

## Coarse-Grained Model for the Alkyl-Chain Family of Imidazolium CnMIM-BF4 Ionic Liquids

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A generic Coarse-Grained (CG) model for to simulate the CnMIM-BF4 ( $n=2,4,6,8,10$ ) series of Ionic Liquids (ILs) is presented. The model builds in previous parametrization strategies Ref. [1,2]. Bulk static and dynamic properties are computed and compared against experimental data. We find that the new CG models provides a good prediction of the IL's properties, and compared favorably with the existing state-of-the-art All-Atom Molecular Dynamics Simulation results. We use our models to investigate the dependence of the thermodynamic properties with the alkyl chain length for different temperatures. The impact of the alkyl chain length on the structure of the ionic liquids, particularly on the mesoscopic structure of the liquid is also shown and quantified via the computation of cluster size distributions. This CG model is also shown to be a promising approach to perform systematic investigations of bulk dynamic properties as well as interfacial phenomena relevant in supercapacitor applications and electro-tunable friction Ref. [3].

### References:

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