Computational Study of MEA adsorption on TiO_2(110) surface

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The adsorption and dissociation of monoethanolamine (MEA) on clean and defective TiO_2(110) surface was investigated with the density functional theory (DFT) calculation. For accurate approximation for defective surface, Hubbard U parameter (4.2eV) for Ti3d was used and open-shell singlet state was applied for two reduced titanium induced by an oxygen vacancy. To consider hydrogen bond and van der Waals effects of MEA and TiO_2(110) surface, the TS method for DFT-D correction was also implemented. To investigate adsorption tendency of MEA, the displacement of titanium, which binds to MEA, and the adsorption energy of MEA was calculated. With the dissociation of hydrogen of hydroxyl group, the bond length of titanium and oxygen of MEA and it became shorter with increase of titanium displacement. It is shown that dissociative adsorption of MEA was preferred in any formation. In particular, the adsorption on oxygen vacancy site was stable than the clean surface adsorption. Among all systems considered, the dissociative adsorption of MEA on defective surface with the Gauche motif was the most stable state with adsorption energy of -3.604eV.