

## Supplementary materials

### *In situ* high temperature X-ray diffraction, transmission electron microscopy and theoretical modeling for the formation of WO<sub>3</sub> crystallites

Suman Pokhrel<sup>1</sup>, Johannes Birkenstock,<sup>2</sup> Arezoo Dianat<sup>3,4</sup>, Janina Zimmermann<sup>3,5</sup>, Marco Schowalter<sup>6</sup>, Andreas Rosenauer<sup>6,7</sup>, L. Colombi Ciacchi<sup>3,7</sup>, L. Mädler<sup>1,7\*</sup>

<sup>1</sup>Foundation Institute of Materials Science (IWT), Department of Production Engineering, University of Bremen, Germany

<sup>2</sup>Central Laboratory for Crystallography and Applied Materials, University of Bremen, Germany

<sup>3</sup>Hybrid Materials Interfaces Group, Department of Production Engineering and Bremen Center for Computational Materials Science, University of Bremen, Germany

<sup>4</sup>Institute for Materials Science, University of Dresden, Germany

<sup>5</sup>Fraunhofer Society Headquarter, Munich, Germany

<sup>6</sup>Institute of Solid State Physics, University of Bremen, Germany

<sup>7</sup>MAPEX Center for Materials and Processes, University of Bremen, Germany

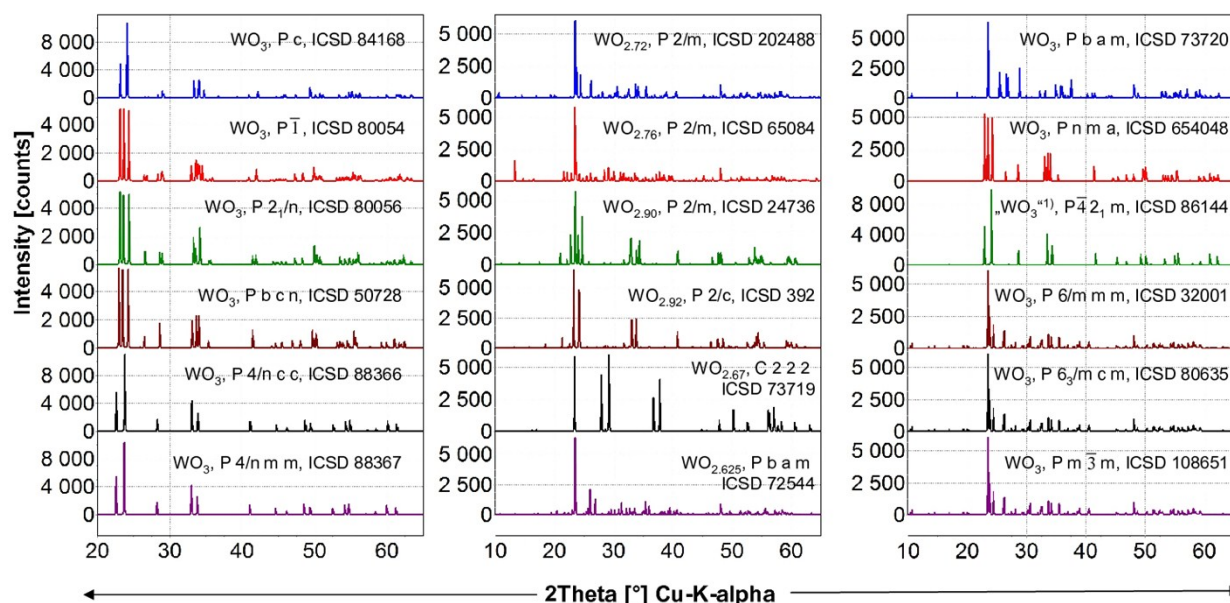


Fig. S1: Calculated XRD patterns for all structurally unique WO<sub>3-x</sub> found in the ICSD (inorganic crystal structure database, FIZ Karlsruhe) together with respective composition and number of the applied ICSD entry. (a) temperature dependent series of stable phases of non deficient WO<sub>3</sub> including the three phases found in the present study, (b) oxygen-deficient phases WO<sub>3-x</sub> (c) other

nominal  $\text{WO}_3$  phases. Among the latter, it was recognized that ICSD entry 86144 is nominally entered as non deficient  $\text{WO}_3$ , while it was clearly characterized as oxygen-deficient  $\text{WO}_{2.9}$  in the related paper of Locherer et al. (1999). The intensities of all patterns are calculated from the ICSD entries referenced in the figure. They are on the same scale and thus represent the proportions they would have in any mixture with equal fractions of this phases<sup>1-4</sup>.

## References

- 1 A. Aird, E. K. H. Salje, *J. Phys: Condensed matter*, 1998, **10**, L377.
- 2 A. Aird, M. C. Domeneghetti, F. Mazzi, V. Tazzoli, E. K. H. Salje, *J. Phys: Condensed matter*, 1998, **10**, L569.
- 3 K. R. Locherer, I. P. Swainson, E. K. H. Salje, *J. Phys.: Cond. Matter*, 1999, **11**, 4143.
- 4 K. R. Locherer, I. P. Swainson, E. K. H. Salje, *J. Phys.: Cond. Matter*, 1999, **11**, 6737.