Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Electronic Supplementary Information

Ab initio theoretical Study of Non-covalent Adsorption of Aromatic Molecules on Boron Nitride Nanotubes

Yu Zhao[1], Xiaojun Wu[2], Jinlong Yang[3] and Xiao Cheng Zeng[1]

[1]Department of Chemistry and Nebraska Center for Materials and Nanoscience, University of Nebraska-Lincoln, Lincoln, Nebraska 68588; [2]Department of Materials of Sciences and Engineering and Hefei National Lab for Physical Science at the Microscale, University of Science and Technology of China, Hefei, 230026, China; [3]Department of Chemical Physics and Hefei National Lab for Physical Sciences at the Microscale, University of Science and Technology of China, Hefei, 230026, China

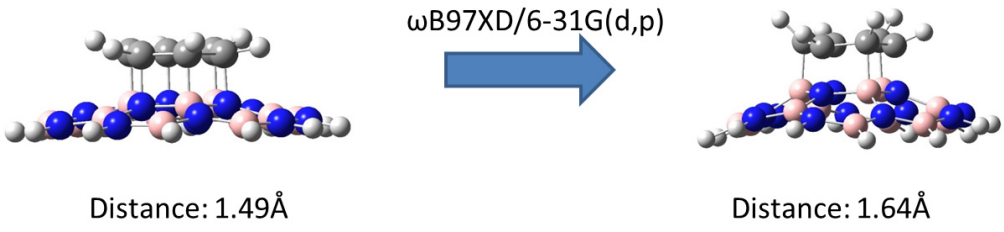

FIG. S1. The initial and optimized structures for benzene covalently bonded to the $(BN)_{12}H_{12}$ piece. The optimization is at ωB97X-D/6-31G(d,p) level of theory. The energy of the local minimum (right panel) is 7.61 eV higher than the ground state shown in the main text.

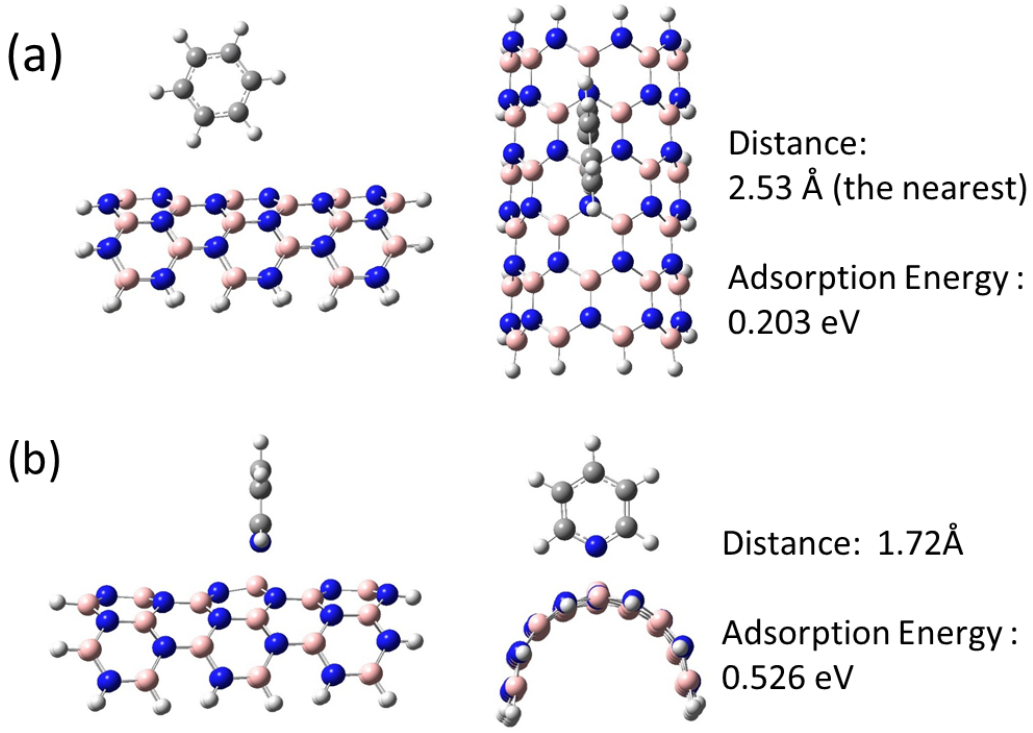

FIG. S2. The optimized structures of (a) a benzene interacting noncovalently with the convex surface of $B_{27}N_{27}H_{20}$ via the C-H-π interaction, and (b) a pyridine covalently bonded to the convex surface of $B_{27}N_{27}H_{20}$. The optimization is performed at ωB97X-D/6-31G(d,p) level of theory as mentioned in the main text.

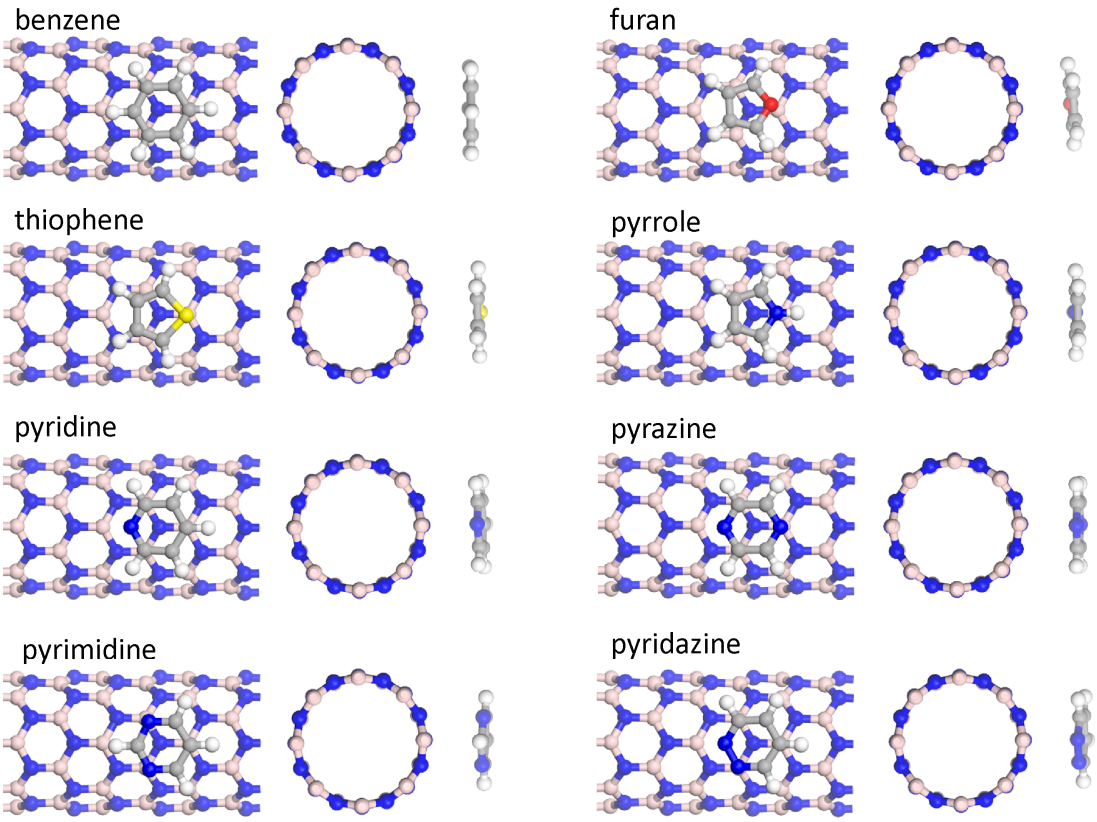

FIG. S3. The side and front view of optimized structures of aromatic ring functionalized BNNTs. The optimization is based on periodic DFT-D method.

Table S1. The summary of BSSE corrected adsorption energy for (8, 0) BNNT, (8, 0) CNT and flat hexagonal BN sheet (*h*-BN), calculated using periodic-DFT-D method by cp2k package [1].

Adsorption Energy (eV/kcal·mol^{-1})	(8,0) BNNT	(8,0) CNT	*h*-BN
C_6H_6	0.380/8.75	0.282/6.49	0.521/12.03
C_5H_5N	0.377/8.70	0.268/6.21	0.595/13.73

[1]: http:// cp2k.berlioz.de, a freely available program to perform atomistic and molecular simulations of solid state, liquid, molecular and biological systems.