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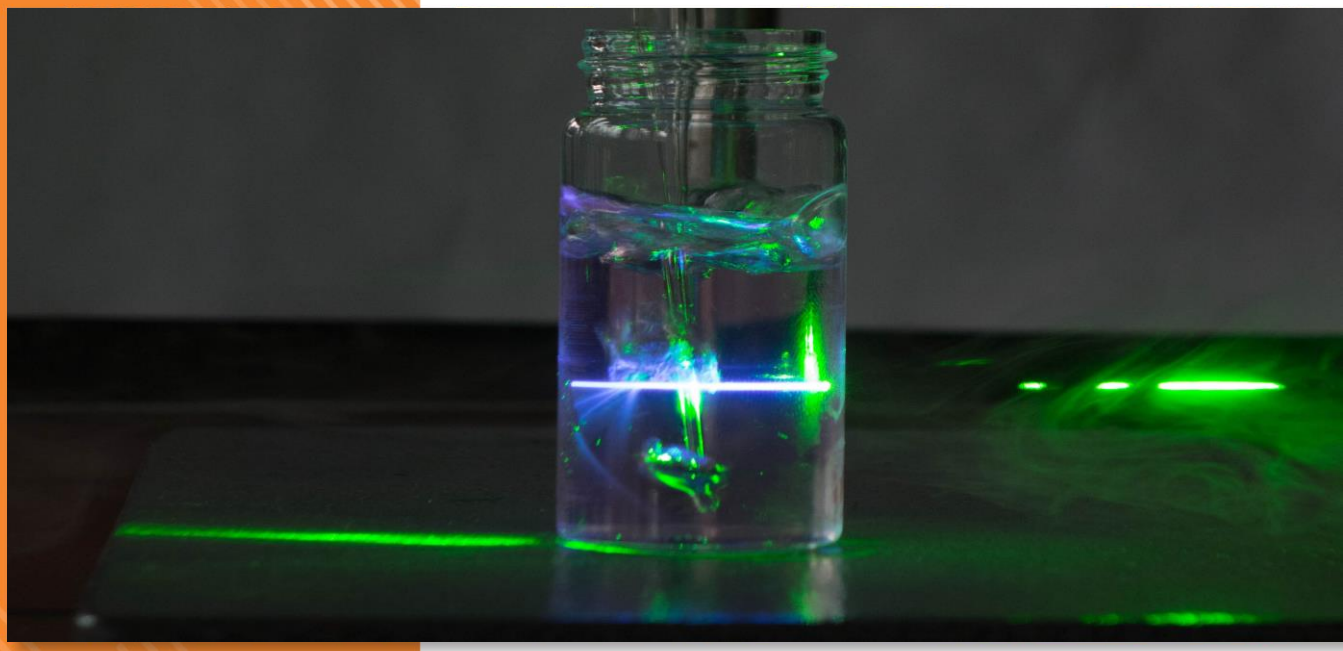

Efficient electronic structure methods for interfaces

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Due to a combination of efficiency and accuracy, density functional theory (DFT) within the Kohn-Sham framework is the most popular method to characterize the electronic structure of molecules and solids. It used extensively in chemistry, physics, and material science to elucidate structural, spectroscopy, and thermodynamic properties. The central quantity in DFT is the exchange-correlation (XC) functional. It comprises all non-classical contributions to the total electronic energy and has to be approximated since the exact functional form is unknown. A large variety of approximations exists and the accuracy of a specific property and a given system often depends strongly on the choice of the XC functional. In particular for very heterogenous systems, such as donor-acceptor systems or hybrid interfaces, an accurate description with existing XC functionals remains challenging. This is mainly due to fixed, system-wide parameters. Another persistent short-coming of DFT is strong correlation between electrons that occurs, e.g., upon bond dissociation or in systems with transition metal centers.

To increase the predictive power of DFT for interfaces, our group develops flexible functionals that adapt to the electronic environment. They are assessed for the description of level alignments at dye-TiO2 interfaces in models for dye sensitized solar cells. Further, strategies to extend this implementation to periodic boundary conditions are devised.

The strong electron-correlation challenge is addressed by introducing a new building block to the functional development: the spherically averaged electron density. In contrast to the electron density and its derivates used to describe the electron-electron interaction so far, the spherically averaged density is a fully nonlocal quantity and contains explicit information on the charge density at two different points in space.

24. Mai 2023
16:00 Uhr
Campus Freudenberg
Hörsaal FZH3

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