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**