Classical and Ab Initio Molecular Dynamics of NaFSI/EMIM-FSI Electrolytes

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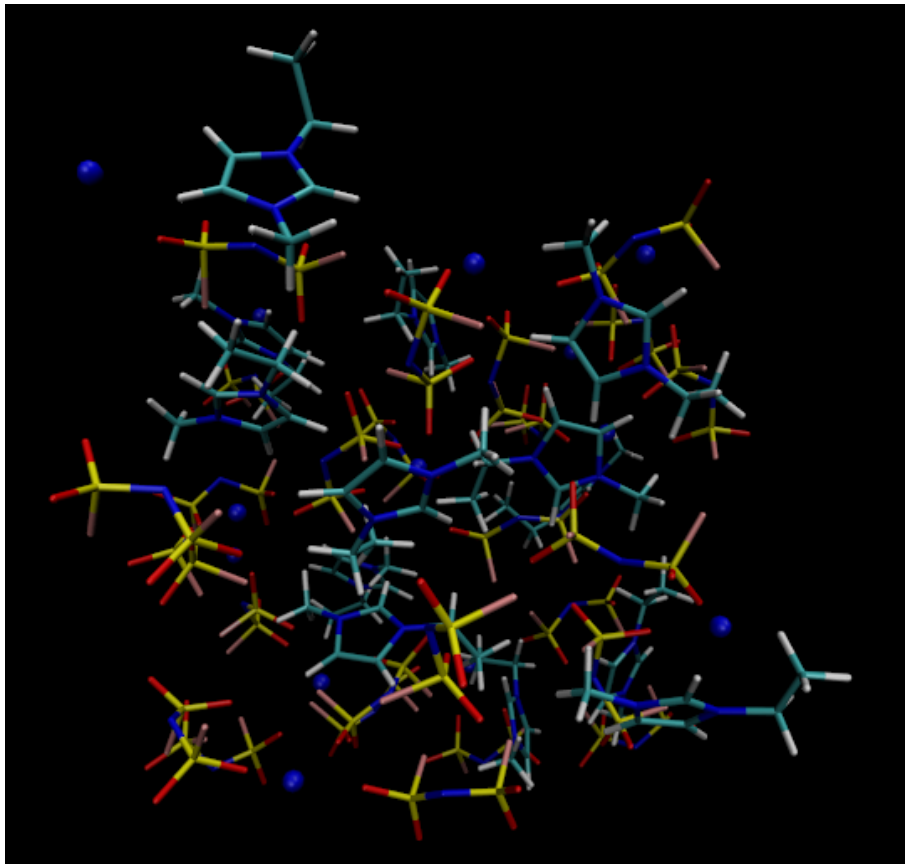
Computational details

1 μs of classical MD trajectory
polarizable and non-polarizable FF

30 *ps* of ab initio MD trajectory
NaFSI mole fraction from 0.0 to 0.5

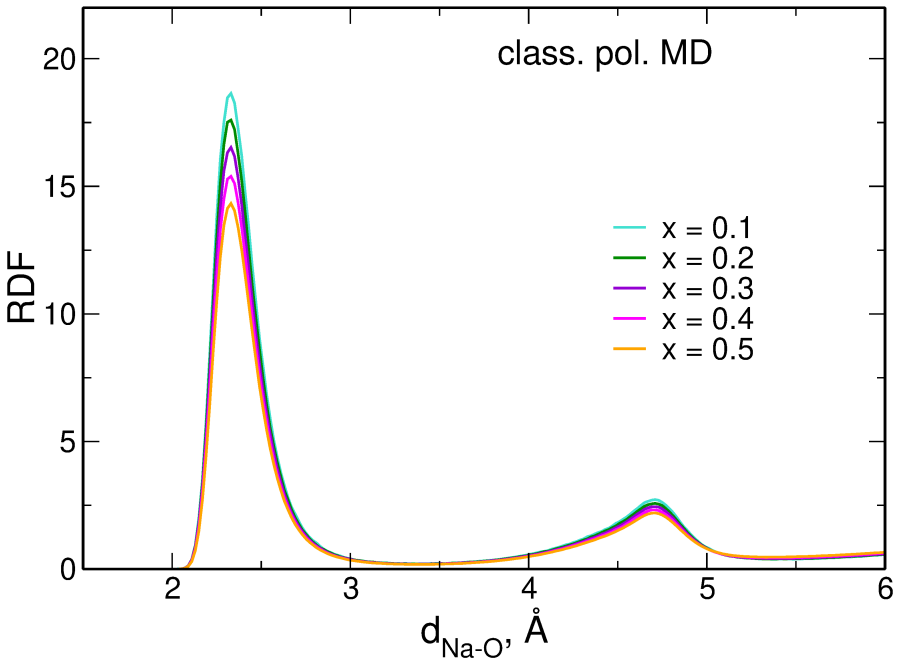
Compared RDFs from classical and ab initio MD trajectories

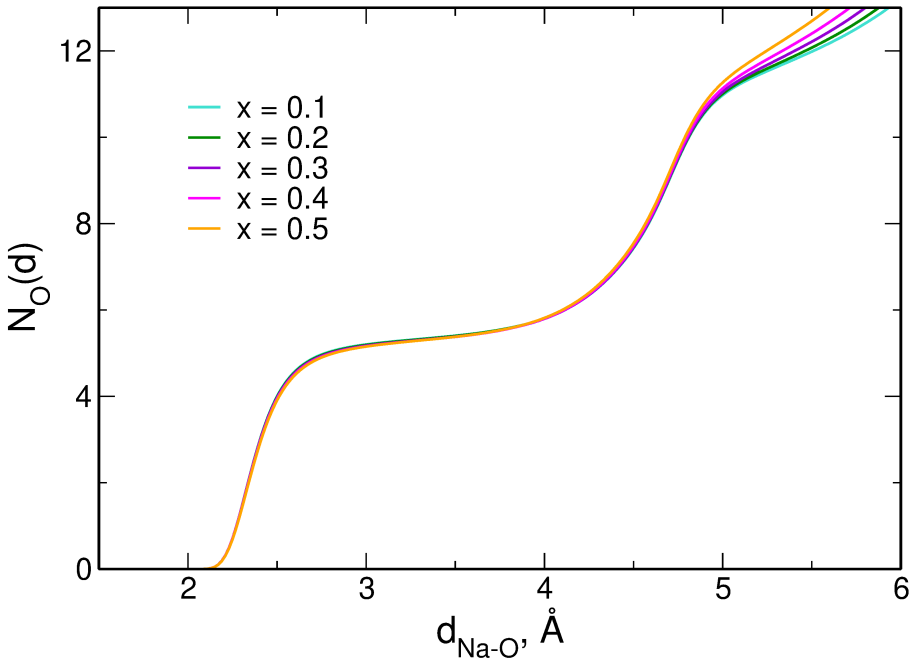
Conductivities and viscosities from classical MD



NaFSI/EMIM-FSI solution with NaFSI mole fraction equal 0.5

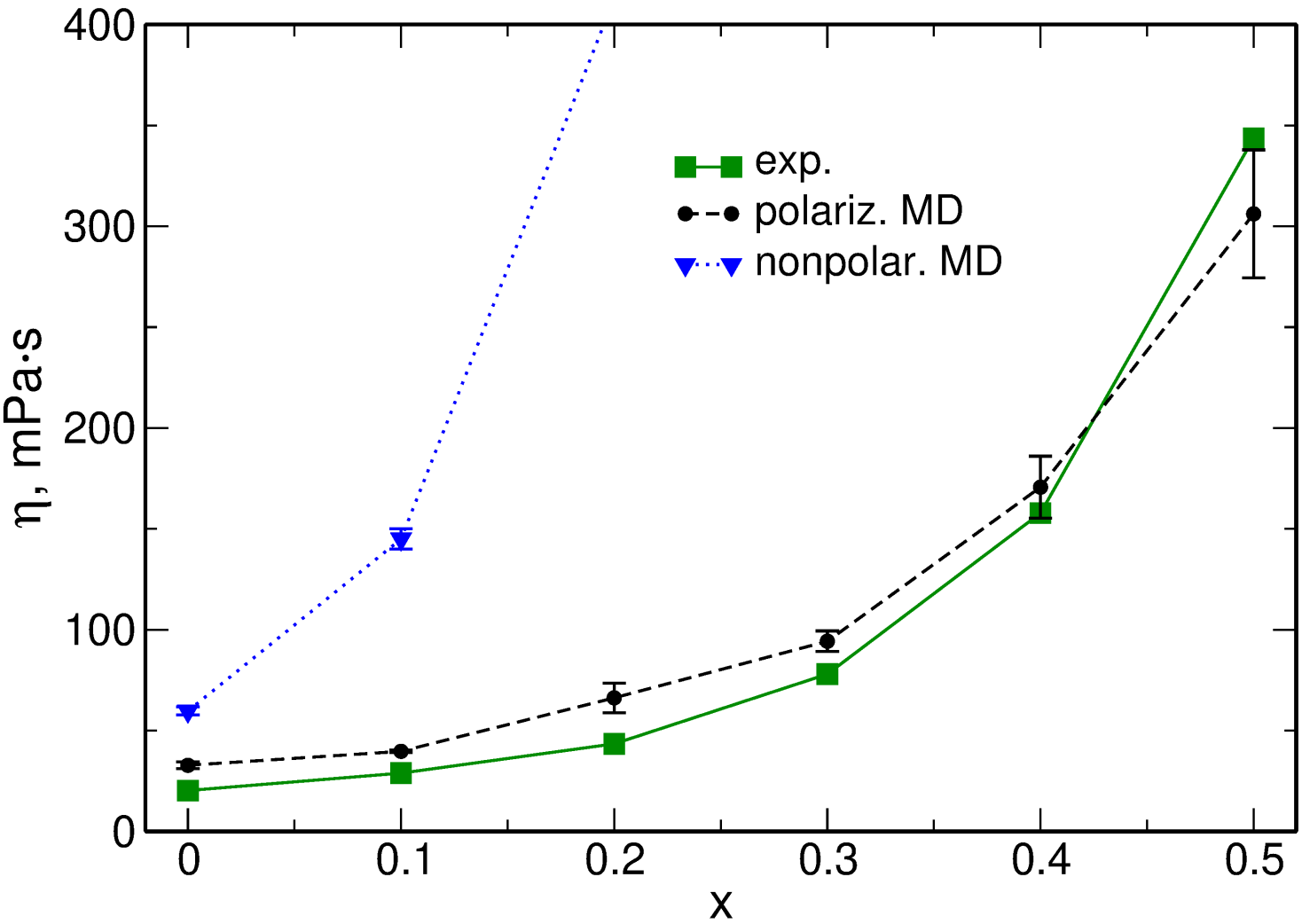
RDF example





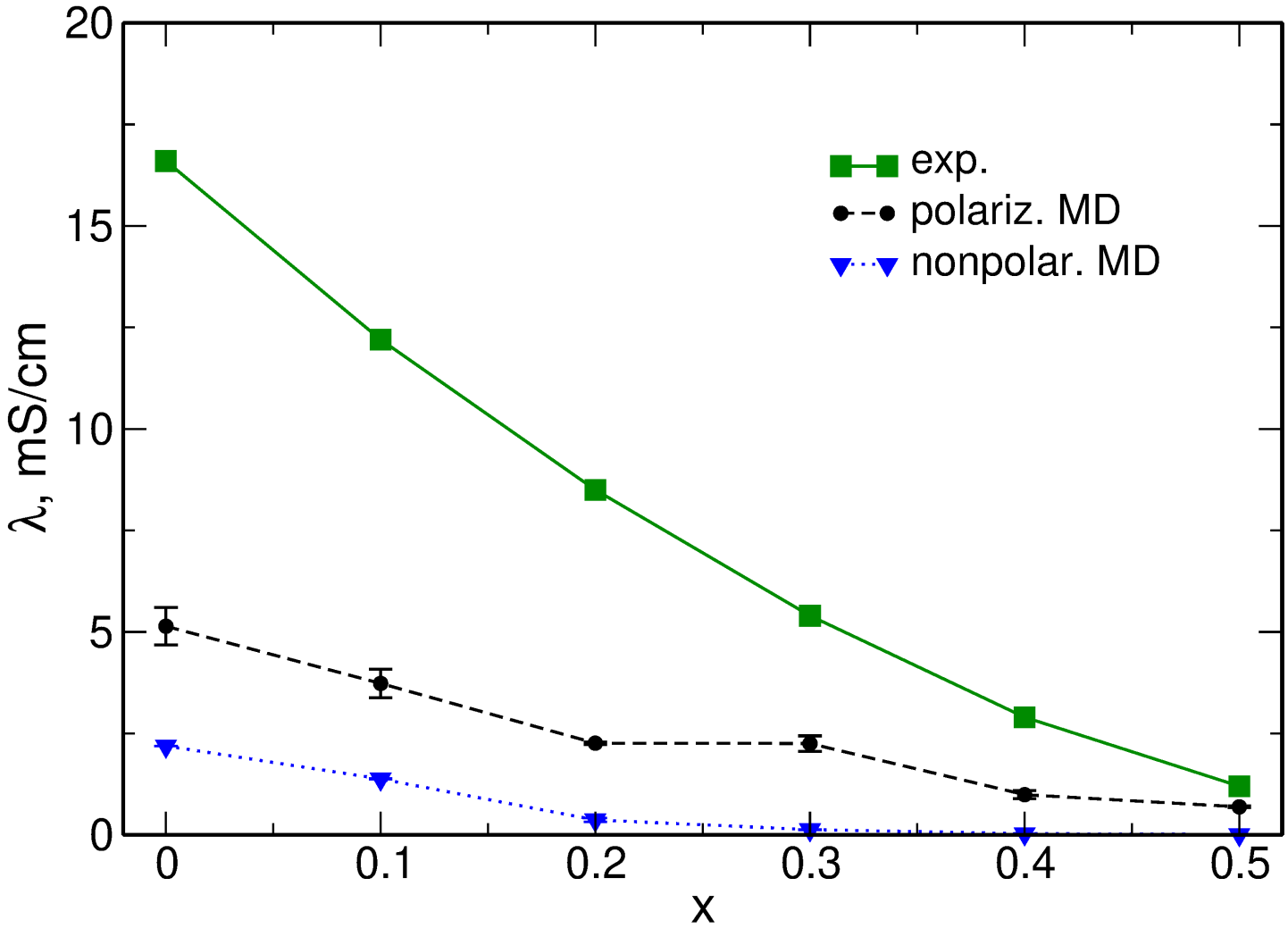
Na-O RDF and its integral obtained from polarizable FF classical MD

Calculated viscosities



Calculated viscosities from classical MD simulations

Calculated conductivities



Calculated conductivities from classical MD simulations