Symposium Energy Landscapes: Statistical Physics of (Spin-)Glasses, Biomolecules, Clusters and Optimization Problems (SYEL)

jointly organized by
the Dynamics and Statistical Physics Division (DY),
the Chemical and Polymer Physics Division (CPP),
the Dielectric Solids Division (DF), and
the Low Temperature Physics Division (TT)

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Overview of Invited Talks and Sessions

(lecture room H1)

Invited Talks

SYEL 1.1	Mon	10:00–10:30	H1	**Energy Landscapes of clusters, glasses, and biomolecules** — •David Wales
SYEL 1.2	Mon	10:30–11:00	H1	**Order parameters and energy landscapes for protein folding and misfolding** — •Steven Plotkin
SYEL 1.3	Mon	11:00–11:30	H1	**Nuclear Spins Reveal the Microscopic Nature of Tunneling Systems in Glasses** — •Christian Enss
SYEL 1.4	Mon	11:30–12:00	H1	**Energy landscapes and phase transitions** — •Lapo Casetti
SYEL 1.5	Mon	12:00–12:30	H1	**Phase transitions in spin glasses** — •Peter Young
SYEL 1.6	Mon	12:30–13:00	H1	**Statistical physics of inverse problems** — •Riccardo Zecchina

Sessions

SYEL 1.1–1.6	Mon	10:00–13:00	H1	**Energy Landscapes: Statistical Physics of (Spin-)Glasses, Biomolecules, Clusters and Optimization Problems (SYEL)**

SYEL 1: Energy Landscapes: Statistical Physics of (Spin-)Glasses, Biomolecules, Clusters and Optimization Problems (SYEL)

Time: Monday 10:00–13:00 Location: H1

Invited Talk SYEL 1.1 Mon 10:00 H1

Energy Landscapes of clusters, glasses, and biomolecules — •David Wales — University Chemical Laboratories, Lensfield Road, Cambridge CB2 1EW

Coarse-graining the potential energy surface into the basins of attraction of local minima, provides a computational framework for investigating structure, dynamics and thermodynamics [1,2]. Steps between local minima form the basis for global optimisation via basin-hopping [3,4] and for calculating thermodynamic properties using the superposition approach and basin-sampling. To treat global dynamics we must include transition states of the potential energy surface, which link local minima via steepest-descent paths. We may then apply the discrete path sampling method [5], which provides access to rate constants for rare events. In large systems the paths between minima with unrelated structures may involve hundreds of stationary points of the potential energy surface. Applications will be presented for a wide variety of atomic and molecular clusters, glass-formers and biomolecules [6-8]. Results for folding, misfolding and aggregation of peptides and proteins illustrate how experimental time and length scales can be addressed for such systems.

[1] DJW, Energy Landscapes, CUP, Cambridge (2003) [2] J. Phys. Chem. B, 110, 20765 (2006) [3] J. Phys. Chem. A, 101, 5111 (1997). [4] Science, 285, 1368 (1999). [5] Mol. Phys., 100 , 3285 (2002); 102, 891 (2004); Int. Rev. Phys. Chem., 25, 237 (2006). [6] Chem. Phys. Lett., 466, 105 (2008). [7] J. Phys. Chem. B, 112, 8760 (2008). [8] J. Chem. Phys., 129, 164507 (2008).

Invited Talk SYEL 1.2 Mon 10:30 H1

Order parameters and energy landscapes for protein folding and misfolding — •Steven Plotkin — Department of Physics and Astronomy, University of British Columbia, 6224 Agricultural Road, Vancouver, B.C. V6T 1Z1, Canada

A fundamental problem of relevance to protein folding and structural comparison of biomolecules is the notion of what *distance* means for higher-dimensional objects such as a polymer. Here we generalize the notion of distance between points to distance between non-crossing space curves to uniquely define the true distance between two biopolymer conformations, and apply this order parameter to the problem of protein folding rates and reaction coordinates. Complementary to the problem of protein folding is the problem of loss of structure gain of toxic function involved in misfolding. Physics-based algorithms based on energy landscape theory can quantify the molecular mechanisms underlying aggregation-related diseases, including ALS and the Prion diseases. Predictions based on such an algorithm that we have developed, which employs both atomistic interactions and surface-area based coarse-graining, have been recently verified by immunological assays and point to diagnostic and therapeutic applications. I will describe the results of our misfolding theory and discuss future directions.

Invited Talk SYEL 1.3 Mon 11:00 H1

Nuclear Spins Reveal the Microscopic Nature of Tunneling Systems in Glasses — •Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, INF 227, 69120 Heidelberg

The low temperature properties of disordered solids, like glasses or crystals with certain substitutional defects are governed by atomic tunneling systems. Until recently it was believed that the dielectric properties of insulating materials devoid of magnetic impurities should not or only very weakly depend on external magnetic fields. Experiments on glasses show in contrast to that a strong magnetic field dependence of the dielectric susceptibility of such materials at ultralow temperatures. We will discuss polarization echo experiments that proof that these effects are caused by tunnelling particles with nuclear magnetic moments. Using isotope substitution we demonstrate the role of nuclear quadrupole and nuclear magnetic dipole moments regarding the magnetic field dependence. We also show that tunnelling particles with nuclear moments can be used as local probes to investigate the microscopic nature of tunnelling systems.

Invited Talk SYEL 1.4 Mon 11:30 H1

Energy landscapes and phase transitions — •Lapo Casetti — Dipartimento di Fisica e Astronomia, Università di Firenze, and INFN, Firenze, Italy

Our current understanding of phase transitions in equilibrium statistical mechanics is remarkable. This notwithstanding, we still do not know which features of the Hamiltonian of a system induce a phase transition.

A natural framework for approaching this problem is energy landscape theory. The potential energy landscape of a classical system is the graph of the potential energy function $V(q_1, \ldots, q_N)$, where the q's are the coordinates of configuration space. The role played by the stationary points of the landscape, where $dV = 0$, is crucial. Remarkably, these are the points where the topology of the level sets of V changes. It has been conjectured that some of these topology changes are related to thermodynamic phase transitions; it has also been shown that the stationary points of V are in one-to-one correspondence with the singularities of the microcanonical entropy at finite N.

Microcanonical singularities at finite N disappear in the thermodynamic limit unless the corresponding stationary points become asymptotically flat. This suggests that thermodynamic phase transitions may be induced by asymptotically flat stationary points of the energy landscape. We discuss some explicit examples of models of physical interest where this idea can be successfully tested.

Invited Talk SYEL 1.5 Mon 12:00 H1

Phase transitions in spin glasses — •Peter Young — Physics Department, University of California, Santa Cruz, CA 95064, USA

This talk will describe recent progress in understanding phase transitions in spin glasses. Whereas the Ising spin glass in zero field is quite well understood, the nature of the transition in the Heisenberg spin glass is much less clear. Another topic of great current interest is whether there is a phase transition in a magnetic field (the de Almeida-Thouless line) for an Ising spin glass. The AT line is argued to exist in the "replica symmetry breaking" (RSB) scenario for the nature of the spin glass state, but not in the "droplet theory". I will discuss results of large-scale Monte Carlo simulations which investigate these questions.

Invited Talk SYEL 1.6 Mon 12:30 H1

Statistical physics of inverse problems — •Riccardo Zecchina — Politecnico di Torino, Italy

We will review some recent results in the statistical mechanics approaches to inverse problems and discuss applications in physics and biology.

Specifically we will show how statistical physics algorithms for inverse Ising, inverse Potts and for the identification of optimal connected sub-graphs of a given network can be used to unveil hidden interactions in biological systems from different types of large scale data.