17th PPEPPD International Conference on Properties and Phase Equilibria for Product and Process Design

11.-15. of May 2025 in Bad Gögging, Germany

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Prof. John O'Connell, University of Virginia, USA
Prof. Pedro de Alcântara Pessoa Filho, University São Paulo, Brazil
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Prof. Sabine Enders, KIT, Germany
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Thank you for our Sponsors:

Conference Program

Sunday, 11. May

15.00 - 21.30 Registration

Opening Session (Chairs: S. Enders, J. Groß)

17.00-19.00 Presentation of Young-Investigator Awardee

Presentation of John Prausnitz-Awardee

19.00-22.00 Welcome reception

Monday, 12. May

8.30-10.30	Invited Presentations (A. Galindo, I. Siepmann) Decision support for sustainable process design: How to evaluate the impact of physical properties and uncertainties?, **Norbert Asprion**, BASF AG, Germany CO_2 Separations with Ionic Liquids, **Joan Brennecke**, University of Texas at Austin	
10.30-11.00	Coffee Break	
11.00 - 12.30	**Phase Equilibria**: W. Chapman. P. Pessoa Filho Phase Behaviour of Methanol + CO_2, M. Trusler, R. Latcham, Imperial College London, UK Combination of Gravimetric Experiments and Molecular Dynamics Simulation: The Road to Accurate Mixture Dew-Point Densities, M. Richter[1], L. Bernardini[1], M. Sekulla[1], M. Kohns[2], M. McLinden[3], [1] TU Chemnitz, Germany [2] RPTU Kaiserslautern, Germany [3] NIST, USA Four-phase equilibrium relation of clathrate hydrate + aqueous + liquefied guest + vapor phases in the carbon dioxide, sulfur hexafluoride, and water ternary system, T. Sugahara[1], T. Ishikawa[1], T. Hirai[1], N. Yoshimoto[2], [1] Osaka University, Japan [2] Yamaguchi University, Japan	**CO_2 Capture**: I. Economou, C. Held Assessment of ionic liquids for carbon dioxide capture through a multiscale approach, S.B. Rodriguez Reartes, F. Llovell, Universitat Rovira i Virgili, Spain CO_2 Capture using Slurry made by Integration of Aqueous and Immobilized Deep Eutectic Solvents, S. Foorginezhad, X. Ji, Lulea University of Technology, Sweden High-Throughput Measurement of CO_2 Properties in Amine-Based Absorbents and Screening Techniques for Accelerating the Development of CO_2 Absorbents, H. Machida, Nagoya University, Japan
12.30 - 14.00	Lunch	
14.00 - 15.30	**Thermodynamics for pharmaceutical applications:** R. Dohrn, M.G. de Angelis Robust phase equilibria in reactive non-ionic and ionic systems relevant to pharmaceutical applications, G. Jackson, F.A. Perdomon, A. Galindo, A. Mitsos, C. Adjiman, Imperial College London, UK Optimization protein stability in lyophilized formulations based on water-activity calculations, C. Brandenbusch, TU Dortmund, Germany Elucidating the Solubility Enhancement of Active Pharmaceutical Ingredients through Hydrotropy: A Case of Local Anesthetics, S. Nasrallah, A. Wendler, M. Minceva, TUM, Germany	**Transport Properties:** X. Lu, E. May Density and Viscosity of Light and Heavy Phases from Mixtures of Bitumen and n-Butane, F.N.T. Duran, F. Schoeggl, H. Yarranton, University of Calgary, Canada Thermodynamic constraints on rate type equations for anomalous diffusion in glassy polymers, F. Doghieri, R. Parchi, G.C. Roda, University of Bologna, Italy Dynamic Light Scattering for the Characterization of Diffusion Processes in Fluid Mixtures and Particulate Systems, A.P. Fröba, FAU, Germany

15.30-16.00	Coffee break
16.00-22.00	Poster Party (P1) with barbecue

Tuesday, 13. May

8.30-10.30	Invited Presentations: G. Sadowski, C. Mc Cabe Tailoring of polymer properties using thermodynamics and mechanics, **Michael Fischlschweiger**, TU Clausthal, Germany Extension of molecular thermodynamics to interface for confined transfer, **Xiaohua Lu**, Nanjing Tech University, China	
10.30-11.00	Coffee Break	
11.00 - 12.30	**Dynamic Processes:** F. Llovell, M. Richter Mechanisms of Droplet Interaction and Interfacial Phenomena in Liquid-Liquid Systems, T. Zeiner[1], M. Singer[1], P. Zimmermann[2], [1] KIT, Germany, [2] BSH, Germany Gas Hydrate Formation Dynamics: Integrating Nucleation and Growth through Chemical Affinity-Based Models, I. Oliveira, C. Costa, A. Barreto Jr., F. Tavares, Federal University of Rio de Janeiro, Brazil Computational Design of Peptides as Detectors, Sensors and Drugs, C. Hall, North Carolina State University, USA	**Thermodynamics for Process Development**: A. Soto, A.P. Fröba CO_2 hydrogenation: new high-pressure equilibrium data for technology improvement, S. Pereda, N. Cotabarrena, F.A. Sanchez, P. Hegel, Universidad Nacional del Sur, Argentina Adsorption Processes of Contaminants of Emerging Concern from Environmental Water, A.B. Pereiro, M.C. Naranjo, J.A. Pulido, J.C. Bastos, J.M.M. Araújo, NOVA University Lisbon, Portugal Design of a Novel Process for the Production of Synthetic Diesel Substitutes from Formaldehyde and n-Butanol/ Isobutanol, J. Burger, L. Winklbauer, TUM, Germany
12.30 - 14.00	Lunch	
14.00 - 19.00	Excursion to Regensburg	
19.00-20.30	Dinner	

Wednesday, 14. May

8.30-10.30	Invited Presentations: H Matsuda, J.C. Hemptiene Presentation of EFCE awardee Thermodynamics of polymeric materials for the energy transition **Maria Grazia De Angelis**, University of Edinburgh, UK,	
10.30-11.00	Coffee Break	
11.00 - 12.30	**New Model Development:** M. Trusler, G.M. Kontogeorgis Thermodynamic Modeling of Rare Earth Elements: Developing Processes for Recovery from Secondary Sources, G. Das, A. Anderko, OLI Systems Inc., USA Validation of Molecular Models via Virial Coefficients and the Virial Equation of State, D. Kofke, R. Suresh, O. Desai, A. Schultz, University at Buffalo, USA A Novel Global Renormalization Group Theory Incorporating Symmetric and Asymmetric Fluctuations on a Cubic Lattice	**Modelling:** M. Fischlschweiger, F.W. Tavares Experimental characterization and thermodynamic modeling of Cryogenic sorption isotherms in amorphous polymers, M. Minelli, V. Signorini, G. Oleari, University of Bologna, Italy Evaluating Square Gradient Theory with Various Equations of State for Correlation and Prediction of Surface Tension, R. Elliott, KFUPM Dhahran, Saudi Arabia Surfing the Molecular Sea with Stochastic Machine Learning: Sigma Profiles as a Digital Chemical Space, D. Abranches[1], E. Maginn[2], Y. Colón[2], [1] University of Aveiro, Portugal, [2] University of Notre Dame, USA

	Model, Y.J. Shih, National Taiwan University, Taiwan	
12.30 - 14.00	Lunch	
14.00 - 17.00	Poster Session (P2) with coffee and cookies	
18.00 - 23.00	Gala Dinner	

Thursday, 15. May

8.30-10.30	Invited Presentations: C. Breitkopf, N. Asprion Framework for a High-Throughput Screening Method to Assess Polymer/Plasticizer Miscibility: The Case of Hydrocarbons in Polyolefins, **Paola Carbone**, Manchester University, UK Ion Trios - A New Paradigm for a 100-Year-Old Stalemate in Aqueous Solution Chemistry? **Eric May**, University of Western Australia,	
10.30-11.00	Coffee Break	
11.00 - 12.30	**Membrans:** J. Brennecke, K. Langenbach Coarse-Grained Molecular Simulation on Mixed Matrix Membranes: MOF Optimum Loading, I. Economou[1], A. Mohamed[1], H.K. Jeong[2], [1] Texas A&M University at Qatar, Qatar, [2] Texas A&M University, USA Molecular dynamics simulation to explore the hybrid adsorption - hydration natural gas capture mechanism of wet MOF fixed bed, Z. Li, J. Kan, N. Li, China University of Petroleum Beijing, China AI promotes the development of high-performance membrane separation materials, Y. Tian, Zhengzhou University, China	**Machine Learning**: E.M. Macado, T. Zeiner Hard-Constraint Neural Networks for Thermodynamically Consistent Property Prediction, T. Specht[1], M. Hoffmann[1], S. Mandt[2], F. Jirasek[1], [1] RPTU Kaiserslautern, Germany [2] University of California Irvine, USA Unlocking the potential of machine learning in co-crystal prediction by a novel approach integrating molecular thermodynamics, Y. Song[1], Y. Ding[1], J. Su[1], J. Li[2], J. Yi[2], [1] Southeast University, Nanjing, China, [2] Jinling Pharmaceutical Co., Ltd., Nanjing, China Predicting shear viscosities of aqueous amine systems using periodic perturbation NEMD simulations and machine learning, L. Gui[1], K. Nehil-Puleo[2], E. Tsochantaris[1], C. McCabe[1], P. Cummings1, [1] Heriot-Watt University, UK [2] Vanderbilt University, USA
12.30 - 13.00	Closing (S. Enders, J. Groß)	
13.00 - 14.00	Lunch	

Additional Events (only by Invitation)

Monday: 18.00-20.00, EFCE Meeting

Wednesday: Lunch Break: IOC Meeting

Poster Program - Poster Session P1 on Monday

	Polymers
1	Thermophysical Properties of Polymer Melts with Dissolved Blowing Agents by Optical Techniques, J.H. Jander, P.S. Schmidt, T. Klein, A.P. Fröba, FAU, Germany
2	Impact of average centrifugation-molecular weight on the polymer molecular weight distribution (MWD) curve, A.A. Jaberi[1], A. Wender[1], N. Ferrando[1], W. Yan[2], J.C. de Hemptinne[1], [1] IFP Energies Nouvelles, France, [2] DTU, Denmark
3	Modelling of shear induced mixing behaviour of polymer blends, J. Jaske, S. Enders, KIT, Germany
4	Inferring equilibrium and pseudo-equilibrium pVT properties of super-glassy polymers from gas solubility data, R. Parchi, G. Pangia, F. Doghieri, University of Bologna, Italy
5	Influence of molecular architecture and semi-crystalline morphology on gas solubility in polyethylene, S. Leube[1], J. Zimmermann[1], M. Fischlschweiger[2], S. Enders[1], [1] KIT, Germany, [2] TU Clausthal, Germany

6	Temperature Dependence of Solubility of Polyethylene in Various Solvents: A Systematic Study for Solvent-based Recycling, J. Yin, TUM, Germany
7	Modelling the solubility of semi-crystalline polyethylene in organic and bioderived solvents using SAFT-γ Mie EoS for plastic recycling, R. Standish[1], J. Yin[2], J. Burger[2], M. Minceva[2], G. Jackson[1], A. Galindo[1], C.S. Adjiman[1], [1] Imperial Collegue London, UK, [2] TUM, Germany
8	D13PEG/Citrate ATPS: From LLE to the complete phase diagram, R. Gómez-Pineda, A. Soto, O. Rodríguez, Universidade de Santiago de Compostela, Spain
9	Recovery of Fish Protein by Aqueous Two-Phase Extraction, Gómez-Pineda, A. Soto, O. Rodríguez, Universidade de Santiago de Compostela, Spain
	Hydrogen
10	A Critical Review of Hydrogen Adsorption on Porous Materials for Energy Storage Applications, M.S. Günther, X. Yang, D. Zipplies, M. Richter, TU Chemnitz, Germany
11	Thermophysical Properties of Liquid Organic Hydrogen Carriers, T.M. Koller, M. Kerscher, J.H. Jander, T. Klein, M.H. Rausch, P. Wasserscheid, A.P. Fröba, FAU, Germany
12	Influence of Gas-Water Interface for Underground Hydrogen Storage, L. Huang, University of Oklahoma, USA
13	Modeling Thermodynamic Properties of Hydrogen-Containing Mixtures Using PC-SAFT, F. Yang, A. Padua, École Normale Supérieure de Lyon, France
14	Bridging Simulation and Reality: 3D Classical Density Functional Theory meets Hydrogen Adsorption, N. Thiele, T. Menzel, R. Stierle, J. Gross, Universität Stuttgart, Germany
	Transport Properties
15	In-situ Mineral Trapping in River Water as a Negative Emission Technology: Experimental Investigation and Modeling of the Reactive Gas-Liquid-Solid Equilibrium, D. Groh, J. Staudt, M. Ibañez, J. Burger, TU Munich, Germany
16	Numerical Simulation of Marangoni Convection in Disperse Liquid-Liquid Systems: Insights and Applications, M. Singer[1], P. Zimmermann[2], T. Zeiner[1], [1] KIT, Germany, [2] BSH Hausgeräte GmbH, Germany
17	Diffusivities in Electrolyte Systems from Dynamic Light Scattering and Molecular Dynamics Simulations, T. Klein, C.J. Kankanamge, A.P. Fröba, FAU, Germany
18	ECCSELLENT Project towards Net-Zero emission: A novel Laboratory for gas sorption, diffusion and transport in polymers for Advanced CCUS Research, V. Signorini, R. Di Carlo, M. Minelli, M.G. Baschetti, G. Burzotta, Z. Maghazeh, University of Bologna, Italy
19	Modeling the Viscosity of Ionic Liquids and Their Mixtures Using ePC-SAFT and Free Volume Theory with an Ion-Based Approach, Z. Zuo[1], X. Lu[2], X. Ji[1], [1] Lulea University of Technology, Sweden, [2] Nanjing Tech University, China
20	Linear nonequilibrium thermodynamics modeling of optimal fluid transport phenomenon in hierarchical Murray materials, J. Cao, X. Ji, X. Feng, X. Lu, Nanjing Tech University, China
21	Predicting Mass Transfer Through Interfaces Using Hydrodynamic Density Functional Theory, B. Bursik, R. Stierle, F. Bender, G. Bauer, J. Gross, University Stuttgart, Germany
22	Entropy Scaling for Thermal conductivity with critical Enhancement for pure substances and mixtures, J. Burkhard, R. Stierle, G. Bauer, J. Groß, Universität Stuttgart, Germany
	New Models
23	Novel Thermodynamic Model for Predicting Isomer Properties and Phase Equilibria, G. Segner[1], P. Zimmermann[2], T. Zeiner[1], [1] KIT, Germany; [2] BSH Hausgeräte GmbH, Germany
24	Revealing the simple structures behind complex fluid states behavior, F. Mayrhuber, Trostberg, Germany
25	Higher order functional approaches in Co-Oriented Fluid Functional Equation for Electrostatic interactions (COFFEE), K. Langenbach[1], J. Marx[1], W.G. Chapman[2], J. Amplatz[1], [1] University of Innsbruck, Austria, [2] Rice University, USA
26	A New Approach for Modeling Nonlinear Hard Chains Based on Perturbation Theory, J. Uceda, A. Mejia, Universidad de Concepcion, Chile
27	Integrating Predictive Assessment of Chemical Stability into Computer Aided Molecular and Process Design, L. Rasspe, K. Leonhard, RWTH Aachen, Germany
28	The influence of intramolecular hydrogen bonding on phase and reaction equilibria, R. Siewert, K. Müller, Universität Rostock, Germany

29	Comparison of multi-parameter Helmholtz and molecular-based equations of state for the description of the density of a gravimetrically prepared LNG-type mixture, D. Tuma[1], D. Lozano-Martín[2], I. Polishuk[3], C.R. Chamorro[2], [1] BAM, Germany [2] Universidad de Valladolid, Spain [3] Ariel University, Israel
30	Grouper: Enabling High-Throughput Simulations with Functional Group Graph Representations in Graph Neural Networks, N. Craven[1], K. Nehil-Puleo[1], C. McCabe[2], P. Cummings[2], [1]Vanderbilt University, USA, [2] Heriot-Watt University, UK
31	Calculation of the vapor-liquid equilibrium and thermodynamic properties of saturated neon by path integral Monte Carlo simulations using ab initio potentials, P. Marienhagen, K. Meier, Helmut-Schmidt-Universität der Bundeswehr Hamburg, Germany
32	A robust SAFT-VR Mie model to address the solubility of F-gases in biomass-derived solvents for refrigeration applications, I. Huenuvil-Pacheco[1], M. Viar[2], G. Zarca[2], A. Urtiaga[2]; A. Mejía[1], F. Llovell[3], [1] Universidad de Concepcion, Chile; [2] Universidad de Cantabria, Chile; [3] Universitat Rovira i Virgili, Spain
33	A Molecular-Based Equation of State for Mixtures of Cylindrically-Symmetric Hard Bodies, N. de Souza, L.F. Franco, University of Campinas, Brazil
34	Predicting thermal conductivity and associated autocorrelation function for simple fluids, I. N. Yapi, O. Haddad, M.B. Amar, J.P. Passarello, Université Sorbonne Paris Nord, France
35	Amonton-like Solid-Liquid Friction Model Considering Slip Length: the Derivation of Corresponding State into Surface by Molecular Parameters, X. Pan, Y. Zhu, X. Lu, Nanjing Tech University, China
36	Optimal strategy for the parameterisation of the association term of SAFT models, H.R. Asmuni[1], N. Ramirez-Velez[1], R. Privat[1], J.N. Jaubert[1], M. Bonnissel[2], S. Ahmed[2], [1] University of Lorraine, France, [2] Gaztransport & Technigaz, Saint-Rémy-lès-Chevreuse, France
37	Evaluation of derivative properties by various thermodynamic models for polar compounds, J. Amanabadi, X. Liang, G.M. Kontogeorgis, DTU, Denmark
38	Interfacial Map for Type II and Type IIa for Lennard-Jones Binary Mixtures, F.A. Figueroa, G. Alonso, A. Mejia, Universidad de Concepcion, Chile
39	A thermodynamic model of fused short hard-sphere chains, S. Dridi[1], M. Abderraba[1], J.P. Passarello[2], [1] IPEST Tunis, [2] University Sorbonne Paris Nord, France
40	Beyond One-fluid Approximations – Symbolic Regression for Mixture Correction in Perturbation Theories, A. Reimer, J. Groß, Universität Stuttgart, Germany
	Phase Equilibria
41	Solubility Enhancement of Active Pharmaceutical Ingredients through Liquid Hydrotrope Addition: A Thermodynamic Analysis, S. Nasrallah, TUM, Germany
42	Phase equilibria for ATPS composed of PEG2k, PVP10k or PVP29k: experimental assessment and PDH+UNIQUAC modelling, P. Velho, J.T. Coelho, C.S. Rebelo, E.A. Macedo, University of Porto, Portugal
43	Strategy for Efficiently Generating Complete VLE Phase Envelopes for Natural Gas Mixtures with Peng-Robinson EoS, V.H. Simões[1], N. Lemes[1], I. de Oliveira[1], A. Young[2], [1] Universidade Federal do Rio de Janeiro, Brazil; 2 Universidade Federal Fluminense, Brazil
44	Implicit differentiation of phase equilibria as a new paradigm in equation of state modeling and molecular design, P. Rehner, ETH Zurich, Switzerland
45	Biobased Polar Green Solvents Use for Oil Desulfurization: Physicochemical Properties, Liquid-Liquid Equilibria and Thermodynamic Modeling, V. Jeřábek; M. Klajmon; Ü. Aslan; K. Řehák, University of Chemistry and Technology Prague, Czech Republic
46	Bubble point pressure measurements for dimethyl ether - 2-methoxyethanol and dimethyl ether - 2-ethoxyethanol, and an activity coefficient model based on a group contribution method, A. Enokido[1]; A.J.X. Lai[2]; T. Tsuji[2]; H. Matsukawa[3]; T. Hoshina[1]; H. Matsukawa[1]; K. Tochigi[1], [1] Nihon University, Japan, [2] Universiti Teknologi Malaysia; [3] Tokyo University of Science, Japan
47	New initialization strategy for two- and three-phase flash calculations in CO_2/water/hydrocarbon mixtures, J. Heringer[1], M. Wapperom[2], C. Secuianu[3], D. Voskov[2], D.V. Nichita[1], [1]University of Pau, France; [2] TU Delft, Netherlands, [3] University Politehnica of Bucharest, Romania
	Deep Eutectic Solvents

48	Effect of water concentration on the microstructures of alkanolamine-based deep eutectic solvents (choline chloride + monoethanolamine), F. Lin[1], X. Lu[1], Y. Zhu[1], X. Ji[2], [1] Nanjing Tech University, China; [2] Lulea University of Technology, Sweden
49	Gas Separation Applications Using Deep Eutectic Solvents: Analysis via soft-SAFT EoS Modeling, L. Alencar[1], S.B. Rodriguez-Reartes[2], F. Llovell[2], F. Tavares[1], [1] Universidade Federal do Rio de Janeiro, Brazil, [2] Universitat Rovira i Virgili, Spain
50	Designing Greener Varnishes using Natural Eutectic Systems, C. Fernandes[1], A. Quirino[1], A. Paiva[1], R. Marques[2], A.R.C. Duarte[1], [1] Nova School of Science and Technology, Brazil; [2] NEON Art Conservation Lda., Brazil
51	Cracking chitin with deep eutectic solvents: A thermodynamic approach, E. Foord, N. Goosen, J. Cripwell, Stellenbosch University, South Africa
	Process Application
52	From Thermodynamic Equilibrium Data to Miniplant-Scale: Integrated Reaction and Separation System for Cyclic Acetals, M. Haas, A. Jupke, RWTH Aachen, Germany
53	On the use of Molecular Dynamics in food processing: behavior of minority compounds in vegetable oil extraction, J.M.C. Madureira[1], P.H.C. Soares[1], M.C. Reis[1], L.C. Kramer Biasi Pagotto[2], P. de Alcântara Pessoa Filho[1], [1] University of São Paulo, Brazil; [2] Center for Research in Energy and Materials, Brazil
54	Integrating Computational Tools for the Ad-Hoc Design of Sustainable Refrigerants, C.G. Albà[1], L.F. Vega[2], F. Llovell[1], [1] Universitat Rovira i Virgili, Spain; [2] Khalifa University of Science and Technology, Abu Dhabi
55	Evaluation of dispersion and aggregation for decanoic acid-modified ceria nanoparticle + organic solvent systems and modeling with activity coefficient models, H. Matsuda[1], R. Yamazaki[1], M. Matsuda[1], N. Yang[2], M. Ota[2]; T. Tomai[2]; H. Inomata[2], [1] Nihon University, Japan; [2] Tohoku University, Japan
56	Comparative Analysis of Different Equations of State (EOS) for Predicting Thermodynamic Properties of Oxygenated Components in Biofuel and Biodiesel Applications, I.B. Jovein[1], M.G. Baschetti[1], F. Galimberti[2], G. Sadowski[3];C. Held[3], F. Doghieri[1], [1] Bologna University, Italy; [2] Eni S.p.A., Italy; [3] TU Dortmund, Germany
57	Extraction based on ionic liquids as a tool to valorize fish by-products, A. Soto, P. Souto-Montero, A. Cáceres, C.A. Pena, E. Rodil, University of Santiago de Compostela, Spain
58	Production of carbon black from the pyrolysis of waste tires: Characterizations, evaluation of thermal conditions and process development, A.O. Goulart, P.C.C. de Araujo, M. Dias Pantolfi, R. M. de Brito Alves, C.A.O. do Nascimento, University of São Paulo, Brazil
59	Modeling and optimization of the compression process in a green ammonia production plant, I. Martínez, D. Lozano-Martín, F. Mato, C. Chamorro, Universidad de Valladolid, Spain
60	Evaluation of Excess Surface Tensions for Binary and Ternary Systems Using ASOG Group Contribution Model, K. Tochigi[1], H. Matsuda[1], T. Tsuji[2], K. Kurihara[1], [1] Nihon University, Japan; [2] Universiti Teknologi Malaysia, Kuala Lumpur
61	Synergistic Enhancement of Thermodynamic Stability of Methane Hydrates using Mixed Promoters, J. Seol, Seoul National University, South Korea
	Experimental
62	New interpretation of NMR relaxation response from MD simulations: Material properties and MRI contrast agents, T.J. Pinheiro dos Santos[1], A.V. Parambathu[2], D.N. Asthagiri[3], P.M. Singer[1], G.J. Hirasaki[1], W.G. Chapman[1], [1] Rice University, USA; [2] University of Delaware, USA; [3] Oak Ridge National Laboratory, USA
63	NMR Fingerprinting and Thermodynamic Modeling of Poorly Specified Mixtures, J. Wagner, Z. Romero, T. Specht, K. Münnemann, H. Hasse, F. Jirasek, RPTU Kaiserslautern, Germany
64	Revealing the essence of large-error slip measured by atomic force microscopy (AFM) from resistance (R) analysis, Z. Liu, L. Mu, X. Lu, Nanjing Tech University, China
65	Automated Vapor-Liquid Equilibrium Measurements with Raman Spectroscopy, C. Busch[1], C. Flake[1], M. Kasterke[2], H.J. Koß[2]; A. Bardow[1], [1] ETH Zürich, Switzerland; [2] RWTH Aachen, Germany

	Carbon Dioxide
1	CO_2 Capture using Slurry made by Integration of Aqueous and Immobilized Deep Eutectic Solvents, S. Foorginezhad, X. Ji, Lulea University of Technology, Sweden
2	Cryo-compressed CO_2 sorption, diffusion and permeation in elastomers for the CO_2 transport value chain, V. Signorini[1], M. Minelli[1], E. Ghiara[2], G. Lazzari[1], R. Di Carlo[1], M.G. Baschetti[1], L. Ansaloni[3], B. Alcock[3], [1] University of Bologna, Italy, [2] Institut de ciencia de Barcelona, Spain; [3] SINTEF, Italy
3	CO_2 capture with hydrophobic natural deep eutectic solvents: PC-SAFT modeling and molecular insights, G. Yu, C. Held, G. Sadowski, TU Dortmund, Germany
4	Experimental and modeling study of adsorption isotherms for CO_2/CH_4 mixtures on activated carbon, A. L. Santos, D. Silva, F. Nascimento, L. Bastos, R. Mirre; S. Vieira de Melo, UFBA, Brazil
5	Algorithms and Thermodynamic Models for CO_2 Capture, A.C. de Lima Neto, E.H. Stenby, W. Yan, DTU, Denmark
6	Influence of subcooling and supersaturation on nucleation kinetics of CO_2 hydrate: a molecular dynamics study, L.Y. Huang; S.T. Lin, National Taiwan University, Taiwan
7	Density Measurements of CO_2 + [(1-x)NaCl + x$CaCl_2$] brines, O.H. Jayeola, M. Cassiede, S. Smith, W. Yan, DTU, Denmark
8	Modeling the adsorption of H_2O and CO_2 on CALF-20 on the basis of a modified equation of state, A.F. Gonçalves[1], E.P. Lyra[1], N. B.C. Santos[2], Y. Magnin[2]; L.F.M. Franco[1], [1] University of Campinas, Brazil [2] TotalEnergies, France
9	Investigation of CO_2 and H_2O adsorption and diffusion in α- and β-CALF20 through molecular simulations, E. Parazzi Lyra[1], A. de Freitas Gonçalves[1], N.B.C. Santos[2], Y. Magnin[2], L.F.M. Franco[1], [1] University of Campinas, Brazil, [2] TotalEnergies, France
10	CO_2/hydrocarbon selectivity of ether-functionalized phosphonium-based ionic liquids and design of the gas separation process, Y. Suzuki[1], K. Isobe[1], D. Kodama[1], T. Sugahara[2], [1] Nihon University, Japan; [2] Osaka University, Japan
11	Systematic screening of amine-based deep eutectic solvents for enhanced CO_2 capture efficiency, Q. Shi; Xi. Ji, Luleå University of Technology, Sweden
12	Phase Equilibria of CO_2-Water and CO_2-Brine at High Temperature: A Multiscale Approach, F.M. Coelho[1]; L.F. Mercier Franco[1], A. Firoozabadi[2], [1]University of Campinas, Brasilia, [2] Rice University, USA
13	The influence of pure compounds' parameters on the phase behavior of systems containing carbon dioxide, J. Heringer[1], S. Sima[2], A.V. Crişciu[2], C. Secuianu[2], D.V. Nichita[1], [1] University of Pau, France, [2] POLITEHNICA Bucharest, Romania
	Artificial Intelligence
14	Development of Ab Initio-based Machine Learning Models to Study Chemical Reactions in Molten Alkali Carbonates and Hydroxides, D. Kussainova, A. Panagiotopoulos, Princeton University, USA
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