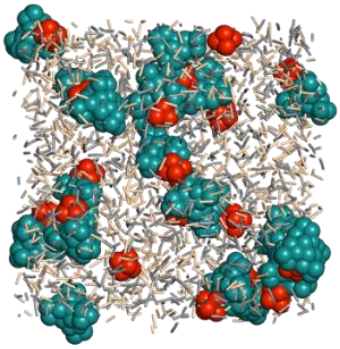
Beyond Arrhenius: Uncovering Driving Forces for Chemical Dynamics

Prof. Ward H. Thompson



A key part of understanding a chemical transformation is determining the size and nature of the barrier involved. The Thompson group has developed theoretical methods for calculating activation energies directly from simulations at a single temperature – *i.e.*, moving beyond an Arrhenius analysis. NSF-REU participants will implement these methods to gain new insight into interesting chemical systems. Of particular interest are CO_2-expanded liquids (CXLs) and electrolytes (CXEs), which are exploited by experimental collaborators as tunable reaction media for catalysis and electrocatalysis. In particular, CXEs (a snapshot of which is shown on the right) have promise for use in electrochemical CO_2 reduction reactions that can convert the greenhouse gas into useful chemical species. Key challenges remain in understanding how to engineer these CXEs, not only through their pressure and temperature dependence, but through modification of the anions and cations that carry the charge. Students will learn fundamental physical chemistry, computer coding, numerical analysis, and molecular dynamics. Dr. Thompson has 8 papers with undergraduate co-authors, 4 of whom were NSF-REU participants.[1-8]

References.

Names of non-KU REU authors are in **bold**; Names of other undergraduates are underlined.

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