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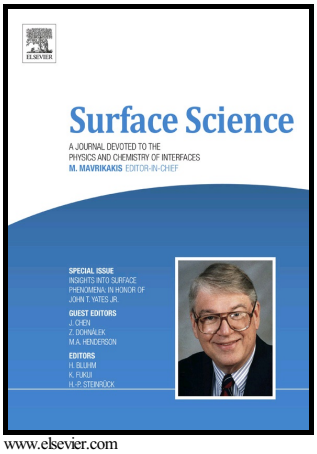

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PII: S0039-6028(16)30369-7
DOI: http://dx.doi.org/10.1016/j.susc.2017.01.004
Reference: SUSC20976

To appear in: *Surface Science*

Received date: 2 August 2016
Revised date: 8 January 2017
Accepted date: 10 January 2017

Cite this article as: Shaobin Yang, Sinan Li, Shuwei Tang, Ding Shen, Wei Dong and Wen Sun, Adsorption, intercalation and diffusion of Na on defective bilayer graphene: a computational study, *Surface Science* http://dx.doi.org/10.1016/j.susc.2017.01.004

Adsorption, intercalation and diffusion of Na on defective bilayer graphene: a computational study

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Abstract

The interaction between inserted/adsorbed Na and the structures of pristine and defective bilayer graphene (BLG) with Stone-Wales (SW), mono-vacancy (MV) and divacancy (DV) defects have been investigated by the first-principles calculations. The computational results show that the intercalation of Na in the interlayer of BLG with DV defects is more energetically favorable than Na adsorption on the surface. The lower formation energies of Na adsorption/intercalation on/in the BLG with DV defect reflect a stronger attraction between Na and DV defects compared with MV and SW defects. A significant charge transfer occurs from Na to near graphene layer(s) of BLG. The adsorption and intercalation of Na not only induce more significant structural distortion into the upper layer graphene with SW defect but also spin polarization for MV and DV defects. The results of migration energy barriers show that Na prefers to diffuse toward the DV site, and the diffusion outward the DV site is more difficult in comparison with the SW and MV defects. As a consequence, more Na atoms would be trapped in the region of the DV defect, leading to larger capacity than SW and MV defects.

Keywords Na-ion battery · Bilayer graphene · First-principles theory · Defects · Diffusion