

Multidimensional Quantum Dynamics of Large Amplitude Motion

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The permanent interest for hydrogen bonds and hydrogen-bond dynamics that has been present in the molecular science community for many decades is motivated both by fundamental questions regarding the quantum tunneling phenomenon and by practical questions concerning dynamical and structural properties of H-bonded systems.

In terms of theory, the quantum nature of the hydrogen and the strong coupling between its motion and that of the molecular framework lead to multidimensional quantum dynamics. In this lecture various aspects of the theoretical simulation of vibrational, vibrational-rotational-tunneling, and ultrafast IR spectra will be discussed. First, on the specific example of carboxylic acid dimers we will show how the broad stationary absorption OH-stretching bands can be understood in terms of multidimensional anharmonic vibrational dynamics [1]. Next, the focus will be on the hydrogen tunneling motion and methods capable of predicting ground and vibrationally excited states tunneling splittings will be presented [2, 3]. We will address questions such as: Does vibrational excitation promotes H-tunneling? Which molecular motions are important for the understanding tunneling motion in the formic acid dimer? At the end ultrafast IR-laser driven H-bonds dynamics will be addressed and simulations of vibrational energy redistributions will be presented.

- [1] I. Matanović, N. Došlić, *Chem. Phys* 338 (2007) 121-126.
- [2] I. Matanović, N. Došlić, O. Kühn, *J. Chem. Phys.* 127 (2007) 014309.
- [3] I. Matanović, N. Došlić, B. R. Johnson, *J. Chem. Phys.* in print.