

## **Structure Prediction of Zinc-Oxide Surfaces**

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To understand the properties of zinc-oxide (ZnO) surfaces, it is of paramount importance to first understand their atomistic structure. Not only do microscopic structural details directly impact the interfacial electronic structure in hybrid inorganic/organic devices, but they must also be expected to indirectly affect (opto) electronic properties through dictating the growth mode of an organic semiconductor deposited onto ZnO. Also a targeted tailoring of the inorganic/organic interface towards application-specific demands, e.g., through introducing self-assembled monolayers (SAMs) of covalently bonded molecules, hinges on a precise knowledge of the resulting surface structure. Here, I will give an overview over ongoing work in project A4, covering progress in (i) structure and stability prediction of bare and SAM-covered ZnO surfaces, (ii) correlating predicted structures with experimentally accessible quantities such as core-level shifts, and (iii) reaction paths and barriers encountered upon functionalizing of ZnO surfaces with SAMs. Time permitting, I will then briefly summarize the status of joint efforts with other projects in CRC 951.