Probing the Effects of Size and Charge on the Hydration Motifs of Polyatomic Anions

Dr. Gregory Tschumper

Castleman Endowed Professor of Discovery
Chemistry, Missouri S&T

Chemistry Seminar on *Interactions of polyatomic anions with water*

Monday February 17 at 4 pm in 126 Schrenk

Please contact Dr. Amitava Choudhury at choudhurya@mst.edu for further information.

Abstract: This work systematically examines a series of negatively charged ions interacting with one or two water molecules (i.e., the monohydrates and dihydrates of trigonal planar BeF_3^-, tetrahedral BF_4^-, trigonal bipyramidal SiF_5^-, octahedral PF_6^- and octahedral SiF_6^{2-}).[1,2,3] The CCSD(T) method and correlation consistent triple-zeta basis sets are used to characterize the structures, energetics and vibrational signatures the interactions. The 2-body:Many-body technique developed in our lab for non-covalent clusters is also being used to examine higher-order hydrates of BeF_3^- and BF_4^-. All monohydrates exhibit a double ionic hydrogen bond motif. For the singly charged ions, the electronic dissociation energy and vibrational perturbations induced by the water-ion interaction increase as the size of the ion decreases. All dihydrate global minima exhibit water-water hydrogen bonding, except for the smallest anion (BeF_3^-). Only in the case of SiF_6^{2-} do dihydrate structures having only water-ion contacts become energetically competitive with the global minimum (relative electronic energies *ca.* 0.1 kcal/mol).

1. Y.A. Abdo and G.S. Tschumper, *J. Phys. Chem A*, **124**, 8744 (2020).
2. L.N. Olive, E.V. Dornshuld, H.F. Schaefer and G.S. Tschumper, *J. Phys. Chem. A*, **127**, 8806 (2023).
3. J.J. Mosely and G.S. Tschumper *J. Phys. Chem. A*, **128,** 5637 (2024).

About the speaker: Prof. Greg Tschumper grew up in southeastern Minnesota and went to college about 30 miles from the family farm. He earned his 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. In 2024, Dr. Tschumper joined the Department of Chemistry at Missouri S&T where he is currently the Donald L. Castleman/FCR Missouri Endowed Professor of Discovery.