Modern Computational Methodologies for new glass developments

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Abstract

This lesson will delve into advanced techniques employed in simulating the structure, properties, and behavior of multicomponent oxide glasses. The discussion will encompass both ab initio methods and classical Molecular Dynamics Simulations, providing participants with a comprehensive understanding of the computational tools driving contemporary glass research.
The presentation will also highlight recent breakthroughs in machine learning potentials tailored for oxide glasses. Attendees will gain insights into how artificial intelligence techniques enhance predictive modeling, contributing to a more efficient and accelerated exploration of novel glass formulations.

Furthermore, the lesson will cover cutting-edge sampling techniques, particularly focusing on metadynamics. The application of metadynamics has proven instrumental in studying crystallization processes originating from silicate melts, offering valuable insights into the dynamics and thermodynamics of glass transformations.

By the end of the session, participants will be equipped with a nuanced understanding of the synergistic application of ab initio simulations, classical Molecular Dynamics, machine learning potentials, and metadynamics in the realm of glass science. This knowledge is poised to catalyze advancements in sustainable glass development, aligning with the overarching theme of the spring school dedicated to a sustainable future for the glass industry.

Keywords: Molecular Dynamics Simulations

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