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@sdnu.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.

Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics. This journal is © the Owner Societies 2024