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The Electronic and Vibrational Structure Of Lanthanide Zirconates

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The lanthanide zirconates are of interest for their use in inert matrix fuels and as nuclear wasteform containment material. For use in these applications, the material's structure must be as resistant as possible to radiation damage, and, therefore, at a basic level, present an electronic and vibrational structure with thermodynamic and mechanical properties that are favourable to long term structural stability under harsh radiation environments. The rare earth zirconates are interesting model systems to explore such problems. This study finds that in these materials the f-electrons 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, however, historically proved rather difficult to model. The full series of lanthanide zirconates was synthesised using solid state techniques and a variety of neutron and synchrotron experiments performed to study the electronic and vibrational structure of this series. In conjunction with a density functional theory (DFT) model, the electronic and vibrational structure is determined and the role of the 4 f electrons to the stability of these interesting materials studied. Unlike the lanthanide titanate series, the interplay between electronic and vibrational character plays the decisive role in determining the fate of the materials stability.

Speakers Gender

Male

Travel Funding

No

Level of Expertise

Expert

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No

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