ENERGETICS OF SMALL CLUSTERS OF ALKALI METALS (Li, Na, AND K) ADSORBED ON GRAPHENE

GAGANDEEP KAUR[1,2], SHUCHI GUPTA[1,3] & KEYA DHARAMVIR[1]

[1]Department of Physics and Centre of Advanced Studies in Physics, Panjab University, Chandigarh, India

[2]Chandigarh Engineering College, Landran, Mohali, Punjab, India

[3]University Institute of Engineering and Technology, Panjab University, Chandigarh, India

ABSTRACT

Graphene has unique properties arising from its honeycomb-lattice structure that could maximize the interaction of adsorbate on the layer. Many experimental methods have been devised to form stable metallic clusters of different sizes. Metal clusters, especially those of alkali-metal atoms Li, Na, and K, have played an important role in the development of cluster physics as a branch of modern physics and chemistry. Moreover metal-graphene contacts would play a crucial role in graphene based electronics.

In this paper, we use a method involving interatomic model potentials to investigate the structure and binding energies of clusters of alkali metal M_n (M=Li, Na, K; n=1, 3), adsorbed on graphene. For M-M interaction, we use Gupta potential while Lennard-Jones potential was used for M-C interactions (C = carbon). We find that for each alkali cluster in the minimum energy configuration, adsorbation at the hollow site on grapheme is favored. Stability of the M_n - graphene system increases with the increase in size of the cluster. All trimers adopted a geometry close to an equilateral triangle with significant changes in bond lengths.

KEYWORDS: Graphene, Metal Clusters, Interatomic Potentials