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Reactivity of TiO₂ Rutile and Anatase Surfaces toward Nitroaromatics SHAO-CHUN LI, ULRIKE DIEBOLD¹, Department of Physics and Engineering physics, Tulane University, New Orleans, LA 70118, USA — The Au-TiO₂ system is a promising catalyst for the synthesis of nitro-aromatic compounds. The adsorption of azobenzene (C₆H₅N-NH₅C₆) and aniline (C₆H₅NH₂) on two single-crystalline TiO₂ surfaces, anatase (101) and rutile (110), has been investigated with scanning tunneling microscopy (STM), low energy electron diffraction (LEED), and X-ray photoemission spectroscopy (XPS), and synchrotron Ultraviolet photoemission (UPS). While azobenzene adsorbs as an intact molecule at low coverages, ordered overlayers of phenyl imide (C₆H₅N) form at saturation coverage, indicating that TiO₂ surfaces cleave the N-N bond even without the presence of Au. The same superstructures, p(1 × 2) on anatase and c(2 × 2) on rutile and the same electronic structures, form upon adsorption of aniline, suggesting the formation of the same, or a very similar, reaction intermediate. These results suggest that the main role of the supported Au in catalytic aniline ↔ azobenzene conversion is the activation of O₂/H₂ for de/hydrogenation reactions.

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