Reaction Mechanisms of Chemical Reduction of Graphene Oxide by Sulfur-Containing Compounds：A DFT Study

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Based on density functional calculations, the mechanisms were identified as reducing epoxide and hydroxyl groups of GO with sulfur-containing compounds as a reducing agent. We also examined the reaction mechanisms of a series of GO structures with different coverage rates and OH:O ratios by sulfur-containing compounds. We provide atomic-level elucidation for the deoxygenation of GO, characterize the product structures, and suggest how to optimize the reaction conditions further.