

**Figure S1.** Side and top views of the relaxed structures of the vertical and parallel configurations of the  $\pi$ -system...2D sheet complexes where  $\pi$ -system = benzene (BNZ)/hexafluorobenzene (HFB) and the 2D sheet = striped borophene (sB)/ $\beta_{12}$  borophene ( $\beta_{12}$ )/pristine graphene (GN) at all possible adsorption sites. The  $\pi$ -system...2D sheet equilibrium distances (d) are given in Å.

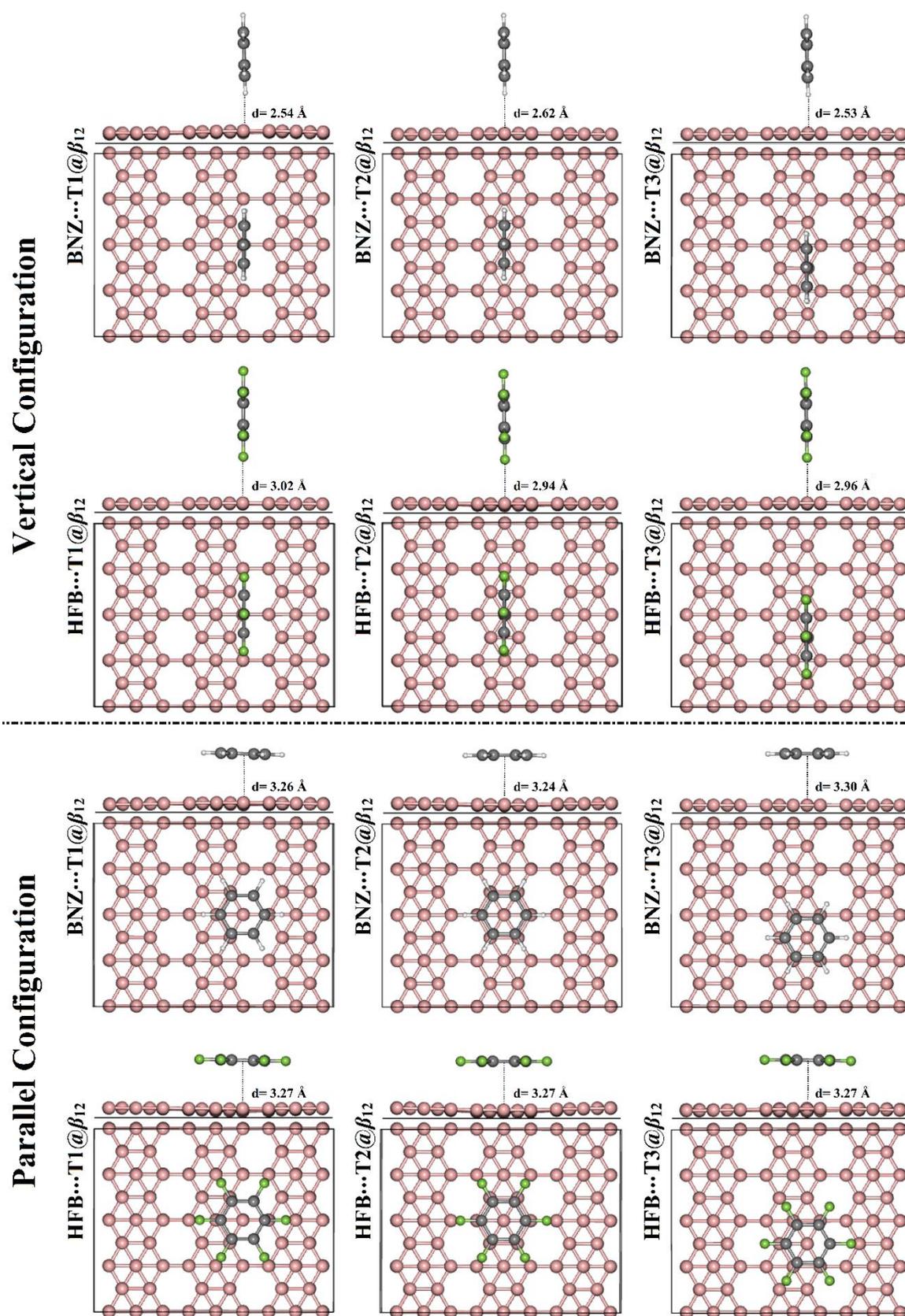


Figure S1. Continued.

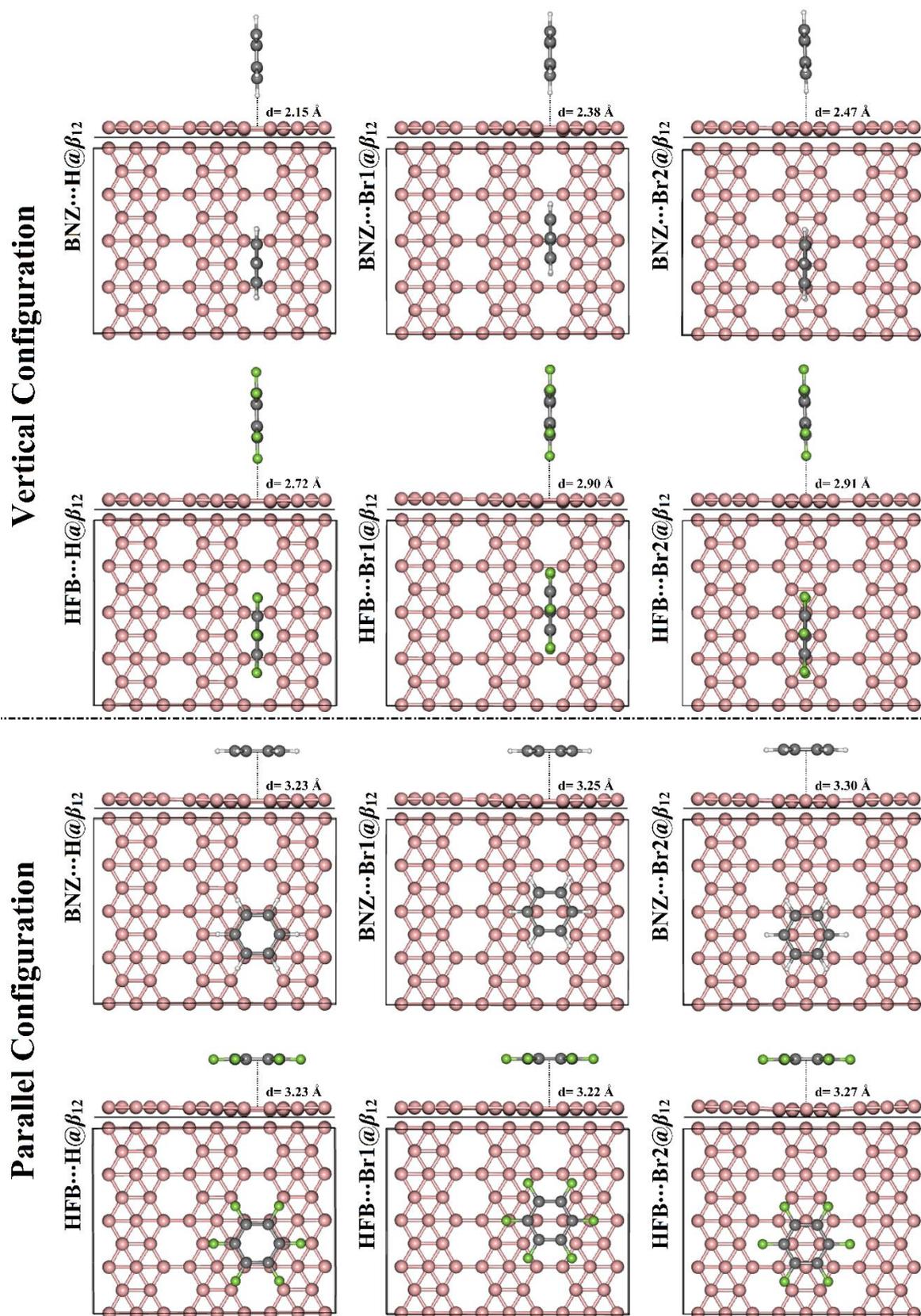


Figure S1. Continued.

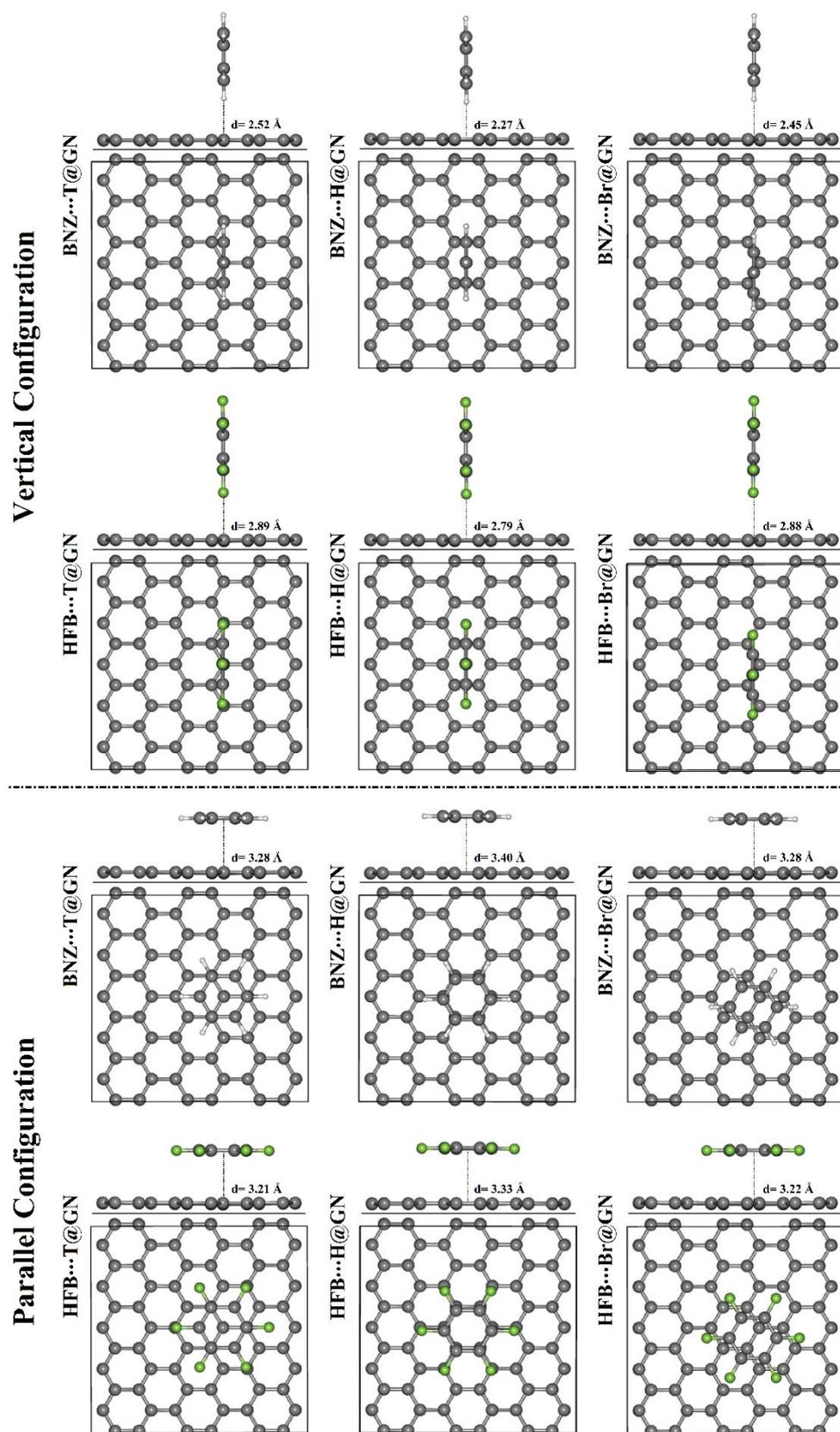


Figure S1. Continued.