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Multiscale Materials Modelling

Tuesday, 29 October 2019 18:20 (50 minutes)

The Multiscale Materials Modelling (MMM) group is part of the recently established cross-departmental Laboratory for Scientific Computing and Modelling, specializing in inter-disciplinary modelling inside and outside PSI.
The MMM group's expertise is in computational chemistry and materials science simulations for a broad range of materials from energy, pharma, and nuclear fields using state-of-the-art tools in the framework of fundamental and applied research. Specific computational tasks include and are not limited to:
• Chemical reactivity: Reaction mechanisms, Homogeneous and heterogeneous catalysis
• Solid state chemistry: Band gap and band structure calculation, Mechanical response of materials, Polymorph stability, Ionic diffusion in structured solids, electronically challenging materials such as nuclear fuels and perovskite architectures
• Energy Viable Materials: Reduction and oxidation potentials, electrode voltages, electro-catalysis
• Characterization: IR, Raman, Optical absorption spectroscopy, X-ray absorption spectroscopy
• Thermodynamical modelling and database generation

Position

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Session Classification: Poster session

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