00 **Apero with poster session**

19:30 **Social dinner**

CASALE | PLANTS FOR A NEW PLANET. SINCE 1921.

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Session 3: Modeling crystals from electrons to large scales

Chair: Claudio Perego (Politecnico di Torino)

09:00-09:30 Matteo Salvalaglio: Reproducible Free Energy Surfaces from Machine-Learned Nucleation Collective Variables

09:30-10:00 Pablo Piaggi: Understanding crystallization with ab initio machine learning simulation

10:00-10:15 Antonino Famulari: Hybrid metal-organic nanocages: structures and properties by a combination of XRay and QM studies

10:15-10:45 **Coffee break**

Session 4: Energy materials

Chair: Annalisa Cardellini (SUPSI)

10:45-11:15 Eliodoro Chiavazzo: On some AI tools for material enhancement and discovery in energy applications

11:15-11:30 Michele Pavone: Phase Equilibria and Solid-State Transitions in P2-Layered Oxides as High-Energy Cathodes for Na-Ion Batteries

11:30-11:45 Paolo de Angelis: Machine Learning Interatomic Potential for Lithium Transport in Solid Electrolyte Interphase: Towards in silico Energy Storage Design

11:45-12:00 Claudio Perego: Modelling Electrode Interface Degradation in Lithium-Ion Batteries

12:00-13:30 **Lunch break**

Session 5: Molecular modeling for sustainable processes

Chair: Matteo Maestri (Politecnico di Milano)

13:30-14:00 Alberto Garbujo: Present and Future of Environmental Catalysis in Industry

14:00-14:30 Dion Vlachos: Molecular and Kinetic Modeling for the Energy Transition

14:30-14:45 Izabela Czekaj: Advanced Molecular Modeling and Catalysis in Biorefineries: Pathways to Sustainable Chemical Technologies

14:45-15:00 Luna Pratali Maffei: Theory-based kinetic modelling for the circular carbon economy: from hydrogen production to carbon materials

15:00-15:15 Izabela Kurzydym: Comparison of ZSM-5 and CLI catalysts with metal dimers (Cu, Fe, Zn) and their sensitivity to poisoning in the DeNOx process - SO2 and NO adsorption matrix

15:15-15:45 **Coffee break**

Session 6: Reaction mechanism discovery

Chair: Daniela Polino (SUPSI)

15:45-16:15 Carlo Cavallotti: On Recent Advancements in Gas Phase Chemical Kinetics: Fundamental Aspects and Applications

16:15-16:45 GiovanniMaria Piccini: Automatic Catalytic Reaction Discovery by Biasing Deep-Learned Skewed Distributions

16:45-17:15 Vanda Glezakou: TBA

17:15-17:30 Simone Perego: Machine Learning-Accelerated DFT Sampling of Dynamical Processes in Catalysis and Materials Science

17:30-17:45 **Closing remarks**