Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Silicon and phosphorus dual doped graphene as the promising metal-free catalysts for oxygen reduction reaction[1] ZHANSHENG LU, SHUO LI, ZONGXIAN YANG, Henan Normal University, RUQIAN WU, University of California Irvine — The pathways of oxygen reduction reaction (ORR) on the metal-free silicon and phosphorus dual doped graphene (Si-P-G) catalyst are systematically investigated based on the dispersion-corrected density functional theory (DFT-D) method. It is found that the Si-P-G can be stable at high temperature from the first-principles molecular dynamics simulation and the local region of dopants displays an important role in the adsorption and reduction of oxygen. Both of the four-electron O_2 direct dissociation and the two-electron OOH dissociation pathways are probable for ORR on the Si-P-G, while the latter pathway is mainly followed by the pathway of the OH hydrogenation into H_2O. For the OOH dissociation pathway, the hydrogenation of O_2 to OOH is the rate-limiting step with a rather small barrier energy of 0.66 eV. The current results indicate that the Si-P-G is a novel metal-free catalyst for ORR, and which is comparable to that of the Pt catalyst.

[1]Work was supported by the National Science Foundation Center for Chemical Innovation on Chemistry at the Space-Time Limit (CaSTL) under Grant No. CHE-1414466, and the National Natural Science Foundation of China (Grant Nos. 51401078, and 11474086)

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Date submitted: 06 Nov 2015 Electronic form version 1.4