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First principle calculation of electronic and optical properties of graphene and mono doped graphene with Ti, Zn, and Ru.

Graphene is a 2-dimensional material that has received a lot of research attention over the last two decades as it is considered to be a revolutionary material for the future due to its superlative properties. Graphene has a zero band gap energy. This research work reports first principle calculations based on Density Functional Theory (DFT) to study the electronic and optical properties of pure graphene and mono doped graphene with Ti, Zn and Ru atoms. The results show that for a pure graphene, the band gap energy is zero. However, when doped with Ti, Zn and Ru atoms, the gaps of the energy were opened. For the doping, the calculated band gap values for the graphene doped with Ti, Zn and Ru are 0.550 eV, 0.713 eV and 0.786 eV, respectively. The results demonstrated that the band gap of graphene can be opened by addition of Ti, Zn and Ru atoms. For the optical properties of the graphene, the doping with the selected atoms weaken the absorption in the visible region and strengthen the absorption in the infrared region.

Apply to be considered for a student ; award (Yes / No)?

Yes

Level for award;(Hons, MSc, PhD, N/A)?

PhD

Consent on use of personal information: Abstract Submission

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