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Electronic and optical properties of single crystal SnS_2: an earth-abundant disulfide photocatalyst.†

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1 Supporting Information

Figure 1 of Supporting Information shows the obtained single crystal X-ray diffraction pattern and the matched sample pattern for this case. The pattern determines the standard hexagonal crystal structure with *P-3m1* symmetry (space group 164) corresponding to the ground state 2H polytype with the lattice constants $a = 3.649$ Å and $c = 5.899$ Å. We note that the 4H SnS_2 structure has a major (0113) peak at 34 °, which we do not see.

Figure 2 shows the first order Laue zone (FOLZ) obtained for the single crystals of SnS_2 at two different contrast settings. The reader is invited to discern the absence of any inner ring formation that would be indicative of polytype impurities in these crystals.

Figure 3 shows the XPS spectrum for the SnS_2 crystals. It is possible to see that very few impurity peaks exist with the exception of relatively small adventitious carbon and oxygen peaks present.

Finally, Figure 4 shows the optical absorption spectra as a function of temperature from Fourier transform infra-red spectrophotometry (FTIR). This figure contains the absorption data plotted as $\alpha^{1/2}$ versus photon energy for indirect gaps, alongside extrapolation to absorption onsets for the temperatures as labelled.

The authors conclude that the analysis performed in this work successfully corresponds to the physical properties of the ground state 2H polytype of SnS_2.

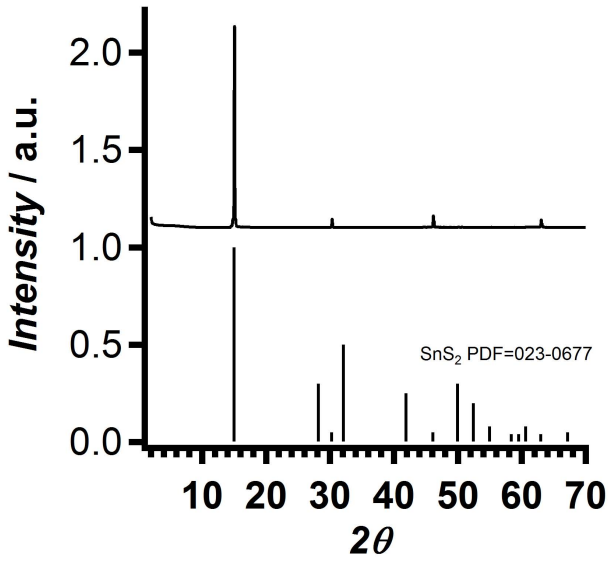

Fig. 1 Single crystal XRD of SnS_2 (top) and the corresponding structure match (bottom).

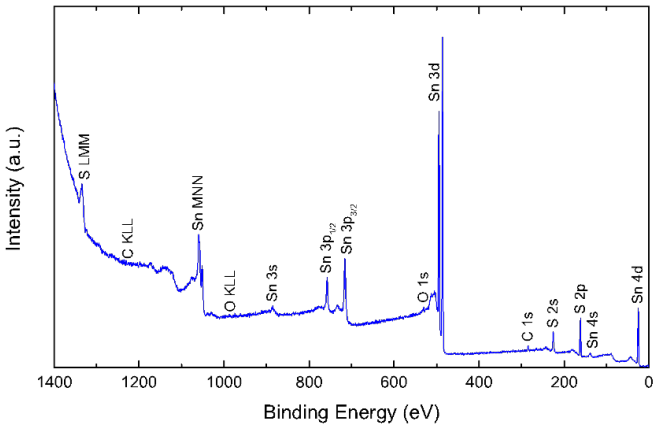

Fig. 3 XPS spectrum for the SnS_2 crystals. Characteristic peaks for Sn and S are present with only minimal adventitious carbon and oxygen contamination.

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† Electronic Supplementary Information (ESI) available: [details of any supplementary information available should be included here]. See DOI: 10.1039/b000000x/

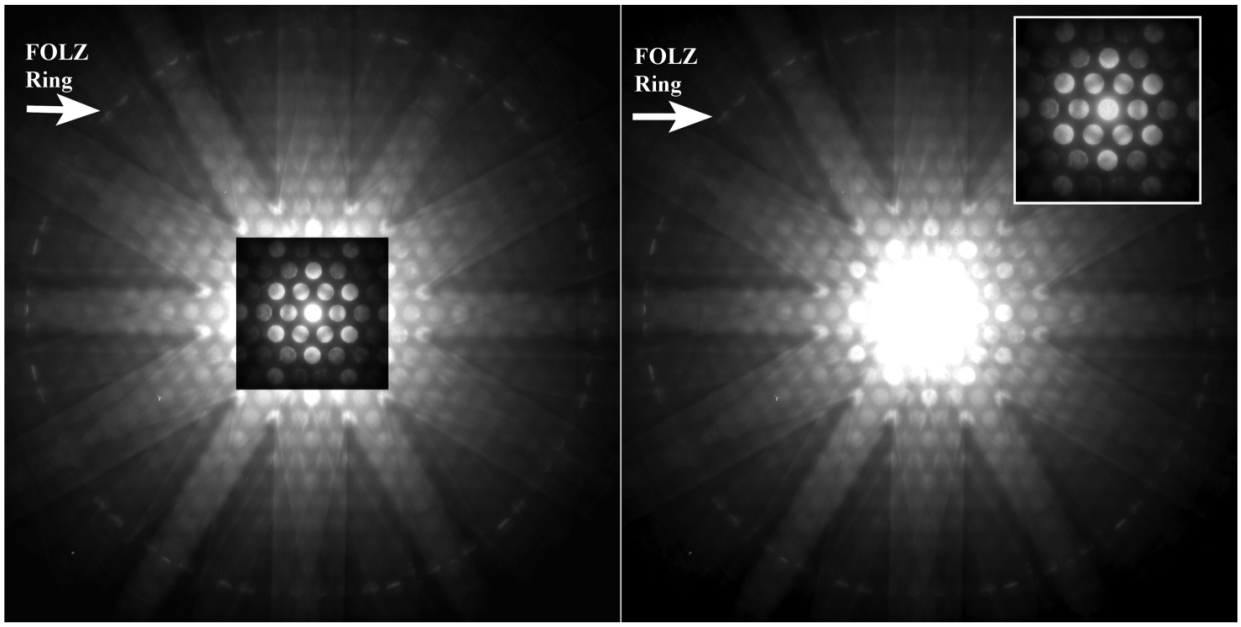

Fig. 2 TEM diffraction patterns for a selected area electron diffraction in the [0001] direction of SnS_2. Two different contrast settings are shown to highlight the absence of inner Laue rings, associated with phase impurities. The FOLZ ring associated with 2H polytype of tin disulfide is highlighted.

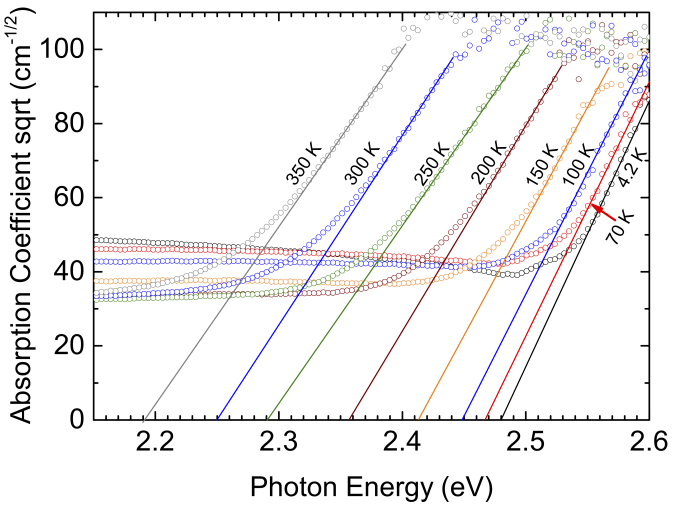

Fig. 4 Optical absorption spectra as a function of temperature containing the absorption data plotted as $\alpha^{1/2}$ versus photon energy.