

Topical Meeting on Molecular Dynamics. VI.

Tuesday, August 23, 2022.

Venue: Royal Danish Academy of Sciences and Letters, H. C. Andersens Boulevard 35,
Copenhagen.

Format: The allocated time for each presentation is 20 minutes, followed by 5 minutes for discussion. A signal will be given by the chair after 15 minutes indicating that five minutes are left.

- 10.30-11.00:** **Registration with coffee and croissants.**
11.00-11.05: Welcome.
- 11.05-11.30: Niels Grønbech-Jensen (UC Davis). *Molecular dynamics algorithms optimized for thermodynamic simulations.*
- 11.30-11.55: Atreyee Banerjee (Max Planck). *Identification of glass transition temperature for polymer melts using data-driven methods.*
- 11.55-12.20: Christian Kjeldbjerg Kristensen (RUC). *Dissipative particle dynamics simulations of ABC miktoarm star terpolymer thin film nanostructures with and without solvent vapor annealing.*
- 12.20-13.00:** **Lunch (40 mins, upstairs).**
- 13.00-13.25: Lorena Zuzic (AU). *Probing the substrate-to-protein proton transfer mechanism of the serotonin transporter.*
- 13.25-13.50: Luise Jacobsen (SDU). *The molecular basis of the antidepressant action of the magic mushroom extract, Psilocin, to the 5-HT_{2A} receptor.*
- 13.50-14.15: Konark Bisht (SDU). *Voltage sensing by dipolar transmembrane peptides.*
- 14.15-14.45:** **Coffee and cake/fruit (30 mins, upstairs).**
- 14.45-15.10 Fabian Schuhmann (UO). *The same, but different, but still the same: structural and dynamical differences of neutrophil elastase and cathepsin G.*
- 15.10-15.35: Christian Jørgensen (AU). *Building multilayer models of the human Stratum Corneum with molecular dynamics.*
- 15.35-16.00: Anders Frederiksen (UO). *Mutational influences on European cryptochrome 4a.*
- 16.00-16.30:** **Coffee and cake/fruit (30 mins, upstairs).**
- 16.30-16.55: Weria Pezeshkian (KU). *Molecular architecture and dynamics of SARS-CoV-2 envelope by integrative modeling.*
- 16.55-17.20: Johanna K. S. Tiemann (KU). *“MDverse”: Shedding a first light onto the dark matter of the MD.*
- 17.20-18.50:** **Poster and beer session (90 mins, upstairs).**
- 19:00-22.00:** **Dinner (Tivolihallen, Vester Voldgade 91, 200 meters from the venue).**

The meeting is organized by *Glass and Time* and supported by the VILLUM Foundation via the *Matter* project at IMFUFA, Department of Science and Environment, Roskilde University.