Mainz Materials Simulation Days (MMSD) 2021

"What Precision is Needed to Create Function: Roles of Defects and Disorder in Hierarchical Structure Formation of Soft Matter"

Program:

Day 1 – Mon June 7

12:30-13:00	Virtual Meetup
13:00-13:10	Welcome - Kurt Kremer

Session 1 (Chair: Robinson Cortes-Huerto)

13:10-14:05 (45+10)	Udo Seifert - From stochastic thermodynamics to the cost of precision
14:05-14:30 (20+5)	Martin Girard - Phase behavior and regulation in cell membranes
14:30-15:00	Coffee break

Session 2 (Chair: Kostas Daoulas)

15:00-15:45 (35+10)	Helen Gleeson - Understanding experiments in liquid crystals
15:45-16:30 (35+10)	Patrick Charbonneau - Characterizing the Disordered Microphases of SALR Models
16:30-17:00	Coffee break
17:00-17:45 (35+10)	Alberta Ferrarini - Defects and elasticity in liquid crystalline systems
17:45-19:45	Poster Session (odds present) + Post-day Discussions

Day 2 – Tue June 8

12:30-13:00 Virtual Meetup

Session 3 (Chair: Omar Valsson)

13:00-13:45 (35+10) Giovanni Pavan - Machine Learning of Defects in Soft Dynamic Assemblies

13:45-14:30 (35+10) Marcus Müller - Kinetics of structure formation in copolymer systems

14:30-15:00 Coffee break

Session 4 (Chair: Peter Virnau)

15:00-15:55 (45+10) Alexander Grosberg - Is the concept of "function" acceptable in statistical mechanics?

15:55-16:20 (20+5) Yani Zhao - Regulation of the phase behavior of intrinsically disordered peptides

16:20-16:50 Coffee break

5) Session 5 (Chair: Giovanni Settani)

16:50-17:35 (35+10) Birgit Strodel - Energy landscapes of conformational switching in intrinsically disordered proteins and protein aggregation

17:35-18:20 (35+10) Peter Tieleman - Molecular dynamics simulations of nanoparticles: structural aspects of lipid nanoparticles for drug delivery and interactions with biological membranes

18:20-20:20 Poster Session (evens present) + Post-day Discussions

Day 3 – Wed June 9

12:30-13:00 Virtual Meetup

Session 6 (Chair: Joseph Rudzinski)

13:00-13:55 (45+10) Bert Meijer - How subtle changes can make a difference: supramolecular chemistry emerges to new levels of fine-tuning

13:55-14:20 (20+5) Giorgia Brancolini - Role of Ionic Strength in the formation of Supramolecular Complexes between Nanoparticles and Proteins

14:20-14:50 Coffee break

Session 7 (Chair: Denis Andrienko)

14:50-15:35 (35+10) Paul Blom - Role of defects in the charge transport of organic semiconductors

15:35-16:00 (20+5) Jasper Michels - Predictive Modelling of Structure Formation in Semiconductor Films Produced by Meniscus-guided Coating

16:00-16:10 Closing Words MMSD - Kostas Daoulas

16:10-17:00 Long coffee break

Special symposium in honor of Kurt Kremer's 65th birthday: "Recent progress in the understanding of entangled systems"

17:00-17:10 Opening words - Burkhard Dünweg

17:10-18:10 (50+10) Jan Smrek - Topological tuning of DNA mobility in entangled solutions of supercoiled plasmids

18:10-19:10 (50+10) Ralf Everaers - Kremer–Grest Models for Commodity Polymer Melts: Linking Theory, Experiment, and Simulation at the Kuhn Scale

19:10-19:15 Closing words - Kurt Kremer