TU Delft
Delft University of Technology


PoreLab
NTNU-UiO Porous Media Laboratory

NTNU
Norwegian University of Science and Technology

April 8th 2022

Computational Methods in Nanothermodynamics

Case studies of porous media, small systems and ionic liquids

08.15: Meet at Onsager meeting room at Gløshaugen (D3-114)

08.25: Welcome by Signe Kjelstrup

Session 1 (Group 1): Thermodynamics of Small Systems

Chair: Øivind Wilhelmsen

Moderator: Sondre Kvalvåg Schnell + Othon Moultos

08.30: Eivind Bering – Entropy Production Beyond the Thermodynamic Limit: Single-Molecule Stretching Simulations

08.45: Shrinjay Sharma – Modelling of Shape Selective Catalysis for Hydroisomerisation Reaction

09.00: Arpenik Kroyan – Molecular Dynamics simulations for RNA: benchmark and folding-stretching experiments

09.15: Mike Pols – Reactive Molecular Dynamics Simulations of Metal Halide Perovskites: Recent Advances in Force Field Parameterization and Applications

09.30-09.45: Coffee break

Session 2 (Group 2): Ionic Liquids

Chair: Thijs Vlugt

Moderator: Anders Lervik + Signe Kjelstrup

09.45: Sebastian Nordby Price – An investigation on the effect of an oscillating Berendsen barostat on the diffusion of particles

10.00: Dominika Wasik – Solubility of CO2 in aqueous formic acid solutions and the effect of adding NaCl studied by molecular simulations

10.15: Øystein Gullbrekken – Charge transport properties in PEO-LiTFSI polymer electrolytes studied by MD

10.30: Parsa Habibi – 2D Boron-Based Materials for Hydrogen Storage: An Ab-Initio Study

10.45-11.00: Coffee break

Session 3 (Group 3): Porous Media

Chair: Dick Bedeaux

Moderator: Sofia Calero

11.00: Vilde Bråten – Equation of Stare for Confined Fluids

11.15: Mert Polat – A major update to Brick-CFCMC: Thermodynamic Integration and Hybrid MD/MC Trial Moves

11.30: Esteban Acuna Yeomans – Characterization of ZIF-8 flexible force fields according to their mechanical and structural properties

11.45: Michael Rauter – Fluid Transport Through Nanoporous Media in the Presence of Phase Transitions

12.00: Bin Fang – The dynamic behavior of gas hydrate dissociation by heating in a confined nanopore: A molecular dynamics simulation study

12.15-13.15: Lunch

Discussions in groups

13.15: We split into three (or six) groups according to sessions and discuss the topics of each session. Rooms: D3-114, E3-108, E2-125B, D3-143 and Porelab-office across the hall.

14.45: We meet back in Onsager (D3-114) and the groups present conclusions from their discussions.

16.00: End

19.00: Dinner at Troll restaurant (Fosenkaia 4A, 7010 Trondheim, Norge)