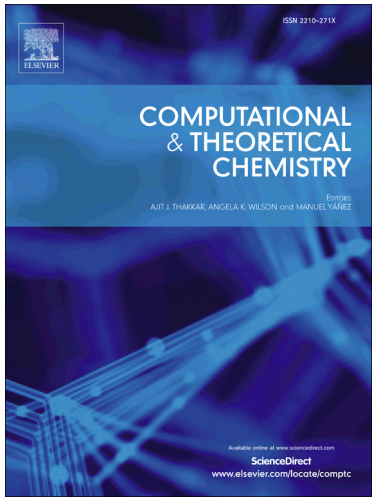

A Comparative Theoretical Study of Methane Adsorption on the Nitrogen, Boron and Lithium Doped Graphene Sheets Including Density Functional Dispersion Correction

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PII: S2210-271X(16)30057-3
DOI: http://dx.doi.org/10.1016/j.comptc.2016.02.019
Reference: COMPTC 2069

To appear in: *Computational & Theoretical Chemistry*

Received Date: 22 February 2016
Accepted Date: 24 February 2016

Please cite this article as: A. Hassani, M.T.H. Mosavian, A. Ahmadpour, N. Farhadian, A Comparative Theoretical Study of Methane Adsorption on the Nitrogen, Boron and Lithium Doped Graphene Sheets Including Density Functional Dispersion Correction, *Computational & Theoretical Chemistry* (2016), doi: http://dx.doi.org/10.1016/j.comptc.2016.02.019

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Abstract

In this study, the adsorption of methane molecules over boron, nitrogen and lithium doped graphene sheet is theoretically studied using density functional theory. Boron and nitrogen atoms are situated in a graphene network in graphitic, pyridinic and defect substitution forms, while Li atoms are placed out of the graphene layer. Density functional theory was applied to prepare the structures with the minimum level of energy by using 6-31 G basis set. DFT-D3 correction was applied to calculate density functional dispersion correction. The results showed that methane molecules were adsorbed on all graphene doped surfaces with physisorption interactions. In addition, simulation results indicated that Li-doped graphene sheet was more reactive than the two other structures in terms of its higher adsorption energy and the medium distance of methane molecule from graphene sheet. Moreover, among various substitution forms of boron and nitrogen atoms in the graphene sheet, graphitic substitution is more stable due to the higher adsorption level of energy. The distribution of the highest occupied molecular orbital of nitrogen and boron substituted graphene showed the polarization nature of the graphene doped sheet in boron and nitrogen while lithium doped graphene was polarized at the adjacent carbons. After methane adsorption, no specific change was observed in highest occupied molecular orbital calculations of graphene sheets, which confirmed the physical adsorption behavior of methane molecule on the graphene doped sheets. In conclusion, Li doped graphene sheet is suggested as an appropriate material in comparison to nitrogen and boron doped structure for enhancing methane storage capacity.

Key words: Graphene doped, Methane Adsorption, Dispersion Correction, Physisorption, HOMO.

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