

Abstract Submitted  
for the MAR11 Meeting of  
The American Physical Society

**The doping mechanism in graphene** RAZVAN A. NISTOR, DENNIS M. NEWNS, GLENN J. MARTYNA, IBM T. J. Watson Research Center — Doping graphene by adsorbing chemical species on its surface is one way to control the carrier concentration of this novel material. Using large-scale *ab initio* simulations and electronic structure calculations, we show the carbon layer acts as a metal catalyst facilitating the disproportionation reaction of adsorbed chemical species on its surface. This reaction leads to the formation of charge transfer complexes which thereby dope the graphene. We also investigate the charge transfer in graphene-silicon and defected graphene-silicon-oxide interfaces. Our microscopic understanding of the doping mechanism in graphene, which brings to light the catalytic power of the material, is important in the development of carbon-based electronics.

Razvan Nistor  
IBM T. J. Watson Research Center

Date submitted: 15 Nov 2010

Electronic form version 1.4