Computational study of optical and electronic properties of metal-decorated Graphene

The computational methods for studying the various properties of nanomaterials like Graphene, have become extremely popular these days. Thanks to the ever increasing processor speeds. These methods include Density functional theory (DFT) and Time dependent density functional theory (TDDFT). DFT can be used to predict the ground state properties like band gap, binding energy, dipole moment etc., and TDDFT can be used to predict the excited state properties like life-time, UV-Visible spectra, emission spectra etc. These results can be used to even validate the experimentally obtained data.

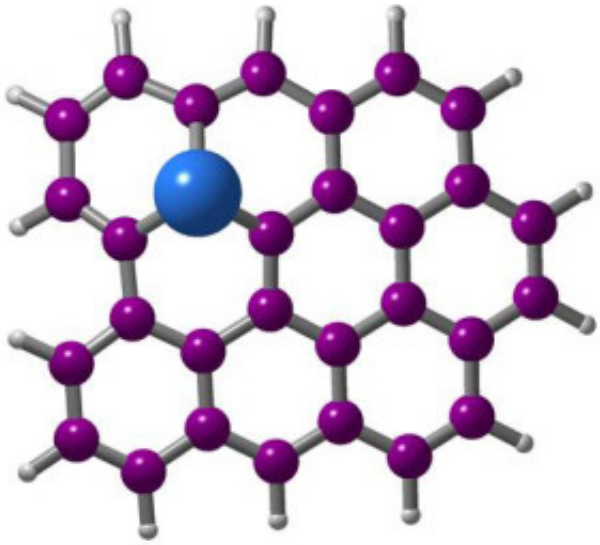

Fig. 1.

Graphene has been extensively studied due to the possibility of tuning its band gap. This can be done, for example, by varying its dimensions/ widths. Additionally, there have been significant research efforts on the optical properties of graphene owing to their huge applications in photonics and optoelectronics ranging from solar cells, light-emitting devices to touch screens, photo-detectors and ultrafast lasers. Recently, the metal decorated/doped graphene has been into limelight due to high variation in optical absorption of pure graphene, on metal doping. In addition metal doping affects the conducting nature of the graphene too.

In the current study, DFT and TDDFT methods have been employed to study the electronic properties, optical absorption and emission in Graphene, both in Pure and single metal atom doped graphene (MGNR). The graphene-metal composites were of the form $C_{29}H_{14}$-X (where X= Ni, Fe, Ti, Co^{+}, Al^{+} and Cu^{+}) (Fig. 1.). The absorption and emission properties were calculated in the

visible range (400-720nm).

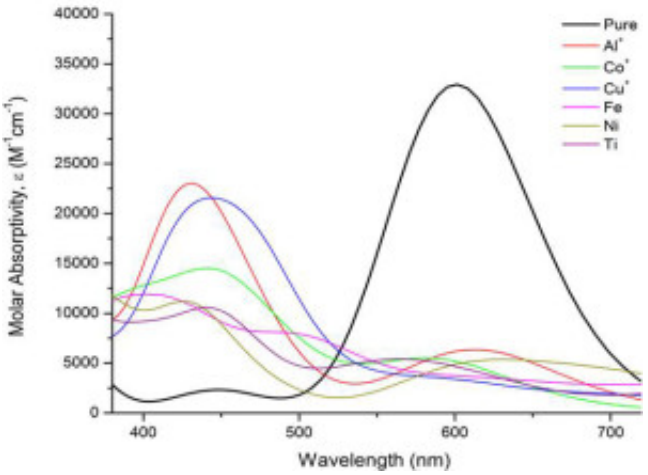

Fig. 2.

Our results show that graphene in its pure form is most stable. Furthermore, amongst the metal doped GNRs, $C_{29}H_{14}$-Co^{+} and $C_{29}H_{14}$-Al^{+} were most and least stable. The metal doping does affect the electronic gap, with the Co^{+} doped GNR with lowest gap. All Graphene structures were found to be semiconducting in nature. It was found that the optical absorption of pure graphene undergoes shift on metal doping (Fig. 2). The absorption of pure graphene around 601nm reduces on doping and increases again around 400nm. The molecular transitions were ascribed to be from ???* orbitals. Emission from the pure graphene was noticed from the lowest excited state. However, in case of the metal doped GNRs, the emission was prominently from the higher excited states. The emission was found to be in the visible range.

These results would improve our understanding of the optical properties of graphene for future applications like photovoltaics or in dye sensitized solar cell (DSSC) applications, where visible-light absorption in the graphene layer is of chief concern.

Publication

Study of Electronic, Optical Absorption and Emission in Pure and Metal-Decorated Graphene Nanoribbons (C29 H14 -X; X=Ni, Fe, Ti, Co(+) , Al(+) , Cu(+)): First Principles Calculations.
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