Stabilization of polar ZnO–surfaces: Validating microscopic models by using CO as a probe molecule

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The determination of the structure of inhomogeneous metal oxide surfaces represents a formidable task. With the present study we demonstrate that using the binding energy of a probe molecule, CO, is a reliable tool to validate structural models for such complex surfaces. Combining several types of first-principles calculations with advanced molecular beam methods we are able to provide conclusive evidence that the polar O-terminated surface of ZnO is either reconstructed or hydrogen-covered. This finding has important consequences for the ongoing discussion on the stabilization mechanism of the electrostatically unstable ("Tasker type 3") polar ZnO surfaces.