

Abstract Submitted
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Monoethanolamine adsorption on TiO₂ (110) for solid supported CO₂ capture¹ DEYU LU, KATHRIN MULLER, Center for Functional Nanomaterials, Brookhaven National Laboratory, SANJAYA SENANAYAKE, Chemistry Department, Brookhaven National Laboratory, DAVID STARR, Center for Functional Nanomaterials, Brookhaven National Laboratory — Solid supported CO₂ capture materials are drawing substantial attention as a promising, cost-effective and environmentally friendly alternative to aqueous amine based CO₂ capture. Recently CO₂ capture was observed from monoethanolamine (MEA) adsorbed TiO₂ powders. In order to facilitate the rational design of future solid CO₂ capture materials, it is very important to understand the interaction between MEA and the TiO₂ surface at the atomic level and how it affects the CO₂ capture capabilities. In this work, we report a combined experimental and theoretical study of MEA adsorption on rutile TiO₂ (110). We found that 1 ML of MEAs can form a stable and ordered pattern on TiO₂ (110). However, the amine group in MEA (the CO₂ capture site) binds preferably to the TiO₂ surface in the gauche mode. The binding energy of the gauche mode is about 0.8 eV larger than the trans mode, where the amine group is free, causing the present MEA/TiO₂ system unable to capture CO₂. We found that this large binding energy difference is originated from a combination of surface donor-acceptor bonds, H-bonds, and dipole-induced dipole interaction. Our study suggests that these effects are key factors to design future amine-based solid supported CO₂ capture materials.

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