# 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 [1], we demonstrate both experimentally and by numerical simulations that the actual symmetry of the rutile phase of TiO2 is orthorhombic, described by the space group *Pnnm*, see Fig. 1, in contrast to the commonly held view that rutile TiO2 has a tetragonal symmetry, described by the space group *P42/mnm* [2, 3]. 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. The symmetry lowering has a small but not negligible influence on the elastic, vibrational, and optical properties of rutile TiO2. The symmetry breaking observed for TiO2 is similar to that reported for β-PbO2 [4].

A diagram of a network

AI-generated content may be incorrect.

**Figure 1.** Schematic view of the *Pnnm* TiO2 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.

[2] Burdett J. K., Hughbanks T., Miller G. J., Richardson J. W. J. & Smith J. V. (1987). *J. Am. Chem. Soc*. **109**, 3639.

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