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A DFT study of low index polar surfaces: the case of SiC and ZnO

GIUSEPPE BRANDINO, GIANCARLO CICERO, Politecnico of Torino, Torino, Italy and CNR-IMEM, Parma, Italy, ALESSANDRA CATELLANI, CNR-IMEM, Parma, Italy — With the advent of nanostructured devices, it appears evident that the role of surface and interface effects may prevail on bulk properties and determine the physical characteristics of the material at the nanoscale: in particular, the understanding of the electronic properties of nanosized structures demands for a proper accurate treatment. Here we report on first principles density functional calculations of the structural and electronic properties of the so called “non-polar” low index surfaces of hexagonal silicon carbide (SiC) and zinc oxide (ZnO), specifically focussing on surface polarity. We first provide an accurate analysis of the macroscopic polarization field as a function of the hexagonality and ionicity of the compound, and then describe in details the properties of the relaxed surfaces. Our predictions nicely compare with recent experimental data on similar SiC and ZnO surfaces: in particular we obtain good agreement between the perpendicular surface dipole component and the experimental work functions values. Moreover, for the first time, we highlight the presence of a strong in-plane dipole component related to dangling bond rearrangement at the surface, which opposes the bulk spontaneous polarization. The decaying behaviour of this dipole inside the slab shows that the presence of surfaces deeply change the polar properties of structures of few nanometers size, while bulk polarization is recovered for thicker systems. Given the importance of surface dipoles in adsorption and functionalization processes, we finally analyze the local surface electric field by employing a simple polar model molecule (HF) as a probe: we describe the interaction in terms of the potential energy surface (PES) experienced by the molecule. This allows us to give a complete description of the surface polarity and to draw conclusions on the most likely adsorption sites of charged and polar species.

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