The Method of Tunneling Currents

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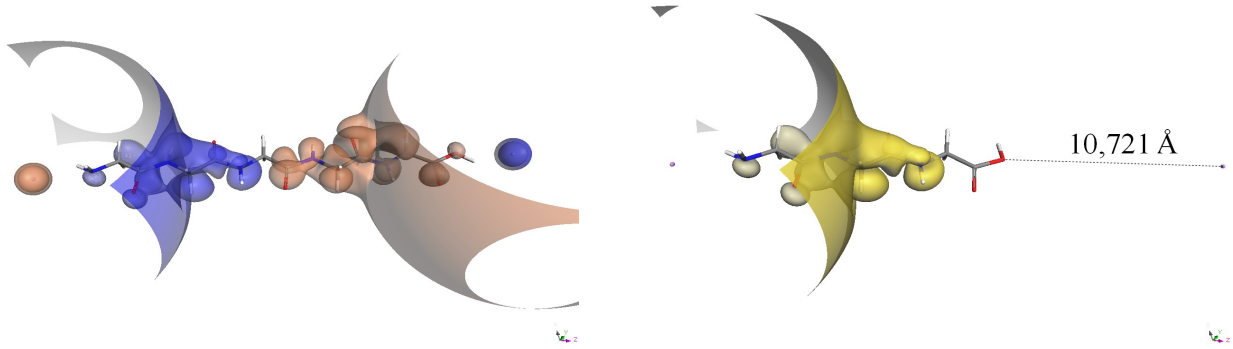

Transition states of electron transfer reactions are stationary states. The description as stationary states allows to apply the Born-Oppenheimer-approximation to the system of interest. Therefore in a series of UHF energy calculations the transition state of an electron transfer reaction can eventually be found by varying an external point charge that acts on the system [1]. The external pointcharge simulates effects of a dipolar medium such as rotations of water molecules on the electronic energy of the redox centers. If two different redox states with same electronic energy can be found, one has found the transition state of the electron transfer reaction. In the transition state an electron can be transferred to the other redox center via tunneling [2]. An analysis of the tunneling process gives insight into the electron transfer reactivity of the system, that means one is able to identify the parts of a system that are (un)necessary for the electron transfer.

By implementing respective formulas [2][3], we will be able to calculate and visualize the vector field of the tunneling flux as well as the electronic coupling of donor- and acceptor states.

[1] X. Zheng, A. Stuchebrukhov, *J. Phys. Chem. B*, **2003**, *107*, 6621-6628.
[2] A. Stuchebrukhov, *Adv. Chem. Phys.*, **2001**, *118*, 1-44.
[3] A. Stuchebrukhov, *Theor. Chem. Acc.*, **2003**, 110, 291-306.