Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Confinement effects on chemical reactions in nanostructured carbon materials AARON GEORGE, Department of Physics, North Carolina State University, MILEN KOSTOV, ERIK SANTISO, KEITH GUBBINS, Department of Chemical Engineering, North Carolina State University, Raleigh, NC 27695, MARCO BUONGIORNO NARDELLI, CHIPS and Department of Physics, North Carolina State University; CCS-CSM, Oak Ridge National Laboratory — Chemical reactions are frequently carried out in nano-structured media, such as micellar or colloidal solutions, nano-porous media, hydrogels or organogels, or in systems involving nano-particles. Nanostructured environments have been shown to enhance reaction rates through a variety of catalytic effects, such as high surface area, interactions with the nano-structure or confinement. In this work, we have used state-of-the-art electronic structure techniques to study the prototypical example of the hydrogen-producing reaction of formaldehyde dissociation ($H_2CO \rightarrow H_2 + CO$) within various configurations of a graphitic pore. Using the Nudged Elastic Band (NEB) method for transition states analysis, we have found that the activation energy of the dissociation can be influenced by the presence of a graphitic pore. In particular, while a graphene surface reduces the activation barrier for the reaction, this catalytic effect is enhanced by the presence of two planar sheets, which mimic the geometry of a nano-pore. These findings will be discussed in terms of the charge transfer and/or polarization mechanism associated with the catalytic process.

Aaron George
Department of Physics, North Carolina State University

Date submitted: 22 Mar 2013 Electronic form version 1.4