

22nd Annual Gibbs Conference on Biothermodynamics

Saturday, October 4 - Tuesday, October 7, 2008

Touch of Nature Environmental Center
Southern Illinois University
Carbondale, Illinois



Organizers

David L. Bain and Jannette Carey

Sponsors

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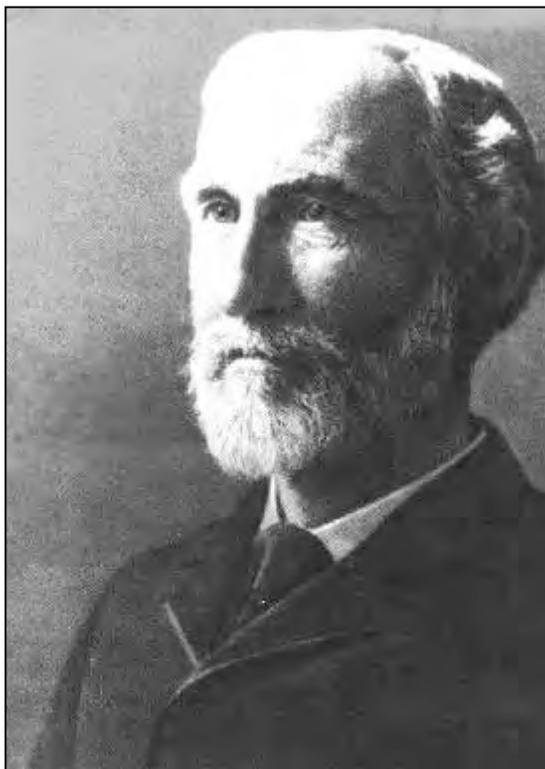
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Cover figure: First direct observation of allosteric structural transition by Felix Haurowitz at Charles University Prague, 1938. Needle-like crystals of oxyhemoglobin with intractably large unit cell were forgotten in the fridge, and turned into irregular purple flecks of deoxyhemoglobin after bacteria consumed all the oxygen (bottom). While Haurowitz later watched the sample in the microscope, red crystalline needles formed again where the surface of the droplet was in contact with air (top). From Perutz, MF. 1990 Mechanisms of cooperativity and allosteric regulation in proteins. Cambridge University Press.

1. The Gibbs Conference on Biothermodynamics

honors the legacy of



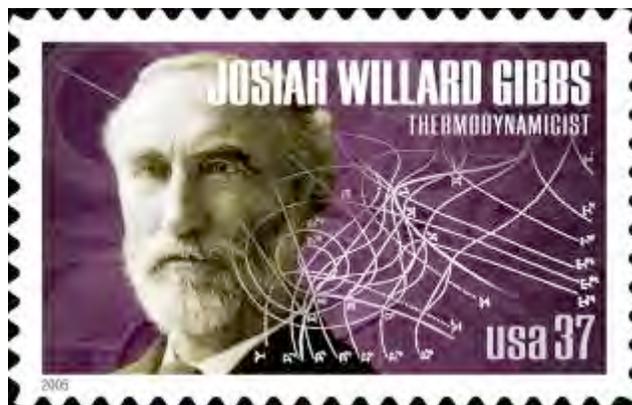
Josiah Willard Gibbs

1839 – 1903

“The greatest thermodynamicist of them all”
–John Fenn, 2002 Nobel Prize in Chemistry



USNS Josiah Willard Gibbs, 1958-1971



USPS Gibbs Stamp, released May 5, 2005

History of the Gibbs Conference on Biothermodynamics

Fall, 1986 1st discussion of the discipline, Thermodynamics in Biological Systems.
Vail, Colorado: Gary Ackers, Wayne Bolen, Ernesto Freire, Stan Gill, Jim Lee

Feb, 1987 2nd discussion of the discipline, Thermodynamics in Biological Systems.
New Orleans: Gary Ackers, Norma Allewell, Wayne Bolen, Ken Breslauer, Ken Dill,
Ernesto Freire, Stan Gill, Jim Lee

Annual Gibbs Conference on Biothermodynamics Touch of Nature Environmental Center, Carbondale, Illinois

- 1st – 1987 Organizers: Jim Lee and Wayne Bolen
- 2nd – 1988 Organizers: Gary Ackers and Michael Johnson
- 3rd – 1989 Organizers: Susan G. Frasier and Michael Johnson
- 4th – 1990 Organizers: Michael Johnson & Marty Straume
- 5th – 1991 Organizers: Gary Ackers & Tim Lohman
Keynote: Ernesto Freire
- 6th – 1992 Organizers: Jim Lee & Tomasz Heyduk
Keynotes: Serge Timasheff & John Schellman
- 7th – 1993 Organizers: Maurice Eftink and Glen Ramsay
Keynotes: Peter von Hippel and Julian Sturtevant
- 8th – 1994 Organizers: Enrico Di Cera and Madeline Shea
Keynotes: Gary Ackers and Kathleen S. Matthews
- 9th – 1995 Organizers: Kenneth P. Murphy and Michael D. Brenowitz
Keynotes: Victor Bloomfield and Mario Amzel
- 10th – 1996 Organizers: Jonathan B. Chaires and Michael L. Doyle
Keynotes: J. Michael Schurr and Allen Minton
- 11th – 1997 Organizers: Dorothy Beckett and Jack Correia
Keynote: Adrian Parsegian
- 12th – 1998 Organizer: Andy Robertson
Keynote: David Draper
- 13th – 1999 Organizers: Bertrand Garcia-Moreno and John Shriver
Keynotes: Wayne Bolen and Gary Ackers
- 14th – 2000 Organizers: George Turner and Kim Sharp
Keynotes: Steve White (replaced Rodney Biltonen)
- 15th – 2001 Organizers: Margaret A. Daugherty and Luis A. Marky
Keynote: George Rose
- 16th – 2002 Organizers: Michael Mossing and George Makhatadze
Keynote: Rodney Biltonin
- 17th – 2003 Organizers: Vince Hilser and Dick Sheardy
Keynote: Jim Lee
- 18th – 2004 Organizers: Doug Barrick and Kathleen Hall
Keynote: Ignacio Tinoco 3

- 19th – 2005 Organizers: Clay Clark and Trevor Creamer
Keynote: Carl Frieden
- 20th – 2006 Organizers: Karen Fleming and Rohit Pappu
Keynotes: Madeline Shea and Timothy Lohman
- 21st – 2007 Organizers: Brian M. Baker and Michael T. Henzl
Keynote: Jamie Williamson
- 22nd – 2008 Organizers: David Bain and Jannette Carey
Keynotes: Dorothy Beckett and Ken Dill

In 2002 The Gibbs Conference on Biothermodynamics incorporated as a mechanism of preserving the philosophy and spirit of the meeting. For a published 10-year history see Ackers and Bolen (1997) "The Gibbs Conference on Biothermodynamics: Origins and evolution." *Biophys. Chem.* **64**, 3-5.

President: Tim Lohman, October, 2007 – October, 2008
President Elect: Luis Marky, October 2008 - October 2009
Secretary: Margaret A. Daugherty, October, 2004 – October, 2008
Treasurer: Michael Johnson, October, 2002 – October, 2008

Past Presidents: Gary Ackers, October, 2001 – October, 2002
Jack Correia, October, 2002 – October, 2003
Wayne Bolen, October, 2003 – October, 2004
Madeline Shea, October, 2004 – October, 2005
Dorothy Beckett, October, 2005 – October, 2006
Jonathan B. Chaires, October, 2006 – October, 2007



The 2007 Gibbs Conference

2. Meeting Schedule

Saturday, October 4, 2008

4:00-7:00 pm Check-In at Little Grassy Lodge

7:00-10:00 pm Reception in Indian Room
Light refreshments/beverages

Sunday October 5, 2008

7:30-8:30 Breakfast in Freeberg Hall

8:45-8:50 Welcome: Timothy Lohman, Gibbs Society President
8:50-8:55 Administrative items: David Bain and Jannette Carey

8:55-9:35 **The Gibbs Conference: A retrospective**
Introduction: Jack Correia
Wayne Bolen (University of Texas Medical Branch, Galveston)

Scientific Session 1: Macromolecular assemblies and interactions

Moderator: Jonathon Renn (University of Notre Dame; Clark Lab)

9:35-10:25 **Keynote Address**
Introduction: George Rose
Ken Dill (University of California San Francisco)
Small-numbers fluctuations in cells and some foundational problems of nonequilibrium statistical thermodynamics

10:25-11:00 Refreshment break

11:00-11:20 T. Lance Min (University of Illinois; Chemla and Golding Labs)
Bacterial swimming studied using an optical trap

11:20-11:40 Deborah Conrady (University of Cincinnati; Herr Lab)
A novel mechanism for intercellular adhesion in Staphylococci

11:40-12:15 Walter Stafford (Boston Biomedical Research Institute)
Treatment of Non-ideality in Sedimentation Velocity Analysis of Self-associating Systems

12:15 **Group photo - location TBA**
Lunch in Freeberg Hall

Scientific session 2: Nucleic acid structure and function

Moderator: Keith Connaghan (University of Colorado Denver; Bain Lab)

- 3:00-3:35 Olke Uhlenbeck (Northwestern University)
Tuning tRNAs for Accurate Translation
- 3:35-3:55 Joshua Blose (Pennsylvania State University; Bevilacqua Lab)
Contributions of molecular mimicry and complementary electrostatics to the increased stability of UNMG and GNRA tetraloops in the context of a CG closing base pair
- 3:55-4:15 Alan Chen (Washington University; Pappu Lab)
Mechanistic studies of monovalent counterion specificity in stabilizing RNA kissing loops
- 4:15-4:35 Refreshment break
- 4:35-5:10 Christopher Fischer (University of Kansas)
*Mechanisms for single-stranded DNA binding and translocation by *S cerevisiae* ISW2*
- 5:10-5:30 Anasuya Roychowdhury (University of Texas Medical Branch; Bujalowski Lab)
*Nucleotide control of replication initiation: NTPase mechanisms of *E. coli* DnaB-DnaC complex*
- 5:30-6:05 Donald Senear (University of California Irvine)
*Indirect Recognition in Site-specific DNA Binding of *E. coli* Integration Host Factor*
- 6:30 Dinner in Freeberg Hall
- 8:00 **Poster session 1:** First author last names A-Kh
Beer/wine in Sledgefoot Hall

Monday, October 6, 2008

- 7:30-8:30 Breakfast in Freeberg Hall
- Scientific session 3: Dynamics and Allostery**
Moderator: Maria Del Mar Ingaramo (University of Maryland;
Beckett Lab)
- 9:00-9:50 **Keynote Address**
Introduction: Olke Uhlenbeck
Dorothy Beckett (University of Maryland)
Flexibility, Allostery and Learning New Tricks
- 9:50-10:10 Michael Feldkamp (University of Iowa; Shea Lab)
Allosteric Interactions of the anti-psychotic drug trifluoperazine with calmodulin
- 10:10-10:30 Danny Miller (University of Kansas Medical Center; Fenton Lab)
H/DX-MS detection of changes in protein dynamics of pyruvate kinase elicited by binding of allosteric versus non-allosteric effector analogs
- 10:30-11:00 Refreshment break
- 11:00-11:20 Francis Insaïdoo (University of Notre Dame; Brian Baker Lab)
Control of T cell receptor recognition by antigen conformational dynamics
- 11:20-11:55 Enrico Di Cera (Washington University)
Allosteric switches: engineering thrombin for anticoagulant activity in vivo
- 12:30 Lunch in Freeberg Hall
- 12:30 Gibbs business meeting: *all previous organizers please attend*

Scientific Session 4: Proteins and Folding

Moderator: Ellen Kloss (Johns Hopkins University; Barrick Lab)

- 3:00-3:35 George Rose (Johns Hopkins University)
Assessing the solvent-dependent surface area of unfolded proteins
- 3:35-3:55 Ignacia Echevarria (Johns Hopkins University; Amzel Lab)
Free energy calculations using Jarzynski's equality for helix-coil transition
- 3:55-4:15 Daniel Kuster (Washington University; Marshall Lab)
From data or dogma? The myth of the ideal α -helix
- 4:15-4:35 Refreshment break
- 4:35-5:10 Ruth Nussinov (National Cancer Institute)
Modeling amyloid conformations and toxic Alzheimer ion channels
- 5:10-5:30 Wei-Feng Xue (University of Leeds; Radford Lab)
Systematic analysis of nucleation-dependent polymerization reveals new insight into the mechanism of amyloid self-assembly
- 5:30-6:05 Juliette Lecomte (Johns Hopkins University)
Heme-protein interactions in cyanobacterial hemoglobins: What a difference a bond makes
- 6:30 Dinner in Freeberg Hall
- 8:00 **Poster session 2:** First author last names KI-Z
Beer/wine Sledgefoot Hall

Tuesday October 7, 2008

7:30-8:30 Breakfast in Freeberg Hall

Scientific Session 5: Macromolecular Stability

Moderator: Susan O'Donnell (University of Iowa; Shea Lab)

9:00-9:35 Bertrand Garcia-Moreno (Johns Hopkins University)
Electrostatic effects in proteins: insights from ionizable groups buried in the hydrophobic interior of proteins

9:35-9:55 Dan Deredge (Louisiana State University; Licata Lab)
Thermodynamic studies of Klenow-DNA binding: the "glutamate effect" is primarily an osmotic effect

9:55-10:30 Yijia Xu (Hunter College)
Switching open and close a subdomain in collagen triple helix

10:30-11:00 Refreshment break

11:00-11:35 Vincent Hilser (University of Texas Medical Branch)
Intrinsic disorder and allostery in an ensemble

11:35-11:55 Olena Ivashyna (Washington University; Schlesinger Lab)
Determination of the oligomeric state of protein BAX during activation in detergent micelles using single-molecule sensitivity and fluorescence techniques

11:55-12:30 Liskin Swint-Kruse (University of Kansas Medical Center)
Subdividing repressor function: DNA binding affinity, selectivity, and allostery can be altered by amino acid substitution of nonconserved residues in a LacI/GalR homologue

12:30 Box lunch and departure