# Electronic structure of photocatalytic materials: doped ZnO and gold-perovskite interfaces.

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Modern environmental applications call for functional surfaces and interfaces that can be used in photocatalysis and electrocatalysis. To this end, we simulate surfaces and interfaces of two widely used materials: doped ZnO and halide perovskites. Using Density-Functional-Theory (DFT) simulations, we focus on the surface of ZnO and the interface of perovskites with gold. For Mn-doped ZnO, we consider various dopant concentrations at the out-most (surface) layer of Zn atoms, while the interior of the material is kept at the ideal wurtzite structure.For each system, we calculate surface energy and surface workfunction. We discuss trends in surface stability and surface electronic structure of this material, as well as its applications in photocatalysis. Gold is used as a cathode in the majority of perovskite solar cells, however a direct gold-perovskite interface is little studied in literature. We perform first-principles calculations for a gold-perovskite interface, focusing on the energetics and the electronic structure of the system.

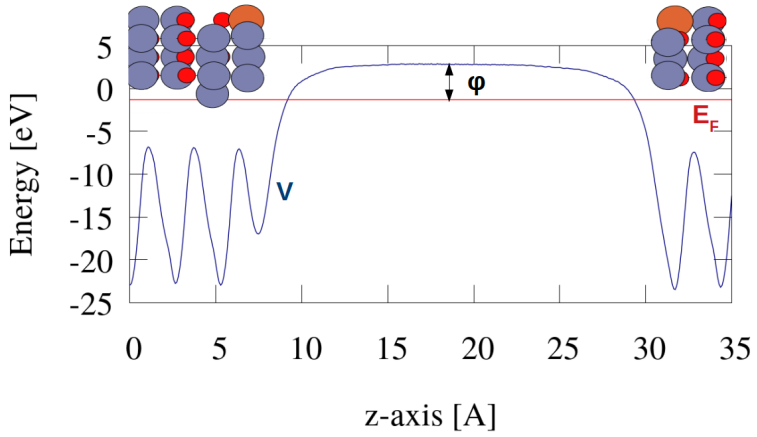


Figure 1: Electronic potential energy as a function of distance from the surface for a periodic simulation of Mn-doped ZnO(0001) slabs. Red, gray and orange spheres represent O, Zn and Mn atoms, respectively. The local potential of the slab (V), Fermi energy (EF) and workfunction () are shown.

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