

NEMD 2026

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

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 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 *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 Almulafeh** (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. Isacson – 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