

2018 Fall Chem 501 Seminar



Dr. David Sherrill

School of Chemistry and
Biochemistry



Thursday – September 27, 2018
Refreshments 3:25pm, Buehler 513
Lecture at 3:45pm, Buehler 555

<http://www.chemistry.gatech.edu/people/sherrill/david/>

Hosted by: Dr. Kostas Vogiatzis

“Quantifying and Visualizing Intermolecular Forces: From Model Systems to Drug Design”

Intermolecular forces govern the properties of liquids, crystal packing forces, protein structure, and drug-protein binding. However, they are still not well understood at a fundamental level. Our group has been developing tools based on quantum mechanics to understand the fundamental nature of non-bonded interactions, especially in organic systems. We have developed very efficient computer software to analyze intermolecular interactions in terms of their fundamental physical components such as electrostatic interactions, and recently we have extended our approach to partition these interactions into interacting pairs of atoms or functional groups. We have applied our new methods to understand cation- π interactions, base stacking in DNA, sulfur- π interactions in proteins, and drug-protein binding.

Dr. C. David Sherrill is a Professor of Chemistry and Biochemistry and a Professor of Computational Science and Engineering at the Georgia Institute of Technology. He obtained his B.S. in Chemistry from MIT in 1992, and his Ph.D. in Chemistry from the University of Georgia in 1996. Dr. Sherrill serves as Associate Director of the Institute for Data Engineering and Science at Georgia Tech, which coordinates efforts in data science, algorithms, and high-performance computing.

He has published over 175 peer-reviewed articles on the development and application of new theoretical methods and new algorithms in computational quantum chemistry. He is a Fellow of the American Association for the Advancement of Science (AAAS), the American Chemical Society, and the American Physical Society, and he has been Associate Editor of the Journal of Chemical Physics since 2009.

In 2017, he was named the Outreach Volunteer of the Year by the Georgia Section of the American Chemical Society for his many years of working with K-12 teachers during National Chemistry Week.