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Bulk-Edge Correspondence of Monolayer Black Phosphorene

We present a theoretical study on the edge state of monolayer black phosphorene (MBP) and its topological origin. The MBP, a single atomic layer of phosphorus, was recently realized by the mechanical exfoliation [1]. The MBP has the buckled honeycomb lattice as shown in Fig. 1, and it has a semiconducting band structure with a finite band gap. It was theoretically shown that the nanoribbon of MBP has edge states for both zigzag edge and armchair edge [2](Fig. 2), in contrast to graphene which has edge states only for zigzag direction[3].

Here we investigate the edge states of MBP from the topological point of view. The study is based on the bulk-edge correspondence [4] between the electric polarization, which is defined by Berry phase, and the existence of localized states at the boundary of the MBP ribbon. We find that the zigzag and armchair edge states originate from the different atomic orbitals, and they have the different center positions in the electric polarization. We actually calculate the Berry phase and Wannier orbitals of MBP, and associate the existence of the edge states with nontrivial topological numbers.

References

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Figures

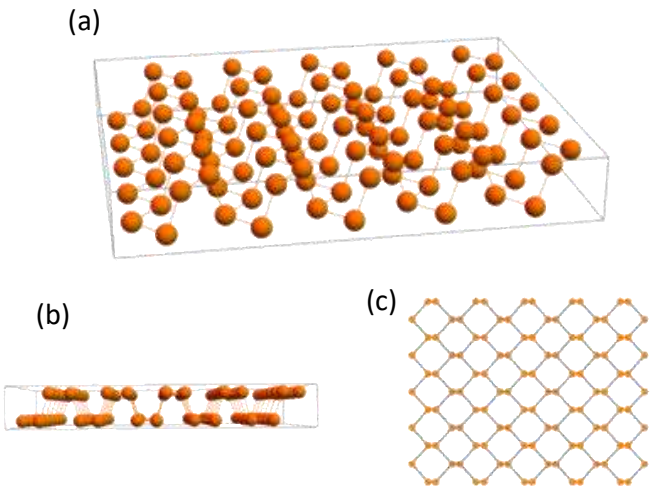

Fig. 1 monolayer black phosphorene

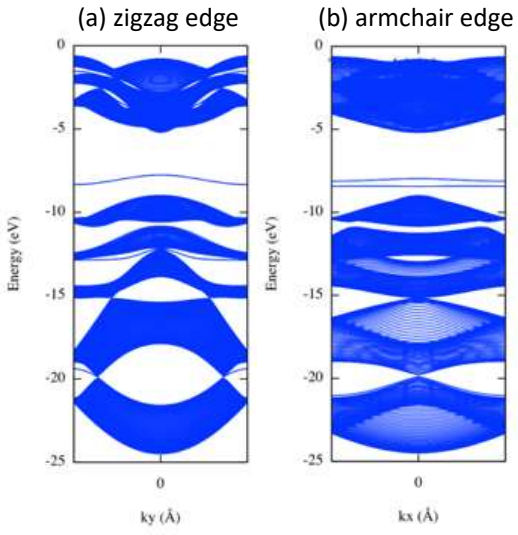

Fig. 2 The band structure