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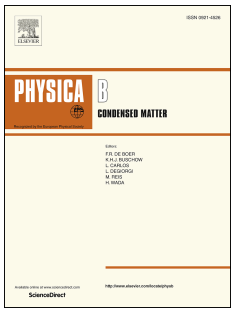

Density functional insights of iodine interaction with graphene and its nanoribbon with zigzag edges

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Density functional insights of iodine interaction with graphene and its nanoribbon with zigzag edges

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Abstract

Graphene, being perfect 2-D structure, exhibits electronic properties which are sensitive to the presence of any impurtiy/adsorbed adatom. In the present work, interaction of I atoms has been investigated with graphene and zigzag graphene nanoribbon (ZGNR) by considering it, as a passivating element as well as an adsorbed adatom. Three different possible combinations of I passivation have been explored which include: one edge I and other edge H passivation (H-ZGNR-I), both edges passivation (I-ZGNR-I) and one edge I passivation while other edge is passivated by H in sp^3 manner (H_2-ZGNR-I). Similarly, three adsorption sites namely top (T), bridge (B) and hole (H) have been considered at ZGNR as well as on planar graphene sheet. It is revealed that passivation of I on ZGNR is energetically favorable and settled in antiferromagnetic (AFM) ground state. Further, it is observed that H-ZGNR-I is the most stable configuration after pristine (H-ZGNR-H) followed by H_2-ZGNR-I and I-ZGNR-I configurations. Our observations show that except I-ZGNR-I, all the structures exhibit magnetic stabilization well above the thermal excitations at room temperature which ensures their applicability for practical applications. Moreover, I adsorption always prefers T site on ZGNR/graphene sheet. Analysis of I migration on 2-D graphene indicates that diffusion barrier is always less than the thermal excitation ($\sim$26 meV) and the diffusion time varies from $\sim$1.5 ps to $\sim$2.2 ps. Present findings suggest for stronger binding of I atoms with ZGNR whereas the same with graphene is comparatively weak and exhibits spontaneous migration.

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