Interface and spin states in armchair graphene nanoribbon junctions

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We present a theoretical analysis, by means of both a pi-tight-binding (TB) mean-field Hubbard model and density functional (DFT) calculations, of interface states emerging at junctions between armchair graphene nanoribbons (AGNRs) with varying widths. By exploring diverse width combinations and alignments, we demonstrate that predicting the number of interface states requires considerations beyond the topological classification alone. Specifically, the width differences and carbon-carbon bonding pattern at the interface play crucial roles (e.g., see Fig. 1 below). We further examine how geometrical deformations (modelled by changing the TB parameters) affect their topological properties and, consequently, the interface states formed. With the help of our open-boundary-conditions self-consistent calculations, we explore the magnetic moments appearing at the interface and how they depend on the number of localized interface-states present. Our findings build on previous work exploring the effect of the topology of the band structure of AGNRs and the appearance of end-states and spin-moments at AGNR boundaries [1,2,3,4,5,6], and contribute to understanding and engineering localized states in AGNR heterojunctions, providing guidelines for manipulating electronic and magnetic properties through structural design.

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References

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Figures

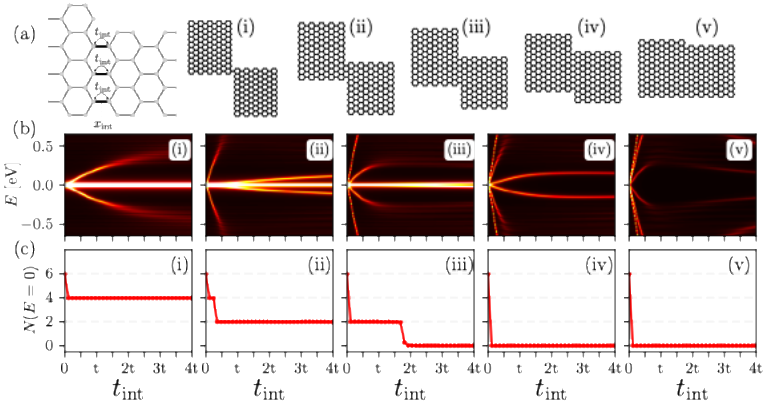

Figure 1: Interface states analysis at type-I 21-19-AGNR heterojunction with different vertical alignments. (a) Sketch of the different structures; (b) DOS in the +/-0.65 eV interval as a function of the inter-ribbon hopping; (c) Number of interface states at zero energy (defined by the DOS integral in the +/-10 meV interval.