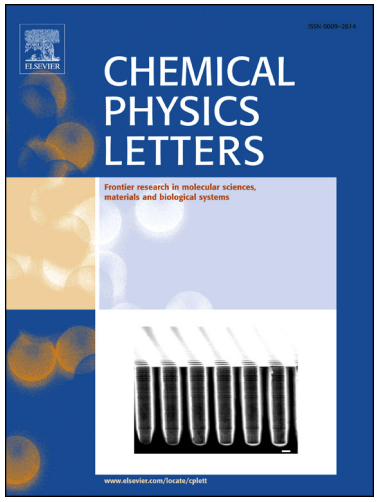

Research paper

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Hydrogen Adsorption in Metal-Decorated Silicon Carbide Nanotubes

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ABSTRACT:

Hydrogen storage for fuel cell is an active area of research and appropriate materials with excellent hydrogen adsorption properties are highly demanded. Nanotubes, having high surface to volume ratio, are promising storage materials for hydrogen. Recently, silicon carbide nanotubes have been predicted as potential materials for future hydrogen storage application, and studies in this area are on going. Here, we report a systematic study on hydrogen adsorption properties in metal (Pt, Ni and Al) decorated silicon carbide nanotubes (SiCNTs) using first principles calculations based on density functional theory. The hydrogen adsorption properties are investigated by calculations of adsorption energy, electronic band structure, density of states (DOS) and Mulliken charge population analysis. Our findings show that hydrogen adsorptions on Pt, Ni and Al-decorated SiCNTs undergo spontaneous exothermic reactions with significant modulation of electronic structure of SiCNTs in all cases. Importantly, according to the Mulliken charge population analysis, dipole-dipole interaction causes chemisorptions of hydrogen in Pt, Ni and Al decorated SiCNTs with formation of chemical bonds. The study is a platform for the development of metal decorated SiCNTs for hydrogen adsorption or hydrogen storage application.