School of Physics

Research project in **Nanoelectronics/Nanotechnology**

Research project in **Theoretical & Computational Solid State**

Resonant inelastic x-ray scattering:
probing chemical bonding in transition metal compounds

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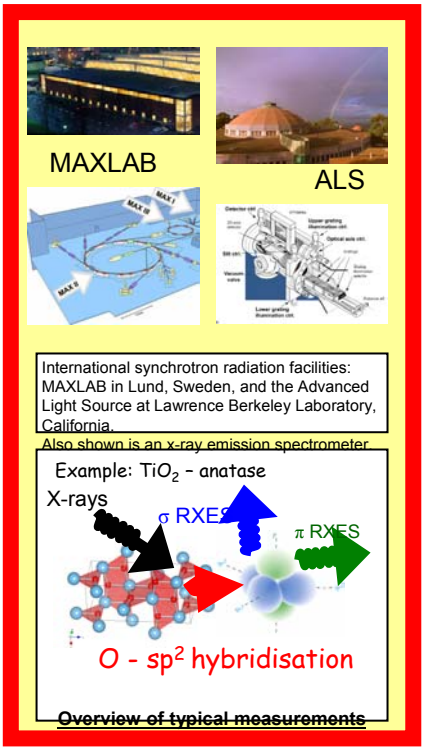
Scientific Background / Current Research

The nature of the chemical bond is of fundamental interest as it is the interplay between the physical structure and chemical bonding in a material which gives rise to the electronic bandstructure and the properties. Photon-in/photon-out **x-ray absorption/emission spectroscopy** or **resonant inelastic x-ray scattering**, is elementally selective and can probe either end of a metal-anion chemical bond in a transition metal fluoride or oxide binary compound, impossible by any other method. This can be exploited in e.g. MnF_2 a rutile transition metal fluoride and prototypical antiferromagnet, as well as other MA_2 systems in which the anion (oxygen or fluorine) is sp^2 hybridised such as in TiO_2 (rutile or anatase). In these due to the anisotropy of the chemical bonding and crystal structure, there is a combination of polarisation dependence (**dichroism**) and **symmetry-** and **state-selectivity** in the observed RIXS/RXES e.g. at the fluorine K edge. This dichroism gives separate probes of the differing occupied σ-like and π-like Metal-Anion-derived orbitals that contribute to the electronic bandstructure in these systems. Measurements at an elementally selective metal L-edge then gives complementary information from the other side of the Metal-Anion chemical bond.

Project

To measure the **symmetry dependent resonant x-ray emission spectroscopy** or **resonant inelastic x-ray scattering** for a variety of structurally similar transition metal fluorides and oxide. We seek to **measure** and **model** this polarisation dependent RXES at the anion K-edge and especially in metal 2p-3d RIXS and observe in detail how this varies with d-shell filling across the transition metal period. We will connect this with **models** of the electronic bandstructure to **derive further insight** into chemical bonding in these materials. These measurements and derived model spectra will in particular be applied to defective TiO_2, *as used in memristors*, to probe the **local defective electronic structure** due to anion (oxygen) vacancies and cation (or Ti^{3+}) interstitials. Bulk single crystal samples of these materials are available and epitaxial thin films will be grown. RXES/RIXS measurements take place at **synchrotron radiation** facilities, such as those at MAXLAB in Sweden, the Swiss Light Source or Advanced Light Source (ALS), Lawrence Berkeley Lab, CA USA.



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Funding

Funding may be possible under HEA PRTLI 5 programme

More information / References