Exploring Edge Magnetism in Oxygen-terminated zigzag Phosphorene Nanoribbons

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Abstract

Few layer black phosphorous, or phosphorene, has been attracting much attention during the last two years due to its very interesting semiconducting properties: a sizable band gap that ranges between 0.3 – 2 eV depending on the number of layers, and very high carrier mobilities of around 10^3 $cm^2V^{-1}s^{-1}$.[1] These properties makes black phosphorous one of the potential candidates, together with transition metal dichalcogenides, to lead the new generation of field-effect transistors.

Similarly to graphene, cutting few layer black phosphorous along different directions leads to edge geometries that can present either metallic or insulating behavior. These edges are highly reactive and tend to adsorb chemical species during the fabrication process modifying the electronic properties of the nanoribbon[2]. In particular, phosphorene nanoribbons are prone to be oxidized when handled in ambient air.[3]

Motivated by recent experimental observations of magnetism in oxidized black phosphorous antidot lattices[4], here we explore by means of first-principles calculations the possibility of inducing edge magnetic moments in zigzag phosphorene nanoribbons (ZZPNR). In contrast to previously reported calculations[5], we find that edge oxidation is key to achieve a strong edge magnetism out of this material, and that such magnetism is very different to that reported previously in zigzag graphene nanoribbons.

References

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Figures

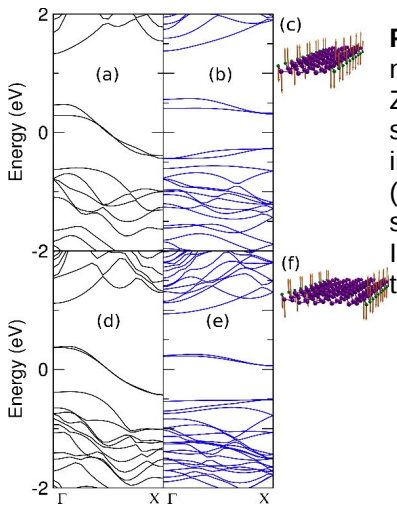

Figure Caption: Band structures of O-terminated zigzag phosphorene nanoribbons of different width. The upper panel correspond to 6l-ZZPNR and the lower one to the 10l-ZZPNR case. The Fermi level is set at E = 0. (a) and (d) are the band structures without spin. It is important to note the presence of a pair of midgap state bands. (b) and (d) are the same bands but including the spin polarization. (c) and (f) show the edge magnetic moments obtained in presence of oxygen. Interestingly, the magnetic moments order antiferromagnetically along the edges and ferromagnetically between adjacent P and O atoms.