



Conference site:

Ruhr-Universität Bochum
ZGH building, room 03/121

Conference phone: 0234-32 29332
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ADVANCED DISCUSSIONS

Application of machine learning and data
science for scale-bridging materials simulation

September 20, 2023

Application of machine learning and data science for scale-bridging materials simulation



8:30-9:00	Welcome / coffee	13:20-15:00	Session 3: Microstructure characterization for multiscale modeling Chair: Alexander Hartmaier
9:00-10:30	Session 1: Atomistic simulations, functional and reactive systems I Chair: Anna Grünebohm	13:20-13:50	Paul Seibert, TU Dresden <i>Reconstructing realistic microstructures using statistical descriptors and data-based approaches</i>
9:00-9:20	Silvana Botti, Faculty of Physics, RUB / ICAMS <i>Machine-learning assisted design of materials for energy</i>	13:50-14:20	Vsevolod Razumovskiy, Materials Center Leoben, Austria <i>Digital material design across length scales</i>
9:20-9:50	Alexandra Goryaeva, CEA Saclay, Paris Saclay, France <i>t.b.a.</i>	14:20-14:40	Pascal Thome, Institute for Materials, RUB <i>Automatic characterization of a large number of optical micrographs by machine learning computer vision techniques</i>
9:50-10:10	Nore Stolte, Theoretical Chemistry, RUB <i>Isotope effects in liquid water at CCSD(T) I</i>	14:40-15:00	Rebecca Janisch, ICAMS <i>From atomistic to effective geometric and continuum description of mechanical interface behavior</i>
10:10-10:30	Matous Mrovec, ICAMS <i>ACE goes ferroelectric</i>	15:00-15:30	Coffee break
10:30-11:00	Coffee break	15:30-17:00	Session 4: Microstructure to property Chair: Fathollah Varnik
11:00-12:20	Session 2: Atomistic simulations, functional and reactive systems II Chair: Markus Stricker	15:30-16:00	Felix Hagemann, Salzgitter Mannesmann GmbH, Salzgitter <i>Machine learning and simulation: Approaches to predicting properties of flat steel material at SZMF</i>
11:00-11:30	Mike Finnis, Imperial College, London, UK <i>Oxygen diffusion in Al</i>	16:00-16:20	Oleg Shchyglo, ICAMS <i>iBain: Intelligent-data-guided process design for fatigue-resistant steel components with bainitic microstructure</i>
11:30-12:00	Stefan Eder, TU Wien, Austria <i>Reactive molecular dynamics simulations: Probing interfacial reaction in sliding contacts</i>	16:20-16:40	Alexander Hartmaier, ICAMS <i>Micromechanical modeling of the fatigue behavior of austenitic steel from additive manufacturing</i>
12:00-12:20	Miguel Marques, ICAMS <i>t.b.a.</i>	16:40-17:00	Irina Roslyakova, Institute for Materials, RUB <i>Data-driven modeling and design of single crystal superalloys</i>
12:20-13:20	Lunch break	17:00-17:30	Final discussion