

## Electronic Supplementary Information

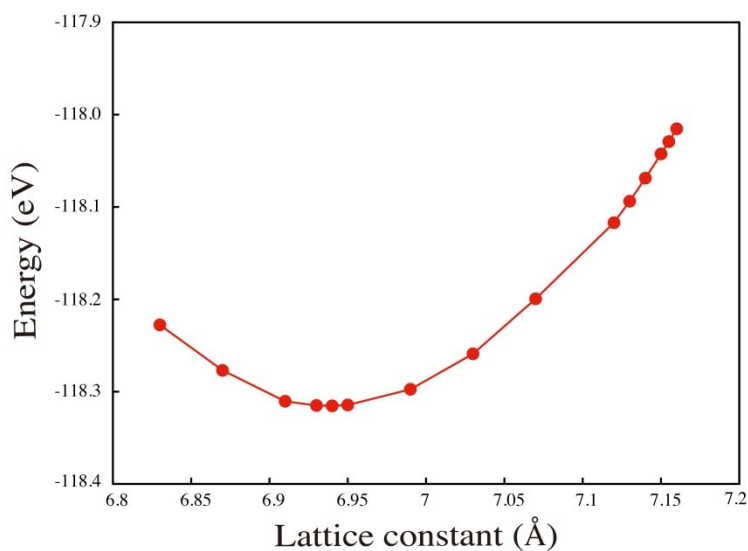
### The origin of enhanced photocatalytic activity of carbon nitride nanotubes: A first-principles study

Qian Gao,<sup>a,b</sup> Shuanglin Hu<sup>\*b</sup>, Yi Du<sup>c</sup> and Zhenpeng Hu<sup>\*a,c</sup>

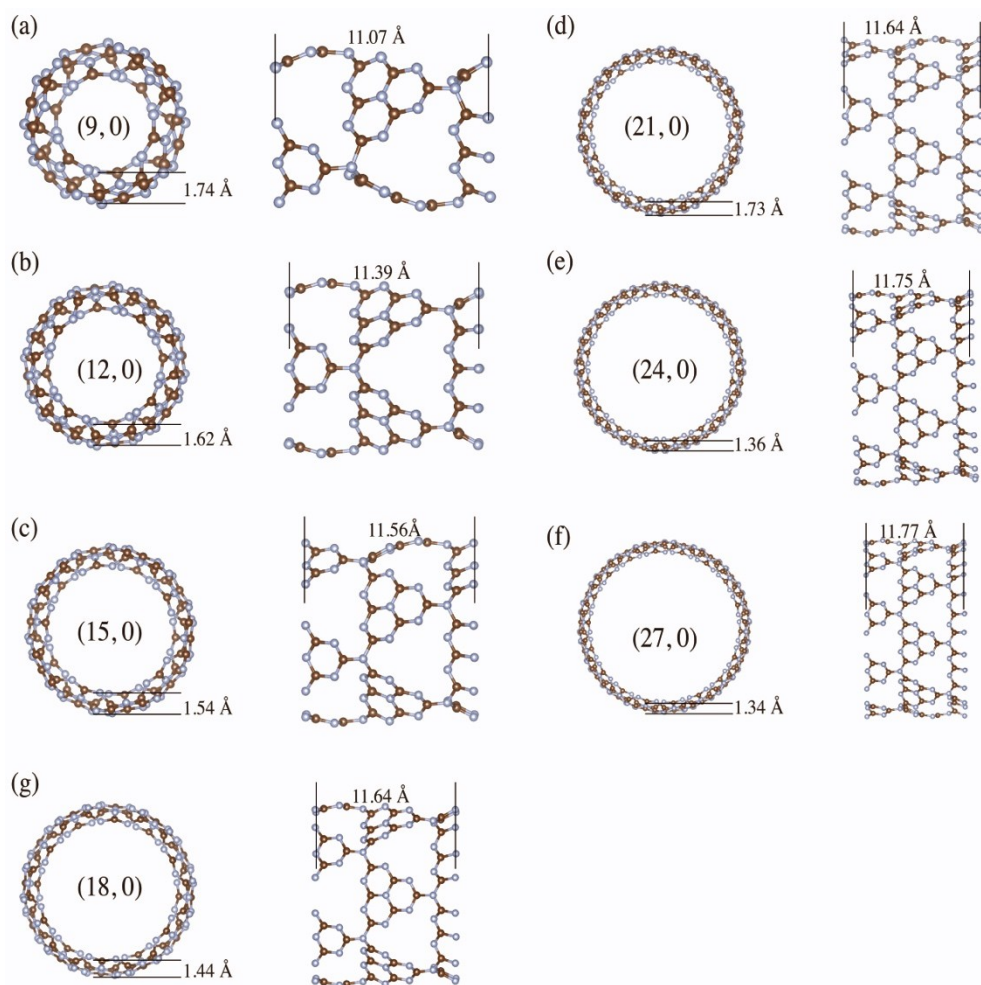
<sup>a</sup>School of Physics, Nankai University, Tianjin 300071, China

<sup>b</sup>Institute of Nuclear Physics and Chemistry, Chinese Academy of Engineering Physics, Mianyang, Sichuan 621900, China

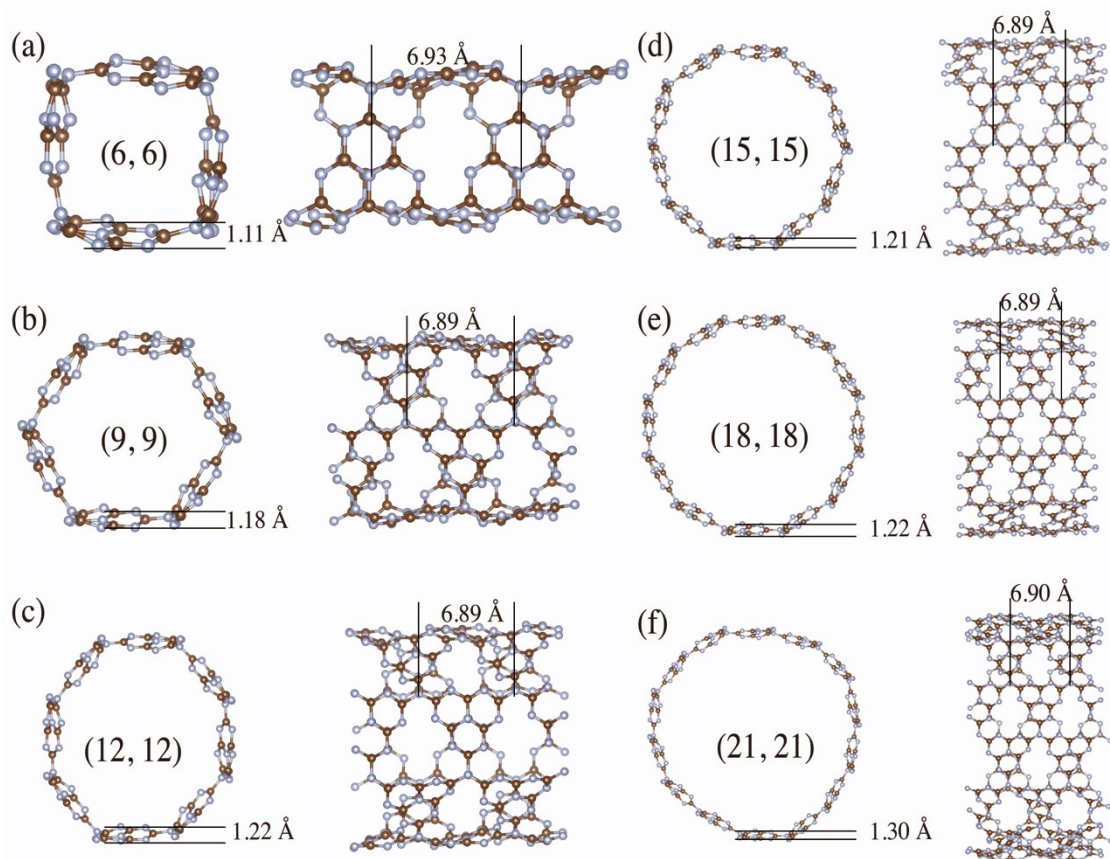
<sup>c</sup>Institute for Superconducting and Electronic Materials, Innovation Campus, University of Wollongong, New South Wales 2522, Australia



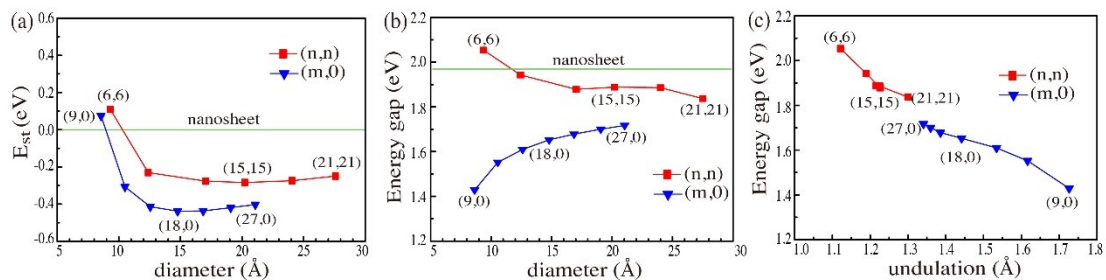
**Figure S1.** Energy profile of a linear scan on the lattice constant of a g-C<sub>3</sub>N<sub>4</sub> monolayer.



**Figure S2.** Top and side views of  $(m, 0)$  CNNTs. The cyan (light) and brown (dark) spheres represent N and C atoms, respectively. The values are the lattice parameters along the periodic direction.



**Figure S3.** Top and side views of  $(n, n)$  CNNTs. The cyan (light) and brown (dark) spheres represent N and C atoms, respectively. The values are the lattice parameters along the periodic direction.



**Figure S4.** The PBE calculated (a) strain energy and (b) energy gap versus the outer diameter of the CNNTs. (c) The PBE calculated energy gap versus the undulation of the CNNTs.