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A Synchrotron Investigation Of The Electronic Structure Of Lanthanide Zirconates RICHARD CLEMENTS, Bragg Insitute, ANSTO and School of Chemistry, The University of Sydney , BRENDAN KENNEDY, School of Chemistry, The University of Sydney, CHRISTOPHER LING, Bragg Institute, ANSTO and School of Chemistry, The University of Sydney, ANTON P.J. STAMPFL, Bragg Institute, ANSTO — abstract- 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 resistant to radiation damage and its thermal, thermodynamic and mechanical properties must be known. The rare earth zirconates are interesting model systems to explore such problems. In such materials the f-electrons may play a localized valence decisive role in determining their thermo-mechanical properties. We have undertaken a synthesis of the full range of the lanthanide zirconate series using solid state techniques. We have performed X-ray photoemission spectroscopy (XPS) and X-ray absorption near edge spectroscopy (XANES) with synchrotron radiation on a selection of the series, in conjunction with a density functional theory (DFT) determination of the electronic structure. -

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