Coverage-dependent adsorption behavior of MEA on TiO_2(110) and its effect on work function

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The adsorption of monoethanolamine (MEA) on rutile TiO_2(110) surface is important for the application on photo-electric devices through the reduction of the work function of TiO_2(110). Thus, we studied coverage-dependent adsorption behavior of MEA on defective and pristine TiO_2(110) surfaces and its effect on work function (Φ) by density functional theory (DFT) calculation. The adsorption energy (ΔE_{ads}) was calculated with various configurations of MEA molecule. The most stable adsorption was found to be the dissociative adsorption of MEA in gauche configuration at the oxygen vacancy site (ΔE_{ads} = -3.604 eV). Also, the work-function drop was the most efficient with this configuration ($\Delta\Phi$ = -1.132 eV). In case of the pristine TiO_2(110) surface, MEA adsorbed on Ti_{5f} rows with gauche or dissociative gauche configuration showed relatively high adsorption energies. Therefore, after oxygen vacancies were fully occupied by MEA, Ti_{5f} rows will be occupied by gauche or dissociative gauche configurations of MEA. It was found that the work function of pristine TiO_2(110) surface gradually decreased with increasing coverage of MEA for both gauche and dissociative gauche forms.