Universität Münster

Fachbereich Physik

Allgemeines Physikalisches Kolloquium

Donnerstag, 16.01.2025 - 16 Uhr c.t.

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Simulating electronic processes in complex molecular systems with embedded ab-initio methods

Complex molecular systems, such as molecular aggregates, thin films, interfaces, solvated dyes, or macromolecules, find a variety of use in electronic devices or biomedical applications. At the heart of their functionality lies an intricate interplay of electronic and structural processes and resolving this interplay – experimentally and computationally – is crucial both for a fundamental understanding and guided material design.
However, as materials become more complex and real-world conditions come into play, accurately simulating these systems becomes a significant computational challenge. Macroscopic phenomena like optical absorption, luminescence, electrical conductivity, and other bulk or surface material properties cannot be fully captured by microscale models alone. As a result, studying electronic excitations in complex disordered systems remains a challenge for ab-initio methods.
Exploiting the, often, localized nature of excitations in such disordered systems makes it possible to construct multiscale embedding models instead, in which the overall system is partitioned into smaller, tractable regions of interest with appropriate interregion couplings.

In my talk, I will discuss several strategies for building such embedded models, including quantum-quantum and quantum-classical embeddings, as well as machine-learning tools. I will focus in particular on showcasing the application to (inverse) photoemission and optical spectroscopy of molecular films for OLEDs, excitonic conversion processes in a polymer-fullerene blend, and charge-transport regulation in polymer-composites.

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Kolloquiums-Kaffee ab 16 Uhr vor dem Hörsaal

Institutsgruppe 1 – HS 2
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