

The 2004 Palke Lecturer

David Chandler (b. 1944) is a Professor of Chemistry at the University of California, Berkeley. After receiving a S.B. Degree in Chemistry from MIT in 1966, and a Ph.D. in Chemical Physics at Harvard in 1969, Chandler began his academic career as an Assistant Professor in 1970 at the Urbana-Champaign campus of the University of Illinois. He rose quickly through the ranks, becoming a full Professor in 1977. Prior to joining the Berkeley faculty in 1986, Chandler spent two years as Professor of Chemistry at the University of Pennsylvania.

Chandler's general area of research is statistical mechanics with particular emphasis devoted to understanding liquids. Early in his career, he worked with Hans Andersen and John Weeks in developing a quantitative description of liquid structure and thermodynamics in terms of molecular packing. Today, this work is known as the WCA theory. To extend this theory to complex fluids, Chandler developed the reference interaction site model (RISM). It describes packing of irregular shaped molecules in the liquid state. Its use in describing polymeric liquids, pioneered by Chandler's student Kenneth Schweizer, is currently the most important application of this model.

With his student Lawrence Pratt, Chandler developed the molecular theory of hydrophobicity. The Pratt-Chandler theory describes in analytical terms the free energy to reorganize water structure in the vicinity of hydrophobic groups. For small hydrophobic groups in water, the most favorable structural rearrangement places water between a pair of hydrophobic particles - a solvent separated hydrophobic bond. Chandler has recently returned to this problem, but with emphasis on extended hydrophobic surfaces. Such surfaces can induce phase transitions and powerful inter-surface interactions over mesoscopic length scales. The onset of this behavior is in the nanometer regime, relevant to structural biology.

Chandler has also developed the statistical mechanical techniques for analyzing chemical equilibrium and chemical dynamics in liquids. He has used these techniques to understand the behavior of electrons in liquids, and has extended these methods into the biophysical realm where he has studied electron transfer in proteins. During the last few years, Chandler and his co-workers Christoph Dellago, Peter Bolhuis and Phillip Geissler have developed the techniques of transition path sampling, permitting the computational study of rare but important events without preconceived knowledge of transition states. Processes investigated with this methodology include weak acid dissociation in water and in clusters and the folding of solvated polymers. Other topics of current interest to Chandler include: self assembly, glasses, aging and dynamics of systems far from equilibrium.

In recognition of his research accomplishments, David Chandler has received a number of awards from various scientific societies and institutions, and he is a member of the National Academy of Sciences. His popular textbook, *Introduction to Modern Statistical Mechanics*, is highly regarded by both students and specialists for its novelty and pedagogy.

The Department of Chemistry & Biochemistry

University of California, Santa Barbara

presents the

5th Annual

W.E. Palke Memorial Lecture

Wednesday, March 10, 2004

Engineering II Pavilion

4:00 P.M.

Reception to follow the lecture in 4606 PSB North

William E. Palke, professor in the UCSB Chemistry Department for 31 years, died on May 10, 1999 from a heart attack. He was 58 years old. To many, he was more than a professor. He was a scientist, colleague, hiking companion, rock climber, and friend.

Professor Palke did his graduate work with W.N. Lipscomb at Harvard, receiving his Ph.D. in 1966. There followed two years of postdoctoral work as an A.A. Noyes Fellow at Caltech where he worked in collaboration with Professor William Goddard. Then in 1968, he came to UCSB as an assistant professor in theoretical chemistry.

His first scientific publication came in 1962 from undergraduate work done with Professor Fred Anson at Caltech. Some 37 years and 84 papers later, his most recent paper appeared in the *Journal of Magnetic Resonance*. Professor Palke was a great collaborator. In our department he was a major resource for many graduate students and co-authored papers with 10 different faculty members.

By and large, the work of Professor Palke fell in five areas. He developed efficient computational methods for determining wave functions used in

evaluating properties of molecules. He sought to understand the quantum details of chemical bonding. He analyzed the different factors that give rise to the barriers to internal rotation in molecules. He applied density functional theory to relate the electron density in molecules to molecular properties. In recent years, he extended the theory of relaxation effects in nuclear magnetic resonance experiments. This work resulted in a set of computer programs that, for the first time, permitted calculation of the spectra exhibited by complicated spin systems interacting in general ways.

Down through the years Professor Palke taught a variety of courses including General Chemistry, Environmental Chemistry, Physical Chemistry, Statistical Mechanics and Quantum Chemistry. He was widely regarded as one of the best teachers in the department. He is sorely missed.



Program

Bill Palke Remembered

J. T. Gerig, Professor of Chemistry, UCSB

Introduction of the 2004 Palke Lecturer

Horia Metiu, Professor of Chemistry and Physics, UCSB

Lecture

"Hydrophobicity at Small and Large Length Scales: Two Faces of Water"

David Chandler

Professor of Chemistry
University of California, Berkeley

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John and Kathryn Kirtley
Amy and Nancy Palke

Contributions to the Palke Lecture fund are welcome at any time and may be addressed to the Chair of the Department of Chemistry and Biochemistry, UCSB.