



**The 27<sup>th</sup> Annual Gibbs Conference on  
Biothermodynamics**

**October 5-8, 2013**

**Organized by**

**James L. Cole and Aron W. Fenton**

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

**Sponsored by**

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The 27<sup>th</sup> Gibbs Conference on Biothermodynamics



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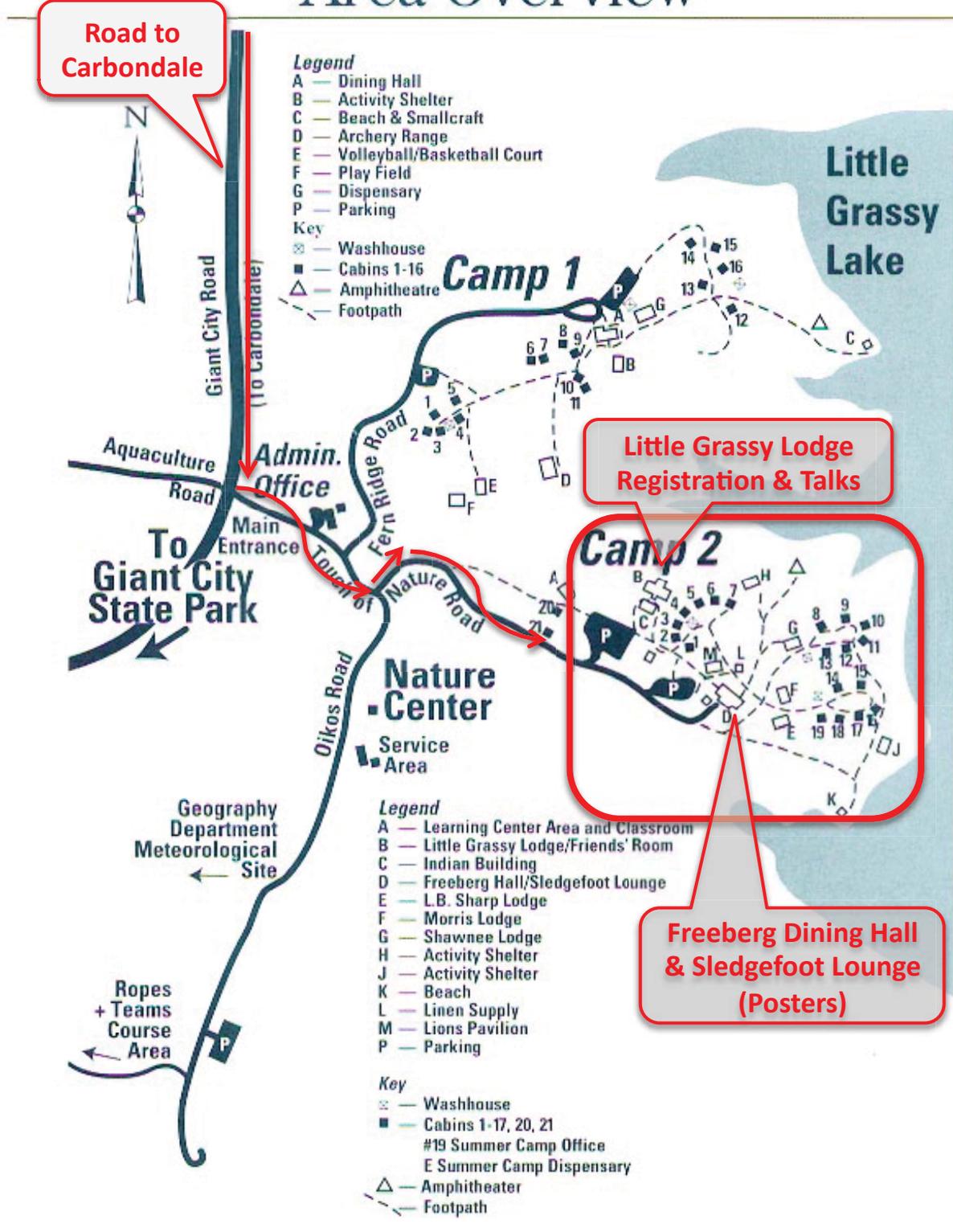
## Sponsors

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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.

## Area Overview



# The Gibbs Conference on Biothermodynamics

## History

*Fall, 1986*

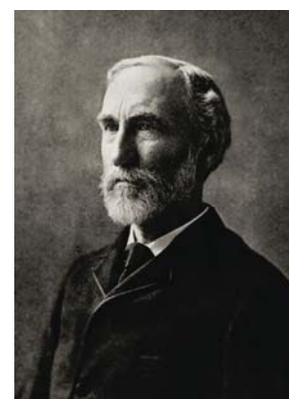
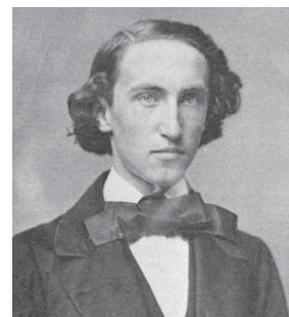
Discussion of the discipline: Thermodynamics in Biological Systems  
At the Gill residence in Vail, Colorado  
Gary Ackers, Wayne Bolen, Ernesto Freire, Stan Gill, Jim Lee

*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, 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

- 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 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.

# 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: David Bain, 2012-2013
- ❖ Vice President: Michael L. Johnson, 2011 - 2013
- ❖ Secretary: Margaret A. Daugherty, 2004 – 2013
- ❖ Treasurer: John J. Correia, March 2011 – October, 2016

## Board of Directors, listed alphabetically

- ❖ David Bain, President
- ❖ Douglas Barrick, Past President
- ❖ John J. Correia, Treasurer
- ❖ Margaret Daugherty, Secretary
- ❖ Michael L. Johnson, Vice President
- ❖ George Makhataдзе, President Elect
- ❖ Madeline Shea

## Past Presidents

|           |                           |
|-----------|---------------------------|
| 2001-2002 | Gary Ackers               |
| 2002-2003 | Jack Correia              |
| 2003-2004 | D. Wayne Bolen            |
| 2004-2005 | Madeline Shea             |
| 2005-2006 | Dorothy Beckett           |
| 2006-2007 | Jonathan (Brad) Chaires   |
| 2007-2008 | Tim Lohman                |
| 2008-2009 | Luis Marky                |
| 2009-2010 | Bertrand Garcia-Moreno E. |
| 2010-2011 | Karen Fleming             |
| 2011-2012 | Doug Barrick              |

## Past Treasurer

|           |                    |
|-----------|--------------------|
| 2001-2011 | Michael L. Johnson |
|-----------|--------------------|

## 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 – Margaret Daugherty  
Saturday Night Thermo Organizers – Liskin Swint-Kruse and Vincent J. LiCata  
With thanks to Alan Teska at the Touch of Nature Conference Center

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

2013 Lecturer – *Bertrand Garcia-Moreno E., Department of Biophysics, Johns Hopkins 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.

## **△Gibbs<sub>27</sub> • Saturday Evening • October 5, 2013**

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 Bazaar – pick up mugs purchased at registration**

### **Saturday night thermo – Event for trainees only**

#### **Faculty Organizers**

Vince LiCata, Louisiana State University & Liskin Swint-Kruse, University of Kansas Medical Center

**Trainee Moderators:** Jaycob Warfel, LiCata Lab, Louisiana State University  
Kate Henderson, Emerson Lab, Mississippi State University

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. **The annexin-lipid party line: Communication between protein and membrane**  
Anika Rannikko, Hinderliter Lab, University of Minnesota - Duluth
2. **Structural and dynamic features underlie the switch of ligand binding specificity in a Tiam1 PDZ domain mutant**  
Xu Liu, Fuentes Lab, University of Iowa
3. **Cyclipostin derivatives as inhibitors of rat hormone sensitive lipase**  
Elena Vasilieva, Dupureur Lab, University of Missouri – St. Louis
4. **Domain interactions in VA I RNA mediate high-affinity PKR binding**  
Katherine Launer-Felty, Cole Lab, University of Connecticut
5. **Distinctive solvation patterns make renal osmolytes diverse**  
Prem Sinha, Rösgen Lab, Penn State College of Medicine
6. **Are proton binding reactions in proteins coupled to local conformational fluctuations?**  
Daniel Richman, Garcia-Moreno Lab, Johns Hopkins University
7. **Calmodulin recognition of anti-parallel nested binding sites in the neuronal voltage-dependent sodium channel Na<sub>v</sub>1.2**  
Mark Miller, Shea Lab, University of Iowa
8. **Contributions of alanine residues to the hydrodynamic radius of p53(1-93)**  
Romel Perez, Whitten Lab, Texas State University

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

7:15 – 8:15 pm     **Career panel – Session open to all trainees**  
Andrew Robertson, National Psoriasis Foundation  
Ana-Maria Soto, Towson University  
Catherine Royer, Rensselaer Polytechnic Institute

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

## **△Gibbs<sub>27</sub> • Sunday Morning • October 6, 2013**

7:00 - 8:15 am      **Breakfast served in Freeberg Hall**

### **Macromolecular Folding and Stability**

8:30 - 8:35 am      **Welcome by David Bain**, Gibbs Society President

*Moderator:*      Giselle Jacobson, Clark Lab, University of Notre Dame

8:35 - 8:50 am      **Introduction to the 27<sup>th</sup> Annual Gibbs Conference Keynote Speaker**  
George Makhatadze, Rensselaer Polytechnic Institute

8:50 – 9:30 am      **Keynote Lecture**  
**Measuring coupling energies in simple proteins and extrapolating to complicated proteins**  
Doug Barrick, Johns Hopkins University

9:30 – 9:45 am      **Capped G-quadruplexes: A model for a looped out motif flanked by duplex DNA**  
Vu Le, Lewis Lab, Mississippi State University

9:45 – 10:00 am      **Probing N-H - - N hydrogen bond “strain” in a conserved N-capping motif**  
Matthew Preimesberger, Lecomte Lab, Johns Hopkins University

10:00 – 10:30 am      **Break – Refreshments in Indian Lodge**

10:30 – 11:00 am      **Studying the folding of individual residues in a small protein**  
Nicholas Fitzkee, Mississippi State University

11:00 – 11:15 am      **Exchange of putrescine<sup>2+</sup> and Mg<sup>2+</sup> in the ion atmosphere of RNA: Contributions to folding and gene regulation**  
Robert Trachman, Draper Lab, Johns Hopkins University

11:15 – 11:45 am      **Tug-of-war between thermodynamic stability and actin-binding function of tandem calponin-homology domains**  
Krishna Mallela, University of Colorado Anschutz Medical Campus

11:45 am              **Conference photo near Freeberg Hall**

11:50 am              **Lunch in Freeberg Hall**

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

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

## $\Delta$ Gibbs<sub>27</sub> • Sunday Afternoon • October 6, 2013

### Nucleic Acids and Their Binding Partners

*Moderator:* Irine Khutsishvili, Marky Lab, University of Nebraska Medical Center

3:00 – 3:30 pm **Structured mRNA induces the ribosome into a hyper-rotated state**  
Peter Cornish, University of Missouri

3:30 – 3:45 pm **How do the different DNA-binding modes of *E. coli* SSB affect function?**  
Vincent Waldman, Lohman Lab, Washington University

3:45 – 4:15 pm **Looking at multicomponent systems with small angle x-ray scattering: Ions around DNA; DNA around proteins**  
Lois Pollack, Cornell University

4:15 – 4:35 pm **Break – Refreshments in Indian Lodge**

4:35 – 4:50 pm **Binding and salt linkages of HIV-1 reverse transcriptase with different DNA and RNA substrates reflect polymerization versus RNase H compatible modes of interaction**  
Hiromi Brown, LiCata Lab, Louisiana State University

4:50 – 5:20 pm **DNA binding behavior of sequence specific polyamides**  
Cynthia Dupureur, University of Missouri - St Louis

5:20 – 5:35 pm **Yeast Rap1 interacts with telomeric sequences with multiple binding modes**  
Erik Feldmann, Galletto Lab, Washington University

5:35 – 6:05 pm **Substrate recognition by human O6-alkylguanine DNA alkyltransferase**  
Michael Fried, University of Kentucky

6:05 – 6:15 pm **General Discussion**

6:15 pm **Dinner in Freeberg Hall**

## $\Delta$ Gibbs<sub>27</sub> • Sunday Evening • October 6, 2013

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.

Sponsors displays in Freeberg (upper level) – near beer, wine and soft drinks

## **△Gibbs<sub>27</sub> • Monday Morning • October 7, 2013**

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

7:00 - 8:15 am      **Breakfast served in Freeberg Hall**

### **Structure / Thermodynamic Correlations**

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

*Moderator:*      Keith Connaghan, Bain Lab, University of Colorado Anschutz Medical Campus

8:35 – 8:50 am      **Introduction to the Gary K. Ackers Lecture in Biothermodynamics**  
David Bain, University of Colorado Anschutz Medical Campus

8:50 – 9:30 am      **5th Annual Gary K. Ackers Lecture**  
**pH-Dependent processes in proteins**  
Bertrand Garcia-Moreno E., Johns Hopkins University

9:30 – 9:45 am      **Impact of pH on the structure and function of neural cadherin**  
Matt Dukes, Pedigo Lab, University of Mississippi

9:45 – 10:00 am      **Revisiting thermodynamic cooperativity: Studying TRBP interactions with double stranded RNA**  
Roderico Acevedo, Showalter Lab, Pennsylvania State University

10:00 – 10:20 am      **Break – Refreshments in Indian Lodge**

10:20 – 10:50 am      **Molecular switches in signaling and disease**  
Linda Nicholson, Cornell University

10:50 – 11:05 am      **Thermodynamics of cationic and anionic surfactant interaction**  
Vytautas Petrauskas, Matulis Lab, Vilnius University

11:05 – 11:35 am      **Structure, dynamics and inhibition of Tiam1 PDZ domain complexes**  
Ernesto Fuentes, University of Iowa

11:35 – 11:40 am      **Vendor introduction**

11:40 am              **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

### **Trainee funding panel**

2:00 – 3:00 pm      **Discussion of trainee fellowship applications - open to all attendees**

Trevor Creamer, University of Kentucky  
Sarah Bondos, Texas A&M Health Science Center  
Dorothy Beckett, University of Maryland

## **ΔGibbs<sub>27</sub> • Monday Afternoon • October 7, 2013**

### **Macromolecular Interactions**

*Moderator:* Clarissa Weaver, Lucius Lab, University of Alabama at Birmingham

3:15 – 3:45 pm **Transition metal homeostasis: Allosteric switching by metal sensor proteins**  
David Giedroc, Indiana University

3:45 – 4:00 pm **Heterotropic linkage between protein-protein and protein RNA interactions determines protein partitioning in the snRNPs**  
Sandra Williams, Hall Lab, Washington University

4:00 – 4:30 pm **Engineering linked-equilibria into protein interfaces to allow regulation of protein interactions**  
James Horn, Northern Illinois University

4:30 – 4:45 pm **Break – Refreshments in Indian Lodge**

4:45 – 5:15 pm **Biophysical studies on the A1 and A3 domain homologues of von Willebrand factor**  
Matthew Auton, Mayo Clinic

5:15 – 5:45 pm **Structure and function of a novel phosphopeptide binding domain from the transcriptional corepressor MINT**  
Rhett Kovall, University of Cincinnati College of Medicine

5:45 – 6:00 pm **Discussion**

6:00 pm **Dinner in Freeberg Hall**

## **ΔGibbs<sub>27</sub> • Monday Night • October 7, 2013**

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<sub>27</sub> • Tuesday Morning • October 8, 2013**

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

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

### **Modeling and Computation**

8:40 – 8:45 am      **Closing announcements by organizers**

*Moderator:*      Catie Shelton, Herr Lab, University of Cincinnati College of Medicine

8:45 – 9:15 am      **Computation and calorimetry: What can we learn from each other?**  
Michael Gilson, University of California-San Diego

9:15 – 9:30 am      **The tertiary architecture of LacI/GalR proteins accommodates multiple networks of functionally important positions**  
Daniel Parente, Swint-Kruse Lab, University of Kansas Medical Center

9:30 – 10:00 am    **Temperature effects on the hydrodynamic radius of intrinsically disordered proteins**  
Steven Whitten, Texas State University

10:00 – 10:20 am   **Break – Refreshments in Indian Lodge**

10:20 – 10:40 am   **Rational design of two proteins with 80% sequence identity but different folds using sequence transplantation**  
Lauren Porter, Potomac Affinity Proteins

10:40 – 10:55 am   **Deletion of the connecting linker between kringle-1 and kringle-2 in prothrombin stabilizes the zymogen in a collapsed conformation**  
Nicola Pozzi, Di Cera Lab, Saint Louis University

10:55 – 11:25 am   **Molecular modeling of the ligand binding free energy and conformational rearrangements in AMPA type glutamate receptors**  
Maria Kurnikova, Carnegie Mellon University

11:25 am            **Box lunch available in Freeberg Hall**

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