**Revisiting the optoelectronic properties of graphene: a dft approach**


## ABSTRACT

Understanding the atomic behaviour of pure graphene is crucial in manipulating its properties for achieving optoelectronics with high absorption indexes and efficiencies. However, previous research employing the DFT approach emphasised its zero-band gap nature, not its unique optical properties. Therefore, this study employed ab initio calculations to revisit the electronic, magnetic, and optical properties of pristine graphene using the WIEN2K code. The results reveal that the PBE-GGA valence and conduction bands cross at -0.7 eV. Our calculations demonstrated that the absorption coefficient of graphene has the strongest light penetration in the parallel direction. Furthermore, our results not only present the best possible propagation of light in pure graphene but also reveal that the linear relationship between the formation of the free electron carriers and the energy absorption is responsible for the high optical conductivity observed in pure graphene, as indicated by the peaks. Lastly, the metallic properties of graphene are reflected by the variation in spin up and down that appears, as evidenced by the total and partial densities of states, and the large refractive index attributed to its high electron mobility confirms its metallic nature.