MAPEX METHODS WORKSHOP II

Computational Materials Science

MAPEX Bremen
Material. Process. Excellence.

17 May 2018 – TAB building (entrance F)

Programme

Session 1	***'atom'***
	Welcome
9:00	**Computational Materials Science in Bremen Across Multiple Time and Size Scales** Lucio Colombi Ciacchi *MAPEX Speaker, Hybrid Materials Interfaces, Production Engineering*
9:15	**Structural Prediction of Biomolecules** Lucio Colombi Ciacchi Hybrid Materials Interfaces, *Production Engineering*
9:45	***discussion and coffee break***
Session 2	***'atom at interface'***
10:00	**Atoms at Materials Interfaces** Massimo Delle Piane *Hybrid Materials Interfaces*, *Production Engineering*
10:30	**Kinetic Monte Carlo (kMC) Calculations for the Prediction of Crystal-Fluid Interactions** Andreas Lüttge *Mineralogy*, *Geosciences*
11:00	***discussion and coffee break***
Session 3	***'electron'***
11:15	**Electrons in 2D Materials, Research Training Group QM^3** Tim Wehling *Institute for Theoretical Physics*, *Physics*
12:00	**Quantum Crystallography and Computational Chemistry in Different Environments** Rumpa Pal, Florian Kleemiß *Institute of Inorganic Chemistry and Crystallography*, *Biology/Chemistry*
12:30	**Electrons at Interfaces** Thomas Frauenheim *Computational Materials Science, Physics*
13:00	***discussion and lunch break***

Session 4	*'continuum'*
14:00	**Spatio-Temporally Resolved Simulation of Fluid Processes** Marc Avila *ZARM, Production Engineering*
14:30	**Numerical Implementation of Continuum Dislocation Dynamics: Crystal Plasticity in Nano- and Micro-Scales** Alireza Ebrahimi *bime, Production Engineering*
15:00	**wrap-up** Susan Köppen, Massimo Delle Piane, Hanna Lührs
15:15	***discussion and coffee break***
15:45	***end***