Magnetic property of porous black phosphorene layer: electric field and edge passivation effect

Arqum Hashmi*, M. Umar Farooq Umar and Jisang Hong
Department of Physics, Pukyong National University

Using the first principles method, we explored the possibility of long range magnetic ordering in two-dimensional porous phosphorene (PP) layer. The self-passivated pore geometry showed a non-magnetic state while the pore geometry with dangling bond at two zigzag edges with the distance of 7.7 Å preferred an anti-ferromagnetic ordering (AFM). The thermodynamic Gibbs free energy calculation revealed that the passivated system was more stable than the pristine PP layer and the O passivation was more favorable than the H passivation. The AFM state was persisted by the oxidation of the edge. Pore to pore magnetic interaction with a distance of 13.5 Å between two pores was found to be remarkably long ranged, and this emerges from the interactions between the magnetic tails of the edge states in the armchair direction. Interestingly, the long range AFM ordering changed to ferromagnetic (FM) ordering by external electric field. Our study implies a possibility that a long range FM ordering in whole 2D phosphorene sheet can be formed if a uniform pore exists in a phosphorene monolayer. The results are noteworthy in the interplay between electric field and electronic spin degree of freedom in phosphorene studies and may also open a promising way to explore phosphorene based spintronics devices.