UNIVERSITÄT DUISBURG ESSEN

Offen im Denken

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Sondertermin: Berufungsvortrag

Simulating the Interfaces of Energy Materials

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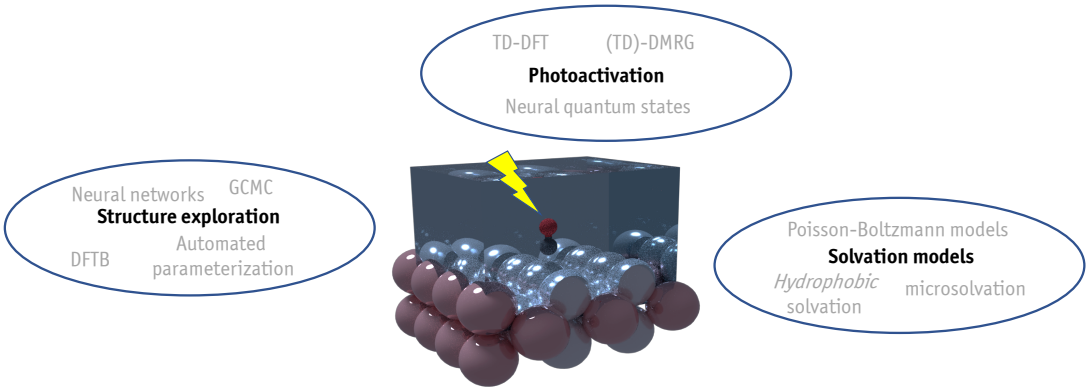

Energy materials, such as catalysts and batteries, are crucial for most technologies that enable a more sustainable economy in the fight against climate change. The relevant processes that define the functionality and lifetime of these materials usually take place at their interface. While the thickness of a solid/gas interface is on the order of 1-2 nm for typical heterogeneous catalysts, it is substantially larger for solid/liquid interfaces in electrocatalysts or the solid-electrolyte interface of batteries. The complex composition of these interfaces and their conformational flexibility leads to a pronounced structural diversity. This and the fact that these interfaces change under *operando* conditions, render investigations of these processes a challenge for experiments and simulations.

In this talk, I will discuss how we approach investigating this structural diversity based on grand-canonical Monte-Carlo sampling with remarkably fast electronic-structure methods and neural networks. I will then discuss approaches for the simulation of solid/liquid interfaces with implicit solvation models and hybrid explicit/implicit microsolvation models. In the final part of the talk, I will outline how we will model photoactivated processes at interfaces and highlight future directions to improve and extend the methodology presented here. I will then briefly discuss how we aim to engage the scientific community by introducing publicly available databases and programs.