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【217】The polar $KTaO_3$ (001) surface: Electronic structure and CO adsorption

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Polar surfaces offer intriguing physical and chemical properties applicable in electronics or catalysis. Cleaving the $KTaO_3$ perovskite along its polar (001) plane provides a well-defined, bulk-terminated surface with KO and TaO_2 terminations. As-cleaved surfaces exhibit a high concentration of in-gap states; these electrons predominantly reside at the TaO_2-terminated parts of the surface. These electrons can affect surface chemistry, as is demonstrated for CO molecules. CO has two adsorption configurations on the TaO_2 termination, and the CO differs in how it couples to the excess electrons. DFT calculations indicate that CO preferentially couples to electron bipolarons.

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