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Characterisation of bonding differences by high-resolution Xray emission and inelastic X-ray scattering techniques

One worldwide recognized strategy to reduce spent nuclear fuel long term radiotoxicity from a geological to a historical time-scale is the P&T (partitioning and transmutation) concept, where Pu and the minor actinides (MA) are separated and reprocessed in the nuclear fuel cycle. P&T requires the separation of trivalent actinides (An(III) = Am and Cm) from the chemically similar trivalent lanthanides (Ln(III)) as some of the latter have large neutron capture cross sections, compromising transmutation efficiency in the nuclear fission process. INE designs and optimizes N-donor ligands with recognized potential for use in the partitioning process. Optimization of the partitioning ligands is a topic of global interest, as the present ligands do not yet fulfil all criteria for application in an industrial process. Such optimization implies basic understanding of the chemical and physical processes responsible for ligand selectivity for An(III) over Ln(III).

The doctoral candidate will apply the innovative high-resolution X-ray emission spectroscopy (HRXES) and inelastic X-ray scattering (IXS) techniques to characterize any subtle bonding differences between the partitioning ligands and the Ln(III) / An(III) cation, which are expected to be the basis for the ligand selectivity. He/She will take part in developing, constructing and commissioning a multi analyzer crystal spectrometer for HRXES and IXS. This instrument will be installed for use at the INE-Beamline dedicated to actinide speciation investigations and the planned CAT-ACT-Beamline for catalysis and actinide research located at the ANKA synchrotron radiation facility, Karlsruhe Institute of Technology (KIT) Campus Nord. The experiments will be performed at ANKA, employing the newly constructed spectrometer, and at external synchrotron sources, e.g., ESRF, SLS. In the first experimental phase, the investigations will focus on a comparative ex-situ study of An and Ln *n*-Pr-BTP complexes in solid and liquid phase. In the second experimental phase, the PhD thesis will concentrate on comparative in-situ HRXES/IXS structural liquid-liquid extraction investigations looking from the An/Ln metal centre or ligand atoms' "point of view".

Required qualification:

Master/Diplom in physics, chemistry or related natural sciences, strong interest in instrumentation, method development and spectroscopy, and good English language skills are required.

<u>Starting date:</u> Immediately

Applications up to: 30.04.2011

KIT is pursuing a gender equality policy. Women are therefore particularly encouraged to apply. If qualified, handicapped applicants will be preferred.

The interested candidates should send a CV and at least one letter of recommendation per mail or E-mail to Tonya Vitova.