Monoethanolamine adsorption on TiO2 (110) for solid supported CO2 capture

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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