Relationship between structural and electronic topology in cove-edged graphene nanoribbons

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Cove-edged zigzag graphene nanoribbons (ZGNR) take their name from zigzag edges with coves formed by removal of one (or more) terminal CH group per length unit on each side of the ZGNR. [1] This structural element controls the electronic properties of these materials. [2] Previously, Lee et al.[3] have shown that cove-edged ZGNRs can be topologically non-trivial depending on their widths and unit cell type. In our work, based on three structural parameters that unambiguously characterize cove-edged ZGNR (Figure 1), we present a general classification scheme, which connects the geometric structure with electronic properties and topology, i.e. whether cove-edged ZGNRs are metallic, topological insulators or trivial semiconductors. This classification scheme is derived from tight-binding calculations. We further show possible ribbon terminations, which should give guidance for future synthetic efforts to realize new topological cove-edged ZGNR with large band gap and to realize topologically protected edge states in these systems.

References

[1] Liu, Junzhi et al., JACS, 137 (2015), 6097-6103.
[2] Wang, Xu et al., JACS, 144 (2021), 228-235.
[3] Lee, Yea-Lee et al., Nano Lett., 18 (2018), 7247-7253.

Figures

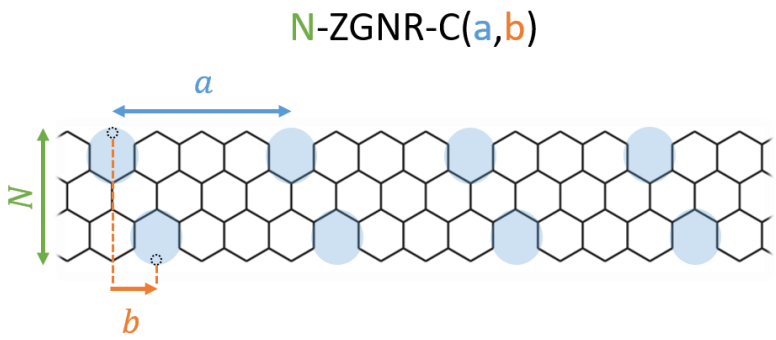

Figure 1: Three structural parameters characterizing cove-edged ZGNR: width N of the ZGNR, the distance a between coves on the same edge, and the offset b between adjacent coves on opposite edges of the ribbon.