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Tuning Electronic and magnetic properties of phosphorene by vacancies and adatoms¹ POOJA SRIVASTAVA, K.P.S.S. HEMBRAM, HIROSHI MIZUSEKI, KWANG-RYEOL LEE, SANG SOO HAN, SEUNGCHUL KIM, Korea Institute of Science and Technology — In the search of novel materials, phosphorene (2D layers of black phosphorus) has been synthesized recently. Intrinsic bandgap, hydrophilicity and anisotropic electron mobility make phosphorene different from graphene and also, its hole mobility is higher than that in MoS_2 . All these properties make it a very promising material for electronics and optoelectronics applications. As with other as-synthesized materials, phosphorene exhibits defects such as vacancies, and these defects can affect the properties of the material significantly. The present work provides a detailed understanding of various vacancy defects (monoand di-vacancies) and their effect on the electronic and magnetic properties of phosphorene. We have also studied the effects of omnipresent non-metallic C/N/O and transition metal (TM) Fe/Co/Ni on the electronic and magnetic properties of phosphorene. We show that, for various adatom adsorbed pristine/defected phosphorene structures the magnetic moment can be tuned via the control of Fermi level. The magnetism for non-metallic adatom adsorbed pristine/defective phosphorene systems can be switch ON/OFF. TM adatoms provide extra flexibility by tuning the magnitude as well.

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