Magnetic anisotropy of Mn, Fe and Co dimers on monolayer phosphorene

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We studied the geometries, electronic structure and magnetic properties of substitutional doping and adsorption of transition metal (Mn, Fe and Co) dimers on phosphorene monolayer. The electronic band structures and magnetic properties were dependent on the doping type and dopant materials. For Mn and Fe substitutional and adsorption dimer, we obtained semiconducting band structures with spin polarization. However, we found a half-metallic feature in Co substitutional dimer while the Co adsorption dimer showed a semiconducting behavior without any spin polarization. The hybridization between TM and phosphorene sheet contributed to suppressing the magnetic moment of TM dimers. For instance, the total magnetic moments of -2.0, 4.24 and 1.28 μ_B/cell for Mn, Fe and Co substitutional dimer were obtained while the Mn and Fe adsorption dimers showed magnetic moments of -1.69 and 0.46 μ_B/cell. We observed that the Mn and Fe substitutional dimers showed an out-of-plane magnetization with magnetocrystalline anisotropy energies (MAEs) of 0.57 and 0.89 meV/cell while an in-plane magnetization with a MAE of 0.58 meV/cell was obtained in Co substitutional dimer. The Mn adsorption dimer still displayed a perpendicular magnetization with a MAE of 0.50 meV/cell. In contrast, the Fe adsorption dimer had an in-plane magnetization with a MAE of 0.11 meV/cell. This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT and future planning (2016R1A2B4006406)