Deciphering the electronic structure of 5-armchair graphene nanoribbons and its topological end-states

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5-armchair graphene nanoribbons (5-AGNRs) are the narrowest from the 3*p*+2 family, with *p* an integer, which are predicted to have the smallest band gaps compared to the other AGNR families [1]. They have been already successfully synthesized with atomic precision, for instance via on-surface synthesis methods [2, 3]. Nevertheless the electronic structure measurements show a substantial discrepancy, with reported band gap ranging from 0.1 eV up to 2.8 eV. Here we performed an extensive characterization of the electronic structure of 5-AGNRs by combining scanning tunneling microscope (STM) and spectroscope (STS) measurements, recorded on both Au(111) substrate and decoupling NaCl layer, with density functional theory (DFT) calculations. We demonstrated the presence of in-gap "end"-states at the termini of finite ribbons that become degenerate and single occupied after reaching a certain ribbon length, explaining the apparent disagreement on the assignment of the band gap on previous studies. We show that these end-states are topological in nature and that they have magnetic character, both theoretically and via STM-tip lifting experiments.

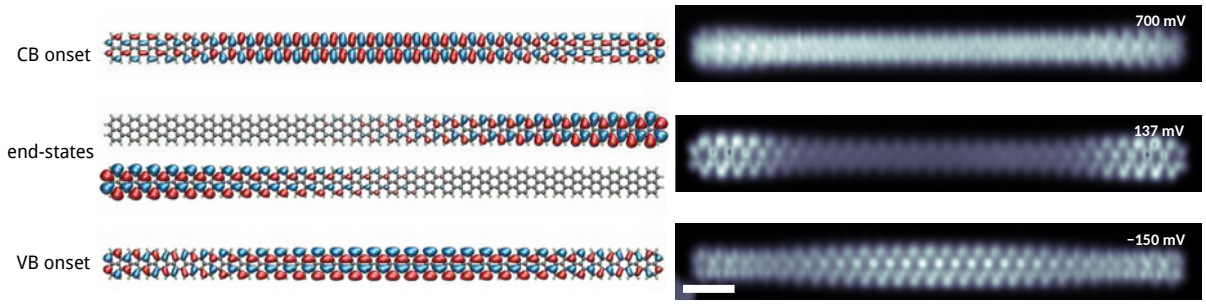

Figure: (left) DFT-calculated 30 unit-cell long 5-AGNR molecular orbitals corresponding to the valence band (VB) and conduction band (CB) onsets and in-gap end-states; (right) Measured constant height dI/dV images (scale bar 1nm).

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[2] A. Kimouche *et al.*, Nat. Commun. **6**, 10177 (2015)
[3] H. Zhang *et al.*, J. Am. Chem. Soc. **137**, 4022 (2015)