



UNIVERSITY OF MINNESOTA
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Department of Chemistry Kolthoff Lectureship in Chemistry

November 5-8, 2012
Professor William Jorgensen

Department of Chemistry, Yale University

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

Faculty Hosts: Jiali Gao & Ilja Siepmann



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.

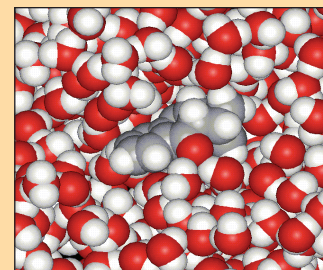
Jorgensen earned a bachelor's degree from Princeton University and a doctorate from Harvard University. His honors include being elected to the National Academy of Sciences, the International Academy of Quantum Molecular Science, the American Academy of Arts and Sciences, and as a fellow of the American 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 1: Modeling Organic and Biomolecular Systems in Solution

3:45 p.m. Monday, November 5
100 Smith Hall

A reception for Professor Jorgensen will be conducted in 117/119 Smith Hall immediately following this lecture. All are welcome to attend.

Research highlights are provided from our work, including development of the TIPnP water models and OPLS-AA force field, QM/MM studies of organic and enzymatic reactions, and computationally guided drug discovery. Calculations of free energy changes have played a central role for locating transition states in solution, elucidating solvent effects on activation barriers, and designing enzyme inhibitors.



[1] Acevedo, O.; Jorgensen, W. L. *Advances in QM/MM Simulations for Organic and Enzymatic Reactions* *Acc. Chem. Res.* **2010**, *43*, 142-151.

[2] Jorgensen, W. L. *Efficient Drug Lead Discovery and Optimization*. *Acc. Chem. Res.* **2009**, *42*, 724-733.

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.

