Interface and spin states in armchair graphene nanoribbon junctions

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Armchair graphene nanoribbons (AGNR) exhibit a fascinating topological nature, which has become a major area of focus in recent years [1]. For instance, wide AGNRs host multiple topological transitions, resulting in the appearence of multiple end states (ES) [2]. In this sense, AGNR heterojunctions provide an interesting platform to explore rich physical phenomena arising from the interplay of topology and geometry, since interfaces between topologically distinct AGNRs are predicted to host half-filled, localized bound states within the energy gap [3].
Here we present a theoretical study of interface states and spin configurations in AGNR heterojunctions of varying widths and alignments. We analyze how interface bonding, width mismatch, and geometrical deformations influence the number and nature of localized electronic states. We show that the number of interface states is directly related to the difference of ES of each AGNR. We also demonstrate that predicting interface states requires consideration beyond topological classification, as the number of carbon-carbon bonds at the junction plays a crucial role. Furthermore, we explore the impact of Coulomb interactions, revealing that spin polarization at the interface is directly linked to the number of localized states. By providing a set of predictive ”rules of thumb,” this study contributes to the design of AGNR-based circuits with tunable electronic and magnetic properties [4].

References

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