Investigating defects in actinides oxides by coupling electronic structure calculations and Positron Annihilation Lifetime Spectroscopy

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Positron Annihilation Lifetime Spectroscopy is a powerful non-destructive technique to investigate vacancy defects in solids (PALS). It relies on the measurement of the positron lifetime in defective materials. Vacancy-type defects are efficient traps for positrons and thus when present in a sample they lead to a strong increase in the positron lifetime. To go further and in particular to assign the measured lifetime components to a particular defect, one needs to compare experiments to simulation. The TC-DFT (Two-Components Density Functional Theory) allows computing positron lifetimes corresponding to atomic-scaled defects [1]. We developed this method in the ABINIT in order to study radiation-defects in UO2 [2,3]. In the present study, we apply this methodology to some mixed actinides oxides: $(U,Ce)O_2$, $(U,Am)O_2$, $(U,Pu)O_2$ and $(U,La)O_2$. When available, we compare our predictions to experimental measurements and try to deduce the effect of the cationic additive on the defects stability in these systems.

References:
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