

Organic and inorganic Gas Sensing Performance of BC₃N₂ monolayer: a first-principles study

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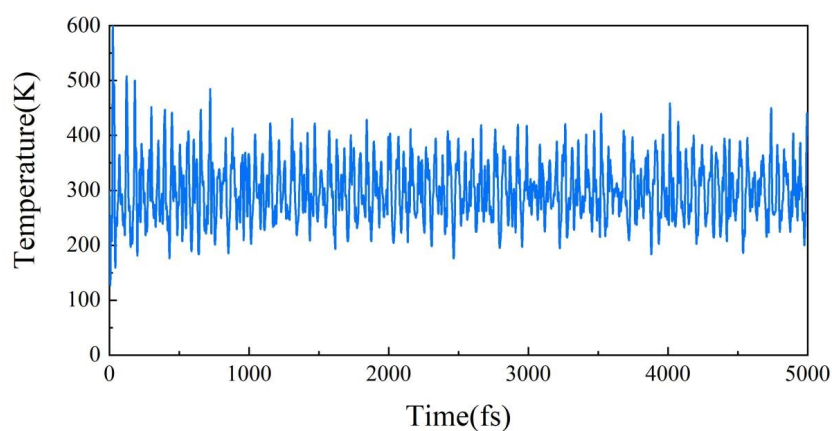


Fig. S1: The molecular dynamics simulation of 2D BC₃N₂ monolayer.

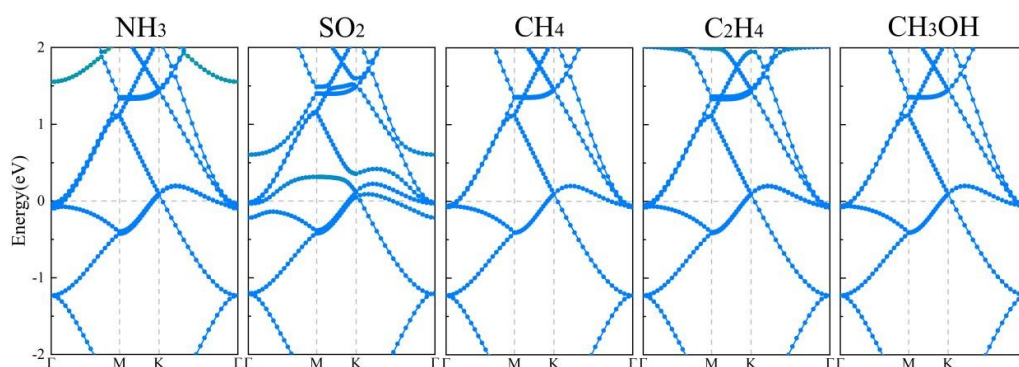


Fig. S2: The band structures of physical adsorption molecules of NH₃ (a), SO₂ (b), CH₄ (c), C₂H₄ (d) and CH₃OH (e) on BC₃N₂ monolayer.

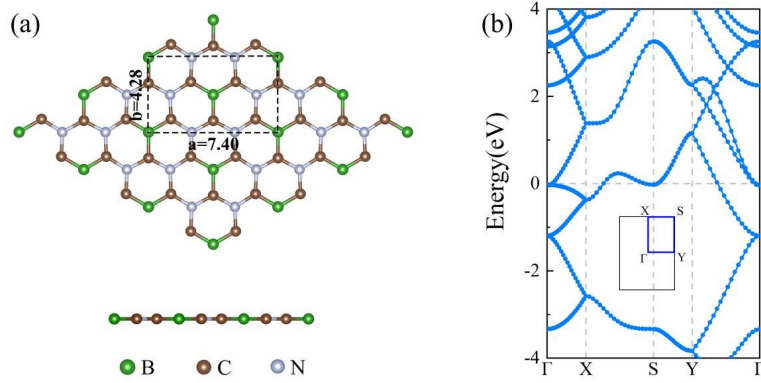


Fig. S3: The rectangled supercell of BC₃N₂ monolayer outlined with black dashed lines (a) and its corresponding electronic band structure (b).

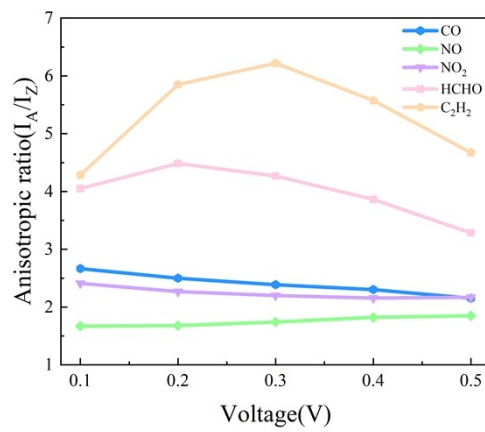


Fig. S4: The anisotropic ratio of the sensitivity of CO, NO, NO₂, HCHO and C₂H₂ along the A direction to that along the Z direction (I_A/I_Z)

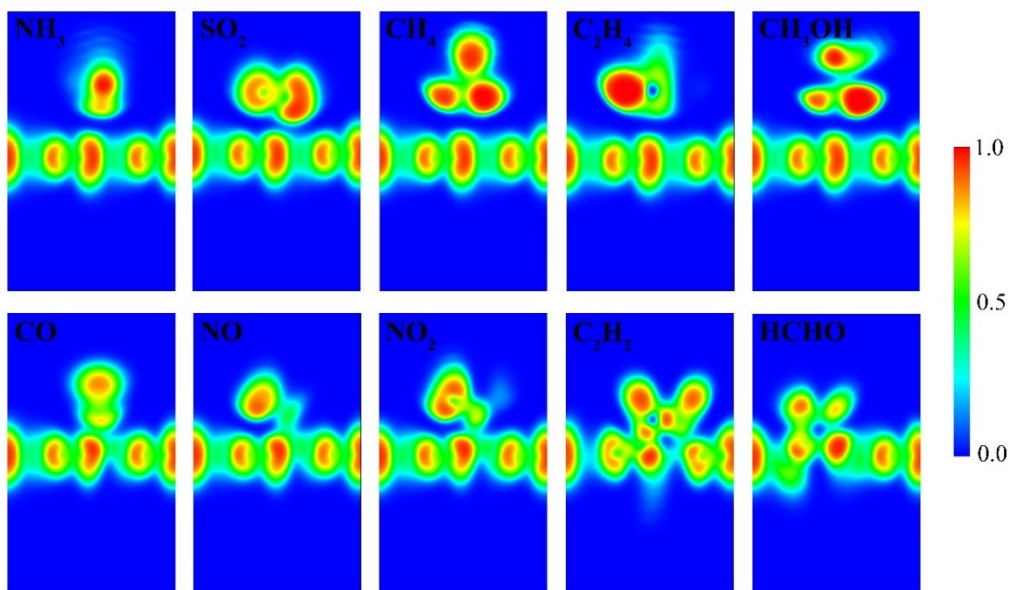


Fig. S5: The ELF maps for gas molecules adsorbed on BC₃N₂ monolayer.