

Abstract Submitted  
for the MAR11 Meeting of  
The American Physical Society

**Oxygen reduction activity of BN decorated bulk defects in graphene** SHYAM KATTEL, BORIS KIEFER, Physics Department, New Mexico State University, PLAMEN ATANASSOV, Chemical and Nuclearing Department, University of New Mexico — We use Density-Functional-Theory to investigate the interaction between  $O_2$  and  $H_2O_2$  with co-doped bulk BN defects in graphene. The results show that the mixed defects are thermodynamically stable in contrast to the nitrogen only defects that need a transition metal for stabilization. The interaction between  $O_2$  and  $H_2O_2$  and the BN defects are found to be very different:  $O_2$  is adsorbed as a molecule on boron with a bond length increase of  $\sim 20\%$ .  $H_2O_2$ , on the other hand, is predicted to adsorb dissociatively to form  $B(OH)_2$ . The predicted binding energy (BE) of  $O_2$  is similar to the N only defects. This observation suggests that BN defects promote the reduction of  $O_2$  to  $H_2O_2$ . However, we also found that the binding energy per OH is  $\sim 75\%$  higher than the corresponding BE for the N only defect. Thus, restoring the catalytic site through OH removal is more difficult as compared to the N only defect. This implies that bulk BN defects are most likely less active than N only defects and edge BN defects which enhance ORR.

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Date submitted: 20 Dec 2010

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