CFEL SCIENCE

SEMINAR

28th January 2016 - 10:00 h

CFEL – Building 99, seminar room I+II (ground floor)

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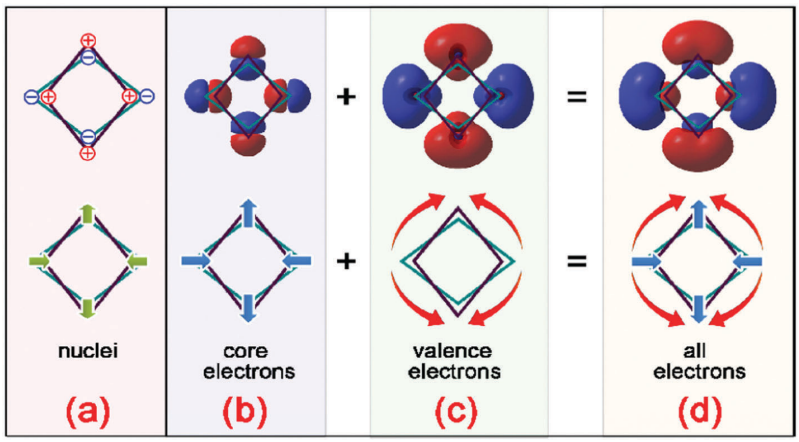
Quantum theory of concerted electronic and nuclear fluxes in molecular dynamics

When molecules vibrate or react from reactants to products, their electrons and nuclei flow. This is known, in principle, already since the day of Schrödinger [1], but many details have been discovered only recently [2], including the answers to question like "Do they flow synchronously? On which time scales? In which directions? How many electrons contribute?", etc. This lecture presents the general quantum theory, focusing on adiabatic processes. Applications are to model systems from Physical, Inorganic, and Organic Chemistry, with increasing complexity: Concerted electronic and nuclear fluxes in vibrating and dissociating $H_2^+(^2\Sigma_g^+, JM=00)$, as an exploding quantum bubble; rhombus-to-rhombus tunneling isomerizations of B_4; and Cope rearrangement of semibullvalene by coherent tunneling. Times associated with these processes range from femtoseconds (H_2^+) over picoseconds (B_4) to kiloseconds (semibullvalene).



[1] E. Schrödinger, Annal. Phys. (Leipzig) 1926, 81, 109
[2] T. Bredtmann, D. J. Diestler, S.-D. Li, J. Manz, J. F. Pérez-Torres, W.-J. Tian, Y.-B. Wu, Y. Yang and H.-J. Zhai, Phys. Chem. Chem. Phys. "Perspective article" (submitted)

Host: Terry Mullins / CFEL Molecular Physics Seminar