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Adsorption of group VA atoms in single and double vacancy of graphene SHYAM KATTEL, BORIS KIEFER, Physics Department, New Mexico State University, PLAMEN ATANASSOV, Chemical and Nuclear Engineering Department, University of New Mexico — Dopants can greatly affect the electronic structure of graphene. In this study we report on the effect of group VA elements associated with single vacancy (SV) and double vacancy (DV) on the electronic structure of graphene. The results of our density-functional-theory (DFT) computations predict strong and exothermic chemisorption of group VA atoms to SV and DV in graphene (M@SV/DV, where M=N, P, As, Sb, or Bi) which leads to large, systematic and diverse effects on its electronic structure. We find that N@SV has a small band gap below Fermi level (E_F) and P@SV has semiconducting and magnetic properties consistent with previous studies. Our preliminary band structure computations show that As@SV induces ∼100% spin polarization close to E_F while Sb@SV and Bi@SV are metallic. In contrast, N@DV has a large spin polarization near E_F while all other DV defects are predicted to be metallic. These results suggest that especially As@SV and N@DV may have interesting applications in spintronics and nanoelectronics.

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