InMoTher 2012
19-20 March 2012

Final Program

Sunday, March 18th		
17:00	***19:00***	***Registration***
		Welcome reception

Monday, March 19th (AM)			
8:30	***9:00***	***Registration***	
9:00	***9:10***	***Opening***	
9:10	**10:00**	***Plenary Lecture*** ***Molecular Simulation of Phase Equilibria: Progress and Challenges.*** Prof. Athanassios Z. PANAGIOTOPOULOS - Princeton University **Chairperson**: Philippe UNGERER - Materials Design	
10:00	***10:30***	***Coffee break***	
		Session 1A (Amphithéâtre Mérieux) **Chairperson**: Maurizio FERMEGLIA - University Of Trieste	**Session 1B (Salle des Thèses)** **Chairperson**: Karel AIM - Institute of Chemical Process Fundamentals of the ASCR
10:30	**11:00**	***Invited Lecture*** ***Application of COSMO-RS in the Design of Ionic Systems.*** Steve LUSTIG - Du Pont	***Invited Lecture*** ***Are there Ways to Improve the Accuracy of predictive Methods in the field of Thermodynamic Properties?*** Rob MEIER - DSM
11:00	**11:20**	***Non-equilibrium Molecular Dynamics Simulation of real Fluids in Nanoporous Materials.*** Martin Thomas HORSCH (ref. 32)	***Molecular Thermodynamics of Quantum Fluids using the SAFT-VR approach with Quantum Corrections.*** Alejandro GIL-VILLEGAS (ref. 22)
11:20	**11:40**	***Heat and Mass Transport through Surfaces.*** Jean-Marc SIMON (ref. 108)	***Modelling of Electrolytes with ePPC-SAFT.*** Justyna ROZMUS (ref. 73)
11:40	**12:00**	***Prediction of physical Properties of CO_2 in ionic Mea/Aqueous Solutions by Molecular Simulation.*** Carlos NIETO DRAGHI (ref. 86)	***gSAFT: Application of the SAFT-g MIE Group Contribution EOS in the Oil/Gas Industry- from academic Research to Industrial Deployment.*** Claire ADJIMAN (ref. 124)
12:00	**12:20**	***Comparison of predicted pKa Values for some Amino-Acids, Dipeptides and Tripeptides, using Cosmo-rs, Chemaxon and Acd/Labs Methods.*** Oumar TOURE (ref. 25)	***Comparison of Performance of the PC-SAFT, Soave-Redlich-Kwong and Peng-Robinson Equations of State in Modelling Vapour-Liquid Equilibria of Binary CO_2 ' 1-Alkanol Mixtures.*** Luis Antonio ROMAN RAMIREZ (ref. 105)
12:20	**12:40**	***Molecular Simulation of Ions in aqueous Solutions.*** Stephan DEUBLEIN (ref. 70)	***Recent Advances in Modelling the Viscosity of Dense Fluids.*** Velisa VESOVIC (ref. 74)
12:40	***13:40***	***Lunch (buffet)***	

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Monday, March 19th (PM)			
13:40	**14:30**	***Plenary Lecture*** ***Equations of state for complex fluids.*** Joachim GROSS - Stuttgart University **Chairperson**: Georgios KONTOGEORGIS - Technical University Of Denmark	
14:30	***14:40***	***Change of room***	
		Session 2A1 ((Amphithéâtre Mérieux) **Chairperson**: Alejandro GIL-VILLEGAS - University of Guanajuato	**Session 2B1 (Salle des Thèses)** **Chairperson:** Carlos NIETO-DRAGHI - IFPEN
14:40	**15:10**	***Invited Lecture*** ***Advanced Models in industrial Praxis: from Process Design to Process Optimization.*** Georgios FOLAS - Satoil	***Invited Lecture*** ***Molecular Thermodynamics- Industrial Applications with Focus on Screening and Extrapolation.*** Manfred HEILIG - BASF
15:10	**15:30**	***Solubility of Pharmaceuticals: a Comparison between a PC-SAFT-Based Approach and NRTL-SAC.*** Theodora SPYRIOUNI (ref. 101)	***Molecular Dynamics Investigation of Triethylene Glycol in hydrated LTA Zeolite ' Emphasis on Evaluation of Potential Models.*** Bjørnar JENSEN (ref. 44)
15:30	**15:50**	***Predicting Phase Equilibria of Oxygenated Compounds Using Molecular Models: Results from the MEMOBIOL Project.*** Rafael LUGO (ref. 82)	***Chemical Potential Calculations in Molecular Dynamics Simulations of Adsorption in Zeolites.*** Charlles ABREU (ref. 59)
15:50	**16:10**	***Nano Tools for Macro Problems: Multiscale Molecular Modeling of Life and Material Sciences.*** Maurizio FERMEGLIA (ref. 92)	***Hydrate Formation in Pipelines and Maximum permittable Water Content in Gas.*** Bjørn KVAMME (ref. 34)
16:10	***16:40***	***Coffee Break***	
		Session 2A2 ((Amphithéâtre Mérieux) **Chairperson**: Ilya POLYSHUK - Ariel University of Toronto	**Session 2B2 (Salle des Thèses)** **Chairperson:** Velisa VESOVIC - Imperial College of London
16:40	**17:00**	***About unexpected Solid-Liquid Phase Diagrams obtained with most of SAFT-like Equations of State.*** Romain PRIVAT (ref. 123)	***Improving the Modeling of compositional Grading in Petroleum Reservoirs: a Molecular Dynamic Approach.*** Guillaume GALLIERO (ref. 122)
17:00	**17:20**	***Efficient Calculation of Fluid Phase Equilibria with Equations of State.*** Ulrich DEITERS (ref. 35)	***Multiphase Equilibrium of Fluids confined in heterogeneous porous Solids.*** Marcelo CASTIER (ref. 107)
17:20	**17:40**	***Application of Lattice Cluster Theory Equation of State for pure Compounds.*** Kai LANGENBACH (ref. 50)	***Improving Molecular Simulation Models of Adsorption in porous Materials: Interdependence between Domains.*** Joel PUIBASSET (ref. 121)
17:40	**18:00**	***Make your Thermodynamic Models available in most Process Simulators.*** Michel PONS (ref. 80)	***Strategy for Multiscaled Micro-emulsion Design with Application in chemical Enhanced Oil Recovery.*** Johannes FRAAIJE (ref. 52)
18:00	***20:00***	***Poster session with Cocktail***	
20:00		***Departure to the Dinner***	

Software Demonstration	**15:10 to 16:10** (In two paralell Sessions) *- Culgi (Ruben Serral Gracia)* *- ProSim (Olivier Baudouin)*	**18:10 to 19:10 :** *InModelia (Patrice Kiener)*

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Tuesday, March 20th			
9:00	**9:50**	***Plenary Lecture*** ***NIST ThermoData Engine: Increasing Value, Preventing "Pollution", Broadening Scope, and Providing Communications for Thermodynamic Property Information.*** Michael FRENKEL - NIST **Chairperson**: Christophe COQUELET - Mines ParisTech	
9:50	***10:20***	***Coffee break***	
		Session 3A (Amphithéâtre Mérieux) **Chairperson**: Philippe ROUSSEAU - Processium Lyon	**Session 3B (Salle des Thèses)** **Chairperson**: Guillaume GALLIERO - University of Pau
10:20	**10:50**	***Invited Lecture*** ***Use of Data in Engineering Company.*** Michael KLEIBER - Uhde GmbH	***Invited Lecture*** ***Ab initio Thermochemistry of Industrial Materials for Energy.*** Pascal RAYBAUD - IFPEN
10:50	**11:10**	***CO_2 Mixture Properties using Equations of States and Molecular Simulations.*** Dimitrios TSANGARIS (ref. 58)	***Coupling Microscopic and Mesoscopic Scales to Calculate Thermodynamic Properties of heterogeneous Fluid Systems including Nanometric Carbon Clusters.*** Emeric BOURASSEAU (ref. 24)
11:10	**11:30**	***Experimental and computational Study on the Liquid - Liquid Equilibrium of Thiophene with ionic Liquids.*** Marta BATISTA (ref. 43)	***Molecular Dynamics Determination of Water-Nanorugged Surfaces Interfacial free Energies.*** Frédéric LEROY (ref. 42)
11:30	**11:50**	***Mesoscopic Simulation of Polyelectrolyte Brushes under Shear.*** Florent GOUJON (ref. 109)	***Prediction of the Surface Tension of Alkane/acid Gases Mixtures with Monte Carlo Molecular Simulations.*** Jean-Claude NEYT (ref. 41)
11:50	**12:10**	***Development of Property Models with uncertainty estimate for Eliable Product-Process Design.*** Amol HUKKERIKAR (ref. 79)	***Solid - Liquid Phase Behavior of Polymer - Solvent Mixtures.*** Michael FISCHLSCHWEIGER (ref. 51)
12:10	**12:30**	***Generalization of SAFT + Cubic Equation of State for predicting and correlating Thermodynamic Properties of heavy organic Substances.*** Ilya POLISHUK (ref. 126)	***Multiscale Modelling of Polymer-Filler Interaction.*** Gaëtan MAUREL (ref. 64)
12:30	**12:50**	***Guiding the Design of ionic Liquids as Substitutes of volatile Organic Solvents: PLS-DA Models for Ecotoxicity (V. Fischeri) Discrimination.*** Manuel ALVAREZ-GUERRA (ref. 85)	***A Stochastic Multi-Scale Modelling Approach of Polymerization Processes.*** Dimitrios MEIMAROGLOU (ref. 69)
12:50	***14:00***	***Lunch (buffet)***	
14:00	**16:00**	***Round-Table discussion*** ***How to improve technology transfer for a faster innovation in molecular thermodynamics*** Moderated by Philippe RICOUX - Total and Mathias BREHELIN - Rhodia	
16:00	**16:15**	**Conference closing**	