Area D: Characterization and Modelling

Symposium D6:

Title: **Atomic Scale Modelling of Advanced Materials – Ab Initio, Molecular Dynamics and Monte-Carlo Simulations**		
Organizer	***Institution***	***Contact email***
Lorenz Romaner	Materials Center Leoben Forschung GmbH	Lorenz.Romaner@mcl.at
Matous Mrovec	Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität Bochum, Germany.	matous.mrovec@icams.ruhr-uni-bochum.de
Marcel Sluiter	Delft University of Technology	m.h.f.sluiter@tudelft.nl

Abstract

Scope: The aim of the symposium is to assess the state of the art in applications of theoretical tools that allow for simulations of materials properties at atomic scale for the knowledge-based design of advanced materials. We will discuss advances and challenges in applications of ab initio calculations, molecular dynamics and Monte-Carlo techniques focusing on a need to carry out simulations at most realistic conditions in which materials operate in tools and devices.

Description: The dominant approach in searching for new materials is experiment. However, it is recognized that the traditional way is too slow, and the goal is to reduce development time and to deploy advanced materials in a more expeditious and economical way. Atomistic simulations allow one to gain far greater insight into physical mechanisms, synthesis, and the properties of materials. Moreover, significant improvement in predictive power of theoretical modeling has led to an expectation of a shift from fully empirical paradigm in materials design to the knowledge-based materials design concept, in which atomistic simulations play an important role. During the symposium, we will discuss theoretical methodologies, starting from the basic concepts of quantum simulations and proceeding along the entire atomistic simulations chain, covering molecular dynamics and Monte-Carlo techniques. Furthermore, the use of new computational data-driven techniques to parametrize interatomic potentials or to extend the time and length scales of atomistic simulations shall be discussed.

Targeted Topics include:

- Novel theoretical approaches allowing for improvement of reliability of theoretical simulations, e.g. improved description of many-electron effects in ab initio simulations
- Ab initio simulations at finite temperature
- Treatment of magnetic effects in atomistic simulations
- Improved coarse-graining techniques for multiscale modeling
- Increasing time and length scales of atomistic simulation
- Data-driven approaches in atomistic simulations, including ML/AI