Short Courses

**Modelling and prediction of speciation in solution and at solid/solution interfaces**

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| **Place***Chimie ParisTech* Engineer School11, Rue Pierre et Marie Curie Paris (France) | **Dates** May 22nd-25th 2018 |

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| **Lecturers**A. Hofmann (Univ. Lille 1 – CNRS, France)G. Lefèvre (Chimie ParisTech – CNRS, France)R. Marsac (Univ. Rennes – CNRS, France) |  **Relevant audience and requirements**Researchers and PhD students who want learn or progress in speciation modelling and simulation.Basics of solution chemistry are required. |

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| **Objectives**The various modules are intended to introduce the use of scientific software for modelling the speciation of elements in solution or adsorbed to a mineral surface. The course consists of three parts: (1) a 2-day introduction to the use of the PHREEQC software to simulate speciation of ions and solids, (2) a 1-day introduction to reactive transport with PHREEQC,(3) a 1-day lecture on surface complexation models and their limitations with examples in PHREEQC.Lectures are given in a computer room to allow parallel hands-on practical sessions with PHREEQC. |

**Program**

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| **Day 1: Introduction to PHREEQC**Thermodynamic data and databases. Use of PHREEQC: input and output files, equilibria in solution. Examples and exercises.**Day 2: Introduction to PHREEQC**Use of PHREEQC: Redox, precipitation/dissolution. Examples and exercises.*Schedule***Days 1-3**: 9:00-16:30**Day 4**: 9:00-15:30 |  | **Day 3: Introduction to adsorption**Ion exchange, basics of surface charge/potential, reactive surface groups in 2-pK model, electrostatic double layer, zeta potential, DLVO theory.**Day 4: Introduction to reactive transport** Transport equations and critical parameters.Coupling between reaction and transport. Modelling in PHREEQC and examples. |
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Registration deadline: March 31st 2018

Form to send to *gregory.lefevre@chimie-paristech.fr*

Given name: Surname/Family name:

Phone: E-mail address:

Address:

Contact details of the person in charge of the payment:

*Fees (including lunches): €1400 (incl. VAT)*

* Diet Restrictions?
* Do you plan to use your own computer (software are free and they will be sent before the courses)? Y / N
* If not, do you prefer a French or English keyboard? F / E