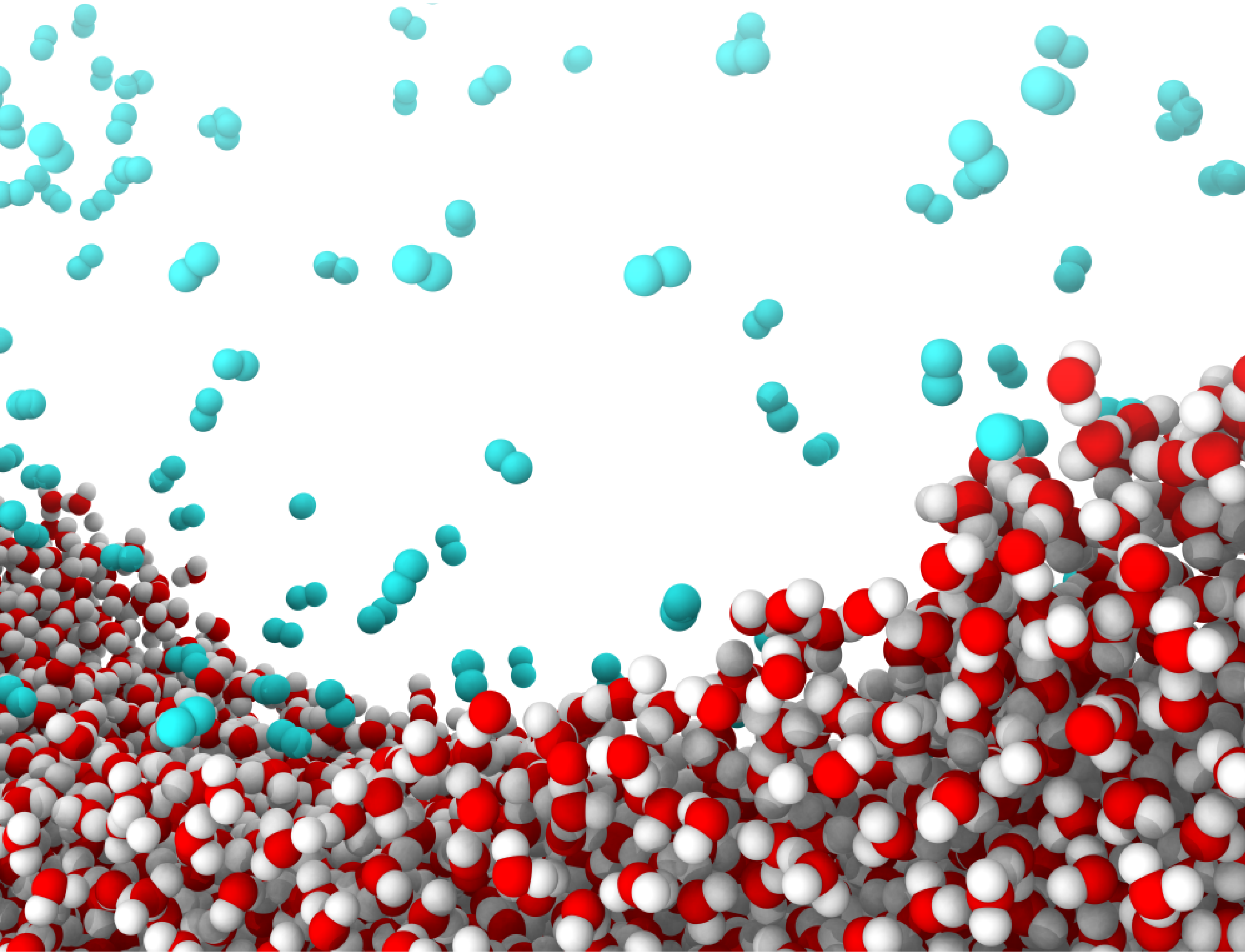
NEMD
2026

5th Non-Equilibrium Molecular Dynamics (NEMD) Conference

6 – 10 July 2026

The University of Edinburgh



About

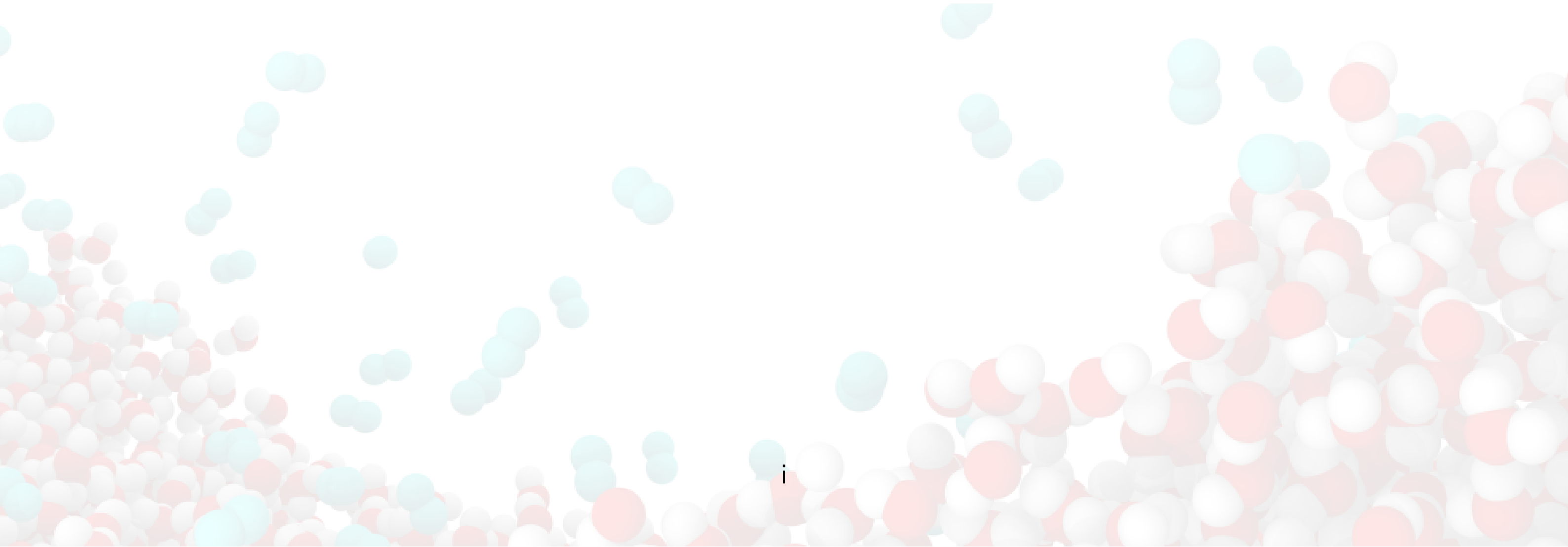
This book of abstracts accompanies the 5th Non-Equilibrium Molecular Dynamics (NEMD) Conference, held at The University of Edinburgh from 8–10 July 2026. The meeting brings together researchers from physics, chemistry, engineering, applied mathematics, and related disciplines to discuss molecular simulation approaches for systems driven away from thermodynamic equilibrium.

The conference programme is organised into five themed oral sessions: NEMD foundations, theory and methods; interfacial thermal transport; coarse-graining, multiscale modelling and functional materials; phase change, wetting and droplets; and rheology and complex fluids. Across these sessions, the programme includes five 40-minute keynote lectures and nineteen 20-minute contributed talks. The poster programme is divided into two poster sessions, each beginning with eight 2-minute lightning talks, followed by time for detailed discussion around the posters.

In addition to the scientific presentations, NEMD 2026 includes dedicated community discussion on the future direction of the field, including funding challenges, collaboration opportunities, and the development of future NEMD meetings. The format is intended to support both focused technical exchange and broader discussion across the NEMD community.

For further information or questions, please contact the conference organising committee:

Dr Rohit Pillai, University of Edinburgh (Chair)
Dr Edward Smith, Brunel University London
Dr Santiago Romero-Vargas Castrillón, University of Edinburgh
Dr Eleonora Ricci, University of Edinburgh
Dr Duncan Dockar, University of Edinburgh
Dr Saikat Datta, Swansea University



Program at a Glance

WEDNESDAY 8 JULY		
09:30–10:10	*Registration & coffee*	
10:10–10:20	*Opening remarks*	
Session I: NEMD Foundations, Theory & Methods		Chair: Edward Smith
10:20–11:00	KEYNOTE **Challenging local equilibrium** **Bjørn Hafskjold** · Norwegian University of Science and Technology, Norway	
11:00–11:20	Revisiting the Green–Kubo relation for friction in nanofluidics **Anna T. Bui** (University of Cambridge, UK), S. J. Cox	
11:20–11:40	Steady-state solutions for nonequilibrium Langevin dynamics **Matthew Dobson** (University of Massachusetts Amherst, USA)	
11:40–12:00	Leveraging machine learning to optimise viscosity prediction in NEMD **Lingfeng Gui** (Heriot-Watt University, UK), E. Medani, P. T. Cummings, C. McCabe	
12:00–13:00	*Lunch*	
Session II: Interfacial Thermal Transport		Chair: Rohit Pillai
13:00–13:40	KEYNOTE **Thermal transfer at metal- and polymer-water interfaces: impact of molecular mobility** **Samy Merabia** · Université Claude Bernard Lyon 1, France	
13:40–14:00	Non-equilibrium thermal energy transfer at structured solid–liquid interface **Kunio Fujiwara** (The University of Osaka, Japan), P. J. Daivis, B. D. Todd	
14:00–14:20	Impact of surface charge on thermo-osmosis **Maxime Boileau** (Université Claude Bernard Lyon 1, France), M. Ouadfel, S. Merabia, L. Joly	
14:20–14:40	Local interfacial thermal conductance and heat-flow anisotropy from NEMD **Fernando Bresme** (Imperial College London, UK), J. D. Olarte-Plata, M. Jiang, A. Chapman	
14:40–15:00	Heat flux for any machine-learning potential: a universal wrapper built on metatomic **Qianjun Xu** (EPFL, Switzerland), G. Fraux, M. Langer	
15:00–15:30	*Coffee*	
15:30–17:00	**Poster Session I**	8 lightning talks (2 min) + browse all posters
THURSDAY 9 JULY		
09:00–09:20	*Welcome refreshments*	
Session III: Coarse-Graining, Multiscale & Functional Materials		Chair: Eleonora Ricci
09:20–10:00	KEYNOTE **Many-body dissipative particle dynamics of non-equilibrium phenomena** **Panagiotis E. Theodorakis** · Polish Academy of Sciences, Warsaw	
10:00–10:20	Coarse-grained NEMD simulations of biointerfaces **Erik Weiand** (Imperial College London, UK), P. M. Cerqueira Diaz, T. Kanesalingam, J. P. Ewen, D. Dini	
10:20–10:40	Mesoscale modelling of lignocellulosic biomass through dissipative particle dynamics **Omololu Fagbiele** (Heriot-Watt University, UK), A. Ozel	
10:40–11:00	*Coffee*	

11:00–11:20	Atomistic investigation of bulk and interfacial properties in high-entropy alloys **Fabiano Tarulli** (Politecnico di Torino, Italy), M. Pellegrino, M. Ganjali Koli, M. Fasano
11:20–11:40	Conformational isomerism tunes refrigeration potential in metal–organic frameworks **Chi Cheng Hong** (University of Edinburgh, UK), W. L. Leung, C. Wilson, M. J. Liddle, R. S. Forgan, J. J. B. Levinsky, A. S. J. S. Mey, C. L. Hobday
11:40–12:00	Non-equilibrium reactive MD of CO_2 permeation in PVAm/PVA membranes **Yuiko Tomita** (University of Tokyo, Japan), R. Togo, I. Kinefuchi
12:00–13:00	*Lunch*
13:00–14:30	**Poster Session II** 8 lightning talks (2 min) + browse all posters

SHAPING NEMD 2027 open to all delegates

14:30–15:00	Panel discussion on funding challenges and opportunities
15:00–15:30	Coffee
15:30–17:00	Collaboration: drafting the proposal together
19:30	Conference dinner The Royal Scots Club, 29–31 Abercromby Place, Edinburgh EH3 6QE

FRIDAY 10 JULY

09:00–09:40	*Welcome refreshments*

Session IV: Phase Change, Wetting & Droplets

Chair: Saikat Datta

09:40–10:20	KEYNOTE **Velocity distribution of water molecules evaporating from a liquid–vapour interface** **Ikuya Kinefuchi** · University of Tokyo, Japan
10:20–10:40	Benchmarking of water models and coarse-graining strategies for high-temperature simulations P. Syroglou, **Konstantinos Ritos** (University of Thessaly, Greece)
10:40–11:00	Molecular-dynamics investigation of kinetic energy in a collapsing cavitation bubble induced by shockwave K. Moriyama, **Shin-ichi Tsuda** (Kyushu University, Japan), S. Watanabe
11:00–11:20	Time-dependent heat-flux analysis during liquid–vapour interfacial adhesion **Hiroki Kusudo** (Tohoku University, Japan), Y. Yamaguchi
11:20–11:40	Smooth-particle-hydrodynamics simulation of spinodal decomposition in a Lennard-Jones fluid **Karl P. Travis** (University of Sheffield, UK), P. J. Daivis
11:40–12:10	*Coffee*

Session V: Rheology & Complex Fluids

Chair: Santiago Romero-Vargas Castrillón

12:10–12:50	KEYNOTE **Interfacial structural and transport properties of fluids at molecular resolution** **Marcello Sega** · University College London, UK
12:50–13:10	TTCF-based analysis of shear-induced microstructure in an aqueous surfactant solution H. Tanaka, **Takeshi Omori** (Osaka Metropolitan University, Japan)
13:10–13:30	Turbulence of dilute solutions of supramolecular polymers F. Serafini, F. Battista, P. Gualtieri, J.-P. Ryckaert, **Carlo Casciola** (Sapienza University of Rome, Italy)
13:30–13:50	Molecular simulation of large-amplitude oscillatory extensional flow **Bharath Ravikumar** (City St George's, University of London, UK), I. K. Karathanassis, M. Gavaises
13:50–14:05	*Closing ceremony*

POSTER PROGRAMME

Note: All posters are displayed on both days

Lightning talks — Poster Session I (Wednesday 8 July)

- **Yashit Verma** (University of Edinburgh, UK), H. Kusumaatmaja – Modelling tight junction formation using coarse-grained molecular dynamics simulations
- **Pengxu Chen** (University of Edinburgh, UK), S. Romero-Vargas Castrillón, R. Pillai, S. Datta – Vibration-driven freeze desalination at the nanoscale
- **Kawa Manmi** (University of Warwick, UK), F. Brosa Planella, M. Landstorfer, C. Pohl – Solid electrolyte interphase model based on non-equilibrium thermodynamics: microscale derivation and upscaling
- **Taher Meydando** (University of Edinburgh, UK), R. Pillai, D. Dockar, L. Gibelli – Determination of nanobubble zeta potential via non-equilibrium molecular dynamics
- **Kseniya Papchenko** (Université de Pau et des Pays de l'Adour, France), E. Ricci, G. Galliero, F. Croccolo – Towards understanding the Soret effect in polymeric liquids
- **Darren Wayne Lim** (University of Cambridge, UK), C. Schran – Do solid phonons play a role in the bounce-to-stick phase transition for liquid nanodroplets on hydrophobic surfaces?
- **Khaled Almulafekh** (University of Edinburgh, UK), E. Ricci – Molecular modelling of anion-exchange membranes
- **Masaharu Yoshida** (Tohoku University, Japan), D. Surblys, T. Ohara – Molecular-scale mechanisms of momentum transport in liquids

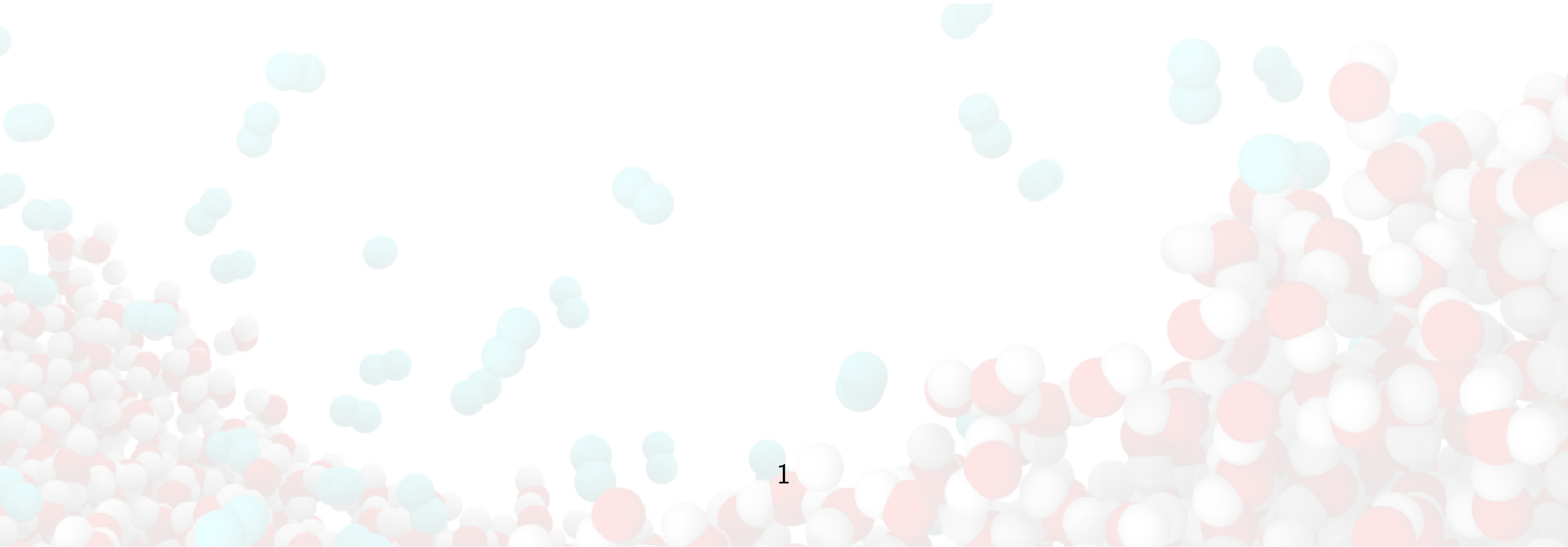
Lightning talks — Poster Session II (Thursday 9 July)

- **Bharath Ravikumar** (City St George's, University of London, UK), I. K. Karathanassis, T. Smith, G. Brown, M. Gavaises – Parameter optimisation of many-body dissipative particle dynamics simulations via machine learning
- **Yeuk Lam Sui** (University of Cambridge, UK) – Predicting the phase diagram of deep eutectic solvents with machine learning interatomic potentials
- **Nikita Allaglo** (École Normale Supérieure, France), C. Scalliet – Disorder-induced memory in liquid–solid friction
- **Tiziano Cavalieri** (University of Edinburgh, UK), E. Ricci – A non-equilibrium approach to molecular modelling of gas transport in a mixed matrix membrane
- **Takumi Tanaka** (Tohoku University, Japan), D. Surblys, T. Ohara – Application of the phantom-wall method to obtain work of adhesion for diverse interfaces
- **Niphredil Klint** (Chalmers University of Technology, Sweden), A. Isacsson – Thermal fluctuations and elastocapillarity in nanoscale Rayleigh–Plateau breakup
- **Thejas Hulikal Chakrapani** (University of Edinburgh, UK), D. Surblys, S. Merabia, R. Pillai – Structure and dynamics of interfacial water govern thermal conductance at graphene–water interfaces
- **Ionuț-Petrișor Ungureanu** (University of Bucharest, Romania), M. Boni, I. R. Andrei, A. Staicu – Interfacial oscillations in binary droplets induced by long-range vapour-mediated interactions

Contents

PART I

Keynote Abstracts



10:20–11:00 |
Wed, 8 July |
Session I

Challenging Local Equilibrium

Bjørn Hafskjold[1]

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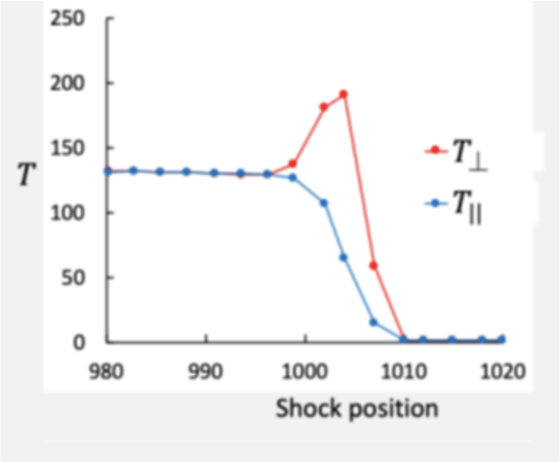

Figure 1: Components of the non-isotropic kinetic temperature in a planar shock front. $T_\perp$ and $T_{||}$ are the temperatures normal to and parallel with the shock plane, respectively.

A common concern in computation of transport coefficients by non-equilibrium molecular dynamics (NEMD) is how one can expect the results to represent real processes with the large driving forces and small systems used in simulations. In the early history of NEMD it turned out that surprisingly strong forces and small systems gave results comparable with hydrodynamic limits. Computers with increasing power eliminated the concern for system size, but the question of linearity in flux-force relations are still of interest.

In this contribution, I will discuss the use of the local-equilibrium assumption (LEA) in non-equilibrium thermodynamics (NET) and three NEMD simulations that challenge the LEA. The fluid model used in the simulations is a Lennard-Jones/spline potential. The three simulations are: (1) a shock wave in a one-component liquid (2) self-diffusion with a NEMD method, and (3) thermo-osmosis and thermodiffusion in a thin membrane.

Shock waves are examples of strongly non-equilibrium processes. An example of the non-isotropic kinetic temperature in the shock front is shown in Figure 1. The NEMD results were compared with solutions of the Navier-Stokes equations and equilibrium thermo-dynamic properties in the shock front, which showed that the LEA is a very good approximation in this case [1].

The self-diffusion simulation was done with mutual diffusion in a fluid with two identical components (a “color experiment”). Large concentration gradients were used to force the system into a state where the deviation from local equilibrium and the non-equilibrium entropy were quantified [2].

The third example is a simulation of thermodiffusion and thermo-osmosis in tight nano-scale membranes. The differences in temperature, pressure, and composition across the membrane were extreme. The LEA was examined and simulation results were analyzed in the NET framework [3].

References

[1] Maltby, T. W.; Hafskjold, B.; Bedeaux, D.; Kjelstrup, S.; Wilhelmsen, Ø. Local equilibrium in liquid phase shock waves. *Phys. Rev. E* **2023**, *107*, 035108.

[2] Kristiansen, K. R.; Hafskjold, B. Local Equilibrium Approximation in Non-Equilibrium Thermodynamics of Diffusion. *Entropy* **2025**, *27*, 400.

[3] Hafskjold, B.; Kjelstrup, S. Thermodiffusion and thermo-osmosis in thin membranes with slit pores. Submitted to *The European Physical Journal E*.

13:00–13:40 |
Wed, 8 July |
Session II

Thermal Transfer at Metal-Water and Polymer-water Interfaces: Impact of Molecular Mobility

O. Gutiérrez[1,2], S. Babaei[3], J. El Hajj[1], Y. Cheragali[3], R. Santamaria[2], C. Loison[1], A. Rajabpour[3] and **S. Merabia**[1]

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[2]Institut de Fisica, Universidad Nacional Autonoma de Mexico, Mexico City, Mexico;
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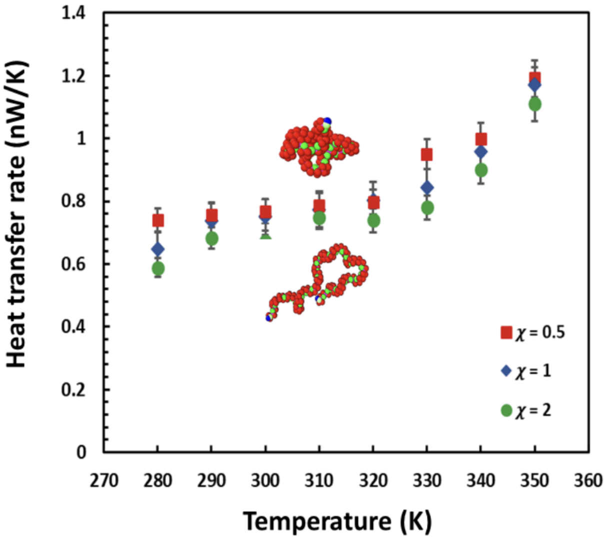

Figure 1: Thermal transfer at PEG-water interfaces [3].

Thermal transport at solid–liquid interfaces finds a broad range of applications in modern cooling devices, management of batteries, and nanoparticle-based thermal therapies. However, a microscopic understanding of thermal transport at these interfaces remains challenging [1]. Here, we propose a decomposition for solid–liquid interfaces separating the thermal conductance into an elastic and an inelastic phonon transport channel [2]. Using non-equilibrium molecular dynamics simulations of model metal–water interfaces with tunable wettability, we show that the inelastic contribution represents more than 40% of the total thermal conductance. We find that the total conductance temperature dependence results from a competition between elastic conductance, which decreases with temperature, and inelastic conductance, which increases with temperature. Furthermore, we demonstrate that the inelastic channel strengthens with increasing molecular mobility in the liquid phase [2].

In a second stage, we employed all-atom molecular dynamics simulations to quantify the interfacial thermal conductance between a polyethylene glycol (PEG) polymer chain and explicit water, see Fig. 1. By tuning the interaction between PEG and water, we investigate how the polymer conformation-collapsed vs. extended-affects interfacial heat transfer. We demonstrate that the effect of polymer conformation can be described by a master curve describing the thermal conductance as a function of temperature [3]. The temperature dependence of interfacial heat transfer is explained by the increase of the mobility of water molecules at high temperatures, and by the change of the secondary structure of hydrogen bonds which occurs around 320 K.

Keywords: interfacial thermal transfer; polymer-water interfaces; metal-water interfaces

References

[1] Chen, J.; Xu, X.; Zhou, J.; Li, B. Interfacial thermal resistance: Past, present, and future. *Rev. Mod. Phys.* **2022**, *94*, 025002.

[2] Gutiérrez, O.; El Hajj, J.; Santamaria, R.; Merabia, S. Anharmonic heat transport at metal–water interfaces: The role of molecular mobility. *Int. J. Heat Mass Transfer* **2026**, *256*, 128066.

[3] Babaei, S.; Cheraghali, Y.; Loison, C.; Rajabpour, A.; Merabia, S. Interfacial Thermal Conductance Between a Polyethylene Glycol Polymer Chain and Water: A Molecular Dynamics Study. *arXiv preprint* **2025**, arXiv:2512.03174.

09:20–10:00 |
Thu, 9 July |
Session III

Many-Body Dissipative Particle Dynamics of Non-Equilibrium Phenomena

Luís H. Carnevale[1], King L. Ng[1], Piotr Deuar[1], Zhizhao Che[2], Michał Klamka[3], Tomasz Bobiński[3] and **Panagiotis E. Theodorakis**[1]

[1]Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warsaw, Poland;
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Many-body dissipative particle dynamics (MDPD) is a particle-based method, which can be employed for simulating various multiphase systems, such as fluids, for example, those having a liquid–air surface in various phenomena, including non-equilibrium, such as droplet break-up or droplet oscillations on vibrating substrates. Moreover, MDPD can be used for studying multicomponent systems, for example, fluids laden with surfactant. In such cases, the method offers advantages, such as the possibility of investigating larger systems for longer times, which could be prohibitive with molecular dynamics (MD) simulation, even when coarse-grained (CG) models are employed.

The presentation will focus on two fluid dynamics phenomena investigated with MDPD. The first refers to the study of the Plateau–Rayleigh instability in liquid threads, where a power law describing the number of satellite droplets as a function of the Ohnesorge and Thermal Capillary numbers has been discovered. The investigation is expanded into systems with sodium dodecyl sulfate (SDS) surfactant, where the role of the latter in the break-up process, both mechanisms and dynamics, is unveiled for surfactant concentration below and above the critical aggregation concentration. In the second part of the presentation, we will focus on a recent study on droplet oscillations caused by a horizontally vibrating substrate. In this case, we have identified three different scenarios (phases I, II, and III), with phase II and III leading to droplet break-up. The boundaries between the different phases have been characterized based on the Capillary and Ohnesorge numbers, thus providing a universal description of droplet oscillation phenomena. Moreover, phase II is particularly interesting, as the growth of instability towards droplet break-up can be characterized by suitable parameters. Finally, the state of the droplet during oscillations has been characterized by measures, such as the number of particle contacts, which can reflect the ‘energy’ of the system in MDPD simulations.

Finally, we will present recent advances and examples related to the ongoing development of the MDPD-MARTINI FF in the Group of Soft Matter and Fluids Physics and future steps in this direction, such as adding more MARTINI-type beads to the interaction matrix and integrating methods developed in the frame of previous work, such as the GoMARTINI approach for proteins and other systems.

This research has been supported by the National Science Centre, Poland, under Grant No.

2019/34/E/ST3/00232. We gratefully acknowledge the Polish high-performance computing infrastructure PLGrid (HPC Center: ACK Cyfronet AGH) for providing computer facilities and support within computational Grant No. PLG/2025/018743. T.B. and M.K. acknowledge the support from Warsaw University of Technology within the Excellence Initiative: Research University (IDUB) program.

09:40–10:20 | Fri, 10 July | Session IV

Velocity Distribution of Water Molecules Evaporating From a Liquid–Vapor Interface

Ikuya Kinefuchi[1], Kohei Sato[2] and Atsuki Fujita[2]

[1]Department of Human and Engineered Environmental Studies, The University of Tokyo, Chiba, Japan;
[2]Department of Mechanical Engineering, The University of Tokyo, Tokyo, Japan

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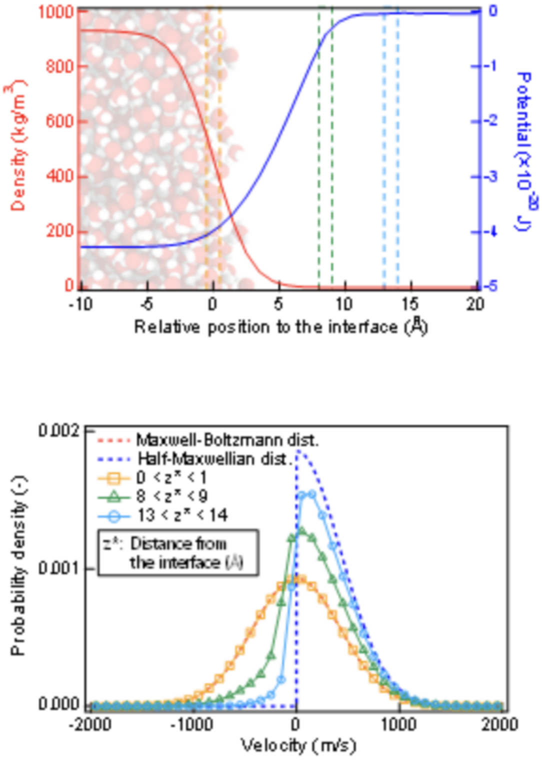

Figure 1: The potential distribution at the liquid-vapor interface (top) and the velocity distribution of evaporating water molecules as a function of the distance from the interface (bottom).

The analysis of gas–liquid two-phase flows with phase change requires boundary conditions at liquid–vapor interfaces that give the mass flux and temperature jump due to evaporation and condensation [1]. A strongly nonequilibrium gas flow region, known as the Knudsen layer, forms in the vicinity of a liquid surface where a net evaporation or condensation flux exists. The boundary conditions for the mass, momentum, and energy fluxes at a gas–liquid interface can be derived by solving nonequilibrium gas flows within the Knudsen layer. However, most analyses conducted so far have assumed that molecules evaporating from a liquid surface follow the Maxwell–Boltzmann distribution, even under nonequilibrium conditions with a net evaporation or condensation flux. Ishiyama et al. [2] demonstrated, using molecular dynamics simulations, that the velocity distribution of evaporating molecules deviates from the half-Maxwellian distribution. Nevertheless, no experimental study has directly measured the velocity distribution of evaporating molecules. Furthermore, establishing accurate interfacial boundary conditions for macroscopic fluid analyses requires a more detailed characterization of the velocity distribution function of evaporating molecules.

In this study, we performed molecular dynamics (MD) simulations of a liquid–vapor interface, in which evaporated molecules were removed at the edge of the computational domain to mimic evaporation into a vacuum. The velocity distribution of evaporating water molecules was obtained as a function of the distance from the liquid–vapor interface. We found that the velocity distribution is heavily influenced by the attractive potential near the liquid surface. The results of the MD simulations were also compared with our molecular beam experiments, where the velocity distribution of D2O (heavy water) molecules was obtained by the time-of-flight method.

Keywords: Liquid-vapor interface; Evaporation; Velocity distribution

References

[1] Aursand, E.; Ytrehus, T. Comparison of kinetic theory evaporation models for liquid thin-films. *Int. J. Multiph. Flow* **2019**, *116*, 67–79.

[2] Ishiyama, T.; Yano, T.; Fujikawa, S. Molecular dynamics study of kinetic boundary condition at an interface between a polyatomic vapor and its condensed phase. *Phys. Fluids* **2004**, *16*, 4713–4726.

12:10–12:50 | Fri, 10 July | Session V

Interfacial structural and transport properties of fluids at molecular resolution

Marcello Sega[1]

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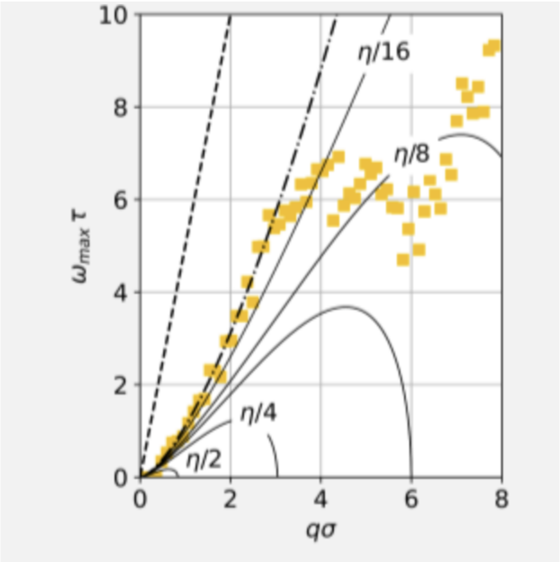

Figure 1: Collective current surface transverse mode (real frequency) in argon,and viscous hydrodynamic predictions for a family of surface viscosities as fraction of the homogeneous fluid viscosity, η.

Viscous response can be viewed as momentum relaxation under different mechanical perturbations. In homogeneous fluids, shear and bulk viscosity reflect transverse and longitudinal stress relaxation, respectively, whereas additional relaxation channels can arise in inhomogeneous systems such as liquid-vapour interfaces.

I will first present recent molecular dynamics results [1] for shear and bulk viscosity in the Virtual Chemistry dataset of organic liquids described by the OPLS and GAFF force fields. Using equilibrium Green–Kubo calculations, we identify chemical classes for which shear viscosity is not reproduced satisfactorily and clarify limitations of current transferable force fields.

Bulk viscosity, also known as volumetric viscosity, remains far less well characterised, with experimental and simulation data available for only a handful of fluids and state points. Our study [1] provides one of the first comprehensive assessments of this property across a broad chemical space and shows that bulk and shear viscosity do not follow the expected mutual trends.

I will then turn to liquid-vapour interfaces and discuss our results for argon, together with recent extensions to water, showing that it is possible to observe surface viscosity in neat liquids, specifically in absence of surfactants, and how surface viscosity emerges in the first molecular surface layer [2]. Bulk-like behaviour, including the occurrence of the usual bulk-like sound mode, emerges already from the dynamics of the second molecular surface layer. I will show two independent methods to estimate the surface viscosity from molecular dynamics simulations [3].

Keywords: viscosity; molecular dynamics; organic liquids

References

[1] Smith, I. D.; Sega, M. Insights from virtual chemistry: Shear and bulk viscosity of organic liquids via molecular simulations. *J. Chem. Phys.* **2025**, *162*, 094502.

[2] Malgaretti, P.; Bafile, U.; Vallauri, R.; Jedlovszky, P.; Sega, M. Surface viscosity in simple liquids. *J. Chem. Phys.* **2023**, *158*, 114705.

[3] Jedlovszky, P.; Sega, M. Surface viscosity of liquid interfaces from Green–Kubo relations. *J. Chem. Phys.* **2024**, *160*, 201101.

PART II

Oral Presentations

11:00–11:20 |
Wed, 8 July |
Session I

Revisiting the Green-Kubo relation for friction in nanofluidics

Anna T. Bui[1], and Stephen J. Cox[2]

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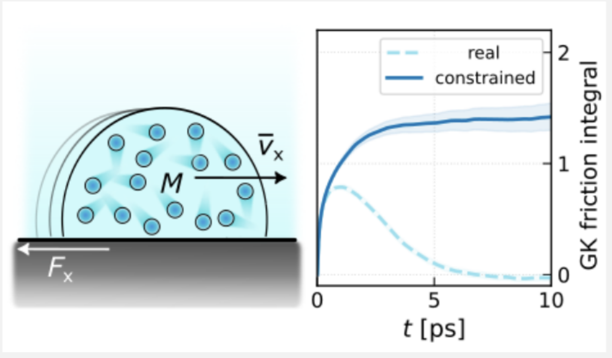

Figure 1: Using real dynamics results in a plateau problem since the force is correlated with the momentum, leading to negative correlation in the force autocorrelation; this causes the GK integral to vanish at long times. Constrained dynamics bypasses this issue by imitating the effect of projected forces, ensuring that the integral plateaus to a finite value

A central aim of statistical mechanics is to establish connections between a system's microscopic fluctuations and its macroscopic response to a perturbation. For non-equilibrium transport properties, this amounts to establishing Green–Kubo (GK) relationships. In hydrodynamics, relating such GK expressions for liquid–solid friction to macroscopic slip boundary conditions has remained a long-standing problem due to two challenges: (i) The GK running integral of the force autocorrelation function decays to zero rather than reaching a well-defined plateau value, and (ii) debates persist on whether such a transport coefficient measures an intrinsic interfacial friction or an effective friction in the system.

Inspired by ideas from the coarse-graining community, we derive a GK relation for liquid–solid friction where the force autocorrelation is sampled with a constraint of momentum conservation in the liquid. Our expression does not suffer from the "plateau problem" and unambiguously measures an effective friction coefficient, in an analogous manner to Stokes' law. We further establish a link between the derived friction coefficient and the hydrodynamic slip length, enabling a straightforward assessment of continuum hydrodynamics across length scales. We find that continuum hydrodynamics describes the simulation results quantitatively for confinement length scales all the way down to 1 nm. Our approach amounts to a straightforward modification to the present standard method of quantifying interfacial friction from molecular simulations, making possible a sensible comparison between surfaces of vastly different slippage.

Keywords: hydrodynamics; non-equilibrium statistical mechanics; nanofluidics

References

[1] Bui, A. T.; Cox, S. J. Revisiting the Greek–Kubo relation for friction in nanofluidics. *J. Chem. Phys.* **2024**, *161*, 201102.

[2] Bui, A. T.; Thiemann, F. L.; Michaelides, A.; Cox, S. J. Classical quantum friction at water–carbon interfaces. *Nano Lett.* **2023**, *23*, 580–587.

[3] Coquinot, B.; Bui, A. T.; Toquer, D.; Michaelides, A.; Kavokine, N.; Cox, S. J.; Bocquet, L. *Nat. Nanotechnol.* **2025**, *20*, 397–403.

11:20–11:40 |
Wed, 8 July |
Session I

Steady-State Solutions for Nonequilibrium Langevin Dynamics

Mattew Dobson[1]

[1]University of Massachusetts Amherst, USA

Corresponding author:

Deforming domain techniques are often applied to simulate molecular flows with steady homogeneous background flows such as shear, elongational, and mixed type flows. Such techniques include the Lees-Edwards boundary conditions for shear flows and Kraynik-Reinelt boundary conditions for elongational flows. This talk will focus on Nonequilibrium Langevin Dynamics with deforming domain boundary conditions where we prove exponential convergence to a steady-state limit cycle and also discuss numerical analysis issues arising with standard integrators.

11:40–12:00 |
Wed, 8 July |
Session I

Leveraging Machine Learning to Optimise Viscosity Prediction in NEMD

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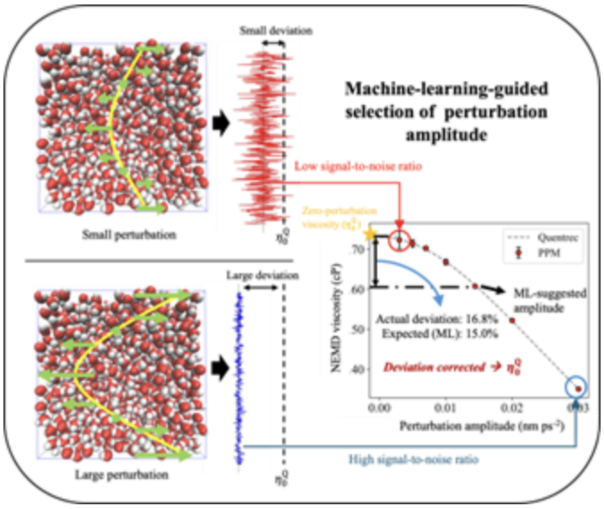

Figure 1: Machine-learning-guided selection of perturbation amplitude for balancing statistical noise and systematic deviation from the zero-perturbation viscosity.

The periodic perturbation method (PPM) [1] is an increasingly adopted non-equilibrium molecular dynamics (NEMD) approach for viscosity prediction. PPM has been shown to offer an efficient and accurate alternative to equilibrium methods across many systems [2]. However, reliable predictions depend critically on selecting an appropriate amplitude for the periodic perturbation. In practice, this amplitude is often chosen empirically or by trial-and-error, which can lead to poor statistical precision (if the perturbation is too weak) or to systematic bias away from the zero-perturbation viscosity (if it is too strong). In this work, using viscosity predictions for 144 organic solvents, we show that Quentrec's local order theory captures the relationship between the measured viscosity and the perturbation amplitude [2]. By extrapolating to the zero-perturbation limit, the zero-perturbation viscosity can be reliably determined. Taking advantage of the analytical form of this relationship, a regime in which the acceleration amplitude is sufficiently small that the viscosity varies only minimally from the zero-perturbation viscosity (e.g., deviation $< 10\%$) can be defined. The amplitude corresponding to a specified relative deviation depends on the nature of the system. This dependence can be captured using machine learning (ML), enabling us to avoid running multiple amplitudes solely to fit Quentrec's equation. Instead, a single NEMD simulation can be run at the amplitude suggested by the ML model. This saves computational expense both by avoiding trial-and-error and by eliminating the need to run NEMD simulations at multiple amplitudes for extrapolation. Ongoing work investigates whether viscosity measured at small acceleration amplitudes can be related to that measured at larger amplitudes via transfer learning, which could minimise the computational expense required to develop accurate machine-learning surrogate models for PPM viscosity prediction.

References

[1] Gosling, E. M.; McDonald, I. R.; Singer, K. On the calculation by molecular dynamics of the shear viscosity of a simple fluid. *Mol. Phys.* **1973**, *26*, 1475–1484.

[2] Gui, L.; Tsochantaris, E.; Nehil-Puleo, K.; Cummings, P. T.; McCabe, C. On the choice of acceleration amplitude for predicting shear viscosity using the periodic perturbation method. *J. Chem. Phys.* **2025**, *163*, 144118.

13:40–14:00 |
Wed, 8 July |
Session II

Non-equilibrium Thermal Energy Transfer at Structured Solid–liquid Interface

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Understanding thermal energy transfer at solid–liquid interface is central for thermal management in various engineering fields. In particular, at the atomic scale, modulating the interfacial thermal resistance (ITR) is one of the essential topics from both thermal science and engineering aspects. The physical origin behind it should be pursued from the atomic perspective; however, heat transfer properties at interfaces at the atomic scale are not well understood when we see it as a non-equilibrium process.

Equilibrium and Non-equilibrium Molecular dynamics (EMD, NEMD) simulations have largely contributed to the advancement of understanding the ITR, and MD is becoming a standard tool for investigating the ITR. In the framework of NEMD, combining with the microscopic expressions of the macroscopic transport equations, we can examine local transport quantities more precisely [1,2,3]; such approach is promising for advancing the understanding of transport phenomena from a standpoint of non-equilibrium transport physics at the atomic scale. Previous study has shown 2D & 3D structures of the heat flux at solid–liquid interfaces with sub-atomic spatial resolutions, although it was limited to a flat surface [3]. Understanding the heat flux structures at structured solid–liquid interfaces would be more important from an engineering perspective.

In this study, we performed a non-equilibrium molecular dynamics simulation for solid–liquid interfacial systems with/without structures under a temperature gradient, and examined thermal energy transfer across the interfaces in detail from an atomistic perspective. The Lennard–Jones potential was adopted in our systems for both the liquid and solid components. In particular, we focused on the heat flux structure in the vicinity of the interface, which was calculated using a method (MoP) [2] based on the microscopic expressions of the macroscopic transport equations. The results showed applicability of the method at extremely small local area in numerical simulations. In addition, unique properties of the local transport quantities were unveiled at structured solid–liquid interfaces.

Keywords: Non-equilibrium molecular dynamics; Thermal energy transfer; Solid–liquid interface

References

[1] Todd, B. D.; Daivis, P. D. *Nonequilibrium Molecular Dynamics: Theory, Algorithms and Applications*; Cambridge University Press: Cambridge, 2017.

[2] Smith, E. R.; Daivis, P. D.; Todd, B. D. Measuring heat flux beyond Fourier's law. *J. Chem. Phys.* **2019**, *150*, 064103.

[3] Fujiwara, K.; Shibahara, M. Thermal transport mechanism at a solid–liquid interface based on the heat flux detected at a subatomic spatial resolution. *Phys. Rev. E* **2022**, *105*, 034803.

14:00–14:20 |
Wed, 8 July |
Session II

Impact of surface charge on thermo-osmosis

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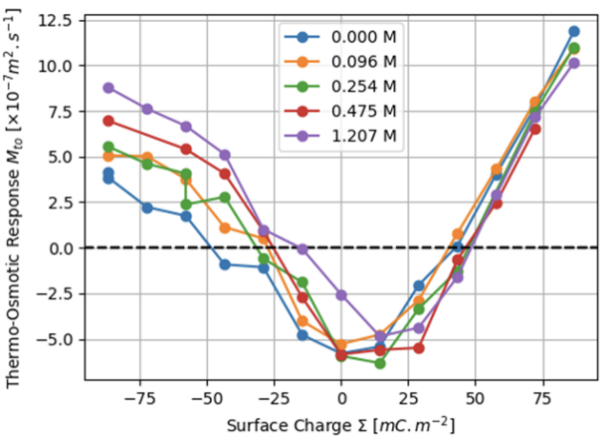

Figure 1: Thermo-osmotic response as a function of surface charge for different solution salt concentrations (in prep.)

Thermo-osmosis refers to the flow of fluids driven by a temperature gradient at liquid-solid interfaces. At the nanoscale, this phenomenon is strongly influenced by interfacial properties such as surface charge. In this work, we investigate the thermo-osmotic response of aqueous NaCl solutions (<1 M) confined between two graphene walls using molecular dynamics simulations. The thermo-osmotic coefficient M_{TO} is expressed as:

$M_{TO} = \frac{\Delta H}{\eta} (\lambda_H + b)$

where ΔH is the interfacial enthalpy excess, η the fluid viscosity, λ_H the characteristic range of the fluid-wall interaction (for common water-solid interfaces) and b the slip length [2].

Two types of simulations are performed to determine these quantities. First, bulk simulation and Green Kubo methods are employed to evaluate the viscosity as a function of the salt concentration. Second, we also modeled an electrolyte confined between two charged graphene layers, in order to evaluate the interfacial enthalpy excess and the slip length as a function of surface charge and concentration. Both types of simulations are performed at room temperature and atmospheric pressure.

Our bulk simulation results indicate that viscosity is only slightly dependent on salt concentration in within the range we explored. However, our simulation results in a confined environment indicate that the excess enthalpy and the slip length are strongly influenced by the surface charge, which affects the thermo-osmotic response (see Figure 1).

We also determined the electrostatic contribution of the excess enthalpy using the Boltzmann-Poisson equation. This study shows the moderate but significant impact of this contribution.

Finally, if time permits, we will also present measurements of the thermo-osmotic response under high temperature conditions.

Keywords: thermoosmosis; solid-liquid friction; electrostatic double layer

References

[1] Würger, A. Thermal non-equilibrium transport in colloids. *Rep. Prog. Phys.* **2010**, *73*, 126601.

[2] Ouadfel, M.; De San Féliciano, M.; Herrero, C.; Merabia, S.; Joly, L. Complex coupling between surface charge and thermo-osmotic phenomena. *Phys. Chem. Chem. Phys.* **2023**, *25*, 24321.

14:20–14:40 |
Wed, 8 July |
Session II

Local Interfacial Thermal Conductance and Heat-Flow Anisotropy from NEMD

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Non-equilibrium molecular dynamics (NEMD) offers a powerful microscopic framework to quantify interfacial heat transport, thermophoresis, and anisotropic heating in nanomaterials, and recent methodological progress, especially the Atomistic Nodal Approach (ANA), enables atomic-resolution mapping of local interfacial thermal conductance (ITC) across complex nanoparticle morphologies, revealing strong heterogeneity linked to surface coordination. Combining NEMD and ANA, we show how Janus nanoparticles with contrasting wettability create sub-nanometre temperature discontinuities and directional heating. Together, these results contribute to establishing universal structure–transport relationships that enable the design of tunable thermal interfaces, thermoplasmonic nanoheaters, and, more generally, systems governed by interfacial temperature gradients.

References

[1] Deshmukh, A.; Zeng, C.; Wilton-Ely, J. D. E. T.; Bresme, F. Interfacial Thermal Transport of Gold Surfaces Coated with Heterogeneous Monolayers in a Binary Solvent. *ACS Appl. Mater. Interfaces* **2025**, *17*, 55564.

[2] Olarte-Plata, J. D.; Bresme, F. Impact of the Interfacial Kapitza Resistance on Colloidal Thermophoresis. *ACS Omega* **2024**, *9*, 43779.

[3] Jiang, M.; Chapman, A.; Olarte-Plata, J. D.; Bresme, F. Controlling Local Thermal Gradients at Molecular Scales with Janus Nanoheaters. *Nanoscale* **2023**, *15*, 10264.

[4] Jiang, M.; Olarte-Plata, J. D.; Bresme, F. Heterogeneous Thermal Conductance of Nanoparticle-fluid Interfaces: An Atomistic Nodal Approach. *J. Chem. Phys.* **2022**, *156*, 044701.

[5] Olarte-Plata, J. D.; Gabriel, J.; Albella, P.; Bresme, F. Spatial Control of Heat Flow at the Nanoscale Using Janus Particles. *ACS Nano* **2022**, *16*, 694.

14:40–15:00 |
Wed, 8 July |
Session II

Heat flux for any machine-learning potential: a universal wrapper built on metatomic

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10:00–10:20 |
THU, 9 July |
Session III

Coarse-Grained NEMD Simulations of Biointerfaces

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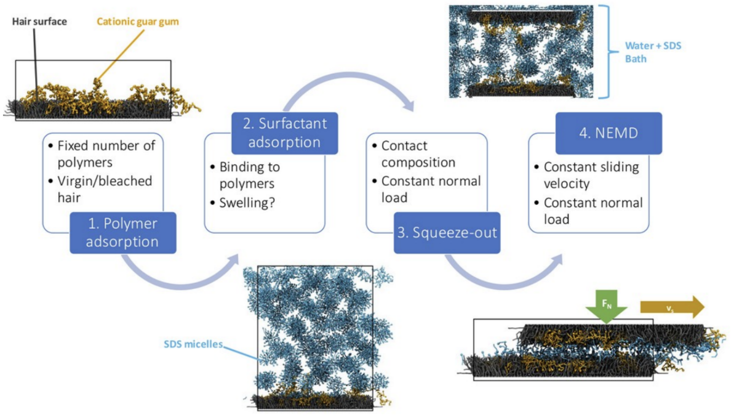

Figure 1: Coarse-grained hair friction screening framework with polyelectrolyte-surfactant layers consisting of adsorption, squeeze-out, and NEMD simulations

Coarse-grained molecular dynamics are a promising alternative to classical MD simulations allowing for accessing larger systems and microscale phenomena. Here, we present coarse-grained models to adsorption and friction phenomena in biointerfaces. We discuss hair care formulation screening frameworks based on hair friction, and how those can be extended to other applications such as textile friction and food tribology.

Tunable friction properties are desirable across a wide range of mechanical systems and are explored across a wide range of industrial applications. In biophysical systems, this is more complex due to the presence of water, macromolecules and macrostructures on substrates and in solution.

Coarse-grained molecular dynamics (CG-MD) are a viable approach compared to all-atom simulations, as systems tens or nanometer up to micrometer scale become accessible.

In this work, we present CG-MD simulations with the MARTINI forcefield for bio-systems[1] to study the friction of healthy and chemically-damaged human hair in the presence of hair care formulations. We present a protocol comprising of adsorption, squeeze-out and NEMD simulations to determine surface coverage, film thickness and friction coefficients in aqueous environments.[2]

Our results suggest systematic increase in friction with increasing surface damage, consistent with AFM experiments.[3] Deposition of cationic surfactants, or exploring synergistic effects from polyelectrolyte-surfactant mixtures is predicted to mitigate such frictional increases, thus explaining the efficacy of hair care formulations at the nanoscale.[2]

We further show how this framework can be extended to study more complex hair formulations, application to nanoscale screening of textile surfaces and mucin proteins in the context of oral/food tribology.[4]

References

[1] Marrink, S. J. et al. The MARTINI force field: coarse grained model for biomolecular simulations. *J. Phys. Chem. B* **2007**, *111*, 7812–7824.

[2] Weiand, E. et al. Boundary lubrication performance of polyelectrolyte-surfactant complexes on biomimetic surfaces. *Langmuir* **2024**, *40*, 7933–7946.

[3] Weiand, E. et al. Nanoscale friction of biomimetic hair surfaces. *Nanoscale* **2023**, *15*, 7086–7104.

[4] Kanesalingam, T. et al. A Coarse-Grained MARTINI Model for Mucins. *J. Chem. Theory Comput.* **2025**, *22*.

10:20–10:40 |
THU, 9 July |
Session III

Mesoscale Modelling of Lignocellulosic Biomass through Dissipative Particle Dynamics: A Bottom-Up Coarse-Graining Approach from Reactive Molecular Dynamics

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Lignocellulosic biomass (LB) is a promising renewable feedstock for the production of biofuels and biochemicals through pyrolysis. However, the multiscale nature of the pyrolysis process spanning across atomistic bond-breaking events through to mesoscale transport phenomena presents significant modelling challenges [1]. While reactive molecular dynamics MD simulations using the ReaxFF force field have provided valuable insights into the atomistic mechanisms of cellulose, hemicellulose and lignin decomposition, these simulations are inherently limited to length scales of a few nanometres and timescales of a few nanoseconds [2], [3], [4]. Bridging this gap at the mesoscale is essential for understanding the collective behaviour of LB components during thermochemical conversion. The aim here is to develop a mesoscale dissipative particle dynamics model for lignocellulosic biomass systematically parametrised from atomistic ReaxFF MD simulation data using a bottom-up coarse-graining methodology. In this study, Reactive MD simulations of cellulose, hemicellulose and lignin pyrolysis were first performed using the ReaxFF force field implemented in LAMMPS, generating a comprehensive database of structural thermodynamics and kinetic properties. A force-matching and inverse Boltzmann coupled coarse-graining scheme was then developed to map the atomistic structures onto DPD bead representations, thereby preserving the chemical identity and connectivity of each component. The DPD conservative interaction parameters were derived from radial distribution [5] and interaction potentials extracted from the atomistic data, while bonded interactions were parametrised to reproduce the conformational statistics for the LB chains. The resulting DPD model reproduces key structural features of the non-reactive LB system, including the spatial organisation of cellulose, hemicellulose and lignin components. Radial distribution functions and density profiles from DPD simulations show good agreement with the atomistic MD references which formed the basis of our reactive LB pyrolysis MD. The model enables simulations at length and time scales approximately two to three orders of magnitude beyond those accessible by atomistic methods whilst retaining the fidelity to the underlyingmolecular interactions. A validated mesoscale DPD framework for lignocellulosic biomass has been established through systematic coarse-graining of atomistic reactive MD. The non-reactive model provided a foundational platform for the development of reactive DPD parameters to simulate LB pyrolysis at the mesoscale, advancing multiscale modelling efforts towards industrially relevant conditions. The approach demonstrates the combination of non-equilibrium atomistic simulations with mesoscale methods to bridge the scale gap in biomass thermochemical conversion modelling.

Keywords: Lignocellulosic biomass; Coarse-graining; Multi-scale simulation.

References

[1] Al-Rumaihi, A. et al. A review of pyrolysis technologies and feedstock: A blending approach for plastic and biomass towards optimum biochar yield. *Renew. Sustain. Energy Rev.* **2022**, *167*, 112715.

[2] Wang, Q. et al. Initial pyrolysis mechanism and product formation of cellulose: An Experimental and Density functional theory (DFT) study. *Sci. Rep.* **2020**, *10*, 3626.

[3] Zhang, T. et al. Initial mechanisms for an overall behavior of lignin pyrolysis through large-scale ReaxFF molecular dynamics simulations. *Energy Fuels* **2016**, *30*, 3140–3150.

[4] Zheng, M. et al. Initial reaction mechanisms of cellulose pyrolysis revealed by ReaxFF molecular dynamics. *Fuel* **2016**, *177*, 130–141.

11:00–11:20 | THU, 9 July | Session III

Atomistic investigation of bulk and interfacial properties in high-entropy alloys

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High-Entropy Alloys (HEAs) are emerging as promising materials for coating applications thanks to their remarkable durability in harsh environments[1]. Experimental evidence has identified two HEA compositions, AlTiMoCrW and CoFeNiMoCr, to address wear and corrosion resistance, respectively. Atomistic molecular dynamics (MD) simulations are performed on medium-entropy precursors, composed of subsets of the target HEA elements, to develop protocols scalable to the full quinary alloys.

Both bulk and interfacial properties are investigated. Each alloy undergoes an initial hybrid MD-Monte Carlo stage[2] to promote potential-driven short-range order, followed by equilibration under controlled thermodynamic conditions to ensure consistent initial states.

Interfacial wetting behavior is studied by coupling crystalline substrates with molten droplets. Substrates are extracted from equilibrated bulk systems, while droplets are melted and shaped prior to interaction. Liquid/vapor surface tension is evaluated via the Kirkwood-Buff formulation[3], while shear viscosity is determined through Linear Response Theory[4]. Droplet spreading dynamics provide access to contact angle evolution, contact line motion, and interfacial friction coefficients.

Mechanical properties are obtained through controlled uniaxial deformation to construct stress–strain responses, enabling extraction of Young's modulus and identification of yield regimes. These results are interpreted in light of composition-dependent stacking-fault energetics, which govern the competition between twinning and slip mechanisms. This approach supports cross-system comparison of stiffness and ductility under conditions relevant to coating applications.

Thermal properties are evaluated from MD using both equilibrium and non-equilibrium approaches. Lattice thermal conductivity is computed via the Green-Kubo formalism from heat-flux autocorrelation functions, capturing bulk phonon transport, while NEMD provides estimates of Kapitza resistance[5] at solid-solid and solid-liquid interfaces. Lattice dynamics are further characterized through the phonon density of states (PDOS), obtained from the Fourier transform of the velocity autocorrelation function, enabling analysis of temperature-dependent effects.

Overall, this work establishes an integrated atomistic framework to relate composition, interfacial behavior, mechanical response, and thermal transport in HEAs. Future scaling to quinary alloys via neural network potentials[6] (NNPs) is currently underway to address the challenges of higher-order chemical complexity.

This project activity is funded by the M2DESCO Horizon EU project (N. 101138397), which aims to produce HEA coatings that are "safe and sustainable by design" by reducing the use of critical metal elements and forever chemicals.

References

[1] Schweidler, S.; Botros, M.; Strauss, F.; Wang, Q.; Ma, Y.; Velasco, L.; Cadilha Marques, G.; Sarkar, A.; Kübel, C.; Hahn, H.; Aghassi-Hagmann, J.; Brezesinski, T.; Breitung, B. High-entropy materials for energy and electronic applications. *Nat. Rev. Mater.* **2024**, *9*, 266–281.

[2] Guo, J.; Haji-Akbari, A.; Palmer, J. C. Hybrid Monte Carlo with LAMMPS. *J. Theor. Comput. Chem.* **2018**, *17*, 1840002.

[3] Kirkwood, J. G.; Buff, F. P. The Statistical Mechanical Theory of Surface Tension. *J. Chem. Phys.* **1949**, *17*, 338–343.

[4] Petravic, J.; Harrowell, P. Linear response theory for thermal conductivity and viscosity in terms of boundary fluctuations. *Phys. Rev. E* **2005**, *71*, 061201.

[5] Swartz, E. T.; Pohl, R. O. Thermal boundary resistance. *Rev. Mod. Phys.* **1989**, *61*, 605–668.

[6] Kocer, E.; Ko, T. W.; Behler, J. Neural Network Potentials: A Concise Overview of Methods. *arXiv preprint* **2021**, arXiv:2107.03727.

11:20–11:40 |
THU, 9 July |
Session III

Conformational Isomerism Tunes Refrigeration Potential in Metal Organic Frameworks

C. C. Hong[1], W. L. Leung[2], C. Wilson[2], M. J. Liddle[2], R. S. Forgan[2], J. J. B. Levinsky[1], A. S. J. S. Mey[1] and C. L. Hobday[1]

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As the effects of climate change become more apparent in the form of rising global temperatures, the necessity for temperature control become more significant.[1] Current refrigerants are low cost and work extremely efficiently but these materials possess very high global warming potentials.[2] A greener alternative is a solid-state approach via barocaloric materials which exhibit large adiabatic temperature and isothermal entropy changes upon compression and decompression cycles.[3]

Metal-organic frameworks (MOFs) are porous, crystalline materials that are highly modular due to the many metal and linker combinations possible.[4] Notably, certain MOFs exhibit the breathing effect wherein the adsorption and desorption of guest molecules are accompanied by a large reversible volume change. From this, they have been recognised as potential barocaloric materials.[5]

My research uses several computational methods to explore and further understand the structure-property relationships in MOFs. We identified the existence of orientational disorder in the linkers which result in conformational isomers in the MIL-53-fum framework series. Using ab initio molecular dynamics, the effects of the isomerism on the framework properties was uncovered. The potential energy surfaces associated with the interconversion of the isomers were then sampled using umbrella sampling. Finally, grand canonical Monte Carlo simulations allowed us to isolate, for the first time, the entropic contributions of guest adsorption from the volumetric or conformational aspects. This revealed the role of breathing and rigid MOFs in refrigeration applications, inform the design of functional materials, and how the barocalorics performance can be tuned with conformational isomerism.

Keywords: Solid-state; MOFs; isomerism; adsorption; refrigeration; caloric

References

[1] Wang, L.; Wang, L.; Li, Y.; Wang, J. A century-long analysis of global warming and earth temperature using a random walk with drift approach. *Decis. Anal. J.* **2023**, *7*, 100237.

[2] Cazorla, C. Novel mechanocaloric materials for solid-state cooling applications. *Appl. Phys. Rev.* **2019**, *6*, 041316.

[3] Moya, X.; Mathur, N. D. Caloric materials for cooling and heating. *Science* **2020**, *370*, 797–803.

[4] Li, B.; Kawakita, Y.; Ohira-Kawamura, S.; Sugahara, T.; Wang, H.; Wang, J.; Chen, Y.; Kawaguchi, S. I.; Kawaguchi, S.; Ohara, K.; Li, K.; Yu, D.; Mole, R.; Hattori, T.; Kikuchi, T.; Yano, S.; Zhang, Z.; Zhang, Z.; Ren, W.; Lin, S.; Sakata, O.; Nakajima, K.; Zhang, Z. Colossal barocaloric effects in plastic crystals. *Nature* **2019**, *567*, 506–510.

[5] García-Ben, J.; López-Beceiro, J.; Artiaga, R.; Salgado-Beceiro, J.; Delgado-Ferreiro, I.; Kolen'ko, Y. V.; Castro-García, S.; Señarís-Rodríguez, M. A.; Sánchez-Andújar, M.; Bermúdez-García, J. M. Discovery of Colossal Breathing-Caloric Effect under Low Applied Pressure in the Hybrid Organic–Inorganic MIL-53(Al) Material. *Chem. Mater.* **2022**, *34*, 3323–3332.

11:40–12:00 |
THU, 9 July |
Session III

Non-Equilibrium Reactive Molecular Dynamics Simulation of CO2 Permeation in PVAm/PVA Facilitated Transport Membranes

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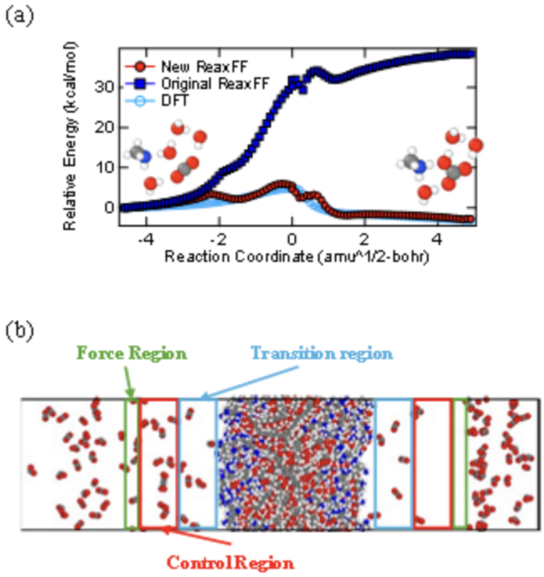

Figure 1: (a) Energy profiles along the reaction pathway calculated by newly developed ReaxFF, original ReaxFF, and DFT with 4 excess H2O molecules. (b) A representative snapshot of the simulation system for CGD-MD.

Facilitated transport membranes [1] based on polyvinylamine/polyvinyl alcohol (PVAm/PVA) composites have emerged as promising materials for CO_2 capture, yet the molecular-level mechanism by which water facilitates CO_2 transport through these membranes remains poorly understood. Two key challenges hinder progress: first, it is experimentally difficult to quantitatively decouple the contributions of solution-diffusion transport and facilitated transport from the measured CO_2 permeation flux; second, analyzing chemical reaction processes at the molecular scale requires first-principles calculations, and kinetic simulations tracking the time evolution of reactions demand prohibitive computational cost. To overcome these limitations, this study combines ReaxFF-based reactive molecular dynamics (MD) simulations with concentration gradient-driven MD (CGD-MD) [2] to investigate the permeation behavior of CO_2 molecules under non-equilibrium conditions.

Figure 1(a) shows the optimization of the ReaxFF force field parameters against the density functional theory (DFT) calculations. To reproduce the chemical reaction between CO_2 and NH_2

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groups in the presence of water, reaction energies calculated with 4 non-reactive H_2O molecules placed in the surrounding environment were used as training data. As a result, the trained parameter set showed good agreement with the DFT results compared to the original ReaxFF parameter set. Furthermore, the trained parameter set reproduced reasonable structural properties in terms of the radial distribution function and density. Figure 1(b) shows the simulation system for CGD-MD, where control regions are placed on both sides of the membrane, and a concentration gradient is imposed by maintaining the CO_2 concentration on the high- and low-concentration sides at their respective target values via force regions.

Keywords: Reactive force field; Facilitated transport membranes; Density functional theory

References

[1] Deng, L.; Hägg, M.-B. Swelling behavior and gas permeation performance of PVAm/PVA blend FSC membrane. *J. Membr. Sci.* **2010**, *363*, 295–301.

[2] Özcan, A.; Perego, C.; Salvalaglio, M.; Parrinello, M.; Yazaydin, A. O. Concentration gradient driven molecular dynamics: a new method for simulations of membrane permeation and separation. *Chem. Sci.* **2017**, *8*, 3858–3865.

10:20–10:40 |
FRI, 10 July |
Session IV

Benchmarking of water models and coarse-graining strategies for high temperature simulations

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Although boiling and cooling generally sound completely different and are placed at two extremes, they are indeed connected. Boiling heat transfer and the boiling crisis represent some of the most complex and industrially consequential phenomena in thermal-fluid science, with direct implications for steam turbine power generation, metallurgical quenching, nuclear reactor cooling, power electronics thermal management, and emerging biomedical applications. Despite extensive experimental, theoretical, and computational research, complete understanding of the critical heat flux transition, the spontaneous and irreversible collapse of nucleate boiling into film boiling and the opposite situation that occurs during metal quenching, remain elusive. The inherently multiscale nature of the problem, spanning molecular interfacial dynamics to macroscopic vapour film formation demands simulation frameworks that are simultaneously accurate and computationally tractable across a wide range of length and time scales.

This work presents a systematic benchmarking and classification of water models and coarse-graining strategies relevant to the molecular simulation of boiling phenomena with emphasis on both physical accuracy and computational efficiency. The atomistic models TIP4P/2005, TIP4P-BGT, OPC, and OPC3 are evaluated against experimental thermodynamic and transport properties, with particular focus on behaviour at elevated temperatures approaching the liquid-vapour coexistence region. This assessment is extended to coarse-grained representations, with an intention to include mW, ML-mW, MARTINI-E, MARTINI 3, and BUMPer, which offer access to the spatial (micrometers) and temporal (microsecond) scales required to study vapour film dynamics and the onset of the boiling crisis. All initial simulations are conducted under equilibrium molecular dynamics conditions (under the boiling point) using LAMMPS, establishing a validated and reliable computational foundation to extend in non-equilibrium molecular dynamics (NEMD) boiling simulations. The long-term objective is to perform NEMD simulations of polymer solutions at high temperatures and various boiling regimes. This in turn will provide us with better understanding of the complex phenomena taking place during boiling heat transfer and improve the accuracy of macroscopic models used in more conventional CFD simulations of industrial applications.

Keywords: Molecular Dynamics; TIP4P/2005; OPC; LAMMPS; mW; MARTINI-E

10:40–11:00 |
FRI, 10 July |
Session IV

Molecular Dynamics Investigation of Kinetic Energy in a Collapsing Cavitation Bubble Induced by Shockwave

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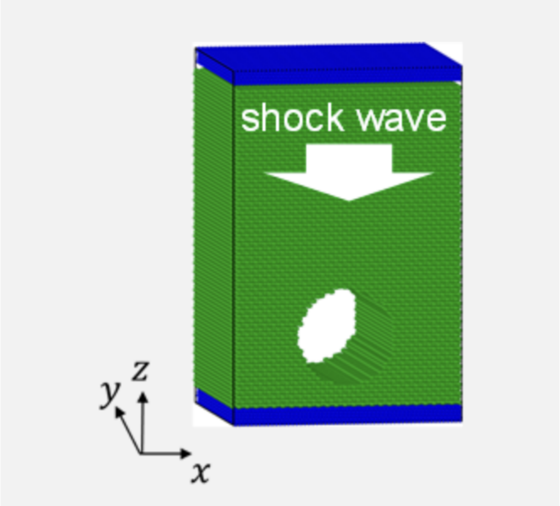

Figure 1: The initial computation domain with a cylindrical cavity (The cavity diameter was set at 10 in the LJ unit).

Collapsing of cavitation bubbles near a wall can cause erosion of the material, which mechanically reduces the lifetime of hydraulic machines such as pumps, water turbines, and propellers. The most important variable in cavitation erosion is the pressure caused by a high-speed collapsing of the cavitation bubbles, while the temperature inside each bubble may be also a key factor that may chemically change the lifetime. However, the latter influence has not been discussed sufficiently compared to the pressure. In addition, the bubble size may be molecular scale when the cavitation bubble diminishes, thus we have an essential question how far the definition of temperature itself, i.e., which can be only defined within a local equilibrium state, is valid. Answering this question would be important because almost all numerical studies for the cavitation bubble collapsing are limited to computation fluid dynamics (CFD) simulations based on the continuum approximation assuming a local equilibrium. In this study, as a simple case, a two-dimensional (cylinder) bubble collapsing induced by a planar shockwave propagation to a solid wall was computed by molecular dynamics (MD) simulations using LAMMPS for particularly investigating the molecular kinetics inside the bubble. The initial computation domain with a cylindrical cavity (bubble) is shown in Fig. 1, and the top wall (blue) reflecting the fluid molecules (green) was used for producing the shockwave propagating to the bottom wall (blue). The fluid was composed of diatomic molecules as the rigid rotor, whose intermolecular interaction was given by

a two-center Lennard-Jones (LJ) potential, and a harmonic potential was applied for the solid wall that was composed of several atomic layers. The standard definition of the temperature was employed for each freedom of the fluid molecules, i.e., translation and rotation of the diatomic molecules. As a result, each temperature for the freedoms significantly showed the different values during the bubble collapsing. It indicates that the equipartition theorem of the molecular kinetic energy is not satisfied, i.e., the local equilibrium cannot be assumed at the collapsing. Separating the translation temperature into each component, it was shown that the component along the shockwave propagation becomes extremely higher than the other translation components. In addition, each kinetic energy distribution for the translation and the rotation was evaluated, and a clear deviation from the Maxwell-Boltzmann distribution was also confirmed. The present results indicate that a non-equilibrium energy transfer, which cannot be estimated by the temperature in typical CFD simulations based on a local equilibrium, should be essentially focused for discussion of the chemical process during the cavitation bubble collapsing.

Keywords: Cavitation Bubble; Collapse; Shock Wave; Kinetic Energy; Non-equilibrium

11:00–11:20 |
FRI, 10 July |
Session IV

Time-dependent heat flux analysis during liquid-vapor interfacial adhesion

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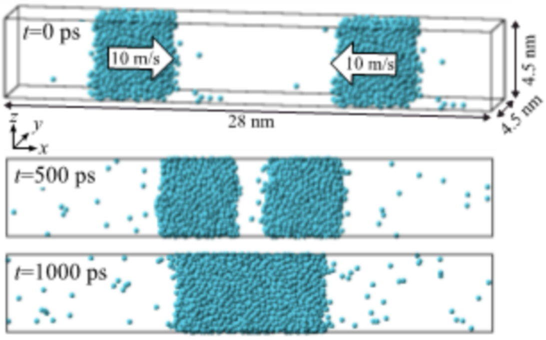

Figure 1: Time series snapshots of a quasi-1D NEMD system of a Lennard-Jones fluid to investigate liquid-vapor interfacial adhesion.

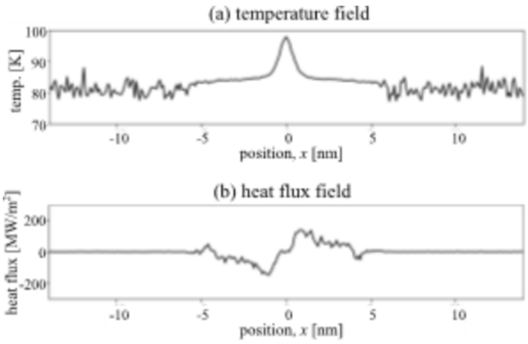

Figure 2: (a) Temperature and (b) heat flux fields at t=500 ps when the two liquid films started to interact during the liquid-vapor interfacial adhesion.

Latent heat is thermal energy released or absorbed during a constant temperature process such as phase transition of bulk. Our previous study revealed that advancing/receding contact line is heating/cooling in the same mechanism as the latent heat of phase change[1]. In the Lagrangian description, the fluid in the vicinity of the dynamic contact line (DCL) changes its interface by moving among the solid-liquid, solid-vapor and liquid-vapor interfaces, which induces the temperature rise/drop at the DCLs.

In this study, we investigate the heat release phenomenon induced in nanoscale during liquid-vapor interfacial adhesion without DCL. We employed unsteady non-equilibrium molecular dynamics (NEMD) simulations of a quasi-1D system with two Argon liquid films of a Lennard-Jones (LJ) fluid as shown in Fig. 1. Specifically, a single liquid film was equilibrated with Nosé-Hoover thermostat at 85K and then duplicated in the x-direction to create a system of two liquid films. Setting this moment as the initial time, we applied a macroscopic speed of 10 m/s to each film in opposite directions to investigate the interfacial adhesion under the NVE ensemble as shown in Fig.1. Furthermore, we performed ensemble averages over 25,000 trials and analyzed heat transport based on the conservation laws.

Figure 2 shows the temperature and heat flux fields at t=500 ps when the two liquid films started to interact during the liquid-vapor interfacial adhesion. Temperature rise between the interfaces was clearly observed, indicating that the interfacial adhesion induced heat release there. Furthermore, the released heat conducted both liquid films as shown in heat flux field.

References

[1] Kusudo, H.; Yamaguchi, Y. The receding contact line cools down during dynamic wetting. *J. Chem. Phys.* **2023**, *159*, 161102.

11:20–11:40 | FRI, 10 July | Session IV

Smooth Particle Hydrodynamics Simulation of Spinodal Decomposition in a Lennard-Jones Fluid

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Smooth Particle Hydrodynamics (SPH) is a particle-based solver of the governing equations of continuum physics introduced in the late 1970s by Lucy, Monaghan and Gingold1,2 for astrophysical applications. The method has since been applied to a diverse range of problems in fluid flow and structural mechanics. Its strength and popularity derive from the simplicity of the algorithm (having a structure similar to Molecular Dynamics) and increased efficiency compared to standard continuum solvers including Finite Element and Computational Fluid Dynamics. A highly promising application of SPH is to solve the equations of linear irreversible thermodynamics, opening up the possibility of studying chemical reactions and spinodal decomposition in liquid mixtures and alloys.

Parameterisation of SPH requires an equation of state, transport properties (fluids), elastic constants, plasticity models (for solids), and a model for surface tension. In the case of plasticity and surface tension, there is a choice of models to employ. Additionally, a wide variety of options exist for the SPH algorithm; choice of kernel (including variable smoothing length), artificial transport for taming numerical instability, kernel corrections, methods to deal with tensile instability and stress rotation being examples.

Given the large number of different ways to construct an SPH solver for a given application, a reliable validation method is highly desirable. The superior choice of validation for SPH involves Molecular Dynamics, a method which is essentially exact for a given choice of forcefield. By matching the equation of state derived from such a forcefield and using transport properties calculated for the same system, an SPH code can be tested to high fidelity. Furthermore, models of surface tension can be compared and evaluated before selecting the best one to use for the production stages of the work

In this presentation we demonstrate a validation scheme for an SPH model of the liquid-vapour transition in a single component Lennard-Jones fluid, quenched deep into the spinodal region of the phase diagram. For simplicity we work in 2-physical dimensions but include some work in 3D. Transport coefficients (shear and bulk viscosity, thermal conductivity) are obtained using Green-Kubo calculations while surface tension is obtained from two independent methods: the liquid ribbon method and the recently introduced gravitational field technique. Each of these methods additional provides the coexisting densities of liquid and vapour to be determined. The Reddy-O'Shea equation of state is used to capture the thermodynamics of the 2D Lennard-Jones system. A 2D SPH solver parameterised entirely from the Molecular Dynamics work is then used to study the dynamically evolving phase separation. This work will improve on previous studies by using a more realistic equation of state, which will guarantee that the equilibrium properties are correct and allow us to quantitatively validate the model of the dynamics.

Keywords: Smooth Particle Hydrodynamics; spinodal decomposition; Lennard-Jones Fluid

References

[1] Lucy, L. B. A numerical approach to the testing of the fission hypothesis. *Astron. J.* **1977**, *82*, 1013–1024.

12:50–13:10 |
FRI, 10 July |
Session V

TTCF based analysis of shear induced microstructure in an aqueous surfactant solution using molecular dynamics

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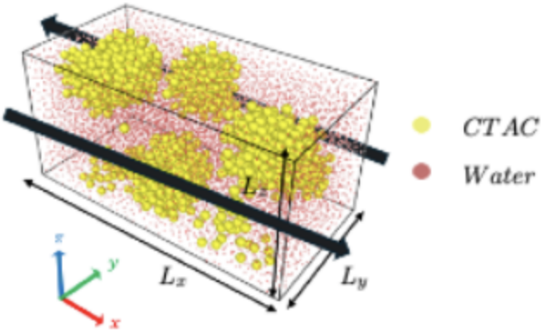

Figure 1: Snapshot of the CTAC distribution under shear. Micelles are formed and elongated along the shear direction, which results in the increase in the shear viscosity.

Understanding the non-Newtonian behaviour of aqueous surfactant solutions is essential for a wide range of engineering applications, such as optimizing flow control in microfluidic systems and achieving drag reduction in pipe flows. Experimental studies [1,2] have shown that surfactant solutions above the critical micelle concentration exhibit a non-monotonic increase in viscosity under shear, which has been attributed to the formation of wormlike micelle structures. However, direct observations via cryo-TEM remain limited, and the underlying mechanisms governing micelle formation and the associated viscosity increase are not yet fully understood.

In this study, we investigate the viscosity and micelle structures in CTAC (cetyltrimethylammonium chloride) solutions under shear (Fig. 1) using coarse-grained molecular dynamics simulations with the Martini force field [3]. To evaluate viscosity over a wide range of shear rates, ensemble averaging was performed using the TTCF approach [4]. Our simulations capture the non-monotonic viscosity increase within specific shear-rate and salt-concentration ranges, in agreement with experimental observations. The relationship between viscosity enhancement and the evolution of micelle structures will also be discussed in detail in the presentation/poster.

Keywords: SIS; viscosity; Martini force field

References

[1] Oda, R.; Panizza, P.; Schmutz, M.; Lequeux, F. Direct Evidence of the Shear-Induced Structure of Wormlike Micelles: Gemini Surfactant 12–2–12. *Langmuir* **1997**, *13*, 6407–6412.

[2] Lu, S.; Mei, Q.; Chen, J.; Wang, Z.; Li, W.; Feng, C.; Dong, J. Cryo-TEM and rheological study on shear-thickening wormlike micelles of zwitterionic/anionic (AHSB/SDS) surfactants. *J. Colloid Interface Sci.* **2022**, *608*, 513–524.

[3] Marrink, S. J.; Risselada, H. J.; Yefimov, S.; Tieleman, D. P.; de Vries, A. H. The MARTINI force field: coarse grained model for biomolecular simulations. *J. Phys. Chem. B* **2007**, *111*, 7812–7824.

[4] Maffioli, L.; Ewen, J. P.; Smith, E. R.; Varghese, S.; Daivis, P. J.; Dini, D.; Todd, B. D. TTCF4LAMMPS: A toolkit for simulation of the non-equilibrium behaviour of molecular fluids at experimentally accessible shear rates. *Comput. Phys. Commun.* **2024**, *300*, 109205.

13:10–13:30 |
FRI, 10 July |
Session V

Turbulence of Dilute Solutions of Supramolecular Polymers

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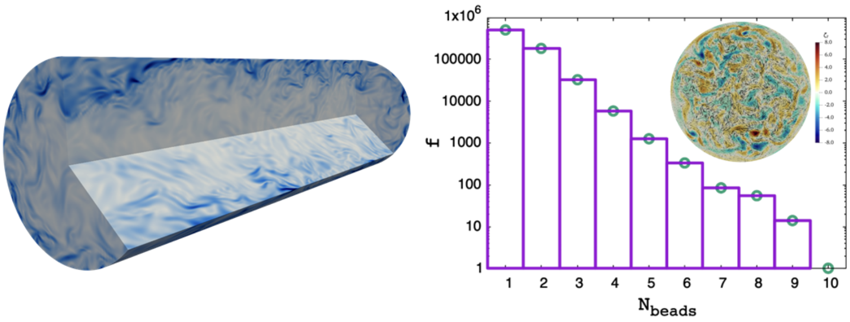

Figure 1: Left: Instantaneous axial velocity isocontours of a polymer-laden turbulent pipe flow. Right: histogram of the polymer chain lengths after scissions-recombination reach a statistical steady state. Inset: Axial vorticity isolcontours in a transverse section, together with the projection of the polymer chains.

It took five decades from Tom's discovery before DNS demonstrated viscoelasticity as crucial in polymer-induced drag reduction (DR) [1,2]. The polymer chain was modeled as a dumbbell with two massless beads connected by a nonlinear spring stretched by the solvent (FENE model). To make the model tractable, the Peterlin approximation was adopted (FENE-P model) to derive the equation for the so-called conformation tensor. Recently, such an approximation was removed by following the dynamics of every single dumbbell [3], and the analysis was extended to multi-bead chains. Covalently bonded polymers suffer from mechanical degradation, eventually rendering them futile. Here, we address supramolecular polymers that can assemble and disassemble under fluctuating, turbulent shear, making them able for sustained DR. Such a polymer system also presents anti-mist properties useful in preventing explosions, e.g., in the event of aircraft crashes. Raggruppa, Grouped objectIn the talk, besides presenting state-of-the-art and new numerical results for the more usual covalently bonded chains, which show the approach's ability to describe the so-called drag-reduction asymptote [4], a statistical mechanics model for self-organizing supramolecular polymers described at a very coarse-grained level is introduced. The model will be illustrated using the prototypical problem of polymer stretching by a uniform shear [5] as a validation step before moving to the more complex case where the polymers' dynamics couple to a turbulent wall-bounded flow. The algorithm for coupling the atomistic polymer model with the background turbulent flow of the solvent, described at the continuum level, will be discussed. Entirely new, still-unpublished results on the statistics of turbulence-induced polymer scissions and recombinations will be presented, together with a discussion of the drag-reducing effect we observe in the simulations after the polymer population reaches a statistically steady distribution.

References

[1] Sureshkumar, R.; Beris, A. N.; Handler, R. A. Direct numerical simulation of the turbulent channel flow of a polymer solution. *Phys. Fluids* **1997**, *9*, 743–755.

[2] De Angelis, E.; Casciola, C. M.; Piva, R. DNS of wall turbulence: dilute polymers and self-sustaining mechanisms. *Comput. Fluids* **2002**, *31*, 495–507.

[3] Serafini, F.; Battista, F.; Gualtieri, P.; Casciola, C. M. Drag reduction in turbulent wall-bounded flows of realistic polymer solutions. *Phys. Rev. Lett.* **2022**, *129*, 104502.

[4] Serafini, F.; Battista, F.; Gualtieri, P.; Casciola, C. M. Universal mean velocity profile in polymeric flows at maximum drag reduction. *Phys. Rev. Fluids* **2025**, *10*, L111301.

[5] Huang, C.-C.; Ryckaert, J.-P.; Xu, H. Structure and dynamics of cylindrical micelles at equilibrium and under shear flow. *Phys. Rev. E* **2009**, *79*, 041501.

13:30–13:50 |
FRI, 10 July |
Session V

Molecular simulation of large amplitude oscillatory extensional flow

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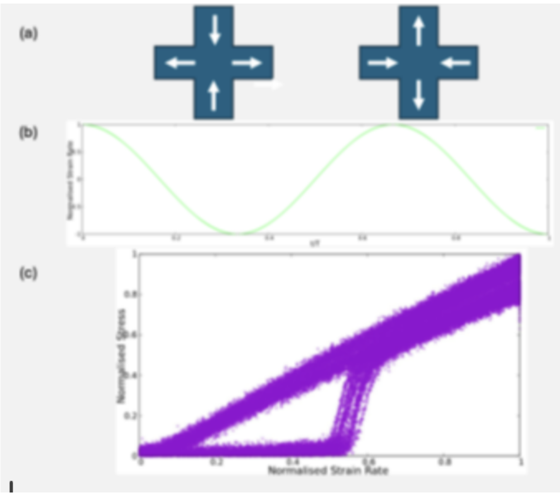

Figure 1: (a) Schematic of the oscillatory extensional flow. (b) Normalised strain rate as a function of time-period. (c) Stress vs Strain Rate for a dilute polymer solution under oscillatory extensional flow.

While large amplitude oscillatory shear (LAOS) tests are ubiquitous to rheological property measurement of complex fluids such as biological fluids, polymer melts, and electrospinning liquids, large amplitude oscillatory extension (LAOE) experiments are still not widely reported. LAOE is particularly useful to understand the material properties of spray cooling liquids, inkjet fluids, and flow through porous media. LAOE for low viscosity fluids are challenging as they are prone to gravitational sagging, necking and filament breakup[1]. This motivates one to explore molecular simulation capabilities to characterise the fluids under LAOE conditions. Molecular dynamics (MD) simulation under steady state extensional flow fields is robustly implemented by Nicholson and Rutledge[2], and is available as a package in LAMMPS simulation software. However, the primary challenge to reproduce the LAOE simulations is to ensure volume conserving deformation of the box. Currently LAMMPS cannot couple dimensions or introduce time dependent strain variables via fix deform command for a consistent extensional strain rate. In this work, we investigate and report the implementation of oscillatory extensional flow simulation via a velocity field in LAMMPS. This research enables the simulation of a true homogeneous oscillatory extensional flow with a correct temperature definition, no density oscillations and an affine velocity field. The non-equilibrium MD simulations are made suitable to extract extensional viscosity harmonics.

Keywords: oscillatory extensional flow; viscoelasticity; LAMMPS

References

[1] Recktenwald, S. M.; John, T. P.; Shen, A. Q.; Poole, R. J.; Fonte, C. P.; Haward, S. J. Large amplitude oscillatory extension (LAOE) of dilute polymer solutions. *J. Non-Newton. Fluid Mech.* **2025**, *342*, 105421.

[2] Nicholson, D. A.; Rutledge, G. C. Molecular simulation of flow-enhanced nucleation in n-eicosane melts under steady shear and uniaxial extension. *J. Chem. Phys.* **2016**, *145*, 244903.

PART III

Poster Presentations

15:30–17:00 |
WED, 8 July |
Poster Session I

Modelling Tight Junction Formation using Coarse-Grained Molecular Dynamics Simulations

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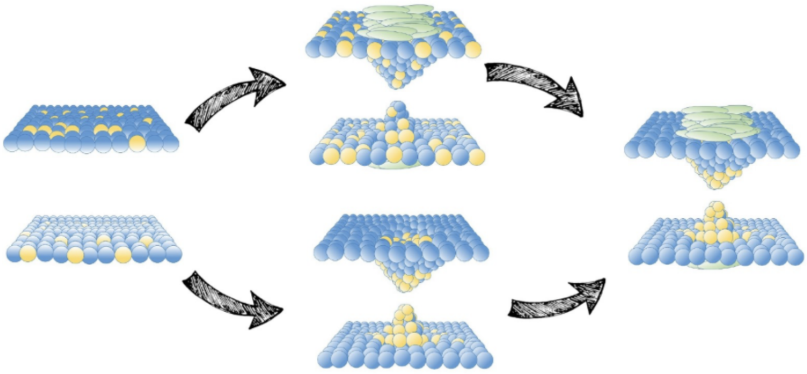

Figure 1: Two alternative pathways that can lead to TJ formation. In the upper pathway, the ZO-1 proteins (green) form 2D condensate which facilitates the aggregation of claudin protein (yellow) to form the TJ. In the second pathway, the Claudin proteins are primarily responsible for the TJ formation, and ZO-1 acts only as a coat layer for the TJ

Biomolecular condensates are membrane-less compartments composed of proteins and RNAs and are formed via liquid-liquid phase separation. These condensates play an important role in cellular organization and biochemical regulation. Increasing evidence suggests that condensates can interact with lipid membranes, influencing morphological changes in them, thus playing a distinct role in cell biology [1]. An important example of mutual remodelling between biomolecular condensates and lipid membranes is Tight Junction (TJ) formation in epithelial cells [2]. Here, we use bespoke coarse-grained MD simulations to investigate different possible pathways for TJ formation (see Figure 1), especially the complex interplay between 2D condensates formed by ZO-1 proteins and Claudin transmembrane proteins. Our results suggest that ZO-1 condensates can heavily influence the aggregation rates of Claudin, which in turn modulates the membrane shape during TJ formation. The analysis of the spatial synchronization of Claudin clusters in two adjacent cells points toward distinct mechanisms for different transmembrane proteins. In the long run, the insights learned may be beneficial for better understanding of condensate functions inside cells as well as applications in synthetic biology, artificial cell research, and therapeutic solutions targeting condensate assemblies

Keywords: Coarse grained MD Simulations; Tight Junction; Computational biophysics

References

[1] Mangiarotti, A.; Siri, M.; Tam, N. W.; Zhao, Z.; Malacrida, L.; Dimova, R. Biomolecular condensates modulate membrane lipid packing and hydration. *Nat. Commun.* **2023**, *14*, 6081.

[2] Pombo-García, K.; Adame-Arana, O.; Martin-Lemaitre, C.; Jülicher, F.; Honigmann, A. Membrane prewetting by condensates promotes tight-junction belt formation. *Nature* **2024**, *632*, 647–655.

15:30–17:00 |
WED, 8 July |
Poster Session I

The structural dynamics and barocaloric response of organic ionic plastic crystals

Rong Wei[1], Phillippa Partridge[1], Chi Cheng Hong[1], Joshua J. B. Levinsky[1], Jennifer M. Pringle[2] and Claire L. Hobday[1]

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Refrigeration systems account for 17% of global electricity consumption. As global temperatures rise, the demand for sustainable cooling technologies continues to increase.[1] Conventional refrigerants are highly efficient but have significant environmental impacts, creating an urgent need for greener alternatives. Barocaloric materials, which undergo large entropy and temperature changes under applied pressure, offer a promising solid-state cooling solution. Organic ionic plastic crystals (OIPCs) are attractive barocaloric materials because they exhibit multiple solid-solid phase transitions that can be driven by pressure. Their interionic interactions are highly tunable, and their characteristic transitions from highly orientationally disordered phases to ordered phases can lead to large entropy changes.[2] However, the microscopic mechanisms governing their phase behaviour remain unclear. (Cyanomethyl)trimethylammonium hexafluorophosphate ($[N_{111CN}][PF_6]$) undergoes a four-step disorder-order transition with notable thermal hysteresis. Understanding the nature of disorder in its high temperature phase is therefore crucial for optimising its barocaloric performance. In this work, ordered models of the disordered high-temperature phase (Phase I) are compared to investigate its structural flexibility. Ab initio molecular dynamics simulations have been performed to examine the dynamic behaviour associated with the phase transitions. The results indicate that Phase I is more dynamically disordered than the other three phases, with pronounced rotational motion of the [PF6]- anions accompanied by weaker dynamic motion of the $[N_{111CN}]^+$ cations. These insights improve the microscopic understanding of OIPCs as next generation solid state refrigerants. Based on AIMD simulations, the project is now progressing towards the training and optimisation of a machine learning potential, which will enable larger scale simulations and more detailed investigation of disorder driven phase behaviour.

Keywords: barocaloric; molecular dynamics; MLIPs

References

[1] Moya, X.; Mathur, N. D. Caloric materials for cooling and heating. *Science* **2020**, *370*, 797–803.

[2] Moya, X.; Kar-Narayan, S.; Mathur, N. D. Caloric materials near ferroic phase transitions. *Nat. Mater.* **2014**, *13*, 439–450.

15:30–17:00 |
WED, 8 July |
Poster Session I

Solid Electrolyte Interphase Model Based on Non-equilibrium Thermodynamics: Microscale Derivation and Upscaling

Kawa Manmi[1,2], Ferran Brosa Planella[1,2], Manuel Landstorfer[3] and Christoph Pohl[3]

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The solid electrolyte interphase (SEI) is a passivation layer that forms on the negative electrode of lithium-ion batteries through irreversible electrolyte decomposition. It governs both initial capacity loss during formation and long-term degradation throughout the battery's lifetime. Despite its importance, most continuum models treat the SEI as a boundary condition rather than a thermodynamic phase with its own transport equations, and the constitutive relations used for transport and interfacial reactions are typically specified empirically rather than derived from a consistent thermodynamic framework. We present a continuum model for SEI formation and growth derived from non-equilibrium thermodynamics [1,2]. The model treats three coupled bulk phases—active electrode, SEI, and electrolyte—each governed by mass and charge conservation with constitutive relations derived from free energy functions. Chemical potentials, incorporating both entropic and enthalpic (Redlich–Kister) contributions, determine all transport properties: diffusion and migration fluxes with thermodynamic factors that ensure consistency between open-circuit voltage, diffusivity, and reaction kinetics. Interfacial reactions at the electrode–SEI and SEI–electrolyte boundaries follow generalised Butler–Volmer kinetics, with the driving forces arising naturally from electrochemical potential differences. The SEI formation reaction is shown to be thermodynamically irreversible, reducing to a Tafel-like form. A moving boundary tracks the growing SEI–electrolyte interface. We derive a reduced ODE system via spatial averaging valid under OCV or low-rate conditions, and present numerical results demonstrating distinct growth regimes—linear, square-root, and logistic saturation—depending on kinetic parameters and electrolyte reservoir size, capturing both active lithium depletion and solvent exhaustion as termination mechanisms [1]. We then derive a macroscale model via asymptotic homogenisation, exploiting the scale separation between the particle-level microstructure and the cell-level geometry. Scaling analysis reveals which physics can be upscaled: electrolyte ion transport and electronic conduction operate at the macroscale, while SEI transport and solid-state lithium diffusion remain intrinsically microscale processes. The resulting homogenised model has a Doyle–Fuller–Newman-like structure, with effective transport coefficients expressed through cell problems on the representative volume element, coupled to a microscale SEI sub-problem with a moving boundary at each particle. Time-dependent porosity evolves as the SEI consumes electrolyte volume. The macroscale structure without SEI has been validated against the standard DFN using published cell parameters [3]; implementation of the full coupled model with SEI growth is ongoing work. harmonics.

Keywords: non-equilibrium thermodynamics; solid electrolyte interphase; asymptotic homogenisation; lithium-ion batteries; moving boundary

References

[1] Landstorfer, M.; Pohl, Ch.; Brosa Planella, F.; Manmi, K. A model for SEI-growth based on non-equilibrium thermodynamics. *WIAS Preprint* **2025**, No. 3250. DOI: 10.20347/WIAS.PREPRINT.3250.

[2] Landstorfer, M.; Ohlberger, M.; Rave, S.; Tacke, M. A modelling framework for efficient reduced order simulations of parametrised lithium-ion battery cells. *Eur. J. Appl. Math.* **2023**, *34*, 554–591.

[3] Chen, C.-H.; Brosa Planella, F.; O'Regan, K.; Gastol, D.; Widanage, W. D.; Kendrick, E. Development of experimental techniques for parameterization of multi-scale lithium-ion battery models. *J. Electrochem. Soc.* **2020**, *167*, 080534.

15:30–17:00 |
WED, 8 July |
Poster Session I

Determination of Nanobubble Zeta Potential via Non-Equilibrium Molecular Dynamics

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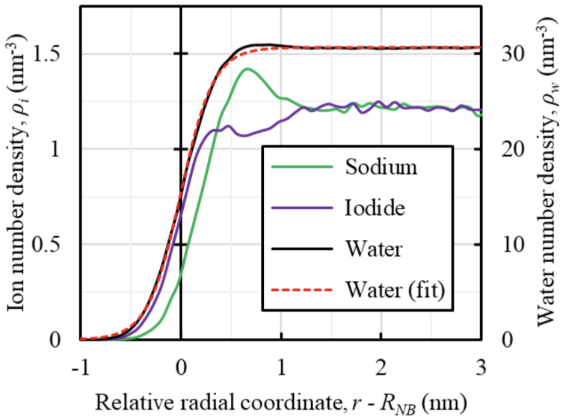

Figure 1: Ion and water number densities as a function of the relative radial distance from the interface ($r - R_{NB} = 0$)

Nanobubbles are defined as bulk spherical gas pockets with diameters $< 1\mu$m, and they possess unique physicochemical properties that have attracted significant industrial interest. For example, their high surface-to-volume ratio, coupled with dominant surface tension, enables nanobubbles to store large volumes of homogeneously distributed gas such as oxygen, which can enhance agricultural yields. Notably, their collapse can generate extreme-velocity jet flows, offering potential for targeted cancer therapies where mechanical force and encapsulated drug delivery combine to destroy malignant cells. Despite their utility, a theoretical paradox exists: due to high internal pressures, a 100 nm radius bubble is predicted to last only 0.1 ms [1], while experimental observations report that nanobubbles can exist for hours or even days [2].

Recent studies suggest that nanobubbles possess a negative surface charge, with a typical zeta potential of approximately $\zeta \sim$ -10 mV. This charge has been proposed as a potential stabilisation mechanism, where electrostatic repulsion may prevent bubble dissolution. Moreover, it suggests that nanobubbles could be manipulated and transported using externally applied electric fields.

Currently, zeta potentiometers take this measurement indirectly, relying on a phenomenon known as electrophoresis where the nanobubble is subjected to an electric field, and its terminal drift velocity is related to its zeta potential via the Smoluchowski equation. However, the accuracy of this approach is not well understood, specifically the relationship between the electrophoretic drift velocity and the ionic layering around the nanobubble.

In this study, we perform Molecular Dynamics (MD) simulations of a nanobubble dissolved in water with sodium and iodide to confirm that ions do adsorb on the interface, where an electric double layer (EDL) forms through the arrangement of ions near the liquid-gas interface, as shown in Figure 1, and we can estimate the zeta potential by fitting respective ionic densities to the Poisson Boltzmann equation.

Furthering this study, we recreate the experimental electrophoresis setup using non-equilibrium MD simulations. By exposing mechanically and chemically equilibrated nanobubbles to an electric field, the resulting electrophoretic mobility can be used to predict another estimate for zeta potential in accordance with experimental methodology. We make comparisons between our two estimates for zeta potential, and comment on the accuracy of electrophoretic-based zeta potentiometers for nanobubble characteristation.

References

[1] Epstein, P. S.; Plesset, M. S. On the Stability of Gas Bubbles in Liquid-Gas Solutions. *J. Chem. Phys.* **1950**, *18*, 1505–1509.

[2] Ma, T.; Kimura, Y.; Yamamoto, H.; Feng, X.; Hirano-Iwata, A.; Niwano, M. Characterization of Bulk Nanobubbles Formed by Using a Porous Alumina Film with Ordered Nanopores. *J. Phys. Chem. B* **2020**, *124*, 5067–5072.

15:30–17:00 |
WED, 8 July |
Poster Session I

Towards understanding the Soret Effect in Polymeric Liquids

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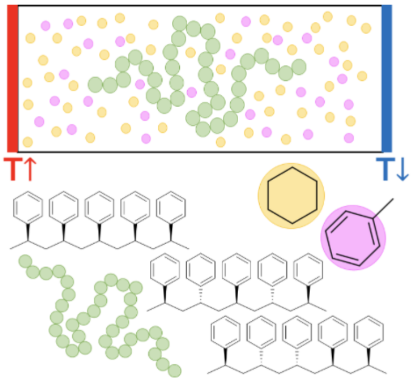

Figure 1. Graphical representation of the present work.

Figure 1

Mass diffusion in complex mixtures can be induced through the application of a suitable temperature gradient. This effect is known under the name of Ludwig-Soret effect, or thermodiffusion, or thermophoresis when referred to biological fluids. The extent and direction of the resulting concentration gradient depends on multiple effects, such as mixture composition and molecular weight difference of components and can be quantified by the Soret coefficient,S_T, also defined as the ratio between the thermodiffusion coefficient,D_T, and the mass diffusion one, D[1,2].

To date, a lot of work has been done to investigate the Soret effect in binary gaseous and liquid mixtures both experimentally and computationally. On the other hand, the investigation of this effect in ternary mixtures and polymeric liquids is still quite limited, but of great practical interest for applications ranging from fluid storage and transport to food processing and biomedical industries [1].

While some effects, like S_T variation with the molecular weight of the polymer, have been investigated for several polymer–solvent systems, other phenomena, like the effect of tacticity or of copolymer structure on the Soret coefficient of great importance for polymer fractionation, are still lacking accurate description. This is due to limited availability of experimental data and intrinsic difficulty associated with investigation of ternary systems or polymeric systems at high polymer concentration.

Here, we use molecular analysis to investigate the Soret effect in polystyrene:toluene:cyclohexane

(PS:Tol:cHex) mixtures. Such mixture represents a suitable model system given the availability of experimental data for syndiotactic PS. Another point of scientific interest is given by opposite sign of S_T for PS:Tol and PS:cHex mixtures, hence the Soret coefficient of the ternary system is expected to be dependent on the Tol:cHex concentration of the binary solvent. Moreover, PS is an ideal candidate to investigate the influence of tacticity on thermodiffusion, providing the link between transport and interaction energy of components in the mixture. Here, we apply the EMD and boundary-driven NEMD to investigate mixtures of isotactic, syndiotactic, and atactic PS at infinite dilution in Tol, cHex, and Tol:cHex at equilibrium and under the effect of the temperature gradient, as shown in Figure 1.

Keywords: thermodiffusion; Soret coefficient; polymeric liquids

References

[1] Vailati, A.; Šeta, B.; Bou-Ali, M. M.; Shevtsova, V. Perspective of research on diffusion: From microgravity to space exploration. *Int. J. Heat Mass Transfer* **2024**, *229*, 125705.

[2] Köhler, W.; Morozov, K. I. The Soret Effect in Liquid Mixtures – A Review. *J. Non-Equilib. Thermodyn.* **2016**, *41*, 151–197.

15:30–17:00 |
WED, 8 July |
Poster Session I

Do solid phonons play a role in the bounce-to-stick phase transition for liquid nanodroplets on hydrophobic surfaces?

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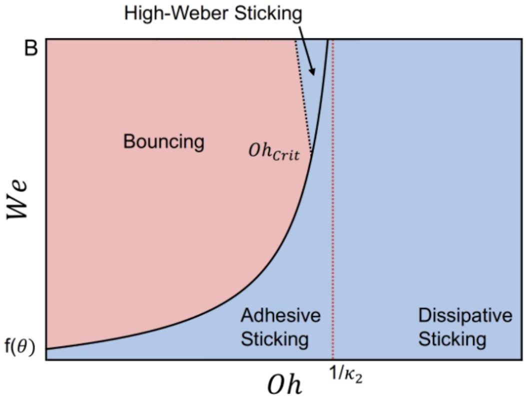

Figure 1: Phase diagram of the dynamical bouncing/sticking behavior of an aqueous microdroplet on a rigid hydrophobic surface, in terms of its Weber (We) and Ohnesorge (Oh) numbers, as reported in Ref. [1].

Whether a given liquid droplet bounces or sticks to a given surface, despite its apparent simplicity, is an important and surprisingly poorly-understood phenomenon. This question plays a critical role in understanding wetting and surface deposition of aerosols in the context of e.g. disease transmission, industrial processes, or other natural phenomena; yet controversy remains as to exactly which factors control this process.

Recent work[1] using finite-element numerical simulations, and supported by experiments, reports that aqueous microdroplets of diameter $30 - 50\mu$m, impinging upon rigid hydrophobic surfaces, either bounce or stick depending only on their Weber and Ohnesorge nondimensional numbers. In particular, it is found that the bouncing/sticking behaviors form a dynamical phase space (see Figure 1), with a primary phase transition indicating a low-velocity sticking mechanism, and a reentrant phase transition indicating a high-velocity sticking mechanism. These transitions are explained through the interplay of surface tension, viscous dissipation, and wetting on a flat rigid surface.

However, it was recently reported that phonons play a significant role in the nanoscale wetting of flexible 2D materials under free-standing conditions, and that mechanical strain has an oversized effect on the water contact angle as a consequence of this phonon coupling.[2] It would therefore be likely that, on a realistic elastic solid surface, the bouncing/sticking behavior of a nanodroplet would be further affected by the coupling between wetting and solid surface phonons, as well as accelerated dissipation through solid phonons dispersing into the bulk. Non-equilibrium molecular dynamics simulation will be critical to study liquid droplets at the nanoscale, where classical continuum methods break down, and how they couple to a realistic solid throughout the bouncing/sticking motion. Such a coupling, if present, is expected to contribute further insight towards nanoscale aerosols, which are currently implicated in certain health and environmental concerns, but also show promise for several industrial processes.

References

[1] McLauchlan, J.; Walker, J. S.; Sanjay, V.; Jalaal, M.; Reid, J. P.; Squires, A. M.; Souslov, A. Bouncing microdroplets on hydrophobic surfaces. *Proc. Natl. Acad. Sci. U.S.A.* **2025**, *122*, e2507309122.

[2] Lim, D. W.; Advincula, X. R.; Witt, W. C.; Thiemann, F. L.; Schran, C. Revealing strain effects on the graphene-water contact angle using a machine learning potential. *arXiv preprint* **2026**, arXiv:2601.20134.

15:30–17:00 |
WED, 8 July |
Poster Session I

Molecular modelling of anion-exchange membranes

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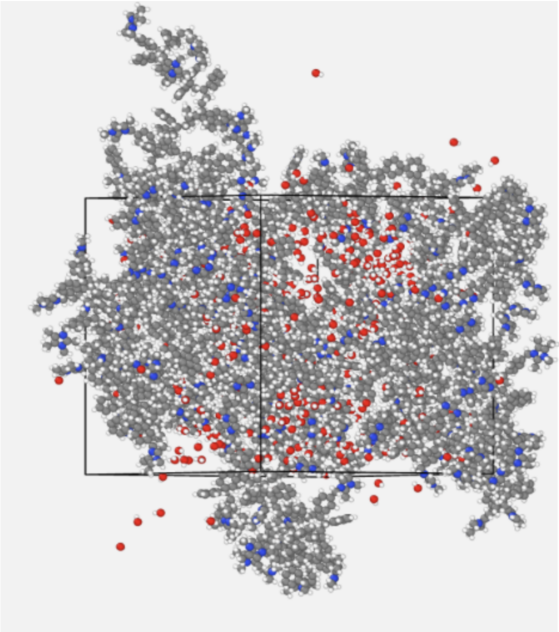

Figure 1: Molecular model of hydrated Sustainion® obtained via the iterative GCMC-MD protocol

To achieve a sustainable, net-zero carbon future, the global energy infrastructure must transition to efficient, clean-energy conversion devices.[1] Fuel cells are central to the development of the hydrogen economy, offering direct and zero-emission power generation.[1] While Proton Exchange Membrane Fuel Cells are well-established, their high costs, driven by platinum catalysts and fluorinated polymers, limit large-scale deployment.[2] Anion Exchange Membrane Fuel Cells (AEMFCs) offer a promising, economical alternative by operating in an alkaline medium that permits the use of abundant, non-precious metal catalysts.[2]

Despite these advantages, the commercial viability of AEMFCs is currently hindered by membrane degradation and conductivity trade-offs, making the rational design of highly durable, high-performance Anion-Exchange Membranes (AEMs) a critical research priority for their commercialisation.[2] In this regard, predictive molecular modelling can provide property estimation and mechanistic insight to inform materials design and selection.

In this work, molecular modelling is applied to study AEM polymers, with the goal to establish robust simulation protocols for the reliable prediction of performance metrics, specifically ionic conductivity and mechanical resistance, as a function of their hydration state.

The protocol is first validated against the dry polymer state, where equilibrium Molecular Dynamics (MD) is used to compute dry density and Young's modulus, ensuring accurate force field selection. Building on this foundation, iterative Grand Canonical Monto Carlo (GCMC) - MD simulations are employed to estimate water uptake and swelling, providing the equilibrated hydrated morphologies (Figure 1) necessary for transport analysis.

Subsequently, a non-equilibrium approach, namely Concentration Gradient Driven Molecular Dynamics[3], is implemented to compute the diffusivity of hydroxide ions and extract ionic conductivity across varying hydration states. This protocol offers an efficient computational framework to accelerate the discovery and design of next-generation AEM materials.

Keywords: Anion Exchange Membranes; Concentration Gradient Driven Molecular Dynamics; Ionic conductivity

References

[1] Staffell, I.; Scamman, D.; Velazquez Abad, A.; Balcombe, P.; Dodds, P. E.; Ekins, P.; Shah, N.; Ward, K. R. The role of hydrogen and fuel cells in the global energy system. *Energy Environ. Sci.* **2019**, *12*, 463–491.

[2] Varcoe, J. R.; Atanassov, P.; Dekel, D. R.; Herring, A. M.; Hickner, M. A.; Kohl, P. A.; Kucernak, A. R.; Mustain, W. E.; Nijmeijer, K.; Scott, K.; Xu, T.; Zhuang, L. Anion-exchange membranes in electrochemical energy systems. *Energy Environ. Sci.* **2014**, *7*, 3135–3191.

[3] Özcan, A.; Perego, C.; Salvalaglio, M.; Parrinello, M.; Yazaydin, A. O. Concentration gradient driven molecular dynamics: a new method for simulations of membrane permeation and separation. *Chem. Sci.* **2017**, *8*, 3858–3865.

15:30–17:00 |
WED, 8 July |
Poster Session I

Molecular-scale mechanisms of momentum transport in liquids

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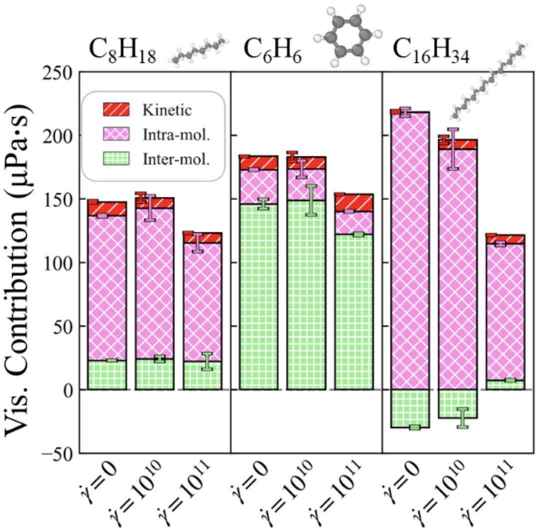

Figure 1: Viscosities of several organic molecules decomposed into Coarse-grained contributions into kinetic, intra-molecular, and inter-molecular interaction. Here, $\dot{\gamma}$ denotes the applied shear rate. For each molecule, the leftmost bar represents the EMD result, while the middle and right bars present the NEMD results at $\dot{\gamma} = 10^{10}\text{s}^{-1}$ and 10^{11}s^{-1}, respectively. Error bars indicate one standard deviation.

Small-molecule liquids can exhibit non-Newtonian behavior, such as shear thinning at high shear rates, yet the microscopic origin of this nonlinear viscosity response remains poorly understood compared with monatomic fluids or entangled polymer melts. In particular, it is still unclear how molecular structure governs the reorganization of momentum transport pathways under shear. Molecular dynamics (MD) simulations provide a powerful framework to address this issue, as they enable direct access to microscopic stress, molecular configurations, and momentum transport under controlled shear conditions. This study aims to elucidate the molecular-scale mechanisms underlying shear-dependent viscosity in liquids of intermediate molecular complexity.

Equilibrium and non-equilibrium molecular dynamics (EMD and NEMD) simulations were performed for a series of liquids with varying molecular rigidity and chain length: H_2O, C_6H_6, and linear alkanes ($C_4H_{10}, C_8H_{18}, C_{16}H_{34}$). Shear viscosity was evaluated under both zero-shear and steady-shear conditions, and the stress tensor was decomposed into kinetic, intra-molecular, and inter-molecular contributions. Shear-induced structural anisotropy and its effect on momentum transport were further characterized using two-dimensional radial distribution functions and spatially resolved stress maps in the flow–gradient plane.

The molecular-level mechanisms governing viscosity and its nonlinear response to shear were elucidated. Figure 1. shows the decomposition of viscosity into kinetic, intra-molecular, and inter-molecular contributions. The response of each contribution to shear differed depending on molecular geometry. C_8H_{18} exhibited polymer-like behavior, in which the intra-molecular contribution decreased with increasing shear rate. C6H6 showed monatomic-like behavior, characterized by a reduction in the inter-molecular contribution. $C_{16}H_{34}$, however, displayed a unique response: although the intramolecular contribution decreased in a polymer-like manner, the inter-molecular contribution increased anomalously under shear. Two-dimensional structural and stress analyses revealed that this anomalous behavior originates from shear-induced molecular anisotropy, which reorganizes momentum transport pathways by suppressing intra-molecular stress transfer while enhancing inter-molecular interactions.

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THU, 9 July |
Poster Session II

Parameter optimisation of many-body dissipative particle dynamics simulations via machine learning

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Many-body dissipative particle dynamics (MDPD) has emerged as the primary mesoscopic model for capillarity, wetting, and vapor–liquid coexistence because its density-dependent conservative term closes the van der Waals loop that standard pairwise DPD cannot. Despite extensive applications, choosing MDPD parameters that yield target thermophysical properties for real liquids remains non-trivial. The scope of machine learning to model MDPD parameters is still left open as analytical expressions do not enforce thermodynamic and hydrodynamic consistency simultaneously. In this work, we perform a thorough investigation to select the ideal machine learning-based regression model connecting the thermophysical properties such as surface tension, pressure, bonded interactions and Schmidt numbers of the liquids to the MDPD model parameters. The relationship between the different parameters and the target properties established by the regression models are explained using SHAP values. The chosen models are subsequently used to optimise the parameters via evolutionary algorithms to provide an automated pathway to perform MDPD simulations. The quality of the models is verified by comparing the target properties of four dielectric thermal fluids formulated by mixing polyisobutylene (PIB) polymer in polyalphaolefin oil (PAO).

Keywords: many-body DPD; machine learning; parameter optimisation

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Poster Session II

Predicting the phase diagram of deep eutectic solvents with machine learning interatomic potentials

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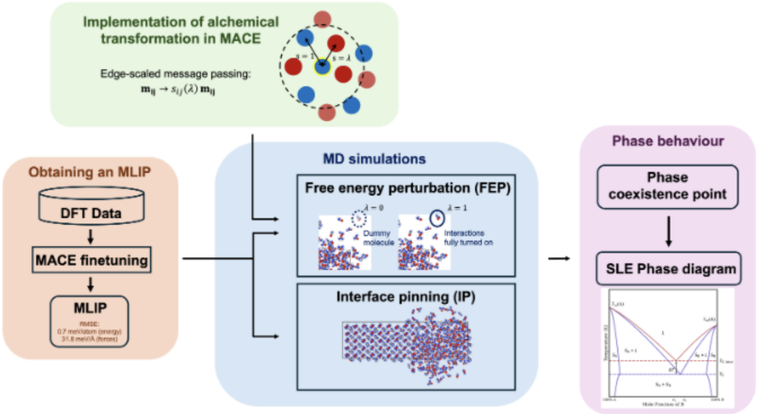

Figure 1. Schematic representation of the computational framework combining MACE with phase coexistence methods

Text Box 1, TextboxDeep eutectic solvents (DES) are ‘designer solvents’ characterised by melting points significantly lower than the predicted ideal eutectic point. Despite two decades of research driven by their low toxicity and ease of preparation, the solid-liquid equilibrium (SLE) and phase diagram of the most studied DES, reline (1:2 choline chloride-urea), remain poorly defined. The most widely utilised and robust classical model for this system [1] is parameterised only for the reline composition. This specific parameterisation makes it non-transferable across the full composition range, where it tends to overestimate densities and incorrectly predict high pressure crystal phases that do not align with experimental observations. While ab initio molecular dynamics (AIMD) provides a reliable alternative, its extreme computational cost makes the determination of phase behaviour prohibitive. This work establishes a framework for computing the phase diagram of reline using machine learning interatomic potentials (MLIPs) that achieve near-DFT accuracy at a substantially reduced computational cost. We developed a fine-tuned potential within the MACE framework [2] using DFT reference data spanning four liquid-state compositions. The resulting model achieves an energy RMSE of 0.7 meV/atom and a force RMSE of 31.8 meV/Å for the liquid test set at untrained compositions. Remarkably, despite being trained exclusively on liquid configurations, the model generalises across the full composition range and accurately describes crystal phases, with energy and force RMSEs of 1.3 meV/atom and 13.1 meV/Å, respectively. Predicted densities align closely with experiments and DFT for both reline and constituent urea and choline chloride crystal polymorphs. Furthermore, the MLIP demonstrates improved stability for urea polymorphs, correctly identifying crystal structures that the classical force field fails to capture. Phase coexistence occurs at the temperature at which the chemical potentials of the solid and liquid phase are equal, which can be located using interface pinning (IP) or free energy perturbation (FEP). In this work, we introduce an alchemical capability in MACE that allows FEP calculations via scaling the edges of the message passing neural network, which leads to continuous scaling of solute-environment interactions. This provides a robust and transferable route to finding the phase behaviour of choline chloride-urea mixture and other multicomponent DES systems.

References

[1] Perkins, S. L.; Painter, P.; Colina, C. M. Molecular Dynamic Simulations and Vibrational Analysis of an Ionic Liquid Analogue. *J. Phys. Chem. B* **2013**, *117*, 10250–10260.

[2] Batatia, I.; Kovács, D. P.; Simm, G. N. C.; Ortner, C.; Csányi, G. MACE: Higher Order Equivariant Message Passing Neural Networks for Fast and Accurate Force Fields. *Adv. Neural Inf. Process. Syst.* **2022**, *35*.

13:00–14:30 |
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Poster Session II

Disorder-induced memory in liquid-solid friction

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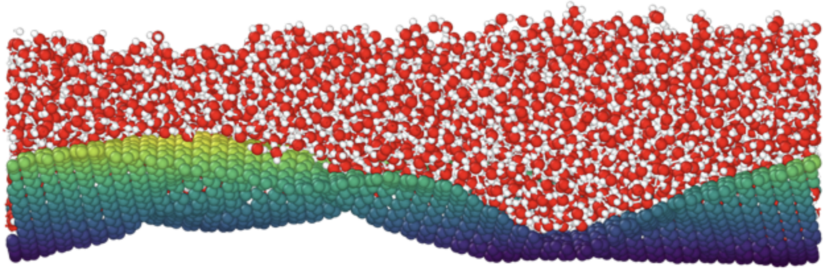

Figure 1: Water on a defective fluctuating graphene sheet. Carbon colors indicate the relative height field of graphene.

Transport in nanofluidic systems is governed by liquid–solid interactions, with interfacial friction playing a central role. While most studies focus on ideal crystalline surfaces, defects can be utilized to engineer tailored dynamical and phononic properties, opening new routes to control interfacial dynamics. As a matter of fact, recent work showed that defects induce a phase transition from dynamic to static rippling in freestanding graphene [1]. In this work, we investigate the interfacial properties of water on a defective fluctuating graphene sheet using equilibrium molecular dynamics simulations. By computing friction coefficients via Green–Kubo relations under controlled momentum constraints, we reveal that defects not only enhance friction but also fundamentally alter its temporal response. Specifically, the latter exhibits a non-monotonic relaxation characterized by an elastic recoil. We show that this effect originates from the interplay between the almost frozen structure of graphene and defect-induced dynamical heterogeneity. Water molecules preferentially populate highly curved active regions which in turn store and release mechanical stress over time. As a result, the force exerted on the liquid displays memory effects, with defective graphene behaving analogously to a "memory foam". We now aim to benchmark such effects using NEMD simulations.

Keywords: interfacial water; graphene; defects; liquid-solid friction; Green-Kubo formula; memory

References

[1] Thiemann, F. L.; Scalliet, C.; Müller, E. A.; Michaelides, A. Defects induce phase transition from dynamic to static rippling in graphene. *Proc. Natl. Acad. Sci. U.S.A.* **2025**, *122*, e2416932122.

13:00–14:30 |
THU, 9 July |
Poster Session II

A Non-Equilibrium Approach to Molecular Modelling of Gas Transport in a Mixed Matrix Membrane

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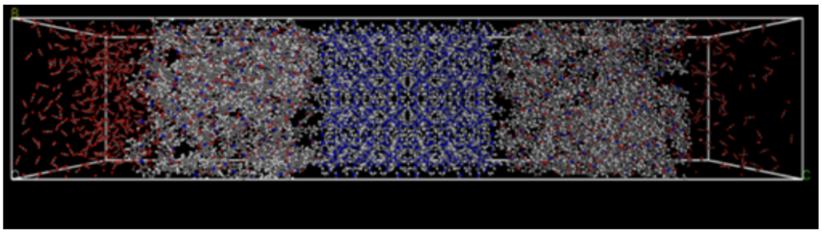

Figure 1: An MMM molecular model, consisting of a ZIF-8 surface slab in between two slabs of Matrimid® polymer, in contact with CO2 gas phases at different concentration on each side

Mixed matrix membranes (MMMs) are composite materials made of a polymeric matrix with porous nanoparticles dispersed within. The possibility to achieve better separation performance is a key feature that make these materials interesting to replace existing commercial dense polymeric membranes. However, the identification of which matrix/filler combination can relevantly improve the separation performance of MMMs for different gas separations is challenging. This is because of the uncertainty related to the prediction of their properties and the lack of theoretical frameworks able to accurately describe the non-idealities that originate at the polymer/filler interface.

In this work, molecular dynamics simulations have been performed to study a MMM made of Matrimid® and ZIF-8 metal organic framework (MOF). A system consisting of a slab of ZIF-8 in between two polymer layers has been built in order to study the transport of gas molecules. All simulations were performed with LAMMPS software and considering a Concentration Gradient Driven Molecular Dynamics approach. This consists in putting the composite system in contact with a gas phase at a given concentration at one side and another gas phase at a lower concentration on the other side as shown in Figure 1. The concentration gradient across the membrane provides the driving force for the transport of the gas molecules during an MD simulation as described by Ozcan A. et al. [1], which mimic a constant pressure permeation test.

The experimental dry polymer density and pure gas sorption and adsorption isotherms in the polymer and filler were obtained from MD and Gran Canonical Monte Carlo simulations. These guided the force field selection and validation of the simulation protocol. Single-phase systems were compared with the composite one in terms of equilibrium and transport properties, density profiles and local dynamics, allowing us to highlight interfacial effects on the polymer packing, chains dynamics, gas transport and gas-polymer-filler interactions.

Keywords: Mixed Matrix Membranes; Concentration Gradient Driven Molecular Dynamics; Gas transport, Gas solubility.

References

[1] Özcan, A.; Perego, C.; Salvalaglio, M.; Parrinello, M.; Yazaydin, A. O. Concentration gradient driven molecular dynamics: a new method for simulations of membrane permeation and separation. *Chem. Sci.* **2017**, *8*, 3858–3865.

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Poster Session II

Application of the phantom-wall method to obtain work of adhesion for diverse interfaces

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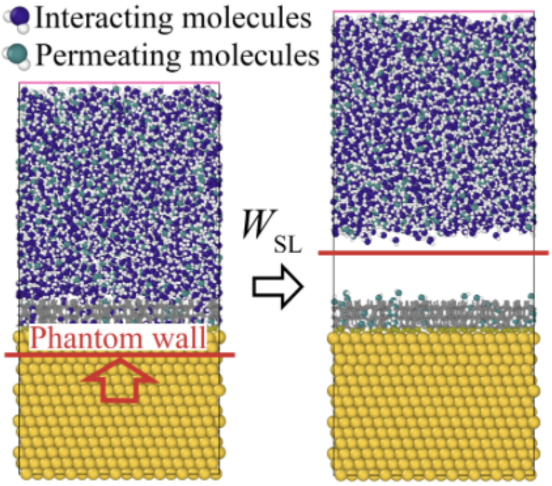

Figure 1: Schematic of the partially permeable phantom-wall method in the Au-SAM-Water system.

Wettability at solid-liquid interfaces can be quantified by the work of adhesion, which is directly obtained from the interfacial free-energy change calculated using thermodynamic integration. The phantom-wall (PW) method is one implementation of thermodynamic integration in molecular dynamics simulations and has been applied to various systems[1-3]. In this method, a phantom wall interacting only with liquid molecules separates the liquid phase from the solid surface. When the PW moves from z_0 to z_1 in a system with pressure p, volume V, and cross-sectional area A, the solid-liquid work of adhesion W_{SL} is evaluated by integrating the pressure exerted on the wall, $p_{\mathrm{w}}(z)$, as

$$W_{\mathrm{SL}} = \int_{z_0}^{z_1} p_{\mathrm{w}}(z)\,dz - \frac{p\Delta V}{A} \tag{1}$$

However, because all liquid molecules are separated by the wall, the effects of vapor pressure and adsorption layers are neglected. In addition, the method is difficult to apply to structurally complex surfaces where liquid molecules penetrate surface structures.

To address these limitations, we introduce a partially permeable PW that interacts with only a fraction of the liquid molecules (Fig. 1). The method was applied to Pt-Ar[4] and Au-SAM-water[3] systems. In the Pt-Ar system, simulations were conducted under both weak and strong solid–liquid interactions. For weak interactions, vapor formation between the PW and the solid surface was observed during the separation, and the vapor density was proportional to the permeability of the PW. For strong interactions, highly permeable walls prevented reversible separation, producing an "unmixing" effect in which only permeating molecules remained below the PW while maintaining a liquid state. This occurs because the loss of entropy of mixing associated with separating interacting and permeating molecules is smaller than the free-energy change required to detach the liquid from the surface. Therefore, the change in entropy of mixing was evaluated to estimate the wall permeability that enables a reversible process. Using a PW with 20% permeability, the work of adhesion was successfully calculated while preserving the adsorption layer on the solid surface.

In the Au-SAM-water system, a self-assembled monolayer (SAM) composed of tripodal triptycene molecules was physically adsorbed on an Au substrate, and some water molecules had permeated into the SAM structure. The suitable PW permeability was similarly estimated from the entropy of mixing, and a 20% permeable PW enabled reversible separation while maintaining the interfacial structure in which water molecules remained in the SAM layer, as shown in the right figure of Fig.1. These results demonstrate that the partially permeable PW extends the applicability of the PW method to diverse interfaces and enables the calculation of the work of adhesion under more realistic interfacial conditions.

References

[1] Leroy, F.; dos Santos, D. J. V. A.; Müller-Plathe, F. Interfacial Excess Free Energies of Solid–Liquid Interfaces by Molecular Dynamics Simulation and Thermodynamic Integration. *Macromol. Rapid Commun.* **2009**, *30*, 864–870.

[2] Saito, T.; Shoji, E.; Kubo, M.; Tsukada, T.; Kikugawa, G.; Surblys, D. Evaluation of the work of adhesion at the interface between a surface-modified metal oxide and an organic solvent using molecular dynamics simulations. *J. Chem. Phys.* **2021**, *154*, 114703.

[3] Imaizumi, T.; Takehara, R.; Surblys, D.; Yamashita, Y.; Yagi, T.; Sanjayan, S.; Shoji, Y.; Ohara, T.; Fukushima, T. Chain and End Group Effects of Self-Assembled Monolayers of Tripodal Molecules on Solid–Liquid Interfacial Thermal Resistance. *Langmuir* **2025**, *41*, 18200–18212.

[4] Yamaguchi, Y.; Kusudo, H.; Surblys, D.; Omori, T.; Kikugawa, G. Interpretation of Young's equation for a liquid droplet on a flat and smooth solid surface: Mechanical and thermodynamic routes with a simple Lennard-Jones liquid. *J. Chem. Phys.* **2019**, *150*, 044701.

Thermal Fluctuations and Elastocapillarity in Nanoscale Rayleigh-Plateau Breakup

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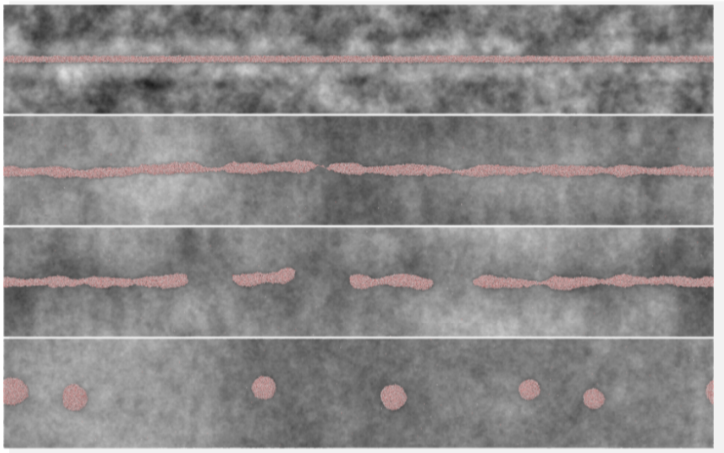

Figure 1: Example of an MD simulation trajectory of SPC/E water on suspended pristine graphene, depicted through four snapshots at different timesteps

A liquid jet, such as a stream of water, will disintegrate and form droplets if the length-to-radius ratio exceeds a critical value. This phenomenon, known as the Rayleigh-Plateau (R-P) instability, occurs due to propagating surface instabilities. Whilst well-understood classically, thermal fluctuations at the nanoscale influence the mechanism and may cause the breakup dynamics to enter a stochastic regime [1]. Furthermore, if a liquid nanoscale cylinder is placed on a highly compliant surface, wetting induced deformations of the underlying material [2] and additional noise from thermally excited flexural phonons [3] will affect the breakup process. We use large-scale molecular dynamics (MD) simulations to examine the dynamics of the R-P instability in the presence of elastocapillary effects at ambient temperatures. Specifically, we study the interactions between SPC/E water and suspended pristine graphene, and investigate the impact of deformations by applying controlled tension, which alters the graphene flexibility. We focus on characterising the breakup profile and instability wavelength, isolating the effects of graphene through a comparison of these results to simulations of water alone.

Keywords: Rayleigh-Plateau instability; graphene; elastocapillarity

References

[1] Eggers, J. Dynamics of Liquid Nanojets. *Phys. Rev. Lett.* **2002**, *89*, 084502.

[2] Kateb, M.; Isacsson, A. Nanoscale Elasto-Capillarity in the Graphene–Water System under Tension: Revisiting the Assumption of a Constant Wetting Angle. *Langmuir* **2023**, *39*, 12610–12617.

[3] Ma, M.; Tocci, G.; Michaelides, A.; Aeppli, G. Fast diffusion of water nanodroplets on graphene. *Nat. Mater.* **2016**, *15*, 66–71.

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THU, 9 July |
Poster Session II

Structure and Dynamics of Interfacial Water Govern Thermal Conductance at Graphene-Water Interfaces

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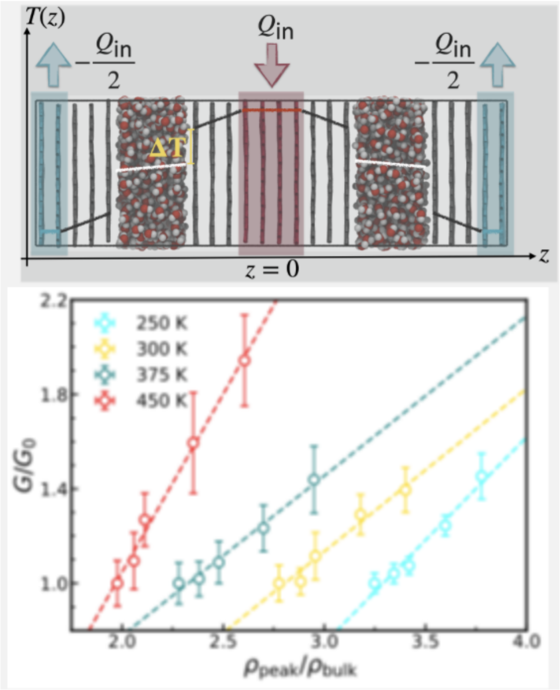

Figure 1: (a) NEMD setup for computing the ITC of a graphene–water interface. Water (O: white, H: red) is confined between parallel graphene sheets (C: black) in a symmetric cell. Heat is injected at the center (rate Q_{in}) and extracted equally at the boundaries, establishing a steady 1D heat flux $q = Q_{in}/2$. The ITC is computed as $G = J/\Delta T$, where $J = q/A$. Here, ΔT is the temperature discontinuity across the graphene-water interface. (b) ITC vs reduced density at different temperatures. G_0 is the conductance at 1 bar for a given temperature.

Interfacial thermal conductance (ITC) at graphene-water interfaces is governed by nanoscale structure and dynamics, yet its microscopic origin remains unclear. Using NEMD, we study ITC over a wide range of temperatures (250-450 K) and pressures (1-5000 bar). For graphene-water interfaces, Alexeev et al. showed that ITC scales with the first peak density, the density of the first hydration layer adjacent to graphene, through the reduced density(ρ_{peak}/ρ_{bulk}), which reflects the number of interfacial heat carriers. This scaling holds when temperature is fixed. However, increasing temperature at a fixed pressure reduces the first peak density, which would suggest lower conductance; instead, we observe an increase in ITC.

We show that the first peak density serves as a proxy for interfacial bonding strength (elastic coupling) between graphene and water. Increasing temperature weakens this coupling while enhancing molecular escape from the first hydration layer, leading to higher perpendicular diffusivity. This increased mobility promotes non-elastic heat transfer through enhanced kinetic energy exchange between first hydration layer and bulk liquid, which enhances conductance.

Taken together, these observations suggest that both interfacial structure and molecular mobility play a coupled role in governing ITC. We explore whether incorporating a transport metric, based on the normalized perpendicular diffusivity, alongside the structural descriptor can reconcile the observed temperature dependence. Initial results are promising, indicating that such a joint metric may help collapse the conductance data. Ongoing work aims to assess the robustness of this approach across a broader range of interfaces.

References

[1] Alexeev, D.; Chen, J.; Walther, J. H.; Giapis, K. P.; Angelikopoulos, P.; Koumoutsakos, P. Kapitza Resistance between Few-Layer Graphene and Water: Liquid Layering Effects. *Nano Lett.* **2015**, *15*, 5744–5749.

13:00–14:30 |
THU, 9 July |
Poster Session II

Interfacial Oscillations in Binary Droplets Induced by Long-Range Vapour-Mediated Interactions

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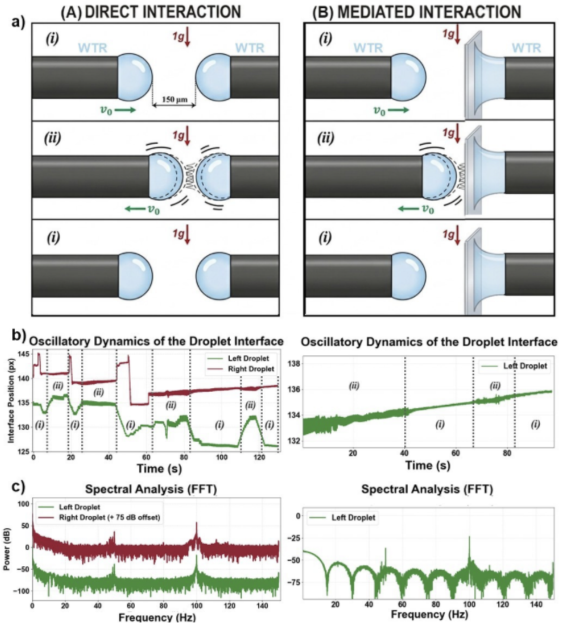

Figure 1: a) Sketch of experimental setup (author's drawing, digitized using AI); b) Subpixel analysis of the droplet interface; c) Interface oscillation frequency analysis.

The vapour-mediated long-range interaction between closely spaced droplets is defined by attractive and repulsive forces. These forces are induced by temperature and surface tension gradients of gas phase separating the liquid interfaces[1,2]. Mass transfer and natural convection facilitate this interaction and contribute to the onset of interfacial instabilities[3]. This study investigates long-range interactions between two hanging droplets and the oscillations induced by their approach and retraction. Two experimental configurations were used to observe both direct and plate-mediated droplet coupling [Figure 1. a)]. Results show that when droplets reach a critical volume ($V \sim 3.8\ \mu L$), correlated with their resonance frequency [Figure 1. c)], they begin to oscillate, with oscillation amplitude increasing as the inter-droplet distance decreases [Figure 1. b)]. Droplets with volumes far from the critical value do not oscillate, while those near it begin to oscillate. A glass plate inserted between the droplets confirms that the interaction is mediated by vapour temperature gradients that drive local surface tension modifications, providing a new perspective on non-contact droplet coupling and contributing to a better understanding of the long-range interaction mechanism.

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Keywords: long-range interactions; interfacial oscillations; vapour-mediated coupling; droplet dynamics

References

[1] Man, X.; Doi, M. Vapor-induced motion of liquid droplets on an inert substrate. *Phys. Rev. Lett.* **2017**, *119*, 044502.

[2] Wen, Y.; Chen, H.; Li, X.; Fang, H. Vapor-induced motion of two pure liquid droplets. *Soft Matter* **2019**, *15*, 2135–2139.

[3] Okhotsimskii, A.; Hozawa, M. Schlieren visualization of natural convection in binary gas–liquid systems. *Chem. Eng. Sci.* **1998**, *53*, 2547–2573.

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