## October 3, 2020 6 pm - 8:15 pm CDT (UTC -5)

## Virtual Saturday Night Thermo Event for trainees only

(the Zoom link for this session will be sent separately to all who registered for SNT)

## Organizers:

Kacey Mersch, University of Iowa Ari Paiz, UT-Southwestern Vince J. LiCata, Louisiana State University Susan Pedigo, University of Mississippi

#### Moderators:

Kacey Mersch, University of Iowa Ari Paiz, UT-Southwestern

6:00 - 7:00 pm Flash Talks

- 1. Tradeoff between Thermostability and DNA-binding Function in Engineered Variants of EnHD

  Lily Schumacher (McCully Lab), Santa Clara University
- 2. Domain Interactions Determine the Conformational Ensemble of SurA Mathis Leblanc (Fleming Lab), Johns Hopkins University
- Conformational analysis of the structural ensemble of the SARS-CoV-2 nucleocapsid protein
   Jasmine Cubuk (Soranno Lab), Washington University in St. Louis
- 4. Development of a Thiol Exchange- and Mass Spectrometry-Based Technique for the Evaluation of Protein Folding Stabilities

  Aurora Cabrera (Fitzgerald Lab), Duke University
- Pressure Effects on the Conformational Transitions of tRNALys3
   Jingiu Wang (Royer Lab), Rensselaer Polytechnic Institute
- 6. Composition-dependent thermodynamics of intracellular phase separation Joshua Riback (Brangwynne Lab), Princeton University

#### Short Break

### 7:15 - 7:45 pm Career Panel

- 7. Jackie Thompson Dillon, *Ph.D.*Associate Scientific Manager at Benson Hill
- Alexandra Schnoes, Ph.D.
   Associate Director of Career and Professional Development iBiology, Inc.
- Donald M. Engelman, Ph.D.
   Chairman of the Scientific Advisory Board of pHLIP, inc.
   Eugene Higgins Professor of Molecular Biophysics and Biochemistry, Yale University

7:45 - 8:15 pm Career Panel Q&A and open discussion

8:15 - Open mixer

Sunday ◆ October 4, 2020 1 pm – 5 pm CDT (UTC -5)			1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
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12:40 pm	Zoom link goes live
1:00 – 1:05 pm	Opening Comments by Organizers
1:05 – 1:10 pm	President's Welcome by Kathleen Hall, Washington University Saint Louis
	12 <sup>th</sup> Annual Gary K. Ackers Lecture
1:10 – 1:20 pm	Introduction to the Gary K. Ackers Lecture in Biothermodynamics  Bertrand García-Moreno, Johns Hopkins University
1:20 – 2:10 pm	12 <sup>th</sup> Annual Gary K. <u>Ackers Lecture</u> Using statistical thermodynamics to understand protein stability and bioinformatics <u>Doug Barrick</u> , Johns Hopkins University
2:10 – 2:20 pm	Ackers Lecture Q&A
2:20 – 2:25 pm	Short Break
	Session I
Moderator Co-moderator	Drake Jensen, <u>Galburt Lab</u> , Washington University Saint Louis Ryan Mahling, <u>Shea Lab</u> , University of Iowa
2:25 – 2:45 pm	Unusual van't Hoff and Arrhenius Barriers to Steps of Transcription Initiation at the   PR Promoter
ASSESSED TO THE REAL PROPERTY.	Dylan Plaskon, Record Lab, University of Wisconsin-Madison
2:45 – 3:05 pm	Energetic dependencies dictate folding mechanism in a complex protein
	Xiuqi Chen, Kaiser Lab, Johns Hopkins University
3:05 – 3:35 pm	Xiuqi Chen, Kaiser Lab, Johns Hopkins University  Protein Folding and Aggregation in the Cellular Environment
	Xiuqi Chen, Kaiser Lab, Johns Hopkins University  Protein Folding and Aggregation in the Cellular Environment  Silvia Cavagnero, University of Wisconsin-Madison
3:05 – 3:35 pm 3:35 – 3:40 pm	Xiuqi Chen, Kaiser Lab, Johns Hopkins University  Protein Folding and Aggregation in the Cellular Environment
	Xiuqi Chen, Kaiser Lab, Johns Hopkins University  Protein Folding and Aggregation in the Cellular Environment  Silvia Cavagnero, University of Wisconsin-Madison  Short Break
3:35 – 3:40 pm Moderator	Xiuqi Chen, Kaiser Lab, Johns Hopkins University  Protein Folding and Aggregation in the Cellular Environment Silvia Cavagnero, University of Wisconsin-Madison  Short Break  Session II  Michael Baxa, Sosnick Lab, University of Chicago
3:35 – 3:40 pm  Moderator Co-moderator	Xiuqi Chen, Kaiser Lab, Johns Hopkins University  Protein Folding and Aggregation in the Cellular Environment Silvia Cavagnero, University of Wisconsin-Madison  Short Break  Session II  Michael Baxa, Sosnick Lab, University of Chicago Mayank Boob, Gruebele Lab, University of Illinois at Urbana-Champaign  How is phase behavior encoded in the sequence of low-complexity domains?
3:35 – 3:40 pm  Moderator Co-moderator 3:40 – 4:00 pm	Protein Folding and Aggregation in the Cellular Environment Silvia Cavagnero, University of Wisconsin-Madison  Short Break  Session II  Michael Baxa, Sosnick Lab, University of Chicago Mayank Boob, Gruebele Lab, University of Illinois at Urbana-Champaign  How is phase behavior encoded in the sequence of low-complexity domains?  Anne Bremer, Mittag Lab, St. Jude Children's Research Hospital  Prolyl isomerase Ess1 engages bivalent RNAPII CTD substrates in a length-dependent manner
3:35 – 3:40 pm  Moderator Co-moderator 3:40 – 4:00 pm  4:00 – 4:20 pm	Xiuqi Chen, Kaiser Lab, Johns Hopkins University  Protein Folding and Aggregation in the Cellular Environment Silvia Cavagnero, University of Wisconsin-Madison  Short Break  Session II  Michael Baxa, Sosnick Lab, University of Chicago Mayank Boob, Gruebele Lab, University of Illinois at Urbana-Champaign  How is phase behavior encoded in the sequence of low-complexity domains?  Anne Bremer, Mittag Lab, St. Jude Children's Research Hospital  Prolyl isomerase Ess1 engages bivalent RNAPII CTD substrates in a length-dependent manner  Tongyin Zheng, Castañeda Lab, Syracuse University  Understanding functions of dysfunctional proteins
3:35 – 3:40 pm  Moderator Co-moderator 3:40 – 4:00 pm  4:00 – 4:20 pm	Protein Folding and Aggregation in the Cellular Environment Silvia Cavagnero, University of Wisconsin-Madison  Short Break  Session II  Michael Baxa, Sosnick Lab, University of Chicago Mayank Boob, Gruebele Lab, University of Illinois at Urbana-Champaign  How is phase behavior encoded in the sequence of low-complexity domains?  Anne Bremer, Mittag Lab, St. Jude Children's Research Hospital  Prolyl isomerase Ess1 engages bivalent RNAPII CTD substrates in a length-dependent manner  Tongyin Zheng, Castañeda Lab, Syracuse University  Understanding functions of dysfunctional proteins Elizabeth Rhoades, University of Pennsylvania

## Monday ♦ October 5, 2020 1 pm – 5 pm CDT (UTC -5)

12:40 pm	Zoom link goes live
1:00 – 1:10 pm	Announcements
Control of the last	Session III
Moderator Co-moderator	Emery Usher, <u>Showalter Lab</u> , Penn State University Melissa Stuchell-Brereton, <u>Soranno Lab</u> , Washington University Saint Louis
1:10 – 1:30 pm	Exploring the biophysics of protein-surface interactions Gabriel Ortega, Plaxco Lab, University of California Santa Barbara
1:30 – 1:50 pm	Thousand-fold nearest-neighbor cooperativity in ligand binding by the dodecameric ring-shaped gene-regulatory protein, Bha TRAP Weicheng Li, Foster Lab, The Ohio State University
1:50 – 2:20 pm	Examining equilibria through conformational ensembles  Lisa Warner, Boise State University
2:20 – 2:25 pm	Short Break Session IV
Moderator Co-moderator	Robb Welty, <u>Walter Lab</u> , University of Michigan Miranda Mecha, <u>Cavagnero Lab</u> , University of Wisconsin
2:25 – 2:45 pm	MELD-Bracket: May the best ligand win!  Emiliano Brini, Dill Lab, Stony Brook University
2:45 – 3:05 pm	Peptide Anchor Modification Allosterically Modulates T Cell Recognition in a TCR Dependent Fashion  Angela R. Smith, Baker Lab, University of Notre Dame
3:05 – 3:35 pm	Biophysics at DOE National Labs  Nathan Baker and Wendy Shaw, Pacific Northwest National Laboratory
3:35 – 3:40 pm	Short Break
	34th Annual Gibbs Conference Keynote Lecture
3:40 – 3:50 pm	Introduction to the 34th Annual Gibbs Conference Keynote Speaker Timothy Lohman, Washington University Saint Louis
3:50 – 4:40 pm	Keynote Lecture But does it bind? RNA, proteins, and salt Kathleen Hall, Washington University Saint Louis
4:40 – 4:50 pm	Keynote Q&A
4:50 – 5:00 pm	Closing Remarks by Organizers and President, Liskin Swint-Kruse, University of Kansas Medical Center
5:15 – 6:00 pm	Virtual Social. A separate Zoom meeting link will be provided via email to all registrants. Breakout rooms will be set up for discussion.
7:00 – 9:00 pm	Virtual Posters. See page 10 for details.

# Sunday, October 4 and Monday, October 5, 2020 7 pm – 9:30 pm CDT (UTC -5)

## Organizers:

Jim Horn, Northern Illinois University
Lydia Kisley, Case Western Reserve University
Ashley De Lio, University of Illinois at Urbana-Champaign
Suman Shrestha, University of Texas at Arlington

Virtual Posters will be presented in Zoom breakout rooms. Sessions I and II will be held on Sunday evening and will feature posters from presenters with last names P to Z; Session I will also feature posters from presenters who are nearing graduation and seeking postdoctoral positions. Sessions III and IV will be held on Monday evening and will feature posters from presenters with last names A to O. Both nights will start at 7:00 pm and conclude at 9:30 pm, with the first session running from 7:00-8:30 and the second session running from 8:00-9:30 pm. Details about how to join the poster session during Gibbs34 will be sent to all conference registrants.

## Poster Session I (Posters 1 - 19)

October 4, 2020 7 pm – 8:30 pm CDT (UTC -5)

Presenting Authors: Job Seekers (\*\*, students looking for a postdoc) and Last Names Starting with Y to Z

- 1\*\* Syeda Tajin Ahmed

  Design rules for tuning protein adsorption on grafted zwitterionic thin films
- 2\*\* Mayank Boob

  TMAO: protecting proteins from feeling the heat
- 3\*\* Aurora Cabrera

  Development of a Thiol Exchange- and Mass Spectrometry-Based Technique for the Evaluation of Protein Folding Stabilities
- 4\*\* Ellen Gagliani
  A Drosophila model of Adams-Oliver Syndrome reveals Notch cofactor titration as a mechanism underlying developmental defects
- 5\*\* Pooja Goswami
  Potential G1/S Transcription Factor Feedback Loop in the Start Transition of Buddying Yeast Probe by
  Scanning Number and Brightness
- 6\*\* Taranpreet Kaur

  Regulation of Interactions at the Surface Dictates Multi-phasic Architecture of Protein-RNA condensates
- 7\*\* Aaron Morgan
  Kinetics of Nucleotide Binding to the gp16 ATPase
- 8\*\* Cristian M Pis Diez
  Persulfide-sensing in a dithiol-based transcriptional regulator impair DNA-binding by the formation of a tetrasulfide crosslink with minor structural perturbation
- 9\*\* Meredith Rickard

  The Impact of Local Environment on Simulated Metabolite Conformations
- 10\*\* Suman Shrestha

  Evolutionary changes in caspase folding landscape

- 11. Yanxing Yang
  Binding of amyloid peptides to lipid bilayers; effects of ions and lipid content
- 12\*\* Liqi Yao

  The Evolution and Mechanism of Enzyme Specificity in Caspase-3
- Alexander Yarawsky

  Determining the mechanism of the Zn-mediated assembly of a functional amyloid-forming protein from Staphylococcus epidermidis
- 14 Shawn Yoshida

  Characterizing the simulated anomalous diffusion of proteins in relation to the nanoporous structure of extracellular matrix-relevant hydrogels
- 15 Feng Yu

  The Dimensions of Intrinsically Disordered Proteins Determine their Solution Sensitivity
- 16 Yafan Yu
  The structural basis for natural competence in Acinetobacter
- 17\*\* Yifan Zhang
  Iron acquisition by Streptococcus pneumoniae: PiuA specifically recognizes tetradentate catechol Felll complexes
- 18 Siwen Zhang

  Probing pressure effects on core packing of a repeat protein using 13C-1H NMR
- 19\*\* Xinji Zhu
  Salt Dependence of the Stability of a Psychrophilic DNA Polymerase

## Poster Session II (Posters 20 - 39)

October 4, 2020 8 pm – 9:30 pm CDT (UTC -5)

Presenting Authors: Last Names Starting with P to W

- 20 Niyati Patel
  Using VHH Single Domain Antibodies as Modules for Protein Thermostability Enhancement
- 21 Marko Popovic
  A thermodynamic insight into viral infections: do viruses in a lytic cycle hijack cell metabolism due to their low Gibbs energy?
- Julien Roche
  Thermodynamic stability of hnRNP A1 low complexity domain revealed by high-pressure NMR
- 23 Riya Samanta
  Investigation of an Allosteric Mechanism from an Evolutionary Perspective
- 24 Emma Schoch
  Stabilization of Dimeric Fbxw7 by Fusion to its Binding Partner Skp1
- 25 Lily Schumacher
  Tradeoff between Thermostability and DNA-binding Function in Engineered Variants of EnHD
- 26 Catherine Scull Co-transcriptional folding of riboswitches
- 27 Sambuddha Sen Characterization of a H2S stress regulator FisR from Acinetobacter baumannii

- Andrews	28	Hossain Shadman
1	11 11 11	A Comparison of the Structural Features of Mammalian and Fish Protamines: a Molecular Dynamics
Sie	17/1/1	Simulation Study
1	29	Corinne Soutar
r (g)	23	Amphotericin B Interactions with Cell Membrane Sterols Revealed by Solid-State NMR
	30	Helena Spikes
	-	Group 14 Metallafluorenes as Solvatochromic Probes of Membrane order
	31	Grace Sullivan
7	3	Unfolding Thermodynamics of an Intramolecular DNA Kissing Complex
日かり		
	32	Sydney Tippelt
		How Hox Proteins Regulate DNA Binding
in	33	Eric Tomko
	-	Functional distinctions between human and yeast TFIIH kinase modules and XPB/Ssl2 dsDNA
		translocase
. 6		The same of the sa
	34	Matias Villarruel  Characterization of the interaction between a truncated homoglable and mambrages in Mysobacterium
		Characterization of the interaction between a truncated hemoglobin and membranes in Mycobacterium tuberculosis
		taborodicolo
	35	Yuhan Wang
6 9	-	Quantifying protein-protein binding interaction in vitro and in cells
7.	36	Jinqiu Wang
	00	Pressure Effects on the Conformational Transitions of tRNALys3
	Sec. On	
	37	Jordan Webb
		Structural Characterization of a Novel Interaction Between the Coregulator NCoA1 and the Notch Transcriptional Activation Complex
	*	Transcriptional Activation Complex
	38	Chamitha Weeramange
A. A.	- W	The Cra-FruK complex alters regulation of central metabolism of γ-proteobacteria
244	39	Riley Workman
The state of	39	Conformational entropies of aqueous and condensed-phase glycine-rich pentapeptides following liquid
gn.	- S	liquid phase separation
	30	
C MAN		Poster Session III (Posters 40 – 58)
Ser. Con		October 5, 2020
		7 pm — 8:30 pm CDT (UTC -5)
		Presenting Authors: Last Names Starting with J to O
	40	Amanda Jons Immobilizing Split GFP Biosensors in Protein Materials: Salt Tunes Analyte Binding and Release
		minipolinzing split or F Diosetisors in Florein Waterials, Salt 1 thes Arialyte billumg and Kelease

- 41 Grant Keller
  Determinants of Antigenicity in Tumor Necepitopes for the Development of Personalized/Multiple
  Peptide Vaccines
- 42 Irine Khutsishvili
  Unfolding Thermodynamics of an RNA Pseudoknot and its DNA Analogs
- 43 Tom Laue IgG Charge

44	Patrick Laughlin Redirecting Self-Assembly of a Virus Capsid: Capsid Assembly Modifiers Stabilize Hexameric Lattice
45	While Destabilizing Native Icosahedral Symmetry  Tosha Laughlin  Engineering Multidirectional pH Dependent Protein-Ligand Interactions using Ionizable Triggers Within Lighted Dimon Interface.
46	Taeho Lee Temperature Dependency of CLC-ec1 dimerization in membranes
47	Josephine Liess Structure and Function of Clostridium perfringens Type IV Pili
48	Jiaqi Ma Dynamic allostery controls the peptide sensitivity of the Ly49C natural killer receptor
49	Upasana Mallimadugula A Parallel Ratchet-Stroke Mechanism Leads to an Optimum Force for Molecular Motor Function
50	Justin Marsee Assessing the Classification of putative PHB depolymerase from B. parapertusis
51	Meranda Masse Contribution of nascent polypeptides of increasing length to the apparent stability of the bacterial ribosome
52	Miranda Mecha Optimal prevention of aggregation is achieved when client proteins fold on the surface of the Hsp70 chaperone: a computational study
53	Alexander Meyer Structure and Function of Clostridium perfringens Type IV Pili
54	Pinaki Misra Early events in light chain aggregation at physiological pH reveal new insights on assembly, stability,
55	and aggregate dissociation Tushar Modi Information propagation in time through allosteric signaling
56	David Moses Probing the Hidden Sensitivity of Intrinsically Disordered Proteins
57	Sarah Mosure Structural basis for heme-dependent NCoR binding to the transcriptional repressor REV-ERB\$
58	Kari Olson The Energetic and Structural Characterization of Dystrophin Spectrin Repeats
	Poster Session IV (Posters 59 - 80) October 5, 2020
	8 pm — 9:30 pm CDT (LTC -5)

Presenting Authors: Last Names Starting with A to H and late-breaking posters

- Ibraheem Alshareedah 59 Phase transition of RNA-protein complexes into ordered permeable hollow condensates
- 60 Jhullian Alston Phase separation propensity of the SARS-CoV-2 nucleocapsid protein

- Chad Brambley 61. Poly(aspartic acid) hydrolase PahZ1KT-1 substrate selectivity is governed by conformational dynamics and non-standard serine active site residue interactions Daiana Capdevila Structural basis of persulfide-sensing specificity in a transcriptional regulator 63 Jasmine Cubuk Conformational analysis of the structural ensemble of the SARS-CoV-2 nucleocapsid (N) protein 64 Moumita Dasgupta Biophysical Characterization of Interactions of T Cell Receptor (TCR) with Viral Antigens derived from Lymphocytic Choriomeningitis Virus (LCMV) 65 Ashley De Lio Lipid Functionalization: the role of charged residues **Gregory Dignon** 66 Solution Conditions to Regulate Protein-Protein Interactions and Monoclonal Antibody Stability and Viscosity Gina El Nesr 67 Predicting Gibbs free energy change of mutations using statistical information and machine learning Melanie Ernst 68 Thermodynamic stability measurements on the ion channel Fluc show an equilibrium reaction in the membrane 69 Joseph Fakhoury Structural and mechanistic characterization of persulfide sensing transcriptional regulators Verna Frasca 70 Characterization of Enzyme Kinetics with Isothermal Titration Calorimetry Richard Gillilan High Pressure Chromatography-Coupled BioSAXS: a tool for Deep Life and Extreme Biophysics 72 Gopika Gopan RNA-protein binding affinity and kinetics in live cells using Fast Relaxation Imaging (FReI) 73 Shawn Gray The Nucleoporin Gle1 promotes ATP binding to the RNA helicase Dbp5 74 Tristan Gunther Kinetics and Mechanism of Transcription Initiation from the Ribosomal RNA Promoter rrnB P1
- 75 Nastaran Hadizadeh Step into the Unresolved: Versatile Tools Towards Real-time Single-molecule Biology
- 76 Wyel Halimeh

  Dependence of Proline Isomerization on the Kinetics of Folding of Anthrax Lethal Factor
- 77 Rachel Hutchinson
  A novel combined approach employing fluorescence-anisotropy decay and microviscometry to explore the cotranslational compaction of nascent proteins
- 78\* Cory Ayres
  Force Pull Quasiequilibrium: Investigating the Impact of Force on TCR/peptide-MHC Stability and Immunological Recognition

