

Supplementary Information (SI)
Electronic and Molecular Adsorption Properties of Pt-doped
BC₆N: An Ab-initio Investigation

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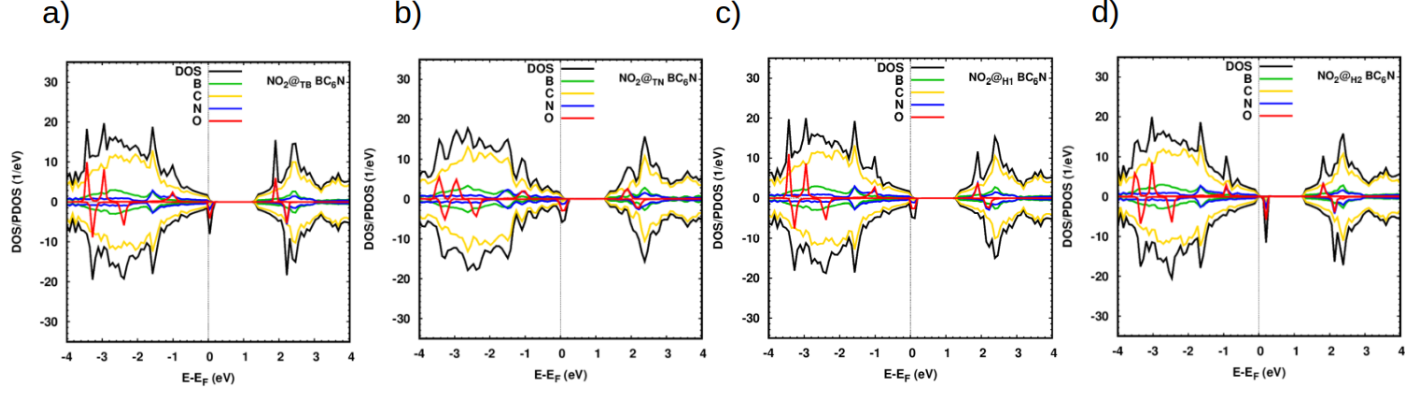


FIG. S 1. DOS/projected DOS (PDOS) of: (a) $\text{NO}_2@_{\text{TB}}\text{BC}_6\text{N}$, (b) $\text{NO}_2@_{\text{TN}}\text{BC}_6\text{N}$, (c) $\text{NO}_2@_{\text{H1}}\text{BC}_6\text{N}$ and (d) $\text{NO}_2@_{\text{H2}}\text{BC}_6\text{N}$.

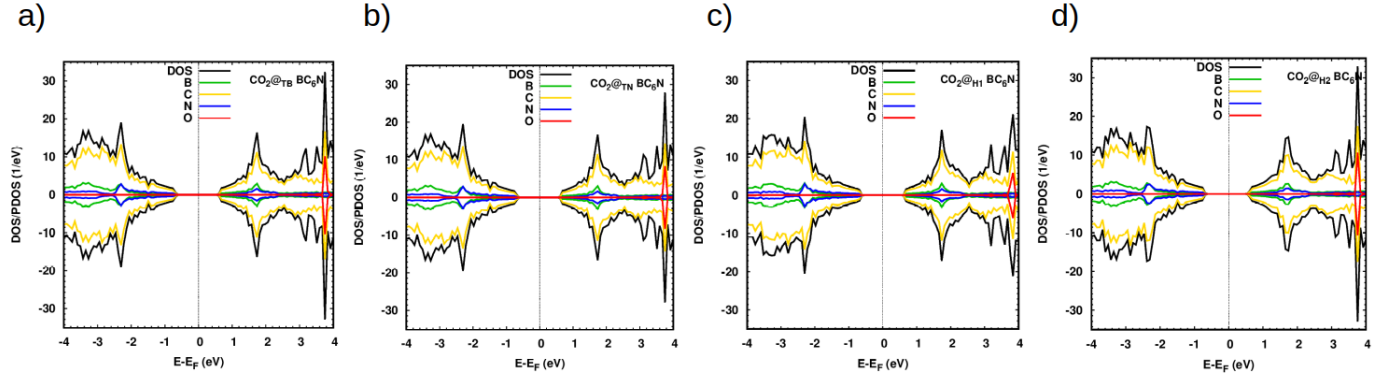


FIG. S 2. DOS/projected DOS (PDOS) of: (a) $\text{CO}_2@_{\text{TB}}\text{BC}_6\text{N}$, (b) $\text{CO}_2@_{\text{TN}}\text{BC}_6\text{N}$, (c) $\text{CO}_2@_{\text{H1}}\text{BC}_6\text{N}$ and (d) $\text{CO}_2@_{\text{H2}}\text{BC}_6\text{N}$.

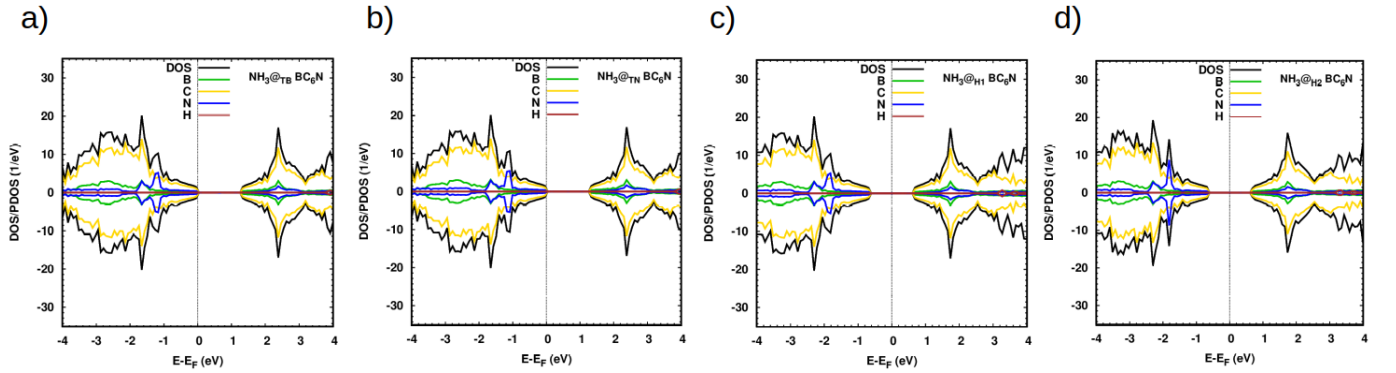


FIG. S 3. DOS/projected DOS (PDOS) of: (a) $\text{NH}_3@_{\text{TB}}\text{BC}_6\text{N}$, (b) $\text{NH}_3@_{\text{TN}}\text{BC}_6\text{N}$, (c) $\text{NH}_3@_{\text{H1}}\text{BC}_6\text{N}$ and (d) $\text{NH}_3@_{\text{H2}}\text{BC}_6\text{N}$.