

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Opening of slit-shaped pores from bending of graphene walls¹

MATTHEW CONNOLLY, University of Missouri-Columbia, CARLOS WEXLER, University of Missouri - Columbia — Graphene has gained particular interest in many areas of research including adsorption. Recent studies have shown deformations in graphene resulting from the pressure of intercalants or edge bonds. In this talk, the opening of slit shaped pores from uniaxial bending of the graphene walls of the pore is examined. The energy functional associated with the deformation from equilibrium shape is minimized to obtain an optimal shape. The minimization is done analytically for a simple model and numerically for various graphene-graphene interaction potentials. The strain induced from bending has been shown to effect the hybridization of carbon bonds within the graphene sheet. The effect of any increase in the number of binding sites due to bending as well as hybridization effects on excess adsorption are studied by Molecular Dynamics simulations.

¹This material is based upon work supported in part by the Department of Energy under Award Nos. DE-FG02-07ER46411, DE-FG36-08GO18142 and DE-AC02-06CH11357.

Matthew Connolly
University of Missouri-Columbia

Date submitted: 17 Nov 2010

Electronic form version 1.4