

Band Structure of Zigzag Phosphorene Nanoribbons: A Tight-Binding Hubbard Model

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The phosphorene nanoribbon (PNR), a one-dimensional analogue of phosphorene, has received considerable attention owing to its remarkable electronic properties. In particular, PNRs with zigzag edge termination [Fig. 1(a)] have been used as the underlying material for introducing novel nanodevices such as quantum switches, pseudospin valves, and spin filters [1-3]. The functioning of these devices is mainly based on electric- or magnetic-field tuning of the so-called midgap energy bands of zigzag phosphorene nanoribbons (ZPNR)s. The midgap bands are a pair of energy bands in electronic band structure of ZPNRs that cross the Fermi level and are far from the other energy bands. Near-equilibrium electronic transport in ZPNRs is governed by the midgap bands with little to no contribution from the other energy bands. This shows that a careful assessment of the ZPNR electronic properties and the performance of ZPNR-based electronic devices requires employing a model that accurately captures the electronic dispersion of midgap bands. The fifteen-nearest-neighbor tight-binding (TB) Hamiltonian proposed by Rudenko *et al.* [4] provides an accurate band dispersion for bulk phosphorene with respect to density functional theory (DFT) calculations. However, if used for ZPNRs, the TB model fails to capture the band structure and, in particular, the midgap-band energy dispersions accurately. In this work, we show that a Hamiltonian that includes the fifteen-nearest-neighbor TB Hamiltonian for bulk phosphorene along with a Hubbard mean-field-approximation term correctly captures the band dispersion of midgap bands in ZPNRs. In particular, the added Hubbard term dramatically modifies the midgap bands dispersion and upon choosing a proper Hubbard potential replicates the midgap bands dispersion obtained from our DFT calculations. The model presented here is a much-needed tool for careful investigation of electronic properties of ZPNRs and provides the platform for credible assessment of ZPNRs as a material for future developments in nanoelectronics.

[1] S. Soleimanikahnoj and I. Knezevic, *Phys. Rev. Applied*, **8**, 064021 (2017).

[2] S. Soleimanikahnoj and I. Knezevic, *JCEL*, **16**, 064021 (2017).

[3] W. Zhou et al., *Physica E*, **94**, 53–58 (2017).

[4] A. Rudenko et al., *Phys. Rev. B*, **92**, 085419 (2015).

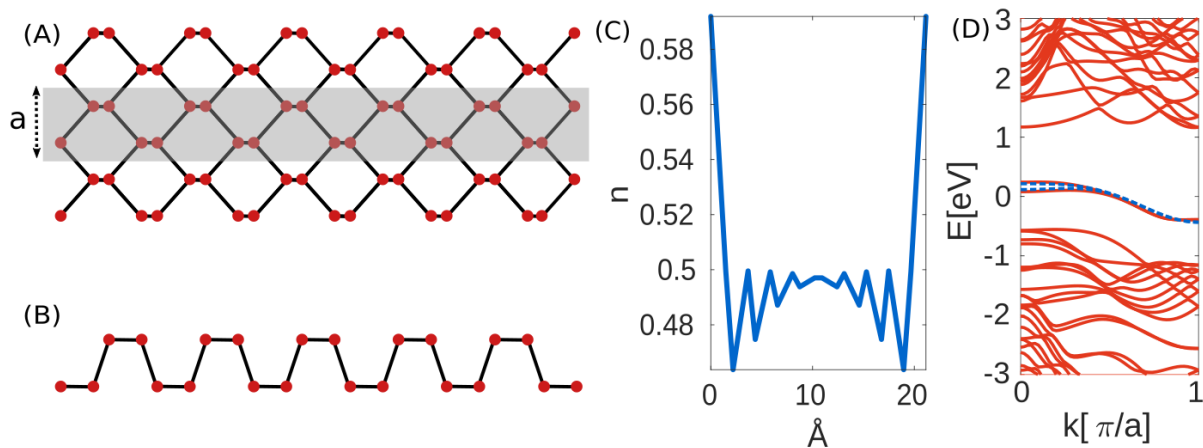


Fig.1: (a) Top view of a single-layer ZPNR. The left and the right edges are zigzag. The gray rectangle denotes a unit cell for this ZPNR. $a = 3.31 \text{ \AA}$ is the length of the unit cell. (b) Side view of a ZPNR. (c) Identical Up-spin and down-spin electron occupation per lattice site across the ribbon. The ribbon is in paramagnetic state. (d) Electronic band structures calculated for the ZPNR in panels (a),(b). Fermi level is at zero energy. Solid-line curves are the band structure from our DFT calculations. Dashed curves are the dispersion of midgap bands obtained from the proposed TB Hubbard model.