

♥ free energy in the woods ♥



26th Annual
Gibbs Conference
on Biothermodynamics

September 22-25, 2012

Organized by:

Patricia L. Clark & Aaron L. Lucius

Touch of Nature Environmental Center
Southern Illinois University
Carbondale, IL

SponSors:

Agilent - Aviv - Chreston - GE Healthcare - Horiba
ISS - JASCO - Micromath - Olis - PTI - UAB Chemistry

Table of Contents

The 26th Annual Gibbs Conference on Biothermodynamics

Introduction

<i>Map of Touch of Nature</i>	2
<i>History and List of Meetings</i>	3
<i>Gibbs Society Governance – Incorporation, Officers, Committees</i>	6
<i>The Gary K. Ackers Lecture in Biothermodynamics</i>	7

Meeting schedule

<i>Saturday, September 22</i>	8
<i>Sunday, September 23</i>	9
<i>Monday, September 24</i>	11
<i>Tuesday, September 25</i>	13

List of Posters

<i>Poster information</i>	14
<i>Session I - Sunday</i>	14-18
<i>Session II - Monday</i>	19-22

Abstracts

<i>Speakers</i>	23-46
<i>Posters – Session I – Sunday Night</i>	47-95
<i>Posters - Session II – Monday Night</i>	96-129

List of participants

<i>Alphabetical</i>	130-146
<i>Directory by Laboratory</i>	147-150

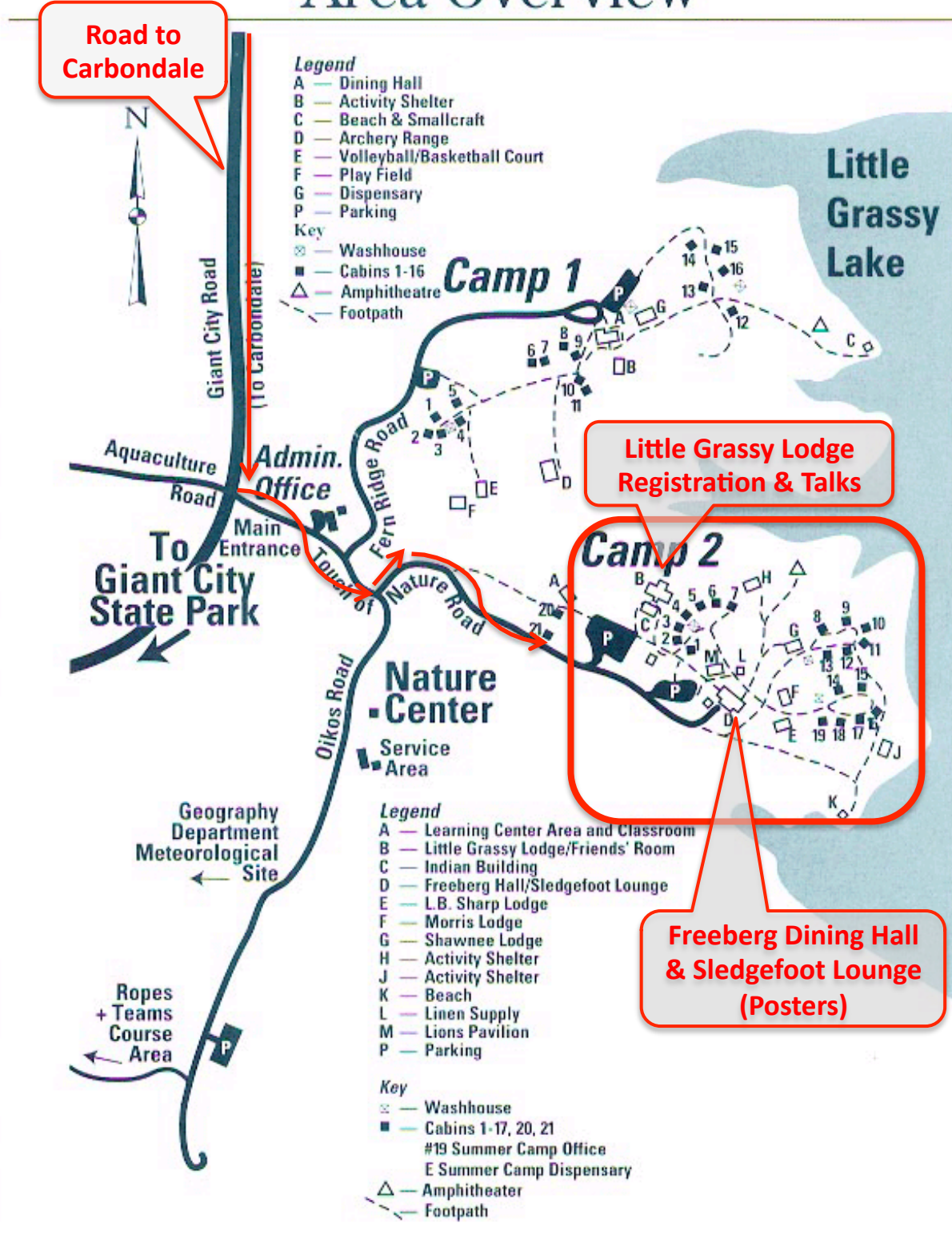
Sponsors

<i>Listing and Product Information</i>	151
--	-----

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

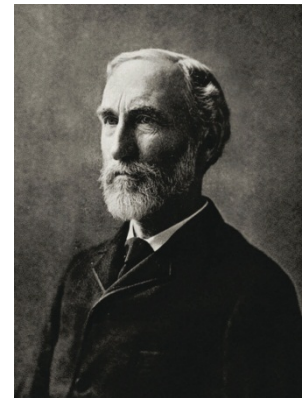
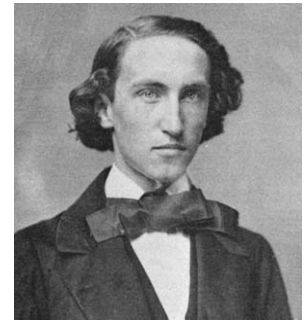
February, 1987

Discussion of the discipline: Thermodynamics in Biological Systems
The Gumbo Shop, New Orleans, LA during the 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)

A complete list of scientific contributions by past organizers to a special issue of *Biophysical Chemistry* commemorating the 25th Gibbs Conference follows the list of meetings.



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 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
Saturday Night Thermo Organizers – Liskin Swint-Kruse and Vincent J. LiCata
Editors of Special Issue of *Biophysical Chemistry* – Enrico Di Cera, Tim Lohman, Jack Correia

2012 Organizers: Patricia L. Clark and Aaron L. Lucius
Keynote Speaker: Terry G. Oas
The Gary K. Ackers Lecture in Biothermodynamics: Enrico Di Cera

Gibbs Society Governance

Incorporation

In 2002, the *Gibbs Society on 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: Doug Barrick, 2011-2012
- ❖ Vice President: Michael L. Johnson, 2010 - 2013
- ❖ Secretary: Margaret A. Daugherty, 2004 – 2013
- ❖ Treasurer: John J. Correia, March 2011 – October, 2016

Board of Directors, listed alphabetically

- ❖ Douglas Barrick, President
- ❖ David Bain, President Elect
- ❖ John J. Correia, Treasurer
- ❖ Margaret Daugherty, Secretary
- ❖ Karen Fleming, Past President
- ❖ Michael L. Johnson, Vice President
- ❖ 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

Past Treasurer

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

Committees & Other Contributions

Ackers Lecturer Selection Committee – James Ching Lee, Chair
Gibbs Society Website Hosting – Karen Fleming (2010 -)
GoogleDocs Application/Registration & PayPal – Nathan Baker and Jack Correia
Mailing List – Margaret Daugherty
Fundraising – Aaron L. Lucius and Jack Correia
Gibbs26 Website Hosting – Patricia Clark
Catering, Wine and Meal Contract – Jack Correia, Patricia L. Clark, and Aaron L. Lucius
With thanks to Alan Teska at the Touch of Nature Conference Center!

4th Annual Gary K. Ackers Lecture

2012 Lecturer – Enrico Di Cera, Edward A. Doisy Department of Biochemistry and Molecular Biology, St. Louis University School of Medicine

This lecture honors the scientific contributions of Gary K. Ackers (1939-2011) to the field of Biological Thermodynamics. He served on the faculty of the University of Virginia, and the 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.

ΔGibbs₂₆ • Saturday Evening • September 22, 2012

4:00 – 10:00 pm

Check-in at Little Grassy Lodge

7:30 – 10 pm

Open Reception in Indian Lodge – Light refreshments, beer, wine and soft drinks

Participants are expected to make dinner arrangements independently.

Gibbs T-shirt Bazaar – Please pay for the shirts ordered during registration.

Saturday Night Thermo – Events for Trainees Only

Faculty Organizers

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

Trainee Moderators *Esther Braselmann, Laboratory of Patricia L. Clark, Notre Dame and Dan Parente,*

Laboratory of Liskin Swint-Kruse, KUMC

5:30 pm

Freeberg Hall – Dinner for trainees who registered in advance

6:00 pm

Flash Talks (Poster Introductions) – Session open to all trainees

1. **Structural Insight into the Recognition of Proteins by RNA Aptamers**
Frances-Camille Solomon Padlan, Brenowitz Lab, Albert Einstein College of Medicine
2. **Biochemical Characterization of Myxococcus xanthus Histidine Kinase-Response Regulator Homologs Reveals Signaling Specificity in Two-Component Systems**
Nitija Tiwari, Fuentes Lab, University of Iowa
3. **An Enthalpic "On/Off Switch" linking DNA binding and nucleotide incorporation activity in Pol I DNA Polymerases**
Hiromi S Brown, LiCata Lab, Louisiana State University
4. **Thermodynamic Stability of the Von Willebrand Factor A3 Domain Assessed by the Urea-Temperature Phase Diagram Method**
Alexander Tischer, Auton Lab, Baylor COM
5. **Engineering T-Cell Receptors to Optimize Anti-Tumor Immunity**
Lance Hellman, Baker Lab, University of Notre Dame
6. **Ligand-induced synthetic prions: detection of a prion intermediate.**
Reagan Meredith, Whitten Lab, Texas State University - San Marcos
7. **Stability of AcrB trimer and function of AcrAB-TolC pump**
Linliang Yu, Wei Lab, University of Kentucky
8. **Thermodynamic studies of the binding of substituted porphyrins to G-quadruplex DNA**
Vu H Le, Lewis Lab, Mississippi State University

7:00 – 7:15 pm

Refreshment Break

7:15 pm

Career Panel – session open to all trainees

Nathan Baker, Pacific Northwest National Laboratory

Kausiki Datta, Hoffman La Roche

Verna Frasca, GE Healthcare

8:15 pm

Adjourn to reception in Indian Lodge

Δ Gibbs₂₆ • Sunday Morning • September 23, 2012

7:00 – 8:15 am Breakfast served in Freeberg Hall

Folding and Disorder

8:20 – 8:25 am **Welcome by Doug Barrick**, Gibbs Society President

Moderator: Frances-Camille Padlan, Brenowitz Lab, Albert Einstein College of Medicine

8:25 – 8:40 am **Introduction to the 26th Annual Gibbs Conference Keynote Speaker**
Patricia L. Clark, University of Notre Dame

8:40 – 9:20 am **Keynote Lecture**
Using kinetics to measure and interpret thermodynamic data: coupled folding & binding and multidomain folding
Terry G. Oas, Duke University

9:20 – 9:40 am **Pathway selection for folding of the leucine-rich repeat protein PP32**
Thuy P. Dao, Barrick Lab, Johns Hopkin University

9:40 – 10:10 am **Virtues of Protein Disorder in Assembly and Regulation of Large Molecular Machines**
Elisar Barbar, Oregon State University

10:10 – 10:30 am Break, delicious Gibbs coffee will be served!

10:30 – 11:00 am **Why is Taq DNA Polymerase so Stable?**
Vince J. LiCata, Louisiana State University

11:00 – 11:20 am **Combining ITC with carbon detected NMR methods to probe folding-upon-binding events involving intrinsically disordered proteins**
Scott A Showalter, Penn State University

11:20 – 11:40 am **Extracting mechanistic information about the Hsp90 molecular chaperone with a model unfolded protein substrate**
Timothy O Street, Agard Lab, UCSF

11:40 – 12:10 pm **Pressure effects on protein folding**
Catherine Ann Royer, INSERM

12:15 pm Conference photo near Freeberg Hall

12:15 pm Lunch in Freeberg Hall

Free time until Late Afternoon Session.
Information about local parks & Attractions is available near the entrance to Little Grassy Lodge.

Δ Gibbs₂₆ • Sunday Afternoon • September 23, 2012

Stability of Macromolecules

Moderator:

Michael J. Harms, Thornton Lab, University of Oregon

3:00 – 3:30 pm

Oxysterol perturbation of lipid bilayers

Nathan A Baker, Pacific Northwest National Laboratory

3:30 – 3:50 pm

Molecular dynamics simulations of electrostatic and hydrophobic interactions in concentrated solutions: significant differences between non-polarizable force fields

Casey T Andrews, Elcock Lab, University of Iowa

3:50 – 4:10 pm

Modeling Autotransporter Folding and Secretion

Igor Drobnak, Clark Lab, University of Notre Dame

4:10 – 4:40 pm

Molecular Mechanism for the Preferential Exclusion of TMAO from Protein Surfaces

Angel E Garcia, Rensselaer Polytechnic Institute

4:40 – 4:55 pm

Break, more delicious Gibbs coffee, trail mix, and more ☺

4:55 – 5:25 pm

Modulation of the protein folding landscape by electrostatic interactions

George Makhatadze, RPI

5:25 – 5:45 pm

Deciphering the ubiquitin “code”: Assembly and solution NMR studies of all-natural polyubiquitin chains of every possible lysine linkage

Carlos A Castaneda, Fushman Lab, University of Maryland, College Park

5:45 – 6:15 pm

Synergies and snags in balancing folding and function of natural and designed beta-trefoil proteins

Elizabeth M Meiering, University of Waterloo

6:15 pm

Dinner in Freeberg Hall

Δ Gibbs₂₆ • Sunday Evening • September 23, 2012

8 – 10 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 Soda

ΔGibbs₂₆ • Monday Morning • September 24, 2012

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 Delicious Breakfast and a healthy serving of recovery in Freeberg Hall

Macromolecular Interactions

8:20 – 8:25 am Announcements by Organizers

Moderator: Kate Hayden, Graves Lab, University of Alabama at Birmingham

8:25 – 8:40 am **Introduction to the Gary K. Ackers Lecture in Biothermodynamics**
Madeline A. Shea, Carver College of Medicine, University of Iowa

8:40 – 9:20 am **4th Annual Gary K. Ackers Lecture in Biothermodynamics**
Conformational selection in trypsin-like proteases
Enrico Di Cera, Saint Louis University

9:20 – 9:40 am ***X. laevis* ISWI remodels nucleosomes through a random-walk**
Koan E M Briggs, Fischer Lab, University of Kansas

9:40 – 10:10 am **Conformational dynamics of a glutamate transporter homologue**
Olga Boudker, Weill Cornell University

10:10 – 10:30 am Break, apples, juice, and delicious Gibbs coffee!

10:30 – 11:00 am **Actin Filament Severing by Cofilin**
Enrique M De La Cruz, Yale University

11:00 – 11:20 am **Allosteric Pathways of Caspase-3**
Christine Cade, Clark Lab, North Carolina State University

11:20 – 11:40 am **Oxidative Footprinting of Fibrillar and Prefibrillar Oligomer Forms of Amyloid Beta**
Alexandra L Klinger, Axelsen Lab, University of Pennsylvania

11:40 – 12:10 pm **Comparative Studies of Allosteric Mechanism**
Jannette Carey, Princeton University

12:15 pm Lunch in Freeberg Hall

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

Free Time until Late Afternoon Session.

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

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

Δ Gibbs₂₆ •Monday Afternoon•September 24, 2012

Complex ASSEMBLIES

- Moderator:* Justin Miller, Lucius Lab, University of Alabama at Birmingham
- 3:00 – 3:30 pm **The assembly and functionalization of protein-based materials composed of a *Drosophila* transcription factor**
Sarah E. Bondos, Texas A&M Health Science Center
- 3:30 – 3:50 pm **Thermodynamic and hydrodynamic examination of ClpB assembly**
Jiabei Lin, Lucius Lab, University of Alabama at Birmingham
- 3:50 – 4:10 pm **Structural & Hydrodynamic Analysis Of A Novel Drug Delivery Vector: ELP[V5G3A2-150]**
Daniel F Lyons, Correia Lab, The University of Mississippi Medical Center
- 4:10 – 4:30 pm Break, trail mix, tea, maybe some cookies...
- 4:30 – 5:00 **Measuring the dimerization free energy of a CLC Cl-/H+ antiporter in lipid bilayers by single molecule fluorescence analysis**
Janice L. Robertson, Brandeis University
- 5:00 – 5:20 pm **Activation of PKR by stem-loop RNAs with flanking ssRNA tails**
Christopher B Mayo, Cole Lab, University of Connecticut
- 5:20 – 5:50 pm **Zinc-dependent protein self-assembly governs intercellular adhesion in Staphylococcal biofilms**
Andrew B. Herr, University of Cincinnati College of Medicine
- 6:00 pm Dinner in Freeberg Hall

Δ Gibbs₂₆ •Monday Evening•September 24, 2012

- 8 – 10 pm **Poster Session II in Sledgefoot (lower level) & Freeberg (upper level)**
Presenters with last name M to Z
Please remove posters before midnight to make room for Monday presenters.
- Sponsors Displays in Freeberg (upper level) – near Beer, Wine and Soda

ΔGibbs₂₆ • Tuesday Morning • September 25, 2012

Checkout - 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

7:00 – 8:15 am	Delicious Breakfast and a healthy serving of recovery in Freeberg Hall
	Protein Ligand Interactions
8:40 am	Closing Announcements by Organizers
<i>Moderator:</i>	Jennifer Starner-Kreinbrink, Clark Lab, Notre Dame
8:45 – 9:15 am	Molecular Recognition by $\alpha\beta$ T cell receptors Brian M Baker, University of Notre Dame
9:15 – 9:35 am	How can a ligand be a positive and negative allosteric effector for the same protein? Hesam N. Motlagh, Hilser Lab, Johns Hopkins University
9:35 – 9:55 am	Dissecting signal recognition and signal control in the MDR regulator, BmrR Herschel Wade, Johns Hopkins University
9:55 – 10:15 am	Break, you know what you're getting
10:15 – 10:45 am	Experimental description of a protein family: Critical experiments for the post-genomic era Liskin Swint-Kruse, The University of Kansas Medical Center
10:45 – 11:05 am	Developing solutes as probes of protein and nucleic acid processes Emily Guinn, Record Lab, University of Wisconsin Madison
11:05 – 11:35 am	Phl p 7: An Uncommonly Stable Polcalcin Michael T Henzl, University of Missouri
11:35 pm	Box lunch available in Freeberg Hall
Checkout	Please leave your room keys at the counter in Little Grassy Lodge