

Intriguing aspects of Defect-Transition Metal Complexes in 2D Phosphorene

Mukul Kabir

*Department of Physics, and Centre for Energy Science,
Indian Institute of Science Education and Research, Pune*

Abstract

Inducing magnetic moment in otherwise nonmagnetic two-dimensional semiconducting materials is the key first step to design spintronic materials. In this talk, we will address the feasibility of inducing such local moment in single-layer phosphorene through 3d transition-metal (TM) doping without affecting its intrinsic semiconducting nature¹. While adjudicating on this subject, all previous studies conveniently neglected TM diffusion. However, we predict that increased TM diffusivity on pristine phosphorene would severely hinder any possibility of controlled magnetism, and thus any application. Here we propose that the point-defects will anchor metals, and exponentially reduce the diffusivity. We further argue that the divacancy complex is imperative in any practical purpose due to their increased thermodynamic stability over monovacancy. For most cases, the defect-transition metal complexes retain the intrinsic semiconducting properties, and also induce a local magnetic moment with large exchange-splitting and spin-flip energies, which are necessary for spintronic applications. Further, we provide a simple microscopic model to describe the local moment formation in these transition metal and defect complexes. Moreover, such metal absorption could completely alter the intrinsic electronic structure of the single-layer phosphorene, and may lead to exotic many-body physics².

[1] R. Babar and M. Kabir, Transition Metal and Vacancy Defect Complexes in Phosphorene: A Spintronic Perspective, *J. Phys. Chem. C* 120, 14991 (2016)

[2] R. Babar and M. Kabir, Engineering Robust and Intrinsic Kondo State in Semiconducting Phosphorene, Unpublished