

**Supplementary Information**  
**for**  
**Influence of Nonmetal Dopants on Charge Separation of Graphitic Carbon Nitride**  
**by Time-Dependent Density Functional Theory**

Tzu-Jen Lin<sup>\*a,b</sup> and Cheng-chau Chiu<sup>c</sup>

\* Corresponding author: [tzujenlin999@gmail.com](mailto:tzujenlin999@gmail.com)

<sup>a</sup> Department of Chemical Engineering, Chung Yuan Christian University, 200 Chung Pei Road, Chung Li District, Taoyuan City, 32023, Taiwan

<sup>b</sup> Luh Hwa Research Center for Circular Economy, 200 Chung Pei Road, Chung Li District, Taoyuan City, 32023, Taiwan

<sup>c</sup> Institute of Atomic and Molecular Sciences, Academia Sinica, Address: No. 1, Roosevelt Rd., Sec. 4, Taipei, 10617, Taiwan

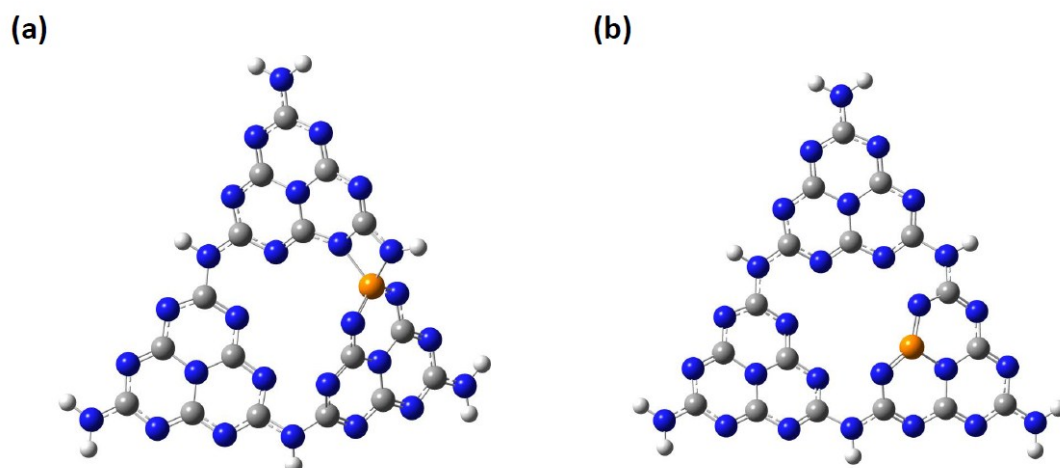


Fig. S1 The optimized ground state structure of the single-phosphorus-doped HT where the phosphorus atom was located at (a) the corner position and (b) the bay position.