

Supplementary Information for: Structural Identification of Single Boron-Doped Graphdiynes by Computational XPS and NEXAFS Spectroscopy.

Hai-Bo Li,^a Jun-Rong Zhang,^{b*} Xiu-Neng Song,^a Chuan-Kui Wang,^a Weijie Hua,^b and Yong Ma^{a,*}

^a School of Physics and Electronics, Shandong Normal University, 250358 Jinan, China.

^b MIIT Key Laboratory of Semiconductor Microstructure and Quantum Sensing, Department of Applied Physics, School of Science, Nanjing University of Science and Technology, 210094 Nanjing, China

* Corresponding authors. E-mail addresses: mayong@sdu.edu.cn (Yong Ma)
E-mail addresses: zhangjr@njust.edu.cn (Jun-Rong Zhang)

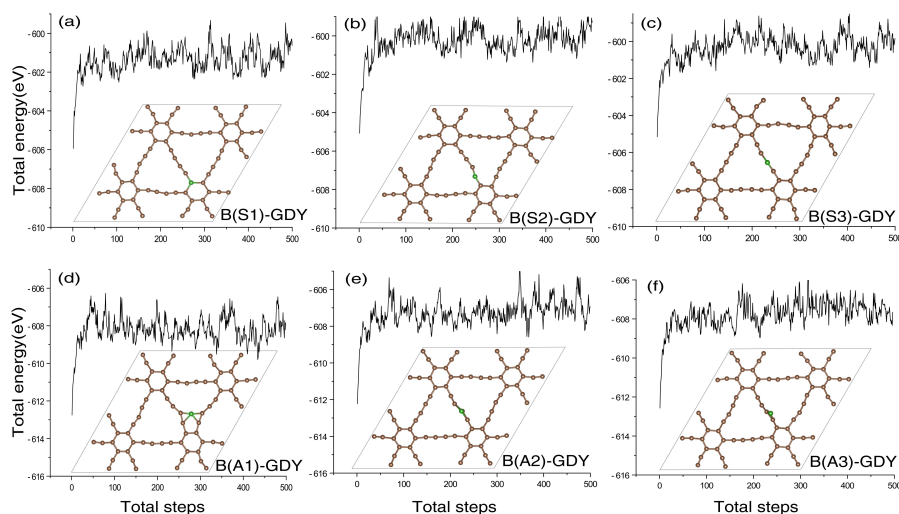


Figure S1. Born-Oppenheimer molecular dynamics (BOMD) production run of six boron-doped graphdiynes at 300 K, and each snapshot of the computational cell after BOMD were shown in the corresponding graph.