

Dienstag, 02.02.2016

Hörsaal D, Chemie Zentralbau, 17:15 Uhr

Sprecher: **Dassia Egorova**
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Thema: **Coherence as a probe of
inseparable electron-nuclear
motion**

Abstract: The breakdown of the Born-Oppenheimer approximation, associated with avoiding crossings and conical intersections of potential-energy surfaces, is known as a driving force in molecular reaction dynamics and ultrafast photochemistry. While its theoretical description is well established, it is still nontrivial to visualize the associated nuclear and electronic motions, and unambiguous interpretations of experimental measurements remain challenging, especially for larger multidimensional systems. Coherence, as a superposition of quantum states, can be explored as a probe of the coupled electron-nuclear motion and represents an observable accessible for both theory and experiment. In the presentation I will consider two examples: excited-state dynamics in pentafluorobenzene and two-dimensional electronic spectroscopy of pentacene crystals. In pentafluorobenzene, the experimentally detected long-lived oscillations can be traced back to the periodic change of excited-state electronic character strongly coupled to the out-of-plane nuclear motion. In pentacene crystals, the detected oscillations shed light on how the electronic process known as singlet fission is accelerated by nuclear dynamics. I will focus on the physical origin of oscillatory signatures in time-resolved signals and on a clear relation of experimental observables to the underlying dynamics.

Organisation: Volker Engel

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Informationen zur Forschergruppe unter: <http://www.for1809.uni-wuerzburg.de>