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Passport:
U.S. Passport; Date of expiration: 24 October 2022;
I anticipate no issues to obtain a visa for Russia in a seven day timeframe
CCP Poster Presentation:
Title: Simulating the Solvation Dynamics of Ionic Liquids
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Abstract:

Molecular dynamics simulations of coumarin 153 (C153) in imidazolium based ionic liquids (ILs) are performed to shed insight into solvation dynamics and compare directly with experimental studies. Solvation dynamics in ILs reveal very complex kinetics over a range of time scales, spanning from femtoseconds to tens of nanoseconds. In order to draw conclusions about the nature of these dynamics an extensive amount of simulation time is necessary for the response function to converge, requiring at least 5 microseconds of MD simulations per ionic system. By employing various decomposition techniques on the simulated solvation dynamic response on a representative set of ILs it is possible to deduce information about the local environment and factors responsible for solvation dynamics and identify any trends that may exist. Thus far, preliminary analysis of the structure in the vicinity of C153 has revealed preferential solvation by the cations despite typically being larger than the anions. However when separating the solvation response into its respective components, it is the smaller and more distant anions that are responsible for a majority of the short and long time response to the sudden charge perturbation. Obtaining insight of solvent dynamics is crucial for our understanding of solvent effects on chemical reactions. Given the multitude of possible combinations of cations and anions, it is absolutely necessary to understand the molecular interactions that are responsible for the macroscopic physicochemical properties of interest.

Relevant References:

(1) Terranova, Z. L.; Corcelli, S. A. "On the Mechanism of Solvation Dynamics in Imidazolium-Based Ionic Liquids," *The Journal of Physical Chemistry B* **Article ASAP.**
(2) **Supplemental Information:** http://zackterranova.com/research