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Polar properties of ZnO nanostructures. GIANCARLO CICERO, Politecnico of Torino, Torino, Italy; CNR-IMEM, Parma, Italy, ANDREA FERRETTI, CNR-S3, Modena, Italy, ALESSANDRA CATELLANI, CNR-IMEM, Parma, Italy — The advent of nanostructured devices critically enhances the role of surface and interface effects on bulk properties and determines the physical characteristics of the material: in particular, the understanding of the electronic properties of nanosized structures requires a proper accurate treatment. Here we report on first principles density functional calculations of the structural and electronic properties of the (1-100) "non-polar" surface of hexagonal zinc oxide (ZnO) and compare the results with those of ZnO nanowires grown along the [0001] direction and analogous exposed cuts, with a diameter range of about 9-23 Å. We discuss the changes in the nanostructures polarity in terms of two contributions, one related to changes in equilibrium lattice parameters at the nanoscale and the other related to surface effects. Variations of other relevant observables such as the piezoelectric response of the nanowire are addressed. We compare our results with those obtained for nanostructures based on materials with different polarity (e.g. SiC and InN).

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