3rd Annual Danish Workshop on Advances in Molecular Simulation

9-10 Dec 2025, AIAS, Aarhus University

Day 1	
8:30-9:00	Registration, coffee, poster set-up
9:00-9:15	Introduction
	Chair: Weria Pezeshkian, KU
9:15-10:00	**Mohsen Sadeghi**, Zuse Institut, Berlin. *Computational biology at the mesoscale: From membrane mechanics to cellular dynamics*
10:00-10:20	**Beatrice Geiger**, NBI, KU. *Membrane necks' split personality: the nuclear envelope under osmotic pressure*
10:20-10:40	**Adria Bravo Vidal**, NBI, KU. *Multi-body fluctuation-induced forces between membrane proteins: insights from mesoscale simulations*
10:40-11:10	Coffee break
	Chair: Anna Duncan, AU
11:10-11:55	**Weria Pezeshkian**, NBI, KU *Multiscale simulation of biomembranes: Bridging the gap between simple models and complex reality*
11:55-12:15	**Amanda Dyrholm Stange**, AU. *Toward a design framework for chemically modified RNA: Integrating cryo-EM, functional assays, and molecular dynamics*
12:15-12:35	**Darian Yang**, KU. *Driving MD sampling with dynamic experimental data for active refinement of conformational ensembles*
12:35-13:15	Lunch
13:15-14:30	Poster session 1
14:30-15:00	Coffee
	Chair: Vincent Nieto, AU
15:00-15:45	**Matteo Degiacomi**, University of Edinburgh. *Learning (from) protein dynamics*
15:45- 16:05	**Lorena Zuzic**, AU. *CHARMM and Amber force fields produce different outcomes in MD simulations of multicomponent systems*
16:05-16:25	**Isabell Lindahl**, NBI, KU. *Who induces what? Exploring membrane curvature generation and sensing of mitochondrial membrane proteins using coarse-grained MD*
17:00	Walk to dinner
18:15	Conference dinner at *Den Gamle By*

Day 2	
8:30-9:00	Coffee, arrival
	Chair: Mikkel Dahl Andreasen, AU
9:00-9:20	**Lasse Messell Desdorf**, AU. *Binding mechanism of NBCn2*
9:20-9:40	**Luise Jacobsen**, SDU. *A novel model for proton transport mediated by Uncoupling Protein 1*
9:40-10:25	**Lucie Delemotte**, SciLifeLab, Stockholm. *Voltage-gated ion channel activation and gating: insights from a family-wide molecular dynamics investigation*
10:25 – 10:55	Coffee break
	Chair: Leonhard Starke, AU
10:55-11:40	**Ilpo Vattulainen**, University of Helsinki. *Cell membrane structures as barriers and operating environments for biological functions*
11:40-12:00	**King Ifashe**, University of Oxford. *Molecular dynamics reveal conformational restriction eliminates cross-reactivity in engineered therapeutic T-Cell receptors*
12:00-12:20	**Ali Asghar Hakami Zanjani**, SDU. *Quantifying membrane geometry in molecular dynamics simulations*
12:20-13:00	Lunch
13:00-14:00	Poster session 2
	Chair: Tommy Rosendahl, AU
14:00-14:20	**Daria Gusew**, KU. *Modeling chemical exchange dynamics in proteins using molecular dynamics simulations and NMR relaxation*
14:20-14:40	**Fabian Schuhmann**, NBI, KU. *TS2CG 2.0 — the membrane builder*
14:40-15:00	**Hassan Ghermezcheshme**, SDU. *Realistic modeling of PET nanoplastics for interactions with a model lipid membrane*
15:00-16:00	Coffee and concluding remarks