**CAN DOPING AND CHARGE MODULATION MAKE BORON-NITROGEN NANO-MATERIALS AN ATTRACTIVE ADSORBENT FOR TOXIC GASES?**

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Chemically boron-nitrogen (BN) nanomaterials are more attractive adsorbent than their organic cousins, as they are composed of Lewis acid (B-sites) and base (N-sites) centers. It is expected that both electron rich and electron deficient gas molecules may be adsorbed at the surface of BN-materials, such as BN-nanotube and nano-sheet, via weak as well as strong chemical bonding. DFT results will be presented based on the adsorption of toxic molecules, such as hydrazine (N2H4) and hydrogen cyanide (HCN), at the surface of BN-nanomaterials. How doping and charge variation (both oxidation and reduction process) change adsorption energies will be discussed.