Science at the Edge
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11:30 BPS 1400

Reactions of Fluorine and Chlorine Atoms with Water and the Water Dimer

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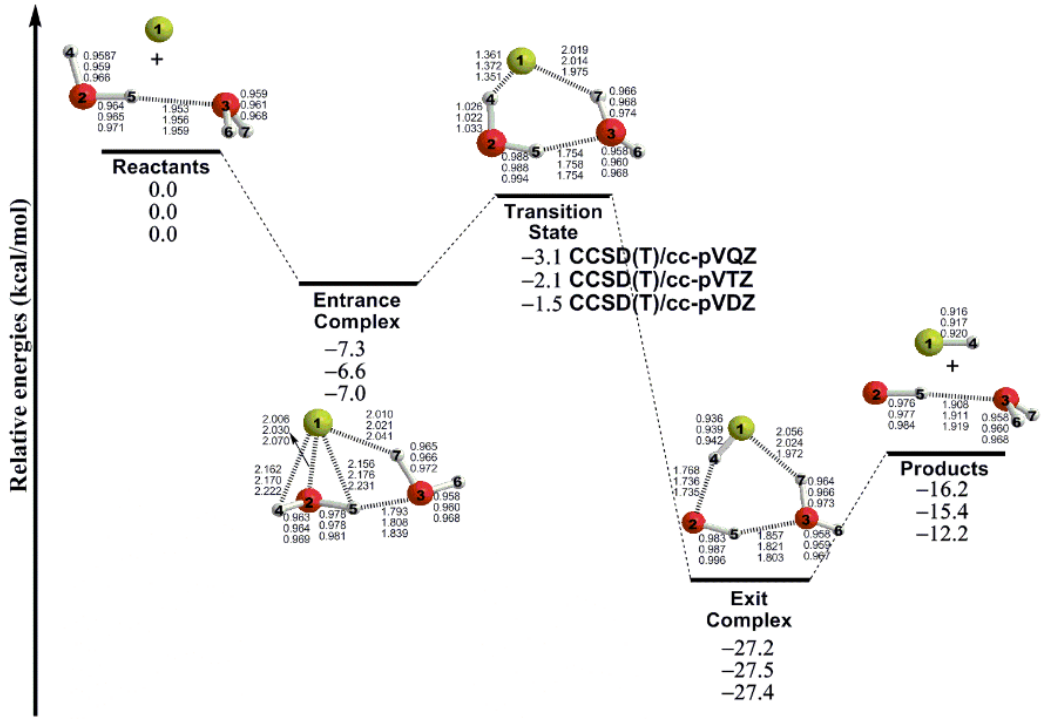
ABSTRACT

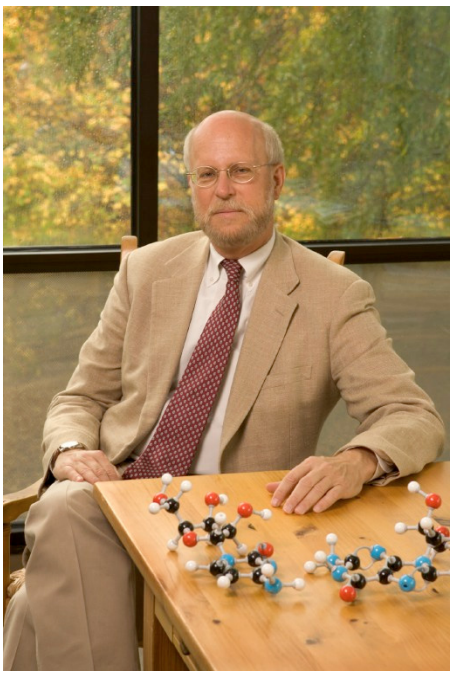
The ubiquitousness of water on our planet makes the study of many of its elementary chemical reactions of fundamental importance, or even of applied importance for atmospheric and combustion chemistry. This lecture will be concerned with some of the simplest reactions of water and the water dimer. Seemingly similar reactions with halogen atoms turn out to have very different energy landscapes and dynamics.

http://www.ccqc.uga.edu/people/member_page.php?id=6



Please contact P. Piecuch (piecuch@chemistry.msu.edu) or R. Ghosh (ghosh@pa.msu.edu) to meet with the speaker

Professor Henry F. Schaefer III



Henry F. Schaefer III was born in Grand Rapids, Michigan. He attended public schools in Syracuse (New York), Menlo Park (California), and Grand Rapids (Michigan), graduating from East Grand Rapids High School in 1962. He received his B.S. degree in chemical physics from the Massachusetts Institute of Technology (1966) and Ph.D. degree in chemical physics from Stanford University (1969). For 18 years (1969-1987) he served as a professor of chemistry at the University of California, Berkeley. During the 1979-1980 academic year he was also Wilfred T. Doherty Professor of Chemistry and inaugural Director of the Institute for Theoretical Chemistry at the University of Texas, Austin. Since 1987 Dr. Schaefer has been Graham Perdue Professor of Chemistry and Director of the Center for Computational Quantum Chemistry at the University of Georgia. In 2004 he became Professor of Chemistry, Emeritus, at the University of California at Berkeley. His other academic appointments include Professeur d'Echange at the University of Paris (1977), Gastprofessur at the Eidgenössische Technische Hochshule (ETH), Zürich (1994, 1995, 1997, 2000, 2002, 2004, 2006, 2008, 2010), David P. Craig Visiting Professor at the Australian National University (1999), and Visiting Professor at the Ludwig Maximilian University (LMU) Munich (2012, 2013). He is the author of more than 1400 scientific publications, with a large majority appearing in the *Journal of Chemical Physics* or the *Journal of the American Chemical Society* or the *Journal of Physical Chemistry*. A total of 300 scientists from 35 countries gathered in Gyeongju, Korea for a six-day conference in February, 2004 with the title "Theory and Applications of Computational Chemistry: A Celebration of 1000 Papers of Professor Henry F. Schaefer III." In May 2010, the University of California at Berkeley hosted a large international conference in Professor Schaefer's honor, the title of the conference being "Molecular Quantum Mechanics: From Methylene to DNA and Beyond." Simultaneous with the Berkeley conference was published the book "Selected Papers of Henry F. Schaefer III," Edited by R. J. Bartlett, T. D. Crawford, M. Head-Gordon, and C. D. Sherrill.

Critical to Professor Schaefer's scientific success has been a brilliant array of students and coworkers; including 63 undergraduate researchers who have published papers with him, 103 successful Ph.D. students, 49 postdoctoral researchers, and 73 visiting professors who have spent substantial time in the Schaefer group. A number of his students have gone on to positions of distinction in industry (Accelrys, Allstate Insurance, American Cyanamid, AstraZeneca, AT&T, Avaya, Bicerano and Associates,

Chemical Abstracts, Clariant, Computational Geosciences, Coraid, DeNovaMed, Deutsche Bank, Dow Chemical, ELANTAS, Electronic Arts, Endress-Hauser, GAUSSIAN, Goodrich, Google, Henkel, Hewlett-Packard, Hughes Aircraft, IBM, Komag, Lehman Brothers, Locus Pharmaceuticals, Materials Design, Mobil Research, Molecular Simulations, Monsanto, OpenEye, OSI Software, Pharmaceutical Research Associates, Polaroid, Proctor & Gamble, Q-CHEM, Reagens Deutschland, Ricoh, Schroedinger, SciCo, Sugen, and WaveSplitter Technologies). Four of his graduated Ph.D.s have started their own companies. Several have gone on to successful careers in government laboratories, including the Australian National University Supercomputer Center, Environmental Protection Agency (EPA), Joint Institute for Laboratory Astrophysics (JILA), Lawrence Livermore National Laboratory, NASA Ames, National Cancer Institute, National Center for Disease Control, National Institutes of Health (Bethesda), National Research Council of Canada (Ottawa), Naval Research Laboratory, Oak Ridge National Laboratory, Pacific Northwest National Laboratory, Pittsburgh Supercomputing Center, Sandia National Laboratories, and the Savannah River National Laboratory. Charles Blahous went directly from his Ph.D. studies with Professor Schaefer to the position of American Physical Society Congressional Scientist Fellow, and eventually to positions of significant importance in the U.S. political system (chief of staff for Senator Alan Simpson of Wyoming and later for Senator Judd Gregg of New Hampshire; and Executive Director of President George W. Bush's Bipartisan Committee to Strengthen Social Security; see Wall Street Journal article April 22, 2005). Dr. Blahous is currently Research Fellow at the Hoover Institution, Stanford University and was recently appointed by President Barack Obama to the Board of Trustees for Social Security and Medicare.

Many of Professor Schaefer's students have accepted professorships in universities, including the University of Alabama at Birmingham, University of Arizona, Budapest University (Hungary), University of California at Merced, City University of New York, Duke University, Emory University, Fatih University (Istanbul, Turkey), Georgia Tech, University of Georgia, University of Giessen (Germany), University of Girona (Spain), University of Grenoble (France), University of Guelph (Ontario), University of Illinois-Chicago, University of Illinois-Urbana, Indian Association for the Cultivation of Science (Calcutta), Indiana University-Purdue University at Indianapolis, Johns Hopkins University, University of Kentucky, University of Manchester (England), University of Marburg (Germany), University of Massachusetts, University of Memphis, University of Michigan, University of Mississippi, National Tsing Hua University (Taiwan), University of North Dakota, Ohio State University, Osaka University (Japan), University of Paris - Sud (France), Pennsylvania State University, University of Pittsburgh, Pohang Institute of Science and Technology (Korea), Portland State University, Rice University, Rikkyo University (Tokyo), Scripps Research Institute, University of South Florida, St. Andrew's University (Scotland), St. Petersburg State University (Russia), Stanford University, University of Stirling (Scotland), University of Stockholm (Sweden), University of Tasmania (Australia), Technical University of Munich (Germany), Texas A&M University, the University of Texas at Arlington, University of Trondheim (Norway), University of Tübingen (Germany), and Virginia Tech.

Professor Schaefer has been invited to present plenary lectures at more than 250 national or international scientific conferences. He has delivered endowed or named lectures or lecture series at more than 50 major universities, including the 1998 Kenneth S. Pitzer Memorial Lecture at Berkeley, the 2001 Israel Pollak Distinguished Lectures at the Technion - Israel Institute of Technology, Haifa, the 2007 C. V. Raman Memorial Lecture in Calcutta, India, and the 2007 Per-Olov Löwdin Lectures at the University of Uppsala, Sweden. He is the recipient of twenty-seven honorary degrees. He was the longest serving Editor-in-Chief of the London-based journal *Molecular Physics* (1995-2005). He was also the longest serving President of the World Association of Theoretical and Computational Chemists, from 1996 to 2005. His service to the chemical community includes the chairmanship of the American Chemical Society's Subdivision of Theoretical Chemistry (1982) and Division of Physical Chemistry (1992). At the 228th National Meeting of the American Chemical Society (Philadelphia, August, 2004) the Division

of Computers in Chemistry and the Division of Physical Chemistry co-sponsored a four-day Symposium in Honor of Henry F. Schaefer's 60th Birthday. The book "Theory and Applications of Computational Chemistry: The First Forty Years" (1308 pages, Elsevier) was published in 2005 in honor of Professor Schaefer.

Professor Schaefer's major awards include the American Chemical Society Award in Pure Chemistry (1979, "for the development of computational quantum chemistry into a reliable quantitative field of chemistry and for prolific exemplary calculations of broad chemical interest"); the American Chemical Society Leo Hendrik Baekeland Award (1983, "for his contributions to computational quantum chemistry and for outstanding applications of this technique to a wide range of chemical problems"); the Schrödinger Medal (1990); the Centenary Medal of the Royal Society of Chemistry (London, 1992, as "the first theoretical chemist successfully to challenge the accepted conclusions of a distinguished experimental group for a polyatomic molecule, namely methylene"); the American Chemical Society Award in Theoretical Chemistry (2003, "for his development of novel and powerful computational methods of electronic structure theory, and their innovative use to solve a host of important chemical problems"). In 2003 he also received the annual American Chemical Society Ira Remsen Award, named after the first chemistry research professor in North America. The Remsen Award citation reads "For work that resulted in more than one hundred distinct, critical theoretical predictions that were subsequently confirmed by experiment and for work that provided a watershed in the field of quantum chemistry, not by reproducing experiment, but using state-of-the-art theory to make new chemical discoveries and, when necessary, to challenge experiment." *The Journal of Physical Chemistry* published a special issue in honor of Professor Schaefer on April 15, 2004. In 2009, the journal *Molecular Physics* published five consecutive issues in honor of Professor Schaefer. He was elected a Fellow of the American Academy of Arts and Sciences in 2004. He was the recipient of the prestigious Joseph O. Hirschfelder Prize of the University of Wisconsin for the academic year 2005-2006. He became a Fellow of the Royal Society of Chemistry (London) in 2005. He was among the inaugural class of Fellows of the American Chemical Society, chosen in 2009. In April 2011 he received the Ide P. Trotter Prize of Texas A&M University. Recent recipients of this prestigious award have been Nobelists Charles Townes, William Phillips, Francis Crick, and Steven Weinberg. In 2012 he received the Alexander von Humboldt Award. On March 29, 2012 Professor Schaefer received the $20,000 SURA Distinguished Scientist Award, given to the outstanding scientist in any field in the southern USA, from Missouri to Texas to Florida to Virginia. On April 5, 2013, at the Chemical Heritage Foundation in Philadelphia, Professor Schaefer received the Chemical Pioneer Award of the American Institute of Chemists.

During the comprehensive period 1981 - 1997 Professor Schaefer was the sixth most highly cited chemist in the world; out of a total of 628,000 chemists whose research was cited. The Science Citation Index reports that by December 31, 2012 his research had been cited more than 53,000 times. Professor Schaefer's Wikipedia H-index is 105. His research involves the use of state-of-the-art computational hardware and theoretical methods to solve important problems in molecular quantum mechanics.