

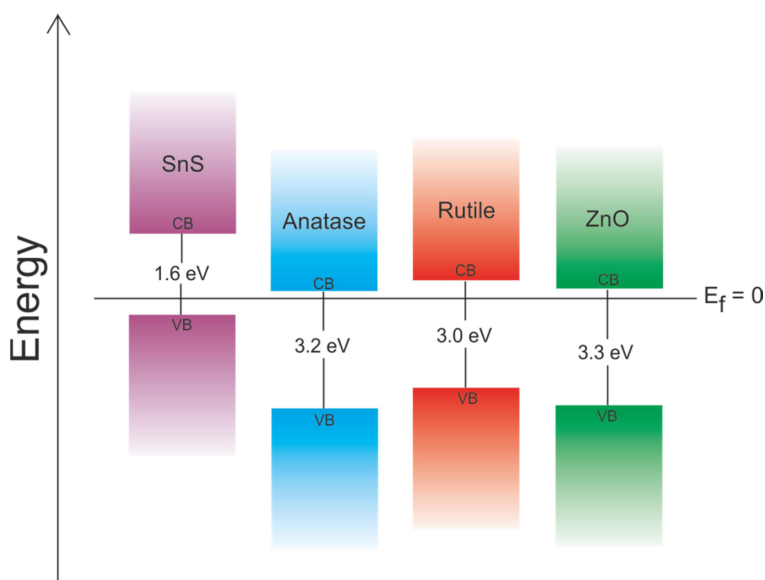
Band alignment analysis of 2D SnS with Anatase (101), Rutile (110), and ZnO (100) by x-ray photoelectron spectroscopy.

Rosemary A. Jones^{1,5}, David Lewis¹, Karen Syres², Aleksander A. Tedstone³, Zheshen Li⁴
Paul O'Brien^{1,3}, Andrew G. Thomas^{1,5}.

1. School of Materials, University of Manchester, UK
2. School of Physical Sciences and Computing, University of Central Lancashire, UK
3. School of Chemistry, University of Manchester, UK
4. Department of Physics and Astronomy, Aarhus University, Denmark
5. Photon Science Institute, University of Manchester, UK

Dye, quantum dot and perovskite sensitised metal oxides are a subject of intensive research. An alternative approach to sensitising surfaces is to use small band gap 2-D materials, such as chalcogenides where the band gap can be tuned by varying the number of layers [1]. In order for such devices to operate the relative positions of valence and conduction bands of the sensitiser and n-type material is important.

Here we report on the measurement of band alignment of 2-D SnS deposited on anatase (101) surface by x-ray photoelectron spectroscopy (XPS). The 2-D SnS was obtained by liquid-phase exfoliation and deposited directly onto an anatase (101) single crystal surface, which had been cleaned under ultra-high vacuum conditions. To determine the alignment the valence band offset for the heterojunction n-TiO₂/p-SnS was measured using soft XPS which gave an overlap of 0.55 eV. Literature values of the band gaps of 2-D SnS (1.6 eV) [1] and anatase TiO₂ (3.2 eV) [2] were used to determine the conduction band position. Analysis shows that the interface between p-SnS and single crystal anatase phase n-TiO₂ has a type II offset. Under the same conditions Rutile (110) and ZnO (100), with bandgaps of 3.0 eV [3] and 3.3 eV [4] respectively, also demonstrated a type II offset interface with 2-D SnS. Rutile (110) and ZnO (100) showed larger overlaps with 2-D SnS of 0.9 eV and 0.7 eV respectively.



- [1.] Jack R. Brent, David J. Lewis, Tommy Lorenz, Edward A. Lewis, Nicky Savjani, Sarah J. Haigh, Gotthard Seifert, Brian Derby, and Paul O'Brien, *J. Am. Chem. Soc.*, **2015**, vol.137, issue 39, 12689–12696.
- [2.] L. Kavan, M. Gräzel, J. Rathousky, and A. Zukal, *J. Electrochem. Soc.* **1996** vol. 143, issue 2, 394-400.
- [3.] B Poumellec, P J Durham and G Y Guo, *J. Phys: Condensed Matter*, **1991** vol. 3, issue 42.
- [4.] S. Major, A. Banerjee, and K.L. Chopra, *Thin Solid Films*, **1983**, vol. 108, no. 3, 333–340.