# Stabilization mechanisms at polar ZnO surfaces in ideal vacuum conditions: a SCC-DFTB study

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We present a study of a variety of surface reconstructions for the most abundant polar ZnO surfaces, namely the Zn-terminated (0001) and the O-terminated ($000\bar{1}$) surfaces [1]. Our method is quantum-mechanical calculations of the tight-binding DFT type. More precisely, we use a SCC-DFTB approach [2] in conjunction with a recently developed parameter set [3]. The applicability, transferability and quality of the chosen set of parameters were thoroughly tested by comparison with results obtained from DFT calculations as well as with earlier experimental and theoretical work, see e.g. [4, 5, 6]. These tests show that, using SCC-DFTB, the polar surfaces of ZnO are described astonishingly well, and at a low computational cost which allows for the investigation of larger - and more realistic - surface structures compared to previous studies. In particular, we find that the different surface terminations demonstrate different reconstruction patterns as a result of minimizing the dipole moment across the surface. At the ZnO(0001) surface, the reconstruction results in a high density of triangular defects with O-terminated step edges, whereas the ZnO($000\bar{1}$) surface favors ordered hexagonal defect patterns. Finally, through an extensive analysis of the SCC-DFTB-generated energetics and electronic structures of surfaces exhibiting many different step defect patterns, we have developed a simple geometric model that manages to predict the favored surface reconstruction patterns for the ZnO(0001) and ZnO($000\bar{1}$) surface terminations.

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