



Virtual Workshop

22/23 November 2021

Multiscale modelling in materials science, chemistry, and biology: How to meet, greet, and beat scale-bridging challenges

Many interesting research problems cover a broad range of time- and length scales, which are a severe challenge for the multiscale methods developed to date. One of them is that these problems are recursive, i.e., events on longer time-scales influence structure and function on shorter time-scales. The aim of this workshop is to address challenges not covered by standard multi-scale simulation methods, highlighting examples from different fields such as friction, organic semiconductors, heterogeneous catalysis and biological function. Leading scientists cover both state-of-the-art and novel simulation concepts and theoretical approaches to address such scale-bridging problems via tailored combinations of quantum-chemical, molecular dynamics, coarse-grained and continuum models.

Contributed talks and poster session

Deadline for abstract submission: End of September 2021

Organizers

M. Elstner, K. Fink, P. Gumbsch, F. Gräter, M. Hochbruck, S. Höfener, W. Klopper, M. Kozłowska, T. Kubar, L. Pastewka, A. Schug, A. Streit, F. Studt, W. Wenzel

Invited speakers

David Beljonne, Universite de Mons, Belgium
Peter Bobbert, Eindhoven University of Technology, Netherlands
Qiang Cui, Boston University, US
James Ewen, Imperial College London, UK
Ding Feng, IBS Center for Multidimensional Carbon Materials, Korea
Geoffroy Hautier, Dartmouth College, US
Ville Kaila, Stockholm University, Sweden
Roland Netz, FU Berlin, Germany
Andela Saric, UCL, UK
Christoph Schütte, FU-Berlin, Germany
Cristiana Di Valentin, University of Milano Bicocca, Italy

For more information, see:

<https://www.compnano.kit.edu/WinterWorkshop2021.php>