PHYSICAL CHEMISTRY SEMINAR

Wednesday, March 6, 2024
10:30-11:30 a.m. BRWN 4102

"Unraveling the Periodic Table, Spanning the Control of Excitation Pathways to Environmental Contaminants"

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Abstract:

Theoretical chemistry provides vital developments to unravel some of our most challenging chemical problems. An ongoing challenge is throughput – how to describe chemical properties well, not just aiming for qualitative accuracy, but quantitative accuracy – but, to do so efficiently. In this talk, a range of computational methodologies, including some we have developed, will be discussed and demonstrated, in terms of their utility towards achieving quantitative or qualitative accuracies in the prediction of thermochemical properties. Our work has spanned the periodic table, and demonstrations throughout the periodic table will be provided. In recent work, we have developed methodologies that enables control of excitation and de-excitation pathways for transition metal species, and in this work, our model systems are relevant to processes targeting replacement of species like ruthenium in solar cells with more earth-abundant species. As well, our group has been well-engaged in per- and polyfluoroalkyl substances (PFAS) research, with a focus upon the modeling of PFAS interactions in a range of environments, with some demonstrations of the impact of methodology choice.

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