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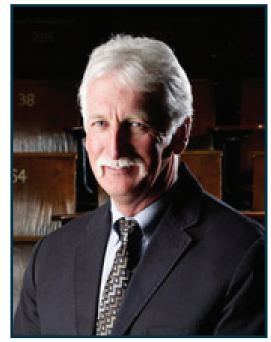
Department of Chemistry
Kolthoff Lectureship in Chemistry

Professor William Jorgensen

Department of Chemistry, Yale University

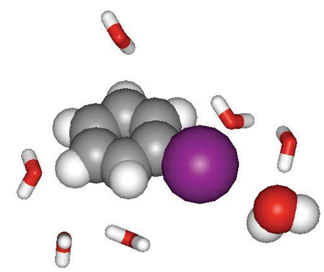
Website: http://www.chem.yale.edu/faculty/jorgensen.html

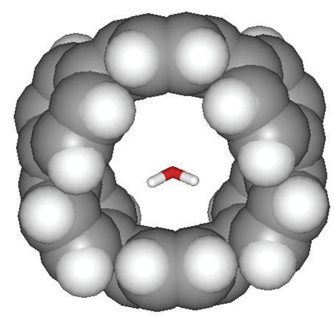


William Jorgensen is the Sterling Professor of Chemistry and Director of the Physical Sciences & Engineering Division at Yale University. He is a pioneer in the field of computational chemistry. His research focuses on organic, medicinal, and computational chemistry, including simulations of organic and enzymatic reactions, computer-aided drug design, and the synthesis and development of therapeutic agents targeting infectious, inflammatory, and hyperproliferative diseases. He has more than 300 publications on his research. Jorgensen earned a bachelor's degree from Princeton University and a doctorate from Harvard University. His honors include being elected to the National Academy of Sciences, the International Academy of Quantum Molecular Science, the American Academy of Arts and Sciences, and as a fellow of the American Chemical Society (ACS), and American Association for the Advancement of Science. He has received the International Academy of Quantum Molecular Sciences Award in Computational Biology, the Sato International Award, the ACS Award for Computers in Chemical and Pharmaceutical Research, and the A.C. Cope Scholar Award. He is editor of the *Journal of Chemical Information and Modeling* and the *Journal of Chemical Theory and Computation*, and holds positions on the editorial advisory boards of several other journals.

Lecture 3: *New Challenges for Modeling Chemistry in Solution*

9:45 a.m. Thursday, November 8, 331 Smith Hall





The correct representation of intermolecular interactions using force fields is essential to their utility in simulations of organic and biomolecular systems as well as new materials. Two issues that have been addressed recently are halogen bonding and the interaction of water and ions with extended π-systems including acenes, graphene, and nanotubes. For halogen bonding, the classical point charge model requires augmentation with a partial positive charge on the C-X axis to represent the σ-hole for aryl chlorides, bromides, and iodides. The enhanced force fields, OPLS-AAx and OPLS/CM1Ax, have been tested in calculations on gas-phase complexes and for free energies of hydration, densities, and heats of vaporization of halobenzenes. For the extended π-systems, the OPLS-AA force field is found to perform very well in comparison to CCSD(T)-level calculations for complexes with a water molecule. However, proper representation of interactions with ions requires addition of polarization such as with inducible dipoles in the OPLS-AAP force field.

Treatment of Halogen Bonding in the OPLS-AA Force Field; Application to Potent Anti-HIV Agents. Jorgensen, W. L.; Schyman, P. J. Chem. Theory Comput. 2012, 8, 3895-1901.

Izaak Maurits Kolthoff was born on February 11, 1894, in Almelo, Holland. He died on March 4, 1993, in St. Paul, Minnesota. In 1911, he entered the University of Utrecht, Holland. He published his first paper on acid titrations in 1915. On the basis of his world-renowned reputation, he was invited to join the faculty of the University of Minnesota's Department of Chemistry in 1927. By the time of his retirement from the University in 1962, he had published approximately 800 papers. He continued to publish approximately 150 more papers until his health failed. His research, covering approximately a dozen areas of chemistry, was recognized by many medals and memberships in learned societies throughout the world, including the National Academy of Sciences and the Nichols Medal of the American Chemical Society. Best known to the general public is his work on synthetic rubber. During World War II, the government established a comprehensive research program at major industrial companies and several universities, including Minnesota. Kolthoff quickly assembled a large research group and made major contributions to the program. Many of Kolthoff's graduate students went on to successful careers in industry and academic life and, in turn, trained many more. In 1982, it was estimated that approximately 1,100 Ph.D. holders could trace their scientific roots to Kolthoff. When the American Chemical Society inaugurated an award for excellence in 1983, he was the first recipient.