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Edge effects in Bilayer Graphene Nanoribbons[1] MATHEUS P. LIMA, ADALBERTO FAZZIO, ANTONIO J. R. DA SILVA, Physics Institute - University of Sao Paulo — We investigate the geometrical and electronic structure of zigzag bilayer graphene nanoribbons (B-ZGNR), with widths that range from $w = 0.6$ to $w = 4.5$ nm. The layers are in the Bernal stacking, which means that there are two types of C atoms, those that are positioned above the center of the hexagons of the other layer, defining a B-sublattice, and those right on top of the C atoms of the other layer, forming an A-sublattice. When we cut the layer along the zigzag edge, there are two possible alignments, α, where the outermost edge atoms belong to the A- sublattice, and β, where the outermost edge atoms belong to the B-sublattice. Thus, only the inter-layer edge interaction differs. We found that the α alignment is energetically favorable, with an inter-layer edges attraction, whereas for the β there is an inter-layer edges repulsion. These edge-related forces cause a deviation from the exact Bernal stacking, resulting in a non-monotonic behavior of the energy gap with the width w for the α B-ZGNR, with a maximum value at $w \approx 3.5nm$. This is a consequence of the competition between bulk and strongly attractive edge interactions. All results were obtained using density functional theory calculations with the inclusion of parametrized van der Waals interactions.

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