

The 28th Annual Gibbs Conference on Biothermodynamics

September 20-23, 2014

Organized by Andrew B. Herr and Steven T. Whitten

Touch of Nature Environmental Center Southern Illinois University, Carbondale, IL

Sponsored by
Avanti • Aviv • Horiba • Jasco • Malvern
NanoTemper • TxSt Chemistry & Biochemistry

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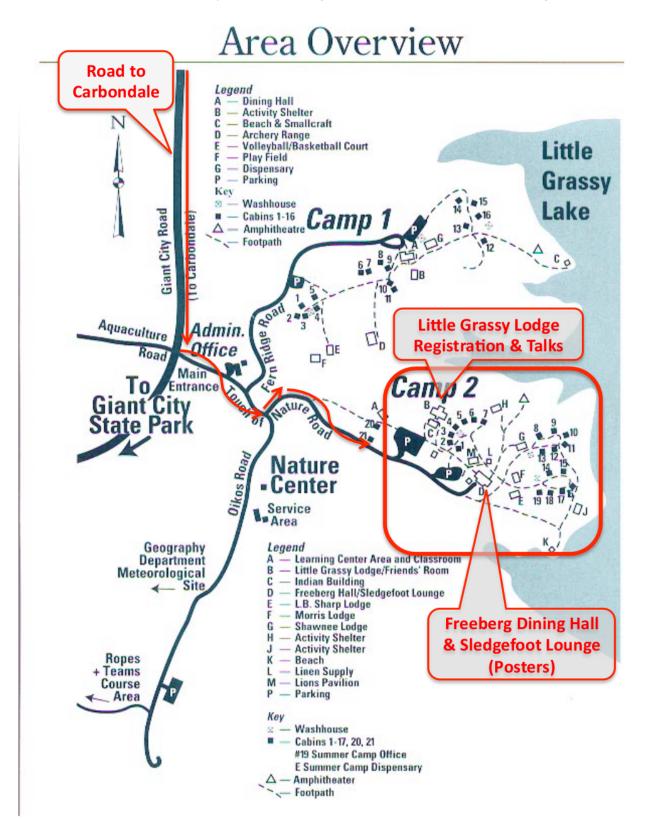
The 28th Gibbs Conference on Biothermodynamics

2014 Gibbs Conference on Biothermodynamics

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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

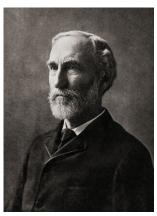
February, 1987

Discussion of the discipline: Thermodynamics in Biological Systems
The Gumbo Shop, New Orleans, LA during the 31st 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, The Gibbs Conference on Biothermodynamics: Origins and Evolution. *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 Introduction: Twenty five years of the Gibbs Conference on Biothermodynamics *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

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 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

1996 Organizers: Jonathan B. Chaires and Michael L. Doyle Keynote Speakers: J. Michael Schurr and Allen Minton

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 and originator of the Society website. Articles of Incorporation and By Laws are available here: http://www.jhu.edu/~gibbs

Current Officers

- ❖ President: George Makhatadze, 2013 2014
- ❖ Vice President: Michael L. Johnson, 2011 2014
- ❖ Secretary: Liskin Swint-Kruse, 2013 2017
- ❖ Treasurer: John J. "Jack" Correia, Oct 2010 Oct 2017

Board of Directors, listed alphabetically

- David Bain, Past President
- Patricia Clark, President Elect
- John J. Correia, Treasurer
- Michael L. Johnson, Vice President
- George Makhatadze, President
- Madeline Shea
- Liskin Swint-Kruse, Secretary

Past Presidents

Gary Ackers
Jack Correia
D. Wayne Bolen
Madeline Shea
Dorothy Beckett
Jonathan (Brad) Chaires
Tim Lohman
Luis Marky
Bertrand Garcia-Moreno E.
Karen Fleming
Doug Barrick
David Bain

Past Treasurer

2001-2011 Michael L. Johnson

Past Secretary

2004-2013 Margaret A. Daugherty

Committees & Other Contributions

Ackers Lecturer Selection Committee – Micheal Brenowitz, Chair Gibbs Society Website Hosting – Karen Fleming (2010 –)
GoogleDocs Application/Registration & PayPal – Nathan Baker and 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

6th Annual Gary K. Ackers Lecture

2014 Lecturer – David E. Draper, Johns Hopkins University and Reed College

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.

△Gibbs₂₈ • Saturday Evening • September 20, 2014

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 Mugs and Caps - pick up at registration

Saturday Night Thermo – Event for trainees only

Faculty Organizers

Vince LiCata, Louisiana State University & Susan Pedigo, University of Mississippi

Trainee Moderators: Liam Hovey, Shea lab, University of Iowa

Jackie Thompson, Carlson lab, University of Kansas Medical Center

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. PP_{II} propensities in IDPs measured by R_h compaction from glycine substitutions Micheal Tarver, Whitten lab, Texas State University
- 2. How does structure influence the folding pathway in GB3? Dinesh Yadav, Fitzkee lab, Mississippi State University
- Functional unfolding in adenylate kinase
 Jeremy Anderson, Hilser lab, Johns Hopkins University
- Single restorative mutations alter stability and fibril formation in an amyloidogenic light chain protein
 Marta Marin-Argany, Ramirez-Alvarado lab, Mayo Clinic
- 5. Thermodynamic studies of metal and substrate binding in taurine dioxygenase Kate Henderson, Emerson lab, Mississippi State University
- 6. Identifying functional mimetics of histone deacetylase using isothermal titration calorimetry

Sophia Robinson, Jin lab, DePaul University

- 7. Allosteric cooperativity of protein kinase A Jonggul Kim, Veglia lab, University of Minnesota
- 8. Simulation of the *salmonella* four-U thermometer to improve AMBER force field parameters

Angelo Setaro, Chen lab, University at Albany, State University of New York

7:00 – 7:15 pm Refreshment break

7:15 – 8:15 pm Career panel – Session open to all trainees

Dr. Nichola Garbett, University of Louisville

Dr. Adrian Whitty, Boston University

Dr. Sukesh Bhaumik, Southern Illinois University

8:15 pm Adjourn to reception in Indian Lodge

Δ Gibbs₂₈ • Sunday Morning • September 21, 2014

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

Membrane Proteins

8:30 – 8:35 am	Welcome by Jack Correia, Gibbs Society Treasurer
Moderator	Venkata Machha, Auton lab, Mayo Clinic
8:35 – 8:50 am	Introduction to the 28 th Annual Gibbs Conference Keynote Speaker Dorothy Beckett, University of Maryland
8:50 – 9:30 am	Keynote Lecture Driving forces for the sorting and folding of outer membrane proteins Karen G. Fleming, Johns Hopkins University
9:30 – 9:50 am	Thermal denaturation of membrane proteins – membrane protein unfolding Zhaoshuai Wang, Wei lab, University of Kentucky
9:50 – 10:10 am	Thermodynamic landscape along the membrane insertion and refolding pathway of the diphtheria toxin T domain Mauricio Vargas-Uribe, Ladokhin lab, University of Kansas Medical Center
10:10 – 10:40 am	Break – Refreshments in Indian Lodge
10:40 – 11:10 am	Exploring the edges of protein folding energy landscapes Patricia L. Clark, University of Notre Dame
11:10 – 11:30 am	Aromatic residues display a modest energetic depth-dependence in lipid bilayers Sarah C. McDonald, Fleming lab, Johns Hopkins University
11:30 am – noon	Membrane-binding thermodynamics explain the mechanism and selectivity of antimicrobial lipopeptides: results from molecular simulation Alan Grossfield, University of Rochester Medical Center
noon	Conference photo near Freeberg Hall
12:05 pm	Lunch in Freeberg Hall

Free Time until Late Afternoon Session.

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

∆Gibbs₂₈ • Sunday Afternoon • September 21, 2014

Biophysical Relationships

Moderator	Catherine Chaton, Herr lab, Cincinnati Children's Hospital Medical Center
3:00 – 3:30 pm	The dark energy of proteins comes to light: motion and conformational entropy in protein function A. Joshua Wand, University of Pennsylvania
3:30 – 3:50 pm	The dynamic basis for negative cooperativity in thymidylate synthase Bradley T. Falk, Lee lab, University of North Carolina at Chapel Hill
3:50 – 4:20 pm	Hemoglobin, more than an honorary enzyme Juliette T.J. Lecomte, Johns Hopkins University
4:20 – 4:50 pm	Break – Refreshments in Indian Lodge
4:50 – 5:10 pm	Ligand binding of a Tiam2 PDZ domain quadruple mutant: thermodynamic and dynamic underpinnings for the switched specificity Xu Liu, Fuentes lab, University of Iowa
5:10 – 5:40 pm	Allosteric control of caspases in cell death and signaling A. Clay Clark, North Carolina State University
5:40 – 6:00 pm	The vWF A3-domain maintains its native fold upon disruption of the disulfide bond: A quantitative analysis applying the urea-temperature phase diagram method Alexander Tischer, Auton lab, Mayo Clinic
6:00 – 6:30 pm	Protein electrostatic network optimization using a polarizable X-ray refinement target and dead-end elimination: improved PCNA structures yield functional insights Michael J. Schnieders, University of Iowa
6:30 – 6:35 pm	General Discussion
6:35 pm	Dinner in Freeberg Hall

△Gibbs₂₈ • Sunday Evening • September 21, 2014

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

∆Gibbs₂₈ • Monday Morning • September 22, 2014

Posters to be presented on Monday night may be mounted as soon as space is available on Sunday night.

Airport Ride Board will be available in Little Grassy Lodge, near check-in window

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

Nucleic Acids

8:30 – 8:35 am	Announcements by Organizers
Moderator	Dinesh Yadav, Fitzkee lab, Mississippi State University
8:35 – 8:50 am	Introduction to the Gary K. Ackers Lecture in Biothermodynamics Kathleen B. Hall, Washington University
8:50 – 9:30 am	6 th Annual Gary K. Ackers Lecture Zen and the art of RNA folding David E. Draper, Johns Hopkins University and Reed College
9:30 – 9:50 am	Revealing transient structures of nucleosomes as DNA unwinds Yujie Chen, Pollack lab, Cornell University
9:50 – 10:10 am	Effect of loop length on the stability of DNA hairpin loops and pseudoknots Calliste Reiling, Marky lab, University of Nebraska Medical Center
10:10 – 10:40 am	Break – Refreshments in Indian Lodge
10:40 – 11:10 am	Yeast Rap1 interacts with dsDNA in multiple binding modes regulated by the wrapping loop and RCT domain Roberto Galletto, Washington University
11:10 – 11:30 am	Sequence-specific incorporation of DNA into protein-based biomaterials Kelly Churion, Bondos lab, Texas A&M Health Science Center
11:30 am – noon	RNA:protein binding, linkage, and allostery Kathleen B. Hall, Washington University
noon – 12:05 pm	Vendor introduction
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.

∆Gibbs₂₈ • Monday Afternoon • September 22, 2014

Macromolecular Complexes

Moderator	James Campbell, Kim lab, Baylor College of Medicine
3:00 – 3:30 pm	Counteracting hyperglycemia by targeting allosteric regulation of liver pyruvate kinase Aron W. Fenton, University of Kansas Medical Center
3:30 – 3:50 pm	Conformational dynamics in tryptophan repressor Balasubramanian Harish, Carey lab, Princeton University
3:50 – 4:20 pm	Modeling coupled protonation and conformational equilibria Jana Shen, University of Maryland at Baltimore
4:20 – 4:50 pm	Break – Refreshments in Indian Lodge
4:50 – 5:10 pm	Breaking the IQ code: deciphering the keys for tight CaM-NaV interaction Dagan C. Marx, Shea lab, University of Iowa
5:10 – 5:40 pm	Upper limits of protein-ligand and protein-protein binding energy Adrian Whitty, Boston University
5:40 – 6:00 pm	Comparative analysis of CSL binding partners by isothermal titration calorimetry Nassif Tabaja, Kovall lab, University of Cincinnati
6:00 – 6:20 pm	DNA binding by RecA from <i>Deinococcus radiodurans</i> and <i>Escherichia coli</i> to short DNA oligomers Jaycob D. Warfel, LiCata lab, Louisiana State University
6:20 – 6:25 pm	General Discussion
6:25 pm	Dinner in Freeberg Hall

\triangle Gibbs₂₈ • Monday Evening • September 22, 2014

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

∆Gibbs₂₈ • Tuesday Morning • September 23, 2014

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

7:30 - 8:30 am **Breakfast served in Freeberg Hall**

Unfolded Micfolded and Disordered Proteins

Unfolded, Misfolded, and Disordered Proteins
Closing announcements by organizers
Micheal Tarver, Whitten lab, Texas State University
Disordered intermediate states: calcineurin Trevor P. Creamer, University of Kentucky
Secondary structure elements and tertiary interactions within the disordered RAM region of the Notch receptor are important for Notch signaling Kathryn Sherry, Barrick lab, Johns Hopkins University
Calculating the contributions from voids and hydration to the change in volume upon protein unfolding Calvin Chen, Makhatadze lab, Rensselaer Polytechnic Institute
Break – Refreshments in Indian Lodge
Biophysics of chemical denaturation Alex S. Holehouse, Pappu lab, Washington University
Dynamics and energy contributions for transport of pertactin through an aerolysin nanopore Benjamin Cressiot, Clark lab, University of Notre Dame
Light chain amyloidosis: a journey from thermodynamics and structural biology to cell toxicity and (hopefully) a cure Marina Ramirez-Alvarado, Mayo Clinic
Box lunch in Freeberg Hall
Please leave your keys at the counter in Little Grassy Lodge