Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.
This journal is © the Owner Societies 2014

Adsorption Properties of Nitrogen Dioxide on Hybrid Carbon and Boron-Nitride Nanotubes

*Haining Liu and C. Heath Turner**

Department of Chemical and Biological Engineering, The University of Alabama, Tuscaloosa, AL 35487-0203

Electronic Supplementary Information

*To whom correspondence should be addressed: hturner@eng.ua.edu
205-348-1733 (phone)
205-348-7558 (fax)

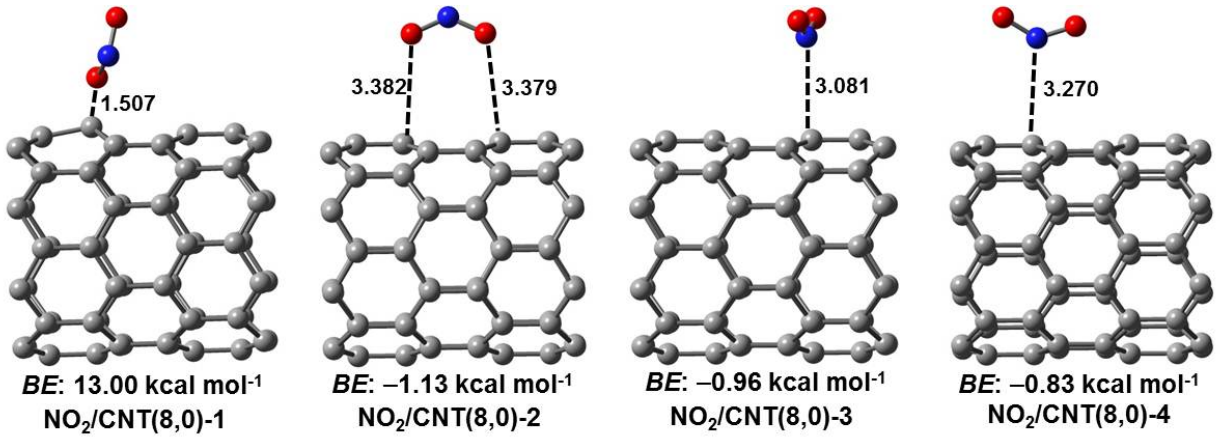

Fig. S1 The optimized structures of the NO_2/CNT(8,0) complexes obtained in this study. Key interaction distances are shown in angstroms. (Color scheme: grey = carbon, blue = nitrogen, pink = boron, red = oxygen)

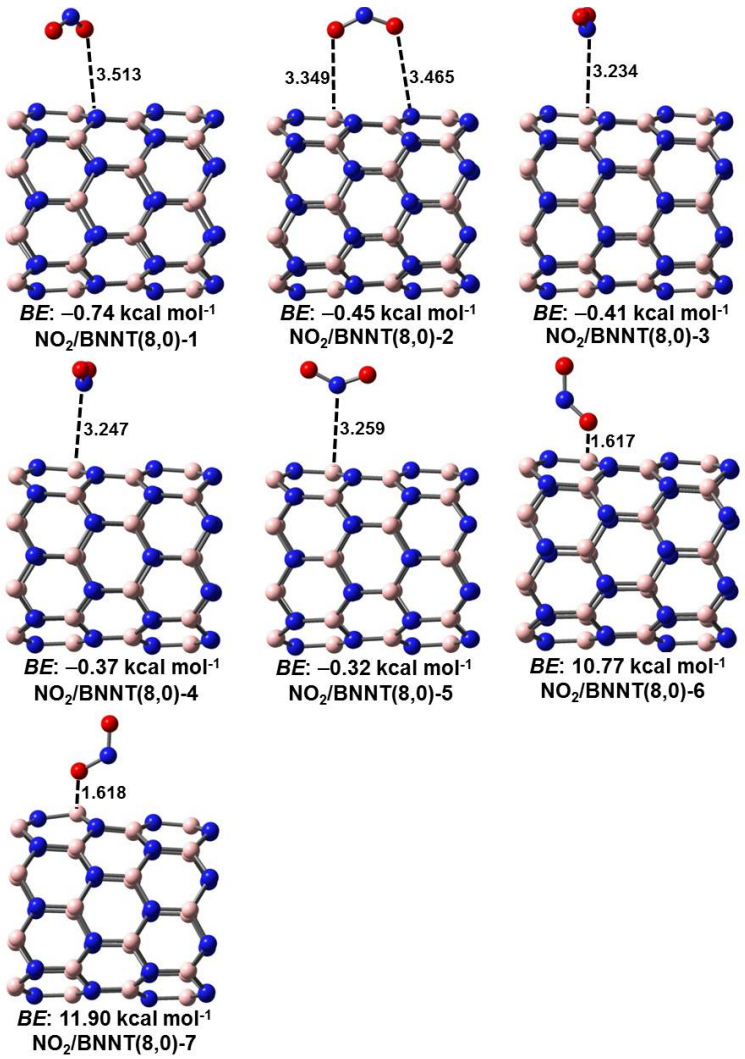

Fig. S2 The optimized structures of the NO_2/BNNT(8,0) complexes obtained in this study. Key interaction distances are shown in angstroms. (Color scheme: grey = carbon, blue = nitrogen, pink = boron, red = oxygen)

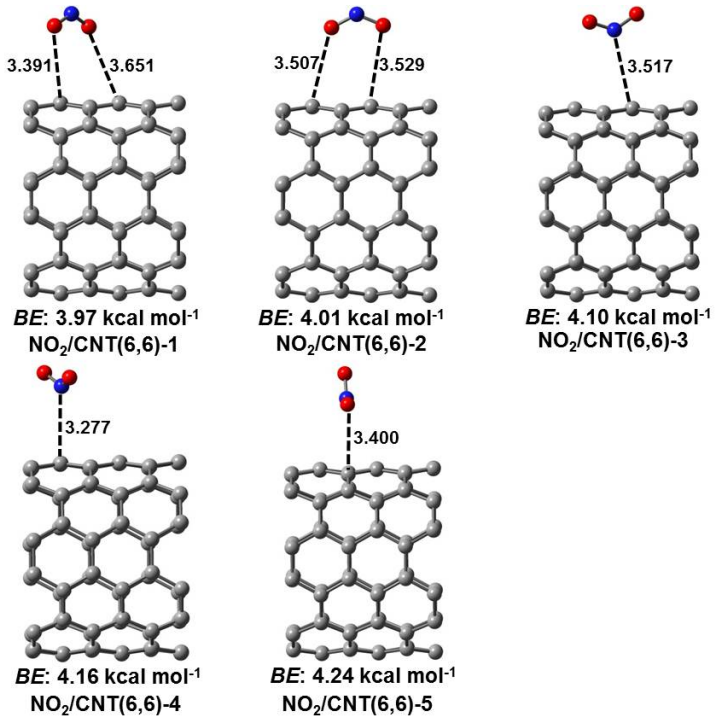

Fig. S3 The optimized structures of the NO_2/CNT(6,6) complexes obtained in this study. Key interaction distances are shown in angstroms. (Color scheme: grey = carbon, blue = nitrogen, pink = boron, red = oxygen)

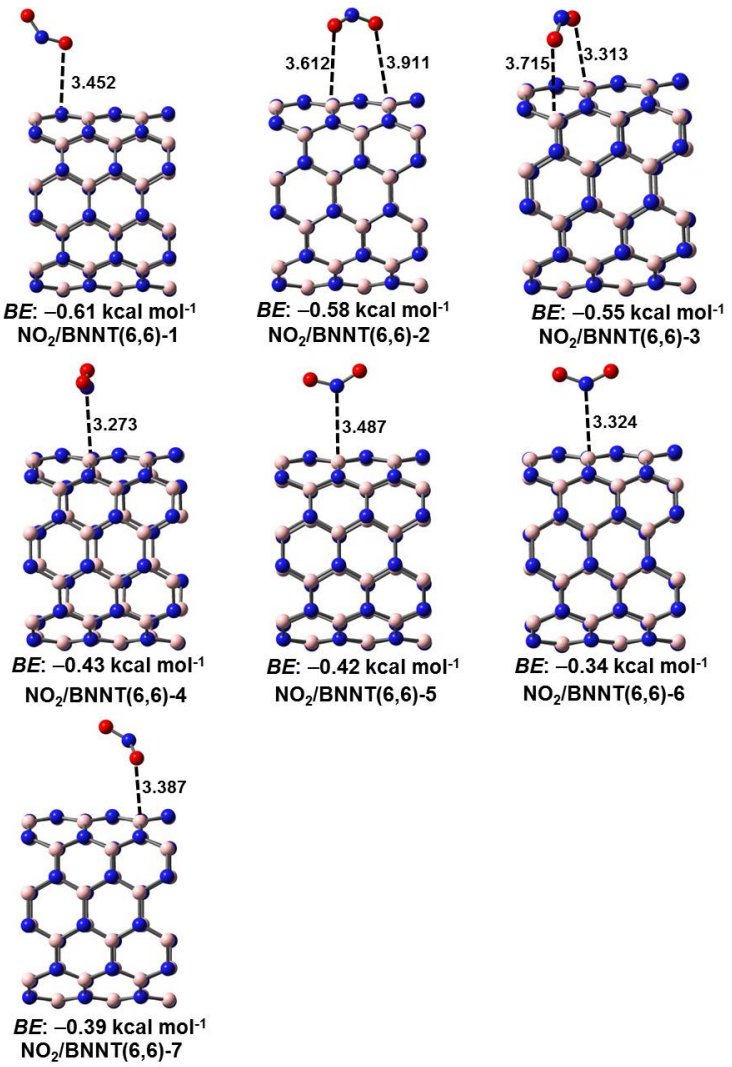

Fig. S4 The optimized structures of the NO_2/BNNT(6,6) complexes obtained in this study. Key interaction distances are shown in angstroms. (Color scheme: grey = carbon, blue = nitrogen, pink = boron, red = oxygen)

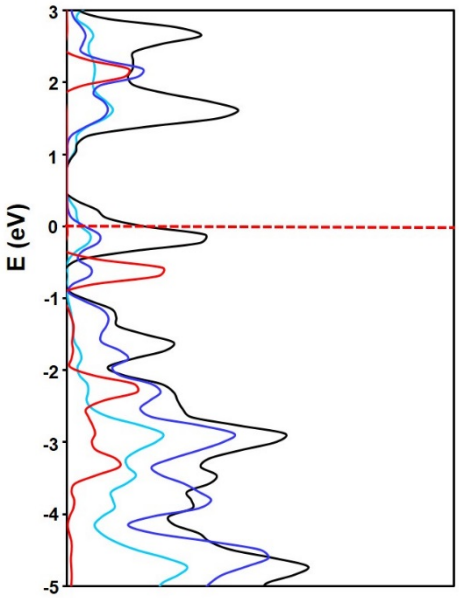

Fig. S5 The calculated projected density of states of NO_2/CBNNT(8,0)-1. Green, black, blue and red curves represent projected B-p, C-p, N-p and O-p states, respectively. The Fermi level (red dashed line) is shifted to 0 eV.

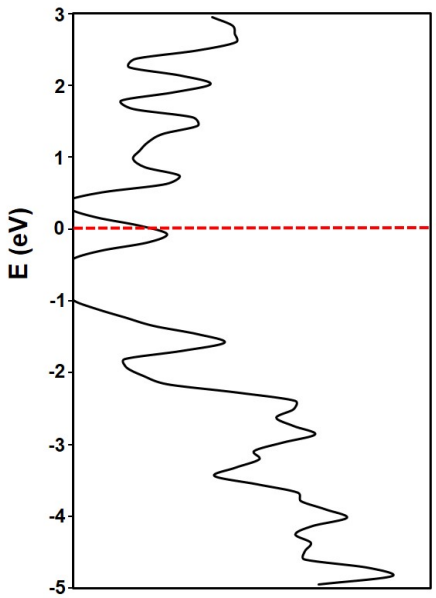

Fig. S6 The calculated total density of states for the complex between NO_2 and a CBNNT with a 2:2 stoichiometric combination of CNT and BNNT segments. The NO_2 orientation is the same as NO_2/CBNNT(8,0)-1 reported in the paper. The Fermi level (red line) is shifted to 0 eV.