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Role of edge states in graphene nano-ribbons: - DFT studies
SUMIT SAXENA, TREVOR A. TYSON, Dept. of Physics, New Jersey Institute of technology, Newark, NJ — We present first principle calculations to study the effect of edge states in graphene nano-ribbons. Spin restricted calculations for graphene nano-ribbons were performed using ground state density functional theory. The plot of electron localization function corresponding to the edge dangling bonds has revealed highly reactive edge states in graphene nano-ribbons. The reactivity of the nano-ribbons with respect to the edge structure is discussed. This study has been supplemented by band structure studies in armchair and zigzag edged graphene nano-ribbon systems. This work is supported in part by NSF DMR-0512196.

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