Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Point and Line Defect-mediated Binding of Metal Nanoparticles to Graphene IOANNA FAMPIOU, ASHWIN RAMASUBRAMANIAM, University of Massachusetts Amherst — The synthesis of well dispersed, size-controlled metal nanoclusters on carbon supports is highly desirable since such clusters have been shown to possess enhanced catalytic activity and selectivity in a variety of chemical reactions. However, metal clusters interact rather weakly with defect-free carbon supports and can coarsen over time leading to loss of surface area and thence catalytic activity. Defects in carbon supports play an important role in enhancing metal-carbon bonding, thereby reducing the propensity for cluster coalescence. Using a combination of density functional theory and empirical potential simulations, we examine the interaction of metal Pt clusters with point (vacancies, holes) and line defects (dislocations, grain boundaries) in graphene. We compare and contrast the binding energies and diffusivities of clusters bound at defects and on pristine graphene. Our results suggest possible avenues for controlling the dispersion of Pt catalyst clusters on carbon supports via defect engineering.

Ashwin Ramasubramaniam
University of Massachusetts Amherst

Date submitted: 19 Nov 2010 Electronic form version 1.4