THE KELLY LECTURE

Arthur Kelly, an alumnus of the university, established the Kelly Fund at Purdue University in 1956. The income from this fund is used to bring outstanding scientists and engineers to the campus for lectures and discussions in the Department of Chemistry and the School of Chemical Engineering.

Pablo Debenedetti

Class of 1950 Professor in Engineering & Applied Science
Princeton University

"Water in Confinement"
Tuesday, March 18, 2008, 3:30 p.m., FRNY G140

"Statistical Characterization of Structure in Complex Systems"
Wednesday, March 19, 2008, 11:30 a.m., FRNY B124

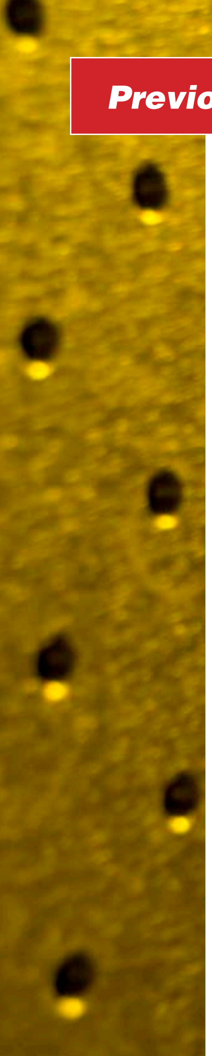
PURDUE UNIVERSITY | SCHOOL OF CHEMICAL ENGINEERING

PURDUE UNIVERSITY

SCHOOL OF CHEMICAL ENGINEERING

Forney Hall of Chemical Engineering
480 Stadium Mall Drive
West Lafayette, IN 47907-2100

2008 KELLY LECTURE



Previous Kelly Lectures in Chemical Engineering

1965 Warren L. McCabe
1966 Arthur Metzner
1967 Olaf A. Hougen
1968 R. Byron Bird
1969 C. Judson King
1970 L.E. Scriven
1971 Charles N. Satterfield
1972 Robert L. Pigford
1973 Andreas Acrivos
1974 John M. Prausnitz
1975 Michel Boudart
1976 Arthur E. Humphery
1977 Rutherford Aris
1978 James J. Carberry
1979 Warren E. Stewart
1980 Paul J. Flory
1981 Neal R. Amundson
1982 William R. Schowalter
1983 Thomas J. Hanratty
1984 Wolfgang M.H. Sachtler
1985 Benjamin G. Levich
1986 Alan S. Michaels
1987 Morton M. Denn
1988 Edward L. Cussler
1989 E.N. Lightfoot
1990 H. Ted Davis
1991 Reuel Shinnar
1992 Robert S. Langer
1993 Arthur W. Westerberg
1994 W. Harmon Ray
1995 Douglas A. Lauffenburger
1996 John H. Seinfeld
1997 Lanny D. Schmidt
1998 Matthew Tirrell
1999 George Stephanopoulos
2000 Robert A. Brown
2001 Gerhard Ertl
2002 Mark E. Davis
2003 Gregory Stephanopoulos
2004 William B. Russel
2005 Special symposium celebrating 40 years
Frank S. Bates
Alexis T. Bell
Ignacio E. Grossmann
Michael L. Shuler
James Wei
2006 Frances H. Arnold
2007 Manfred Morari

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Professor Pablo Debenedetti is the Class of 1950 Professor in Engineering and Applied Science at Princeton University. He completed his undergraduate studies at the University of Buenos Aires (1978), and obtained MS (1981) and Ph.D. degrees (1985), all in Chemical Engineering, at the Massachusetts Institute of Technology. Between 1978 and 1980 he was a process development engineer with O. De Nora, Impianti Elettrochimici in Milan, Italy.

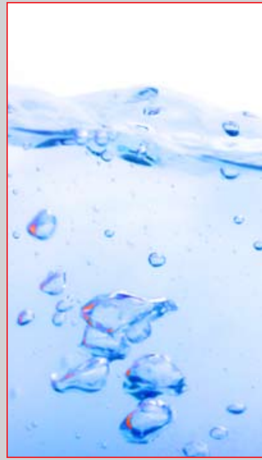
Pablo Debenedetti's research interests include glasses and amorphous materials, water and aqueous solutions, nucleation, metastability and protein thermodynamics. The author of one book, *Metastable Liquids*, and more than 160 scientific articles, he is the recipient of the National Science Foundation's Presidential Young Investigator Award (1987), the Camille and Henry Dreyfus Teacher-Scholar Award (1989), a Guggenheim Memorial Foundation Fellowship (1991), the Professional Progress Award from the American Institute of Chemical Engineers (1997), the John M. Prausnitz Award in Applied Chemical Thermodynamics (2001), and the American Chemical Society's Joel Hildebrand Award on the Theoretical and Experimental Chemistry of Liquids (2008). He has also delivered named lectures at many prominent institutions.

Professor Debenedetti is a member of the National Academy of Engineering. He currently serves on the National Academies' Board on Chemical Sciences and Technology and is an Associate Editor of the AIChE Journal.

"WATER IN CONFINEMENT"

Tuesday, March 18, 2008, 3:30 p.m., FRNY G140

Confining surfaces that contain thin water films are ubiquitous in biology, engineering and materials science. Understanding the effects of surfaces on the dynamics, structure and thermodynamics of proximal water is of interest in applications ranging from lab-on-a-chip technologies to the design of super-hydrophobic surfaces. Molecular simulation is a powerful tool for probing the behavior of water in nano-scale confinement. Careful tuning of surface hydrophobicity and hydrophilicity leads to the formation of a variety of layered phases, allows sensitive control of the mechanical properties of amorphous films, and provides fundamental insight on the importance of drying transitions near atomically-smooth and biological confining environments. The microscopic detail obtained from simulation, augmented by a rigorous thermodynamic framework, enables the rational analysis of experimental observations and facilitates the engineering design of new materials.



"STATISTICAL CHARACTERIZATION OF STRUCTURE IN COMPLEX SYSTEMS"

Wednesday, March 19, 2008, 11:30 a.m., FRNY B124

Systems with many degrees of freedom cannot be described taxonomically (e.g., enumeration of local energy minima in a glass or a protein). The statistical description of such systems will be illustrated by means of two examples. One deals with the protein design problem, where the goal is to find the sequence of amino acids that folds into a target structure. The *sequence landscape* constructed by a flat-histogram Monte Carlo algorithm displays novel phase transitions in sequence space, whose possible biological relevance remains an open question. In the second example, the analysis of order in particle packings leads to the notion of an *order map*, in which the state of the system is described by order parameters that quantify its statistical geometry. Striking regularities emerge in the order map as the spectrum of liquid and glassy behavior ranging from simple (atomic) to complex (associating) is traversed. The order map emerges as a useful organizing principle in the study of structure, dynamics and thermodynamics of liquids and glasses.