

Lithium and magnesium dispersion on boron doped graphene

Luís M. Almeida, Vitor B. Torres

Department of Physics and I3N, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal
lma@ua.pt

Abstract

One promising way to store molecular hydrogen at high level of gravimetric density capable of satisfying the very demanding requirements of light-duty fuel cell vehicles is the use of graphene or graphitic type of materials.

The hydrogen storage on graphene can be improved by decorating metallic atoms on its surface [1]. Lithium and magnesium atoms, that have already proven to increase hydrogen adsorption, could be used to satisfy the low gravimetric density hydrogen storage.

In order to disperse metallic atoms on graphene or expanded graphite their binding energies to graphene must be higher than the bulk metal cohesive energies. For magnesium and lithium the calculated binding energies to graphene are higher than their bulk metal cohesive energies. Because of this they have a tendency to cluster preventing them to disperse on graphene. However, the boron doping or boron substituted graphene [2,3] creates an electron deficient system that bound lithium atoms helping the resulting ions to disperse due to coulomb repulsion.

We calculate the binding energies of lithium and magnesium to graphene and boron doped graphene type materials using ab-initio density functional theory methods. In these simulations we used a boron concentration of about 5% in substitutional positions. The binding energies of lithium to these structures are found to be higher than lithium bulk cohesive energy even for high proportion of Li:B and not changing much from relative location of Li atoms to boron defect. On the other hand the effect of boron doping to the dispersion of magnesium in graphene is not so strong.

References

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