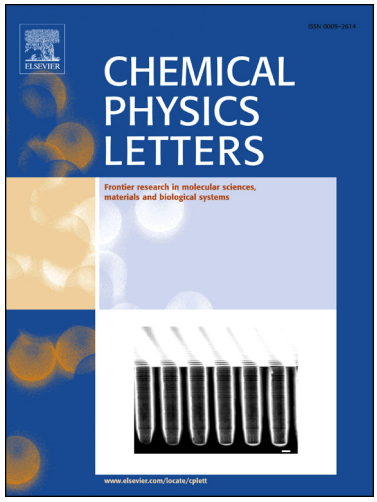

Research paper

Lithium adsorption on heteroatom mono and dual doped graphene

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Lithium adsorption on heteroatom mono and dual doped graphene.

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Abstract

Herein, we studied the interaction of lithium with monodoped (X) and dual-doped graphene (XY), X=Al, Si, P and S and Y=B, N and O. Dual-doping is the best choice to modulate the interaction of lithium with graphene. The strongest interaction with lithium was observed for SN-dual-doped graphene, while S-doped and N-doped graphene displayed the weakest interactions. With regards to the electronic properties, for some systems Li adsorption opened a band-gap, while for others restored the Dirac cones and the semimetallic character at the K-point. Therefore, Li-doping is a useful tool to fine-tune the band gap in mono and dual-doped graphene.

Keywords: carbon nanomaterials, adsorption, graphene, density functional calculations, doping.

1. Introduction

There is a large body of evidence which indicates that ripples, charge puddles and substrates can be used to modulate the interactions between graphene and atoms or molecules. For example, the experimental investigations of Fan et al.[1] showed that either the sodium atoms intercalated between graphene and the SiO_2 support, or the ripples which naturally occur in 2D crystals, have a similar effect: the addition of aryl diazonium salts is facilitated. Inert substrates like cubic BN or alkyl terminated groups do not affect the chemistry of graphene, while SiO_2 and Al_2O_3 have the opposite effect [2]. Much attention has been dedicated to the study of alkali/graphene nanocomposites, because they constitute one of the simplest examples of charge doping of graphene. Density functional calculations demonstrated that Li [3], K [4] and artificial charges [5-6] increase the interaction energy between graphene and free radicals, as well as with Au nanoparticles [7]. A similar effect can be found for strong electron withdrawing molecules such as F4-