Topical Meeting on Molecular Dynamics. V.

Program: Wednesday, August 25, 2021.

Venue: Royal Danish Academy of Sciences and Letters, H. C. Andersens Boulevard 35, 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 after 15 mins.

COVID-19 information: A Corona-pas is required for all participants (e.g., vaccination, negative test).

10.30-11.00:	**Registration with coffee and croissants.**
11.00-11.05:	Welcome.
11.05-11.30:	Himanshu Khandelia (SDU). *Use of Molecular Dynamics in virtual teaching.*
11.30-11.55:	Tao Du (AAU). *Predicting fracture propensity in amorphous Alumina from its static structure using MD and machine learning.*
11.55-12.20:	Peter Knudsen (RUC). *Quantifying dynamical and structural invariance in a simple molten salt model.*
12.20-13.00:	**Lunch (40 mins, upstairs).**
13.00-13.25:	Luise Jacobsen (UOL). *Development of an improved and automated virtual drug screening procedure.*
13.25-13.50:	Frederik Thomasen (KU). *Interplay of folded domains and the disordered low-complexity domain in mediating hnRNPA1 phase separation.*
13.50-14.15:	Maja Hanić (UOL). *Computational reconstruction and analysis of structural model of avian Cryptochrome 4.*
14.15-14.45:	**Coffee and cake/fruit (30 mins, upstairs).**
14.45-15.10:	Konark Bisht (SDU). *Twitching motility in confined geometries.*
15.10-15.35:	Heloisa Bordallo (KU). *Dynamical accuracy of water models on supercooling.*
15.35-16.00:	Giulio Tesei (KU). *Modelling liquid-liquid phase behaviour of intrinsically-disordered proteins based on data-driven optimisation of conformational properties*
16.00-16.30:	**Coffee and cake/fruit (30 mins, upstairs).**
16.30-16.55:	VM Hridya (SDU). *Probing viscosity dependence of rate: Internal friction or lack of friction?*
16.55-17.20:	Dorthe Posselt (RUC). *Solvent vapor annealing of nanostructured block copolymer thin films – Experiments and DPD simulations.*
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).**