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Quantum dynamics study of the H_2 molecule confined in Single-Walled Carbon Nanotubes

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Synopsis The quantum dynamics of the hydrogen molecule confined in carbon nanotubes is studied using the MCTDH algorithm. Novel insights on the coupling between the different degrees of freedom are found and discussed for this system.

The ever more important need to store low density gases, either potential fuels like H_2 or CH_4 or known pollutants such as NH_3 or other greenhouse gases, has been a driving force in the last few years for the study of novel materials with the capability to keep molecules adsorbed both efficiently and reversibly. Most of these new devices are based on nanostructured materials, such as zeolites, metal-organic frameworks and carbon nanotubes[1][2][3]. These solids present a huge surface-volume relation, and more importantly some substances have been seen to have a higher preference to be adsorbed in them than in regular surfaces. The study of this phenomenon has led to the discovery of important distortions in the energies and internal structure of the captured molecules. These effects are now known as *quantum confinement*. A deep understanding of the quantum confinement effects at a fundamental level would definitely help to the discovery and design of better storage devices. Moreover, it could help to develop other kind of devices, such as *quantum sievings*[4], or even open the way to the use of these materials to control chemical reactions, taking advantage of the distortions generated on the confined species[5].

In the present work we study the dynamics of the hydrogen molecule confined in the hollow cavity of a (8,0) Single-Walled Carbon nanotube. This is the narrowest carbon nanotube in which adsorption of hydrogen is energetically favourable, according to Molecular Dynamics studies[6]. Therefore, its cavity can be seen as being quasi one-dimensional and confinement effects are expected to be very important. The Multiconfiguration Time-dependent Hartree (MCTDH) method[7] has been used to perform the dynamic study in a rigorous and fully quantum approach. The study of the system allowed us to see that the confinement in nanometric cavities affects deeply to the dynamical structure of the trapped molecule, due to the tight potentials and the increase of the coupling between the different degrees of freedom.

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