WWU MÜNSTER

FACHBEREICH PHYSIK

Allgemeines Physikalisches Kolloquium

Donnerstag, 26.01.2023 um 16 Uhr c.t.

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Atomistic Insight into Light-Responsive Functional Materials by Multiscale Modelling

Considering living organisms, the embedding of molecular switching units into well-defined matrices is fundamental to achieve complex and tunable functionalities. Inspired by biological prototypes, a molecular-based design of functional materials for applications such as sensing and photonic materials is thus a promising approach. However, to rationally develop corresponding responsive and functional materials, a detailed picture of both structural and dynamic properties of responsive molecular units, which are embedded into hierarchical architectures, is needed. Atomistic simulations can provide such a detailed insight. Based on this, fundamental aspects can be deciphered, which enables to guide the development of these materials. I will showcase the potential of theoretical investigations by giving a selective overview of our activities on developing and applying theoretical methods to investigate the dynamics of stimuli-responsive systems at different time and length scales. In particular, I will present an on-the-fly training algorithm to parametrize, based on quantum mechanical calculations, interatomic potentials. By a guided and non-guided phase space sampling, relevant reference data are automatically and continuously generated and included into the parametrization of the potentials.[1] Atomistic simulations based on these interatomic potentials will be presented, which enabled us to decipher, for example, the operation mechanism of molecular machines embedded into a Metal-Organic Framework. These atomistic studies revealed a dynamic and cooperative interplay of these machineries within the periodic matrix. [2] By identifying parameters dominating individual and collective motion, our investigations promote the development of responsive and functional materials.

References:
[1] E. Kolodzeiski, S. Amirjalayer, *J. Chem. Theory Comput.*, **2021**, 17, 7010.
[2] E. Kolodzeiski, S. Amirjalayer, *Science Adv.*, **2022**, 8, eabn4426.

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