Sonderforschungsbereich 1277
Emergent Relativistic Effects in Condensed Matter -
From Fundamental Aspects to Electronic Functionality

SFB-Seminar

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Thema: Photodynamics of light harvesting molecules: energy transfer, localization, molecular scrambling and state-specific vibrations

Abstract
Solar energy conversion starts with the harvest of light, and its efficacy depends on the spatial transfer of the light energy to where it can be transduced into other forms of energy. Harnessing solar power as a clean energy source requires the continuous development of new synthetic materials that can harvest photon energy and transport it without significant losses.

We investigate photoexcited dynamics and relaxation pathways in a variety of light-harvesting molecules using Non-Adiabatic Excited State Molecular Dynamics (NA-ESMD). We aim to achieve a detailed comprehension of the ultrafast intramolecular electronic and vibrational energy transfer that takes place after photoexcitation. Within our NA-ESMD framework, direct nonadiabatic molecular dynamics simulations can be applied to describe photoinduced dynamics in large organic conjugated molecules involving multiple coupled electronic excited states. Such NA-ESMD simulations are performed by combining the molecular dynamics with quantum transitions (MDQT) approach with “on the fly” analytical calculations of excited state energies, gradients, and non-adiabatic couplings terms.

With chemically-controlled branched architectures, dendrimers are ideally suited for light harvesting, since they consist of arrays of chromophores with relative positioning and orientations to create energy gradients and to spatially focus excitation energies. The spatial localization of the energy delimits its efficacy and has been a point of intense research for synthetic light harvesters. We therefore present results of combined theoretical experimental studies elucidating ultrafast electronic energy transfer on different phenylene-ethynylene dendrimers (PPE), leading to either unidirectional energy transfer onto an energy sink including an ultrafast collapse of the photoexcited wave function and exciton self-trapping on different units including an ultrafast spatial scrambling among isoenergetic chromophore units.

Besides, the use of multiconfigurational Ehrenfest method is discussed and compared to surface-hopping approach in this kind of molecules.

Gastgeber: Prof. Dr. John Lupton