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## The 30<sup>th</sup> Gibbs Conference on Biothermodynamics

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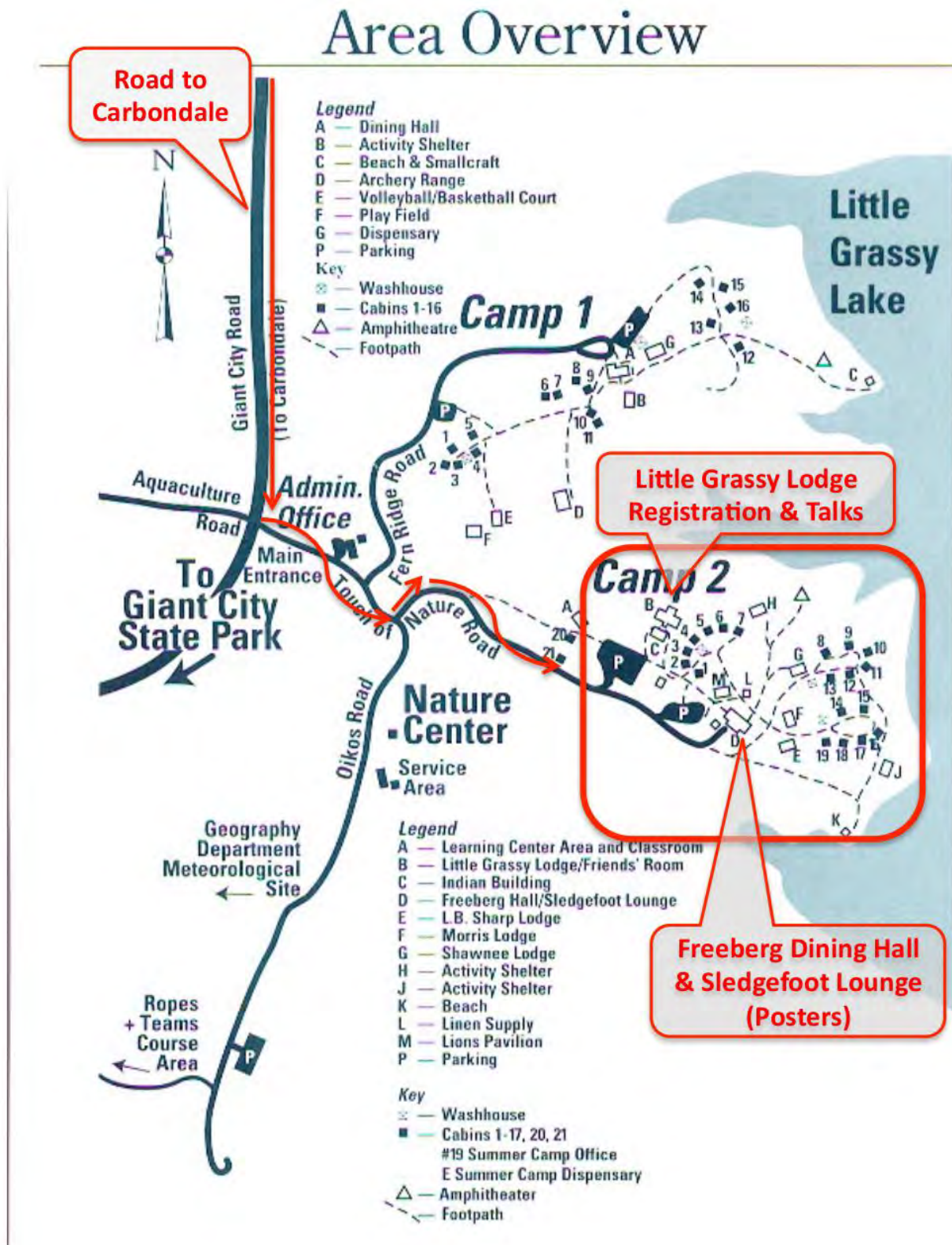
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# Map of Touch of Nature Environmental Center

Most of the Gibbs Conference activities will be held in “Camp 2” as shown in the map below. Cell phone reception is extremely limited; parking lots are popular places for making calls.



# The Gibbs Conference on Biothermodynamics

## History

*Fall, 1986*

Discussion of the discipline: Thermodynamics in Biological Systems  
At the Gill residence in Vail, Colorado

Gary Ackers, Wayne Bolen, Ernesto Freire, Stan Gill, Jim Lee

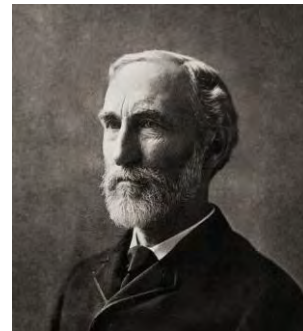
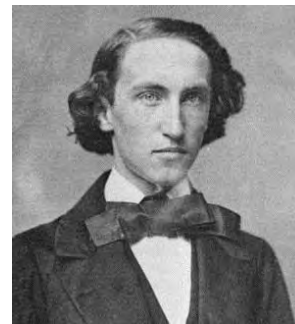
*February, 1987*

Discussion of the discipline: Thermodynamics in Biological Systems  
The Gumbo Shop, New Orleans, LA during the 31<sup>st</sup> Annual Biophysical  
Society Meeting - Gary Ackers, Norma Allewell, Wayne Bolen, Ken

Breslauer, Ken Dill, Ernesto Freire, Stan Gill, Jim Lee

A history of the first ten years of the meeting was provided by Ackers GK and Bolen DW in the article entitled "The Gibbs Conference on Biothermodynamics: Origins and Evolution" published in *Biophysical Chemistry* **64** (1997) 3-5 (doi:10.1016/S0301-4622(96)02246-6).

An update is provided by Shea, MA, Correia, JJ, and Brenowitz, MD, entitled "Introduction: Twenty five years of the Gibbs Conference on Biothermodynamics" available in *Biophysical Chemistry* **159** (2011) 1-5 (doi:10.1016/j.bpc.2011.07.002).



## Meetings

All meetings have been held at the Touch of Nature Environmental Center associated with Southern Illinois University – Carbondale. From 1987 through 1993, all of the speakers in the scientific sessions were students or postdoctoral fellows.

- 1987 Organizers: Jim Lee and Wayne Bolen  
Philosophical Talks: Gary K. Ackers and Ken Dill
- 1988 Organizers: Gary Ackers and Michael Johnson
- 1989 Organizers: Susan G. Frasier and Michael Johnson
- 1990 Organizers: Michael Johnson and Marty Straume
- 1991 Organizers: Gary Ackers and Tim Lohman  
Keynote Speaker: Ernesto Freire
- 1992 Organizers: Jim Lee and Tomasz Heyduk  
Keynote Speakers: Serge Timasheff and John Schellman
- 1993 Organizers: Maurice Eftink and Glen Ramsay  
Keynote Speakers: Peter von Hippel and Julian Sturtevant
- 1994 Organizers: Enrico Di Cera and Madeline Shea  
Keynote Speakers: Gary Ackers and Kathleen S. Matthews
- 1995 Organizers: Kenneth P. Murphy and Michael D. Brenowitz  
Keynote Speakers: Victor Bloomfield and Mario Amzel
- 1996 Organizers: Jonathan B. Chaires and Michael L. Doyle  
Keynote Speakers: J. Michael Schurr and Allen Minton
- 1997 Organizers: Dorothy Beckett and Jack Correia  
Keynote Speaker: Adrian Parsegian

- 1998 Organizer: Andy Robertson  
Keynote Speaker: David Draper
- 1999 Organizers: Bertrand Garcia-Moreno E. and John Shriver  
Keynote Speakers: Wayne Bolen and Gary Ackers
- 2000 Organizers: George Turner and Kim Sharp  
Keynote Speaker: Steve White
- 2001 Organizers: Margaret A. Daugherty and Luis A. Marky  
Keynote Speaker: George Rose
- 2002 Organizers: Michael Mossing and George Makhatadze  
Keynote Speaker: Rodney Biltonen
- 2003 Organizers: Vince Hilser and Dick Sheardy  
Keynote Speaker: Jim Lee
- 2004 Organizers: Doug Barrick and Kathleen Hall  
Keynote Speaker: Nacho Tinoco
- 2005 Organizers: Trevor Creamer and Clay Clark  
Keynote Speaker: Carl Frieden
- 2006 Organizers: Karen Fleming and Rohit V. Pappu  
Keynote Speakers: Madeline A. Shea and Timothy Lohman
- 2007 Organizers: Brian M. Baker and Michael T. Henzl  
Keynote Speaker: Jamie Williamson
- 2008 Organizers: Jannette Carey and David Bain  
Keynote Speakers: Dorothy Beckett and Ken Dill
- 2009 Organizers: Nathan Baker and Liskin Swint-Kruse  
Keynote Speaker: Linda Jen-Jacobson  
The Gary K. Ackers Lecture in Biothermodynamics: Michael Brenowitz
- 2010 Organizers: Elisar Barbar and Vince LiCata  
Keynote Speaker: C. Nick Pace  
The Gary K. Ackers Lecture in Biothermodynamics: Timothy Lohman
- 2011 Organizers: Gibbs Society of Board of Directors  
Keynote Speaker: Bertrand Garcia-Moreno E.  
The Gary K. Ackers Lecture in Biothermodynamics: Madeline Shea  
Editors of Special Issue of *Biophysical Chemistry* – Enrico Di Cera, Tim Lohman, Jack Correia
- 2012 Organizers: Aaron L. Lucius and Patricia L. Clark  
Keynote Speaker: Terry G. Oas  
The Gary K. Ackers Lecture in Biothermodynamics: Enrico Di Cera
- 2013 Organizers: James L. Cole and Aron W. Fenton  
Keynote Speaker: Doug Barrick  
The Gary K. Ackers Lecture in Biothermodynamics: Bertrand Garcia-Moreno E.
- 2014 Organizers: Andrew B. Herr and Steven T. Whitten  
Keynote Speaker: Karen G. Fleming  
The Gary K. Ackers Lecture in Biothermodynamics: David E. Draper
- 2015 Organizers: Ernesto J. Fuentes and James R. Horn  
Keynote Speaker: Rohit V. Pappu  
The Gary K. Ackers Lecture in Biothermodynamics: Walter S. Englander
- 2016 Organizers: Sarah Bondos and Nick Fitzkee  
Keynote Speaker: Patricia Clark  
The Gary K. Ackers Lecture in Biothermodynamics: Ken Dill

## Gibbs Society Governance

### Incorporation

In 2002, the Gibbs Society of Biological Thermodynamics incorporated in the Commonwealth of Virginia, under the guidance of Michael L. Johnson, then Treasurer of the Society. Articles of Incorporation and By Laws are available here: <http://www.jhu.edu/~gibbs>

### Current Officers

- ❖ President: Vince LiCata, 2015 – 2016
- ❖ Vice President: Michael L. Johnson, 2010 – 2016
- ❖ President Elect: James Cole, 2015-2016
- ❖ Secretary: Liskin Swint-Kruse, 2013 – 2016
- ❖ Treasurer: John J. “Jack” Correia, 2010 – 2017

### Board of Directors, listed alphabetically

- ❖ Patricia Clark
- ❖ James Cole
- ❖ John J. “Jack” Correia
- ❖ Michael Johnson
- ❖ Vince LiCata
- ❖ Madeline Shea
- ❖ Liskin Swint-Kruse

### Past Presidents

2001-2002	Gary K. Ackers	2008-2009	Luis A. Marky
2002-2003	J. Jack Correia	2009-2010	Bertrand Garcia-Moreno E.
2003-2004	D. Wayne Bolen	2010-2011	Karen G. Fleming
2004-2005	Madeline A. Shea	2011-2012	Doug Barrick
2005-2006	Dorothy Beckett	2012-2013	David L. Bain
2006-2007	J. Brad Chaires	2013-2014	George I. Makhatadze
2007-2008	Tim M. Lohman	2014-2015	Patricia Clark

### Past Treasurer

2001-2011 Michael L. Johnson

### Past Secretary

2004-2013 Margaret A. Daugherty

### Committees & Other Contributions

Ackers Lecturer Selection Committee – Madeline A. Shea, Chair  
Gibbs Society Website Hosting – Karen G. Fleming (2010 – present)  
GoogleDocs Application/Registration & PayPal – Nathan A. Baker and J. Jack Correia  
Mailing List – Liskin Swint-Kruse  
Saturday Night Thermo Organizers – Susan Pedigo and Vincent J. LiCata  
With thanks to Alan Teska at the Touch of Nature Conference Center

## Confidentiality Statement

Please remember that the abstracts for this meeting are confidential material and may contain unpublished results. They will not be posted online. Please ask permission from the authors before taking photos of posters. Please do not record the talks unless a speaker has given you permission.

## 8<sup>th</sup> Annual Gary K. Ackers Lecture

2016 Lecturer – Ken Dill, Stony Brook University

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This lecture honors the scientific contributions of Gary K. Ackers (1939-2011) to the field of Biological Thermodynamics. He served on the faculty at the University of Virginia, Johns Hopkins University and the Washington University School of Medicine. He was a Fellow of the Biophysical Society and was one of the founding organizers of the Gibbs Conference.

Gary demonstrated a lifelong commitment to the growth and development of an intellectual community of scholars devoted to furthering the field of biothermodynamics. Gary was an active member of the Biophysical Society throughout his career and served as President of the Society, as well as Organizer of the annual meeting. While on the faculty of the University of Virginia, he was a leader in the graduate biophysics training program. When on the faculty in the Department of Biology at the Johns Hopkins University, he conceived and organized the Institute for Biophysical Studies of Macromolecular Assemblies, a university-wide training program in molecular biophysics that has continued for decades. While at Johns Hopkins, he also played a leading role in the establishment of the Gibbs Conference on Biothermodynamics, an annual meeting organized to promote innovative development of biophysical principles applied to current problems in biology and to train the next generation of molecular biophysicists to tackle hard problems rigorously. After moving to St. Louis to chair the Department of Biochemistry and Molecular Biophysics at Washington University, he spearheaded a new graduate program in biophysics and hired many faculty who have joined the community of regular contributors to the Gibbs Conference.

Gary was a pioneer in the development of methods and application of principles of equilibrium thermodynamics to the study of linkage in complex macromolecular assemblies. Studies from his laboratory on the energetics of self-association and ligand binding in human hemoglobin proved unequivocally that the classic and elegant MWC model of intersubunit allostery was insufficient to explain cooperative oxygen binding: the position, as well as the number, of ligands matters. His contributions in this area greatly enhanced our understanding of the relationship between structure, energy and function in hemoglobin, and in multimeric allosteric systems in general. By probing ever more deeply into the molecular mechanism of cooperativity, he demonstrated a beautiful, useful, and general strategy for dissecting functional energetics in macromolecular assemblies.

His quantitative study of the interactions between proteins and nucleic acids in the bacteriophage lambda system included the development of quantitative DNase footprinting methods for measuring free energies of repressor-operator interactions. The footprinting assay remains an effective tool for measuring the extremely tight binding constants that are often encountered in site-specific interactions between proteins and nucleic acids. Those studies paved the way for similar methods to study protein-nucleic acid interactions in more complex systems, including time-resolved studies of the kinetics of RNA folding. Based on his experimental studies of phage lambda, his group developed statistical thermodynamic models to simulate the lysogenic-to-lytic growth switch: the series of macromolecular events that determine the fate of bacteriophage lambda during infection of *E. coli*. This work demonstrated how a complex biological function could be predicted quantitatively, strictly from the kinetics of transcription and translation, and the Gibbs free energy of interactions between the key macromolecular components in the genetic switch.

During Gary's early career, he developed methods to measure association constants in self-associating systems based on analytical gel permeation chromatography. Those methods have since become standard tools in the field. His group was also responsible for modifications of the cryo-gel electrophoresis methods, moving from applying them to hemoglobin to protein-DNA interactions. These contributions focused on developing the capacity to quantify intermediate states that are only transiently populated during the course of a biochemical process. His more than 200 articles and chapters changed our view of the molecular mechanisms that govern complex biochemical reactions.

## **ΔGibbs 30 • Saturday Evening • September 24, 2016**

4:00 – 10:00 pm      **Check-in at Little Grassy Lodge**

7:30 – 10:00 pm      **Open Reception in Indian Lodge – Light refreshments, beer, wine, and soft drinks**  
Participants are expected to make dinner arrangements independently

**Gibbs T-shirts and Mugs – pick up at registration**

### **Saturday Night Thermo – Event for trainees only**

**Faculty Organizers:** Vince J. LiCata, Louisiana State University and Susan Pedigo, University of Mississippi

**Trainee Moderators:** Christopher Fox, Pedigo Lab and Tod Baker, LiCata Lab

5:30 pm                **Freeberg Hall – Dinner for trainees who registered in advance**

6:00 – 7:00 pm      **Flash Talks (Poster Introductions) – Session open to all trainees**

- 1. Toward a Phase Diagram for the Rational Design of Ligand-Induced Folding and Allosteric Interactions Dynamics in a Family of De Novo Heme-Binding Helical Bundles**  
Joseph Brisendine, Koder Lab, The City College of New York
- 2. The Perplexing Cooperative Folding of a Low Sequence Complexity, Poly-Proline 2 Protein Lacking a Hydrophobic Core**  
Michael Baxa, Sosnick Lab, The University of Chicago
- 3. Multivalency in Intrinsically Disordered ASCIZ**  
Sarah Clark, Barbar Lab, Oregon State University
- 4. Cooperative Folding of tRNA<sup>phe</sup> in Cellular Conditions Arises from Destabilization of Intermediates and Stabilization of the Full Length RNA**  
Kathleen Leamy, Bevilacqua Lab, The Pennsylvania State University
- 5. Side Chain Hydrophobicity Scale Using the Tilted Beta-Barrel PagP**  
Dagan Marx, Fleming Lab, Johns Hopkins University
- 6. Biophysical Characterization of G-Quadruplex Capped by Flanking Duplex Ends: A Model for Human c-MYC NHE-III<sub>1</sub>**  
Amanda Metz, E. Lewis Lab, Mississippi State University
- 7. Interaction of RIG-I-like Receptors with Polyubiquitin Chains**  
David Mouser, Cole Lab, University of Connecticut
- 8. The von Willebrand Factor A1-Collagen III Interaction is Independent of Conformation and Type 2 von Willebrand Disease Phenotype**  
Venkata Machha, Auton Lab, Mayo Clinic

7:00 – 7:15 pm      **Refreshment break**

7:15 – 8:15 pm      **Career panel – Session open to all trainees**  
Dr. Randy Wadkins, University of Mississippi, Biophysical Society Congressional Fellow  
Dr. Randy Forsyth, Shire  
Dr. Michaelleen Doucleff, National Public Radio Correspondent

8:15 pm                **Adjourn to reception in Indian Lodge**

## **ΔGibbs 30 • Sunday Morning • September 25, 2016**

7:00 – 8:30 am **Breakfast served in Freeberg Hall**

### **Thermodynamics of Energy Landscapes**

8:30 – 8:35 am **President's Welcome by Vince LiCata, Louisiana State University**

*Moderator* Jingheng Wang, Beckett Lab, University of Maryland

8:35 – 8:50 am **Introduction to the 30<sup>th</sup> Annual Gibbs Conference Keynote Speaker**  
Karen Fleming, Johns Hopkins University

8:50 – 9:50 am **Keynote Lecture**  
**Protein Folding Away From Equilibrium**  
Patricia Clark, University of Notre Dame

9:50 – 10:20 am **Break – Refreshments in Indian Lodge**

10:20 – 10:40 am **Re-parameterization of Protein Force Fields Guided by Osmotic Coefficient Measurements from Molecular Dynamics Simulations**  
Mark Miller, Elcock Lab, University of Iowa

10:40 – 11:10 am **The Role of Protein Self-Association and Liquid-Liquid Phase Separation in the Formation of Membrane-less Organelles**  
Tanja Mittag, St. Jude's Hospital

11:10 – 11:30 am **Quantifying Amide-Amide and Amide-Hydrocarbon Interactions: Implications for Hydrogen Bonding,  $n - \pi^*$  and Other Amide Group Interactions of Protein Folding and Assembly**  
Xian Cheng, Record Lab, University of Wisconsin-Madison

11:30 – 12:00 pm **Mapping Protein Folding Landscapes Using High Pressure NMR**  
Catherine Royer, Rensselaer Polytechnic Institute

12:00 pm **Conference photo near Freeberg Hall**

12:10 pm **Lunch in Freeberg Hall**

### **Workshop: Science and Communication**

This optional workshop will cover three perspectives on the importance of communicating scientific ideas effectively, both to our colleagues and the general public.

*Moderator* Nishant Singh, Baker Lab, University of Notre Dame

1:15 – 1:45 pm **Try Science Advocacy. You Might be Surprised...**  
Ken Dill, Stony Brook University

1:45 – 2:15 pm **How to Communicate Science Effectively**  
Michaeleen Doucleff, National Public Radio

2:15 – 2:45 pm **AAAS Science & Technology Congressional Fellowship Sponsored by the Biophysical Society: What I Learned as a Congressional Staffer**  
Randy Wadkins, University of Mississippi

### **Free Time until Late Afternoon Session.**

Information about local parks and attractions is available near the entrance to Little Grassy Lodge.



## **ΔGibbs 30 • Sunday Afternoon • September 25, 2016**

### **Thermodynamics of Function and Catalysis**

- Moderator* Melvin Thomas III, C. Clark Lab, University of Texas at Arlington
- 3:00 – 3:30 pm **Crowding Activates the Hsp90 Molecular Chaperone**  
Timo Street, Brandeis University
- 3:30 – 3:50 pm **Multiple Pathways of Large Subunit Ribosome Assembly Observed in Cells Expressing Helicase Inactive DbpA**  
Riley Gentry, Koculli Lab, University of Central Florida
- 3:50 – 4:20 pm **GroEL Actively Stimulates Folding of the Endogenous Substrate Protein PepQ**  
Hays Rye, Texas A&M University
- 4:20 – 4:50 pm **Break – Refreshments in Indian Lodge**
- 4:50 – 5:20 pm **Visualizing Structural Ensembles with Small-Angle X-Ray Scattering**  
Lois Pollack, Cornell University
- 5:20 – 5:40 pm ***Saccharomyces cerevisiae* Hsp104 is a Non-processive Polypeptide Translocase**  
Clarissa Weaver, Lucius Lab, University of Alabama at Birmingham
- 5:40 – 6:00 pm **Chemo-mechanical Pushing of Single Stranded DNA Binding Proteins Along Single Stranded DNA**  
Joshua Sokoloski, Lohman Lab, Washington University in Saint Louis
- 6:00—6:10 pm **General Discussion**
- 6:15 pm **Dinner in Freeberg Hall**



## **ΔGibbs 30 • Sunday Evening • September 25, 2016**

- 8:00 – 10:00 pm **Poster Session I in Sledgefoot (lower level) & Freeberg (upper level)**  
Presenters with last name A to L
- Please remove posters before midnight to make room for Monday presenters
- Sponsor's displays in Freeberg (upper level) – near beer, wine, and soft drinks

## **ΔGibbs 30 • Monday Morning • September 26, 2016**

Posters to be presented on Monday night may be mounted as soon as space is available on Sunday night. The Airport Ride Board will be available in Little Grassy Lodge, near the check-in window.

7:00 – 8:30 am      **Breakfast served in Freeberg Hall**

### **Thermodynamics of Folding and Assemblies**

8:30 – 8:35 am      **Announcements by Organizers**

*Moderator*      Calliste Reiling-Steffensmeier, Marky Lab, University of Nebraska Medical Center

8:35 – 8:50 am      **Introduction to the Gary K. Ackers Lecture in Biothermodynamics**  
Doug Barrick, Johns Hopkins University

8:50 – 9:50 am      **8<sup>th</sup> Annual Gary K. Ackers Lecture**  
**Cellular Growth Laws are a Manifestation of Protein Physical Chemistry**  
Ken Dill, Stony Brook University

9:50 – 10:20 am      **Break – Refreshments in Indian Lodge**

10:20 – 10:50 am      **MeCP2, the Protein, Still Surprises**  
Michael Brenowitz, Albert Einstein College of Medicine

10:50 – 11:20 am      **Mechanism for Activation of the Antiviral Kinase PKR**  
Jim Cole, University of Connecticut

11:20 – 11:40 am      **Phosphorylation Induces Sequence-specific Conformational Switches in the RNA Polymerase II C-Terminal Domain**  
Eric Gibbs, Showalter Lab, The Pennsylvania State University

11:40 – 12:00 pm      **A Network of Polar Asparagines Provides Coupling Between Repeats in Leucine-Rich Repeat Proteins**  
Sean Klein, Barrick Lab, Johns Hopkins University

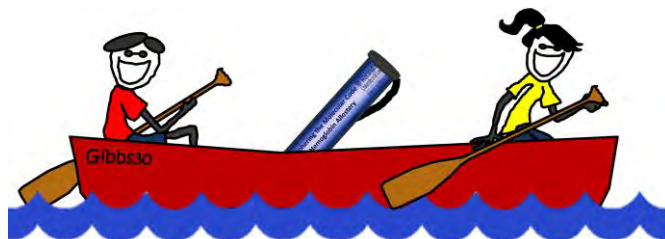
12:00 - noon      **Introduction of Conference Sponsors**

12:05 pm      **Lunch in Freeberg Hall**

1:00 – 2:00 pm      **Meeting of Past Organizers – Indian Building**  
Refreshment area will be unavailable to other meeting attendees during this time

### **Free Time until Late Afternoon Session.**

Information about local parks and attractions is available near the entrance to Little Grassy Lodge.



## **ΔGibbs 30 • Monday Afternoon • September 26, 2016**

### **Thermodynamics of Disorder and Allostery**

- Moderator* Robb Welty, Hall Lab, Washington University School of Medicine
- 3:00 – 3:30 pm **Probing Transient Partial Unfolding in Proteins by Native-State Proteolysis**  
Chiwook Park, Purdue University
- 3:30 – 3:50 pm **The Intrinsically Disordered Proline/Glycine-Rich Region of the Biofilm Adhesion Protein Aap Forms an Extended Stalk with High Polyproline Type II Helix Propensity**  
Alexander Yarawsky, Herr Lab, University of Cincinnati
- 3:50 – 4:20 pm **Regulation of Dynamic Protein Assemblies: A Novel Structural Interplay Between Protein Disorder, Phosphorylation, and Isoform Specificity**  
Elisar Barbar, Oregon State University
- 4:20 – 4:50 pm **Break – Refreshments in Indian Lodge**
- 4:50 – 5:10 pm **Contributions of Local Stability and Conformational Heterogeneity to pH-dependent Myristoyl Switching**  
Duncan MacKenzie, Meiering Lab, University of Waterloo
- 5:10 – 5:40 pm **Rheostats and Toggle Switches for Modifying Protein Function**  
Liskin Swint-Kruse, Kansas University Medical Center
- 5:40 – 6:00 pm **Dissecting Mechanisms of Allostery by Quantifying Correlations in Disorder and Structure**  
Sukrit Singh, Bowman Lab, Washington University in Saint Louis
- 6:00 – 6:10 pm **General Discussion**
- 6:15 pm **Dinner in Freeberg Hall**

## **ΔGibbs 30 • Monday Evening • September 26, 2016**

- 8:00 – 10:00 pm **Poster Session II in Sledgefoot (lower level) & Freeberg (upper level)**  
Presenters with last name M to Z
- Sponsors displays in Freeberg (upper level) – near beer, wine, and soft drinks

## **ΔGibbs 30 • Tuesday Morning • September 27, 2016**

Check-out: Please leave your room keys at the counter in the lobby of the Little Grassy Lodge. The Airport Ride Board will be available in Little Grassy Lodge, near the check-in window.

7:00 – 8:30 am **Breakfast served in Freeberg Hall**

### **Thermodynamics of Design and Membranes**

8:30 – 8:35 am **Closing Announcements by Organizers**

*Moderator* Kacey Mersch, Robertson Lab, University of Iowa

8:35 – 9:05 am **DNA in Tight Spaces: Linking Structure, Stability and Protection in Cation-Packaged DNA**

Jason DeRouchey, University of Kentucky

9:05 – 9:25 am **The Role of Protein Folding Factors in the Biogenesis of Outer Membrane Proteins**

Ashlee Plummer, Fleming Lab, Johns Hopkins University

9:25 – 9:45 am **Twister Ribozyme: A New Twist in RNA Folding and Catalysis**

Subrata Panja, Woodson Lab, Johns Hopkins University

9:45 – 10:15 am **Break – Refreshments in Indian Lodge**

10:15 – 10:45 am **Nuclear Receptor Functional Energetics and Transcriptional Regulation**

David Bain, University of Colorado Anschutz Medical Campus

10:45 – 11:05 am **Exploring the Multiple Binding Modes of  $[\text{Ru}(\text{II})(\text{L})(\text{phen})_2]^{2+}$  Analogs with B-DNA**

Clinton Mikek, E. Lewis Lab, Mississippi State University

11:05 – 11:25 pm **Tracing the Evolution of Peptide Binding Specificity in the S100 Protein Family Using Phage Display and Deep Sequencing**

Luke Wheeler, Harms Lab, University of Oregon

11:25 – 11:55 am **Towards Self-reporting Fluorescent Biosensors using Leave-One-Out Green Fluorescent Protein**

Chris Bystroff, Rensselaer Polytechnic Institute

11:55 – 12:00 pm **Closing Remarks by Organizers and President**

12:00 pm **Box lunch in Freeberg Hall**

Check-out Please leave your keys at the counter in Little Grassy Lodge

