

Abstract Submitted
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Origin of minute magnetic moments in spin-orbit coupled zigzag Phosphorene monolayer¹ KASHMIRI BARUAH, SUSHANT KUMAR BEHERA, PRITAM DEB, Department of Physics, Tezpur University, Tezpur-784028, India — We predict signature of induced magnetism in the electronic band structure of phosphorene monolayer in the presence of external magnetic field using *ab initio* density functional theory approach with inclusion of the spin-orbit coupling. We derive a tight-binding (TB) Hamiltonian [*Phys. Rev. B* **89**(201408), 2014] with minimum energy including spin-orbit coupling for two dimensional phosphorene monolayer. Applying an external magnetic field in antiferromagnetic order in the ranges where the structure is still stable, leads to the appearance of minute magnetic moments on phosphorous atom. Moreover, we examine the effect of spin polarization on zigzag phosphorene monolayer (PML) and the development of intrinsic moments of the corresponding active edge states when the system is simulated under external antiferromagnetic ordering. In case of PML, up to a value of $0.023 \mu_b$ per formula unit is few orders of magnitude larger than the ferromagnetic ordering of external magnetic field.

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