



Société Française  
de Génie des Procédés  
Des réponses aux défis  
industriels du XXI<sup>ème</sup> siècle

**PROCESSNET**  
EINE INITIATIVE VON DECHEMA UND VDI-6VC

**EFE**  
ENS DE LYON

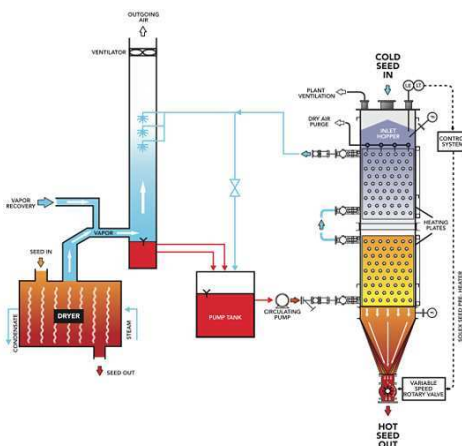
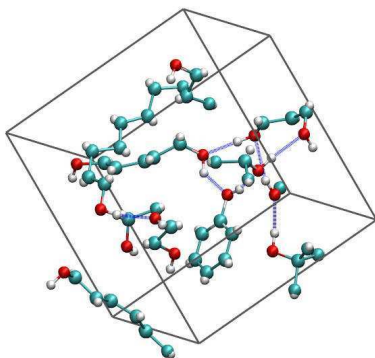
*are pleased to announce:*

# InMoTher 2012

**Industrial use of Molecular Thermodynamics**

19 – 20 March 2012

*Molecular tools for*



*an improved process design*

All information at:

<http://www.congres-sfgp.eu/inmother2012>

Contact: [secretariat@sfgp.asso.fr](mailto:secretariat@sfgp.asso.fr)



held under the auspices of the:  
**EFCE Working Party**  
**on Thermodynamics and Transport Properties**

# Objectives

The *improved understanding of molecular-scale phenomena* opens up an immense field of *new possible applications for the chemical industry and beyond*. Recent efforts in this field have resulted in models, simulation methods, and tools which not only allow academic problems to be solved but also contribute substantially towards industrial research and development. They open up routes to gain insight and improve processes which up until now could only be dealt with empirically.

This workshop is aimed at providing industrial experts with a clear vision of the opportunities that lie within this rapidly developing *interdisciplinary field*, where efforts from natural sciences and engineering are combined. It represents a unique opportunity to gain an overview of the state of research and its applications in the development of engineering models. There will be a number of *review lectures*, along with a large number of examples of *success stories* where these new technologies have been implemented.

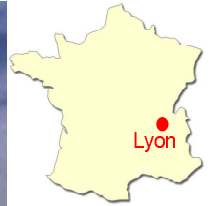
# Major topics

*Industrial case-studies and state of the art reviews* are the primary objectives of the workshop. They will be related to industrial applications of molecular simulation and molecular thermodynamics by the use of molecular calculation tools, molecular equations of state as well as experimental data giving information at either the *microscopic* or the *macroscopic* scale. Major areas of interest are:

- MD/MC simulation methods and tools (force fields)
- Coupling molecular tools and equations of state
- Use of multiscale tools in experimental research
- Process and solvent design for sustainable processes
- Nanoscale processes
- Porous media, surfaces treatment, heterogeneous catalysis
- Water treatment
- CO<sub>2</sub> capture and storage
- Electrolyte applications
- Biomolecules and polymers
- Reactive systems

# Location

In Lyon, France,  
a high gastronomy place in the heart  
of the Rhône-Alpes region.



**The workshop is hosted by the renowned**  
***Ecole Normale Supérieure***



**Address:**

15 parvis René Descartes  
69007 Lyon - FRANCE



# Important deadlines and participation fees

## Deadlines:

- **15 April 2011:** Call for papers
- **1 October 2011:** Abstract submission deadline
- **1 December 2011:** Registration opens
- **15 December 2011:** Acceptance/rejection of abstracts - notification to authors
- **6 January 2012:** Preliminary program
- **19-20 March 2012:** Workshop

## Participation fees:

- |                                 |                             |
|---------------------------------|-----------------------------|
| ■ <b>Industrial participant</b> | <b>500 € (VAT included)</b> |
| ■ <b>Academic participant</b>   | <b>400 € (VAT included)</b> |
| ■ <b>Students</b>               | <b>250 € (VAT included)</b> |

A discount of 100 € will be granted to the members of any of the following societies: DECHEMA, VDI-GVC, SFGP, EFCE, SCF and to holders of an EFCE passport. A copy of a card member will be requested.

- |                           |                                     |
|---------------------------|-------------------------------------|
| ■ <b>Exhibition Stand</b> | <b>1000 € (VAT 19.6 % excluded)</b> |
|---------------------------|-------------------------------------|

## Committees

### **Organized by (alphabetically)**

**Jean-Charles de Hemptinne  
Raphaël Huyghe  
Jean-Noël Jaubert  
Patrice Méheux  
Pascal Rousseaux  
Richard Sass  
Anne-Gaëlle Vilatte**

### **Scientific committee (alphabetically)**

**Jean-Charles de Hemptinne  
Jean-Luc Dubois  
Ioannis Economou  
Hans Hasse  
Eric Hendriks  
Günter Olf  
Gabriele Sadowski  
Philippe Sautet  
Philippe Ungerer**

**We hope to see you all in Lyon in Spring 2012 !**