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Correlation between Bonding Geometry and Band Gap States at Organic – inorganic interfaces: Catechol on Rutile TiO_2 (110)

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Adsorbate-induced band gap states in semiconductors are of particular interest due to the potential of increased light absorption and photoreactivity. A combined theoretical (DFT) and experimental (STM, photoemission) study of the molecular-scale factors involved in the formation of gap states in TiO_2 is presented. Using the organic catechol on rutile $TiO_2(110)$ as a model system it is found that the bonding geometry strongly affects the molecular electronic structure. At saturation catechol forms an ordered 4×1 overlayer. This structure is attributed to catechol adsorbed on rows of surface Ti atoms with the molecular plane tilted from the surface normal by about $\pm 27^\circ$ in an alternating fashion. In the lowest-energy structure one of the two terminal OH groups at each catechol dissociates and the O binds to a surface Ti atom in a monodentate configuration, while the other OH group forms a H-bond to the next catechol neighbor. Through proton exchange with the surface this structure transforms into one where both OH groups dissociate and the catechol is bound to two surface Ti in a bidentate configuration. Only bidendate catechol introduces states in the band gap of TiO_2.

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