56e A Simple Chemical View of Relaxations at (110) Surfaces of Rutile Structure-Type Oxides

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First-principles electronic structure calculations have been used to examine the geometric and electronic structure of the bulk and (110) surface of two rutile structure-type oxides: stannic oxide, SnO_2, and stishovite, SiO_2. Examination of the 3D valence charge density distributions and the electron localization function (ELF) provides a simple view of the electronic structure in terms of local electron bond pairs and lone pairs. For stoichiometric (110) surfaces, variations in the spatial distribution of electron pairs about the oxygen anions can be interpreted in simple chemical terms as rehybridization of surface oxygen anions, and the driving force for relaxations can be understood qualitatively in terms of the simple valence shell electron pair repulsion (VSEPR) model, independent of the nature of the cation in the structure. For the case of SnO_2, the stability of highly oxygen-deficient surfaces can be understood in terms of the coordination chemistry of the surface Sn cations.