Advancing Fundamental Molten Salt Modeling using Ultrafast Spectroscopy

PI: Alexander Bataller – NCSU
CoPI: Benjamin Beeler – NCSU
Collaborator: Amanda Leong, Virginia Tech

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ABSTRACT:

An important need for developing molten salt reactors (MSRs) and pyroprocessing facilities is the ability to predict molten salt properties across a large temperature and compositional parameter space. One method utilized in the field features molecular dynamics simulations to obtain equilibrium properties, which are then compared to experimental measurements (e.g., electrical conductivity). More recent efforts include *ab initio* molecular dynamics (AIMD) for simulating local structure, which are then validated against x-ray and/or neutron scattering experiments. While this methodology has demonstrated success, an important output of AIMD simulations has not been utilized nor validated in advancing our fundamental understanding of molten salts, namely, the ion kinetics. The information provided by ion kinetics is directly related to the atomic interactions, and thus dictates many of the macroscopic phenomena of interest to the MSR community (e.g., thermal and electrical transport). Ionic motion in molten salts occurs on the femtosecond-to-picosecond timescales, which necessitates ultrafast spectroscopic techniques for their interrogation. The overarching goal of the proposed research is to advance our fundamental understanding of molten salts by combining ultrafast spectroscopic experiments with high fidelity atomistic simulations. To achieve this goal, the proposed research will introduce a new experimental technique to the study of molten salts that will directly measure ion kinetics, specifically, terahertz time-domain spectroscopy (THz-TDS). The complex refractive index obtained from THz-TDS will then be compared to the results of AIMD simulations and prior experimental structural studies. Our proposed methodology will be applied in progression of salt complexity including $MgCl_2$, NaCl-$MgCl_2$, and finally NaCl-$MgCl_2$-UCl_3, where the ternary salt is relevant to MSR fast reactors as a fuel salt.