Gulf-edged zigzag graphene nanoribbons (ZGNR-Gs): potential nanoelectronic materials with structure-imposed electronic topology

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Gulf-edged zigzag graphene nanoribbons (ZGNR-Gs) are a family of graphene nanoribbons exhibiting interesting electronic and topological properties. As shown in Figure 1, they can be thought of as ZGNRs with 2*M*-1 connected C atoms removed on both zigzag edges in a periodical manner, and then saturated with H atoms again to maintain the trivalency of sp^2 carbons. If $M = 0$, the systems is a standard ZGNR[1] (Figure 1(a)), if $M = 1$, so-called cove-edge ZGNRs are formed[2-4] (Figure 1(b)), and if $M > 1$, the general family of ZGNR-Gs is formed (Figure 1(c)). Following our previous work[4], electronic and topological properties of ZGNR-Gs are discussed as highly controlled by their geometric structure. With four structural parameters and the inversion centre placed at unit-cell boundaries, all ZGNR-Gs can be easily classified as either metallic, topological or trivial semiconductors. Moreover, unlike cove-edged ZGNRs, there is no steric repulsion between hydrogen atoms at the edges, making ZGNR-Gs perfectly planar systems. The planarity of ZGNR-Gs make them better candidates for on-surface synthesis and electronic devices. Hence, we further investigated their properties with tight-binding (TB) method and density functional theory (DFT) and demonstrated possible structures, including hetero-junctions, for experimental considerations.

References

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Figures

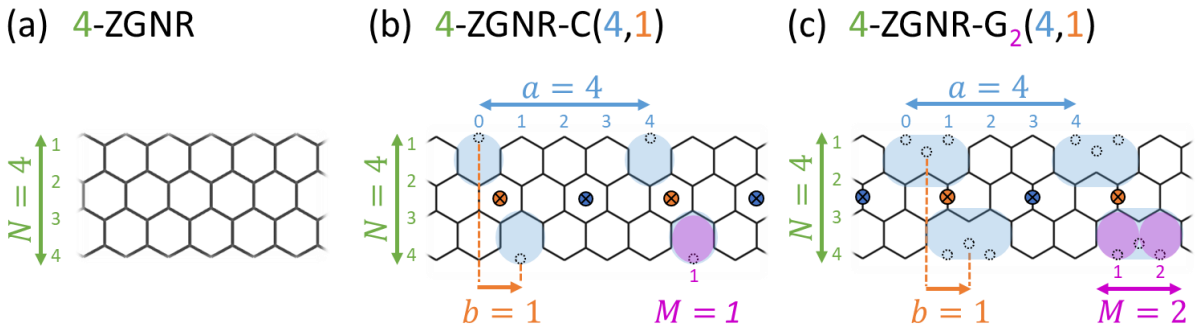

Figure 1: Schematic representations of (a) zigzag graphene nanoribbon (ZGNR) (b) cove-edged ZGNR (ZGNR-C) and (c) gulf-edged ZGNR (ZGNR-G). Width N, gulf size M, gulf distance a, and offset b are structural parameters. Orange and blue cross dots label two distinguish inversion centres in ZGNR-Cs and ZGNR-Gs.