

Using multi-edge HERFD-XAS to study the uranium electronic structure in MUO_3 ($\text{M} = \text{K}, \text{Na}, \text{Rb}$)

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The attractiveness of uranium is not only due to their high relevance on safety and economic performance of the nuclear power plant but also from a fundamental point of view. Indeed, uranium can induce very versatile physico-chemical properties due to the wide range of possible oxidation states offered by its $[\text{Rn}]7s^26d^15f^3$ electronic ground state configuration. Additionally, uranium 5f electrons show an apparent duality in localization, being often found in radially dispersed and hybridized bands in the vicinity of the Fermi level, whereas sometimes they remain localized [1-2].

The understanding of this duality is difficult both experimentally owing to the natural radioactivity of uranium, and, theoretically because calculations are extremely complicated because of comparable magnitudes of the crystal field, spin-orbit coupling and the electron-electron repulsion interactions. The influence of the latter effect can be significantly reduced by exploring pure pentavalent $\text{U}^{(\text{V})}$ compounds. Indeed, the $\text{U}^{(\text{V})}$ valence state corresponds to a simpler electronic configuration $[\text{Rn}]5f^1$, where no electron-electron repulsion interactions are expected, at least within the 5f shells.

In this contribution, we will discuss our comprehensive analysis of multi-edge high energy resolution fluorescence detected X-ray absorption data obtained at the uranium L_1 -edge, L_3 -edge and M_4 -edge for $\text{MU}^{(\text{V})}\text{O}_3$ perovskite compounds with $\text{M} = \text{K}, \text{Na}$ and Rb .

The uranium valence electronic structure was evaluated by comparing theoretical calculations with experimental data, giving the opportunity to directly extract for example the crystal field splitting of U-6d electrons in KUO_3 [3].

[1] Guziewicz et al., Phys. Rev. B 69 (2004) 045102.

[2] Y. A. Teterin et al., Russ. Chem. Rev. 73 (2004) 541.

[3] Bes et al., J. Synch. Rad. 29 (2022) 21.