Horst Köppel, J Phys Chem Biophys 2018, Volume 8
DOI: 10.4172/2161-0398-C3-033

5th International Conference on

Physical and Theoretical Chemistry

October 11- 13, 2018 | Edinburgh, Scotland

Horst Köppel

University of Heidelberg, Germany

Non adiabatic molecular dynamics following photoexcitation: an *ab initio* quantum approach

The author will present an overview over the theoretical work on molecular dynamics following photoexcitation in the visible or UV spectral range. This carries the system to an electronically excited state with a potential energy surface (PES) differing from that of the electronic ground state. A rich variety of vibrational and related processes will thus be initiated which can proceed on a single or several of the many different excited-state PESs. If some of these PESs are close in energy they interact and the nuclear motion on them does not proceed independently. This is the realm of nonadiabatic molecular dynamics which has been in the focus of interest of spectroscopists and physical and theoretical chemists for many years. It is of fundamental importance for many different excited-state processes in biology, chemistry and physics (such as charge transfer, photochemical rearrangements etc.). A typical scenario are so-called conical intersections of potential energy surfaces where different PES become degenerate upon variation of two nuclear coordinates. Systems treated by us recently comprise SO_2, small polyenes like butadiene or hexatriene or the benzene cation. Key features of the systems and methods used will be highlighted in the talk.

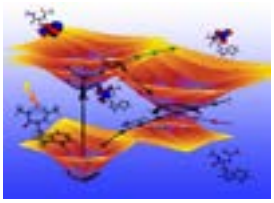

Figure 1: Schematic representation of two conical inter-sections and their associated photochemical reaction pathways.

Recent Publications

1. Teller E (1941) The crossing of potential surfaces. Journal of Physical Chemistry. 41(1):109-116.
2. H Köppel, W Domcke and L S Cederbaum (1984) Multimode Molecular dynamics Beyond the Born-Oppenheimer approximation. In Advances in Chemical Physics. 57:59-246.
3. W Domcke, D R Yarkony and H Köppel, Eds. (2011) Conical Intersections: Theory, Computation and Experiment. In Advanced Series in Physical Chemistry. World Scientific. Pages:768. Doi:10.1142/7803.
4. C Lévêque et al. (2013) *Ab initio* quantum study of the photodynamics and absorption spectrum of SO_2. The Journal of Chemical Physics. 138(4): 044320.
5. A Komainda et al. 2016) *Ab initio* benchmark study of nonadiabatic S1-S2 photodynamics of cis-and trans-hexatriene. The Journal of Physical Chemistry A. 120(33):6541-6556.

Biography

Horst Köppel has been a Senior Lecturer, and later Professor of Theoretical Chemistry at Heidelberg University since 1991. His research interests focuses on the theory of the Jahn-Teller effect, molecular excited state processes and vibrational structure in electronic spectra; special focus is on phenomena which cannot be described within the conventional Born-Oppenheimer separation of electronic and nuclear motions. He has authored and coauthored about 250 peer-reviewed original research papers, edited three books with topical reviews and organized several conferences in the field.

horst.koeppel@pci.uni-heidelberg.de