# Correlation between bonding geometry and band gap states at organic-inorganic interfaces: catechol on rutile $TiO_2$ (110)

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**Supplemental Computational Results:**

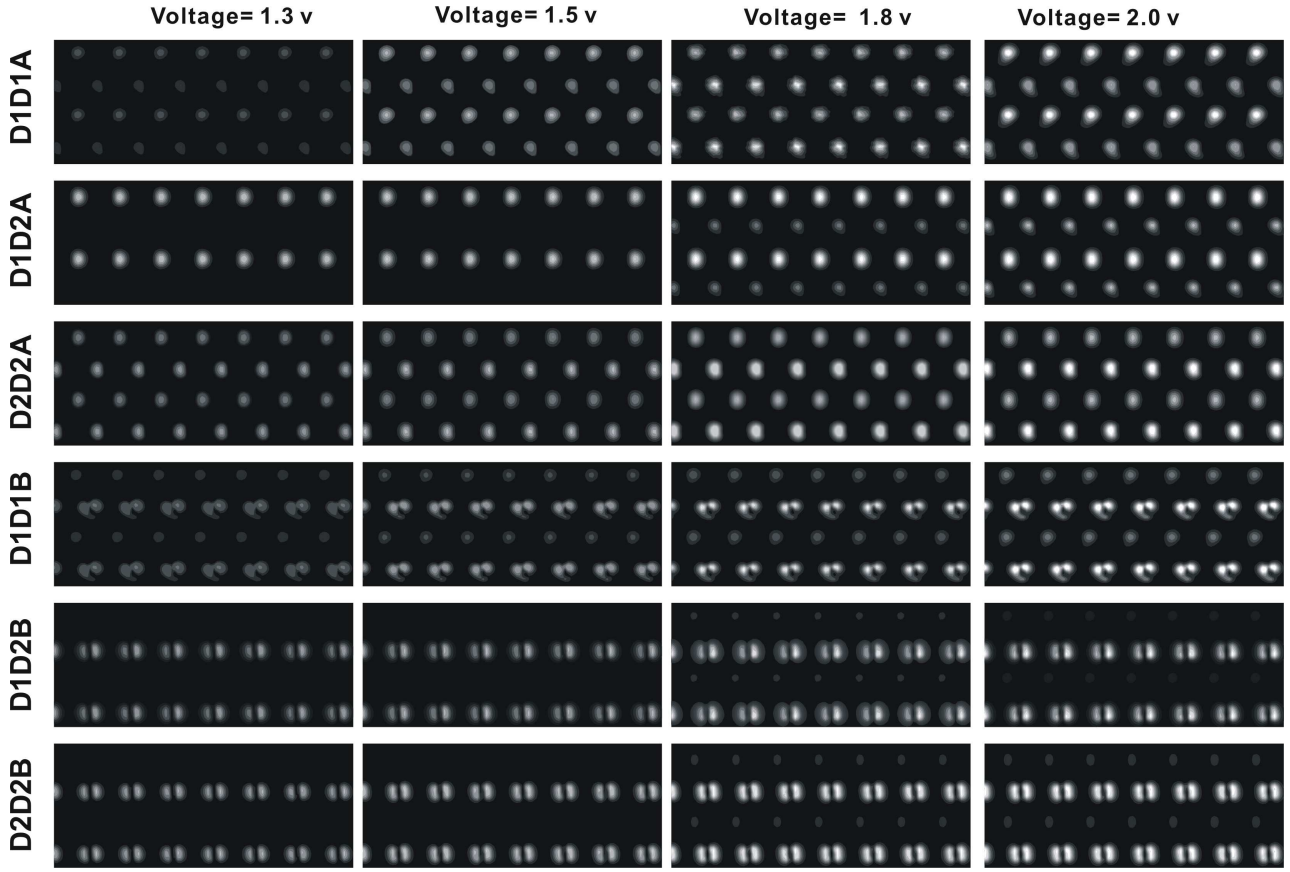


**Figure S1:** Simulated empty state STM images as a function of bias (V=1.3, 1.5, 1.8 and 2.0 eV) for the structures in Fig.2. The same contrast scale is used for all the images. Bias voltages are referenced to the Fermi level, $E_F$. Note that, while $E_F$ is located in the vicinity of the conduction band minimum in slightly-reduced $TiO_2$ samples, it is located at the valence band maximum in the theoretical calculations.

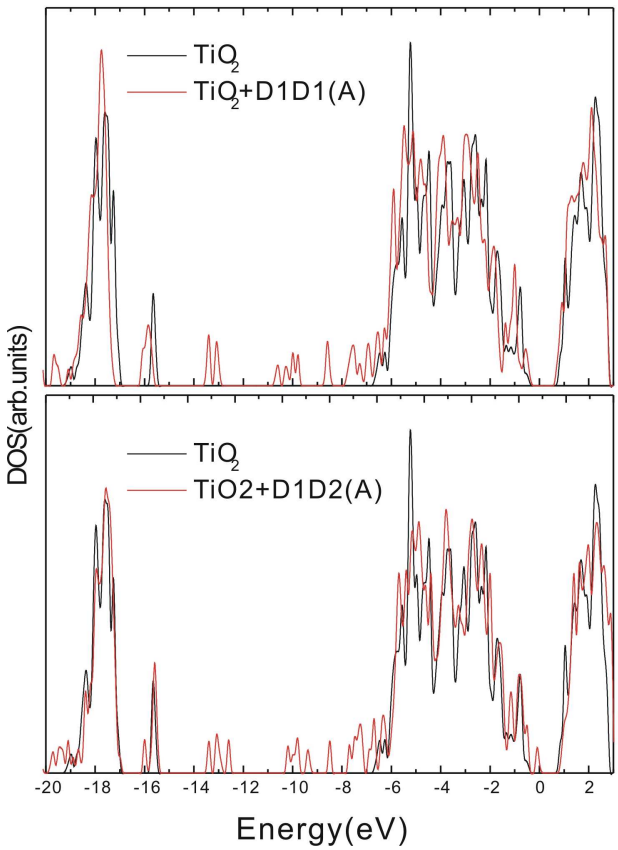


**Figure S2.** Total DOS of a 4 × 1 overlayer of catechol/$TiO_2$ (110) in D1_D1(A) and D1_D2(A) configuration. States well below the O-2p valence band are shown. The DOS for the clean surface is also reported (black curve).