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Atomic structure of progressively reduced graphene oxide VIVEK SHENOY, AKBAR BAGRI, RASSIN GRANTAB, NIKHIL MEDHEKAR, Brown University — Using molecular dynamics simulations, we have studied the evolution of epoxy and hydroxyl functional groups on graphene oxide (GO) during high temperature thermal reduction. We find that the reduced GO sheets are characterized by a large number of stable hole-like defects formed by breaking of C-C bonds in the basal plane. These defects are always decorated by the carbonyl (C=O) groups and are formed due to the strain in the basal plane created by epoxy and hydroxyl functional groups that are located close to each other. With very few exceptions, the carbonyl groups that are observed in Raman spectroscopy and other experimental studies are generally attributed to the C=O terminations of the edges. However, our study using first principles calculations and a reactive force field approach clearly shows that the formation of carbonyl groups within the graphene basal plane is energetically favorable compared to other well-known functional groups such as epoxies and ethers. We have identified the specific reaction mechanisms that lead to the formation of these holes starting from particular initial configurations of epoxy and hydroxyl functional groups. These configurations can be readily found on GO sheets with random distribution of epoxy and hydroxyl groups and do not require an ordered arrangement of any particular functional groups.

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