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A Synchrotron Investigation Of The Electronic Structure Of Lanthanide Zirconates

The lanthanide zirconates are of interest for use in inert matrix fuels and nuclear wasteforms. For use in these applications, the material's structure must be as impervious as possible to radiation damage, and, therefore, its thermal, thermodynamic, and mechanical properties, at a basic sciences level, must be known to make any sort of real-world predictions. The rare earth zirconates are interesting model systems to explore such problems. In these materials the f-electrons may play a localized-valence decisive role in determining their thermo-mechanical properties making them an intriguing model for the interplay between the localised and delocalised valence nature of such oxide materials, the full understanding of which may also lead to novel material development. The f-electronic structure has historically proved difficult to model, however.

We have synthesised the full series of lanthanide zirconates using solid state techniques. We have performed X-ray photoemission spectroscopy (XPS), valence band photoemission, and X-ray absorption near edge spectroscopy (XANES) with synchrotron radiation on a selection of the series. XANES has shown to be very sensitive to the Zr coordination environment. In conjunction with a density functional theory (DFT) model, we have determined the electronic structure and the role of the 4f electrons to the stability of these interesting materials.

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