

Molecular modeling of hydrogen storage in carbon nanotubes: a combined molecular dynamics/ab initio orbital study

Pricl, Fermeglia, Ferrone, Coslanich, Paneni, Romanel

Interest in hydrogen as an environmentally clean fuel has recently grown up in view of decreasing fossil fuel supply. One of the main proposed application of hydrogen is its use as ecologically clean fuel in transportation. In spite of the lack of a convenient, lightweight but cost-effective on-board storage at present, the Daimler Chrysler Corp. announced that they would place the first fuel cell vehicles on the market during the next few years. Single-wall carbon nanotubes (SWNTs) seem to be convenient adsorbent materials that could form the basis of technologically viable hydrogen storage systems. Two main modes of hydrogen storage in carbon nanotubes have been proposed: physisorption, making use of nonbonding interactions between the hydrogen and carbon atoms, and chemisorption, taking place by hydrogenation of the nanotube carbon atoms. Nevertheless, the progress in this domain is hampered by several factors, among which we annoverate its novelty, and poor reproducibility or misinterpretation of the results obtained by various groups. Not secondary by importance, is the deleterious effect exerted by carbon monoxide co-adsorption, and eventual desorption of carbon dioxide, which act as poison with respect to hydrogen adsorption, competing for binding sites. Accordingly, in this work we present the results obtained by the application of different molecular modeling techniques, based on molecular dynamics and ab initio calculations, to the study of hydrogen storage in SWNTs.