Calculating Vibrationally Averaged Molecular Properties with Multicomponent Methods

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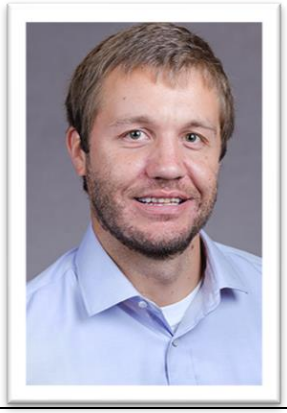

Chemistry Seminar on *Calculation of Molecular properties*

Monday March 31 at 4 pm in 126 Schrenk

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

Abstract: Multicomponent methods are a rapidly emerging class of quantum-chemistry methods that inherently and directly include nuclear quantum effects such as zero-point energy and nuclear delocalization in quantum-chemistry calculations. Such nuclear quantum effects are often important when comparing experimentally measured molecular properties to those calculated theoretically. As an example, theoretically calculated rotational constants commonly change by 0.5% when vibrational averaging effects arising from zero-point energy are included. As accuracy with 0.1% of the measured value is normally needed to assist experimental studies, their inclusion in calculations is essential. In this talk, we will pedagogically introduce the multicomponent formalism, discuss our recent implementations of wave function-based multicomponent methods, and demonstrate how these methods can calculate accurate vibrationally averaged molecular properties such as geometries and rotational constants. Finally, we will show how multicomponent methods have the same computational scaling with respect to system size and similar working equations as the standard methods of quantum chemistry. These similarities make multicomponent methods ideally suited to include nuclear quantum effects in computationally chemistry calculations for a wide range of systems and by a diverse cohort of computational chemistry users.

About the speaker: Kurt R. Brorsen is an Assistant Professor of Chemistry at the University of Missouri-Columbia. He received his Ph.D. in Physical Chemistry from Iowa State University in 2014 in the group of Mark S. Gordon. He was a postdoctoral research associate at the University of Illinois Urbana-Champaign in the group of Sharon Hammes-Schiffer from 2014-2018. His research focuses on the development of new theoretical quantum-chemistry methods. Current research interests include the development of new multicomponent methods for the inclusion of nuclear quantum effects in computational-chemistry calculations, the application of selected configuration interaction methods to novel systems, and computational studies of precursors for oxidative molecular layer deposition.