

Topical Meeting on Molecular Dynamics. IV.

Final Program: Tuesday, August 25, 2020.

Venue: Royal Danish Academy of Sciences, H. C. Andersens Boulevard 35, DK-1553 Copenhagen.

Format: 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.

COVID-19 information: As you probably know, Denmark has lately seen an increase in the number of COVID-19 cases. The restaurant in the evening is a cozy family restaurant, and we can therefore not ensure enough distance amongst all dinning participants. The organizers have therefore decided to **require** that all participants attending the dinner take a COVID-19 test before the meeting.

We moreover *encourage* all participants to wear a mask during the meeting, and will provide two masks for each participant as well as personal hand sanitizers.

- 10.30-11.00:** **Registration with coffee and croissants.**
 11.00-11.05: Welcome.
- 11.05-11.30: Alberto Imparato (AU). *The out-of-equilibrium Frenkel-Kontorova model.*
- 11.30-11.55: Simone Orioli (KU). *Digging out buried residues: a story of phosphorylation.*
- 11.55-12.20: Ida Friis (SDU). *Modeling the effect of ion-induced shock waves and DNA breakage with the reactive CHARMM force field.*
- 12.20-13.00:** **Lunch (40 mins, upstairs).**
- 13.00-13.25: Andreas Haahr Larsen (Oxford). *Binding of calcium-independent C2 domains to lipid membranes: a multi-scale molecular dynamics study.*
- 13.25-13.50: Ali Asghar Hakami Zanjani (SDU). *Annexin A4 Trimers Induce High Curvature on Plasma Membrane.*
- 13.50-14.15: Solvej Knudsen (RUC). *Hydrodynamics of the Lennard-Jones system in view of its hidden scale invariance.*
- 14.15-14.45:** **Coffee and cake/fruit (30 mins, upstairs).**
- 14.45-15.10: Sowmya Indrakumar (KU). *Combining NMR and molecular simulations to characterize the complex between the growth hormone receptor and Lyn kinase.*
- 15.10-15.35: Saeed Mehri (RUC). *Computer Simulation Confirms Single-Parameter Aging.*
- 15.35-16.00: Fabian Schuhmann (UOL). *User-friendly peptide modeler for biophysical applications.*
- 16.00-16.30:** **Coffee and cake/fruit (30 mins, upstairs).**

- 16.30-16.55: Kay Schaller (DTU). *Computing Cellulase Kinetics with a Multi-Domain Linear Interaction Energy Approach.*
- 16.55-17.20: Søren Toxvaerd (RUC). *Molecular Dynamics: Isaac Newton's discrete dynamics.*
- 17.20-18.50: Poster and beer session (90 mins, upstairs).
- 19:00-22.00: Dinner (Tivolihallen, 200 meters from the venue).**