



# 10<sup>th</sup> Joint Meeting of UNIFAC Consortium and DDBST User Meeting



## Timetable

<b>Location:</b>	<b>Sept. 17<sup>th</sup> (Monday)</b>	<b>Café &amp; Bar Celona, Markt 4, Oldenburg</b> <a href="http://www.cafe-bar-celona.de">www.cafe-bar-celona.de</a>
	<b>Sept. 18<sup>th</sup> (Tuesday)</b>	<b>TGO Technologie- und Gründerzentrum Oldenburg GmbH, Seminar Room IV Marie-Curie-Str. 1, Oldenburg</b>
	<b>Sept. 19<sup>th</sup> (Wednesday)</b>	<b>DDBST, Marie-Curie-Str. 10 D-26129 Oldenburg</b>

### Monday, September 17<sup>th</sup>

19.30 Informal Get-Together at Café & Bar Celona, Markt 4, Oldenburg  
(Phone: +49 (0) 441 2489525)

### Tuesday, September 18<sup>th</sup>

#### 09.00 Reception

09.30 

- Welcome
- Introduction
- Time schedule
- Overview of the work of consortium and DDBST

 Prof. Dr. Jürgen Gmehling

10.00 DDB and DDB Software Package From 2011 to 2012 and Beyond Prof. h.c. Dr. Jürgen Rarey

10.30-10.50 The Status and Development of VTPR Group Contribution Equation of State Dr. Bastian Schmid

11.00-11.20 Solvent Selection for Liquid-Liquid Extraction and Absorption Andre Schedemann

#### 11.30 Coffee Break / Photo Shooting

11.50-12.05 *Simulis Thermodynamics: just one more thermodynamic package?* Olivier Baudouin  
**ProSim SA**

12.10-12.25 *Modification of fragmentation rules* Dr. Kai Fischer  
Dr. Eric Hendriks  
**Shell**

12.30-12.45 *Modified Trouton's rule for estimation, correlation and evaluation of vapor pressure* Dr. Paul Mathias  
**Fluor Enterprises Inc.**

#### 12.50 Lunch Break

13.30-13.45 *An unexpected model choice* Dr. Michael Kleiber  
**ThyssenKrupp Uhde GmbH**

13.50-14.05 *Overview of Invensys Implementation (and How to Use) of the UNIFAC Consortium Models* Francisco J. Braña-Mulero  
**Simsco-Esscor**

14.10-14.25 *Reliable Process Modelling with Accurate Thermophysical Property Data and Models* Dr. Richard Sass  
**DECHEMA e.V.**

14.30-14.45 *COSMO-X  
A new concept to model 3-dim. structure* Dr. Gerard Krooshof  
**DSM Chemical Technology**

14.50 Current State of the Revision and Extension of UNIFAC, Mod. UNIFAC and PSRK Group Contribution Equation of State Dr. Dana Constantinescu

15.10 Consortium Session Dr. Dana Constantinescu  

- Delivery 2012
- Customization files
- Future plans
- Discussion

 Prof. Dr. Jürgen Gmehling

#### 15.20 Coffee Break

15.30-16.25 DDB-Session In Depth Presentation of New Developments Prof. h.c. Dr. Jürgen Rarey  
Co-workers of DDBST

17.00 Laboratory Tour LTP

19.30 **Dinner**  
Rodizio Restaurant  
(Rodizio Lazador Brazil  
<http://www.rodizio-oldenburg.de/>)  
Pferdemarkt 16, 26121 Oldenburg  
Phone: +49 (0) 441 8007433

### Wednesday, September 19<sup>th</sup>

#### 09.00 Reception

09.30-13.00 Hands-On Workshop Co-workers of DDBST

- Dortmund Data Bank (DDB)
  - DDB Software Package (DDBSP)
- Small group or individual hands-on introduction to various features of DDB and DDBSP. Several topics are offered but this session is open to customer specific questions:
- Process Simulation Parameter Verification Using DDB/DDBSP
  - Physical Property Estimation and Critical Evaluation of Method Reliability
  - Pure Component and Mixture Data Regression
  - Data and Parameter Import/Export
  - DDBSP with AspenPlus and Pro II

09.30-18.00 Private appointment with co-workers of DDBST and LTP

14.00-16.00 Hands-On Workshop (continued) Co-workers of DDBST