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Computational Studies for Reduced Graphene Oxide in Alcohol- and Hydrogen-Rich Environments RAMIN ABOLFATH, CHENG GONG, MUGE ACIK, YVES CHABAL, KYEONGJAE CHO, University of Texas at Dallas — We employ *ab-initio* molecular dynamic simulations to analyze the chemical reaction mechanisms for the oxygen removal process of graphene oxide upon annealing in the presence of water molecules and compare various thermal pathways in alcohol- and hydrogen-rich environments. Our first principles calculation shows damage-repair mechanisms of sp^2-C bonds in the etch holes of reduced graphene oxide and formation of dangling and/or sp^3-C bonds. The initial oxygen-abstraction results in the propagation of broken bonds and multi-site sp^2-C bond damage driven by the cascade of chemical reactions. The interplay between the environmentally induced damages and self-repair mechanisms of sp^2-C bonds determines the quality of the sheets after chemical treatments in alcohols or with hydrogen-rich environment. Water molecules form C=O and C-H bonds in the etch holes. We show that the alcohol- and hydrogen-rich environment provide an efficient transformation of C=O to the C-O bonds, and the removal of oxygen that is rarely observed with alcohol-rich environment alone.

Ramin Abolfath
U. Texas at Dallas

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