

Seminar im Rahmen des GRK 2078

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Date: Tuesday, February 2, 2021
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Title: **Tailored Scale-Bridging Approaches to Computational Nanoscience**

Abstract

The last decades brought a massive development of simulation methods for materials science, chemistry and soft matter applications, now being efficient and accurate for the targeted application area. Despite their numerous successful applications, these methods are mostly limited to a certain time- and length scale and a plethora of scientific questions remain, which are not or cannot be addressed by such approaches. Common scale-bridging approaches either apply techniques like bottom-up parametrization or parameter passing, which rely on an intrinsic time-scale separation of the scientific problem, or they are based on the combination of simulation methods, as e.g. in QM/MM approaches. The latter, although successfully bridging a broad range of scales in space, are limited to the time-scale of the computationally most expensive method. Many interesting research problems, however, integrate a broad range of time-scales and being recursive in nature, i.e. events on a longer time scale determine structure and function on a short time-scale. Prominent examples are conformationally gated biochemical reactions in proteins. In this RTG we want to systematically investigate problems, which are not addressable by standard tools from the quantum chemistry toolbox. The research is organized into seven projects, where five projects address scientific challenges like friction, materials aging, material design and biological function, which so far cannot be approached by single computational methods or standard multiscale approaches.

Alle Interessenten sind herzlich eingeladen.

Prof. Dr.-Ing. Thomas Böhlke
(Sprecher des GRK 2078)