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Orthorhombic Symmetry and Anisotropic Properties of Rutile TiO2

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The symmetry of the material is an important factor determining its properties. In this work, we demonstrate [1] both experimentally and by numerical simulations that the actual symmetry of the rutile phase of TiO2 is CaCl2-type [2] orthorhombic, described with space group Pnnm, in contrast to what it is commonly believed that rutile TiO2 has a tetragonal symmetry [2-4], described with space group P42/mnm. We present very precise first-principles calculations for the determination of the structural properties of rutile TiO2 and highlight the relevance of using the revised regularized SCAN meta-GGA density functional for the interpretation and analysis of neutron and synchrotron radiation diffraction measurements. We showed that symmetry lowering is present in both lattice constants and atomic positions. The lowering of the symmetry has a small but not negligible influence on the elastic, vibrational, and optical properties of rutile TiO2. Results are discussed in the context of analogous lower symmetry structure description in other rutile-type compounds: β-PbO2 [5], β-MnO2 [6] and MnF2 [6].
References:
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