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Direct assessment of the acidity of individual surface hydroxyls on $In_2O_3(111)$

Non-contact atomic force microscopy is a versatile tool to investigate properties of individual atoms or molecules. Here we report a novel approach to determine the acidity of individual surface hydroxyls, which is directly linked to the proton affinity (PA) of the involved O atoms. The PA - the tendency to gain or lose a proton - is crucial *e.g.* in acid-base catalysis and the electro- and photocatalytic splitting of water.
The testcase of this study is the stoichiometric $In_2O_3(111)$ surface, which has four inequivalent surface O atoms $O_S(\alpha\text{-}\delta)$. Water dissociation leads to a pair of OH groups: the surface $O_SH(\beta)$ and the water O_WH. The remaining surface O atoms $O(\alpha, \gamma, \delta)$ can be protonated via manipulation with the tip. We probe the strength of their H bond with a functionalized tip of a nc-AFM via *F*(z)-spectroscopy and find quantitative agreement with density-functional theory (DFT) calculations. By relating the results to known PAs of gas-phase molecules, we can calibrate our data and determine the PA of different surface sites of $In_2O_3(111)$ with atomic precision. Measurements on hydroxylated TiO_2 and zirconia extend our method to other oxides. The trends of the site-specific PA values agree well with the expectations based on area-averaging techniques.

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