Electronic Supplementary Information

Structural interpretation of SnO_2 nanocrystals of different morphologies synthesized by microwave irradiation and hydrothermal methods

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1. Preparation of different SnO_2 nanostructures:

1.1 Preparation of SnO_2 nanparticles

Previously, we have reported the microwave assisted synthesis of SnO_2 nanoparticles.[37] In a typical procedure, tin (IV) acetate (0.375 mmol; 0.134 g) was dissolved in a mixture of oleic acid (2.2 ml) and oleyl amine (3.6 ml). The resulting solution was heated at 110°C for 5 minutes under vigorous stirring. After heating, Tin (IV) acetate was dissolved and a yellowish viscous solution was obtained. After cooling to room temperature, the viscous solution was transferred to a microwave tube of 10 ml capacity. The tube was inserted into a mono-mode microwave reactor with power set 200 W at 120°C for 5 minutes. After the reaction, the resulting solution was diluted by chloroform. A white precipitate was obtained which was dissolved in chloroform and then it was re-precipitated by adding ethanol. Finally, the white precipitate was centrifuged and washed several times by ethanol. The obtained precipitate was finally dried in an oven at 60°C over night to get the final product as greyish white powder.

1.2 Preparation of SnO_2 nanospheres by microwave irradiation method using ionic liquid

About 0.175 g of $SnCl_4 \cdot H_2O$ was dissolved in 10 ml of deionised water. To this solution about 0.2 g of NaOH and 0.5 g of an ionic liquid $(BMIm)BF_4$ were added. A clear solution was obtained. After stirring the solution for 30 minutes, the resulting solution was placed in a microwave tube of 10 ml capacity. The tube was inserted in a mono-mode microwave reactor with power set 200 W at 120°C for 45 minutes. After the reaction was

completed, the solution was cooled down to room temperature. A white suspension was obtained which was centrifuged and washed several times by distilled water. The obtained precipitate was finally dried in an oven at 70°C for 2h. to get the final product as white powder.

1.3 Preparation of SnO_2 nanorods by hydrothermal method

Previously, we have also reported the hydrothermal synthesis of SnO_2 nanorods.[37] In a typical procedure, about 0.525 g (1.5 mmol) of $SnCl_4 \cdot 5H_2O$ was dissolved in 10 ml of water. About 0.7 g of NaOH was dissolved in 20 ml water and 20 ml ethanol was added to this solution to make a 1:1 basic mixture of alcohol and water. This mixture was added drop wise to the $SnCl_4 \cdot 5H_2O$ solution with continuous stirring. A white cloudy suspension was slowly formed at acidic pH. This white suspension slowly disappeared with increasing pH and a clear solution was obtained at pH range 11–12. The clear solution was placed in a Teflon lined steel chamber of 110 ml capacity and the steel chamber was placed inside an oven and heated at 180°C for 12 h. After the reaction was completed, the steel chamber was air-cooled to room temperature. The products were then collected and washed with distilled water and ethanol several times to remove the impurities. The obtained white powdery product was then dried in an oven overnight at 60°C to get the final product as a white powder.

1.4 Preparation of SnO_2 nanopyramides by hydrothermal method

The synthesis of SnO_2 nanopyramides by hydrothermal method is reported by Das et al.[38] We used this method with slight modification. In a typical procedure, about 2.1 g of $SnCl_2 \cdot 2H_2O$ was dissolved in a mixture of 10 ml of distilled water and 10 ml of ethanol. About 2.0 g of NaOH was also dissolved in 10 ml water and 10 ml ethanol was added to this solution to make a 1:1 basic mixture of alcohol and water. Now this basis mixture was added slowly to the $SnCl_2 \cdot 2H_2O$ solution with continuous stirring. The resulting solution was placed in a Teflon lined steel chamber of 50 ml capacity and the steel chamber was placed inside an oven and heated at 180°C for 10 h. After the reaction was complete, the steel chamber was air-cooled to room temperature. The products were then collected and washed with distilled water and ethanol several times to remove the impurities. The obtained white powdery product was then dried in an oven overnight at 60°C to get the final product as a white powder.

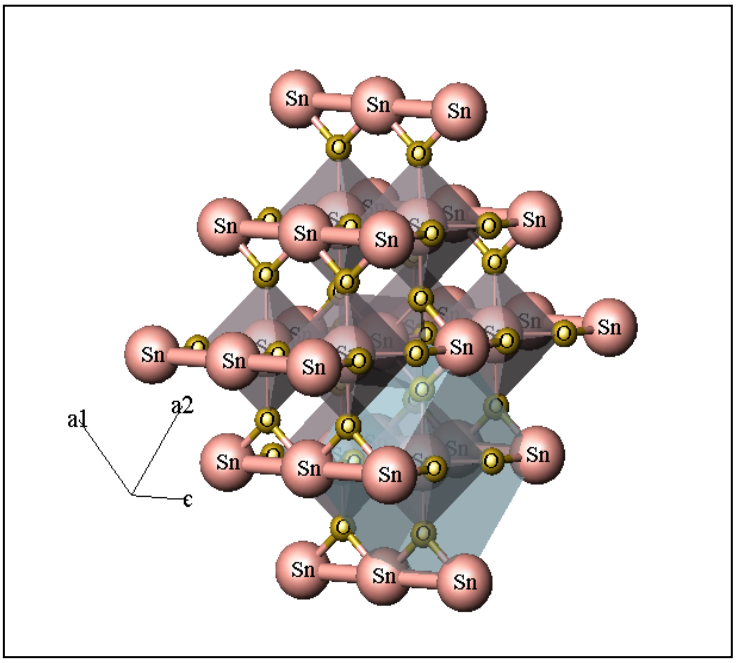

Figure S1. Atomic structure of tetragonal (ICSD database no. 154960) SnO_2 phase with SnO_6 octahedra.

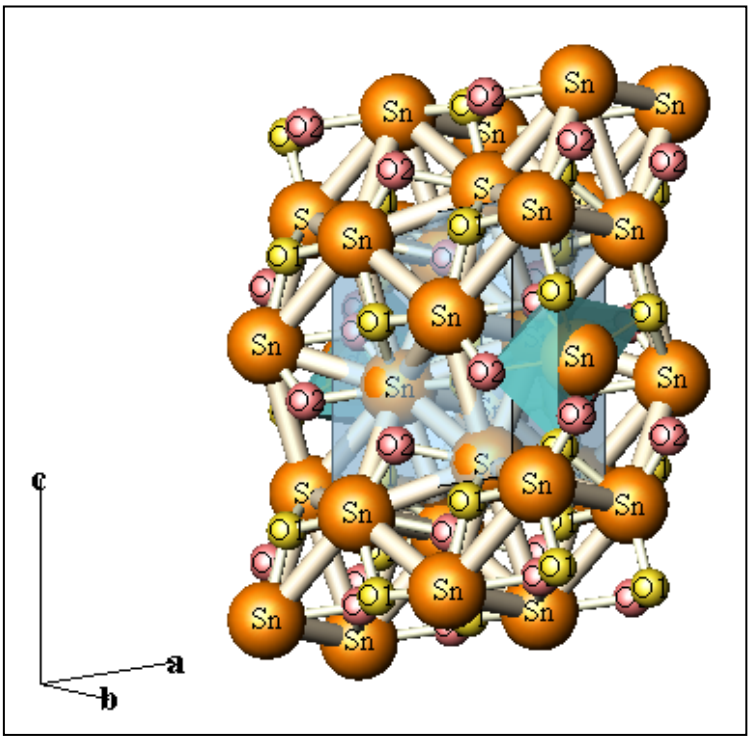

Figure S2. Atomic structure of orthorhombic-I (ICSD database no. 181283) SnO_2 phase with tilted octahedra.

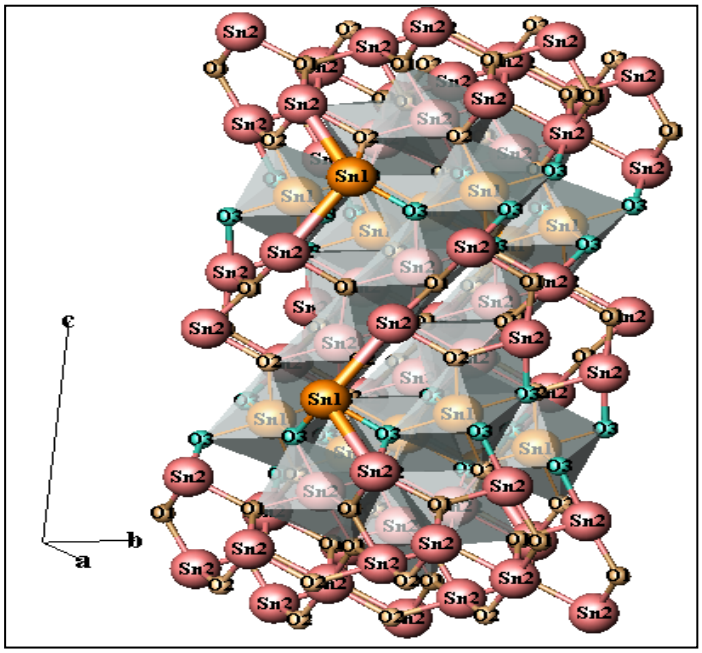

Figure S3. Atomic structure of orthorhombic-II (ICSD database no. 62199) SnO_2 phase with less tilted SnO_6 octahedra.

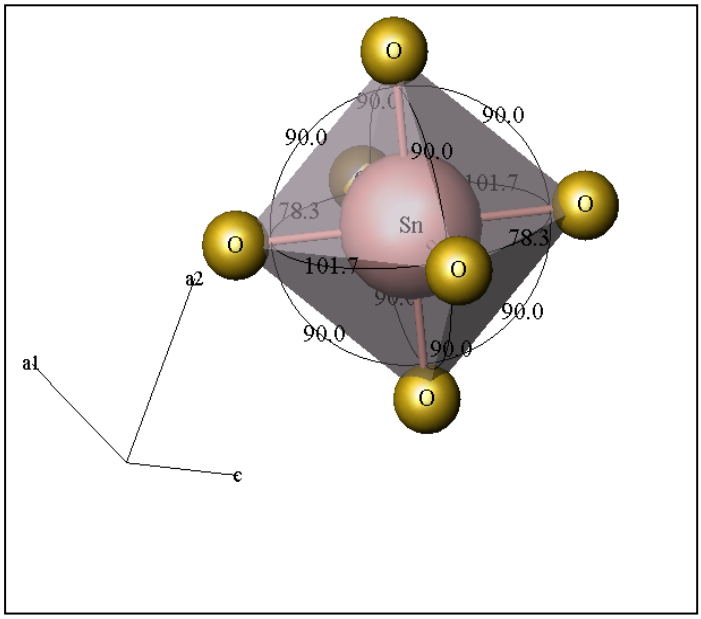

Figure S4. Individual SnO_6 octahedron with different bond angles of tetragonal (ICSD database no. 154960) SnO_2 phase.

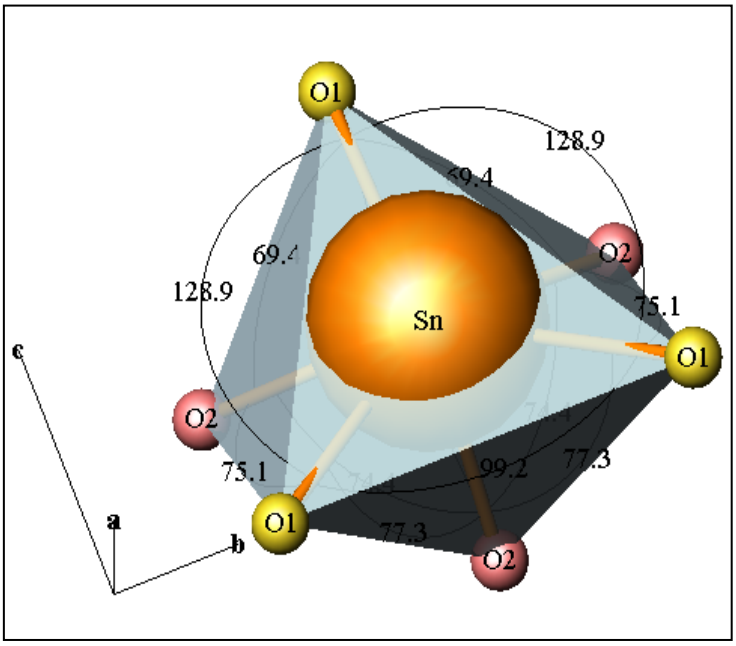

Figure S5. Formation of tilted octahedron due to asymmetrical Sn-O bond lengths and bond angles of orthorhombic-I (ICSD database no. 181283) SnO_2 phase.

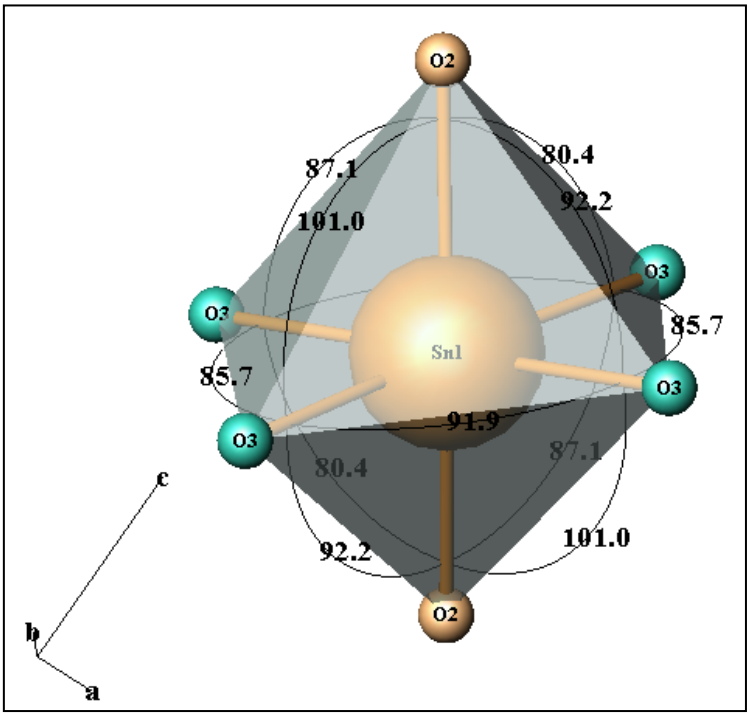

Figure S6. Formation of less tilted octahedron due to almost symmetrical Sn-O bond lengths and bong angles of orthorhombic-II (ICSD database no. 62199) SnO_2 phase.