Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Kinetic and chemical stability of graphene oxide layers SI ZHOU, Georgia Institute of Technology, School of Physics, ANGELO BONGIORNO, Georgia Institute of Technology, School of Chemistry and Biochemistry, BONGIORNO'S LAB TEAM — Chemical functionalization of graphene holds great promise to open new applications of graphene in technology. Here we combine density functional theory (DFT) and Monte Carlo calculations to study both the stability and structure of graphene layers functionalized with epoxide and hydroxyl species. Our calculations show that sparse functionalizations of graphene are unstable in air at room temperature. However, oxygen groups diffuse and are prone to form dense agglomerates. To investigate these phenomena, we use DFT calculations to first map the interaction of functionalities on graphene, and then to device a simple energy scheme to both compute the Gibbs free energy of formation of arbitrary functionalizations of graphene and predict the structure resulting from diffusion and agglomeration processes. We find that the stability of graphene oxide increases for increasing both the O:C ratio and ageing time. The structure of the aged layers consists of a non-homogeneous phase of highly oxidized regions surrounded by areas of pristine graphene. Within the oxidized domains, formation of energetically stable motifs reduces the likelihood of occurrence of decomposition reactions, thereby enhancing the kinetic stability of the oxidized layer.

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Date submitted: 12 Nov 2013 Electronic form version 1.4