TECHNISCHE UNIVERSITÄT WIEN

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IAP-SEMINAR

ANNOUNCEMENT

Date: **Tuesday, 26.4.2016**
Time: **16:00 p.m.**
Location: **Technische Universität Wien, Institut für Angewandte Physik, E134**
yellow tower „B“, 5th floor, Sem.R. DB gelb 05 B (room number DB05L03), 1040 Wien, Wiedner Hauptstraße 8-10

Lecturer: **Univ.Prof. Dr. Leticia González**
University of Vienna, Institute of Theoretical Chemistry

Subject: **All you need is light: Photochemistry from first principles**

Abstract: One particular challenge of Chemistry is to understand processes driven by light [1]. From the theoretical point of view, the study of photochemistry means calculating electronically excited states but also investigating the relaxation pathways that a molecule follows after being illuminated with light. Only after the natural dynamics of a molecular system is explained it is even possible to manipulate light-induced processes using light particularly shaped. In our group we employ ab initio quantum chemical methods, typically multiconfigurational ones, to first explore the excited states which are populated after a system is irradiated, and then to characterize the potential energy surfaces that the molecule can visit induced by light. A more detailed picture of the light-induced relaxation pathways is obtained with a time-dependent analysis. Here we employ ab initio molecular dynamics, where the electronic structure is treated quantum mechanically but the nuclear motion is subject to classical mechanics. In this case, we put special emphasis on treating on the same footing nonadiabatic and spin-orbit couplings to allow both internal conversion and intersystem crossing, respectively [2]. Several examples to exemplify the methods above will be presented.

[1] L. González, D. Escudero, and L. Serrano-Andrés. Progress and challenges in the calculation of electronic excited states. Chem. Phys. Chem. 13, 28-51, (2012)

[2]] M. Richter, P. Marquetand, J. González-Vázquez, I. Sola, and L. González. SHARC - ab initio molecular dynamics with surface hopping in the adiabatic representation including arbitrary couplings. J. Chem. Theory Comput., 7,1253 (2011).

All interested colleagues are welcome to this seminar lecture
(45 minutes presentation followed by discussion).

U. Diebold e.h.
(Seminar-Chairperson)

H. Störi e.h.
(LVA-Leiter)