

## **Announcements**

### **17TH IUPAC CONFERENCE ON CHEMICAL THERMODYNAMICS**

**Rostock, Germany**

*July 28–August 2, 2002*

#### **Participants:**

Scientists from research institutions, universities, and the chemical industry active in the area of chemical thermodynamics and chemical engineering are invited to attend the conference.

#### **Topics:**

Plenary lectures, invited lectures, and short oral and poster contributions will be presented in the following symposia:

- Molecular Simulations of Fluids and Statistical Thermodynamics
- Phase Equilibria, Supercritical Mixtures, and Separation Techniques Including Polymer Systems
- Electrolyte Solutions and Nonelectrolyte Mixtures Including Reactive Systems
- Thermodynamic Properties of New and Advanced Materials
- Organized Solutions, Surface and Colloid Chemistry
- Thermochemistry, Calorimetry, and Molecular Energetics Including the Laehnwitz Seminar on Calorimetry
- Theoretical Aspects and Technical Application

#### **Additional workshops:**

- Third International Workshop on Thermochemical, Thermodynamical, and Transport Properties of Halogenated Hydrocarbons and Mixtures

- Material and Energy Transport in Dense Membranes
- Properties of Ionic Liquids and Their Application in Chemical Engineering

**Local organization:**

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**Further information:**

Web site: <http://icct.chemie.uni-rostock.de>

## FIRST INDUSTRIAL FLUID PROPERTIES SIMULATION CHALLENGE

The Computational Molecular Science and Engineering Forum (<http://www.comsef.aiche.org/>) of the American Institute of Chemical Engineers (AIChE) has established an open competition for scientists and engineers to use molecular simulation methods to calculate results for specific sets of posed problems. The primary goal of the Industrial Fluid Properties Simulation Challenge is to obtain an in-depth and objective assessment of our current abilities and inabilities to predict thermophysical properties of industrially challenging fluids using computer simulation. Another goal of this competition is to help drive development of molecular simulation methodology toward a closer alignment with the needs of the chemical industry. We anticipate that this challenge will be an annual event.

**The competition began in November 2001, when the problems were announced. Entries are due no later than September 3, 2002.** Full details are available at <http://www.cstl.nist.gov/FluidSimulationChallenge>. Participants must register at this web site to ensure that their proposed methodology is eligible. Two half-day sessions at the 2002 Annual Meeting of the AIChE in Indianapolis (November 3–8, 2002) will be held to discuss the results and announce the winners. The winners will be presented with an award and prize at the AIChE meeting. It is anticipated that significant monetary prizes will be provided by industrial donors.

Industry is seeking successful methods, based on molecular simulation techniques, for the prediction of properties of fluids and mixtures. This challenge is geared in part toward ensuring the relevance of academic simulation activities to industrial requirements. Successful participants will have the opportunity to transfer their methods to industry.

This competition is a result of the Workshop on Simulation Methods to Predict the Thermophysical Properties of Fluids (<http://www.ctcms.nist.gov/~fstarr/ptpfms/home.html>).

All inquiries should be directed to

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Competition Committee Chair

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## ECTP-2002: THE SIXTEENTH EUROPEAN CONFERENCE FOR THERMOPHYSICAL PROPERTIES

Imperial College of Science, Technology and Medicine, London, United Kingdom

September 1–4, 2002

*About the Conference.* ECTP-2002 will be the 16th meeting in a series of conferences on thermophysical properties which are held in Europe every 3 years. The conference will be held at Imperial College, London, and is coorganized by Imperial College and the U.K. National Physical Laboratory. The scope of the meeting will include measurement, theory, modeling and applications of the thermophysical properties of materials. Full details may be found at the conference web site:

<http://www.ectp.npl.co.uk>

Please note that the web site will be used for registration, abstract submission, and further notices relating to the conference. To receive further announcements (by E-mail), please preregister at the web site now.

*Topics.* The conference will encompass the following general topics.

- Solids (including refractory, metallic, powdered, granular, and thin-film materials, ceramics, composites, polymers, and soft solids)
- Fluids (including gases, liquids, near-critical and supercritical fluids, aqueous systems, phase equilibria, and equations of state)

In addition, the meeting will feature the following special interest topics.

- Biological and Medical Applications
- Large-Scale Computation
- Materials at the Small Scale
- Petroleum Fluids
- Process Design and Engineering Applications

*Format.* The format of the conference will involve plenary lectures, invited and contributed papers (20-minute oral presentations), and poster sessions. It is hoped to have no more than two parallel sessions.

*Plenary Lecturers.* The following speakers have accepted invitations to present plenary lectures.

- Dr. Steve Garwood (Rolls Royce plc)
- Professor Dominic Tildesley (Unilever Research plc)
- Professor Geoff Maitland (Schlumberger Cambridge Research)

*Registration and Accommodations.* Registration and accommodation reservations will be handled through the conference web site. Full details, including prices, will be published at the web site.

*Contributed Papers and Posters.* Extended (two-page) abstracts, due 1 February 2002, will form the basis for acceptance of contributed papers and posters. Authors will be notified of the outcome of the review process by 8 March 2002. Final manuscripts should be submitted by 28 June 2002. Accepted papers will be reviewed for publication as appropriate in one of the following mainstream journals.

- *International Journal of Thermophysics*
- *Fluid Phase Equilibria*
- *High Temperatures–High Pressures*

Full details including an abstract template are given at the conference web site.

*Deadlines and Further Information.* Deadlines are as follows.

Abstract submission: 1 February 2002

Acceptance notification: by 8 March 2002

Registration/payment: 1 April 2002

Papers in final form: 28 June 2002

Further information is given at the conference web site (<http://www.ectp.npl.co.uk>), and the local organizers may be contacted by E-mail at [ectp@npl.co.uk](mailto:ectp@npl.co.uk).

*Local Organizing Committee.* The organizing committee is as follows.

John Redgrove (NPL)

David Robinson (NPL)

J. P. Martin Trusler (Imperial College)

Velisa Vesovic (Imperial College)

William A. Wakeham (University of Southampton)

*Scientific Programme Committee.* The program committee is as follows.

Dr. K. V. Aim (Czech Republic)

Prof. M. J. Assael (Greece)

Prof. E. Behar (France)  
Dr. A. N. Burgess (UK)  
Dr. J. H. Dymond (UK)  
Prof. I. Egry (Germany)  
Prof. J. Fricke (Germany)  
Dr. N. Glen (UK)  
Dr. A. R. H. Goodwin (USA)  
Dr. S. Gustafsson (Sweden)  
Dr. W. M. Haynes (USA)  
Dr. K. Keller (Germany)  
Prof. A. Leipertz (Germany)  
Prof. T. W. de Loos (The Netherlands)  
Prof. G. C. Maitland (UK)  
Prof. E. Matteoli (Italy)  
Prof. A. Nagashima (Japan)  
Prof. G. Neuer (Germany)  
Dr. P. Nesvadba (UK)  
Dr. P. Quested (UK)  
Dr. J. Redgrove (UK)  
Dr. F. Righini (Italy)  
Dr. R. Rusby (UK)  
Prof. J.-F. Sacadura (France)  
Prof. E. H. Stenby (Denmark)  
Prof. R. Taylor (UK)  
Prof. J. P. M. Trusler (UK)  
Dr. V. Vesovic (UK)  
Prof. W. A. Wakeham (UK)  
Prof. K. Watanabe