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Density-functional study of the structure and stability of ZnO surfaces

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An extensive theoretical investigation of the nonpolar $(10\bar{1}0)$ and $(11\bar{2}0)$ surfaces as well as the polar zinc-terminated (0001)-Zn and oxygen-terminated $(000\bar{1})$-O surfaces of ZnO is presented. Particular attention is given to the convergence properties of various parameters such as basis set, *k*-point mesh, slab thickness, or relaxation constraints within local-density and generalized-gradient approximation pseudopotential calculations using both plane-wave and mixed-basis sets. The pros and cons of different approaches to deal with the stability problem of the polar surfaces are discussed. Reliable results for the structural relaxations and the energetics of these surfaces are presented and compared to previous theoretical and experimental data, which are also concisely reviewed and commented.