

# High energy resolution X-ray spectroscopy in the Tender and Hard X-ray ranges

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In recent years, scientists have progressively recognized the role of electronic structure in the characterization of the chemical and physical properties of materials. High-energy resolution X-ray spectroscopy emerged as a promising direction because this method can probe material properties at the atomic and molecular levels<sup>1,2</sup>. Such experiments are performed at the synchrotron facilities, which offer a number of unique advantages. One of them is the element-selectivity using the energy of incident X-rays, which can be tuned and thus allows one to probe electronic transitions on a very small amount of sample without vacuum conditions. Moreover, synchrotron methods are non-destructive and bulk sensitive to the materials being studied.

This contribution will provide an overview of the recently performed studies<sup>2–11</sup> at the Rossendorf Beamline (ROBL) of the European Synchrotron (ESRF) in Grenoble (France). This innovative and worldwide unique experimental station was used to study actinide systems by several experimental methods: X-ray absorption spectroscopy in high energy resolution fluorescence detection (HERFD) mode, Resonant Inelastic X-ray Scattering (RIXS) at the An L<sub>3</sub> and M<sub>4,5</sub> edge and X-ray diffraction (XRD). I will show that the experimental data, analysed by electronic structure calculations are able to a) provide fingerprint information on the actinide oxidation state and ground state character b) probe 5f occupancy, non-stoichiometry, and defects c) investigate the local symmetry and effects of the crystal field<sup>4,5,7–12</sup>. It might be of interest for fundamental research in chemistry and physics as well as for applied science.

## References:

- 1 K. O. Kvashnina and S. M. Butorin, High-energy resolution X-ray spectroscopy at actinide M 4,5 and ligand K edges: what we know, what we want to know, and what we can know, *Chem. Commun.*, 2022, **58**, 327–342.
- 2 K. O. Kvashnina, S. M. Butorin, P. Martin and P. Glatzel, Chemical State of Complex Uranium Oxides, *Phys. Rev. Lett.*, 2013, **111**, 253002.
- 3 K. O. Kvashnina, Y. O. Kvashnin and S. M. Butorin, Role of resonant inelastic X-ray scattering in high-resolution core-level spectroscopy of actinide materials, *J. Electron Spectros. Relat. Phenomena*, 2014, **194**, 27–36.
- 4 E. Gerber, A. Y. Romanchuk, S. Weiss, S. Bauters, B. Schacherl, T. Vitova, R. Hübner, S. Shams Aldin Azzam, D. Detollenaere, D. Banerjee, S. M. Butorin, S. N. Kalmykov and K. O. Kvashnina, Insight into the structure–property relationship of UO<sub>2</sub> nanoparticles, *Inorg. Chem. Front.*, 2021, **8**, 1102–1110.
- 5 Z. Pan, B. Bártoová, T. LaGrange, S. M. Butorin, N. C. Hyatt, M. C. Stennett, K. O. Kvashnina and R. Bernier-Latmani, Nanoscale mechanism of UO<sub>2</sub> formation through uranium reduction by magnetite, *Nat. Commun.*, 2020, **11**, 4001.
- 6 L. Amidani, T. V. Plakhova, A. Y. Romanchuk, E. Gerber, S. Weiss, A. Efimenko, C. J. Sahle, S. M. Butorin, S. N. Kalmykov and K. O. Kvashnina, Understanding the size effects on the electronic structure of ThO<sub>2</sub> nanoparticles, *Phys. Chem. Chem. Phys.*, 2019, **21**, 10635–10643.
- 7 L. Amidani, G. B. M. Vaughan, T. V. Plakhova, A. Y. Romanchuk, E. Gerber, R. Svetogorov, S. Weiss, Y. Joly, S. N. Kalmykov and K. O. Kvashnina, The Application of HEXS and HERFD XANES for Accurate Structural Characterisation of Actinide Nanomaterials: The Case of ThO<sub>2</sub>, *Chem. – A Eur. J.*, 2021, **27**, 252–263.

- 8 L. Amidani, M. Retegan, A. Volkova, K. Popa, P. M. Martin and K. O. Kvashnina, Probing the Local Coordination of Hexavalent Uranium and the Splitting of 5f Orbitals Induced by Chemical Bonding, *Inorg. Chem.*, 2021, **60**, 16286–16293.
- 9 K. O. Kvashnina, A. Y. Romanchuk, I. Pidchenko, L. Amidani, E. Gerber, A. Trigub, A. Rossberg, S. Weiss, K. Popa, O. Walter, R. Caciuffo, A. C. Scheinost, S. M. Butorin and S. N. Kalmykov, A Novel Metastable Pentavalent Plutonium Solid Phase on the Pathway from Aqueous Plutonium(VI) to PuO<sub>2</sub> Nanoparticles, *Angew. Chemie Int. Ed.*, 2019, **58**, 17558–17562.
- 10 E. Gerber, A. Y. Romanchuk, S. Weiss, A. Kuzenkova, M. O. J. Y. Hunault, S. Bauters, A. Egorov, S. M. Butorin, S. N. Kalmykov and K. O. Kvashnina, To form or not to form: PuO<sub>2</sub> nanoparticles at acidic pH, *Environ. Sci. Nano*, 2022, **9**, 1509–1518.
- 11 E. Gerber, A. Y. Romanchuk, I. Pidchenko, L. Amidani, A. Rossberg, C. Hennig, G. B. M. Vaughan, A. Trigub, T. Egorova, S. Bauters, T. Plakhova, M. O. J. Y. Hunault, S. Weiss, S. M. Butorin, A. C. Scheinost, S. N. Kalmykov and K. O. Kvashnina, The missing pieces of the PuO<sub>2</sub> nanoparticle puzzle, *Nanoscale*, 2020, **12**, 18039–18048.
- 12 I. Pidchenko, J. März, M. O. J. Y. Hunault, S. Bauters, S. M. Butorin and K. O. Kvashnina, Synthesis, Structural, and Electronic Properties of  $K_4PuVI O_2(CO_3)_3(cr)$ : An Environmentally Relevant Plutonium Carbonate Complex, *Inorg. Chem.*, 2020, **59**, 11889–11893.