13th International Conference on Properties and Phase Equilibria for Products and Process Design

26 – 30 May 2013, Iguazu Falls, Argentina and Brazil

WELCOME

On behalf of the International Organizing Committee of PPEPPD 2013, we welcome you to the thirteenth edition of the internationally recognized conference on Properties and Phase Equilibria for Product and Process Design. This is the first time that PPEPPD is held in the southern hemisphere. It is our greatest pleasure to host all of you in the beautiful and peaceful surroundings of Iguazu and hope that the meeting can renew traditional collaborations and open opportunities for many new contacts, research projects and friendship.

We are very pleased for the interest shown in this conference and are delighted to have received many fine contributed papers from different parts of the world.

We want to express our gratitude to the International Organizing Committee and to the Scientific Advisory Board for their invaluable support. Our deepest thanks go to the Local Organizing Committee, and particularly to Selva Pereda and Lucio Cardozo Filho, for solving countless problems with readiness, competence and good mood. We also wish to acknowledge Gastón Greco for the graphical design of printed material and web page.

We are most pleased to have a very distinguished group of invited speakers. We thank them for their willingness to participate and for their contribution to the excellence of the meeting. We also deeply appreciate the participation of leader companies in the two workshops of the conference and the attendance of professionals from industry. Last but not least, we thank the government agencies, institutions and industrial sponsors for the financial support to this conference. Without any doubt, the interaction between the industrial, academic and public sectors is an essential step in the creation and growth of technological knowledge for the benefit of society.

Welcome to Iguazu and many tanks to each of you for making PPEPPD 2013 possible!

Fred and Susana

COMMITTEES

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SPONSORSHIP AND SUPPORT

The Organizing Committee acknowledges the sponsorship and support of:

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Materials Design

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RADIX, Brazil

SCIENOMICS

May 1st, 2013

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ABOUT PPEPPD

PPEPPD Conferences started in USA in the 1970´s to promote the contact between theoreticians and practitioners in the area of properties and phase equilibrium for product and process design. The motivation and spirits of the first PPEPPD conference have been kept over more than 30 years of uninterrupted triennial editions:
1977: Asilomar, California, USA
1980: Berlin, Germany
1983: Callaway Gardens, Georgia, USA
1986: Elsinore, Denmark
1989: Banff, Alberta, Canada
1992: Cortina d'Ampezzo, Italy
1995: Aspen, Colorado, USA
1998: Nordwijkerhout, Netherlands
2001: Kurashiki, Japan
2004: Snowbird, Utah, USA
2007: Hersonissos, Crete, Greece
2010: Suzhou, China

PPEPPD 2013

PPEPPD 2013 takes place in the Iguazu Falls surroundings. The Iguazu Falls are on the frontier between Argentina, Brazil and Paraguay. They have been selected as one of the new 7 natural wonders of the world. An impressive volume of water of the Iguazu river falls from a height of 70 meters, forming 275 waterfalls, along a length of 2.7 Km. The National Parks within the falls area preserve the exuberant subtropical vegetation which surrounds the Falls and their inhabitants (parrots, humming-birds, toucans, yaguaretes, tapirs, capybaras, lynxes, ant-eaters and pumas).
The conference hotel Loi Suites is located in the subtropical jungle of Iryapu, 15 minutes far from the Iguazu falls. Set deep in the heart of the jungle the Hotel was built with extreme respect for nature, preserving native trees and most of the jungle.

SCOPE AND TOPICS

Fundamentals

- Thermodynamics and phase equilibria (experimental & modeling)
- Transport properties and crystallization science
- Surfaces, interfaces and confinement effects
- Quantum computation and force fields
- Molecular simulation and multiscale simulation

Processing and Applications

- Agrochemicals and biomass
- Gas&Oil downstream and upstream, petrochemicals
- Renewable energy
- Product and process engineering
- Novel reaction and separation technologies (ionic liquids and electrolyte systems, gas hydrates, etc)
- Pharmaceuticals and cosmetics
- Biological systems
- Food and functional food processing
- Materials (polymers, metals, inorganic solids and liquid crystals)
- Nanoscience and nanotechnology
- Environment, sustainability and risk management

JOHN M. PRAUSNITZ AWARD

This will be the sixth award in the John M. Prausnitz series instituted in 1998. The sixth John M. Prausnitz award for outstanding achievement in Applied Chemical Thermodynamics will be awarded to Professor Peter Cummings from the Department of Chemical and Biomolecular Engineering, Vanderbilt University, Nashville, USA. Professor Cummings is awarded for his outstanding research accomplishments in the study of water and aqueous solutions in bulk and at interfaces, and the elucidation of the molecular basis for phase transitions in nano-confined fluids.

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List of previous J. M. Prausnitz awardees:

PPEPPD 1998: Prof. Athanassios Panagiotopoulos, University of Maryland, USA
PPEPPD 2001: Prof. Pablo Debenedetti, Princeton University, USA
PPEPPD 2004: Prof. David Kofke, University of Buffalo, USA
PPEPPD 2007: Prof. Joan Brennecke, University of Notre Dame, USA
PPEPPD 2010: Prof. Theodore Randolph. University of Colorado, USA

SPECIAL ISSUE OF FLUID PHASE EQUILIBRIA

The Editors of Fluid Phase Equilibria have arranged for publication of the PPEPPD 2013 Conference Proceedings as a Special Issue of FPE. John O'Connell will be the principal handling Editor, while Clare McCabe and Theo de Loos will provide editorial support.
All submissions for the Special Issue must have been presented at the Conference and use the Special Issue portal that is being set up on the Elsevier EES System. Log in as author to http://ees.elsevier.com/fpe/, click on "Submit New Manuscript", and choose article type "Special Issue: PPEPPD 2013".
Formatting must follow the FPE Guide for Authors. Submissions with new experimental data must follow the "New procedures for articles reporting thermophysical properties", Fluid Phase Equilibria, Volume 340, 25 February 2013, Page iii. The normal process of review and decision for FPE submissions will be followed by the Editor.
To achieve publication during 2013, all papers must be accepted by October 1, 2013. Only manuscripts submitted by July 15 will be assured of being in the Proceedings, though papers submitted after this time can be considered for regular FPE issues.

Technical Program

SUNDAY MAY 26th

15:00-21:30 Registration
18:30-20:00 Welcome reception
20:00-20:10 Opening ceremony

Chair: *Thanos Panagiotopoulos*

20:10-21:00 **Key note address:** Nanoscale drying and hydration phenomena: Fundamentals and applications, ***Pablo Debenedetti*** *(Princeton University, USA)*

MONDAY MAY 27th

Chairs: *Marcelo Castier and Sabine Enders*

8:30-9:15 **Invited lecture:** Diffusion, annealing and all that jazz: How to approach them when they are anomalous? ***Constantino Tsallis*** *(Centro Brasileiro de Pesquisas Físicas, Brazil)*

9:15-9:40 SAFT EOS model of electrolytes for scale and corrosion applications at extreme high temperatures and pressures; *Kenneth Cox and Walter Chapmann (Rice University, USA)*

9:40-10:05 Molecular simulation of aqueous electrolytes; *William Smith, Filip Moucka and Ivo Nezbeda (University of Ontario, Canada)*

10:05-10:35 Coffee break

Chairs: *Joan Brennecke and Yoshio Iwai*

10:35-11:20 **Invited lecture:** Platonic and archimedean geometries in elastic membranes, ***Mónica Olvera de la Cruz*** *(Northwestern University, USA)*

11:20-11:45 Multiscale modeling for phospholipid bilayer simulations, *Carol Hall and Emily Curtis (North Carolina State University, USA)*

11:45-12:10 Fluid and nanoparticle transport in lipid bilayer membranes using coarse grained molecular dynamics simulations, *Bo Song, Cynthia Jameson and Sohail Murad (University of Illinois at Chicago, USA)*

12:10-12:35 Insights on solid-liquid equilibrium operations in the downstream processing of proteins, *Luis Fernando Mercier Franco and Pedro de Alcântara Pessôa Filho (Universidade de São Paulo, Brazil)*

12:35-14:00 Lunch

14:00-16:00 **Parallel workshops**

Workshop 1: Properties of non-conventional gas and oil resources

Workshop 2: Molecular simulation for industrial applications

16:00-16:30 Coffee break

Chairs: *Keith Gubbins and Vladimir Nichita*

17:00-17:45 **Invited lecture:** Entropy and self assembly, ***Daan Frenkel*** *(University of Cambridge, UK)*

17:45-18:10 PC SAFT parameters from ab-initio calculations, *Kai Leonhard, Muhammad Umer and Katja Albers (RWTH Aachen University, Germany)*

18:10-18:35 The A in SAFT: Investigating the association contributions within a Wertheim TPT1 treatment, *Simon Dufal, Andrew Haslam, Thomas Lafitte, Amparo Galindo and George Jackson (Imperial College London, UK)*

18:35-20:00 Dinner

20:00-22:00 **Poster Session I**

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TUESDAY MAY 28th

Chairs: *Jean-Noël Jaubert and Walter Chapmann*

8:30-9:15 **Invited lecture:** Hydrocarbon thermophysical properties: Unexpected frontiers, ***John Shaw*** *(Univesity of Alberta, Canada)*

9:15-9:40 Molecule-based assay characterization methodology for correlation and prediction of properties for crude oil and petroleum fractions, *Chau-Chyun Chen (Aspen Technology, Inc.)*

9:40-10:25 **Invited lecture:** From classical to solar fuels: trends and needs in research, ***Sophie Jullian*** *(IFP Energies Nouvelles, France)*

10:30-12:30 **Poster Session II** (including coffee break)

12:30-13:30 Lunch

13:30-18:00 Excursion to the water falls

18:30-21:00 Dinner at the National Park: barbecue (asado al asador)

WEDNESDAY MAY 29th

Chairs: *Antonio Marcilla Gomis and Theo de Loos*

8:30-9:15 **Invited lecture:** Describing water with computer simulations, ***Carlos Vega de las Heras*** *(Universidad Complutense de Madrid, Spain)*

9:15-9:40 Mesoscale solubilization in aqueous solutions of hydrotropes, *Deepa Subramanian, Jeffery B. Klauda, BoualemHammouda and Mikhail Anisimov (University of Maryland, College Park, USA)*

9:40-10:05 Separation of ethanol and other oxygenates from aqueous solutions: Molecular-level insights for extraction and sorption processes, *Ilja Siepmann, Peng Bai, Samuel L. Keasler and Deeksha Jain (University of Minnesota, USA)*

10:05-10:35 Coffee break

Chairs: *Gabriele Sadowski and Mauricio Futran*

10:35-11:20 **Invited lecture:** Physical property data @ BASF - Relevance and future challenges, ***Bernd Eck*** *(BASF, Germany)*

11:20-11:45 Chiral room-temperature ionic liquids: Insight from molecular dynamics simulations, *M. Lísal, Z. Chval, J. Storch, P. Izák and Karel Aim (Institute of Chemical Process Fundamentals, Academy of Science, Czech Republic)*

11:45-12:10 Temperature effects in crystal structure prediction, *M. Vasileiadis, Claire Adjiman and C.C. Pantelides (Imperial College London, UK)*

12:10-12:35 Cocrystal free energy surfaces and phase diagrams, *Richard McClurg (SSCI division of Aptuit, USA)*

12:35-14:00 Lunch

Chairs: *Carol Hall and Martin Trusler*

14:00-14:45 **Prausnitz award lecture:** Understanding the large and complex by focusing on the small and simple: A statistical mechanic's approach, ***Peter Cummings*** *(Vanderbilt University, USA)*

14:45-15:10 Evolution of methane gas during hydrate dissociation, *S. Alireza Bagherzadeh, Peter Englezos, Saman Alavi and John A. Ripmeester (University of British Columbia, Canada)*

15:10-15:35 Some examples of the contribution of applied thermodynamics to CO_2-capture technology, *Paul Mathias (Fluor Corporation)*

15:35-16:00 Coffee break

16:00-18:00 **Poster Session III**

18:30-22:00 Conference dinner

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THURSDAY MAY 30th

Chair: *Xiaohua Lu and John O´Connell*

8:30-9:15 **Invited lecture:** From multiscale modeling to meso-science — A chemical engineering perspective, ***Jinghai Li****, (Chinese Academy of Science, China)*

9:15-9:40 Measuring and correlating diffusivity in polymer-solvent systems, *Ronald Danner (The Pennsylvania State University, USA)*

9:40-10:05 Bending rigidity of a diblock copolymer membrane containing weak polyelectrolyte sub chains and pH-induced shape transitions of copolymer's aggregates in solution, *Alexei Victorov (St.Petersburg State University, Russian Federation)*

10:05-10:35 Coffee break

Chair: *Cor Peters and Selva Pereda*

10:35-11:00 Synergic effects of imidazolium ionic liquids on surfactant mixed micelles for inducing micro/mesoporous materials, *FeiGao, ZijunBian, Jun Hu, Honglai Liu and Ying Hu (East China University of Science and Technology, China)*

11:00-11:25 Thermodynamic study of hydrogen production from glycerol via supercritical water reforming, *Laura Rovetto, Martin E. Frontane and L.E. Moyano (IDTQ, Universidad Nacional de Cordoba, Argentina)*

11:25-12:10 **Invited lecture:** The process of phase design, ***Esteban Brignole****, (PLAPIQUI, Universidad Nacional del Sur, Argentina)*

12:10-12:25 Presentation of PPEPPD 2016, ***Eugenia Macedo****, (University of Porto, Portugal)*

12:25-12:40 Closing ceremony

12:40-14:00 Lunch

WORKSHOPS

Properties of non-conventional gas and oil resources

- Introduction: **Dr. Ricardo C. Pinto**, Petrobras
- Oil Sands / Shale Gas / Acid Gas: What is it? Estimated reserves. Challenges for production and required properties measurement and new estimation methods. Will commercial software packages meet these new requirements? **Dr. Marco Satyro**, Virtual Materials Group Inc.
- Pre-salt oil resources: What is it? Estimated reserves. Challenges for production and properties measurement/estimation. Will commercial softwares meet these new requirements? Molecular simulation as a tool for properties estimation: **Eng. Cassiano Aimoli**, Petrobras
- Panel discussion
- Concluding remarks: **Dr. Ricardo C. Pinto**, Petrobras

Molecular Simulation for Industrial Applications

- Introduction, open-source packages for Molecular Dynamics on CPUs and GPUs: **Prof. Athanassios Z. Panagiotopoulos**, Princeton University
- Availability and limitations of open-source software packages for Monte Carlo calculations of phase equilibria and adsorption: **Prof. J. Ilja Siepmann**, Univ. of Minnesota
- Novel applications of molecular modelling: adsorption and diffusivity in coal models, properties of oxygen-bearing molecules from ligno-cellulosic biomass, mechanical properties of polymer materials MY-PhU-XR: **Dr. Marianna Yannourakou**, Materials Design
- Panel discussion
- Concluding remarks: **Dr. Sophie Jullian**, IFP-EN

ORAL PRESENTATIONS

Speakers are expected to use Power Point presentations or similar. Laptop computers will be available for presenters. Speakers are kindly asked to be in the main conference room ten minutes before their session and to check in advance their files with the technical staff.

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POSTERS

Most of the PPEPPD technical contributions will be presented in posters sessions. Three posters sessions will be held on Monday evening, Tuesday morning and Wednesday afternoon. Presenters should hang their posters before the session begins and remove them once the session is over.

CONFERENCE DOCUMENTS

A pendrive will be provided to the conference participants at registration. The unit contains PDF documents with the technical program, list of participants, abstracts and full texts submitted electronically through the conference website.

EXCURSION AND SOCIAL EVENTS

A welcome cocktail is scheduled for Sunday May 26th from 18:30 to 20:00. We will gather at the lobby terrace.

On Tuesday May 28th conference participants and accompanying persons are invited to join us for the conference excursion to the Iguazu waterfalls. Buses will take us to the Argentinean National Park at 1:30 pm. Dinner that night will be served at a restaurant within the national park. Visitors and local participants will enjoy a typical Argentinean barbecue (asado al asador).

The conference dinner will take place on Wednesday May 29th at Hotel Loi Suits.

Poster Session I

Chairs: *Lucio Cardozo Filho and Marcelo Zabaloy*

ID-004 **Study on kinetics of alkalescent fiber FFA-1 adsorbing glyphosate from production waste water of glyphosate**
C. Zhou, G. Li, D. Jiang
Zhengzhou University, China

ID-010 **Salt-forming regions of seawater type solution in the nonequilibrium state of fractional crystalization processes**
H. Zhou, Y. Bao, L. Huangfu, C. Zhang
Tianjin University of Science and Technology, China

ID-014 **Monte Carlo simulation on phase equilibrium for dimethyl carbonate synthesis system**
Y. Pan, A. Xuan, Y. Wu, Z. Yan, Z. Chen, T. Xu
Wuhan Institute of Technology, China

ID-015 **Investigating the metastability and structural transitions of clathrate hydrates**
G. Grim, D. Sloan, C. Koh, A. Sum
Colorado School of Mines, United States

ID-016 **Predictions of hydrate formation for systems containing hydrogen**
Q. Ma, G. Chen, C. Sun, X. Guo, L. Yang, B. Liu
China University of Petroleum-Beijing, China

ID-017 **A comprehensive approach for describing the interfacial properties of carbon dioxide + decane and carbon dioxide + eicosane mixtures**
A. Mejía, H. Segura, M. Cartes, E.A. Müller
Universidad de Concepción, Chile

ID-018 **A new approach to the semi-continuous thermodynamics of hydrocarbon mixtures**
M. Petitfrere, D.V. Nichita, F. Montel
University of Pau and CNRS, France

ID-023 **Modeling drug solubility in polymers**
A. Prudic, T. Kleetz, Y. Ji, G. Sadowski
TU Dortmund, Germany

ID-029 **Application of Lattice – Cluster Theory EOS to mixtures**
K. Langenbach, D. Browarzik, S. Enders
TU Berlin, Germany

ID-032 **Solubility of solids in supercritical fluid using a fourth order virial equation of state**
S. J. Pai, Y. C. Bae
Hanyang University, Republic of Korea

ID-035 **Fundamental structure-dynamics relationships in confined aqueous electrolytes**
A. Striolo
University of Oklahoma, United States

ID-036 **Measurement of wax appearance temperature (WAT) for Malaysian crude oils with hyperbranched polymers under CO_2 pressurization**
K. B. M. Sabil, B. Emirhanov, A. A. Ekaputra, A. Hosseini Pour
Universiti Teknologi PETRONAS, Malaysia

ID-041 **Design of equipment replacement and maintenance strategy with Life Cycle Assessment (LCA) on energy neutralization for waste water treatment plant**
G. Xu, M. Yoo
Invensys Operation System, United States

ID-045 **Molecular structure based property modeling: Development/improvement of property models through a systematic property-data-model analysis**
A. Hukkerikar, B. Sarup, G. Sin, R. Gani
Technical University of Denmark, Denmark

ID-046 **Improvement of departure function based predictions for liquid phase heat capacity of hydrocarbons**
N. Dadgostar, J. M. Shaw
University of Alberta, Canada

ID-047 **Phase behavior for carbon dioxide + cyclopentane derivative mixed hydrate systems**
Y. Matsumoto, T. Makino, T. Sugahara, K. Ohgaki
Osaka University, Japan

ID-049 **Effect of solvation with salting effect on solubilities of volatile organic compounds**
H. Nishiumi, H. Ogasawara, K. Ago, D. Kodama
Hosei University, Japan

ID-050 **Phase-change ionic liquids for CO_2 capture: Measurements and modeling of phase behavior**
L. Simoni, S. Seo, K. Graber, M.k Stadtherr, J. Brennecke
University of Notre Dame, United States

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ID-051 **Effect of surfactant on DMSO transport across water/hexane interface by molecular dynamics simulation**
Y.-F. Hu, W.-J. Lv, S.-L. Zhao, H. Liu, H.-L. Wang
East China University of Science and Technology, China

ID-052 **Reaction and diffusion kinetics investigation on melt polycondensation of fiber-grade poly(trimethylene terephthalate) in scale-up reactor**
Z.-Y. Sun, Z.-X. Wu, J.-H. Wei
Technology Research Institute of Shanghai Huayi Group, China

ID-054 **Prediction of solid hydrocarbon solubilities in water with the NRTL-PR model**
J. Escandell, I. Raspo, E. Neau
CNRS - Aix-Marseille University, France

ID-056 **Phase behaviour of CO_2 with liquid crystals**
M. de Groen, H. Matsuda, T.J.H. Vlugt, T.W. de Loos
Delft University of Technology, Netherlands

ID-058 **Compositional analysis and hydrate dissociation condition measurements for $CH_4 + C_2H_4 + C_2H_6 + N_2$ gas mixtures in diesel oil + water + anti- agglomerant emulsion system**
B. Liu, H. Liu, L. Mu, G. Chen, C. Sun, L. Yang
China University of Petroleum, Beijing, China

ID-061 **Influences on the stability of collagen triple-helix**
S. Schweizer, L. Subramanian, X. Krokidis
Scienomics, Paris, France

ID-062 **Pure component and phase equilibrium properties prediction in processes involving edible oils and biodiesel production**
L. Cunico, R. Ceriani, B. Sarup, R. Gani
Technical University of Denmark, Denmark

ID-064 **Hydrogen solubility in triolein and propane solubility in oleic acid for second generation BDF synthesis by use of hydrodeoxygenation reaction**
T. Tsuji, K. Ohya, T. Hoshina, T. Hiaki, K. Maeda, K. Hidetoshi, M. Osako
Nihon University, Japan

ID-066 **Quantifying the choreography of molecules in the nucleation and growth of clathrate hydrates**
A. Sum, D. Wu, B. Barnes
Colorado School of Mines, United States

ID-069 **Discussion around the paradigm of ideal mixtures with emphasis on the definition of the property changes on mixing**
R. Privat, J.-N. Jaubert
ENSIC - LRGP, France

ID-070 **Modeling and simulation of polyethylene waxes using PC-SAFT equation of state**
Y. Guerrieri, G. Costa, M. Embiruçu
Universidade Federal da Bahia,Salvador, Bahia, Brazil

ID-074 **The design of titanium dioxide surface chemistry by molecular modeling**
L. Huang, K. Gubbins
North Carolina State University, United States

ID-077 **Separation of methyl acetate–methanol azeotropic mixture using ionic liquid entrainers**
V. Dohnal, E. Baránková, A. Blahut
Institute of Chemical Technology, Prague, Czech Republic

ID-081 **CO_2 absorption properties, densities, viscosities and electrical conductivities of ethylimidazolium and 1-ethyl-3-methylimidazolium ionic liquids**
T. Makino, Y. Masuda, M. Kanakubo, T. Umecky, A. Suzuki
National Institute of Advanced Industrial Science and Technology, Japan

ID-084 **Interfacial properties and phase behavior of polar solvent systems. Modeling with PCP-SAFT combined with Density Gradient Theory**
E. Schäfer, S. Enders, G. Sadowski
TU Berlin, Germany

ID-085 **Explicit equation improving the temperature vs. composition VLE calculations for binary and ternary azeotropic and non azeotropic systems.**
A. Marcilla, J. A. Reyes-Labarta, M. del Mar Olaya
University of Alicante, Spain

ID-086 **A new continuous flow apparatus for bubble point measurements at high temperature and pressure**
P. Haimi, P. Uusi-Kyyny, M. Saajanlehto, M. Pakkanen, V. Alopaeus
Aalto University, Finland

ID-088 **CO_2 capture/separation using choline chloride-based ionic liquids**
X. Ji, Y. Xie, Y. Zhang, X. Lu
Lulea University of Technology, Sweden

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ID-090 **Improving the energy balance for the supercritical transesterification of triglycerides in carbon dioxide and methanol**
L. Soh, J. Curry, E. Beckman, M. Eckelman, J. Zimmerman
Yale University, United States

ID-099 **Vapour-liquid and solid-vapour-liquid equilibria of the systems (CO_2 + H_2) and (CO_2 + N_2) at temperatures between (218 and 303) K and at pressures up to 15 MPa**
N. McGlashan, O. Fandiño Torres, J. P. Trusler, D. Vega-Maza
Imperial College London, United Kingdom

ID-130 **Simulation of the separation of CO_2/CH_4 mixtures with nanoporous adsorbents: The effect of pore architecture and chemical composition**
L. Lu, X. Wu, W. Cao, E. Müller, Y. Zhu, L. Cai, X. Lu
Nanjing University of Technology, China

ID-155 **Solid-liquid equilibrium in ternary mixtures of ethyl esters: Experimental study and thermodynamic modeling**
M. D. Robustillo Fuentes, D. F. Barbosa, A. J. de Almeida Meirelles, P. de Alcantara Pessoa Filho
UFRN, Brazil

ID-185 **Solubility of supercritical CO_2 in protic ammonium ionic liquids**
L. M. Costa de Oliveira, L. Cardozo, V. Ferreira Cabral, C. da Silva, M. Iglesias, S. Mattedi
Federal University of Bahia, Brazil

ID-195 **Thermodynamic properties of aqueous solutions of multiple salts using the Q-electrolattice equation of state**
A. Zuber, R. F. Checoni, M. Castier
Texas A&M University at Qatar, Qatar

ID-223 **Thermodynamics of the aqueous solubility of calcium salts in the presence of compressed carbon dioxide**
I. Mejia, G. Bolaños
Universidad del Valle, Colombia

ID-229 **Force and osmotic second virial coefficient for dissimilar globular proteins immersed in electrolyte solutions**
M. Simões Santos, E. Rocha de Almeida Lima, F. Wanderley Tavares, E. Chalbaud Biscaia Jr.
Universidade do Estado do Rio de Janeiro - UERJ, Brazil

ID-233 **Generation of characteristic maps of the fluid phase behavior of ternary systems**
G. Pisoni, M. Cismondi, M. S. Zabaloy
PLAPIQUI Universidad Nacional del Sur, CONICET, Argentina

ID-271 **Group-contribution modeling of gas solubility in polar and associating solvents**
M. Gonzalez Prieto, F. Sanchez, S. Pereda, E. A. Brignole
PLAPIQUI Universidad Nacional del Sur, CONICET, Argentina

ID-278 **Developing an accurate generic description of association interactions in fluids of molecules formed from Mie segments within the Wertheim TPT1 approach**
S. Dufal, A. J. Haslam, T. Lafitte, A. Galindo, G. Jackson
Imperial College London, U.K.

ID-283 **Modeling of complexfluids using the GC-SAFT-VR based equation of state**
G. Das, J. D. Haley, C. McCabe
Vanderbilt University, USA

ID-285 **Effect of lithium tetrafluoroborate on the solubility of CO_2 in [bmim][BF_4]**
S. Durano Arnó, S. Lucas, A. Shariati, C. J. Peters
Delft University of Technology, Netherlands

Poster Session II

Chairs: *Pablo Hegel and Papa Ndiaye*

ID-019 **Robust and efficient Trust-Region based stability analysis and equilibrium flash calculations**
M. Petitfrere, D. V. Nichita
University of Pau and Total, France

ID-067 **Experimental evaluation of the efficacy of ice structuring proteins as natural gas hydrate inhibitors**
N. Daraboina, C. Malmos, N. Von Solms
Technical University of Denmark, Denmark

ID-071 **New method to detect asphaltene deposition due to CO_2 injection**
N. Silva, V. Oliveira, M. Souza, G. Costa
Universidade Federal da Bahia, Federação, Salvador, Bahia, Brazil

ID-095 **CO_2 separation from biogas using nano-porous materials**
G. Shen, X. Lu, X. Ji
Lulea University of Technology, Sweden

ID-096 **Carbon dioxide sequestration and hydrogen storage in TBAB and TBAF semi-clathrate hydrates: Kinetics and crystal evolution by *in situ* Raman spectroscopy**
A. Torres Trueba, I. R. Radovic, J. F. Zevenbergen, C. J. Peters, M. C. Kroon
Delft University of Technology, Netherlands

ID-097 **Probing the structure of xenon clathrate hydrates: Implications to phase equilibria of clathrate hydrates**
P. Lafond, A. Sum
Colorado School of Mines, United States

ID-098 **Phase equilibrium and thermophysical property measurements of binary mixtures of trimethylbutylammonium bis(trifluoromethylsulfonyl)imide with ethanol, 1-propanol and dimethylformamide**
M. Massel, A.-L. Revelli, E. Paharik, R. R. Novak, J. F. Brennecke
University of Notre Dame, United States

ID-101 **Quantitative measurements of CH_4 production from CH_4 hydrates with the injection of CO_2**
B. R. Lee, E. D. Sloan, C. Koh, A. Sum
Colorado School of Mines, United States

ID-103 **NIST ThermoData Engine: Generating reliable thermodynamic property data for chemical process and product design**
M. Frenkel
National Institute of Standards and Technology, United States

ID-111 **Solubility of CO_2, CH_4 and other low molecular weight hydrocarbons in ionic liquids**
M. T. Mota Martinez, M. C. Kroon, C. J. Peters
Petroleum Institute, United Arab Emirates

ID-112 **Removal of small hydrocarbons (ethane, propane) from natural gas streams using the ionic liquid 1-ethyl-3 -methylimidazolium tris(pentafluoroethyl)trifluorophosphate**
M. Althuluth, M. Kroon, C. J. Peters
Delft University of Technology, Netherlands

ID-113 **Phase equilibrium for clathrate hydrate formed with methane and octafluorocyclopentene**
K. Murayama, K. Tezuka, S. Takeya, R. Ohmura
Keio University, Japan

ID-115 **Excess diffusion coefficients in mixtures of carbon dioxide and organic solvent under pressure**
T. Funazukuri, C.-Y. Kong
Chuo University, Japan

ID-116 **Comparison of correlations for viscosity prediction**
S. Pinheiro, G. Tarantino, L. C. Santos, L. M. Gois, C. A. Pires, S. Mattedi
Federal University of Bahia, Brazil

ID-118 **A comparison of dissolution processes of monosodium glutamate in aqueous solution and water-ethanol solution probed by Raman spectroscopy**
C. Liu, N. Wu, X. Ji, X. lu
Nanjing University of Technology, China

ID-119 **Determination of vapor-liquid equilibria at elevated pressures using ebulliometer**
H. Taguchi, T. Nakakubo, H. Matsuda, K. Kurihara, K. Tochigi
Nihon University, Japan

ID-120 **Generation and counterion valance controlled aggregation of surface charged PAMAM dendrimers**
D. Sun, J. Zhou
South China University of Technology, China

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ID-121 **Liquid-crystal behavior of hard-sphere chains provided with a linear and a fully-flexible segment**
B. Oyarzun, T. W. de Loos, T. J. H. Vlugt
Delft University of Technology, Netherlands

ID-125 **Automated characterisation of complete liquid-liquid equilibria**
D. Dechambre, A. Bardow, L. Greiner, K. Leonhard
Aachen University, Germany

ID-126 **Modeling of dielectric properties with an associating equation of state**
B. Maribo-Mogensen, G. Kontogeorgis, K. Thomsen
Technical University of Denmark, Denmark

ID-127 **Separation design of switchable ionic liquid based on DBU-glycerol-CO_2 in biorefinery process**
E. Sapei, A. Ostonen, P. Uusi-Kyyny, V. Alopaeus
Aalto University School of Science and Technology, Finland

ID-128 **An equation of state for solid-liquid-vapor equilibrium applied to the air distillation process**
P. Stringari, M. Campestrini, C. Coquelet, P. Arpentinier
MINES ParisTech, Laboratoire CEP/TEP, France

ID-129 **Influence of molecule architecture on phase equilibria**
K. Langenbach, D. Browarzik, M. Fischlschweiger, C. Browarzik, S. Enders
TU Berlin, Germany

ID-132 **Molecular dynamics studies of aqueous amphiphilic systems using a SAFT-γ Coarse Grained Force Field**
O. Lobanova, C. Avendaño, T. Lafitte, C. Herdes, E. Santiso, G. Jackson, E. Müller
Imperial College London, United Kingdom

ID-137 **Multiscale modeling and simulation of protein adsorption at interfaces**
J. Zhou
South China University of Technology, China

ID-138 **Modelling the solubility of active pharmaceutical ingredients in solvents and solvent mixtures with the SAFT-γ Mie group contribution approach**
V. Papaioannou, C. S. Adjiman, G. Jackson, A. Galindo
Imperial College London, United Kingdom

ID-139 **Application of the statistical associating fluid theory for potentials of variable range (SAFT-VR) coupled with renormalization-group (RG) theory to model the phase equilibria and second-derivative properties of fluids**
E. Forte, F. Llovell, L. F. Vega, J. P. M. Trusler, A. Galindo
Imperial College London, United Kingdom

ID-140 **Investigation of oil spill absorbents using different Materials**
J. F. K. Xiang, A. F. Alta'ee, K. M. Sabil
Universiti Teknologi PETRONAS, Malaysia

ID-141 **Mutual diffusion in the ternary mixture water + methanol + ethanol and its binary subsystems**
J. Vrabec, G. Guevara-Carrion, S. Parez, H. Hasse
Univrsity of Paderborn, Germany

ID-142 **Cycle Life Analysis for nutrient removal processes**
G. Ontiveros, E. Campanella
INTEC - FICH (Universidad Nacional del Litoral), Argentina

ID-150 **Evaluation of different contribution methods over the performance of Peng-Robinson and CPA equation of state in the prediciton of ELV of triglycerides and fatty esters +alcohol**
S. Arvelos, L. Rade, E. Watanabe, C. Hori, L. Romanielo
Universidade Federal de Uberlândia, Brazil

ID-151 **Mechanism and rate of formation of polyglutamine oligomers**
A. Fluitt, J. de Pablo
University of Wisconsin-Madison, United States

ID-154 **Expanding the Aspen Plus applications by the use of external models. Case study: Thermodynamic models for electrolyte solutions**
D. Freitas, Y. Guerrieri
Universidade Federal da Bahia, Brazil

ID-157 **Salt solubility data for sodium chloride and mono ethylene glycol aqueous systems from 293.15 to 403.15 K**
P. Alves Sobrinho, L.R.P. Nobre, H.P.C. Ferreira, A.L.N. Mota, C.S. Figueiredo, J.R.P. Ciambelli, O. Chiavone Filho, R.O. Santana, J. F. Nascimento
UFRN, Brazil

ID-158 **Molecular design of soft materials using classical density functional theory**
Z. Feng, B.Marshall, K. Gong, D. Ballal, K. Cox, W. Chapman
Rice University, United States

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ID-165 **Estimation of protein stability thermodynamics from minimum structural information**
J. O'Connell, M. Fan, E. Fernandez
University of Virginia, United States

ID-169 **Phase behavior and properties of Athabasca bitumen-toluene - water mixtures**
M. J. Mohammad J. Amani, M. R. Gray, J. M. Shaw
University of Alberta, Canada

ID-170 **Equilibrium liquid-vapor data obtained by CO_2 + dichloromethane + medroxy-progesterone system and thermodynamic model**
W. Machado Giufrida, L. Ferrera Pinto, G. Duenhas Machado, L. Cardozo Filho, V. Ferreira Cabrail, M. Kunita
State University of Maringá - UEM, Brazil

ID-175 **A new process for biodiesel purification using pressurized carbon dioxide**
A. M. Escorsim, C. Soares Cordeiro, M. Lúcio Corazza, P. Matar Ndiaye, L. Pereira Ramos
Universidade Federal do Paraná, Brazil

ID-176 **Synthesis, physico-chemical and transport properties for two ionic liquids based on stearate anion**
D. F. Santos, L. J. Marques Martfeld, M. A. Iglesias, E. Franceschi, S. Mattedi
Federal University of Bahia, Brazil

ID-188 **Correlation of phase equilibria by concentration dependent surface area parameter model**
Y. Iwai, I. Taniguchi
Kyushu University, Japan

ID-189 **Solubility of CO_2 in [(1 – x)NaCl + x KCl](aq) or $CaCl_2$(aq) or $MgCl_2$(aq) at temperatures from (308 to 423) K and at pressures up to 40 MPa.**
J.P. Martin Trusler, D. Tong, D. Vega-Maza
Imperial College London, United Kingdom

ID-192 **Behavior of water at different interfaces and under nanoconfinement**
G. Appignanesi, J. A. Rodríguez Fris, L. Alarcón, S. Accordino, M. Morini, M. B. Sierra, J. M. Montes de Oca
INQUISUR - Universidad Nacional del Sur - CONICET, Argentina

ID-211 **Study of the formation of clathrate of CO_2 in the presence of alkanolamines**
S. Ceja-Castillo, M. E. Rebolledo-Libreros, A. Trejo
Instituto Mexicano del Petróleo, México

ID-236 **Thermodynamic sound speed of multiphase systems using the Peng-Robinson, Mattedi-Tavares-Castier, and PC-SAFT equations of state**
M. Z. Sheriff, S. Taha, M. Castier
Texas A&M University at Qatar, Qatar

ID-243 **Kinetics of salt dissolution and precipitation in aqueous solution containing glycol using image analysis**
A. Barreto Jr, F. Wanderley Tavares, C. Senna Figueiredo, F. Cajaiba da Silva
UFRJ, Brazil

ID-265 **Modeling the phase diagrams of mixtures containing ionic liquids with PC-SAFT equation of state**
Y. Chen, F. Mutelet, J.-N. Jaubert
Université de Lorraine, France

ID-273 **Phase equilibrium engineering of jojoba oil extraction with liquid CO_2 + propane**
C. Palla, P. Hegel, S. Pereda, G. Mabe, E.A. Brignole
PLAPIQUI Universidad Nacional del Sur, CONICET, Argentina

ID-286 **Investigation of the high pressure solubility of CO in 1-alkyl-3-methylimidazolium bis(trifuoromethylsulfonyl)amide for gas separations**
S. Raeissi, L. J. Florusse, C. J. Peters,
Shiraz University, Iran

Poster Session III

Chairs: *Gustavo Appignanesi and Silvana Mattedi*

ID-026 **Thermodynamic properties of aqueous protein solutions: Measurements and ePC-SAFT modeling**
C. Held, G. Sadowski
TU Dortmund University, Germany

ID-039 **Development of a comprehensive framework for surfactant selection and design for emulsion based chemical product design**
M. Mattei, G. M. Kontogeorgis, R. Gani
CAPEC, Technical University of Denmark, Denmark

ID-048 **Measurement of local composition and phase behavior of organic compounds in porous inorganic media using multi-element acoustic sensors**
M. Cassiede, J. M. Shaw
University of Alberta, Canada

ID-073 **A fractal approach on predicting gas hydrate phase equilibria in porous media**
S.-L. Li, C.-Y. Sun, G.-J. Chen, B. Liu, Q.-L. Ma, L.-Y. Yang
China University of Petroleum, Beijing, China

ID-079 **Separation of methanol–dimethyl carbonate azeotropic mixture using ionic liquid 1-ethyl-3-methylimidazolium tetracyanoborate**
A. Blahut, V. Dohnal
Institute of Chemical Technology, Prague, Czech Republic

ID-080 **Improvement of the PPR78 model in the prediction of excess-enthalpy and excess-heat capacity data**
J.-N. Jaubert, R. Privat
ENSIC - LRGP, France

ID-089 **Vapor–liquid equilibria in the polymer + solvent systems containing lower concentrations of solute at normal or reduced pressures**
J. Pavlicek, G. Bogdanic, I. Wichterle
Acad. Sci. Czech Rep., Czech Republic

ID-091 **Novel aqueous two phase system based on a hyperbranched polymer**
A. Kulaguin-Chicaroux, T. Zeiner
TU Dortmund, Germany

ID-094 **Tuning of equation-of-state – The critical importance of sequence in tuning**
K. H. Yee, A. F. Alta'ee, K. M. Sabil
Universiti Teknologi PETRONAS, Malaysia

ID-104 **Systematic optimization for an OPLS-like force field and its application to hydrofluorocarbons**
K. Kroenlein, E. Paulechka, A. Kazakov, M. Frenkel
National Institute of Standards and Technology, United States

ID-108 **Increasing the energy storage capacity of clathrate hydrates with hydrogen and methane**
Y. Matsumoto, R. G. Grim, T. Sugahara, K. Ohgaki, E. D. Sloan, C. A. Koh, A. K. Sum
Colorado School of Mines, United States

ID-114 **Phase equilibrium for structure H hydrate formed in difluoromethane + 3,3-dimethyl-2-butanone + water system**
T. Watanabe, R. Ohmura
Keio university, Japan

ID-147 **Biogas upgrading processes analysis using statistical design of experiments**
B. Morero, E. Campanella
INTEC - FICH (Universidad Nacional del Litoral), Argentina

ID-149 **Osmotic dehydration of cupuaçu: obtaining the diffusion coefficient of mass transfer based on a chemical potential model and optimal conditions of osmotic treatment**
S. de Souza Castro, G. Paiva Chaves, M. A. Chaves, S. Mattedi
Federal University of Bahia / State University of Southwest of Bahia, Brazil

ID-173 **Determination high-pressure vapor-liquid equilibrium data for systems involving carbon dioxide + (R,S)-1,2-isopropylidene glycerol (Solketal) + oleic acid**
A. F. Zanete, L. Ferrera Pinto, W. Machado Giufrida, L. Cardozo Filho, V. Ferreira Cabrail, R. O. Mendonça Alves de Souza
State University of Maringá - UEM, Brazil

ID-186 **Phase equilibrium measurements and thermodynamic modeling for the systems carbon dioxide + hexanol (or pentanol) at high pressures**
L. Pereira, P. Gashi, A. Scheer, P. Ndiaye, M. L. Corazza
UFPR, Brazil

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ID-196 **Application of the CPA equation of state to [BF_4]- ionic liquids and their mixtures**
F. Maia, I. Tsivintzelis, O. Rodríguez, E. Macedo, G. Kontogeorgis
FEUP, Portugal

ID-199 **Study of the behavior of mixtures ethanol + water + ionic liquid using cubic equations of state**
J. da Paixao Lopes dos Santos, G. F. da Silva, I. Quintela Matos
Universidade Federal de Sergipe, Brazil

ID-201 **Molecular simulations of nanoconfined water behaviors in silt pore: The effect of pore wall interfacial properties**
Y. Zhu, L. Zhang, X. Lu, L. Lu, X. Wu
Nanjing University of Technology, Nanjing, China

ID-202 **Determination and correlation of excess molar enthalpies of the binary carbon dioxide + ethyl acetate system at temperatures from (298.15 to 308.15) K and pressures from (5.0 to 7.0) MPa**
K. Kurihara, Y. Nakamura, T. Okamoto, Y. Itazu, H. Matsuda, K. Tochigi
Nihon University, Japan

ID-204 **Measurements and modeling of phase equilibrium of systems containing polar chemicals**
M. Frost, N. von Solms, G. M. Kontogeorgis
Technical University of Denmark, Denmark

ID-205 **High pressure phase behavior modeling of asymmetric methane + n-alkane binary systems with the RKPR EOS**
M. V. Galdo, M. Gomez, J. M. Milanesio, M. Cismondi Duarte
IDTQ-PLAPIQUI (UNC); Phasety, Argentina

ID-206 **High-pressure phase equilibria of active pharmaceutical ingredients in solvent-supercritical CO_2 mixture**
A.-L. Revelli, S. Laugier, P. Subra-Paternault, A. Erriguible
Université Bordeaux 1, France

ID-207 **High pressure phase behavior modeling of asymmetric ethane + n-alkane binary systems with the RKPR EOS**
N. G. Tassin, S. Zúñiga, M. Yanes, M. Cismondi Duarte
IDTQ-PLAPIQUI (UNC); Phasety, Argentina

ID-209 **Gas solubility of CO_2 in aqueous solutions of diethanolamine with 1-amino-2-propanol**
J. R. Hernandez, M. E. Rebolledo-Libreros, A. Trejo
Instituto Mexicano del Petróleo, México

ID-213 **Liquid-liquid equilibria for pseudoternary mixtures of mono-, di- and triglycerides from palm stearin with (ethanol+water) at 340.16 K**
E. Sánchez, C. Pardo, G. Bolaños
Universidad del Valle, Colombia

ID-214 **Describing the liquid crystalline phase and ordering behaviour of solutions of the polypeptide PBLG with a generalised Onsager-van der Waals approach**
L. Wu, E. A. Müller, G. Jackson
Imperial College London, United Kingdom

ID-215 **Liquid-liquid equilibria of binary systems {benzene + [x-mim][NTf2] ionic liquid}: Experimental data and thermodynamic modeling using a group contribution equation of state**
E. J. González, E. Macedo, Á. Domínguez, S. B. Bottini, S. Pereda
University of Porto, Portugal

ID-220 **Theory and simulations of polymer functionalized nanoparticles**
A Jayaraman, T Martin
University of Colorado Boulder, United States

ID-221 **Correlation of speed of sound by an atomic contribution model and measurements for pyrolysis bio-oil compounds**
D Cunha, M Paredes, R Reis
UERJ, Brazil

ID-222 **Ion dynamics near a charged electrode including ion specific effects through a transient Poisson-Nernst-Planck model**
P Alijó, F Tavares, E Biscaia Jr., A Secchi
PEQ/COPPE/UFRJ, Brazil

ID-224 **Prediction of activity coefficients of mixtures including components of pyrolysis bio-oils**
D Cunha, M Tavares, C Costa, R Reis, M Paredes
UERJ, Brazil

ID-228 **Molecular dynamics simulations of gas diffusion in polymer membranes**
R. Caputo Domingues da Silva, C. Rubber de Almeida Abreu, F. W. Tavares
Universidade Federal do Rio de Janeiro, Brazil

ID-231 **A parameterization approach for equation of state models: The case of water-hydrocarbon binary systems**
J. I. Ramello, S. B. Rodriguez-Reartes, M. Cismondi, M. S. Zabaloy
PLAPIQUI Universidad Nacional del Sur, CONICET, Argentina

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ID-234 **Measurement and calculation of solubilities for the organic metal complexes in supercritical carbon dioxide**
M. Haruki, M. Ohara, M. Morioka, S. Kihara, S. Takishima
Hiroshima University, Japan

ID-235 **Phase equilibrium of fluids confined in porous media from an extended Peng-Robinson equation of state**
L. Travalloni, F. W. Tavares, M. Castier
Texas A&M University at Qatar, Qatar

ID-237 **A NIR probe monitoring transitional phase inversion of emulsions**
R. Charin, F. W. Tavares, M. Nele de Souza
Federal University of Rio de Janeiro, Brazil

ID-239 **Integrated experimental and computational studies of energy-relevant interfaces**
P. Cummings, G. Feng, S. Li, D. Wesolowski
Vanderbilt University, United States

ID-246 **Phase transitions of liquids in nano-pores; the ice structures stabilized by the confinement**
M. Kempinski, M. Jazdzewska, M. Sliwinska-Bartkowiak, Y. Long, K. Gubbins
Mickiewicz University, Poland

ID-253 **Determination and prediction of solubilities of active pharmaceutical ingredients in selected organic solvents**
H. Matsuda, M. Tomioka, K. Mori, K. Kurihara, K. Tochigi, K. Tomono
Nihon University, Japan

ID-262 **Investigation on dissolution of amorphous solid dispersions for poorly water-soluble drugs in a hydrophilic polymer with a chemical potential gradient model**
Y. H. Ji, R. Paus, A. Prudic, G. Sadowski
TU Dortmund, Germany

ID-264 **Thermodynamic characterization of oxygenated based ionic liquids**
F. Mutelet, P. Carre, A. Skrzypczak, J.-N. Jaubert
Université de Lorraine, France

ID-267 **QM - CAMD: Advances in computer-aided molecular design of solvents for reactions**
E. Siougkrou, A. Galindo, C. S. Adjiman
Imperial College London, UK

ID-268 **Phase behavior of model asphaltene + toluene + carbon Dioxide**
B. Breure, S. Soroush, T. de Loos, C. J. Peters
The Petroleum Institute, United Arab Emirates, and Eindhoven University of Technology, The Netherlands

ID-269 **Thermodynamic model for process design, simulation and optimization in the production of biodiesel**
N. Cotabarren, P. Hegel, S. Pereda, E. A. Brignole
PLAPIQUI Universidad Nacional del Sur, CONICET, Argentina

ID-270 **Molecular design of solvents for sustainable chemical processes**
J. Scilipoti, M. Cismondi, E. A. Brignole
PLAPIQUI Universidad Nacional del Sur, CONICET, Argentina

ID-281 **Self-oscillation of the temperature of a material under irradiation**
P. Selyshchev
University of Pretoria, South Africa

ID-282 **The impact of environmental effects on the structure and conductance of molecular junctions**
W. French, C. R. Iacovella, P. Cummings
Vanderbilt University, USA

ID-284 **Modeling and experimental study of the phase behavior of a five-component model gas condensate**
A. Shariati, E. J.M. Straver, L. J. Florusse, C. J. Peters
Shiraz University, Iran

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