

NEMD 2026

5th Non-Equilibrium Molecular Dynamics Conference, University of Edinburgh (8–10 July)

WEDNESDAY 8 JULY

09:00–09:45 *Registration & coffee*

09:45–10:00 *Opening remarks*

Session I: NEMD Foundations, Theory & Methods

Chair: Edward Smith

10:00–10:40 **KEYNOTE**

Challenging local equilibrium

Bjørn Hafskjold · Norwegian University of Science and Technology, Norway

- 10:40–11:00 Revisiting the Green–Kubo relation for friction in nanofluidics
Anna T. Bui (University of Cambridge, UK), S. J. Cox
- 11:00–11:20 Steady-state solutions for nonequilibrium Langevin dynamics
Matthew Dobson (University of Massachusetts Amherst, USA)
- 11:20–11:40 Leveraging machine learning to optimise viscosity prediction in NEMD
Lingfeng Gui (Heriot-Watt University, UK), E. Medani, P. T. Cummings, C. McCabe
- 11:40–12:00 The Molecular Simulation Design Framework (MoSDeF): capabilities and applications
C. Jones, N. C. Craven, C. McCabe, **Peter T. Cummings** (Heriot-Watt University, UK)

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. Davis, B. D. Todd
- 14:00–14:20 Time-dependent heat-flux analysis during liquid–vapour interfacial adhesion
Hiroki Kusudo (Tohoku University, Japan), Y. Yamaguchi
- 14:20–14:40 Heat flux for any machine-learning potential: a universal wrapper built on metatomic
Qianjun Xu (EPFL, Switzerland), G. Fraux, M. Langer

14:40–15:10 *Coffee*

15:10–16:40 Poster Session I

7 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 Weiland (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 CO₂ 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 AND BEYOND *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

08:50–09:10 *Welcome refreshments*

Session IV: Phase Change, Wetting & Droplets

Chair: Saikat Datta

09:10–09:50 **KEYNOTE**

Velocity distribution of water molecules evaporating from a liquid–vapour interface

Ikuya Kinefuchi · University of Tokyo, Japan

- 09:50–10:10 Benchmarking of water models and coarse-graining strategies for high-temperature simulations
P. Syroglou, **Konstantinos Ritos** (University of Thessaly, Greece)
- 10:10–10:30 Molecular-dynamics investigation of kinetic energy in a collapsing cavitation bubble induced by shockwave
K. Moriyama, **Shin-ichi Tsuda** (Kyushu University, Japan), S. Watanabe
- 10:30–10:50 Local interfacial thermal conductance and heat-flow anisotropy from NEMD
Fernando Bresme (Imperial College London, UK), J. D. Olarte-Plata, M. Jiang, A. Chapman
- 10:50–11:10 Smooth-particle-hydrodynamics simulation of spinodal decomposition in a Lennard-Jones fluid
Karl P. Travis (University of Sheffield, UK), P. J. Daivis

11:10–11:40 *Coffee*

Session V: Rheology & Complex Fluids

Chair: Santiago Romero-Vargas Castrillón

11:40–12:20 **KEYNOTE**

Interfacial structural and transport properties of fluids at molecular resolution

Marcello Sega · University College London, UK

- 12:20–12:40 TTCF-based analysis of shear-induced microstructure in an aqueous surfactant solution
H. Tanaka, **Takeshi Omori** (Osaka Metropolitan University, Japan)
- 12:40–13:00 Turbulence of dilute solutions of supramolecular polymers
F. Serafini, F. Battista, P. Gualtieri, J.-P. Ryckaert, **Carlo Casciola** (Sapienza University of Rome, Italy)
- 13:00–13:20 Molecular simulation of large-amplitude oscillatory extensional flow
Bharath Ravikumar (City St George's, University of London, UK), I. K. Karathanassis, M. Gavaises

13:20–13:35 *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
- **Rong Wei** (University of Edinburgh, UK), P. Partridge, C. C. Hong, J. J. B. Levinsky, J. M. Pringle, C. L. Hobday – The structural dynamics and barocaloric response of organic ionic plastic crystals
- **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 Almulafekeh** (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 Cavaliere** (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
- **Zhibo Deng** (Imperial College London, UK), J. M. Seddon, F. Bresme – Thermal gradients drive cholesterol partitioning and heat transport in lipid bilayers
- **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