On Infrared Induced Proton Transfer in Solution

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In condensed phase, a vibrationally excited reactant is usually considered to dissipate its excitation into the environment by vibrational energy relaxation before any chemical reaction can occur. However, it has been suggested [1,2] that for the hydrofluoric weak acid in aqueous solution, the proton transfer acid dissociation could be mode-selectively driven via absorption of an infrared photon: in this case, the solvent would assist the reaction. To study this reaction, we have developed a mixed quantum/classical molecular dynamics approach with non-adiabatic transitions[3,4,5], to account for both the bond breaking/forming in the reacting $FH\cdots OH_2$ dimer and for the quantum character of the high frequency F-H vibration. We will assess the feasibility of this infrared-induced proton transfer, which depends on other issues too, such as e.g. a sufficiently slow vibration-to-vibration energy transfer from the excited HF stretch to the vibrations of the solvent water molecules[6].

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