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Theoretical investigation of manganese adsorption on graphene and graphane: A first-principles comparative study

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Abstract

Within the framework of spin-polarized generalized gradient approximation (sigma GGA) of the density functional theory (DFT) and pseudopotential method, the structural, magnetic, and electronic properties of graphene and graphane upon the adsorption of manganese atoms have been theoretically investigated. In contrast to the recent results (New J. Phys. 12, 063020 (2010)), Mn atom has been found to be adsorbed on a hollow-site configuration and no appreciable indication to substitute one of the C atoms of the graphene sheet. Unlike the recent results on Mn-doped graphane (Carbon 48, 3901 (2010)), the Mn adatom prefers to adsorb on the top of a carbon atom, forming a bridge with the uppermost hydrogen atoms. The magnetic moment of the Mn-doped graphene is found to be larger than that of the Mn-doped graphane. The structural parameters and electronic properties of both Mn-doped graphene and Mn-doped graphane are determined and compared with the available data. (c) 2011 Elsevier B.V. All rights reserved.

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