Phase transitions of H_2 adsorbed on the surface of single carbon nanotubes

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We calculated, by means of the Diffusion Monte Carlo technique, the complete phase diagram of H_2 adsorbed outside single armchair carbon nanotubes whith index in the range from (5,5) to (16,16), and for hydrogen densities up to a single layer completion. In all cases, but the (16,16) one , the ground state was an incomensurate solid, formed by the arrangement of the hydrogen molecules in circumferences with planes perpendicular to the z axix of the nanotube. For each tube, there is only one of such phases stable in the density range considered, except in the case of the (5,5) and (6,6) tubes, in which two of these incommensurate solids are separated by novel first order phase transitions. In the (16,16) tube, the ground state is a commensurate solid similar to the one found in graphene.