



STEM RESEARCH

2021 Virtual HBCU-UP/CREST PI-PD Meeting

Analyzing Imidazolium-Based Ionic Liquid Systems Using C-D Vibrational Labels on Cations



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All findings and opinions are those of the authors, not necessarily of the funding agency or AAAS.



Project Overview

Ionic liquids are entirely made of ions. Typically made of large organic cation in combination with inorganic/organic anions

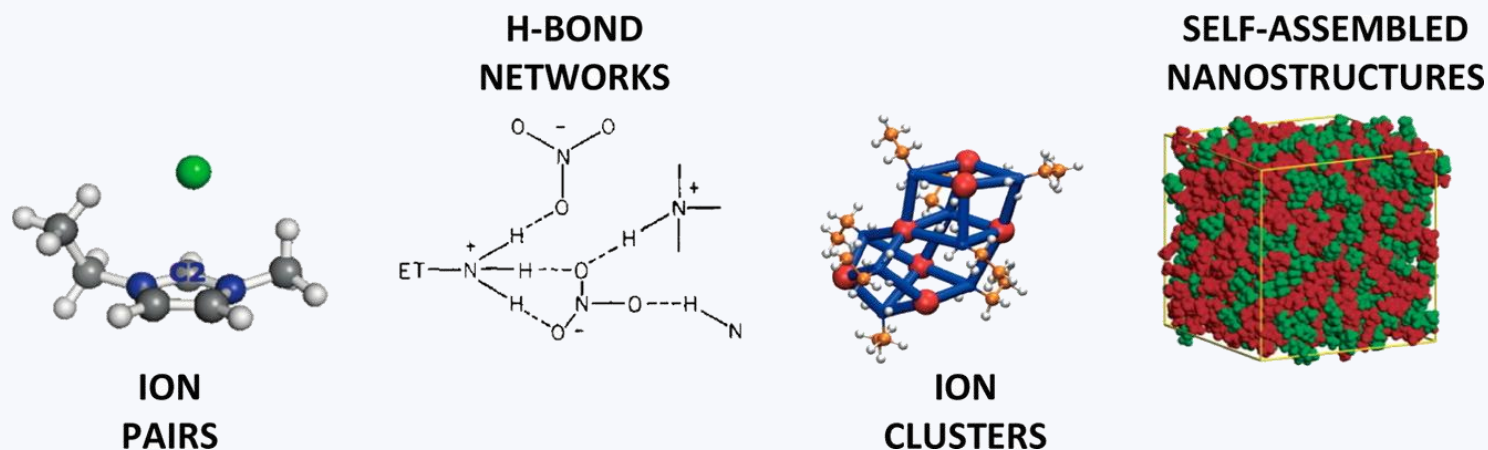


Figure 1: Ionic liquid microenvironment is complex.

Objectives

1. Temperature-dependent restructuring of the ionic liquid
2. The nature of molecular solvent-ionic liquid interactions
3. Gas uptake mechanisms

Source : Canongia Lopes & Padua *J. Phys. Chem. B*, 2006.
Hunt et al. *Chem. Soc. Rev. B*, 2015.



Successes

C2-D band in [EMIM][BF₄] has a striking thermal profile

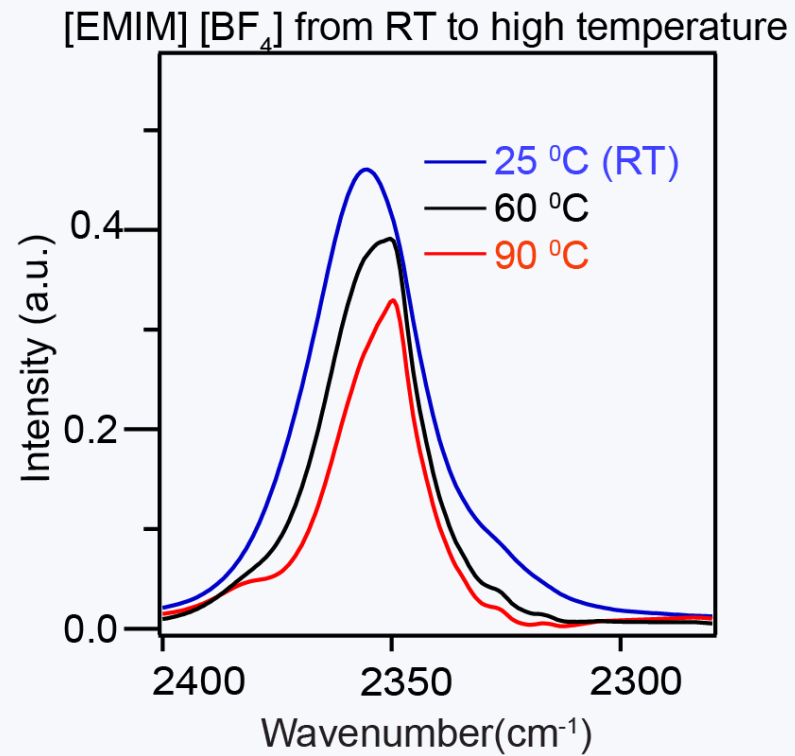
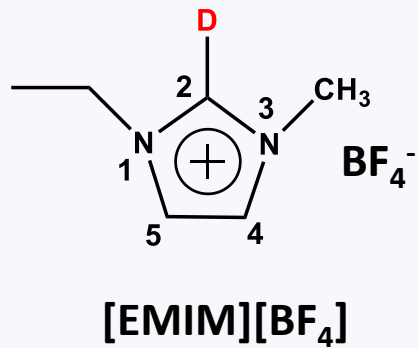


Figure 1: Temperature-dependent studies shows

Implications

- On heating, imidazolium-based ionic liquids can assume ordered structure. Such behavior is counterintuitive as molecular solvent tends to disorganize on heating.



Identified Gap(s)

It is not clear from our studies the molecular origin of the observed ordering with heating.

We have to enhance our computational methods to align with the observed infrared changes