Laboratoire de Modélisation, de Thermodynamique et de Thermochimie
Direction de l'Energie Nucléaire
Département de Physico-Chimie
Service de la Corrosion et du Comportement des Matériaux dans leur Environnement
CEA Saclay
91191 Gif-sur-Yvette

Keywords **:** thermodynamics, CALPHAD (Calculation of PHAse Diagram) method, fluorides, oxifluorides, ab initio calculations, chemical process engineering

Principal Investigators : Sylvie Chatain, Jean-Louis Flèche, Jean-Marc Borgard

Thermodynamics of fluoride compounds for front end nuclear fuel cycle

Approach

Background:

- Thermodynamic behaviour of fluoride compounds (condensed and gaseous phases) involved in front end nuclear fuel cycle, more precisely during the conversion and deconversion process

Aims:

- Thermodynamic support to interpret and understand the experimental results obtained in the laboratory and at industrial scale
- Optimisation of the management of fluoride compounds in the nuclear fuel cycle

Methods:

- Thermodynamic databases establishment using the CALPHAD (CALculation PHAse Diagram) method

- Thermodynamic properties calculations of solid and gaseous compounds deduced from ab initio calculations using the Density Functional Theory

- Chemical process engineering calculations with prosim code

Collaborations (academic, industrial):

AREVA-COMURHEX,
Laboratoire Commun de Recherche « Chimie du fluor » Université Blaise Pascal – Clermont-Ferrand/CNRS/COMURHEX

Solid UO_2F_2 heat capacity