Abstract Submitted
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Density functional theory calculations on the effects of oxygen adsorption on graphene in the presence of defects FAISAL MEHMOOD, WEIJIE LU, JOHN J. BOECKL, RUTH PACHTER, Air Force Research Laboratory, Materials & Manufacturing Directorate, Wright-Patterson Air Force Base, Ohio 45433 — Density functional theory calculations were carried out to investigate effects of oxygen adsorption on the electronic and optical properties of single layer graphene (SLG) in the presence of defects. Stone-Wales and single and double vacancy defects, also including the 555-777 and 5555-6-7777, were considered. Analysis of changes upon oxygen adsorption will be reported in detail, regarding morphology, binding energies and electronic structure, as compared to pristine SLGs, for pure GGA, hybrid and van der Waals corrected functionals. Nudged elastic band calculations of various pathways were investigated in order to understand the diffusion and dissociation of oxygen on SLGs in the presence of defects. Calculation of the optical response carried out at different levels of theory will be discussed, using both hybrid and long-range corrected hybrid functionals, with consideration of comparison to experimental characterization. Finally, implications of the effects of oxygen adsorption on graphene in the presence of defects for aspects of catalyst-free growth or electron transport will be suggested.

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