Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Graphene on Silicon Dioxide: Band gap modulation via substrate surface chemistry PHILIP SHEMELLA, SAROJ K. NAYAK, Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, Troy, NY — We have studied the electronic structure of graphene deposited on a SiO_2 surface using density functional methods. The band structure of the graphene monolayer strongly depends on surface characteristics of the underlying SiO_2 surface: for an oxygen-terminated surface, the monolayer exhibits a finite energy band gap while the band gap is closed when the oxygen atoms on the substrate are passivated with hydrogen atoms. We find that at least a graphene bilayer is required for a near zero energy gap when deposited on a substrate without H-passivation. Our results are discussed in the light of recent experiments.

Philip Shemella

Date submitted: 21 Nov 2008 Electronic form version 1.4