Unlocking Atomic Insights into the Next Generation of Solvents for Biological Applications

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Ionic liquids (ILs) have shown significant potential across various scientific fields, offering innovative solutions to longstanding challenges[1]. Since experimental methods alone are not sufficient to understand the behaviour of ILs at the atomic scale, this project employs molecular dynamics (MD) simulations to investigate ILs by providing detailed insights into the structural and dynamic properties of ILs with atomic resolution, which are not accessible experimentally. This study will examine both polarizable force fields, which offer improved accuracy by accounting for electronic polarization[2], and classical force fields that offer greater computational efficiency and compatibility with biomolecular systems. This balance makes the approach practical for future studies.

This research focuses specifically on the protic IL ethylammonium nitrate (EAN) with extensive availability of experimental data. We systematically compare a range of force fields for neat EAN and validate the prediction results against experimentally measured properties to identify the most accurate model. The goal is to extend the simulation to EAN-water and other IL-water combinations. Importantly, our simulations also extend to concentrations not yet studied experimentally, providing new data to support future experimental work and solvent design.

As the final goal of this part of the research, the optimal force field will be used to explore different combinations of IL cations and anions in water at different concentrations, enabling the design of IL-based solvents with particular properties for specific applications. This research contributes to predictive IL design and helps bridge the gap between simulation and experiment, with relevance to a wide range of industries, including pharmaceutical and biotechnological applications.

References:

1. Greaves, T. L.; Drummond, C. J. Protic Ionic Liquids: Properties and Applications. Chemical Reviews. **2008**, 108, 206–237.
2. Goloviznina, K.; Padua, A. A. H.; et al. Polarizable Force Fields for Ionic Liquids: A Review. J. Mol. Liq. **2019**, 276, 812–835.

I hold a master's degree in Organic Chemistry, focusing on the synthesis of pharmaceutical-based novel compounds, with over 7 years of R&D experience in pharmaceutical industries, to apply my academic knowledge to real-world challenges. To complement my experimental background and broaden my scientific capability, I chose to pursue a PhD in Computational Chemistry, focusing on molecular dynamics simulations of ionic liquids to improve biomolecules' adaptability in pharmaceutical applications. I have authored four publications and presentations at international conferences.