Orthorhombic symmetry and anisotropic properties of rutile TiO_2

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The symmetry of the material is an important factor determining its properties. In this work [1], we demonstrate both experimentally and by numerical simulations that the actual symmetry of the rutile phase of TiO_2 is orthorhombic, described by the space group *Pnnm*, see Fig. 1, in contrast to the commonly held view that rutile TiO_2 has a tetragonal symmetry, described by the space group $P4_2/mnm$ [2, 3]. We present very precise first-principles calculations for the determination of the structural properties of rutile TiO_2 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. The symmetry lowering has a small but not negligible influence on the elastic, vibrational, and optical properties of rutile TiO_2. The symmetry breaking observed for TiO_2 is similar to that reported for β-PbO_2 [4].

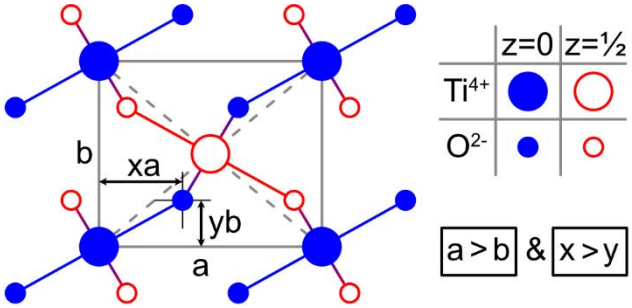

Figure 1. Schematic view of the *Pnnm* TiO_2 unit cell along the *c*-axis.Note the correlation of the oxygen atom position with the unit cell parameters.

[1] Gonzalez Szwacki N., Fabrykiewicz P., Sosnowska I., Fauth F., Suard E. & Przeniosło R. (2023). *J. Phys. Chem. C* **127**, 19240.

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