

The Role of Electrolyte Structure and Dynamics in Organic Redox Flow Battery: Molecular Dynamics Simulation

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Organic redox flow batteries offer a sustainable option for stationary energy storage [1]. However, optimizing battery efficiency and stability requires an understanding of the electrolyte behavior at the molecular level [2]. The structures and dynamics of electrolyte solutions were studied using classical molecular dynamics simulations and experiments in tandem. The simulations are performed with the LAMMPS software [3] using the nonpolarizable OPLS-AA force field [4] for all the neat molecular solvents and the CL&P force field for ionic liquids [5]. First, we characterized the bulk properties of the solvents (acetonitrile, 3-methoxypropionitrile) and of their mixtures with the ionic liquid EMIMTFSI. We compared the simulated structure factors from our model to the experimental X-ray scattering data. To further verify the model, we compared simulated transport properties (such as viscosity, diffusion coefficients, and ionic conductivity) and dielectric spectra to the experimental data to gain a full picture of how ions and molecules are transported.

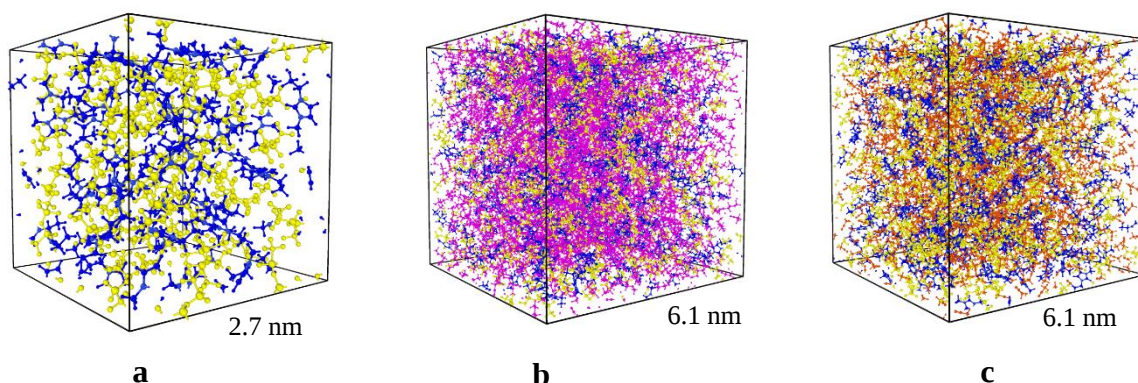


Figure 2. Graphical snapshot of molecular dynamics simulation a) pure EMIMTFSI, b) Acetonitrile + EMIMTFSI (20% ionic liquid), c) 3-methoxypropionitrile + EMIMTFSI (20% ionic liquid). (EMIM: blue, TFSI: yellow, Acetonitrile: pink, 3MPN: Orange.)

The simulations offer key insights into ion solvation, ion pairing, the role of solvent composition in larger-scale molecular ordering, and how the structures of ions and molecules dictate the dynamic behavior of the electrolyte. Future stages of this research will incorporate redox-active species and electrode–electrolyte interfaces, enabling us to gain deeper insight, address challenges such as the prevention of crossover, and ultimately improve battery performance.

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