Poster

Order-disorder control in functional oxides

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The exploitable properties of many functional materials (e.g., their electronic, magnetic, or dielectric properties) are intimately linked to their atomic structure. Investigating the order-disorder transitions of various metal oxide systems can elucidate the physical behaviour observed. This project focuses on the synthesis of both well understood and novel polycrystalline and single-crystal samples of materials exhibiting the *defect pyrochlore* structure, allowing for the measurement of their physical properties, such as conductivity, magnetism, and heat capacity. The correlation of structure with properties can be probed using a combination of Bragg crystallography (powder and single crystal), total scattering or PDF measurements and single crystal diffuse scatter [1].

Of particular interest are a class of metal oxides called *defect pyrochlores* or *β-pyrochlores* of the structure $AMM'O_6$. These materials can exhibit a wide range of functional properties such as metal-insulator transitions, multiferroic behaviour and thermoelectricity. The *A* cation in these materials is a large and low valency metal, while the M and M' cations are smaller higher valency metals, allowing for tuning of their physical properties by substitution for different metal cations. The materials contain a variety of structures varying from cubic and orthorhombic down to monoclinic. Investigation of the symmetry lowering mechanisms and local order-disorder mechanisms will provide greater detail on the reasons for the behaviour of metal oxides and allow for tuning of physical properties for specific functions [2].

In addition, investigations into materials based on $BiMSbO_6$ (*M* = *Ti or* Sn) were carried out due to interest in Bi^{3+} existing on an unusual crystallographic site (*16d* / 0.5, 0.5, 0.5). These materials had shown useful in photocatalysis applications but detailed investigations of the crystal structures of these materials was lacking, therefore, thorough crystallographic experiments were carried out to probe this system and illuminate the true nature of the order-disorder within the materials [3].

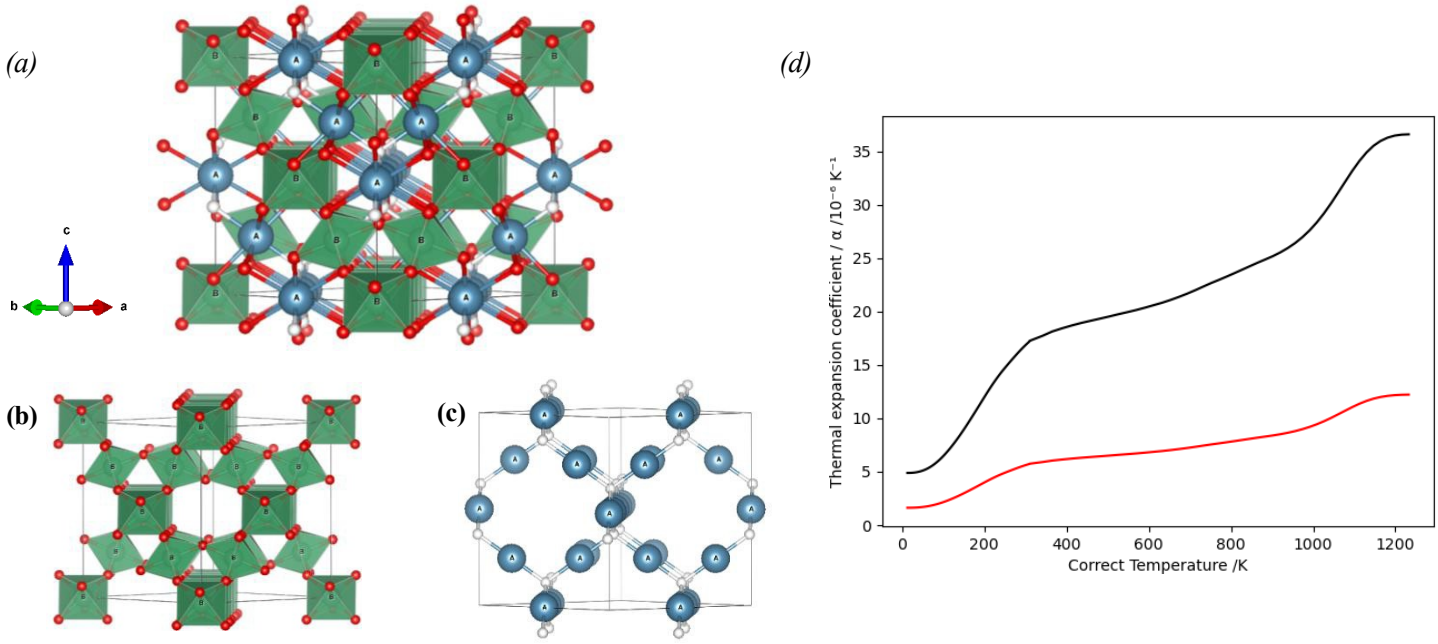

Figure 1. (a) The α-pyrochlore structure $Ca_2Nb_2O_7$, visualised using VESTA, where the blue spheres represent *Ca*, the green spheres represent *Nb*, the red spheres represent *O* at the *X* site, and the white spheres represent *O* at the *Y* site. (b) The B_2X_6 network of corner sharing NbO_6 tetrahedra. (c) The A_2Y network of corner sharing Ca_4O tetrahedra. (d) Plot of thermal expansion of $BiTiSbO_6$ against temperature in terms of volume (black) and *a* cell parameter (red).

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