

**Post-doctoral position (thermochemistry, *Quantum* chemistry)
Reactivity of iodine and ruthenium in case of severe nuclear accident**

Skills	PhD in materials and molecular modelling, knowledge in thermochemistry
Location and duration	Lille (France), 2 years
Date of availability	January 2016
Salary	~2100 euros nets / month

Frame

During a severe accident, which happens to a nuclear facility, the radionuclides coming from the fuel fission can be released outside. Iodine and ruthenium are of particular importance because they are high contributors to radiological consequences. Within the framework of the call for projects titled "RSNR", regarding nuclear safety and radioprotection improvements, the MIRE (Mitigation Releases to the Environment) project was selected⁽ⁱ⁾. This post-doctorate is part of the MIRE project of 6 years duration (2013-2019). One objective of the MIRE project is to better understand iodine and ruthenium behaviors in severe accident conditions. Iodine is present in the nuclear containment building either under aerosol or gaseous form. Iodine oxides are formed by oxidation of molecular iodine and organic iodides. Chemical speciation of the iodine oxides remains to determine in severe accident conditions. Concerning ruthenium, after being released from melt fuel, ruthenium is mainly deposited under RuO₂ form with possible revaporisation under RuO₃ or RuO₄.

Sujet

The works consist in:

- From existing thermodynamic data in the literature relative to the I_xO_yN_z (iodine oxides and nitrosiles) species, a compilation and a critical review of these data have to be performed;
- To carry out some chemical equilibrium computations to determine the main stable species and their phases in representative conditions of a severe accident;
- To make a sensibility analysis to check if the associated uncertainties may impact the equilibrium results and need or not to be refined;
- If impact of uncertainties is important, some theoretical computations will be performed to determine/check the thermodynamic data;
- To do some kinetic simulations (out of equilibrium) with the existing data.

During the second year, a kinetic study of the reaction involving RuO₂ deposits and carbon dioxide: RuO₂(cond) + CO₂ → RuO₃(g) + CO₂, will be performed.

This study will be conducted with theoretical chemistry tool in order to calculate the rate constants. Some extrapolations will be made to estimate the potential impact of this reaction to outside releases in case of accident.

Collaborations

The post-doctorate will have relationships with two laboratories:

- The LETR (<http://www.irsn.fr/FR/Larecherche/Organisation/equipes/surete-nucleaire/LETR/>), located in the nuclear centre of Cadarache.. This laboratory is a part of IRSN (Institute of Radioprotection and Nuclear safety) French public expert of the nuclear risks.
- The PC2A (<http://pc2a.univ-lille1.fr/>) is a research unit associated to CNRS (UMR 8522) and depending on Lille 1 University..

Contacts

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Please send CV + motivation letter.

ⁱ (<http://investissement-avenir.gouvernement.fr/sites/default/files/user/20130517%20CP%20RSNR.pdf>)