DFT APPROACH TO STUDY SINGLE LAYER AND BILAYER GRAPHENE NANOFLAKES ELECTRONICS PROPERTIES

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Abstract

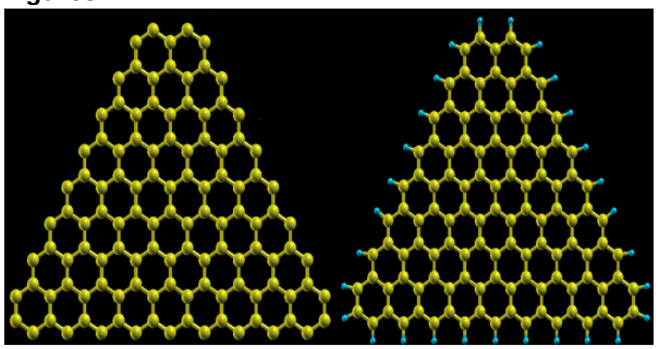
First principle modeling is computational theoretical modeling method used in physics, chemistry, and material science to investigate electronic properties of nanomaterials. Nevertheless, there have been very limited studies on the electronic property of single layer and bilayer graphene nano-flakes by using first principle modeling. Therefore, current research aims to investigate the electronic properties of single layer and bilayer of graphene sheets with different shapes and geometry, by using computational quantum physics modeling which is cost- effective and reliable. Generally, different amount of graphene layer and different amounts of carbon atoms within the edges as well as various shapes of nano-flakes will affect the Fermi energy level and total energy of the system. The structure is then be modelled in terms of electron density by using the density functional theory (DFT)[2]. The computational methodology will employ DFT within the Kohn Sham frame work coded in the Quantum ESPRESSO suite of open source computer codes. Generally, DFT equation $\mathbf{E} = \sum_i^N \boldsymbol{\varepsilon}_i - \frac{1}{2} \int\int \frac{\rho(r)\rho(r')}{|r-r'|} \mathbf{dr}\ \mathbf{d}r' + E_{xc}[\rho] - \int v_{xc}(r)\rho(r)dr$ is

used to the study for fermi energy calculation. DFT is used to investigate electronics properties in graphene nanoflakes with either armchair (AC) or zigzag (ZZ) edges, as well as without passivation and with passivation.

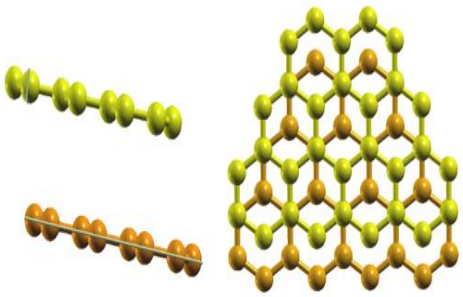
References

[1] Novoselov, K. S.; Geim, A. K.; Morozov, S. V.; Jiang, D.; Zhang, Y.; Dubonos, S. V.; Grigorieva, I. V.; Firsov, A. A., Science, **306 (5696)** (2004) 666–669.
[2] Karaush, Nataliya N., Baryshnikov, Gleb V., Minaev, Boris F., Chemical Physics Letters, 612, (2014) 229- 233

Figures



(a) C_{115} (Radical) $C_{115}H_{29}$ (With Hydrogen Termination)



(a) AB Bernel (b) Bilayer graphene nanoflakes Trapezium geometry