Ab Initio Insights on the Effect of Embedding Lanthanide Atoms on Nitrogenized Holey Doped Graphene (G-C2N)

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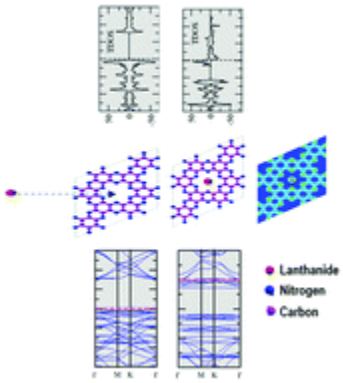
Abstract

Within the density functional theory formalism with the Hubbard correction (DFT+*U*) we explore how the structural, electronic and magnetic properties of nitrogenated holey doped graphene (g-C_2N) can be tuned through embedding of lanthanide atoms. The lanthanide atoms considered in this study were Nd, Pm, Sm, Eu, Gd, Er, Tm, Yb and Lu. With the exception of Yb and Lu embedding for which a reduction in band gap (red shift) was observed, lanthanide ion embedding was found to lead to g-C_2N exhibiting half metallicity. The calculated binding energies indicate that it is possible to embed lanthanide atoms into the matrix of g-C_2N and from the calculated clustering energies, lanthanide atoms were found to exhibit dispersive distribution void of cluster formation. Lanthanide ion embedding lowered the workfunction of g-C_2N and also lead to g-C_2N being magnetic. This study provides significant insights that can be used in the realization of 2D nanoscale devices for electronic, thermionic and spintronic applications.



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