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Structural Corrugation of Graphene Oxides (C_2O Phase)[1]
UDAGAMAGE WIJEWARDENA, Georgia State University, SHIRNECE BROWN, Clark Atlanta University, RAMESH MANI, Georgia State University, XIAO-QIAN WANG, Clark Atlanta University — Although there are a lot of theoretical investigations on Graphene oxides (GO) configurations,[2,3,4] an in-depth explanation of the experimental observations in GO is still not there. The challenge is connected to inhomogeneous nature of the oxidation. We studied the structural, electronic, and vibrational properties of graphene oxide employing a particle swarm optimization search along with density functional theory calculations. Here we report a novel low-energy semiconducting configuration for the C_2O phase of graphene oxide that consists of a combination of 1,2 and 1,3-epoxides as well as carbonyl functional groups running along the armchair direction. A thorough examination of the corrugation and bonding reveals unique features of the new conformation which are in reasonable agreement with experimental observations. Our findings shed light on structural and electronic properties that are important for future improvement of graphene-based nanodevices.

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