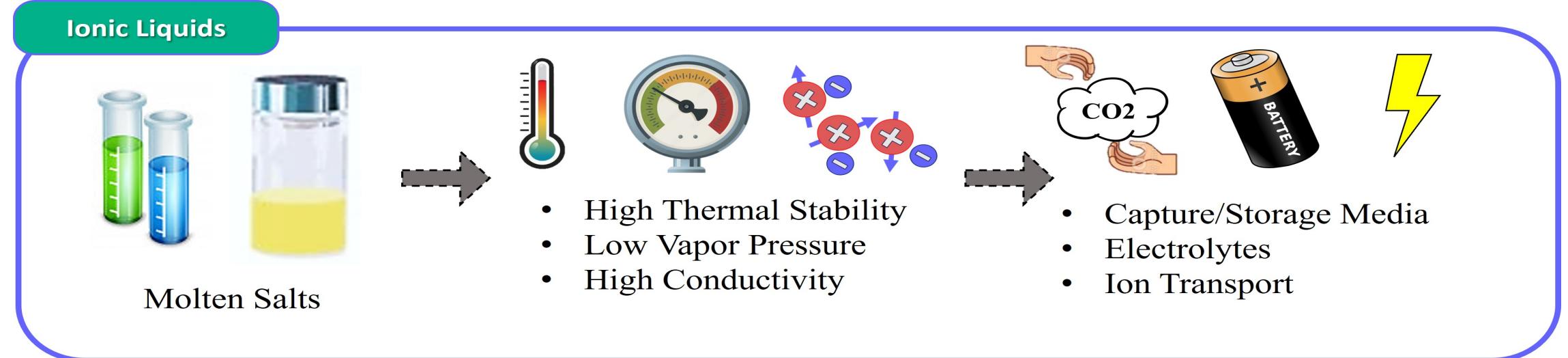


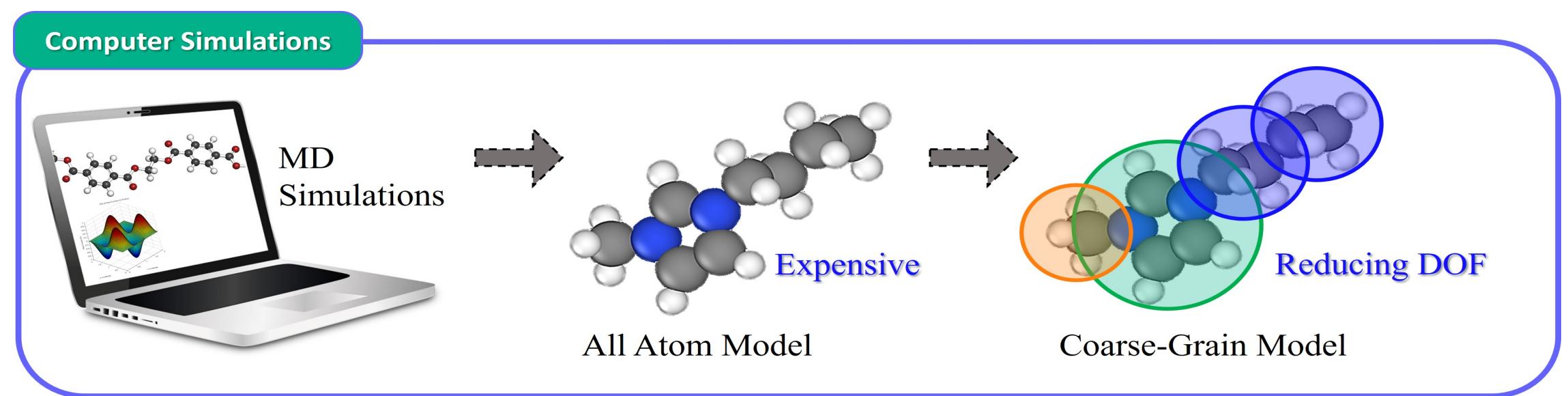
Analyzing Dielectric Constants & Electrostatic Energies of Ionic Liquids : Mean-Field Theory and Stockmayer Fluid Simulation

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Background



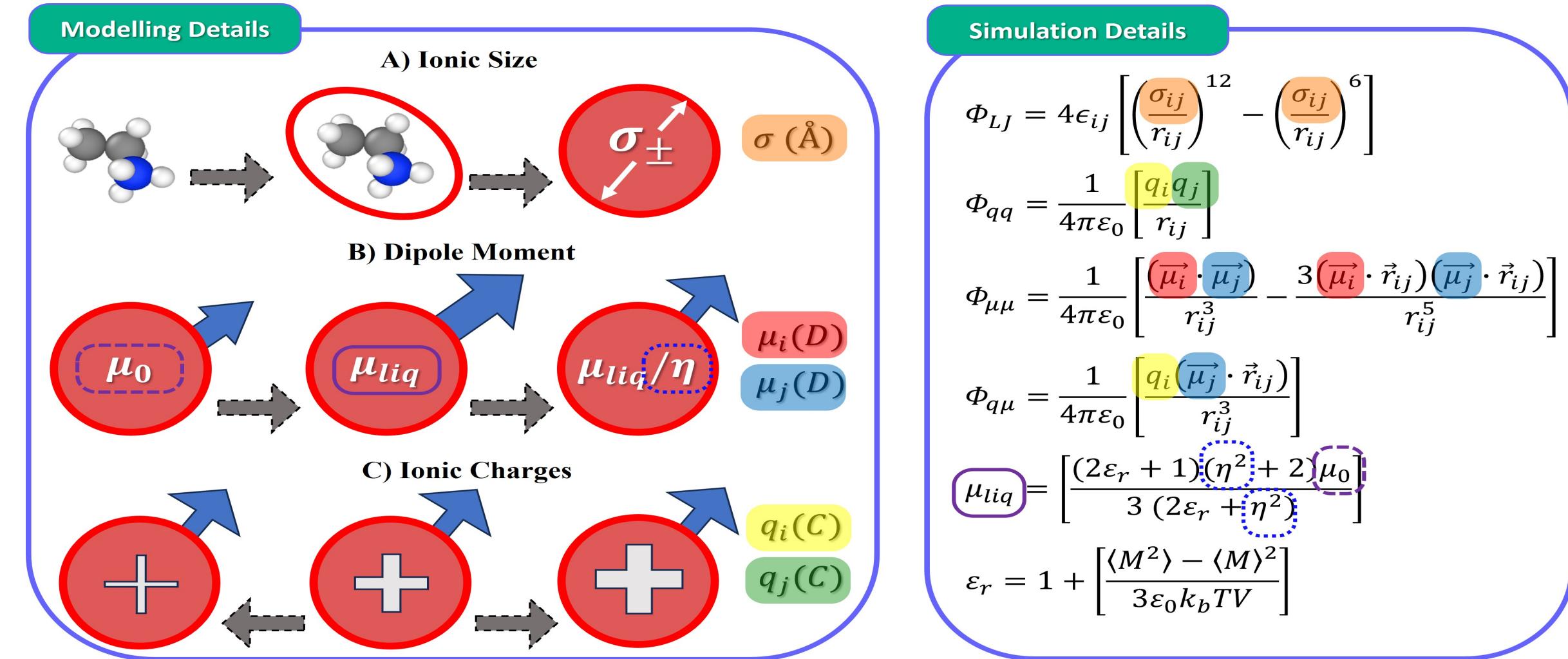
The Ionic Liquids (ILs) are molten salts at room temperature that possess remarkable properties, making them suitable for many applications. Our knowledge of IL dynamics and mechanisms is limited. MD simulations for such large systems can be used as one of the solutions to understand the processes involving these.



In such studies, an all-atom approach is traditionally used, but it is computationally expensive, and statistical noise is a problem. To reduce model's complexity and computational cost, coarse-grain approaches were developed.

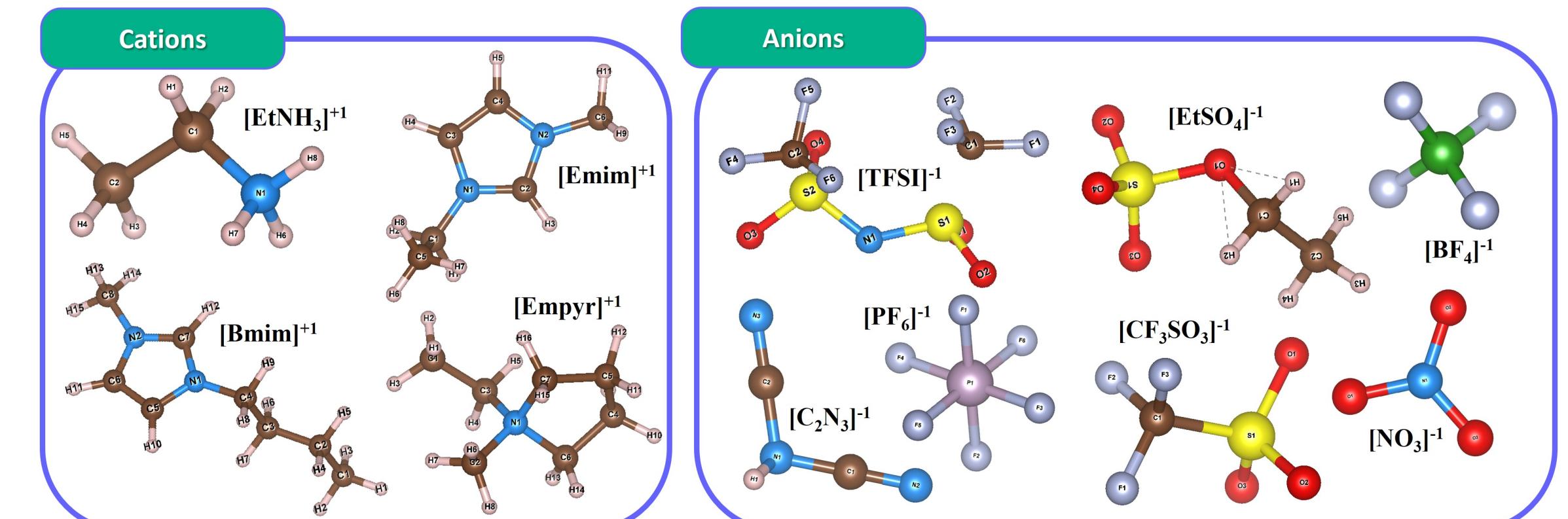
Modeling & Methodology

The Coarse-Grain Stockmayer Fluid Model treats ions as Lennard-Jones spheres carrying point charges with embedded dipole moments. Charges and dipoles interact among themselves with defined potentials.



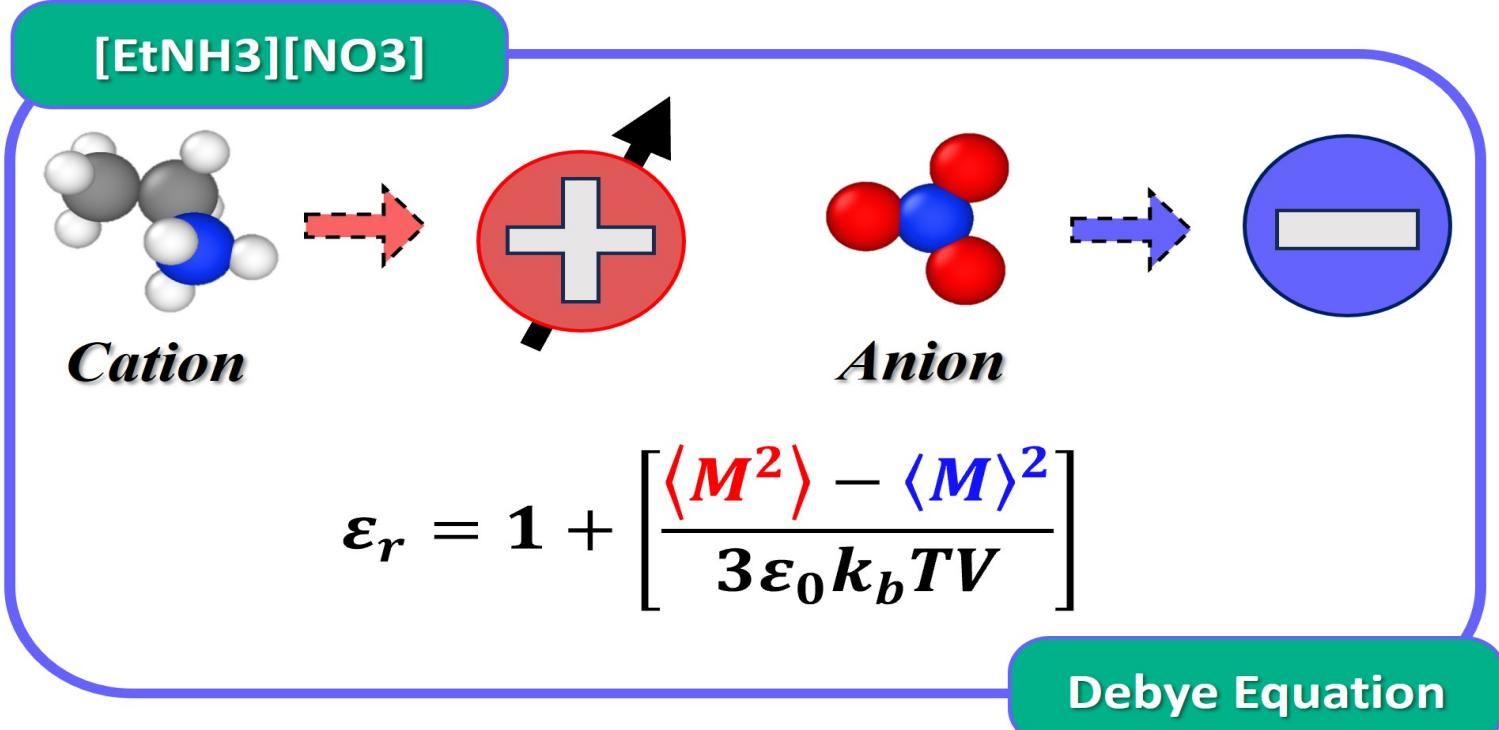
The CGSF is a simple, non-implicit model that accurately captures the behaviour and properties of ILs.

Ionic Liquids Under Investigation



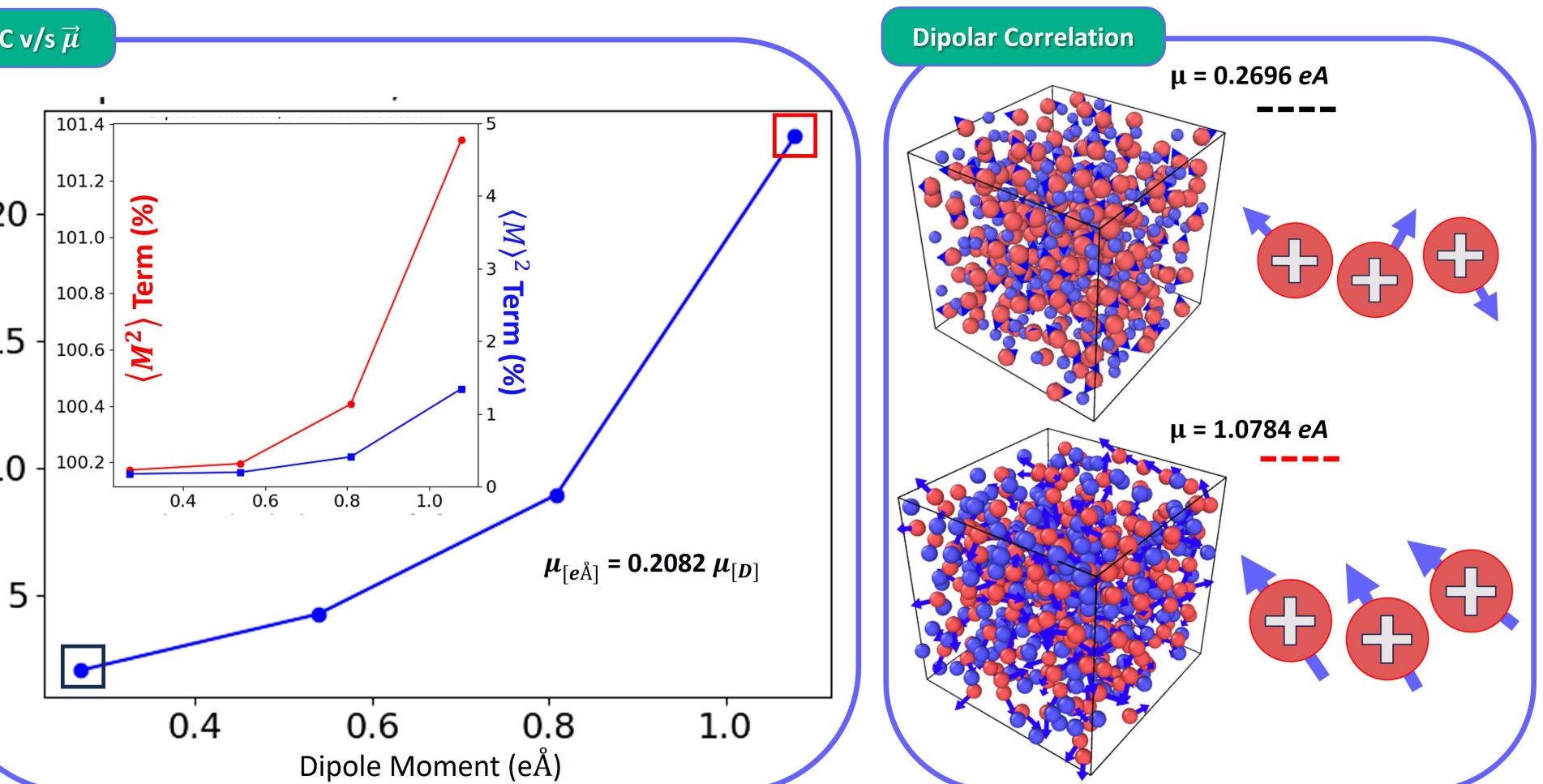
Our modeling efforts focused on a few organic cations and organic/inorganic anions which are often used as candidate ILs in many applications.

Dielectric Constant & Model Parameters

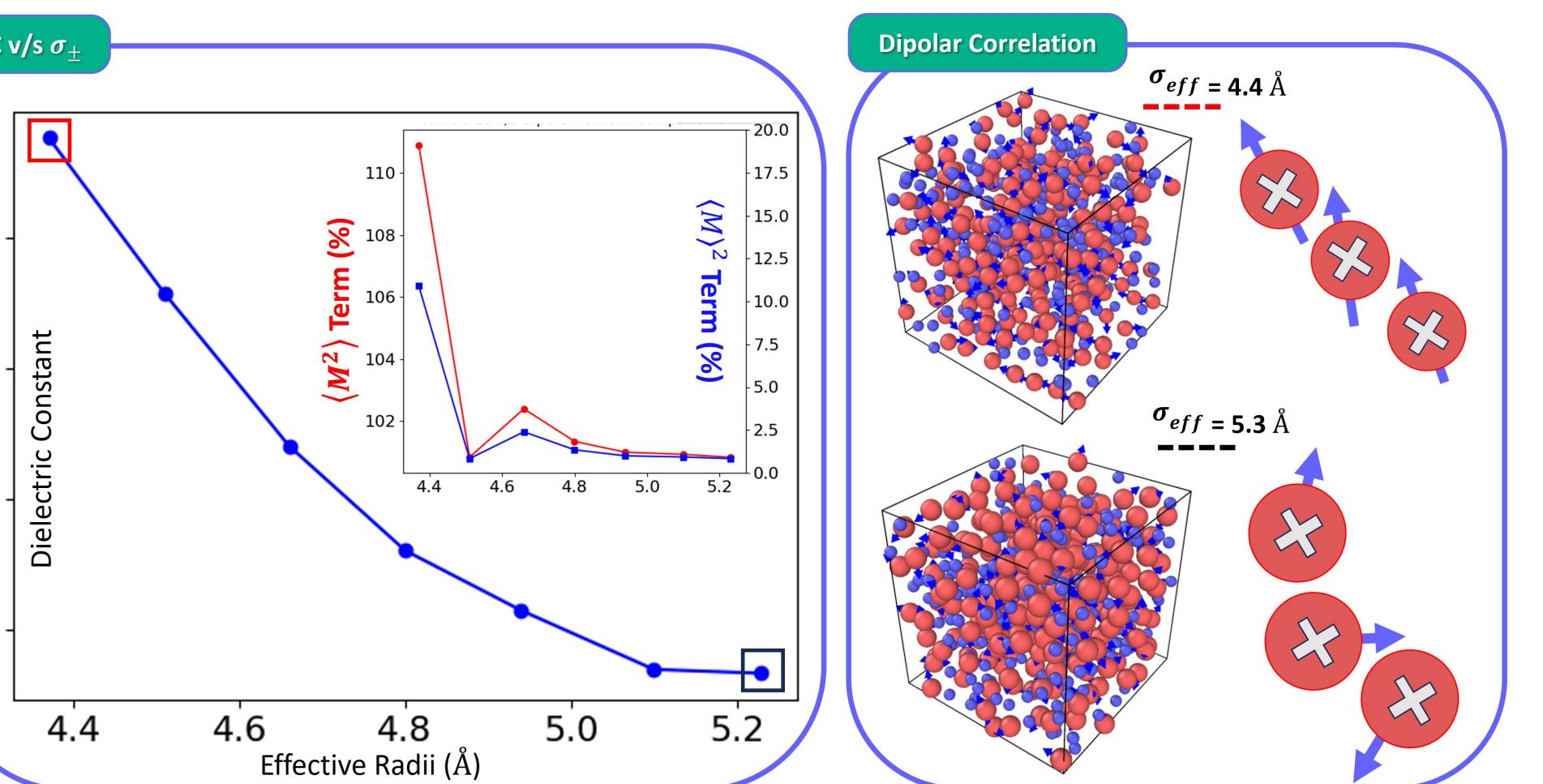


Dipolar moments and dipolar interactions make up the overall DC in our model. The red term can be attributed to dipolar correlations while the blue term corresponds to dipolar orientations. In an isotropic system, the blue term is negligible and contributes only upto 3-5%.

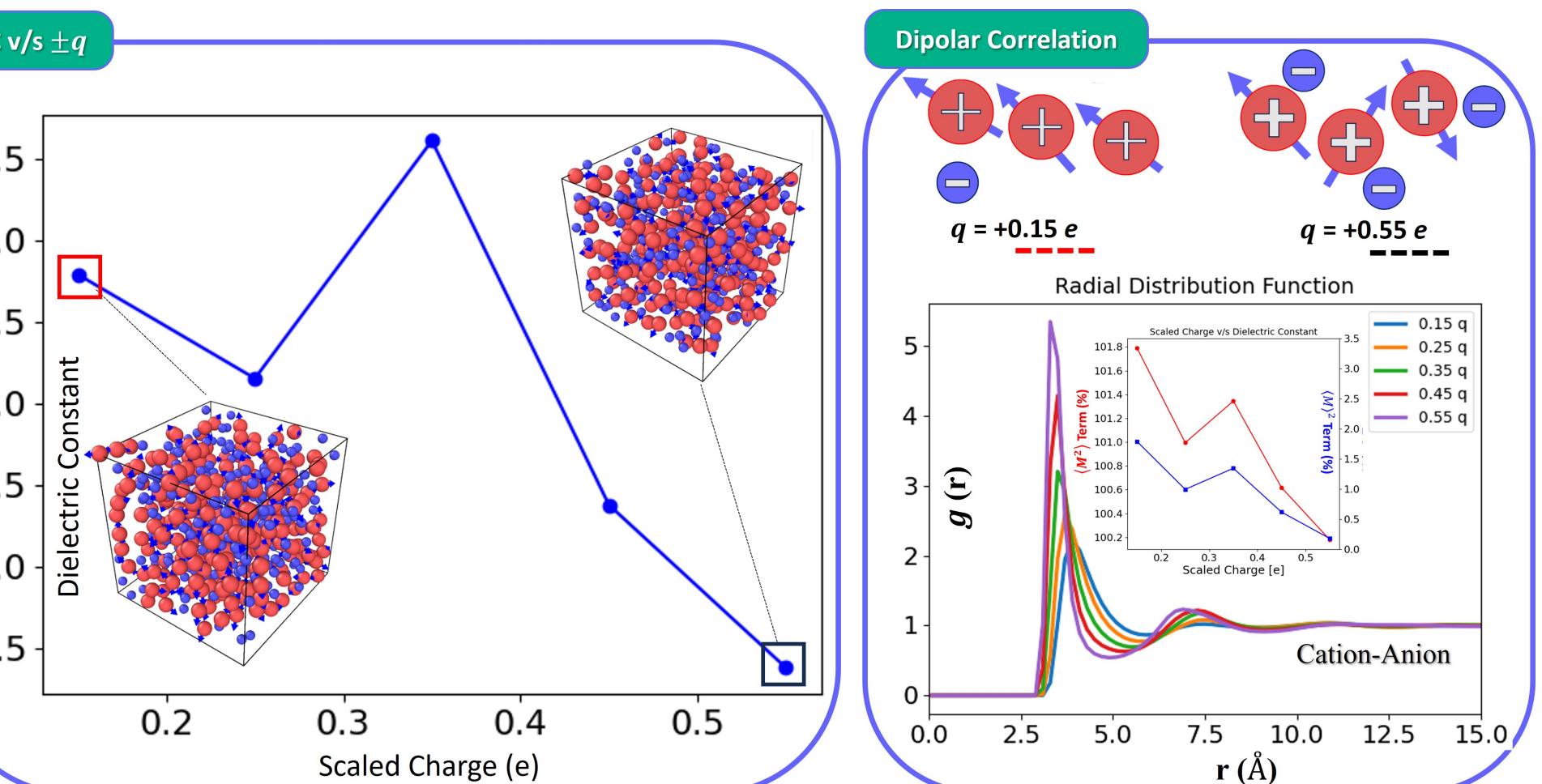
Dependence on Dipole Moment



Dependence on Ionic Size



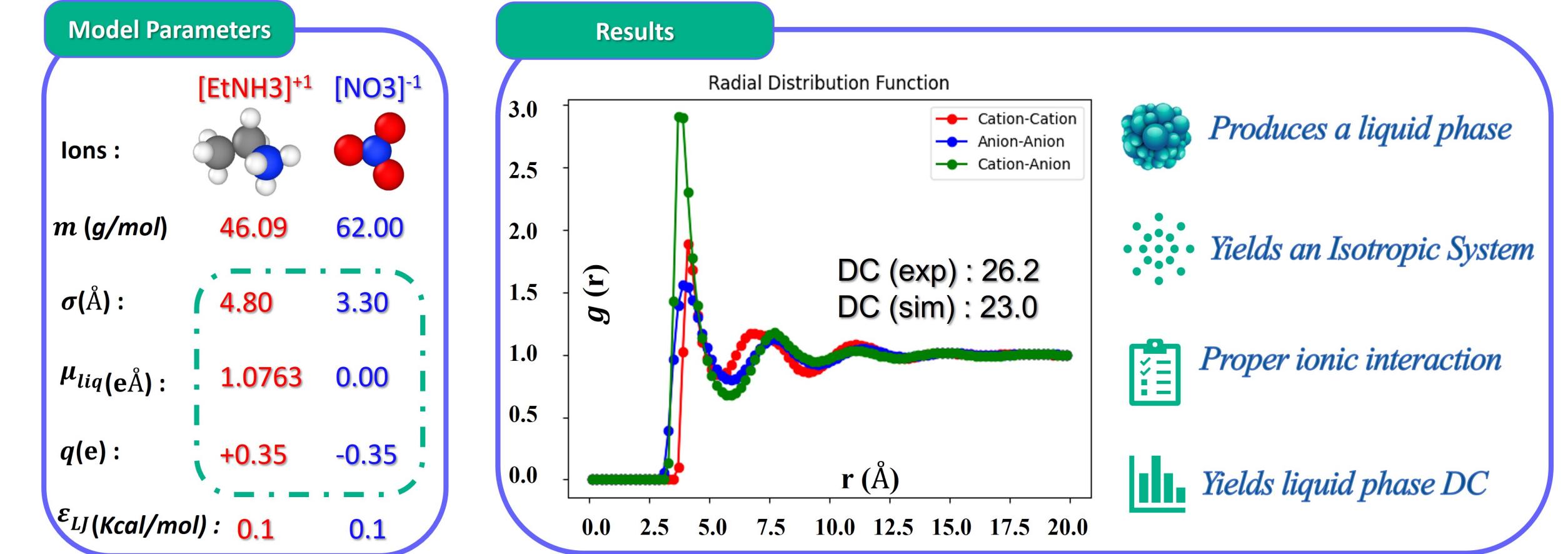
Dependence on Ionic Charge



In order to achieve optimal results, the three model parameters must be chosen within the extreme bounds. A system that is isotropic should be ensured to have proper dipolar correlation and ionic interaction.

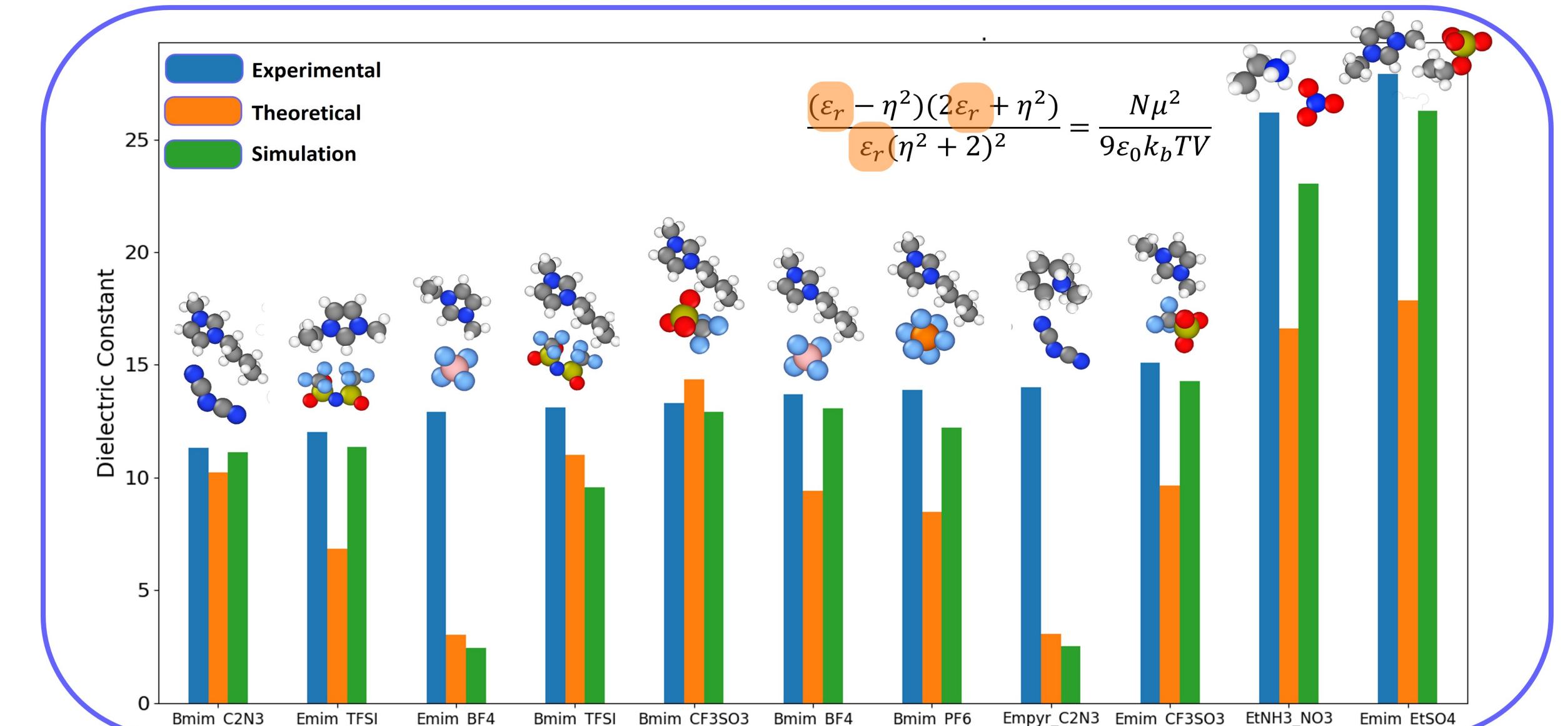
Results : Optimal Set of Model Parameters

Model Parameters	
Ions :	$[\text{EtNH}_3]^+$ $[\text{NO}_3]^-$
$m \text{ (g/mol)}$:	46.09 62.00
$\sigma(\text{\AA})$:	4.80 3.30
$\mu_{liq}(\text{eA})$:	1.0763 0.00
$q(e)$:	+0.35 -0.35
$\epsilon_{IJ}(\text{Kcal/mol})$:	0.1 0.1



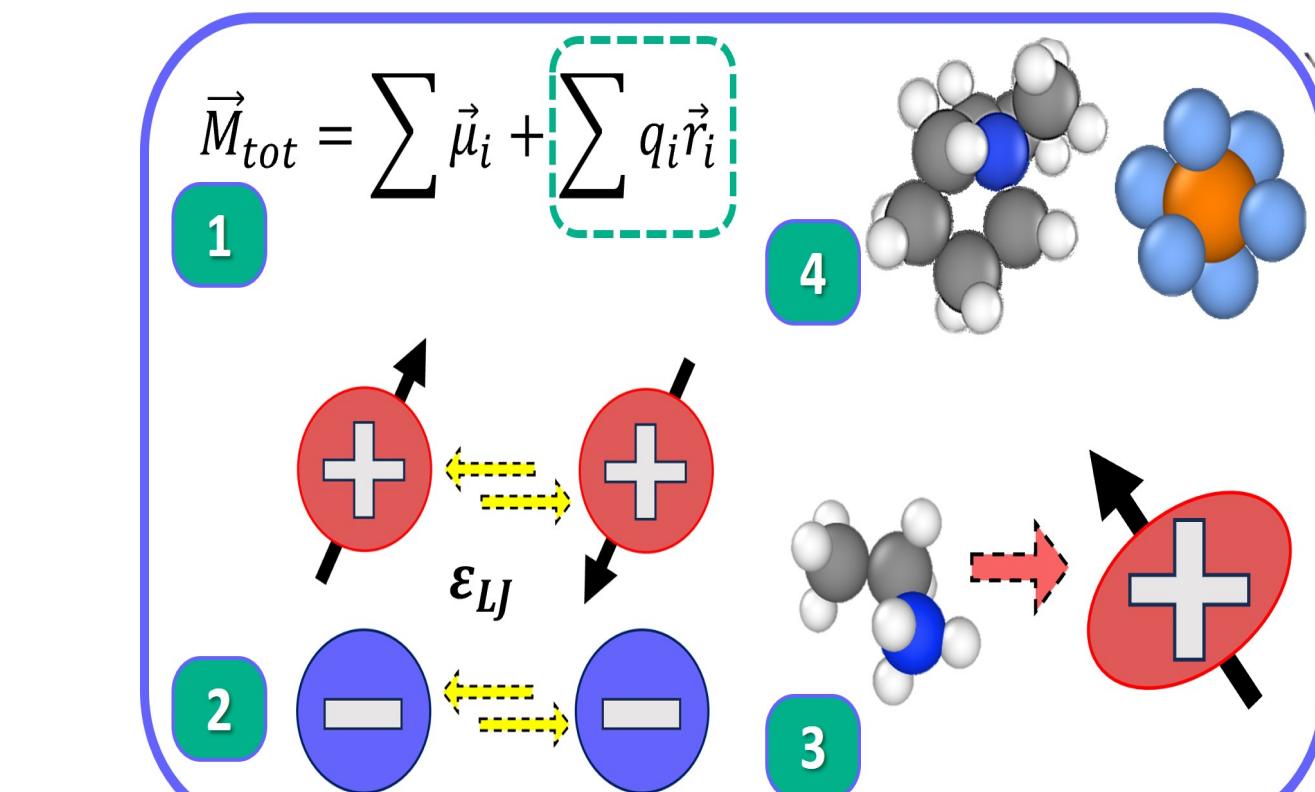
MD simulations were run for 250 cation-anion pairs at room temperature and unit atmospheric pressure using an optimal set of parameters. In addition to the experimental value of dielectric constant, we were able to accurately capture the behavior of Ethylammonium Nitrate IL.

Validating Model : Capturing Different IL Species



The model was extended to 11 species of Ionic Liquid, and we got accurate results 9/11 times. The model was validated by comparing the simulation results with experimental data and with Onsager's theory.

Future Work



Acknowledgement

