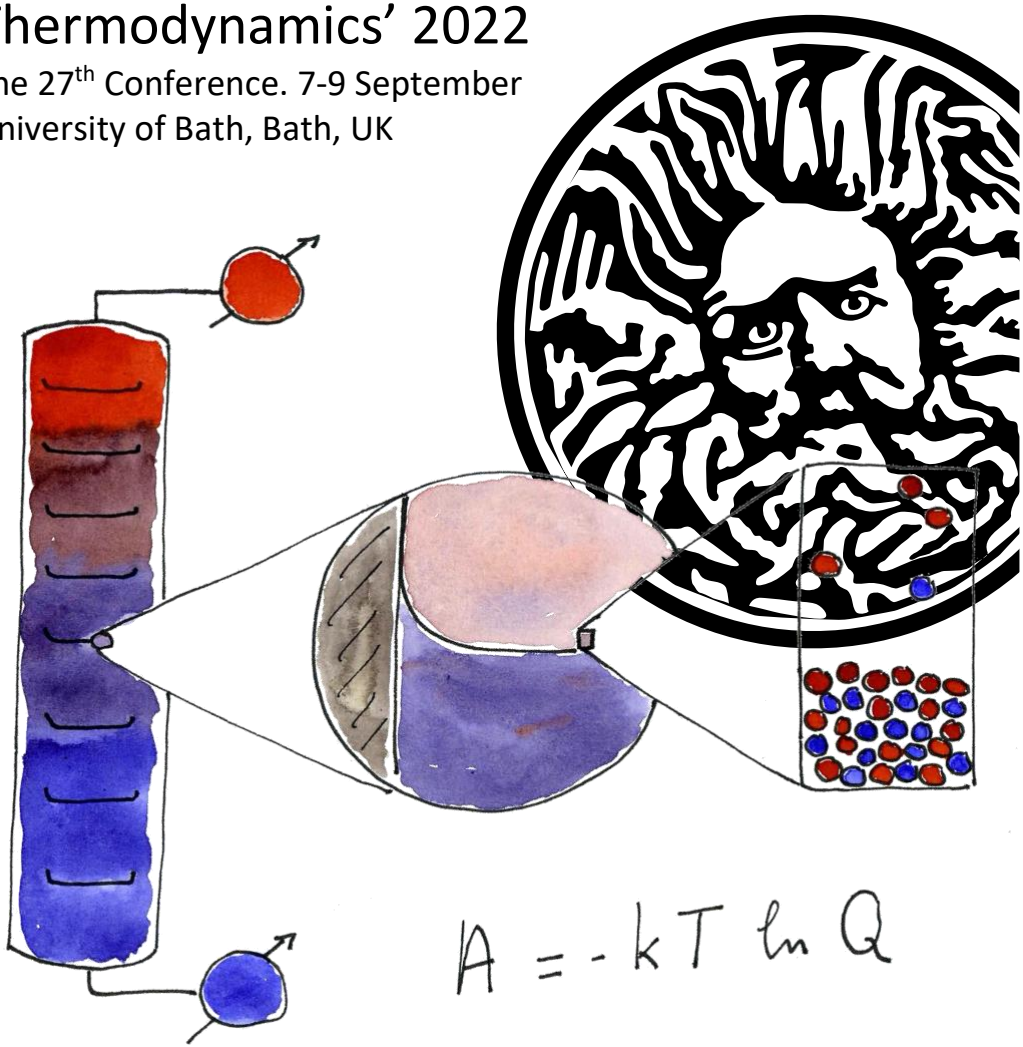
Thermodynamics' 2022

The 27th Conference. 7-9 September
University of Bath, Bath, UK



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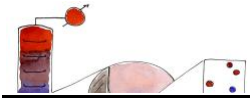

The 27th Thermodynamics Conference
University of Bath
7-9 September 2022

www.thermodynamics2022.org

A meeting of the Statistical Mechanics and Thermodynamics Group (SMGT) of the Faraday Division of the Royal Society of Chemistry (RSC)

Please address all correspondence to the conference chair:
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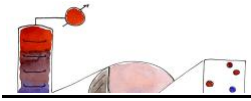


About the conference

Since 1964, initiated by Harold Springall, championed throughout the 1960s and 1970s by Max McGlashan and Sir John Rowlinson, the Thermodynamics Conference Series (TSC) has been devoted to showcasing scientific and engineering contributions encompassing the research subjects of chemistry, physics, biology, chemical engineering, petroleum engineering, and materials science. TSC is an excellent platform for science dissemination among world-class researcher, early career and students. The scientific themes include:

- Advances in molecular simulation
- Interfacial and confined phenomena
- Engineered self-assembly
- Carbon capture and other industrial applications
- Non-equilibrium thermodynamics
- Challenges and advances in fluid phase equilibria

International Scientific Committee

Prof. Felipe J. Blas (University of Huelva, Spain)
Prof. Fernando Bresme (Imperial College London, UK)
Prof. João A. P. Coutinho (University of Aveiro, Portugal)
Prof. Peter T. Cummings (Vanderbilt University, USA)
Prof. Ioannis Economou (Texas A&M University at Qatar)
Prof. Amparo Galindo (Imperial College London, UK).
Prof. Alejandro Gil-Villegas (University of Guanajuato, Mexico)
Prof. George Jackson (Imperial College London, UK)
Prof. Katsumi Kaneko (Shinshu University, Japan)
Prof. Andres Mejía (University of Concepcion, Chile)
Dr Othon Moultos (TU Delft, The Netherlands)
Prof. Thijs J.H. Vlugt (TU Delft, The Netherlands)

Local Organizing Committee

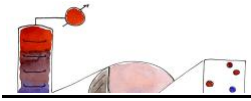
Dr Bernardo Castro-Dominguez (University of Bath, UK)
Dr Carmelo Herdes (Chair, University of Bath, UK)
Dr Hannah Leese (University of Bath, UK)
Prof. Tim Mays (University of Bath, UK)
Prof. Steve Parker (University of Bath, UK)
Mrs. Carolina Salter (University of Bath, UK)
Prof. Nigel Wilding (University of Bristol, UK)

Venue

The campus map, in your delegate package, shows parking, buildings and department locations. The main conference' activities will take place in **The Chancellors' Building** (grid reference C4) including its foyer, lecture rooms CB 1.10 and CB 1.11, in level 1 and a meeting/working room in CB 3.1 level 3. Lunch will be served in the **Lime Tree** (D3).

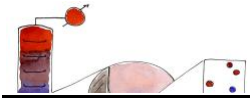
Schedule

The Chancellors' Building (CB)			
CB Foyer 1	CB 1.10	CB 1.11	Lime Tree
CB 3.1 available meeting/working room all days			
Wednesday, 7th September 2022			
11:00	Registration		
13:00	**Welcome** **Vice-Chancellor and President,** Prof. Ian White DL FREng **Conference Chair,** Dr Carmelo Herdes		
13:10	**Invited Talk** *A machine-learning enabled framework for design of sustainable plastics* **Prof. Juan de Pablo** Chair: Prof. Amparo Galindo		
13:50	**Invited Talk** *Thermodynamics meets pharmaceutical development* **Prof. Gabriele Sadowski** Chair: Dr Bernardo Castro-Dominguez		
14:30	Coffee break		
15:30	**Short oral I** **S1 – S10** Chair: Dr Fèlix Llovell	**Short oral II** **S11 – S20** Chair: Dr Susana Figueroa-Gerstenmaier	
16:20	Poster session I with drinks & canapés		



Thursday, 8th September 2022		
9:00	**Molecular Physics Lecture** *Quantum molecular thermodynamics* **Prof. Alejandro Gil-Villegas** Chair: Prof. George Jackson	
9:40	**Christopher Wormald Award** *Properties of low-dimensional materials explored with machine learning potentials* **Dr Fabian L. Thiemann** Chair: Prof. Tim Mays	
10:20	Coffee break	
10:50	**Oral I** **O1 – O6** Chair: Prof. Erich A. Müller	**Oral II** **O7 – O12** Chair: Dr Miguel Jorge
12:20	Lunch	
13:20	**IChemE Guggenheim Medal** *Gas hydrates in energy and carbon capture applications* **Prof. Carolyn A. Koh** Chair: Prof. Alberto Striolo	
14:00	**Invited Talk** *Non-equilibrium interactions and phase separation in active systems* **Prof. Ignacio Pagonabarraga** Chair: Prof. Steve Parker	
14:40	**Short oral III** **S21 – S28** Chair: Dr Carlos Nieto-Draghi	**Short oral IV** **S29 – S36** Chair: Dr Carlos Avendano
15:20	Group photo	
15:40	Poster session II with drinks & canapés	
19:00	Reception at The Roman Baths and Gala Dinner at The Pump Room	

Friday, 9th September 2022		
9:00	**Lennard-Jones Lectureship** *Active matter: a new approach to mechanobiology?* **Prof. Julia Yeomans** Chair: Prof. Nigel Wilding	
9:40	**Invited Talk** *Describing ionic systems: how important are partial charges, charge transfer and polarisability?* **Prof. Patricia Hunt** Chair: Dr Hannah Leese	
10:20	Coffee break	
10:50	**Oral III** **O13 – O18** Chair: Prof. Keith E. Gubbins	**Oral IV** **O19 – O24** Chair: Prof. Eduardo Filipe
12:20	Lunch	
13:20	**Invited Talk** *Unusual behaviour of the interfacial properties for fluid mixtures* **Prof. Andrés Mejía** Chair: Prof. Felipe J. Blas	
14:00	**Invited Talk** *Understanding thermodynamic and thermophysical property data measurement* **Prof. Cara Schwarz** Chair: Prof. João Coutinho	
14:40	Coffee break	
15:10	**Oral V** **O25 -O30** Chair: Prof. Ioannis Economou	**Oral VI** **O31 -O36** Chair: Dr Erik Santiso
16:40	**Entropy Young Researcher Poster Award** **Thermodynamics 2024 announcement** Prof. Amparo Galindo	
16:50	**Closing remarks** Dr Carmelo Herdes	



Invited and plenary talks

All invited and plenary talks are of 40 min. (including questions and discussion) and delivered in CB1.10.

Invited talks:

Wed 7 at 13:10. *A machine-learning enabled framework for design of sustainable plastics,* Juan de Pablo, The University of Chicago.
Chair: Amparo Galindo.

Wed 7 at 13:50. *Thermodynamics meets pharmaceutical development,* Gabriele Sadowski, TU Dortmund.
Chair: Bernardo Castro-Dominguez.

Thu 8 at 14:00. *Non-equilibrium interactions and phase separation in active systems,* Ignacio Pagonabarraga, CECAM.
Chair: Steve Parker.

Fri 9 at 9:40. *Describing ionic systems: how important are partial charges, charge transfer and polarisability?* Patricia Hunt, Victoria University of Wellington.
Chair: Hannah Leese.

Fri 9 at 13:20. *Unusual behaviour of the interfacial properties for fluid mixtures,* Andrés Mejía, Universidad de Concepción.
Chair: Felipe J. Blas.

Fri 9 at 14:00. *Understanding thermodynamic and thermophysical property data measurement,* Cara Schwarz, Stellenbosch University.
Chair: João Coutinho.

Plenary talks:
Thu 8 at 9:00. **Molecular Physics Lecture.** *Quantum molecular thermodynamics,* Alejandro Gil-Villegas, Universidad de Guanajuato.
Chair: George Jackson.

Thu 8 at 9:40. **Christopher Wormald Award.** *Properties of low-dimensional materials explored with machine learning potentials,* Fabian L. Thiemann, Imperial College London.
Chair: Tim Mays.

Thu 8 at 13:20. **IChemE Guggenheim Medal.** *Gas hydrates in energy and carbon capture applications,* Carolyn A. Koh, Colorado School of Mines.
Chair: Alberto Striolo.

Fri 9 at 9:00. **Lennard-Jones Lectureship.** *Active matter: a new approach to mechanobiology?* Julia Yeomans, University of Oxford.
Chair: Nigel Wilding.

Oral presentations
These presentations will take place in **parallel** in CB1.10 and CB1.11. 15 min. are allocated for each talk including Q&A. All speakers should provide their presentation via email thermodynamicsconference@bath.ac.uk by the 6th September 2022.

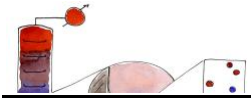
Advances in molecular simulation
Carbon capture and other industrial applications
Challenges and advances in fluid phase equilibria
Engineered self-assembly
Interfacial and confined phenomena
Non-equilibrium thermodynamics

Oral I	Chair: E.A. Müller		Thu, CB1.10, 10:50
O01	Phase behaviour of square-well dimers, trimers, chains and polygons	F. del Río	Universidad Autónoma Metropolitana
O02	Assessment of the Perturbed Chain-Statistical Associating Fluid Theory Equation of State against a Benchmark Database of High-Quality Binary-System Data. Pure Predictions and the Effect of Binary Interaction Parameter and Induced Association	I. Economou	Texas A&M University at Qatar
O03	Thermodynamic modeling of electrolyte solutions	G. Kontogeorgis	Technical University of Denmark
O04	Thermodynamic properties of water from SAFT and CPA equations of state: Comprehensive assessment	I. Nezbeda	J E Purkinje University
O05	Tailoring the phase diagram of discotic mesogens	A. Cuetos	Pablo de Olavide University
O06	Measuring local composition with 129Xe NMR spectroscopy: probing nano-structured mixtures of hydrogenated and perfluorinated alcohols	E. Filipe	Universidade de Lisboa
Oral II	**Chair: M. Jorge**		**Thu, CB1.11, 10:50**
O07	Kinetic control of competing nuclei within a system of interacting dimers on square lattice	D. Mandal	University of Warwick
O08	Lattice model of fluid transport in mixed matrix membranes	T. Yuan	University of Manchester
O09	Transport Properties of Binary Mixtures of Simple Fluids:	D. Fertig	TU Kaiserslautern

O10	Interpretation by Conformal Solution Theory and Quantification by Entropy Scaling Prediction of the Glass Transition Temperature of Polymeric Amorphous Solid Dispersions	L. Gil-Rojo	KIT
O11	Transport coefficients from Einstein-Helfand relation in Dissipative Particle Dynamics with energy conservation	D. C. Malaspina	Universitat Rovira i Virgili
O12	The use of Boundary Driven Non-equilibrium Molecular dynamics to determine transport diffusivities of mixtures in nanopores and study the effect of surface rugosity on transport	W. Xu	Imperial College London
Oral III	**Chair: K.E. Gubbins**		**Fri, CB1.10, 10:50**
O13	Structure-Function Relations for Hydrate Inhibitors	A. Striolo	University College London
O14	Simulation of the Carbon Dioxide Hydrate-Water Interfacial Energy	F. J. Blas	Universidad de Huelva
O15	Spatial control of interfacial heat transport using Janus nanoparticles	F. Bresme	Imperial College London
O16	The role of the solvent in crystal nucleation from solution	E. Santiso	NC State University
O17	Quantum effects of hydrogen storage in ε-phase syndiotactic polystyrene through adsorption	K. Arriola Gonzalez	University of Guanajuato
O18	Using many-body dissipative particle dynamics to predict the surface tension of pure and mixed systems	R. Hendrikse	Durham University

Oral IV	Chair: E. Filipe		Fri, CB1.11, 10:50
O19	Modelling of Dipolar Contributions to the Helmholtz Energy	J. Staubach	TU Kaiserslautern
O20	Enthalpy of dissociation of the mixed methane + propane sII hydrate along the three-phase equilibrium line	I. Tsimpanogiannis	CERTH
O21	Using thermodynamic models to describe water's anomalous behavior - Successes and Challenges	E. Tsochantaris	Technical University of Denmark
O22	Speed of sound measurements in hydrogen using a new cylindrical resonator at pressures up to 100 MPa	C. Wedler	Imperial College London
O23	A new class of descriptors for nanoporous materials and its applications to Classification and CO_2 gas adsorption into zeolites	C. Nieto-Draghi	IFP Energies Nouvelles
O24	6FDA-DAM mixed matrix membranes for challenging gas separations: insights from molecular simulation with realistic force fields	M. Spera	Texas A&M University at Qatar
Oral V	**Chair: I. Economou**		**Fri, CB1.10, 15:10**
O25	Computation of Thermodynamic and Transport Properties of H_2/O_2 Alkaline Aqueous Electrolyte Solutions using Molecular Simulation	P. Habibi	Delft University of Technology
O26	Thermophysical Characterization of Deep Eutectic Solvents for Practical Applications in Greenhouse Gas Capture and Separation	F. Llovell	Universitat Rovira i Virgili

O27	The role of thermodynamics in the design of membrane separation processes for energy and environmental applications	M. G. de Angelis	University of Edinburgh
O28	Casimir contribution to the interfacial Hamiltonian for 3D wetting	J. Romero-Enrique	Universidad de Sevilla
O29	Nucleation in first order phase transitions starting from the top	E. Sanz	University Complutense of Madrid
O30	Molecular dynamics of preferential adsorption in mixed alkali-halide electrolytes at graphene electrodes	M. Lisal	The Czech Academy of Sciences
Oral VI	**Chair: E. Santiso**		**Fri, CB1.11, 15:10**
O31	Predicting the Dielectric Constant and Dipole Moment of Liquids and Mixtures	M. Jorge	University of Strathclyde
O32	Unveiling the capacity of ionic and anionic surfactants for oil extraction in silica/water interfaces through coarse-grain molecular dynamic simulations	G. Perez-Sanchez	CICECO, University of Aveiro
O33	Calculation of thermodynamic properties of simple fluids by Monte Carlo simulations with ab initio potentials	K. Meier	Universität der Bundeswehr
O34	Atomistic Simulation Framework for Molten Salt Vapor-Liquid Equilibrium	W. R. Smith	University of Guelph
O35	Neutron scattering calculation for coarse-grained models	G. Jimenez - Serratos	STFC Hartree Centre
O36	Simulations of bent liquid crystal dimers: approaches to studying the twist-bend (NTB) nematic phase	M. Wilson	Durham University



Short oral presentations

Parallel presentations of 5 min. without allocated time for questions. Short orals with *associated posters* are noted. All speakers should provide their presentation via email thermodynamicsconference@bath.ac.uk by the 6th September 2022.

Short oral I		Chair: F. Llovell	Wed, 15:30, CB1.10
S01 *P05*	Long-time relaxation dynamics in nematic and smectic liquid crystals of soft repulsive colloidal rods	D. Cywiak	University of Guanajuato
S02 *P08*	Reproducibility of Molecular Simulation Computer Experiments	F. Fleckenstein	TU Kaiserslautern
S03 *P10*	Featurizing MOF pores for Machine Learning on Adsorption	A. Gopalan	University of Manchester
S04 *P13*	Dielectric Properties of Model Fluids from Molecular Dynamics and Perturbation Theories	M. Kohns	TU Kaiserslautern
S05 *P14*	All-atom simulations of surfactants at water-oil and water-vacuum interfaces	J. Li	Durham University
S06 *P29*	A Polarization-Consistent Approach to Force Field Development for Solutions and Mixtures	M. Jorge	University of Strathclyde
S07 *P26*	Molecular simulations as a powerful tool to design sustainable approaches for membrane gas separations	K. Papchenko	University of Edinburgh

S08 *P30*	Sticky-MARTINI – A Reactive Coarse-Grained Model for Self-Assembly in Materials Synthesis	J. Gomes	CICECO, University of Aveiro
S09 *P37*	Nanoscopic study on carvone-terpene based natural deep eutectic solvents	S. Rozas	Burgos University
S10 *P89*	A hop, skip, and jump: Computer simulations of water diffusion through organic corrosion protection coatings	C. Wand	University of Exeter
Short oral II	**Chair: S. Figueroa-Gerstenmaier**		**Wed, 15:30, CB1.11**
S11 *P41*	Mesoscale Simulation of Clay Particle Agglomeration in Aqueous Solutions	T. Le	University College London
S12 *P45*	Thermodynamic modeling of the nature of speciation and phase behavior of binary and ternary mixtures of formaldehyde, water and methanol	M. Wehbe	Imperial College London
S13 *P56*	An approach for modelling simultaneous fluid-phase and reaction equilibria in non-ionic and ionic systems via Lagrangian duality: The reactive HELD algorithm	F. Perdomo	Imperial College London
S14 *P60*	A simple pair potential that gives rise to an intriguing phase diagram	K. Travis	University of Sheffield

S15 *P47*	SAFT-gamma Mie molecular modelling of active pharmaceutical ingredients and solvents; solubility calculation	T. Bernet	Imperial College London
S16 *P52*	Evaluation of thermodynamic properties in hydrogen/oxygen mixture modelled by Lennard-Jones fluid	H. Nagashima	University of the Ryukyus
S17 *P70*	Time-dependent Interfacial Properties of Reacting Liquid-Liquid Mixtures	S. Enders	KIT
S18 *P31*	Interfacial tension of structural variations of alkyl polyglucosides surfactants	H. Cardenas	Imperial College London
S19 *P67*	Interdigitated aggregation of polymer-surfactant system: A coarse-grained molecular dynamics study	M. Bhendale	Indian Institute of Technology Kanpur
S20 *P77*	Simulating solvent extraction from metal-organic frameworks using transition matrix GCMC	J. Manning	University of Manchester
Short oral III	**Chair: C. Nieto-Draghi**		**Thu, 14:40, CB1.10**
S21 *P39*	Wettability of graphite under 2D confinement	Z. Wei	The University of Manchester
S22 *P90*	Atomistic simulation study of amino-acid functionalized Ni-CPO-27 membrane for desalination	F. Li	University College London

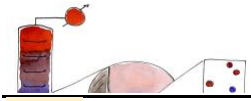
S23 *P91*	Mass Transfer through Vapor-Liquid Interfaces of Binary Mixtures studied by Non-Stationary Molecular Dynamics Simulations	D. Schaefer	TU Kaiserslautern
S24 *P92*	Exploration of Free Energy Landscapes of Perfluorooctanoic Acid Adsorption from Water in All-Silica Zeolites	M. Zhang	University College London
S25 *P93*	The influence of tie-molecules and microstructure on the fluid solubility in semi-crystalline polymers	M. Valsecchi	Imperial College London
S26	Investigation of response time, structure and microrheology of an ER fluid of cubic particles via Dynamic Monte Carlo simulations	L. Tonti	The University of Manchester
S27 *P94*	Polarisation of water under thermal fields: the effect of the molecular dipole and quadrupole moments	A. Chapman	Imperial College London
S28	Fitting a square peg in a round hole: multi-property parametrization of Mie Fluids.	G. Chaparro	Imperial College London
Short oral IV		**Chair: C. Avendano**	**Thu, 14:40, CB1.11**
S29	Exploring cavitation and fracture in HTPB polymer blends	G. Jimenez-Serratos	STFC Hartree Centre

S30 *P25*	Hydrogen Bonded Configurations in Liquid Water and Their Correlation with Local Tetrahedral Structures	A. Vinod Muthachikavil	Technical University of Denmark
S31 *P20*	Understanding the stabilizing effect of histidine on monoclonal antibody aggregation	S. Saurabh	Imperial College London
S32	Solubility prediction of binary and ternary amino-acid mixtures using the SAFT-γ Mie group-contribution approach	A. Alyazidi	Imperial College London
S33 *P48*	The Madrid-2019 force field for electrolytes in water: An extension to the ions F-, Br-, I-, Rb+ and Cs+	S. Blazquez	Universidad Complutense de Madrid
S34	Numerical simulations of the liquid-vapor coexistence curve of square-well dimer fluids	F. Sastre	Universidad de Huelva
S35	Role of molecular theory in investigating phase and interfacial properties of azeotropic blends of fluorinated refrigerants	C. Albà	Universitat Rovira i Virgili
S36	Molecular Dynamics Simulation Study of Heat Transfer Across Solid-Fluid Interfaces: the Kapitza Resistance	S. Stephan	TU Kaiserslautern

Posters

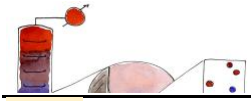
Posters sessions will be held on Wednesday and Thursday afternoons, in the CB Foyer 1. The boards will be available in the morning before the poster session. Presenters are requested to remove their posters immediately at the end of each session. The suggested size of the poster is A0 in portrait orientation.

Poster session I		**Wed, 16:20, CB Foyer1&2**
P01	Exploring the Phase Behaviour of Hard-Sphere Dimers	O. Adesida
P02	Free Energy Surfaces from sets of asynchronous enhanced molecular dynamics simulations subject to multiple biases	A. Bjola
P03	Representing atomistic nucleation rates as a one-dimensional system	K. Blow
P04	Use of Artificial Neural Networks to correlate Mie fluid PVT and transport properties data	G. Chaparro
P05 *S01*	Long-time relaxation dynamics in nematic and smectic liquid crystals of soft repulsive colloidal rods	D. Cywiak
P06	A Molecular Dynamic simulation study of Polyethylene and the Transport Behavior of Hydrogen in the Polymer System	C. Divine-Ayela
P07	Molecular Dynamics Simulation of Spike Proteins of the SARS-CoV-2 Virus	F. Fleckenstein
P08 *S02*	Reproducibility of Molecular Simulation Computer Experiments	F. Fleckenstein
P09	Predicting thermochemical formation properties in solids	R. Fromsejer
P10 *S03*	Featurizing MOF pores for Machine Learning on Adsorption	A. Gopalan
P11	Design of Sugar-Based Surfactants Through Molecular Modelling	M. Kamrul Bahrin



P12	Thermophysical properties prediction: towards a generic coarse grained force field	S. Khennache
P13 *S04*	Dielectric Properties of Model Fluids from Molecular Dynamics and Perturbation Theories	M. Kohns
P14 *S05*	All-atom simulations of surfactants at water-oil and water-vacuum interfaces	J. Li
P15	Machine learning of critical micelle concentrations enhanced by surrogate molecular dynamics	A. Moriarty
P16	Vapor pressures and vapor phase compositions of choline chloride urea and choline chloride ethylene glycol deep eutectic solvents from molecular simulation	O. Moultos
P17	Modelling of complex fluids combining many-body Dissipative Particle Dynamics and molecular-based equations of state	J. O'Connor
P18	Rydberg-type electronic excited states in sodium-doped water clusters	R. Pasca
P19	A novel coarse-grain molecular dynamic simulation framework to unravel the impact of ionic liquids in TX-114 micellar solutions	G. Perez-Sanchez
P20 *S31*	Understanding the stabilizing effect of histidine on monoclonal antibody aggregation	S. Saurabh
P21	A Set of Molecular Models for Alkali Nitrates in Aqueous Solution	D. Schaefer
P22	Employing the SAFT-g-mie equation of state to model long chained polyalkylglycols in water solution through molecular dynamics simulations	G. Silva
P23	Extending the MolMod Database to Transferable Force Fields	S. Stephan
P24	CBD and scCO2: A molecular dynamics interaction study	F. Vásquez

P25 *S30*	Hydrogen Bonded Configurations in Liquid Water and Their Correlation with Local Tetrahedral Structures	A. Vinod Muthachikavil
P26 *S07*	Molecular simulations as a powerful tool to design sustainable approaches for membrane gas separations	K. Papchenko
P27	Molecular Dynamics Simulation of the Equilibrium Phase For CO2 Hydrate-Salty Water System	A. Díaz Acosta
P28	Molecular screening of adsorbents for sustainable and wearable hemodialysis	T. Fabiani
P29 *S06*	A Polarization-Consistent Approach to Force Field Development for Solutions and Mixtures	M. Jorge
P30 *S08*	Sticky-MARTINI – A Reactive Coarse-Grained Model for Self-Assembly in Materials Synthesis	J. Gomes
P31 *S18*	Interfacial tension of structural variations of alkyl polyglucosides surfactants	H. Cardenas
P32	Characterization of methane hydrate crystallization inside a silica pore using Molecular Dynamics	A. Fernandez-Fernandez
P33	Synergetic effects due to salt/surfactant/additives/oil on interfacial tension	T. Kobayashi
P34	Phase equilibria and interfacial properties of thermodynamic hydrate promoters from computer simulation	C. Romero Guzmán
P35	The role of surface ionisation in the hydration-induced swelling of graphene oxide (GO) membranes	M. Shaharudin
P36	Bulk liquid phase and interfacial behaviour of cineole – based deep eutectic solvents with regards to carbon dioxide	S. Rozas
P37 *S09*	Nanoscopic study on carvone-terpene based natural deep eutectic solvents	S. Rozas



P38	Thermodynamics and kinetics of biomolecular condensation from finite-size nucleation simulations	L. Li
P39 *S21*	Wettability of graphite under 2D confinement	Z. Wei
P40	Investigating the synergistic role of additives on the CO2 hydrates with atomistic modelling	X. Cai
P41 *S11*	Mesoscale Simulation of Clay Particle Agglomeration in Aqueous Solutions	T. Le
P42	Modelling Salt Solubility, pH, and CO2 Solubility in Aqueous and Organic Solutions Using ePC-SAFT	D. Pabsch
P43	Effect of alternative fuels on CO2 and other gas emissions resulting from the cement industry	I. Tsimpanogiannis
P44	The Determination of Equation of State (EoS) Parameters Using Machine Learning Methods: A Case Study of The Sanchez-Lacombe EoS.	H. Ismaeel
P45 *S12*	Thermodynamic modelling of the nature of speciation and phase behaviour of binary and ternary mixtures of formaldehyde, water and methanol	M. Wehbe
P46	Membrane Separation of Racemic Mixtures: A Molecular Dynamics Study	J. Skvara
P47 *S15*	SAFT-gamma Mie molecular modelling of active pharmaceutical ingredients and solvents; solubility calculation	T. Bernet
P48 *S33*	The Madrid-2019 force field for electrolytes in water: An extension to the ions F-, Br-, I-, Rb+ and Cs+	S. Blazquez
P49	Wertheim theory quantum associating fluid models	A. Gil-Villegas

P50	Osmotic phase equilibrium by using the chemical potential of the solvent. Application to the thermodynamics of dilute solutions	J. Gómez-Estévez
Poster session II		**Thu, 15:40, CB Foyer1&2**
P51	Is Stokes-Einstein relation valid for the description of intra-diffusivity of hydrogen and oxygen in liquid water?	O. Moultos
P52 *S16*	Evaluation of thermodynamic properties in hydrogen/oxygen mixture modelled by Lennard-Jones fluid	H. Nagashima
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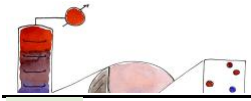

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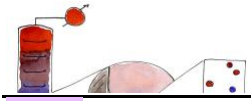

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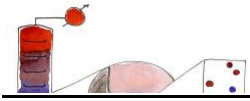
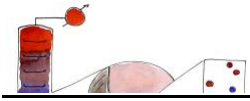
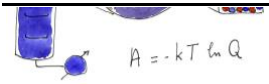



A = - kT ln Q

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