SFB1242

SFB 1242 Nichtgleichgewichtsdynamik kondensierter Materie in der Zeitdomäne

UNIVERSITÄT DUISBURG ESSEN

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Electronic excitations: Optical properties, femto-second dynamics, and materials selection

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Using and probing materials oftentimes involves techniques that create or analyze electronic excited states. Recent experimental advances allow studying these, as well as their femto-second real-time dynamics, with unprecedented accuracy and high time resolution. Interpretation of such experiments, however, relies on solid theoretical and fundamental understanding. First-principles theoretical-spectroscopy, e.g. based on many-body perturbation and time-dependent density functional theory, can provide such an accurate description, as I will illustrate in this talk for several recent, successful examples: Using these electronic-structure methods, we facilitated optical crystal-structure identification, provided deep understanding of light absorption for organo-metal halides, and explored the enhancement of defect diffusion by hot electrons under radiation conditions. Since the predictive accuracy of these techniques depends on physical and numerical approximations, I will also discuss our efforts in addressing deficiencies, such as the description of dielectric screening and explain how we bridge multiple time scales from ultrafast electron dynamics to atomic diffusion. In addition, I will describe how incorporating online databases into computational research on excited electronic states can side-step the problem of high computational cost associated with first-principles simulations and, thus, facilitate materials selection for semiconductor heterojunctions.

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

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