

Getting Down to the Fundamentals of Hydrogen Bonding, Halogen Bonding and Other Non-Covalent Interactions with Computational Quantum Chemistry

Greg Tschumper

Professor

Department of Chemistry and Biochemistry, University
of Mississippi

Chemistry
Seminar on
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Fundamentals of
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Computational
Quantum Chemistry

**Tuesday
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Schrenk**

Please contact
Dr. Garry Grubbs at
grubbsg@mst.edu for
further information.

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Abstract: Non-covalent interactions (hydrogen bonding, halogen bonding, π -stacking, London dispersion forces, etc.) provide some of the motivation and impetus for the work that is the focus of this talk. They play important and sometimes leading roles in chemical, physical and biological processes ranging from solvation and molecular recognition to the directed assembly of supramolecular architectures and even the structure/function of many biological macromolecules. The first part of this presentation will provide a qualitative introduction to and conceptual overview of convergent approaches to quantum mechanical (QM) ab initio electronic structure calculations to help decode much of the jargon used in the field and to demonstrate established procedures for computing the “right answers for the right reasons”. Although these accurate and reliable QM methods have imparted tremendous insight into the structures, energetics and spectroscopic signatures of small molecular clusters held together by relatively weak non-covalent interactions, the associated computational demands often prohibit their routine application to larger molecular systems. This context will set the stage for a discussion of new theoretical methods being developed in our lab to overcome some of these bottlenecks by taking advantage of the many-body expansion for non-covalent clusters and of some recent applications to illustrate the benefits of this theoretical approach.

About the speaker: Prof. Greg Tschumper earned B.S. degree at Winona State University where he pursued majors in chemistry and mathematics. After being introduced to quantum chemistry research during an NSF REU program with Prof. Mark Hoffmann at the University of North Dakota, Dr. Tschumper went on to graduate school at the University of Georgia where he obtained his Ph.D. in chemistry under the direction of Prof. Fritz Schaefer. Dr. Tschumper joined the Department of Chemistry and Biochemistry at the University of Mississippi (“Ole Miss”) in 2001 after post-doctoral appointments at ETH-Zürich with Prof. Martin Quack and at Emory University with Prof. Keiji Morokuma. Dr. Tschumper was the recipient of the University of Mississippi’s Cora Lee Graham Award for Outstanding Teacher of Freshmen in 2009 and the Faculty Achievement Award in 2015. In 2017, Prof. Tschumper became chair of the department. Dr. Tschumper was elected a full member of Sigma Xi, The Scientific Research Honor Society in 2020, as well as a fellow of the American Association for the Advancement of Science (AAAS) in 2021. He was named the university’s recipient of the 2021 SEC Faculty Achievement Award and the 2021 Distinguished Research and Creative Achievement Award. The latter is the highest honor for faculty success and outstanding accomplishment in research, scholarship and creative activity at the University of Mississippi.