Haiku graphene nanoribbons with tunable topology

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Recent advances on surface-assisted synthesis open the door to engineering topological phases in atomically precise graphene nanoribbons (GNRs). However, to fully exploit their potential, a rational design is needed to achieve GNRs with optimal properties for spintronics or quantum computing applications.

Here we explore a novel family of armchair GNRs, which we name haiku-AGNRs, consisting of 5- and 7-atom wide segments. Based on ab initio simulations, we predict a tunable topological phase dependent on the density of the 7-atom wide segments, with the concomitant emergence or quenching of topological end and interface states [1]. Moreover, we derive a generalized Su-Schrieffer-Heeger (SSH) model that allows to treat haiku-AGNRs of technologically relevant lengths, thus providing valuable information for the devise of future experiments. Finally, we also present some results for B-doped periodic haiku-AGNRs in comparison with experiments performed at Prof. Pascual's lab in nanoGUNE, San Sebastian (Spain) [2].

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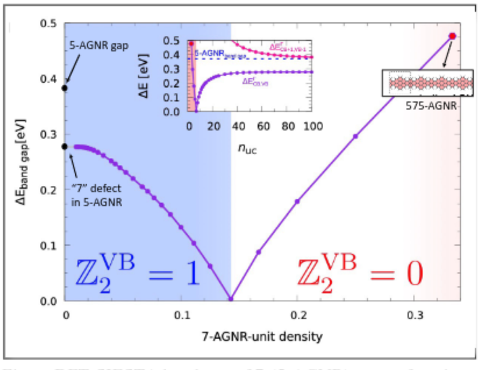

Fig. **1**. DFT-SIESTA band gap of 7-(5-AGNR)$_{nuc}$ as a function of the density ($1/n_{uc}$) of 7 widenings for periodic haiku ribbons with supercells containing n_{uc} 5-AGNR unit cells. The band gap closes separating the topological and the trivial phases. The inset highlights the presence of a defect level localized around isolated 7-widenings for very dilute systems. Notice that the labels 575-AGNR and 7-(5-AGNR)$_3$ denote the same system.

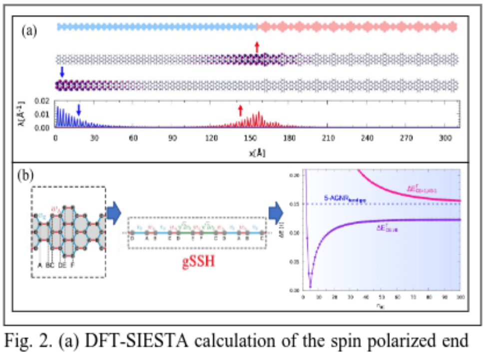

Fig. 2. (a) DFT-SIESTA calculation of the spin polarized end states appearing at the boundaries of the 5-AGNR portion of a mixed 5-AGNR/575-AGNR long ribbon. (b) Same as the inset in Fig. 1 but computed with a simple SSH model derived from a first-neighbors π-tight-binding description.