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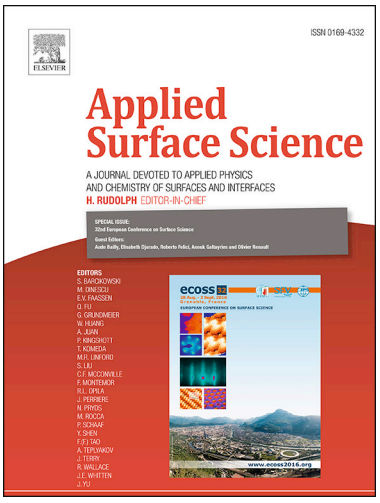

Full Length Article

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A DFT investigation on group 8B transition metal–doped silicon carbide nanotubes for hydrogen storage application

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ABSTRACT

The binding of group 8B transition metal (TMs) on silicon carbide nanotubes (SiCNT) hydrogenated edges and the adsorption of hydrogen molecule on the pristine and TM–doped SiCNTs were investigated using the density functional theory method. The B3LYP/LanL2DZ method was employed in all calculations for the considered structural, adsorption, and electronic properties. The Os atom doping on the SiCNT is found to be the strongest binding. The hydrogen molecule displays a weak interaction with pristine SiCNT, whereas it has a strong interaction with TM–doped SiCNTs in which the Os–doped SiCNT shows the strongest interaction with the hydrogen molecule. The improvement in the adsorption abilities of hydrogen molecule onto TM–doped SiCNTs is due to the protruding structure and the induced charge transfer between TM–doped SiCNT and hydrogen molecule. These observations point out that TM–doped SiCNTs are highly sensitive toward hydrogen molecule. Moreover, the adsorptions of 2–5 hydrogen