

Polyoxotitanate clusters in sol-gel TiO₂ ?

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Sol-gel preparations of nanocrystalline titania photocatalysts often proceed through the initial formation of a precursor phase that is X-ray amorphous. That is, the powder X-ray diffraction pattern comprises only very broad humps. The precursor phase generally has to be heated at temperatures above 300°C to obtain nanocrystalline titania, usually with the anatase structure. In contrast to the amorphous appearance of the diffraction pattern, the pair distribution function (PDF) for the precursor phase is rich in peaks extending beyond 0.7 nm. Previous studies have attempted to fit the PDF of the precursor phase using structure models based on sub-nanometre clusters of different TiO₂ polymorphs, but without success. In this presentation we consider models based on polyoxotitanate clusters. The different reported crystalline polyoxotitanates will be reviewed and the results of fitting different clusters to the experimental PDF data will be presented.