A theoretical study of the H_2 storage by confinement inside carbon nanotubes

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Abstract

Theoritical calculations have been achieved to study te interaction between confined H2 molecule, along the nanotube axis and perpendicular to it, and a armchair (n,n) Single Walled Carbon Nanotubes using the Density Functional Theory (DFT) method with the CAM-B3LYP functional and STO-SG basis sets.

References:

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