Symposium Computational Challenges in Scale-Bridging Modeling of Materials (SYMM)

jointly organized by
the Biological Physics Division (BP),
the Chemical Physics Division (CPP),
the Dynamics and Statistical Physics Division (DY) and
the Metal and Materials Physics Division (MM)

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The vision of predicting and designing materials properties purely on the base of computer simulations poses a great challenge that requires a synergetic effort from different disciplines in view of the growing requirements of new products and technologies. Currently, major efforts are directed towards accurately and yet efficiently simulating new materials for biotechnology, nanosensorics, organic electronics and polymer based applications. Combined methodologies comprising first-principle, molecular dynamics, Monte Carlo simulations of atomistic or coarse-grained material models, and finite element or other continuum-scale methods are conventionally used to describe organic/bio/polymeric systems. Atomistic simulations, however, are still restricted to the nanometer scale due to the computational expense, while the materials properties of interest mostly manifest themselves on the macroscale. Therefore, developing new methods for scale-bridging simulations of materials is a central task for the upcoming exascale computing era.

This symposium aims at bringing together prominent representatives from different computational material design communities to shape an overall picture of the complex problem of large-scale computer simulations. Invited speakers will represent various relevant disciplines, ranging from biological, polymer, and solid state physics to quantum chemistry and mechanical engineering. We expect this symposium to attract a diverse and large group of physicists working in different fields of condensed matter physics, and to define the most promising routes of how to computationally address the challenge of rationally understanding and designing emerging materials.

Overview of Invited Talks and Sessions

(Lecture Room H1)

Invited Talks

SYMM 1.1	Thu	9:30–10:00	H1	**Challenges for first-principles based computation of properties of oxide materials** — •Karsten Albe
SYMM 1.2	Thu	10:00–10:30	H1	**Deformation and Fracture of Solids: Tough Nuts at Atomic and Continuum Scales** — •Peter Gumbsch, Matous Mrovec, Kinshuk Srivastava, Daniel Weygand
SYMM 1.3	Thu	10:30–11:00	H1	**Crucial Issues and Future Directions of Through-Process Modeling** — •Guenter Gottstein
SYMM 1.4	Thu	11:00–11:30	H1	**Adaptive Resolution Simulations for Soft Matter: Applications and New Developments** — •Kurt Kremer
SYMM 1.5	Thu	11:30–12:00	H1	**Materials by design** — •Markus Buehler

Sessions

SYMM 1.1–1.5	Thu	9:30–12:00	H1	**Computational Challenges in Scale-Bridging Modeling of Materials**

SYMM 1: Computational Challenges in Scale-Bridging Modeling of Materials

Time: Thursday 9:30–12:00 Location: H1

Invited Talk SYMM 1.1 Thu 9:30 H1

Challenges for first-principles based computation of properties of oxide materials — •Karsten Albe — TU Darmstadt, FB 11, FG Materialmodellierung, Petersenstr. 32, D-64287 Darmstadt

Calculations based on density functional theory (DFT) have been the mainstay of theoretical studies of the properties of semiconductor and oxide materials over the past few decades. Despite of their significant successes, challenges remain in adapting these methods for predictive simulations that are quantitatively useful in predicting complex device properties. Increasing computing power and improved theoretical methods taking advantage of ever more powerful computer hardware offer the possibility that computational modelling may finally allow a virtual materials design by truly predictive simulations. In this contribution, I will give examples for successes and failures in calculating bulk, point defect and surface properties of transparent conducting as well as ferroelectric oxides and describe the remaining challenges.

Invited Talk SYMM 1.2 Thu 10:00 H1

Deformation and Fracture of Solids: Tough Nuts at Atomic and Continuum Scales — •Peter Gumbsch[1,2], Matous Mrovec[1,2], Kinshuk Srivastava[1], and Daniel Weygand[1] — [1]Institut for Applied Materials IAM, Karlsruhe Institute of Technology KIT — [2]Fraunhofer IWM, Freiburg

Multiscale modeling of deformation processes in crystalline materials poses several challenges although the basic physical process, the motion of dislocations, is well understood. I will use the deformation of single crystalline alpha-iron to illustrate these challenges.

To feed dislocation dynamics with realistic atomistic information requires a reliable and computationally efficient description of the atomic interactions. We use a recently developed magnetic bond-order potential (BOP). Dislocation mobility laws for discrete dislocation dynamics (DDD) studies of large dislocation ensembles then require consideration of the full local stress state in a mesoscopic mobility law since it turned out that the effect of non-glide stresses and orientation of the applied loading is crucial for capturing the non-Schmid behavior.

Averaging the behavior of discrete dislocations into continuum mechanical equations is even more difficult. It requires a homogenization of the dislocation fields including a description of their multiplication and mutual interaction. The mathematical framework for such a continuum field theory is still not available. I will present a kinematically consistent continuum description of the dynamics of curved dislocation systems as a first approach to such a continuum field theory.

Invited Talk SYMM 1.3 Thu 10:30 H1

Crucial Issues and Future Directions of Through-Process Modeling — •Guenter Gottstein — RWTH Aachen University, Institut of Physical Metallurgy and Metal Physics, Aachen, Germany

Computer simulation of materials processing and properties has advanced to an established field and indispensible research topic in materials science and engineering during the past decade. Moreover, it has grown to a powerful and accepted tool for commercial alloy and process development. While the general theory has been laid out, physics based scale-bridging modeling approaches have been developed and are currently employed also in industrial environments, flexible interfacing has become available and automated simulation is currently being tested, there are still bottlenecks that impede the ease of application and the predictive power of these tools and urgently need to be addressed. Such needs include reliable experimental databases, the bridging of knowledge gaps on critical phenomena like nucleation, interacting microstructural evolution processes that require vastly different computation times, inverse modeling algorithms etc. Finally, despite of the remarkable advances in available computer power, computer simulation still suffers from too low computational speed to address statistically significant system sizes and to lend itself to process control. More recent concepts will be introduced, in particular in view of the changing philosophy of computer architecture and the increasing availability of massively parallel computing power, which may actually require a departure from conventional and established modeling concepts.

Invited Talk SYMM 1.4 Thu 11:00 H1

Adaptive Resolution Simulations for Soft Matter: Applications and New Developments — •Kurt Kremer — Max Planck Institute for Polymer Research

The relation between atomistic structure, architecture, molecular weight and material properties is a basic concern of modern soft matter science. A typical additional focus is on surface and interface aspects or the relation between structure and function in nanoscopic molecular assemblies. Here computer simulations on different levels of resolution play an increasingly important role. To progress further, adaptive schemes are being developed, which allow for a free exchange of particles (atoms, molecules) between the different levels of resolution. The lecture will concentrate on these methods to couple particle based simulations. In addition first approaches to connect particle based simulations to continuum as well as to include quantum effects will be presented. Furthermore the extension to open systems MD as well as new recent methodology advances will be explained. A general review on the first part can be found in M. Praprotnik, L. Delle Site, and K. Kremer, Ann. Rev. Phys. Chem. 59, (2008) and recent advances in S. Fritsch et al. Phys. Rev. Lett. 108, 170602 (2012)

Invited Talk SYMM 1.5 Thu 11:30 H1

Materials by design — •Markus Buehler — MIT, 77 Mass. Ave, Cambridge, MA 02139

Biological materials are synthesized, controlled and used for an astonishing variety of purposes including structural support, force generation, mass transport, catalysis, or energy conversion. By incorporating concepts from biology and engineering, computational modeling has led the way in identifying the core principles that link the molecular structure of biomaterials at scales of nanometers to physiological scales at the level of tissues. The use of the world's fastest supercomputers allows us to predict properties of complex materials from first principles, realized in a multiscale modeling approach that spans massive ranges in scale. Combined with experimental studies, such in silico models allow us to simulate disease, understand catastrophic failure of tissues, and enable us to translate concepts from the living world into material designs that blur the distinction between the living and non-living systems. We discuss challenges and opportunities in new methods of scale bridging.