

## Non-equilibrium molecular dynamics school: Tuesday, July, 12th

*Speaker setup: 9:00 - 9:25 AM*

09:25 - 09:30				Welcome
09:30 - 10:15	Peter	Daivis	RMIT University	Non-equilibrium thermodynamics - basics
10:15 - 11:00	Peter	Daivis	RMIT University	Non-equilibrium thermodynamics - extensions

*Morning Tea: 11:00 - 11:30 AM*

11:30 - 12:15	Billy	Todd	Swinburne University	Homogeneous atomistic systems
12:15 - 13:00	Billy	Todd	Swinburne University	Inhomogeneous systems

*Lunch: 13:00 - 14:00*

14:00 - 15:30				Software setup & Tutorial 1
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*Afternoon Tea: 15:30 - 16:00*

16:00 -17:00				Tutorial 2
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## Advanced scattering and microscopy school: Wednesday, July, 13th

*Speaker setup: 9:00 - 9:25 AM*

Session 1				
09:25 - 09:30				Welcome
09:30 - 10:15	David	Paganin	Monash University	Ghost-imaging using x rays and neutrons
10:15 - 11:00	Alison	Funston	Monash University	Scanning near-field optical microscopy (title TBC)

*Morning Tea: 11:00 - 11:30 AM*

*Speaker setup*

Session 2				
11:30 - 12:15	Susie	Seibt	Australian Synchrotron, ANSTO	Anything goes: SAXS/WAXS at the Australian Synchrotron
12:15 - 13:00	Andrew	Clulow	Australian Synchrotron, ANSTO	Small Angle Scattering from Solutions

*Lunch: 13:00 - 14:00*

*Speaker setup*

Session 3				
14:00 - 14:45	Andrew	Martin	RMIT	Introduction to fluctuation scattering: a new way to probe disordered 3D structure at advanced x-ray light sources.
14:45 - 15:30	Rico/Leonie	Tabor/V'ant Hag	Monash University	SANS and USANS

*Afternoon Tea: 15:30 - 16:00*

*Speaker setup*

Session 4				
16:00 -16:45	Timothy	Petersen	Monash University	Hybrid reverse Monte Carlo modelling
16:45 - 17:00				Wrap-up remarks/closing

**Meeting Day 1: Thursday, July, 14th***Speaker setup: 8:30 - 9:00 AM***Session 1: Colloids**

09:00 - 09:10

Welcome

09:10 - 09:40

Asaph

Widmer-Cooper

University of Sydney

The Thermodynamic Origins of Chiral Twist in Monolayer Assemblies of Rod-like Colloids

09:40 - 10:10

Amelia

Liu

Monash University

Local stability and local structure of colloidal glasses

10:10 - 10:40

Gerd

Schroeder-Turk

Murdoch University

TBA

*Morning Tea: 10:40 - 11:10 AM**Speaker setup***Session 2: Scattering**

11:10 - 11:40

David

Paganin

Monash University

Fokker-Planck equation for optical beams

11:40 - 12:10

Jing

Fu

Monash University

Recent advances in nanoscale tomography of soft matters

12:10 - 12:40

Andrew

Martin

RMIT University

Introducing the Pair-Angle Distribution Function: measuring multi-atom statistics of disordered materials

*Lunch: 12:40 - 14:00**Speaker setup***Session 3 A: Simulations - Principles**

14:00 - 14:30

Ellie

Hajizadeh

University of Melbourne

ML-based optimisation for accelerated and targeted multiscale soft matter design

14:30 - 15:00

David

Huang

University of Adelaide

Systematic coarse-graining of molecular simulation models with anisotropic particles

15:00 - 15:30

Luca

Maffioli

Swinburne University of Technology

Measuring the response of highly confined fluids in a Couette flow: the TTCF formalism

*Afternoon Tea: 15:30 - 16:00**Speaker setup***Session 3 B: Simulations - Principles**

16:00 -16:30

Stephen

Sanderson

University of Queensland

Machine learning a Time-Local Fluctuation Theorem for non-equilibrium steady-states

16:30 - 17:00

Tim

Duignan

University of Queensland

Accurate first principles simulation of salt water using deep learning.

*Informal Dinner***Meeting Day 2: Friday, July, 15th***Speaker setup: 8:30 - 9:00 AM***Session 5: Active Matter**

09:00 - 09:30

Prabhakar

Ranganathan

Monash University

Cluster and conquer: invasion of a soft substrate by colonies of rod-shaped cells

09:30 - 10:00

Rahil

Valani

University of Adelaide

Generating active matter from strange attractors

10:00 - 10:30

Shibu

Saw

Roskilde University

Role of the configurational temperature in active-matter models

*Morning Tea: 10:30 - 11:00**Speaker setup***Session 6 A: Simulations - Applications**

11:00 - 11:30

Shern

Tee

University of Queensland

When Is A Supercapacitor Like A Protein?

11:30 - 12:00

Mikhail

Suyetin

Karlsruhe Institute of Technology

Proof of concept: Molecular Dynamics study of memory nanodevice based on Zn-MOF-74.

12:00 - 12:30

Dominic

Robe

Monash University

Linear viscoelasticity of associating star polymers

*Lunch: 12:30 - 14:00**Speaker setup***Session 6 B: Simulations - Applications**

14:00 - 14:20

Patrick

Adams

RMIT University

Using the pair-angle distribution function to analyse protein structure.

14:20 - 14:40

Isaac

Pincus

Monash University

Modelling dilute solutions of semiflexible polymers with excluded-volume and hydrodynamic interactions

14:40 - 15:00

Silpa

Mariya

Monash University

Are soft dendrimers dynamically equivalent to hard spheres?

15:00 - 15:20

Michael

Rinaudo

University of Sydney

Simulating nanoparticle superlattices with Molecular Dynamics

*Afternoon Tea: 15:20 - 15:40**Speaker setup***Session 6 C: Simulations - Applications**

15:40 -16:00

Sobin

Alosious

Swinburne University of Technology

The effect of electrostatic interactions on Kapitza resistance in nano-confined water.

16:00 - 16:20

Christian

Zuluaga-Bedoya

University of Queensland

Entry resistance in flexible zeolitic nanosheets

16:20 - 16:40

Kyle

Stevens

University of Newcastle

Lennard-Jones potential and continuum modelling for heterogeneous molecules

16:40 - 17:00

Marltan

Wilson

University of Adelaide

General high-dimensional neural networks for anisotropic coarse-grained molecular simulation models

17:00 - 17:20

Sleebea

Varghesi

Screenshot

Swinburne University of Technology

Improved methodology to compute the intrinsic friction coefficient at solid-liquid interfaces

17:20 - 17:30

Close