Organic Redox Flow Batteries: Simulation of Polymeric Membranes

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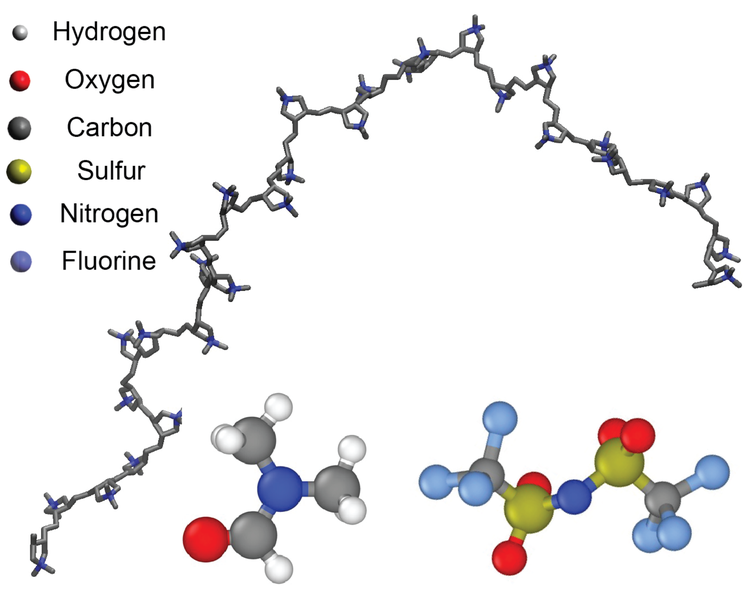
1. Introduction

Organic redox flow batteries (ORFBs) present a promising avenue for sustainable energy storage due to their superior charge density compared to conventional redox flow batteries (RFBs). Their capabilities position them as strong candidates for large-scale energy storage solutions. However, this emergent field requires significant effort to optimize performance. In this study, we mainly utilize classical molecular dynamics (MD) simulations to elucidate and quantify the properties of potential ORFB candidates. We focus on the nanostructural, mechanical, and transport characteristics of membranes in various electrolyte solutions, as well as their interfacial interactions.

2. Building the Models

Solvents: DMF (for casting the membrane), DMF C_3H_7NO
Polymeric Membrane: Polydiallydimethylammonium PDADMA-(anion). Cis and trans Isomers $(C_8H_{16}N)_n^+$
Anion: Bis(Trifluoromethylsulfonyl)imide TFSI$^-$.$(CF_3SO_2)_2N^-$

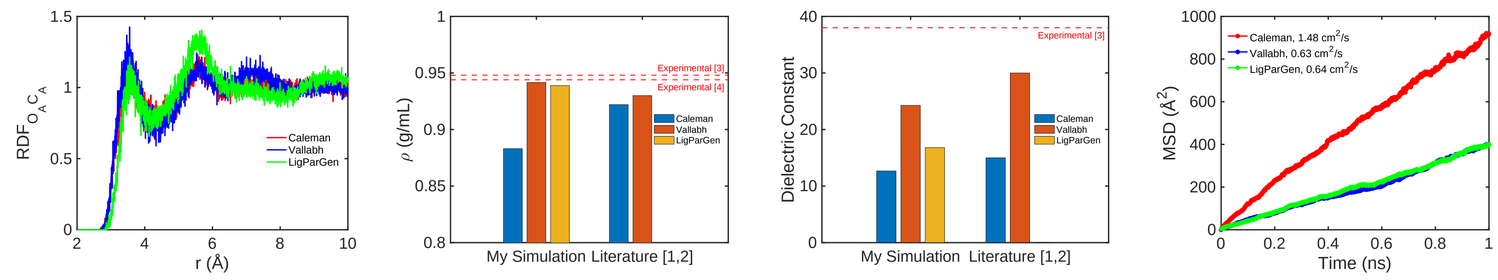


3. Methods

Molecular dynamics simulations are conducted using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS), with the non-polarizable OPLS-AA and CL&P force field [5, 6].

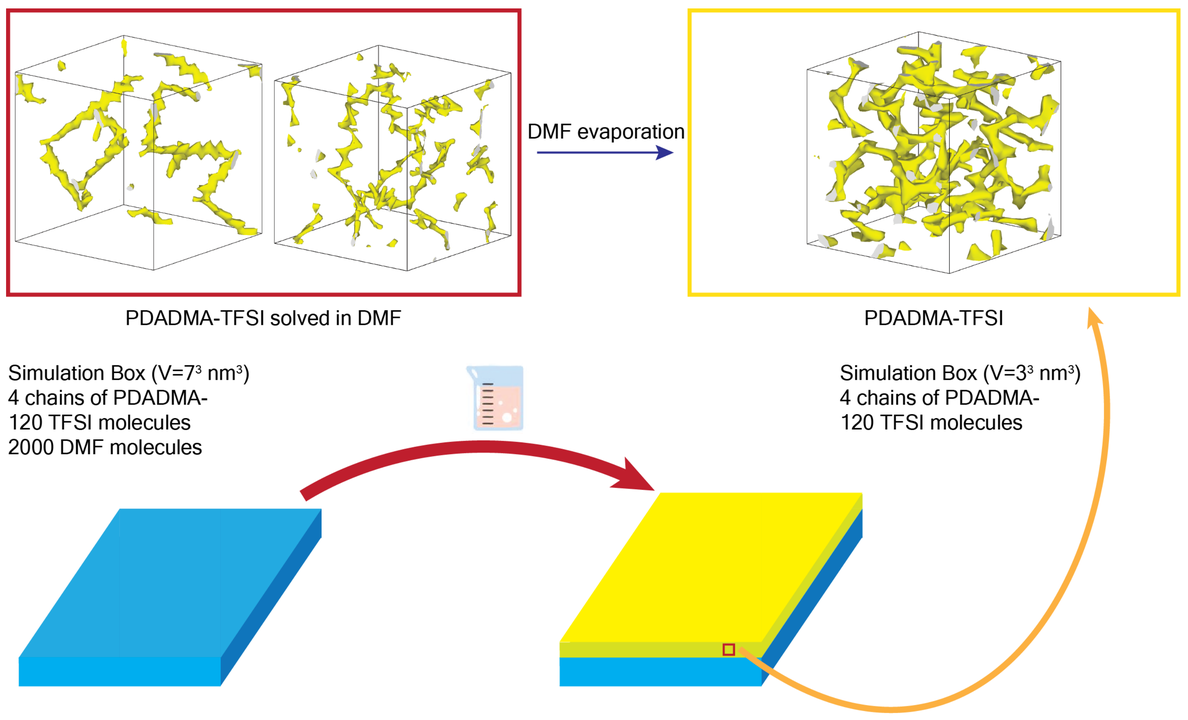
4. DMF Models

We aim to use the optimized the simulation parameters to accurately represent the density, dielectric coefficient, diffusivity, and nanoscale structure orientation of DMF molecules. The plots in this section illustrate a good agreement between our simulations and the literature. Based on the comparison of the different partial charges proposed for DMF, we will use the partial charges suggested by Vallabh [1, 2, 3, 4].

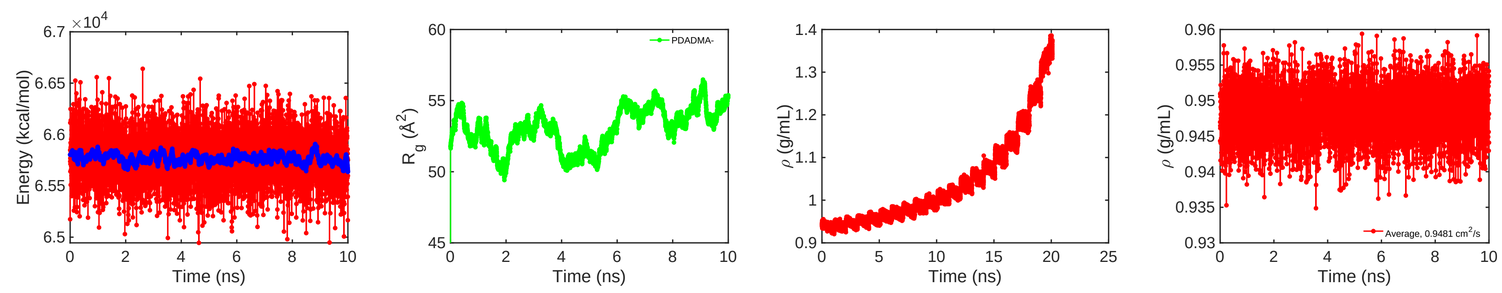


5. Perspective on the Fabrication of the Membrane

This process has been inspired by experimental fabrication methods. The first step involves simulating PDADMA-TFSI in a DMF solution to achieve a relaxed orientation of the polymer. The next step is to evaporate the solvent (DMF), followed by a final energy relaxation of the remaining PDADMA-TFSI in the simulation box.

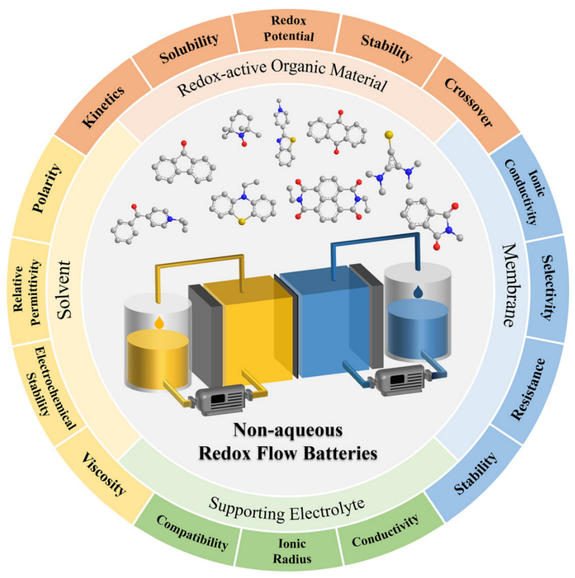


Sudden changes in the radius of gyration of the polymer indicate a phase transformation in the energy relaxation of the PDADMA-TFSI solution in DMF. This suggests performing the simulation over a longer duration.



6. Application

This polymer will serve as a membrane separating the electrolyte solution in organic redox flow batteries. Here, we present different components of the ORFBs [7].



7. Acknowledgment

Financial support from the European Union Horizon Europe Research and Innovation programme under the Marie Skłodowska Curie Industrial Doctoral Network [101119913] “StoreAge” is gratefully acknowledged.

8. Contacts Information

LinkedIn Website Poster PDF

9. References

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