B-Doped Graphene as Catalyst to Improve Charge Rate of Lithium-Air Battery

Xiaodong Ren, Jinzhen Zhu, Fuming Du, Jianjun Liu*, Wenqing Zhang

State Key Laboratory of High Performance Ceramics and Superfine Microstructures, Shanghai Institute of Ceramics, Chinese Academy of Sciences, Shanghai 200050, China

* Corresponding email: jliu@mail.sic.ac.cn

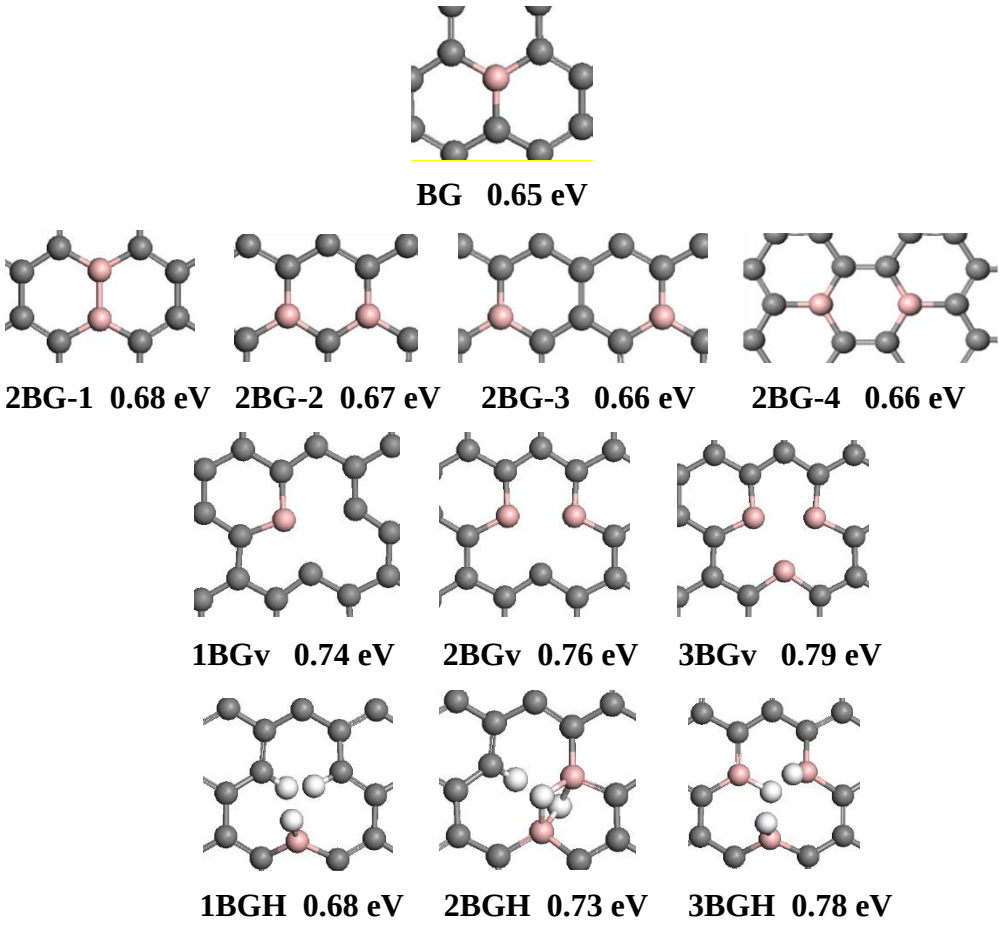

Figure S1, several calculated structures for B-doped graphene model and their formation energies, which are calculated by $F = \frac{1}{N}[E_{slab} - N_C U_C - N_B U_B - N_H U_H]$, with N=N_C+N_B, $U_C = E_{CH_4} - 2E_{H_2} - \Delta G_{CH_4}$, $U_B = E_{BH_3} - 3/2E_{H_2} - \Delta G_{BH_3}$, and $U_H = 1/2E_{H_2}$; N_C and N_B are total number of C and B atoms, respectively; E_{slab} is the total energy calculated for the slab model; E_{CH_4}, E_{BH_3}, and E_{H_2} are calculated total energy for CH_4, BH_3 and H_2; $\Delta G_{CH_4}$and $\Delta G_{BH_3}$are experimental synthesis enthalpies for CH_4, and BH_3.[1]

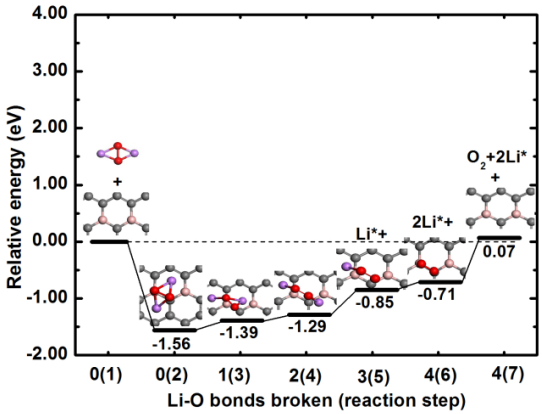

Figure S2, The calculated free energy profiles of Li_2O_2 decomposition reaction paths on 2B-doped graphene.

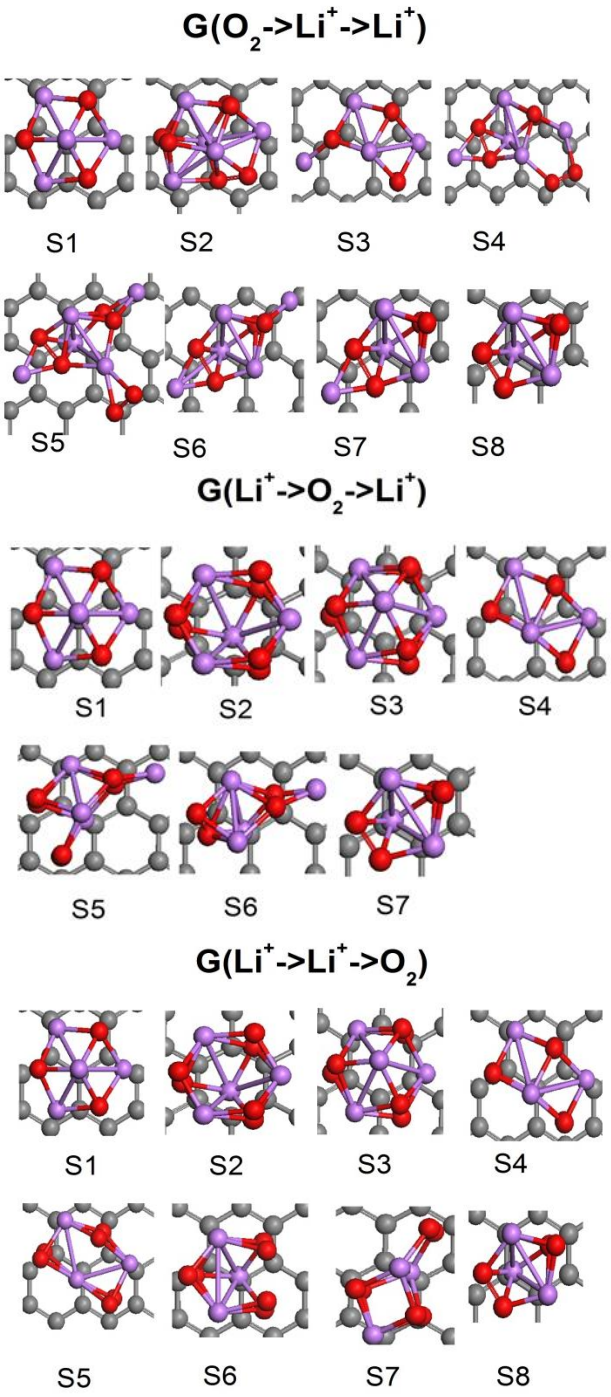

Figure S3, The calculated structures of intermediates of oxygen evolution reaction paths starting from Li_5O_6 on graphene. Sn (n=1,2,3……8) represents step number. For the $G(O_2->Li^+->Li^+)$ path, S1 is the absorption structure of Li_5O_6 on the substrate; then S2-S5 are steps of structural adjustment with Li-O bonds broken; S6 is the O_2 evolution step; S7 is the structure after Li decomposes and S8 is the structure after another Li decomposes. For the other two paths, they are similar but the sequence of O_2 evolution and Li desorption is different. All the intermediates are considered based on the principle that as fewer Li-O bonds are broken as possible to guarantee the energy cost between steps is lowest.

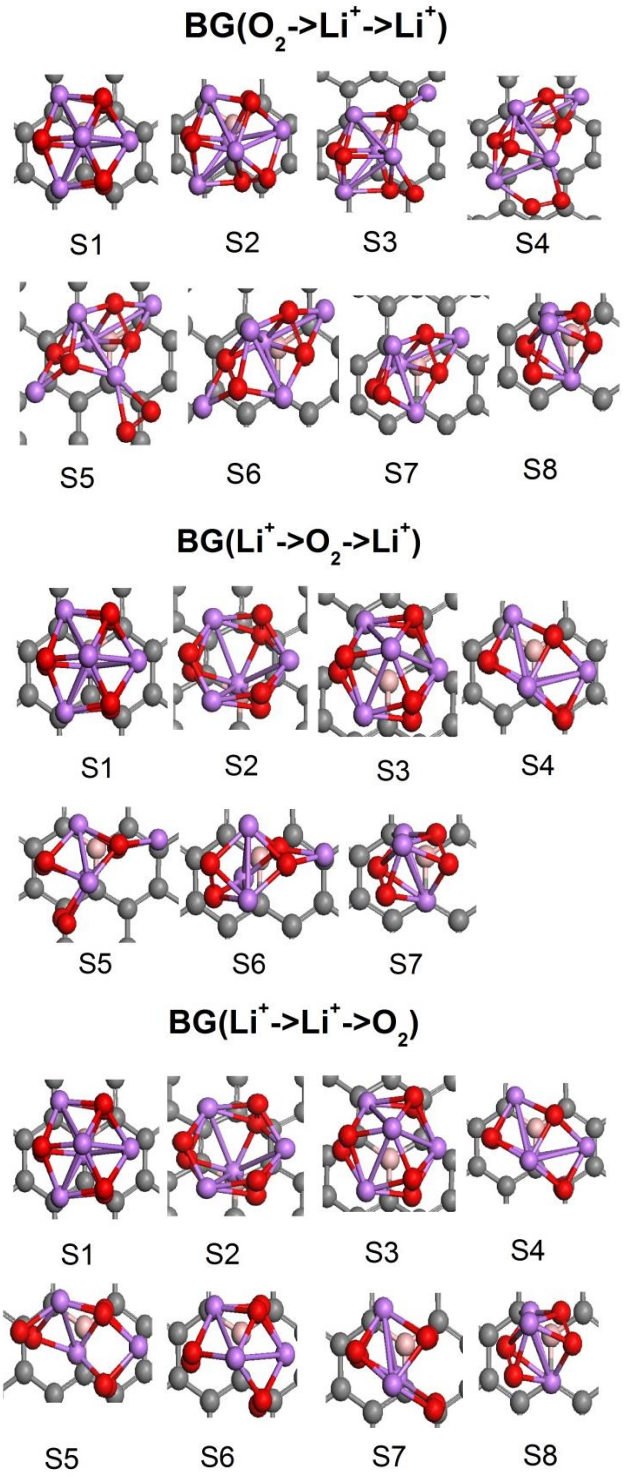

Figure S4, the calculated structures of intermediates of oxygen evolution reaction paths starting from Li_5O_6 on B-doped graphene. Detailed descriptions are similar to that of Figure S3.

Reference

[1] J. A. Manion, R. E. Huie, R. D. Levin, D. R. Burgess Jr., V. L. Orkin, W. Tsang, W. S. McGivern, J. W. Hudgens, V. D. Knyazev, D. B. Atkinson, E. Chai, A. M. Tereza, C.-Y. Lin, T. C. Allison, W. G. Mallard, F. Westley, J. T. Herron, R. F. Hampson, and D. H. Frizzell, NIST Chemical Kinetics Database, NIST Standard Reference Database 17, Version 7.0 (Web Version), Release 1.6.8, Data version 2013.03, National Institute of Standards and Technology, Gaithersburg, Maryland, 20899-8320. Web address: http://kinetics.nist.gov/