Large-scale SCC-DFTB calculations of reconstructed polar ZnO surfaces

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Large-scale SCC-DFTB calculations of reconstructed polar ZnO surfaces

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Abstract

We present a theoretical study of a range of surface defects for the most abundant polar ZnO(0001)/(000$\bar{1}$) surfaces using a tight binding approach with self-consistent charges (SCC-DFTB). We find that a combination of triangular pits at the Zn-terminated surface and a strongly ordered hexagonal defect pattern at the O-terminated surface constitutes a very stable reconstruction, in excellent agreement with experimental findings. On the whole, the SCC-DFTB method describes the polar surfaces of ZnO very well, and at a low computational cost which allows for the investigation of larger - and more realistic - surface structures compared to previous studies. Such large-scale calculations show that, at the Zn-terminated surface, the reconstruction results in a high density of one-layer deep triangular pit-like defects and surface vacancies which allow for a high configurational freedom and a vast variety of defect motifs. We also present extensive tests of the performance of the SCC-DFTB method in comparison with DFT results.

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