# Jörn Manz教授講演会

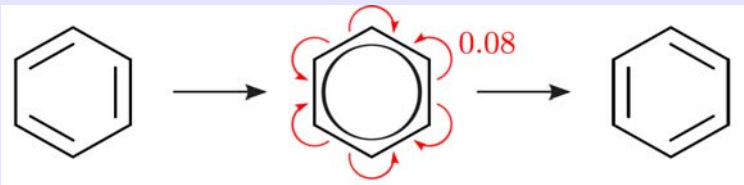
Freie Universität Berlin

Taiyuan, China

# Intramolecular fluxes: from tunneling to charge migration or from kiloseconds to attoseconds

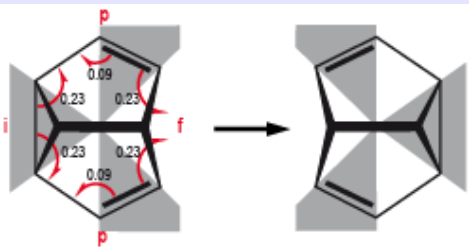
日時 : 2016年 7月11日(月)  16:00 ～17:15
場所 :化学専攻第3講義室

Manz教授は分子の励起状態ダイナミクスなどに関する量子動力学理論研究の第一人者で，分子中のトンネル電子移動やcharge migrationの話をしていただきます。




Recently, adiabatic attosecond charge migration (AACM) has been monitored and simulated for the first time, with application to the oriented iodoacetylene cation where AACM starts from the initial superposition of the ground ($\varphi_0$) and an electronic excited ($\varphi_1$) state [1]. Here, we develop the theory for electronic fluxes during AACM in ring-shaped molecules, with application to oriented benzene prepared in the superposition of the ground and first excited singlet states. The initial state and its time evolution is analogous to coherent tunneling where $\varphi_0$ and $\varphi_1$ have different meanings, however, i.e. they denote the wavefunctions of the lowest tunneling doublet. This analogy suggests to transfer the theory of electronic fluxes during coherent tunneling [2] to AACM, with suitable modifications which account for (i) the different time scales, (ii) the different electronic states, and which make use of (iii) the preparation of the initial state for AACM by a linearly polarized laser pulse. Application to benzene yields the multi-directional angular electronic flux with pincer-motion type pattern during AACM - this unequivocal result confirms a previous working hypothesis [3]. Moreover, the theory of AACM allows to quantify the electronic flux i.e. the maximum number of electrons ( out of 42 ) which flow concertedly during AACM in benzene is 6*0.08 = 0.48 [4].


[1] P.M. Kraus et al., Science 350(2015)790.
[2] T. Bredtmann et al., Phys. Chem. Chem. Phys. 17(2015) 29421 (Perspective Article).
[3] I. S. Ulusoy, M. Nest, J. Am. Chem. Soc. 133(2011)20230.
[4] G. Hermann et al., J. Phys. Chem. A (2016).



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