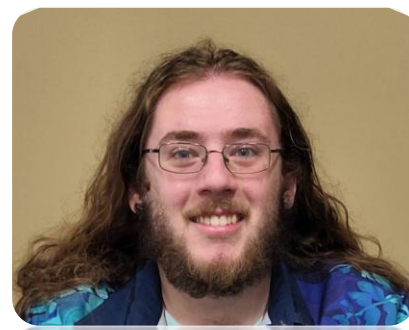


MISSOURI S&T Chemistry Seminar

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Monday, 21st September 2026

4:00 pm at 126 Schrenk Hall

Examination of Barrier Heights, Barrier Widths, and Tunneling Probabilities for Concerted Proton Transfer in Hydrogen-Bonded Clusters of HF, H₂O, and HCl

Bio: Max Tucker is a third-year Ph.D. student in the Tschumper Group where he conducts research using rigorous computational chemistry methods. His work focuses on studying hydrogen bonding interactions and proton transfer in clusters of acids and bases with water, with the goal of gaining insight into the interplay of molecules that are involved in many fundamental chemical processes. He earned his Bachelor of Science in Chemistry and Mathematics from Washington College, Maryland, USA. Max is passionate about using math and physics to elucidate the underlying interactions that are at the heart of many areas of chemistry.

Abstract: Tunneling is a purely quantum mechanical process in which a particle, such as an electron, nucleus, or atom, may pass through a barrier that it would classically be unable to overcome. This phenomenon has wide-ranging applications, from microscopy to electrical engineering to quantum computing. Hydrogen, being the lightest element, is the atom that has the greatest probability to tunnel, and the breaking and reforming of covalent bonds containing hydrogen via this tunneling process, such as in proton transfer reactions, has garnered much interest. This work uses rigorously calibrated quantum chemistry methods to compute parameters relevant to the proton tunneling probability in homogeneous and heterogeneous hydrogen-bonded clusters of HF, H₂O, and HCl.

In the first part of this talk, the physics and mathematics underlying many of the utilized computational methods are explained, with a summary of typical basis sets and methods, both DFT and *ab initio*, that are used in the field. Following this introduction, a discussion of hydrogen atom tunneling in several reactions involving organic molecules is provided, including background on the tunneling splitting observed for the formic acid dimer and the tunneling control of the methylhydroxycarbene tautomerization reaction.

Finally, concerted proton transfer pathways in hydrogen-bonded clusters of HF, H₂O, and HCl are examined. The aforementioned parameters related to the tunneling probability of the proton, including barrier heights, barrier widths, effective masses, and collision energies, are discussed. The Wentzel-Kramers-Brillouin (WKB) approximation is introduced as an effective model for describing the tunneling in these clusters, and a quantitative examination of the probabilities associated with this process is provided. Broader ramifications, including potential connections to experimental spectroscopic analysis, are discussed at the end of the talk.