Layering Structure Formation in Ionic Liquids at Ionic Liquid / Vacuum Interface

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Problem:

Current approaches to coarse-grain molecular dynamics fail to accurately predict dynamics due to neglection of friction and forcefields, and numerous degrees of freedom.

Hypothesis:

Applying the molecular modeling simulation approach for coarse grain molecules will accurately produce the structure and dynamics of the ionic liquid found through experimentation.

Introduction:

Simulation accurately produces structure by emulating the ionic liquid at an atomic level.

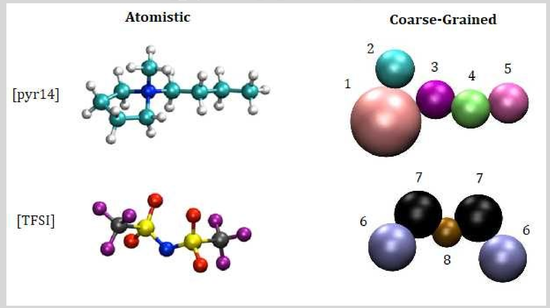
Current coarse-grain molecular dynamics (CGMD) methods do not accurately predict the dynamic properties of diffusion coefficient and radial distribution.

New coarse-grain simulation approach has been applied to predict both diffusion coefficient and radial distribution of ionic liquids.

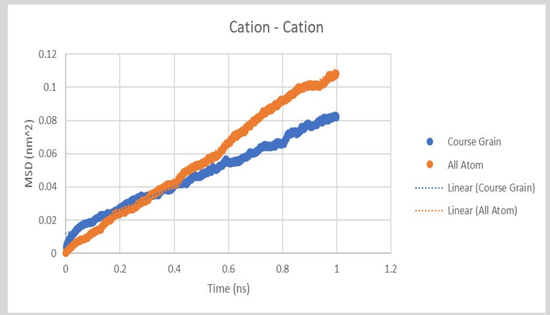
CGMD simulations compared with all-atom MD results show the accuracy of the new method.

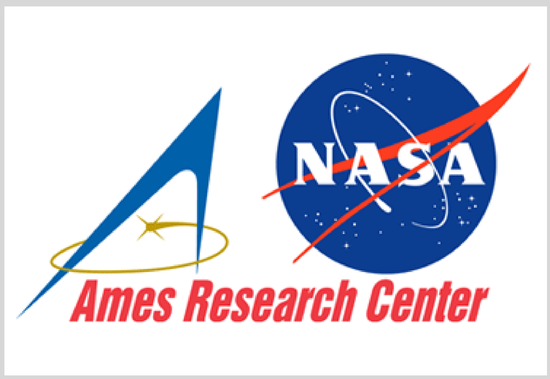
Results:

Coarse-Grain Molecular Dynamics
[pyr14] [TFSI]

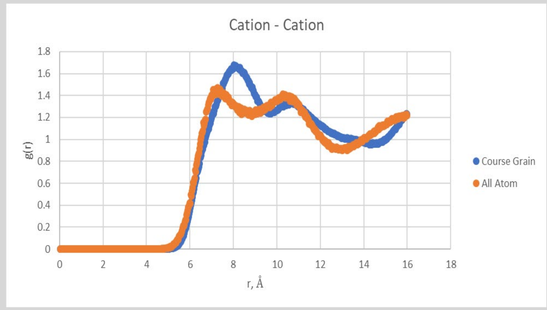


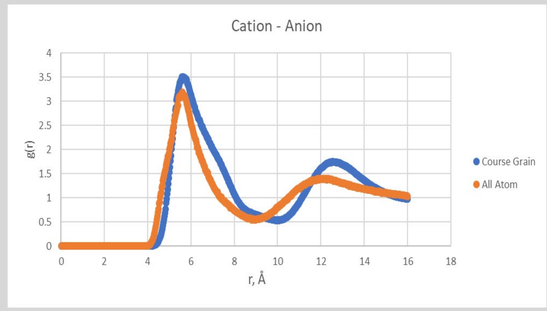
Self-Diffusion Plots:

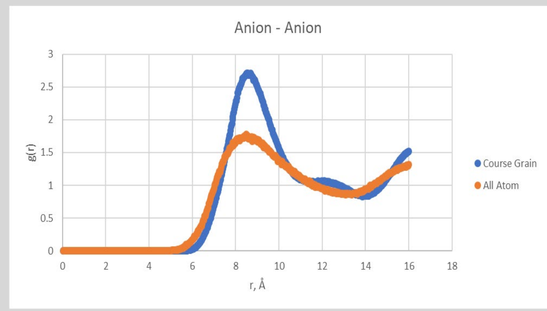




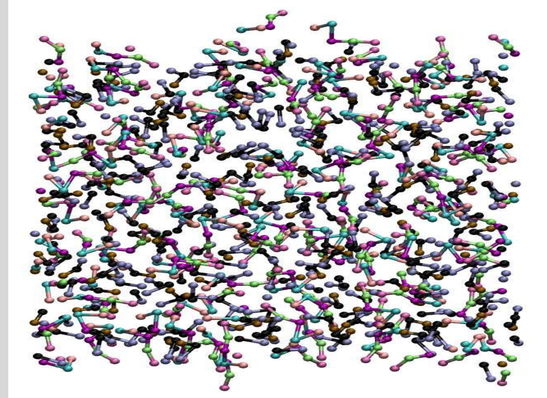
Radial Distribution Functions:







Ionic Liquid/Vacuum CGMD



Results:

Diffusion coefficient and radial distributing function were derived by simulation, and plotted as a function distance between molecules over time.

The diffusion coefficient was determined using the following equation:

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

Conclusions:

The coarse-grain model for ionic liquid has been developed.

By simulating the coarse-grain model, structure and dynamics were predicted accurately, and were consistent with those obtained through all-atom simulations.

Preliminary simulations for ionic liquid vacuum interface have been conducted.

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References:

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