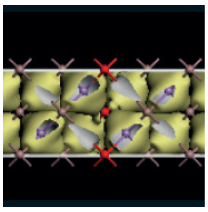

P:28 Electric field modulation of phosphorene nanoribbons' electronic properties

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Black phosphorus can be peeled down to a few monolayers by mechanical exfoliation [1]. The resulting two-dimensional structure is referred to as phosphorene. Single-layer phosphorene has a direct band gap of 1.45 eV at the Γ point of a rectangular Brillouin zone [1]. The gap remains direct in multilayer phosphorene, which makes this material suitable for electronic and optoelectronic applications [2]. The gap decreases with increasing number of layers and reaches a value of 0.3 eV in the bulk [3]. Furthermore, the puckered crystal structure in phosphorene leads to a high tunability of the bandstructure by strain and electric field. For instance, applying an electric field normal to the layers reduces the band gap due to a giant Stark effect [4]. The bandgap closes at a critical electric field, which marks a transition from a moderate-gap semiconductor to a semimetal. This bandgap closing is associated with the emergence of remarkable topological properties of biased phosphorene, as well as drastic changes in its electronic behavior [5]. Although the effect of electric field on electronic properties of multilayer layer phosphorene is un- derstood, the possible use of electric field mod- ulation in tuning the electronic characteristics of phosphorene-based nanostructures is fairly unex- plored.

In this paper, we investigate the tunability of the electronic properties of phosphorene nanoribbons (PNRs) by an external electric field. In PNRs, edge termination plays an important role in determin- ing electronic dispersion. In particular, PNRs with zigzag and skewed armchair edges are metallic while other edge terminations lead to insulating behavior. Focusing on metallic multilayer PNRs, we show that there are twofold-degenerate bands within the bulk gap, which govern electronic transport. The wave functions associated with these bands are localized near the ribbon edges. We propose a dual- edge-gate structure that affects these midgap states and drives the conducting-to-insulating transition in single layer and bilayer PNRs, thus enabling field- effect transistor action compatible with modern na- noelectronics, and potentially leading to new PNR- based devices.

The bandstrcture of bilayer phosphorene is de- scribed by a fifteen-nearest neighbors tight binding Hamiltonian [6]. The band structures of a bilayer zigzag PNRs (ZPNRs) is shown in Fig. 1(a). One can see the presence of midgap bands (red curves) completely detached from the other bands (shown in blue). For ZPNRs, each layer of phosphorene contributes one band of twofold-degenerate midgap states, making a total of four midgap states for bilayer ZPNRs. The ribbon is metallic, since the Fermi level (dashed line) passes through the midgap bands and is energetically far from the other states. Consequently, charge transport is governed by the midgap states. The probability density associated with the wave function for the midgap state at k = 0, marked in Fig. 1(a), is plotted along the width in Fig. 1(d). The probability density peaks near the edges and decays towards the bulk. Hence, charge transport in ZPNRs should be controllable by apply- ing a perpendicular electric field to the edges, where the electrons in midgap states around the Fermi level are likely to reside. When a perpendicular elec- tric field is applied to the edges of metallic PNRs [solid line boxes in Fig. 1(d)], it strongly affects the midgap state which have a high probability density right under the gate. This leads to a energetic shift of midgap states, proportional to the amplitude of the field [see Fig. 1(b)]. Increasing the field beyond a critical value leads to a complete separation of the midgap bads and a transition to insulating behavior [see Fig. 1(c)]. At the conference, we will discuss several device structures that rely on the tunability of midgap states by edge gates.

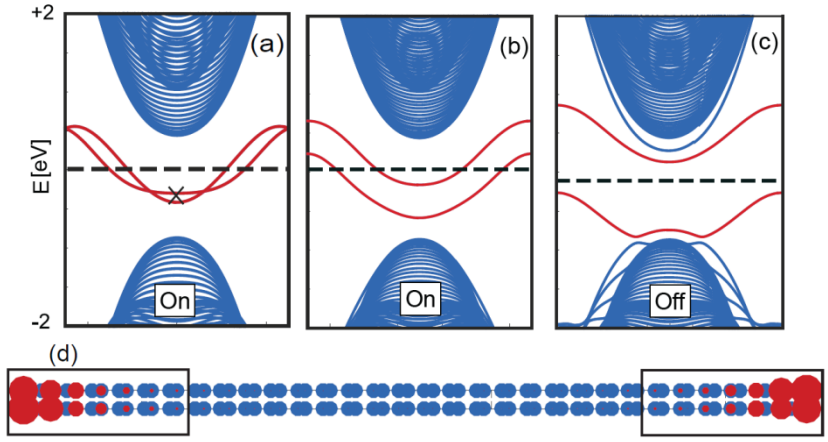

Fig. 1: (a) Band structure of an unbiased bilayer zigzag PNR. (b) Band structure of a zigzag bilayer PNR when the electric field applied to the edges is nonzero but below the critical value. (c) Band structure of zigzag bilayer PNR beyond the critical electric field. (d) On-site probability density of the state whose energy is marked by ”x” in panel (a). The red circles denote the probability density, with the larger circles representing higher probability density.

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