Program

The allocated time for a talk is 20 minutes, followed by 5 minutes for discussion. A signal will be given by the chair five minutes before the discussion should begin.

10.30-11.00: Registration
11.00-11.05: Thomas Schrøder (RUC): Welcome
11.05-11.30: Himanshu Khandelia (SDU): *Free energy calculations of ion transport and cholesterol flips*
11.30-11.55: Jens Walther (DTU): *Heat transfer of graphene - a molecular dynamics study*
11.55-12.20: Kristoffer Enøe Johansson (KU): *Molecular dynamics with tailor-made force fields for pharmaceutical materials science*

12.20:13.05: Lunch (45 minutes; upstairs)

13.05-13.30: Wouter Boomsma (KU): *Mixing Molecular Dynamics and Monte Carlo*
13.30-13.55: Lorenzo Costigliola (RUC): *Freezing and melting line invariants of the Lennard-Jones system*
13.55-14.20: Nicholas Bailey (RUC)*: Isomorphic scaling properties of zero-temperature plastic flows*

14.20-14.40: Coffee (20 minutes; upstairs)

14.40-15.05: Tine Frederiksen (DTU): *A Glucagon-like peptide 1 analogue and its interactions with the endogenous receptor*
15.05-15.30: Ilia Solov'yov (SDU): *Using MD to unravel problems in Quantum Biology*
15.30-15.55: Alberto Imparato (AU): *Energy transfer in molecular devices*
15.55-16.20: Claire Lemarchand (RUC): *From nanoaggregate to non-Newtonian behavior of Cooee bitumen: a non-equilibrium molecular dynamics study*

16.20-16.45: Coffee (25 minutes; upstairs)

16.45-17.10: Jakob Schiøtz (DTU): *The Atomic Simulation Environment for automated atomistic simulations*
17.10-17.35: Ole Juul Andersen (AU): *Reactive center loop insertion in alpha-1 antitrypsin captured by accelerated molecular dynamics simulation*
17.35-18.00: Erik Lindahl (SU/KTH): *Merging Molecular Dynamics Simulations & Electrophysiology to Unravel Allosteric Modulation in the Nervous System*

18.00-19.00: Poster session with beer (upstairs)

19:15- 21.00: Dinner (upstairs)