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Transition Metal and Vacancy Defect Complexes in Phosphorene
MUKUL KABIR, ROHIT BABAR, Department of Physics, Indian Institute of Science Education and Research, Pune 411008, India — Inducing magnetic moment in otherwise nonmagnetic two-dimensional semiconducting materials is the first step to design spintronic material. Here, we study the adsorption of transition-metals on pristine and defected phosphorene, within density functional theory. We predict that increased transition-meal diffusivity on the pristine phosphorene would hinder controlled magnetism. In contrast, point-defects anchor the transiton-metal to reduce metal diffusivity. The di-vacancy complex is more important in this context due to their increased thermodynamic stability over the mono-vacancy. For most cases, the defect-transition metal complexes retain the intrinsic semiconducting properties, and induce a local moment. We provide a simple microscopic model which describe the local moment of these transition metal and defect complexes.

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