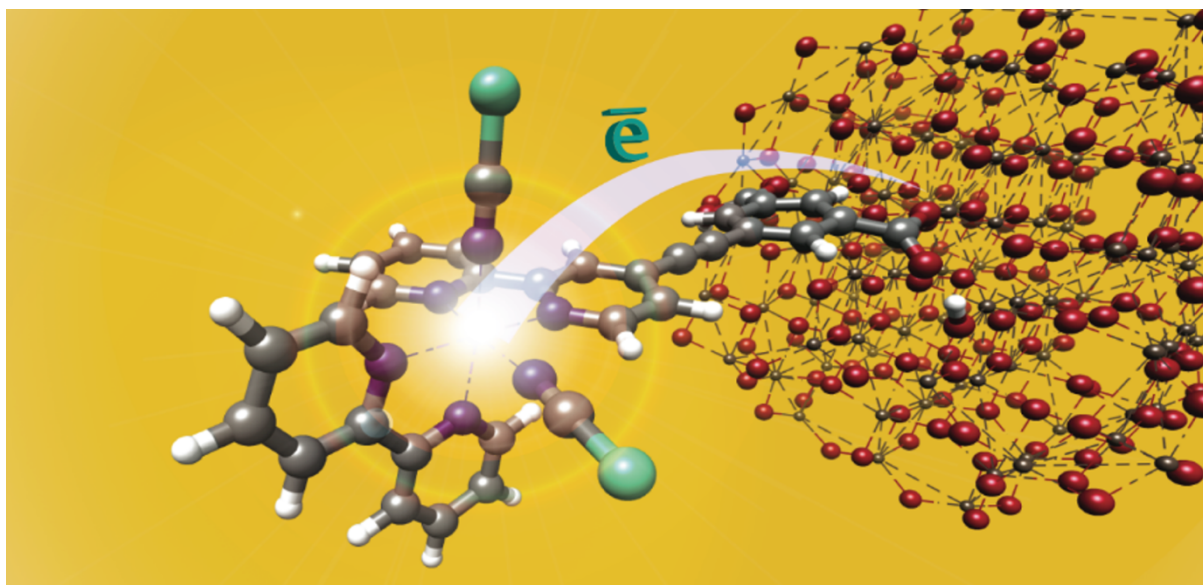


Computational Nanoscience and Ultrafast Reaction Dynamics



Method tags: modelling/simulations, ultrafast spectroscopy, molecular dynamics

Scientific tags: surface growth and reactivity, solar energy conversion, (photo)catalysis

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We investigate solar energy conversion dynamics and other light-induced reactions in a wide range of nanomaterials using a combination of atomistic modelling and time-resolved spectroscopy. Our research covers both traditional nanomaterial systems such as atomistic simulations of semiconductor surface growth and reactivity during photo-assisted Atomic Layer Deposition (photo-ALD), as well as the ultrafast dynamics of photoredox processes in solution as a key step for emerging molecular-based solar fuels and related photocatalytic processes.

We are happy to offer master thesis projects within this research area focussing on (i) atomistic modelling of semiconductor growth and surface reactivity, or (ii) mechanistic studies of photoredox dynamics in light-harvesting systems based on a combination of time-resolved optical spectroscopy and modelling.