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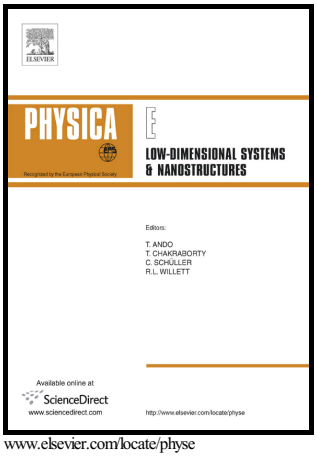

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PII: S1386-9477(17)30342-9
DOI: http://dx.doi.org/10.1016/j.physe.2017.06.021
Reference: PHYSE12843

To appear in: *Physica E: Low-dimensional Systems and Nanostructures*

Received date: 8 March 2017
Revised date: 16 June 2017
Accepted date: 21 June 2017

Cite this article as: Wenjiang Liu, Cheng Zhang, Mingsen Deng and Shaohong Cai, The Structural and Electronic Properties of Metal Atoms Adsorbed on Graphene, *Physica E: Low-dimensional Systems and Nanostructures* http://dx.doi.org/10.1016/j.physe.2017.06.021

The Structural and Electronic Properties of Metal Atoms Adsorbed on Graphene

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Abstract:

Based on density functional theory (DFT), we studied the structural and electronic properties of seven different metal atoms adsorbed on graphene (*M*+graphene). The geometries, adsorption energies, density of states (DOS), band structures, electronic dipole moment, magnetic moment and work function (WF) of *M*+graphene were calculated. The adsorption energies ΔE indicated that *Li*, *Na*, *K*, *Ca* and *Fe* adsorbed on graphene were tending to form stable structures. However, diffusion would occur on *Cu* and *Ag* adsorbed on graphene. In addition, the electronic structure near the Fermi level of graphene was significantly affected by *Fe* (*Cu* and *Ag*), compared with *Li* (*Na*, *K* and *Ca*). The electronic dipole moment and magnetic moment of *M*+graphene were sensitive to the adsorbed metal atoms. Moreover, we found electropositive (electronegative) adsorption can decrease (increase) the WF of the surface. Specially, the WF of *Ag*+graphene and *Fe*+graphene would increase because surface dipole moment make a contribution to electron.

1. Introduction

Due to the special two-dimensional geometry, graphenes, which have a single atom layer thickness, has