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Surface Coverage and Metallicity of ZnO Surfaces from First-Principles Calculations XIAO ZHANG, ANDRE SCHLEIFE, University of Illinois, Urbana-Champaign, THE SCHLEIFE RESEARCH GROUP TEAM — Zinc oxide (ZnO) surfaces are widely used in different applications such as catalysis, biosensing, and solar cells. These surfaces are, in many cases, chemically terminated by hydroxyl groups. In experiment, a transition of the ZnO surface electronic properties from semiconducting to metallic was reported upon increasing the hydroxyl coverage to more than approximately 80 %. The reason for this transition is not well understood yet. We report on first-principles calculations based on density functional theory for the ZnO $[10\bar{1}0]$ surface, taking different amounts of hydroxyl coverage into account. We calculated band structures for fully relaxed configurations and verified the existence of this transition. However, we only find the fully covered surface to be metallic. We thus explore the possibility for clustering of the surface-terminating hydroxyl groups based on total-energy calculations. We also found that the valence band maximum consists of oxygen p states from both the surface hydroxyl groups and the surface oxygen atoms of the material. The main contribution to the metallicity is found to be from the hydroxyl groups.

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