

A quantum-mechanical study of the adsorption of prototype dye molecules on rutile-TiO₂(110): A comparison between Catechol and Isonicotinic Acid.

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I. SUPPORTING MATERIALS

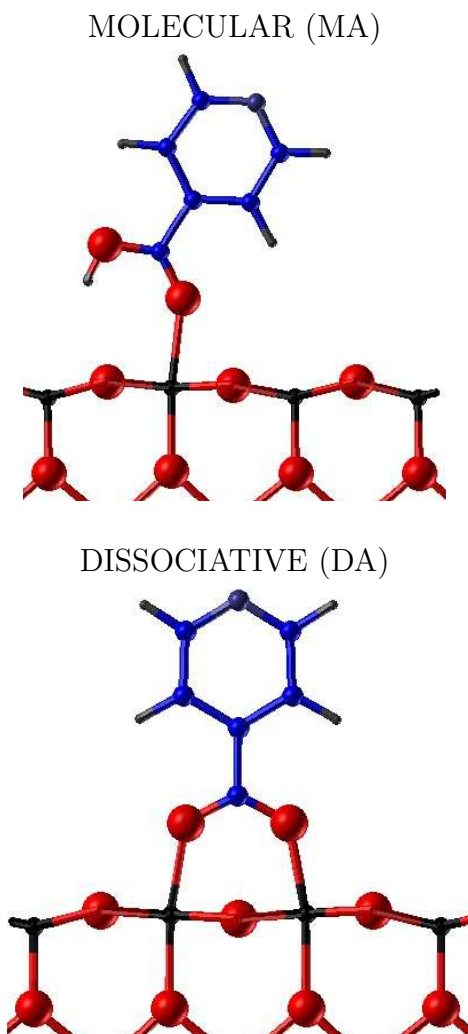


FIG. 1: Ball and stick representation of the adsorption modes of the isonicotinic acid molecule on rutile TiO_2 (110) surface: Molecular Adsorption mode (MA) and Dissociative Adsorption (BDA). Ti atoms are represented in black, O in red, C in blue, H in grey, and N in dark blue.

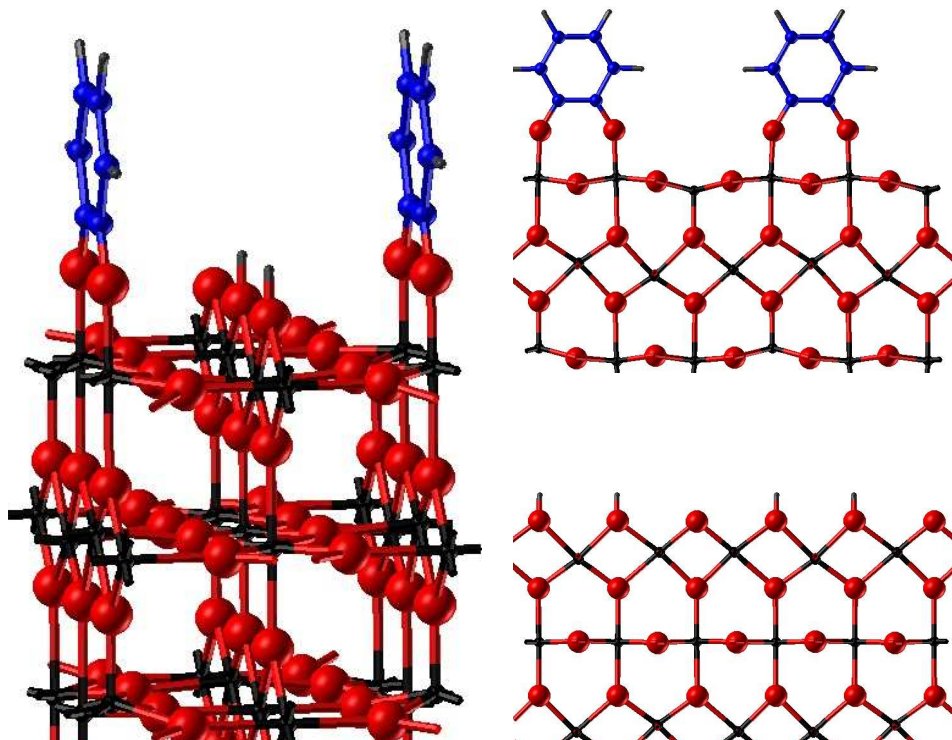


FIG. 2: Bidentate Dissociative Adsorption mode (BDA) for catechol molecule on rutile TiO₂ (110) surface.

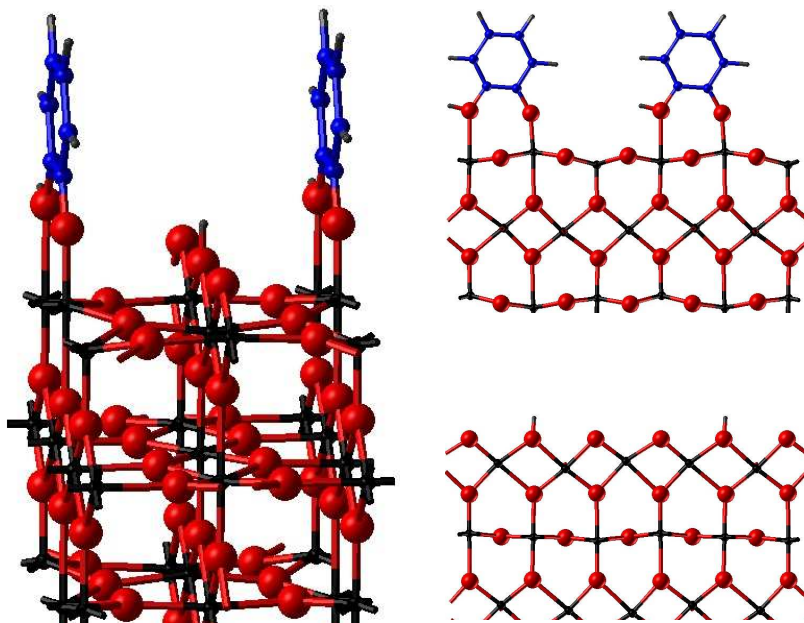


FIG. 3: Monodentate Dissociative Adsorption mode (MDA) for catechol molecule on rutile TiO_2 (110) surface.

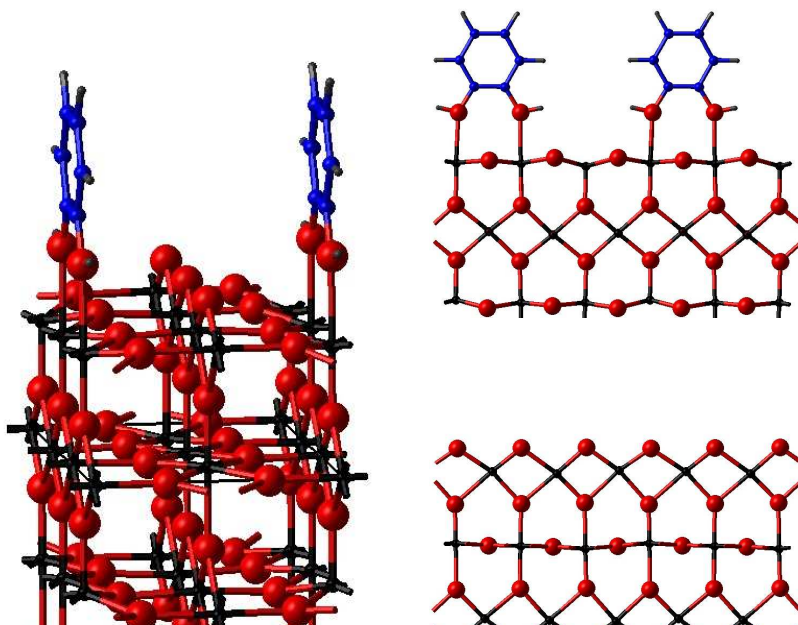


FIG. 4: Molecular Adsorption mode (MA) for catechol molecule on rutile TiO₂ (110) surface.

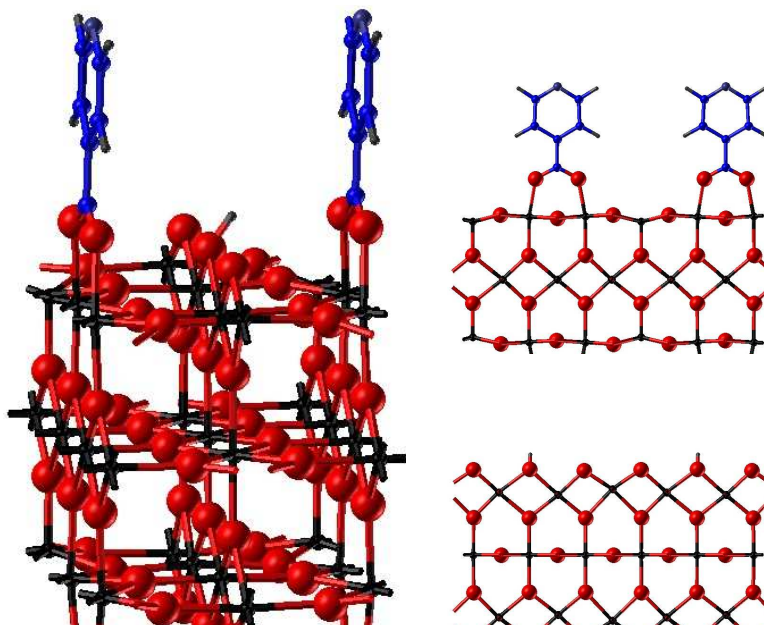


FIG. 5: Dissociative Adsorption mode (DA) for isonicotinic acid molecule on rutile TiO₂ (110) surface.

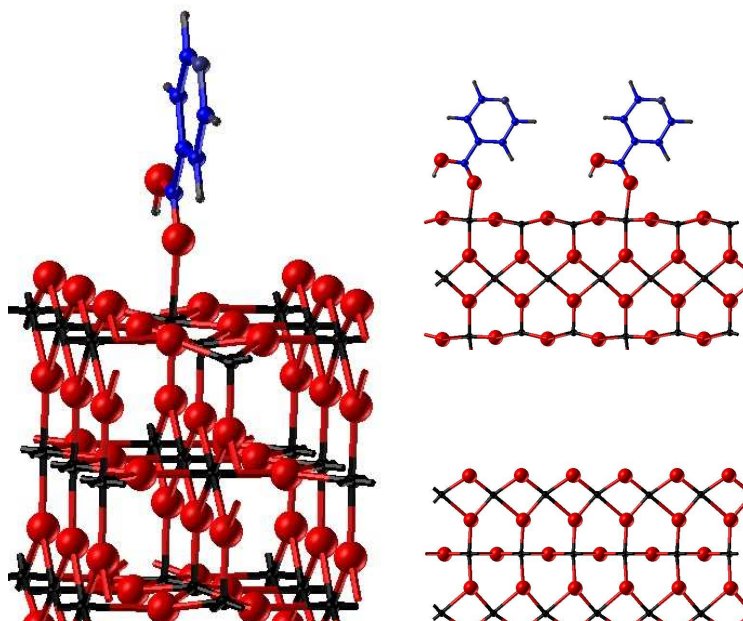


FIG. 6: Molecular Adsorption mode (MA) for isonicotinic acid molecule on rutile TiO₂ (110) surface.