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Hydrogen Diffusion along SWCNTs: Time-scale Separation and Tunneling Effects

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The role of nanostructured materials in both fundamental and applied research is ever increasing due to their interesting and unique properties, from catalysis to electronics [1,2]. A specific field of interest is the understanding and development of storage devices for light gases, specially for energy applications (hydrogen) or environmental reasons (CO2, H2S). Carbon nanotubes have been largely studied with the idea of designing possible storage devices for H2 since the late 1990s [3]. However, a complete quantum dynamics description of the diffusion mechanism inside these structures is still lacking.

Here we present a quantum mechanical study of the diffusion of the H2 molecule along a narrow (8,0) Single-walled Carbon Nanotube (SWCNT). Following previous works by our group [4] we have modelled the system considering all the degrees of freedom (DOFs, internal and translational) of the hydrogen molecule and a rigid nanostructure. The cylindrical shape of the potential energy surface, showing five bound DOFs and one unbound DOF, has prompted us to develop an exact diabatization formalism separating two sets of weakly coupled degrees of freedom: on one hand, the unbound coordinate corresponding to the motion of the center of mass of H2 along the nanotube's axis, and in the other the remaining 5 DOFs, which are effectively confined by the nanostructure. By applying a complete separability assumption to the confined and unbound DOFs we have also developed an adiabatic approximation to the Hamiltonian, which increases the algorithm efficiency while maintaining the accuracy of the results. Both approaches have been employed to simulate Hydrogen diffusion along the SWCNT at temperatures in the 45-135 K range. The computational advantages provided by both method have enabled us to propagate the wave function beyond 15 picoseconds using the State Averaged - MCTDH [5] code, revealing a remarkable resonant structure as well as a noticeable tunnelling effect.

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