

Abstract Submitted  
for the MAR10 Meeting of  
The American Physical Society

**Atomic and Electronic Structure of Graphene Oxide**<sup>1</sup> SUMIT SAXENA, TREVOR A. TYSON, Department of Physics, New Jersey Institute of Technology, SHOBHA SHUKLA, Department of Electrical Engineering, University at Buffalo, State University of New York at Buffalo, EZANA NEGUSSE, Department of Physics, Montana State University, HAIYAN CHEN, Department of Physics, New Jersey Institute of Technology, JAIMIN BAI, Oak Ridge National Laboratory, P. N. PRASAD, Department of Chemistry, University at Buffalo, State University of New York at Buffalo — We have investigated the atomic structure of graphene oxide by DFT calculations. Our spin restricted ab-initio density functional calculations have shown that the oxygen link to the graphene basal plane using epoxide bonds. The flat graphene sheets are found to deform by buckling due to formation of C – O – C linkages normal to the plane of the graphene sheets. The calculations were compared with x-ray diffraction and x-ray spectroscopic measurements. Tentative models of the structure are proposed based on the combined DFT and experimental data.

<sup>1</sup>This work is supported in part by NSF DMR-051219.

Sumit Saxena  
Department of Physics, New Jersey Institute of Technology

Date submitted: 18 Nov 2009

Electronic form version 1.4