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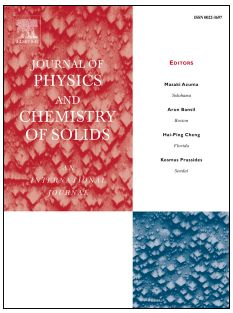

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Adsorption of Water on Fluorinated Graphene

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ABSTRACT

In this paper, we investigate the adsorption of water monomer on fluorinated graphene using state-of-the-art first-principles methods within the framework of density functional theory (DFT). Four different types of methods are employed to describe the van der Waals (vdW) interactions between water molecule and the carbon surface: The traditional DFT calculations within the generalized gradient approximation (GGA), and three additional types of calculations using respectively the semi-empirical DFT-D2 method, the original van der Waals density functional (vdW-DF) method, and one of its variants — the optPBE-vdW method. Two situations and totally four adsorption configurations are considered. Compared with the adsorption on pristine graphene, the adsorption energies of water on fluorinated graphene are significantly increased, and the orientations of water diploe moment are notably changed. The most stable configuration is found to stay right above the top site of the C atom which is bonded with F, and the dipole moment of water molecule aligns spontaneously along the surface normal.

Keywords: Water, Fluorinated Graphene, Adsorption, First-principles Calculations, van der Waals Interactions

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