Ultrafast Vibrational Spectroscopy of Ionic Liquids: Insight into Carbon Capture, Chemical Reactions, and Energy Storage

Abstract:

Ionic liquids are complex solvents. Due to their unique properties, they are being explored for applications as carbon capture absorbents, electrolytes, and energy storage media. From a fundamental perspective, ionic liquids are at the forefront of research because of their structural and dynamical heterogeneity. Many important physical and chemical properties are dictated by the solvation shell around a molecule. The solvation shells are characterized by structure with short length-scales and dynamics on femtosecond to picosecond time-scales, which makes them difficult to observe with many conventional spectroscopies. Ultrafast vibrational spectroscopy, however, can measure the dynamics of the solvation shell around molecules directly. Here, we use ultrafast 2D-IR spectroscopy and supporting theory to explore the dynamics of ionic liquids relevant to several important applications. The vibrations of CO$_2$ report carbon capture from the carbon dioxide's point of view. Thiocyanate, SCN$^-$, displays that dynamics in soft confinement depend strongly on the size and charge of the reverse micelle. Azides partition in different ionic liquid domains due to their hydrogen bonding patterns, which may explain reaction rates and selectivities. Finally, borohydrides may provide a platform for studying hydride transfer reactions in ionic liquids.