SFB1242

SFB 1242 Nichtgleichgewichtsdynamik kondensierter Materie in der Zeitdomäne

UNIVERSITÄT DUISBURG ESSEN

Open-Minded

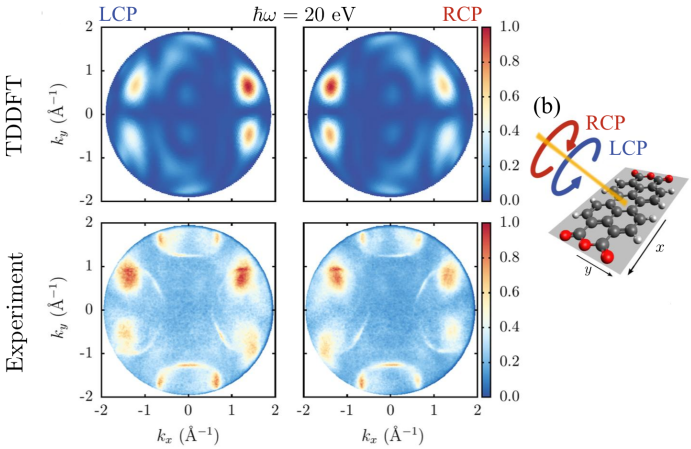
02.02.2021 / 10 Uhr c.t.

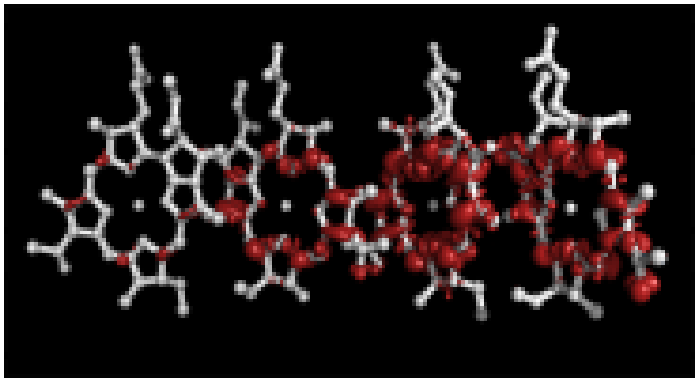
Studying energy- and charge transfer processes in real-time: A density functional perspective

Prof. Dr. Stephan Kümmel

Universität Bayreuth

The interaction of light with condensed matter systems governs many different physical processes, ranging from hallmark quantum mechanical effects such as photoemission up to the process of photosynthesis in natural light harvesting systems. Energy- and charge- transfer steps are decisive in such processes. In this talk we take a look at how such processes can be simulated from first principles in real time with Time-Dependent Density Functional Theory. We will see that one can follow the time evolution of the electron density through space and thus, e.g., understand how the polarization of light shapes photoemission signals, and how energy is transferred between the chromophores in the light-harvesting apparatus of photosynthetic bacteria. However, we will also need to take a look at the intricacies that come along with a density-based description of quantum mechanics and the related quest for the proper balance between computational effort and accuracy.





Two examples for results from real-time simulations of electron dynamics. Left: Angular resolved photoemission signals from a model organic semiconductor for different orientations of the light polarization. Right: Excitation energy spreading through an array of bacteriochlorophyll chromophores

Für diese Zeit steht eine Kinderbetreuung nach vorheriger Anmeldung zur Verfügung.

Contact: Prof. Dr. Björn Sothmann, Faculty of Physics
Phone: +49 (203) 37-91578 / Mail: bjoerns@thp.uni-due.de