Coarse-Graining of Ionic Liquid Electrolytes to Deliver Accurate Dynamics at the Mesoscale

By: Amber Pitt and Lexi Parks

Mentor Dr. Sergiy Markutsya, Department of Mechanical Engineering, UK

Grand Challenge:

The engineering grand challenge in this project is ***Engineer the Tools of Scientific Discovery***. Specifically, how engineering will help us explore the universe. This research has direct applications in lithium-ion battery power and efficiency.

Problem:

Current coarse-grain molecular dynamics methods accurately predict structure but not dynamic properties such as diffusion coefficient and radial distribution function.

Hypothesis:

Application of new coarse-grain method will accurately predict both structure and dynamic properties of ionic liquids when compared to reference atomic molecular dynamics simulation.

Introduction:

Molecular dynamics (MD) is a powerful tool in predicting structure and dynamic properties of systems at the atomic scale.

More efficient methods, such as coarse-grain molecular dynamics, can be used instead.

Current coarse-grain molecular dynamics (CGMD) methods do not accurately predict the dynamic properties of diffusion coefficient and radial distribution.

This new coarse-grain method does predict both diffusion coefficient and radial distribution of ionic liquids.

CGMD simulations show the accuracy of this new method.

Coarse-Grain Molecular Dynamics vs. All Atom Molecular Dynamics

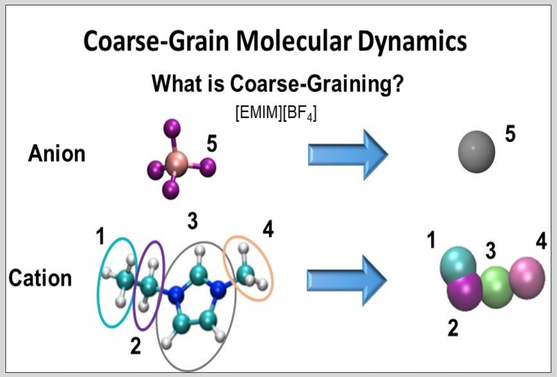

Figure 1. All-atom cation and anion molecules and corresponding coarse-grained model.

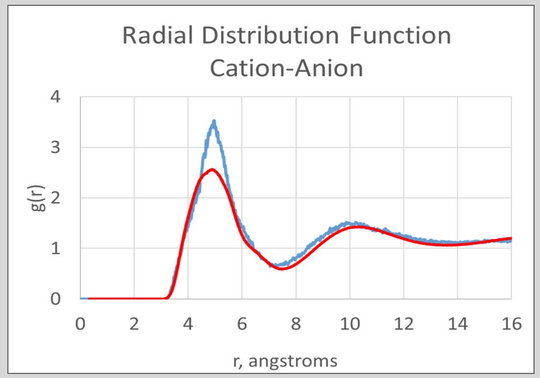

Figure 2. Radial distribution function of the cation-anion pair from the coarse-grained model (blue line) and the all-atom model (red line).

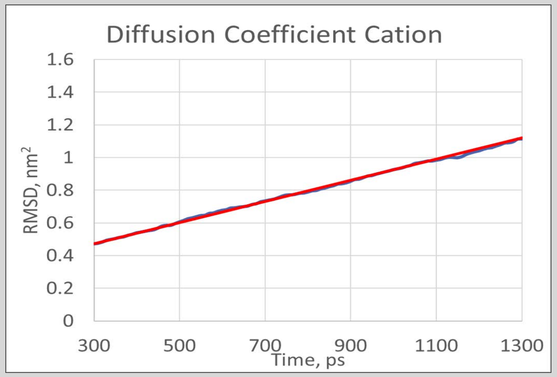

Figure 3. Diffusion coefficient of the cation from the coarse-grained model (blue line) and the all-atom model (red line).

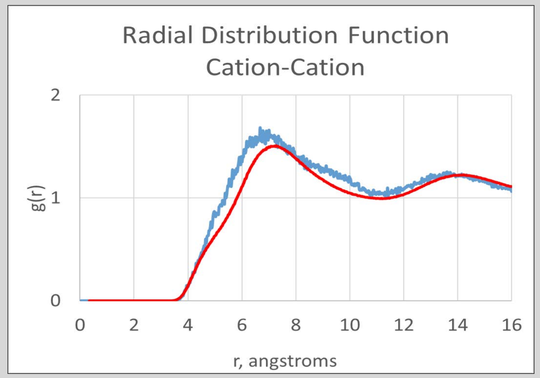

Figure 4. Radial distribution function of the cation-cation pair from the coarse-grained model (blue line) and the all-atom model (red line)

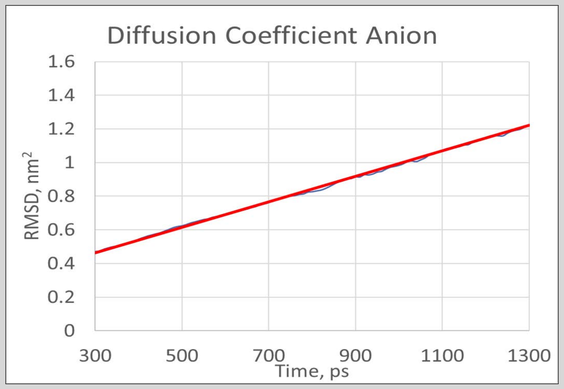

Figure 5. Diffusion coefficient of the anion from the coarse-grained model (blue line) and the all-atom model (red line).

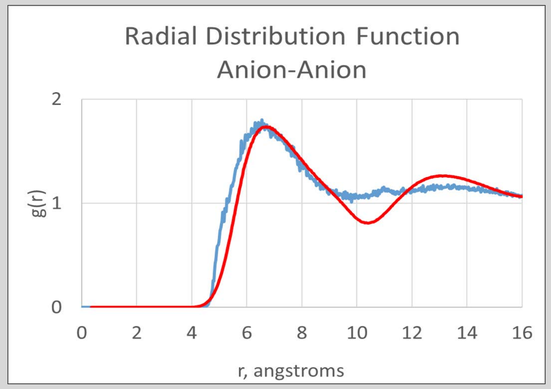

Figure 6. Radial distribution function of the anion-anion pair from the coarse-grained model (blue line) and the all-atom model (red line).

Results:

Diffusion coefficient and radial distribution function are calculated for CGMD and compared to the same parameters obtained from MD simulation.

The following equation was used to determine the diffusion coefficient:

$$\left\langle \left(\boldsymbol{r}(\boldsymbol{t}) - \boldsymbol{r}(\boldsymbol{0})\right)^{2} \right\rangle = \boldsymbol{6Dt}$$

Conclusions:

CGMD method has been successfully applied to ionic liquid electrolytes. This CGMD method accurately represents dynamic properties of coarse-grained model of ionic-liquid electrolytes.

Retained accurate representation of CG structure of ionic liquid electrolytes

The diffusion coefficient lines up perfectly, while the radial distribution function is a close approximation.

Acknowledgements:

Dr. Jeffery Seay, Department of Chemical Engineering, UK

University of Kentucky, College of Engineering

University of Kentucky, Honors Scholars Program

References:

Wang, et. al. 'Multiscale Coarse-Graining of Ionic Liquids', J. Chem. Phys, 110 (2006).

Wang, et. al. 'Multiscale coarse-grained simulations of ionic liquids: comparison of three approaches to derive effective potentials', Phys. Chem. Chem. Phys., 2013, 15, 7701

Merlet, et al. "New Coarse-Grained Models of Imidazolium Ionic Liquids for Bulk and Interfacial Molecular Simulations." *The Journal of Physical Chemistry C*, vol. 116, no. 14, 2012, pp. 7687–7693., doi:10.1021/jp3008877.

Markutsya, et. Al. The Journal of Chemical Physics 141, 174107 (2014); doi: 10.1063/1.4898625