Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Enhanced catalytic reactivity of graphene and h-BN by selective substitution JUNHAO LIN, BIN WANG, SOKRATES PANTELIDES, Physics department, Vanderbilt University — Recent experiments have demonstrated that nitrogen-doped graphene is an efficient metal-free catalyst for the oxygen reduction reaction in fuel cells, but the underlying mechanism still needs to be explored. Using first-principles calculations, we find that in N-doped graphene oxygen molecules can only dissociate at carbon atoms surrounded by nitrogen. We attribute the enhanced chemical reactivity of these carbon atoms to the strong localized states near the Fermi level, which results from misalignment of pz orbitals of nitrogen and carbon atoms. We further show that the dissociation of oxygen molecules can also occur in hydrogenated graphene and h-BN based on the same mechanism. Therefore, we propose a generic way for functionalization of graphene to achieve enhanced catalytic reactivity.

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Date submitted: 17 Dec 2012 Electronic form version 1.4