EUROPEAN COOPERATION IN SCIENCE AND TECHNOLOGY

COST Action CM1206

WG 2 Newsletter 2 – September 2014

Members

Thank you very much to all the researchers that have contacted us to be part of WG2! At the moment we have more than 80 members from 19 different countries in Working group 2 (WG2) making our group the largest of all in our COST action CM1206.

If you have not yet done so, please register in the web page www.usc.es/exil and choose to LOG IN. Please do not forget to complete your *Researcher Profile* (link at the bottom of the homepage) – this will help other colleagues to know you and your work better.

You can *also* subscribe to *other working groups* of this COST Action. Nevertheless, please also inform the leaders of that working group since the webpage does not do this automatically.

If you need a letter of confirmation that you are already member of WG2, please let us know:

Margarida Costa-Gomes: margarida.costa-gomes@univ-bpclermont.fr
Christian Schröder: christian.schroeder@univie.ac.at

Discussion Forum

The discussion forum for WG2 is located at http://www.usc.es/exil/forum/3

You can find here:

1. Periodic newsletters
2. Presentations of our Workgroup sessions
3. Guide lines to propose a *Research Action* in WG2.

Furthermore, you may advertise your recent papers, start a discussion, ask or offer short term missions or place job opportunities. You may also make suggestions.

COST CM1206 Meetings

The second Managing Committee (MC) meeting took place after the EUCHEM 2014 on Molten Salts and Ionic Liquids in Tallinn:

1. The new chair of the COST EXIL action is Prof. Rasmus FEHRMANN from DTU Copenhagen, Denmark, he replaces Prof. MUDRING that moved to a position at the Iowa State University in the USA. The Vice-chair, Res. Prof. Catherine SANTINI from CNRS Lyon, France remains.

2. The budget of the second year was discussed. It has been decided to increase the money for *Short Term Scientific Missions (STSM)* to 40k€ for the second year.
3. A strategic core member meeting is scheduled in Dresden after the Advanced Fluids Conference in Autumn 2014.

Recent Scientific Meetings

1. **Multiscale modelling of ionic liquids: from quantum methods to coarse-grained models.**
   CECAM/COST EXIL Sponsored Workshop, EPFL, Lausanne, Switzerland, 4-6 June 2014.
   Organizers: Prof. PADUA and Prof. CANONGIA LOPES

This workshop covered multiple scales in simulations from quantum-chemical studies on hydrogen bonding, other interactions and reaction rates, to mixed QM/MM studies, non-polarizable and polarizable MD simulations and to coarse-grained approaches. Please check the web site for the complete program: www.cecam.org/workshop-1052.html.

2. **ILSEPT2 – 2nd Int. Conference on Ionic Liquids in Separation and Purification Technology.**
   The Westin Harbour Castle, Toronto, Canada, June29 – July 2 2014.
   Organizers: Dr. SHIFLETT, Prof. MAGINN

The aim of the this conference was to provide a forum for researchers in academia and industry to share and discuss their cutting edge results on the use of ionic liquids in separation applications. The conference covered different topics: Ionic liquids as advanced materials; applications of ionic liquids; process modelling and fundamental studies; laboratory to commercialization. Please check the web site for an overview of the complete program: http://www.ilsept.com/

3. **27th ESAT – European Seminar on Applied Thermodynamics.**
   Eindhoven University of Technology, The Netherlands, 6-9 July 2014.
   Organizers: Prof. KROON, Prof. PETERS, Prof. VIUGT

The general scientific topics of ESAT 2014 comprise experimental and theoretical thermodynamics, phase equilibria and molecular simulations. Some of the invited speakers are specialists on the physical chemistry of ionic liquids and several oral communications were presented on the equilibrium and transport properties of ionic liquids as well as on the prediction of their physical-chemical properties. Please check the web site for more detailed information: www.**esat2014**.org/

4. **EUCHEM2014 – Molten Salts and Ionic Liquids XXV.**
   Tallinn, Estonia, 6-11 July 2014.
   Organizer: Prof. KOEL

The EUCHEM 2014 in Tallinn (http://euchem2014.ttu.ee) concentrated on electrochemical studies and their applications. The last day of this conference was dedicated to workgroup session of our COST action CM1206. In WG2, Prof. Varela presented the ongoing work of our Research Action "Electrostatics of ionic liquids and their mixtures".

5. **248th ACS National Meeting & Exhibition. PHYS: Physical Chemistry of Ionic Liquids.**
   San Francisco, USA, 10-14 August 2014.
   Organizers: Prof. CASTNER, Dr. WISHART, Prof. MARGULIS, PROF. MAGINN

During this symposium of the ACS National Meeting, the latest advances in the physical chemistry of ionic liquids were presented. A range of topics was covered including the relationships between ionic liquid structure and physical and transport properties, volatility and thermal stability, electron transfer, photolysis and radiolysis, ultrafast to ultra-slow spectroscopy, separations and solubility, interfaces with bulk and nanomaterials, and catalysis.

6. **Gordon Research Conference on Green Chemistry – Industrial Successes and Challenges**
   The Chinese University of Hong Kong, Hong Kong, China, July 27 – Aug 1, 2014.
   Chairs: Prof. SEDDON, Prof. HARMER; Vice-chairs: Prof. KRUPER, Prof. QUADRELLI

This GRC featured recent green processes implemented on an industrial scale, the emphasis on academic-industrial collaboration, and the discussion of the green chemical challenges for the future. The sessions were chaired and selected by recognized global leaders in the oil and gas industry, biomass processing, the polymer industry, comestibles, the pharmaceutical industry, green energy, and education and communication. The opening keynotes discussed the greening of organic synthesis and the consumer industry, and the final session will focus on Global Green Challenges for the future. For more information, please check the web site of this GRC. http://www.grc.org/programs.aspx?year=2014&program=greenchem

7. **ICCT SAIChE Conference 2014.**
   Durban, South Africa, July 27 – Aug 1, 2014.
   Chairs: Prof. HLATSHWAYO, Prof. RAMJUGERNATH

ICCT is the most renowned conference on chemical thermodynamics and is hosted by IACT every two years. This year the conference included a session on Thermodynamics of Ionic Liquids. Please check the web site for more information: http://www.icctsaiche2014.co.za/

8. **Gordon Research Conference on Ionic Liquids – Solvents, Materials, or Medicines?**
   Sunday River Resort, Newry, ME, USA, 17 – 22 Aug, 2014.
   Chair: Prof. ROGERS; Vice-chair: Prof. MUDRING

This GRC highlighted many of the emerging themes which are becoming quite important worldwide and represented an opportunity to meet and discuss these and other major topics in the field of ionic liquids with international experts. Representatives from large and small industry provided insights into key issues such as scale-up, costs, availability, registration, and other key parameters needed to plan new ventures.

9. **ECTP2014 – European Conference on Thermophysical Properties**
   Porto, Portugal, Aug 31 – Sept 4, 2014.
   Chairs: Prof. SANTOS, Prof. COUTINHO

As stated by the chairs, the ECTP2024 provided a forum for academic European scientists and industrial researchers to meet and exchange valuable experiences in the field of thermophysical

properties of a wide variety of systems covering fluids and solids. The conference included oral and poster presentations in the topics: Energy; electronic materials; ionic liquids. For more information, please check the web site: http://ectp2014.fc.up.pt/

Next Scientific Meetings

1. **7th Green Solvents conference: Advanced fluids in science and application**

   Dresden, Germany, October 2014

   www.dechema.de/gsfs2014

2. **.4th International Workshop on Ionic Liquids – Advanced Energy Applications**

   Tarragona, Spain, January 2015.

   http://www.crever.urv.cat/

   Our next workgroup session will probably take place in this gathering.

Short term missions

In the first year of CM1206, 15 short term missions were initiated in WG2. They are listed, for your information in the following Table and we have divided them into four scientific areas:

Title	From	To	Area
Heterogeneous dynamics of ILs studied by polarizable MD simulations	Padua (France)	Schröder (Austria)	Simulation/Modelling
Interactions and structure in IL solutions	Costa Gomes (France)	Welton/Hunt (UK)	Simulation/Modelling
Point-induced dipoles and Drude oscillators	Heuer (Germany)	Schröder (Austria)	Simulation/Modelling
Estimation of thermodynamic properties	Mikkola (Finland)	Verevkin (Germany)	Simulation/Modelling
CO_2 solubility in C_2mim based ILs	Stark (Germany)	Fernandez (Spain)	Solubility/Phase behaviour
Solubility of CO_2 and methane in C_4mim $FeCl_4$	Mudring (Germany)	Costa Gomes (France)	Solubility/Phase behaviour
CO_2 solubility in IL mixtures	Paulechka (Belarus)	Costa Gomes (France)	Solubility/Phase behaviour
Activity coefficients of terpenoids in IL	Coutinho (Portugal)	Domanska (Poland)	Solubility/Phase behaviour
Thermal analysis of eutectic mixtures	Soto (Spain)	Smiglak (Poland)	Solubility/Phase behaviour
Liquid-liquid equilibria based on phosphonium ILs	King (Finland)	Soto (Spain)	Solubility/Phase behaviour
Phase behavior of mixtures IL / volatile fatty acids	Kroon (Netherlands)	Rathke (Germany)	Solubility/Phase behaviour
Investigation of EAN / DMSO mixtures	Kirchner (Germany)	Triolo (Italy)	Solubility/Phase behaviour
Dynamics of ILs by solvation and photon correlation spectroscopy	Rivera (Spain)	Blochowicz (Germany)	Spectroscopy
X-ray photoelectron spectroscopy of worn surfaces with ILs	Fernandez (Spain)	Reichelt (Germany)	Spectroscopy
Viscosimetric characterization of ILs at high pressures	Fernandez (Spain)	Assael (Greece)	Transport properties

The average duration of all short term missions in CM1206 was 47 days. The reports of these short term missions will not be made public since the data are not published yet. However, if you are interested in one of these topics, you may contact us and we will give you the email address of the corresponding principal investigators. We encourage you to make your students apply for a short term mission. The next deadline will be Nov 1st. Please follow the instruction given on our homepage.

Research Actions in WG2

1. "Electrostatics of ionic liquids and their mixtures"

Our first action concerns electrostatics of ionic liquids and their mixtures chaired by L.M. Varela (luismiguel.varela@usc.es) and O. Cabeza (oscabe@udc.es). This is a joint study between theoretician and experimenter. For more information visit http://www.usc.es/exil/node/28.

2. "Database on physico-chemical properties of ionic liquids"

Our second topic is a reliable database on the physic-chemical properties of ionic liquids. At the last MC meeting in Tallinn we came to the conclusion, that our own resources are too limited to start a new database but we would like to contribute to the efforts of IUPAC. Consequently, our second action chaired by Magdalena Bendova (bendova@icpf.cas.cz) concerns the systematic study of relevant physico-chemical properties. Furthermore, ILthermo (http://ilthermo.boulder.nist.gov/) is reactivated. Please have a look.

3. "New polarizable force field on ionic liquids"

The third action would like to combine our efforts to make a new polarizable force field on the basis of the well-known non-polarizable force field of Prof. Canongia Lopes and Padua. In a first step, we are developing a force field conversion tool. This tool reads force field information from AMBER, CHARMM, DL_POLY or GROMACS and converts it in a readable XML file structure. This structure will be used for a general force field data base. Our tool is also capable of writing force field files for the above mentioned MD programs on the basis of the XML file. This way, force fields can be exchanged between groups using different MD programs. For further information please contact Christian Schröder (christian.schroeder@univie.ac.at).