Band gap opening of doped graphene Stone Wales defects: simulation study

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We implemented density functional theory to investigate the electronic properties of doped graphene Stone Wales defects. We found that the band gap of nitrogen doped graphene with different orientations of Stone Wales defect could be tuned. The obtained band gap results strongly depend not only on the specific location of the doped atom, but also on the orientations of Stone Wales defects. The symmetrical density of states is an indication that the total magnetic moment was zero as the valence electrons grouped in pairs. In addition, we performed charge analysis for all nitrogen doped graphene Stone Wales defects structures and it can be observed that the carbon atoms are more electronegative compared to nitrogen atoms, which obtain all the valence electrons. The transferred charge from nitrogen atom is largely localized on the carbon atoms lying in close proximity of the dopant atom.

Keywords: Graphene, Stone Wales defects, nitrogen doping, electronic properties, density functional theory and charge density.

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