



## Intrinsically Disordered Protein Regions in the Context of Polymer Physics

DoubleTree Hotel -215 S Illinois Ave. Oak Ridge, TN 37830 – Salon A

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### Tuesday, September 10, 2019

Time	Topic	Presenter	Place
8:00 – 9:00 AM	Working Breakfast: Welcome, Overview, Introductions, Scope of Workshop, Organizational, Q&A	Hans Christen (NSD Director) Volker Urban	Salon A
9:00 – 9:45 AM	Synergy between polymer and IDP studies	Andreas Stadler	Salon A
9:45 – 10:30 AM	Probing the Liquid-like Structure of the Nucleolus; Integrative Approaches including SANS	Richard Kriwacki	Salon A
10:30 – 11:00 AM	Break & Open Discussion		Salon A
11:00 – 11:30 AM	Molecular simulations as a predictive tool for IDPs, and as an aid to interpreting smFRET and scattering experiments	Robert Best	Salon A
11:30 – 12:00 PM	Associative polymers under the guise of disordered protein segments: conformation, dynamics and assembly.	Erik Martin	Salon A
12:00 – 12:15 PM	Workshop Picture		Salon A
12:15 – 1:30 PM	Working Lunch: Overview of the Spallation Neutron Source Second Target Station	Ken Herwig	Salon A
1:30 – 2:00 PM	Metal-ions Impart Assembling Functionality to Intrinsically Disordered Protein Tau	Cyrus Safinya	Salon A



## Tuesday, September 10, 2019

Time	Topic	Presenter	Place
2:00 – 2:30 PM	The importance of measuring the solvent quality of unfolded proteins.	Tobin Sosnick	Salon A
2:30 – 3:00 PM	Controllable Activation of Nanoscale Dynamics in a Disordered Protein Alters Binding Kinetics.	Zimei Bu	Salon A
3:00 – 3:30 PM	Coffee Break & Open Discussion		Salon A
3:30 – 4:00 PM	Polymer effects modulate binding affinities in disordered proteins	Hagen Hofmann	Salon A
4:00 – 4:30 PM	Validation of macromolecular flexibility in solution by small angle X-ray scattering (SAXS)	Michal Hammel	Salon A
4:30 – 5:30 PM	Open Discussion	Jeremy Smith	Salon A
5:30 – 6:00 PM	Transfer/ Shuttle to Dinner		
6:00 – 9:00 PM	Working Dinner: A Multimodal Small-Angle Neutron Scattering Instrument for Biological Systems Science at Second Target Station	Shuo Qian & Omar Demerdash	Calhoun's

## Wednesday, September 11, 2019

Time	Topic	Presenter	Place
8:00 – 8:30 AM	Working Breakfast: Summary of Day 1 & Overview for Day 2	Workshop Organizers	Salon A
8:30 – 9:15 AM	From polymer dynamics to protein dynamics: How far can we go?	Alexei Sokolov	Salon A
9:15 – 10:00 AM	Modeling Polymers on Multiple Time and Length Scales	Gary Grest	Salon A



**OAK RIDGE**  
National Laboratory

# AGENDA

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## Wednesday, September 11, 2019

Time	Topic	Presenter	Place
10:00 – 10:30 AM	Modeling IDPs using enhanced sampling molecular dynamics simulations	Utsab Shrestha	Salon A
10:30 – 11:00 AM	Break & Open Discussion		Salon A
11:00 – 11:30 AM	Role of Sequence-Encoded Non-Covalent Interactions in the Structure and Self-Assembly of Synthetic Heteropolymers	Donghui Zhang	Salon A
11:30 – 12:00 PM	Short-time dynamics of therapeutic monoclonal antibodies in solution	Yun Liu	Salon A
12:00 – 12:30 PM	Experimental and Computational Bio-Dynamics of Multi-Domain Macromolecules	Laura Stingaciu	Salon A
12:30 – 1:15 pm	Working Lunch	Hugh O'Neill	Salon A
1:15 – 1:45 PM	Discussion: Defining Requirements for Neutron Techniques for IDR Research	Workshop Organizers	Salon A
1:45 – 2:00 PM	Workshop Summary & Outlook	Workshop Organizers	Salon A
2:00 – 4:00 PM	Lab Tours of SNS		SNS
4:00 PM	End of Workshop		