INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

ICAMS Seminar

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Stretching the limits of first principles: Structure prediction, dynamics and spectroscopy from large surfaces to biomolecules

Quantum-mechanical first principles (e.g., density-functional theory) provide us with an enormously successful, essentially accurate computational framework for the potential energy surface that governs materials or molecular properties, chemical reactions etc. One of the ongoing challenges is that we can reach benchmark-level accuracy for small systems (few-atom molecules) relatively easily, but pushing the same benchmark accuracy out to large systems -- when it matters – is an ongoing challenge.

This talk focuses on two areas where high accuracy for relatively large structure sizes (hundreds or thousands of atoms) is indeed desirable, if it can be had: (i) The structure, stability and dynamics in biomolecular systems, where relatively weak interactions (e.g., Hydrogen bonds, van der Waals) make a critical difference, and (ii) surface reconstruction at a larger scale, where the physically relevant structure of an interface is determined by relatively small (per atom) energy contributions.

We use all-electron electronic structure theory as implemented in the FHI-aims code to meet these challenges. Numeric atom-centered basis sets provide essentially converged numerical accuracy for the task at hand, and efficient parallelization up to massively parallel architectures (hundreds or thousands of processors) allows us to reach the relevant system sizes. In particular, we address the possible bottleneck of an algebraic eigenvalue solver (Kohn-Sham equations) on massively parallel machines. On the biomolecular side, we focus on polyalanine molecules (5-20 aminoacids) large enough to form secondary or tertiary structure, where accurate vacuum experiments (IR spectroscopy) are available for quantitative comparisons to experiment. Regarding surface reconstruction, we address the structure and thermodynamic stability of commensurate, graphene-like reconstructions that form on SiC(111).