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MICHAEL L. KLEIN, PH.D..

EXPLORING NATURE'S DESIGN OF
VOLTAGE GATED ION CHANNELS VIA COMPUTATION

OCTOBER 24, 2013
4:00 P.M.
208 LIGHT HALL

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Upcoming Discovery Lecture:

HAROLD E. VARMUS, M.D.
National Cancer Institute

November 21, 2013
208 Light Hall / 4:00 P.M.

VANDERBILT  UNIVERSITY
MEDICAL CENTER

EXPLORING NATURE'S DESIGN OF VOLTAGE GATED ION CHANNELS VIA COMPUTATION

I will present an overview of the significant advances in the understanding the mechanism of action of voltage gated ion channels since the recent determination of x-ray structures of several prokaryotic voltage-gated potassium and sodium channels and their subsequent investigation using high performance computation and modeling. In contrast to what was learned from potassium selective channels, studies of the available sodium channel structures point to a conduction mechanism where partially hydrated sodium ions can explore pore lining sites while being loosely coupled to other ions and water. Discrimination of sodium over other ionic species has also been the subject of intense research revealing the weakly-selective nature of sodium channel structures. Though the characterization of conduction and selectivity within prokaryotic channels holds promise to ultimately shed light on the structure-function interplay of more complex and pharmacologically relevant mammalian channels, much still remains to be done to fully understand the structure and function of these intriguing nanoscale molecular machines.



MICHAEL L. KLEIN, PH.D.

**DEAN, COLLEGE OF SCIENCE AND TECHNOLOGY
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**LAURA H. CARNELL PROFESSOR OF SCIENCE
MEMBER, NATIONAL ACADEMY OF SCIENCES**

Michael L. Klein received his B.Sc. and Ph.D. degrees in Chemistry from the University of Bristol UK and was a postdoctoral research fellow in Italy, UK, and USA before joining the Chemistry Division of NRCC in Ottawa, Canada, where he rose through the ranks from Associate to Principal Research Officer. In 1987, he returned to the USA as Professor of Chemistry at the University of Pennsylvania, where from 1993 he was the Hepburn Professor of Physical Science and Director of the Laboratory for Research on the Structure of Matter, one of the US leading materials science research labs. In 2009, he moved to Temple University as the Laura H. Carnell Professor of Science and Director of the Institute for Computational Molecular Science. His research involves using computer simulation to probe the behavior of molecular assemblies. His pioneering contributions range from physical chemistry and biophysics to drug discovery and chemical biology, with recent emphasis on understanding nature's design of voltage gated ion channels. His researches have been honored with awards from the American Chemical Society, American Physical Society; European Physical Society; Royal Society of Chemistry UK; Chemical Research Society of India and The World Academy of Science. He is a member of the National Academy of Sciences and a Fellow of the Royal Society of London. He was recently elected an honorary fellow of Trinity College, Cambridge UK. He is currently Dean of the College of Science & Technology at Temple University.
