# Table of Contents

## The 30th Gibbs Conference on Biothermodynamics

### Introduction

- Map of Touch of Nature ................................................................. 2
- History and List of Meetings .......................................................... 3-4
- Gibbs Society Governance – Incorporation, Officers, Committees ......................................................... 5
- Confidentiality Statement .................................................................. 5
- The Gary K. Ackers Lecture in Biothermodynamics ........................................ 6

### Meeting Schedule

- Saturday, September 24 ........................................................................ 7
- Sunday, September 25 .......................................................................... 8-9
- Monday, September 26 ......................................................................... 10-11
- Tuesday, September 27 .......................................................................... 12

### List of Posters

- Poster Information ........................................................................... 13
- Session I, Sunday .............................................................................. 13
- Session II, Monday ........................................................................... 17

### Abstracts

- Speakers ............................................................................................ 21
- Posters ............................................................................................. 51

### List of Participants

- Alphabetical List of Participants ......................................................... 173
- Participants by Lab ........................................................................... 185

### Sponsors

- Listing and Product Information ......................................................... 189
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


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-Jacobsen
    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

Board of Directors, listed alphabetically
- Patricia Clark
- James Cole
- John J. “Jack” Correia
- Michael Johnson
- Vince LiCata
- Madeline Shea
- Liskin Swint-Kruse

Past Presidents
- 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. Makhadadze

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
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.
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.
Gibbs 30 • Saturday Evening • September 24, 2016

4:00 – 10:00 pm  Check-in at Little Grassly 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\textsubscript{phe} 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;
   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 Doucelff, National Public Radio Correspondent

8:15 pm  Adjourn to reception in Indian Lodge
Gibbs 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 30th 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 – π* 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.
**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

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**Gibbs 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
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  8th 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.
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

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
**Gibbs 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 Anschultz Medical Campus

10:45 – 11:05 am  Exploring the Multiple Binding Modes of [Ru(II)(L)(phen)]₂⁺ Analogs with B-DNA

Clinton Mikek, E. Lewis Lab, Mississippi State University

11:05 – 11:25 am  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