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전산모사를 이용한 탄소나노튜브의 수소 검지 연구
Density-functional study on the hydrogen sensing mechanism of Carbon Nanotubes

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Based on the computer simulation using density functional theory (DFT), we propose a mechanism for the sensing of hydrogen gas on carbon nanotubes(CNT). At first, the binding energy of H to a (10,0) CNT is calculated at various coverage case, and the amount of charge transfer and the conductivity change through CNT is also discussed.
As is well known, the hydrogen molecule does not adsorb on the CNT surface. But hydrogen molecules can bind to the CNT surface by the medium of Pd atom. We also discuss about the possibility of dissociative adsorption of hydrogen on the Pd-CNT system.