

Supplementary Data

Table S1. Reaction enthalpy (ΔH_f in kcal/mol) of deprotonated pentachlorophenol (pcp-H)/deprotonated 6-OH-BDE-47 (6ohbde47-H) adsorbed by the zigzag (9,0) and (18,0) boron nitride nanotubes decorated with CePc₂, EuPc₂, TbPc₂ and YbPc₂ complexes

| ΔH_f | | | | ΔH_f | | | |
|-------------------------|-------------|--------------------------------------|---------------------------|-------------------------|-------------|--------------------------------------|---------------------------|
| | | | (kcal mol ⁻¹) | | | | (kcal mol ⁻¹) |
| BN90_CePc ₂ | +pcp-H | →BN90_CePc ₂ _pcp-H | -5.2061 | BN90_TbPc ₂ | +pcp-H | →BN90_TbPc ₂ _pcp-H | -1.8587 |
| BN90_CePc ₂ | +6ohbde47-H | →BN90_CePc ₂ _6ohbde47-H | 7.4113 | BN90_TbPc ₂ | +6ohbde47-H | →BN90_TbPc ₂ _6ohbde47-H | 9.3292 |
| BN180_CePc ₂ | +pcp-H | →BN180_CePc ₂ _pcp-H | 2.5082 | BN180_TbPc ₂ | +pcp-H | →BN180_TbPc ₂ _pcp-H | 3.4442 |
| BN180_CePc ₂ | +6ohbde47-H | →BN180_CePc ₂ _6ohbde47-H | 6.6059 | BN180_TbPc ₂ | +6ohbde47-H | →BN180_TbPc ₂ _6ohbde47-H | 8.9916 |
| BN90_EuPc ₂ | +pcp-H | →BN90_EuPc ₂ _pcp-H | -2.1945 | BN90_YbPc ₂ | +pcp-H | →BN90_YbPc ₂ _pcp-H | -0.5749 |
| BN90_EuPc ₂ | +6ohbde47-H | →BN90_EuPc ₂ _6ohbde47-H | 9.2920 | BN90_YbPc ₂ | +6ohbde47-H | →BN90_YbPc ₂ _6ohbde47-H | 10.2177 |
| BN180_EuPc ₂ | +pcp-H | →BN180_EuPc ₂ _pcp-H | 3.2563 | BN180_YbPc ₂ | +pcp-H | →BN180_YbPc ₂ _pcp-H | 3.6879 |
| BN180_EuPc ₂ | +6ohbde47-H | →BN180_EuPc ₂ _6ohbde47-H | 8.8058 | BN180_YbPc ₂ | +6ohbde47-H | →BN180_YbPc ₂ _6ohbde47-H | 9.0798 |

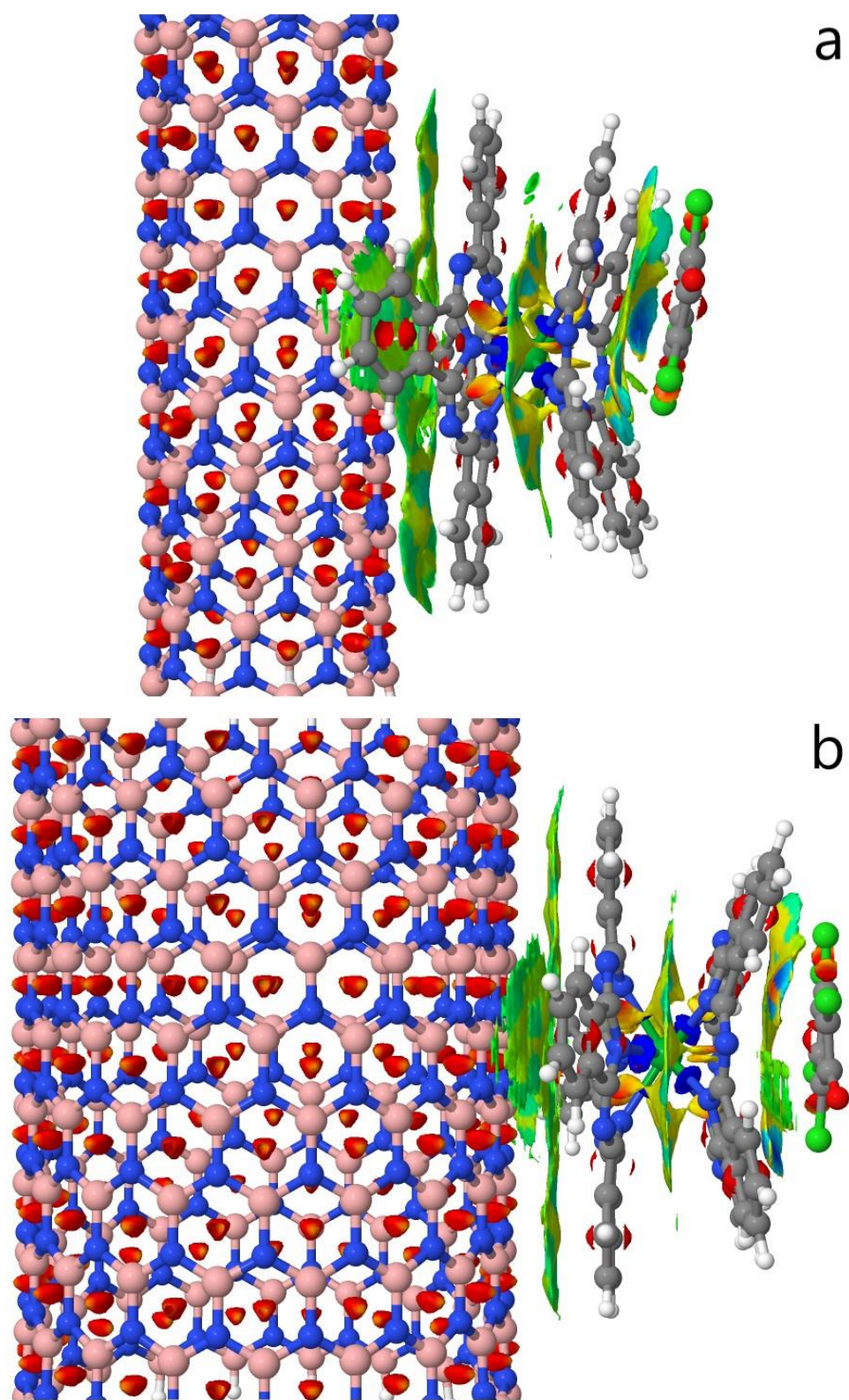


Figure S1. Non-covalent interaction between deprotonated pentachlorophenol (pcp-H) and the zigzag (a) (9,0) (b) (18,0) boron nitride nanotube decorated with YbPc₂ complex.

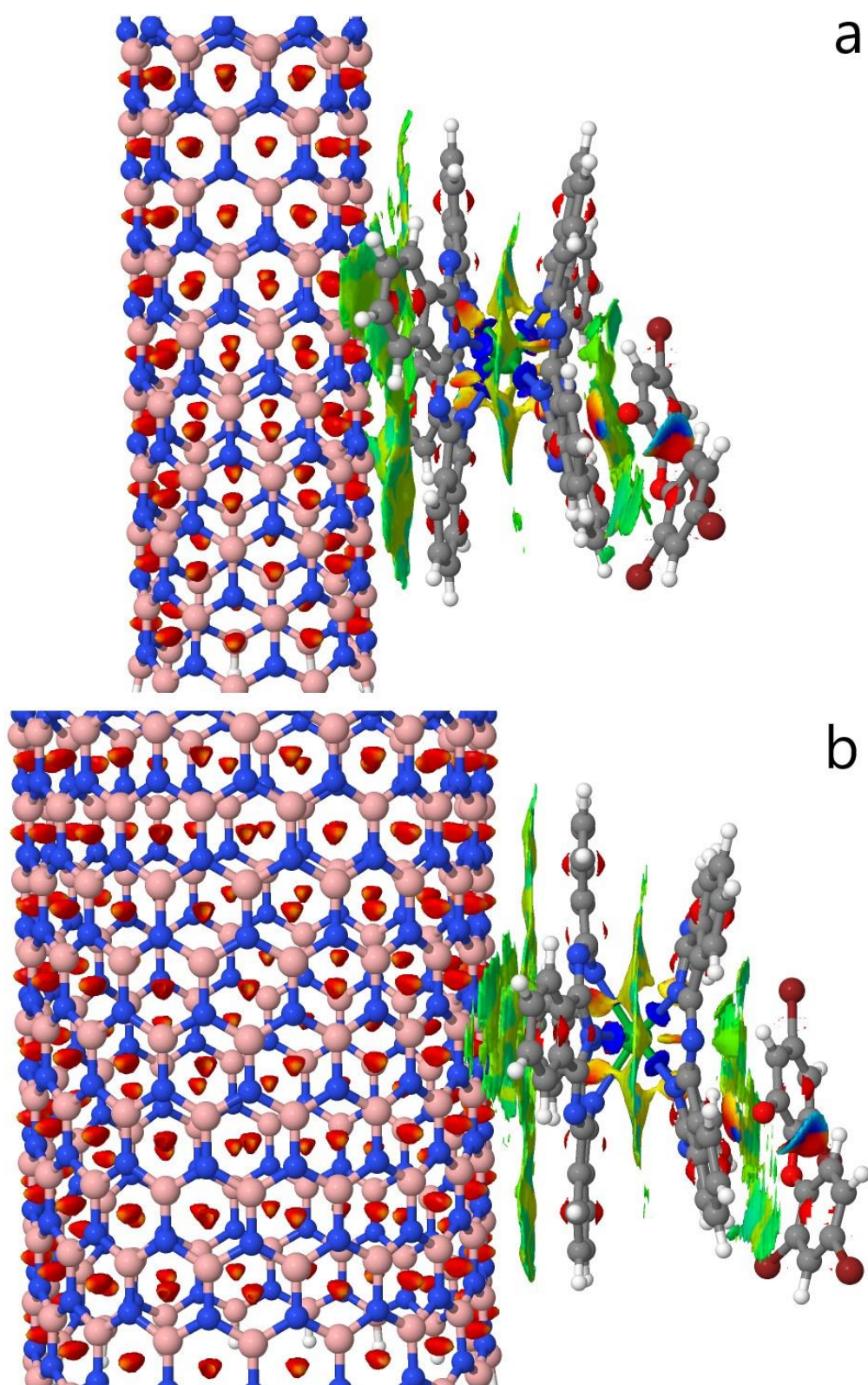


Figure S2. Non-covalent interaction between deprotonated 6-OH-BDE-47 (6ohbde47-H) and the zigzag (a) (9,0) (b) (18,0) boron nitride nanotube decorated with YbPc₂ complex.

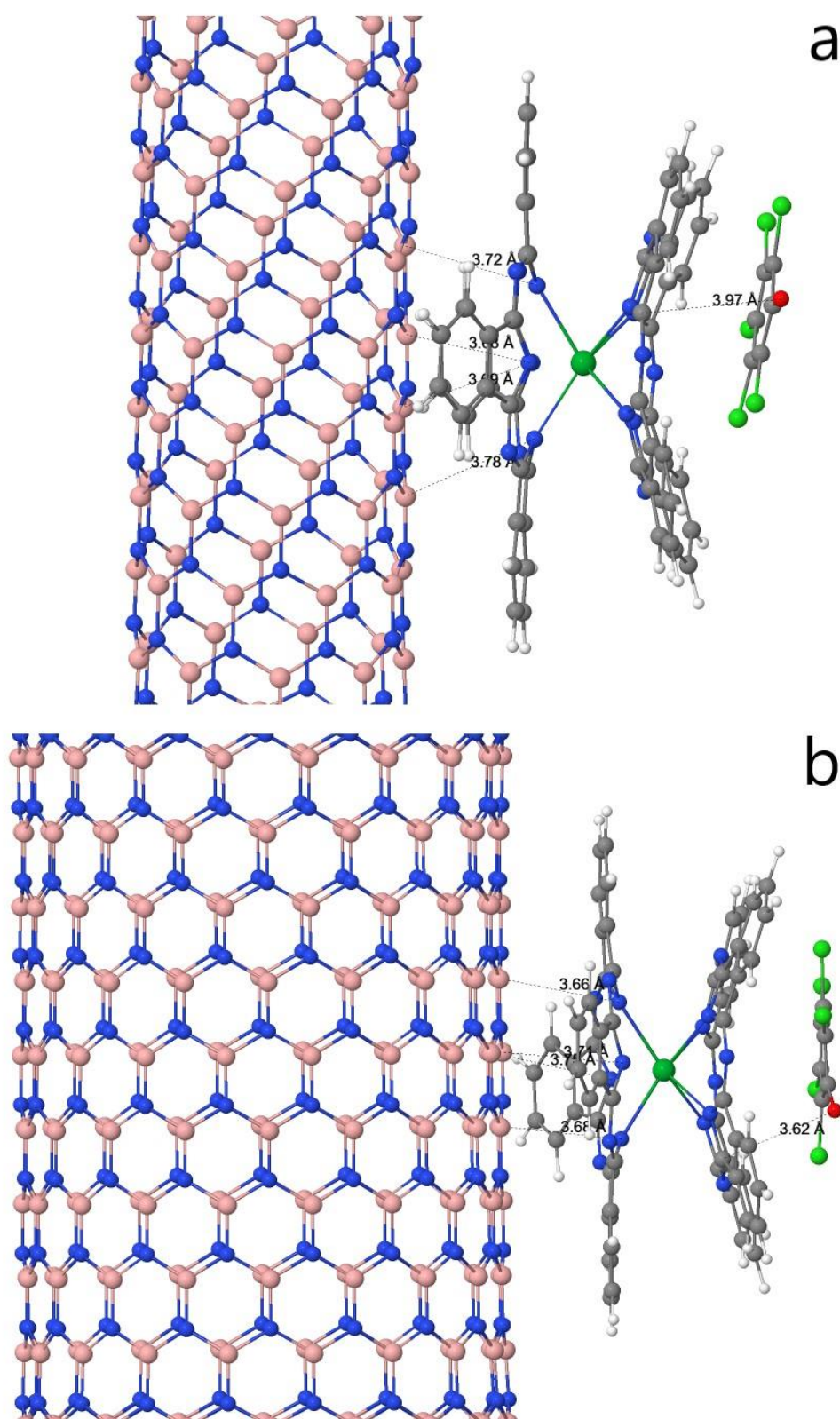


Figure S3. Equilibrium structures of deprotonated pentachlorophenol (pcp-H) adsorbed on the zigzag (a) (9,0) (b) (18,0) boron nitride nanotube decorated with YbPc₂ complex.

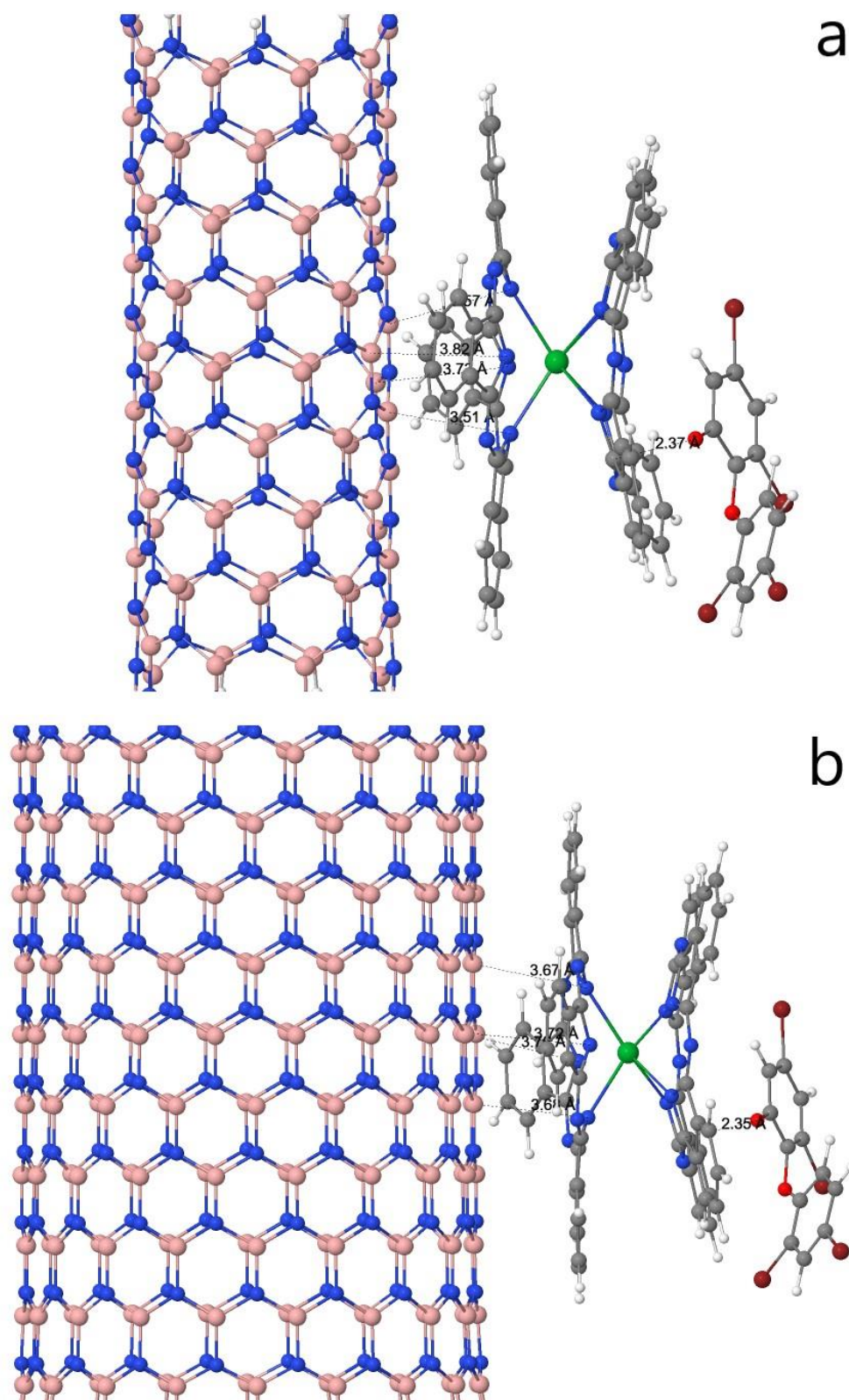


Figure S4. Equilibrium structures of deprotonated 6-OH-BDE-47 (6ohbde47-H) adsorbed on the zigzag (a) (9,0) (b) (18,0) boron nitride nanotube decorated with YbPc₂ complex.