

Abstract Submitted  
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**Structural and magnetic stabilization of edges of layered zigzag graphene nanoribbons**<sup>1</sup> JUN-QIANG LU, University of Puerto Rico at Mayaguez, YANNA ZHANG, XIAO-LI LU, YONGJIN JIANG, BOTAO TENG, Zhejiang Normal University — We report first-principle study on structural and magnetic stabilization of bilayer and trilayer zigzag graphene nanoribbons with two different edge alignments. Our results showed that (I) structural deformation only happens in layered ZGNRs with  $\alpha$ -alignment edges; the ground state of the bi-layered ZGNR with  $\alpha$ -alignment edges is nonmagnetic; while that of the tri-layered ZGNR with  $\alpha$ -alignment edges is magnetic even with structural deformation; (II) layered ZGNRs with  $\beta$ -alignment edges are always flat and have magnetic ground states; (III) the intra-layer magnetic order in a layered ZGNR is always antiferromagnetic near each edge regardless of edge alignment and number of layers, as long as its ground state is magnetic; (IV) with the increasing of the number of layers, the magnetic order of the ground states can be complex and non-collinear.

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