DFT study of gas-phase adsorption of benzotriazole on Cu(111), Cu(100), Cu(110), and low coordinated defects thereon

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Supplementary Information

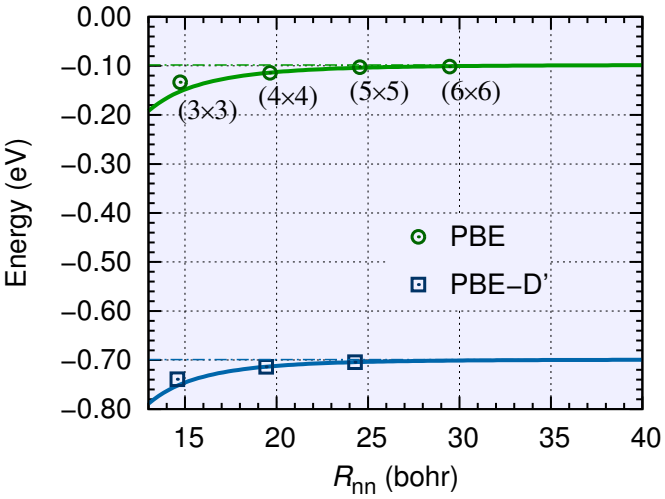

Fig. S1 The PBE and PBE-D' calculated physisorption energies of BTAH on Cu(111) as a function of R_{nn}. Thin dash-dotted horizontal lines indicate the corresponding extrapolated zero-coverage ($R_{nn} = \infty$) values.

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