

Abstract Submitted
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Actinide oxides under pressure LEON PETIT, Daresbury Laboratory, MALCOLM STOCKS, Oak Ridge National Laboratory, MARTIN LUEDERS, ZDZISLAWA SZOTEK, WALTER TEMMERMAN, Daresbury Laboratory, AXEL SVANE, Aarhus University — We use the self-interaction corrected local spin density approximation to investigate the oxidation of actinide dioxides under pressure. The methodology enables us to determine the ground state valency configuration of the actinide 5f electrons and to study the localization/delocalization transition that occurs under pressure. We argue that this delocalization facilitates the oxidation of the actinide dioxides and present results for the estimated transition pressures.

Leon Petit
Daresbury Laboratory

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