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Title:

Pauling's Rules for Oxide Surfaces

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Abstract:

Determination of surface structures currently requires careful measurement and computationally expensive methods since, unlike bulk crystals, guiding principles for generating surface structural hypotheses are frequently lacking. Herein, we discuss the applicability of Pauling's rules as a set of guidelines for surface structures. The wealth of solved reconstructions on SrTiO₃ (100), (110), and (111) are considered, as well as nanostructures on these surfaces and a few other ABO₃ oxide materials. These rules are found to explain atomic arrangements for reconstructions and thin films just as they apply to bulk oxide materials. Using this data and Pauling's rules, the fundamental structural units of reconstructions and their arrangement are discussed.

Keywords: oxide surfaces, surface structure, perovskite oxides, surface reconstructions, reconstructions, strontium titanate

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