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An Ab-initio Study of Folded Armchair Graphene Nanoribbons
ADAM IAIZZI, Ithaca College, NAM LEE, LILIA WOODS, University of South Florida — We present a first principles approach to the characterization of armchair graphene nanoribbons folded along their long axis using density functional theory, along with ultrasoft psuedopotentials and the local density approximation for the exchange-correlation functional. Based on past studies, we anticipate that folding nanoribbons will produces changes in the band structure, possibly turning normally semiconducting nanoribbons into metallic nanowires. We determine the energy required to produce a number of different folded structures from nanoribbons as well as the energy and band structure as a function of width in single-fold structures. Ribbons as narrow as 13 carbon atoms formed stable folded structures.

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