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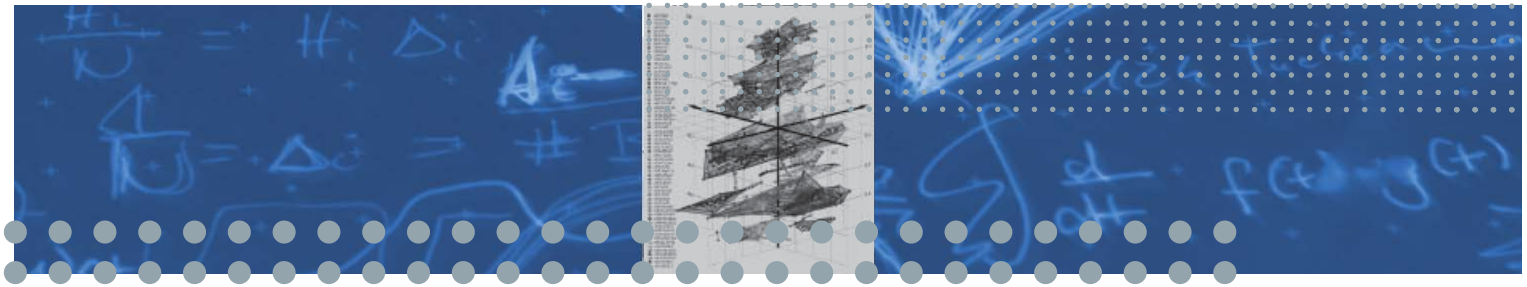

ADVANCED DISCUSSION
Materials Design

ICAMS
INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

Materials Design

1st day, Monday May 2, 2016

09:45	Arrival / Coffee
10:00	Opening
10:05-10:50	*N. Marzari (EPFL, Lausanne):* An industrial age for materials simulations
10:50-11:35	*N. Hatcher (QuesTek, Evanston):* *Materials by Design*®: Developing and deploying novel high performance alloys using integrated computational materials engineering
11:35-11:55	*T. Hammerschmidt (ICAMS):* Robust crystal-structure prediction with structure maps
11:55-13:00	Lunch break
13:00-13:45	*E. George (ZGH, Ruhr-Universität Bochum):* How useful is entropy maximization in structural materials design?
13:45-14:05	*J. Rogal (ICAMS):* Capturing the kinetics of complex phase boundary migration: An adaptive kinetic Monte Carlo study
14:05-14:25	*R. Janisch (ICAMS):* Constitutive relationships for interfaces from atomistic simulations
14:25-14:45	*M. Boeff (ICAMS):* Investigation of the influence of microstructure on fatigue crack initiation and growth using crystal plasticity simulations
14:45-15:15	Coffee
15:15-16:00	*S. Weber (Bergische Universität Wuppertal):* Development of high thermal conductivity steels
16:00-16:20	*J. Wang (ICAMS):* First-principles study of carbon segregation in bcc-Fe symmetrical tilt grain boundaries
16:20-16:40	*H. Ganesan (ICAMS):* Carbon segregation in ferritic iron using a coupled Molecular Dynamics and Monte Carlo approach
16:40-17:00	*M. Staadt (ICAMS):* Sampling atomic and magnetic degrees of freedom in Fe using bond-order potentials
17:00-17:20	*T. Chakraborty (ICAMS):* Prediction of the martensite start temperature for the design of high-temperature shape memory alloys
17:20	End
18:30	Dinner

2nd day, Tuesday May 3, 2016

09:45	Arrival / Coffee
10:00-10:45	*A. Ludwig (Ruhr-Universität Bochum):* Combinatorial and high-throughput methods for the design of new materials
10:45-11:05	*J. Albina (ICAMS):* Modeling the structural stability during delithiation in battery materials from first-principles
11:05-11:25	*T. Schablitzki (ICAMS):* Temperature programmed desorption spectra for 3D materials
11:25-11:45	*I. Roslyakova (ICAMS):* Automated data processing and its application to creep experiments
11:45-13:00	Lunch break
13:00-13:45	*Y. Wang (Ohio State University, Columbus):* Hidden pathway and defect generation during structural phase transformations
13:45-14:05	*A. Monas (ICAMS):* Mg-base alloy modelling: from solidification to mechanical testing
14:05-14:25	*M. Stratmann (ICAMS):* Unifying the CALPHAD sublattice model and the phase-field model with finite interface dissipation
14:25-14:45	*R. Darvishi Kamachali (ICAMS):* Microstructure design in precipitation-hardened alloys
14:45-15:00	Concluding remarks
15:00	End