

# First-Principles Study of Gas Molecule Adsorption on C-doped Zigzag Phosphorene Nanoribbons

Shuai Yang <sup>1</sup>, Zhiyong Wang <sup>1,\*</sup>, Xueqiong Dai <sup>2</sup>, Jianrong Xiao <sup>1</sup>, Mengqiu Long <sup>3</sup> and Tong Chen <sup>4</sup>

<sup>1</sup> College of Science, Guilin University of Technology, Guilin 541008, China; 102017875@glut.edu.cn (S.Y.); xjr@glut.edu.cn (J.X.)

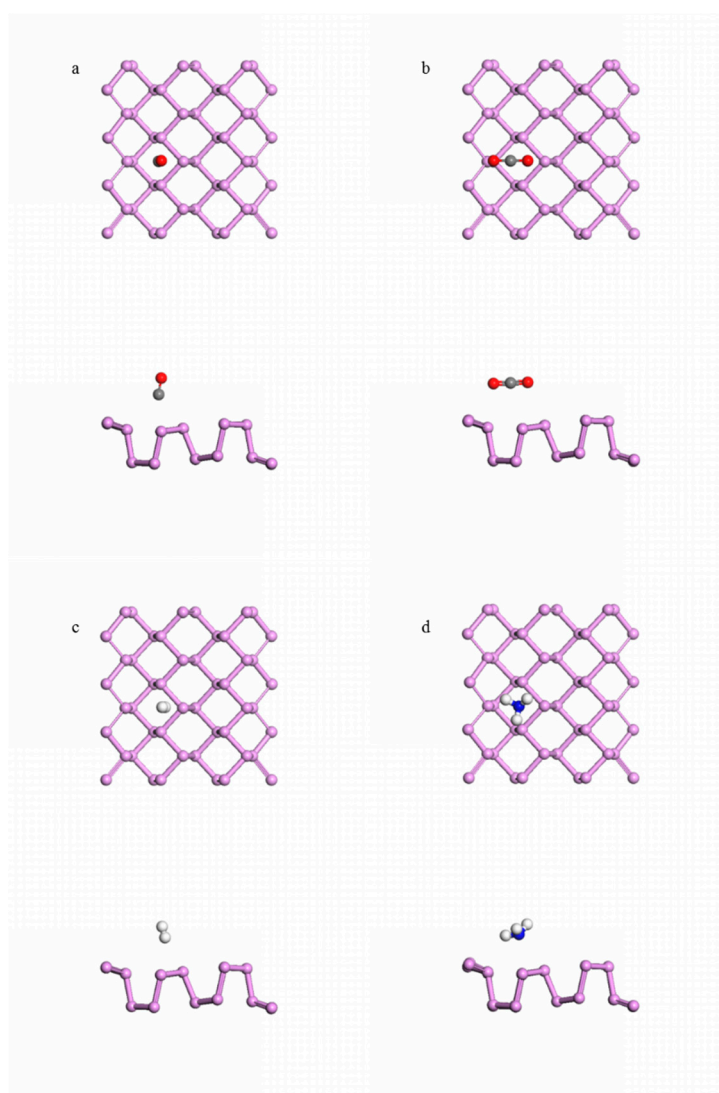
<sup>2</sup> Modern Education Technology Center, Guilin University of Technology, Guilin 541008, China; daisy@glut.edu.cn

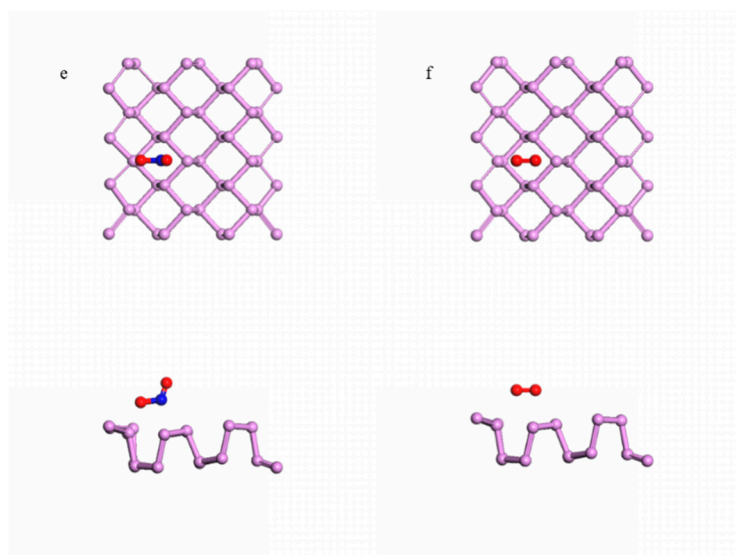
<sup>3</sup> Hunan Key laboratory of Super Micro-structure and Ultrafast Process, Central South University, Changsha 410083, China; mqlong@csu.edu.cn

<sup>4</sup> School of Energy and Mechanical Engineering, Jiangxi University of Science and Technology, Nanchang 330013, China; chentong@jxust.edu.cn

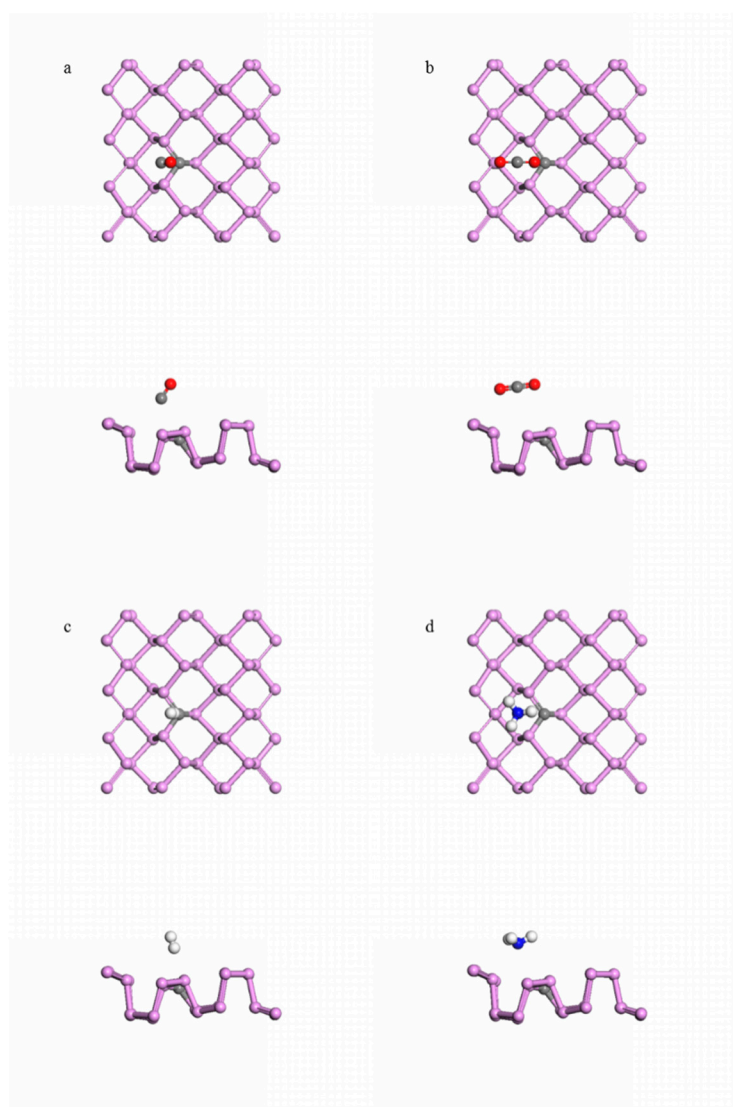
\* Correspondence: zhiyongwang@glut.edu.cn

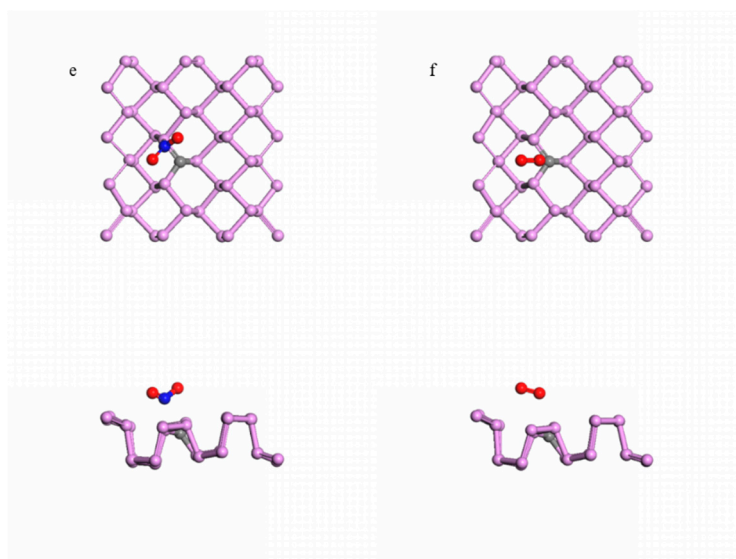
## Supplementary Materials





**Figure S1.** Models of the (a) CO, (b) CO<sub>2</sub>, (c) H<sub>2</sub>, (d) NH<sub>3</sub>, (e) NO<sub>2</sub> and (f) O<sub>2</sub> gas adsorbed on the pristine phosphorene. The purple, red, gray, blue and white balls represent P, O, C, N and H atoms, respectively.





**Figure S2.** Models of the (a) CO, (b) CO<sub>2</sub>, (c) H<sub>2</sub>, (d) NH<sub>3</sub>, (e) NO<sub>2</sub> and (f) O<sub>2</sub> gas adsorbed on the C doped phosphorene. The purple, red, gray, blue and white balls represent P, O, C, N and H atoms, respectively.