A DFT study of Li adsorption in a GeC bilayer for Li-ion batteries

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INTRODUCTION

Bidimensional (2D) materials like graphene have awaken great interest in battery research given their large surface-per-volume ratio and chemical tunability, which has made them the focus of diverse theoretical studies addressing their interaction with Li atoms and their Li-storage capacity. Most studies consider an isolated monolayer, although in most cases, synthesis of isolated monolayers is still a technological challenge. Considering the scarcity of works that study the effect of the presence of a second layer in the Li-adsorption capacity, and also the emergence of van der Waals heterostructures, we study, within the Density Functional Theory formalism, the interaction of Li atoms with a germanium carbide (GeC) bilayer.

EXPERIMENTAL/THEORETICAL STUDY

Density Functional Theory, as implemented in the SIESTA package[1], is used to find the electronic ground state of the systems. The GGA-PBE approximation is used to model the electronic exchange and correlation. Structural optimizations are used to find stable configurations of the Li-bilayer systems, through a conjugate gradient algorithm implemented in SIESTA.

The germanium carbide (GeC) bilayer is modeled by a 100 atom supercell, composed of two stacked graphene-like monolayers of 5×5 primitive cells. The Li atoms are placed at the interlayer space, close to the "bottom" or "top" layers, to study the effect of the different local environments on their adsorption characteristics.

RESULTS AND DISCUSSION

The results show that the so-called AB layer stacking is more favorable than AA one. Also, the interaction of the GeC bilayer with the Li atoms causes a shifting of the Ge atoms from the former monolayer plane, but no important distortion is found until 6 Li atoms per supercell are adsorbed. Three Li atoms at either the top or bottom monolayer make the system metallic, but 4 and 6 Li atoms adsorbed on both monolayers lead to a semiconducting system with a band gap close to 0.5eV. Furthermore, the adsorbed Li atoms tend to form flat clusters at the midpoint of the interlayer space.

CONCLUSION

Results obtained so far show favorable interactions of the GeC bilayer with Li atoms at its interlayer space, suggesting that layered GeC systems are an interesting option for anodes in Li-ion batteries. We think that these results contribute to the ongoing search for more efficient Li-storage systems and anodes for Li-ion batteries.

REFERENCES

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