universität innsbruck

Institut für Ionenphysik
und Angewandte Physik

BritInn

Academic Network Britain-Innsbruck

Institutsseminar

Watching Fundamental Chemistry as it Happens Using Lasers and Computers

Prof. Graham A. Worth

Head of Computational Chemistry Virtual Section
And
Head of Physical Chemistry Section
University College London – United Kingdom

Time-resolved spectroscopy using techniques such as pump-probe pulsed lasers can reveal details of reactivity and chemical reactions as they occur. Of particular interest to me are photo-activated processes. Here, knowing the competition between different possible pathways is key to understanding the behaviour of molecules and the properties of materials after they absorb light. What are termed non-adiabatic transitions, where a system is able to to change electronic state instantaneously in a non-radiative process, have been shown to play a special role. They are important in a range of photo-chemical and photo-physical systems, including the photochemistry of many organic molecules and even providing the photo-stability of DNA bases and the photoswitching of chromophores inside proteins. To help understand what is seen in the experiments, and provide a molecular picture for the signal obtained, computer simulations are indispensable. These processes happen on the femto- to pico-second timescale. At these short time-scales, the quantum nature of matter cannot be ignored and we need to solve the time-dependent Schroedinger equation. Over the last couple of decades, we have been developing a computer code to accurately solve this equation for a range of systems. In this talk I will describe the aims and basic ideas of the fundamental research into nuclear motion, with examples that demonstrate present capabilities and knowledge in how molecules behave after absorbing a photon.

Hörsaal G **17:15 Uhr** **19.02.2020**