**Defects and doping limits in $SnO_2$**

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Transparent conducting oxides (TCOs) are compounds which combine the normally mutually exclusive properties of transparency and conductivity. Most highly transparent materials, such as glass, behave as insulators with high electrical resistivities of > $10^{10}$ Ω cm, whereas materials with low resistivities ($10^{-4}$-$10^{-7}$ Ω cm), such as metals, do not transmit visible light. The combination of both properties in a single material is thus quite an unusual phenomenon and TCOs have proved indispensable in the development of optoelectronic devices such as solar cells, flat panel displays and light emitting diodes. [1-3] $SnO_2$ has long been known to display *n*-type TCO properties when oxygen-deficient or doped with donor cations such as Sb or anions such as F. The origin of the observed conductivity is not clear with hydrogen being suggested as the source of conductivity. In addition, Sb can take on two different oxidation states making its role in conductivity more complicated. *p*-type $SnO_2$ has also been investigated through acceptor doping (e.g. N and group 13 cations), although it is not clear what the electronic nature of the defects formed is, or indeed, if *p*-type $SnO_2$ can be formed. While modelling studies have been performed to look at defects in $SnO_2$, none of these have suitably taken into account the band gap which is underestimated by DFT by approximately 3.0 eV, making the understanding of charged defects impossible.

In this project, the grand challenge is to investigate the origin of conductivity in the bulk and on the surfaces of *n*-type $SnO_2$ using a hybrid-DFT approach, which will remove any band gap issues. We will carry out a consistent study on the effect of intrinsic and extrinsic defects in the bulk and at the surfaces of $SnO_2$ utilising a hybrid functional that successfully predicts the fundamental band gap of $SnO_2$ without the need for any empirical parameters. We will investigate the microscopic origins of the doping limits associated with both current and alternative *n*-type dopants and examine co-doping strategies to boost conductivity. The possibility of *p*-type $SnO_2$, specifically examining the most popular acceptor dopants in the literature to date, will be addressed. We will study the origin of the electron accumulation layers on $SnO_2$ surfaces by analysing the role of surface and subsurface native defects.