Abstract Submitted
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Vacancy vacancy interactions in graphene using first principles calculations[1] PRIYA FRANCIS, University of Pune, Pune 411007, India, CHIRANJIB MAJUMDER, Bhabha Atomic Research Center, Mumbai 400085, India, S.V. GHAISAS, University of Pune, Pune 411007, India — We employ first principles calculations to study the defect induced magnetism on monolayer graphene sheet. Removal of single, double and triple carbon atoms from a 6 $\times$ 6 monolayer graphene sheet gives magnetic moment (MM) comparable with those reported in the literature. For single vacancy defect, MM value lies in between 1.4 and 1.6 μ_B, depending on the type of lattice atoms (α or β). For triple vacancy, MM is 1.04 μ_B. Detailed study of double vacancy in graphene layer with a removal of similar and different type of lattice atoms gives interesting results in terms of magnetic moment as well as in spin density distributions. For double vacancy our study gives magnetic moment values 0 and 3 μ_B, depending on the position and lattice type of the removed atoms. Our study reveals that removal of near by same lattice type atoms (α type) also leads to 0 magnetic moment, same as that of the removal of different lattice type atoms (α and β, irrespective of the distances). Here the distance between the removed two α type atoms is 2.46 Å.

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