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Coverage-dependent adsorption behavior of monoethanolamine on TiO_2 (110)

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Understanding adsorption behavior organic molecules at oxide surfaces is very important for the application of organic-inorganic hybrid materials. Recently, monoethanolamine (MEA) adsorbed on TiO_2 surface has received great interests because it can lower the work function of TiO_2 in photo-electronic devices such as OLED and solar cells. In this study, we investigated the role of surface defects in adsorption behaviors of MEA at the rutile TiO_2 (110) surface by combined study of scanning tunneling microscopy and density functional theory calculations. Our results revealed that oxygen vacancy is the most stable adsorption site for MEA on TiO_2 (110) surface at low coverage. As coverage increases, the oxygen vacancies are occupied with the molecules and MEA molecules start to adsorb at Ti rows at higher coverages. Our results show that the defects at oxide surfaces and the intermolecular interactions are important factors for determining stable adsorption structure of MEA at TiO_2 (110) surfaces.

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