Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Catalytic selectivity of Transition Metal Functionalized 2-Dimensional Graphene SHYAM KATTEL, BORIS KIEFER, Physics Department, New Mexico State University, PLAMEN ATANASSOV, Department of Chemical and Nuclear Engineering, University of New Mexico — Energy production is expected to be one of the most significant challenges in the 21^{st} century. Therefore it is important to develop and explore routes that reduce the dependence on fossil fuels and ensure energy security for future generations. We have performed DFT calculation of binding of small molecules on graphene sheets as mediated by chemisorbed transition metals (TM). The preliminary results show that molecules like N_2, CO and O_2 form stable bonds with the TM. In contrast, H_2O_2 decomposes and forms a stable TM-$(OH)_2$ complex. These two different behaviors may explain selectivity of some carbon based catalytic materials toward O_2. In either case the charge density is affected only locally and hence electronic transport properties are likely dominated by the underlying carbon structure. However, the results also support the notion that the use of the 6 – 8 orders of magnitude more abundant 3^{rd} row TM's in energy generation may form a viable alternative to expensive and comparatively rare transition elements such as platinum.

Shyam Kattel

Date submitted: 19 Nov 2009 Electronic form version 1.4