# Solvation of $Mg^{2+}$ Ions in $Mg(TFSI)_2$–Dimethoxyethane Electrolytes: a Molecular Dynamics Study

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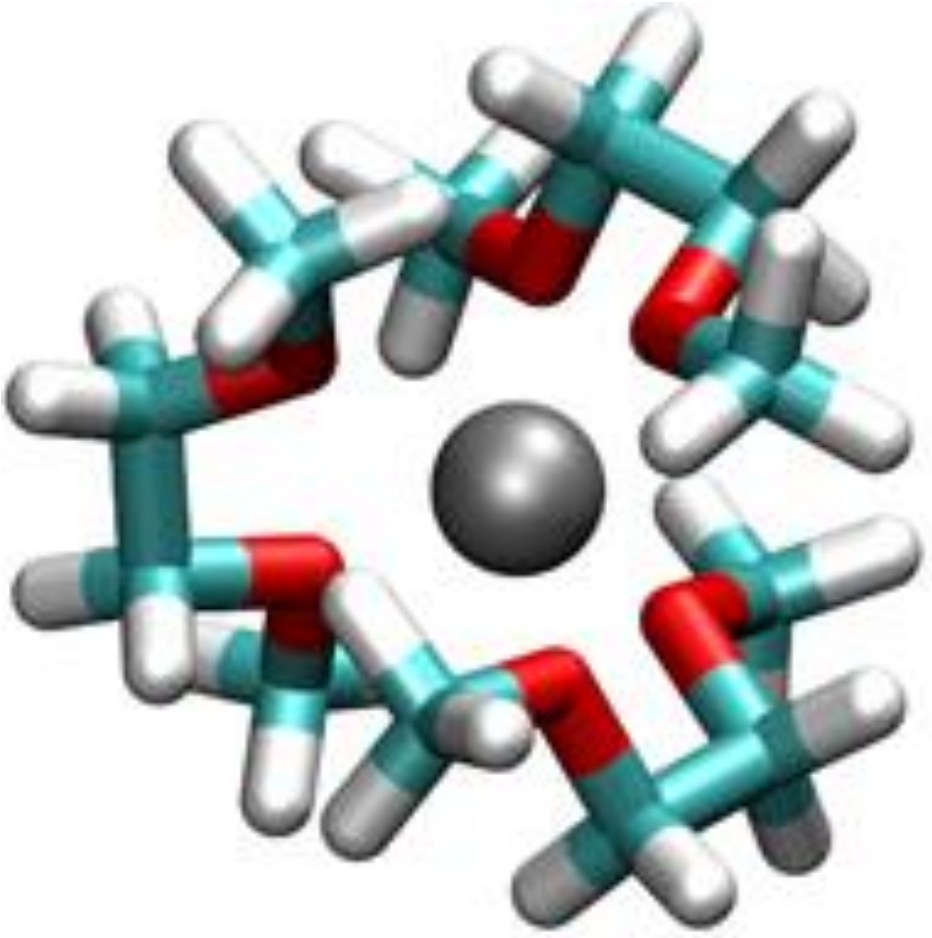
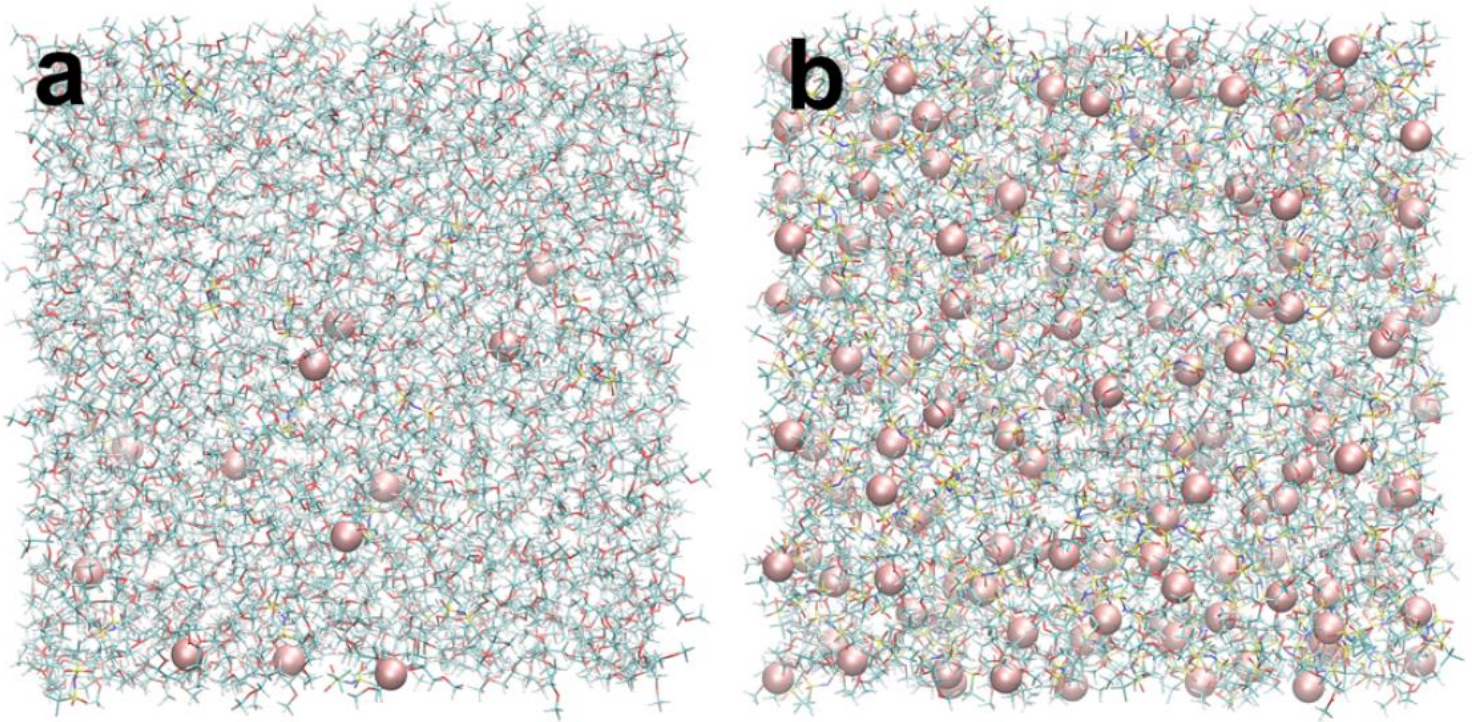


# Investigated systems

-solutions of $Mg(N(SO_2CF_3)_2)_2$ in dimethoxyethane

$Mg(TFSI)_2$ DME

-classical molecular dynamics simulations in NAMD
-150 ns of trajectory for each of 5 systems in 2 FF's
-aprox. 800 000 of normalized walltime hours




snapshots of simulation boxes for c = 0.1 M (a) and c = 1.2 M (b). $Mg^{2+}$ ions are shown as spheres.

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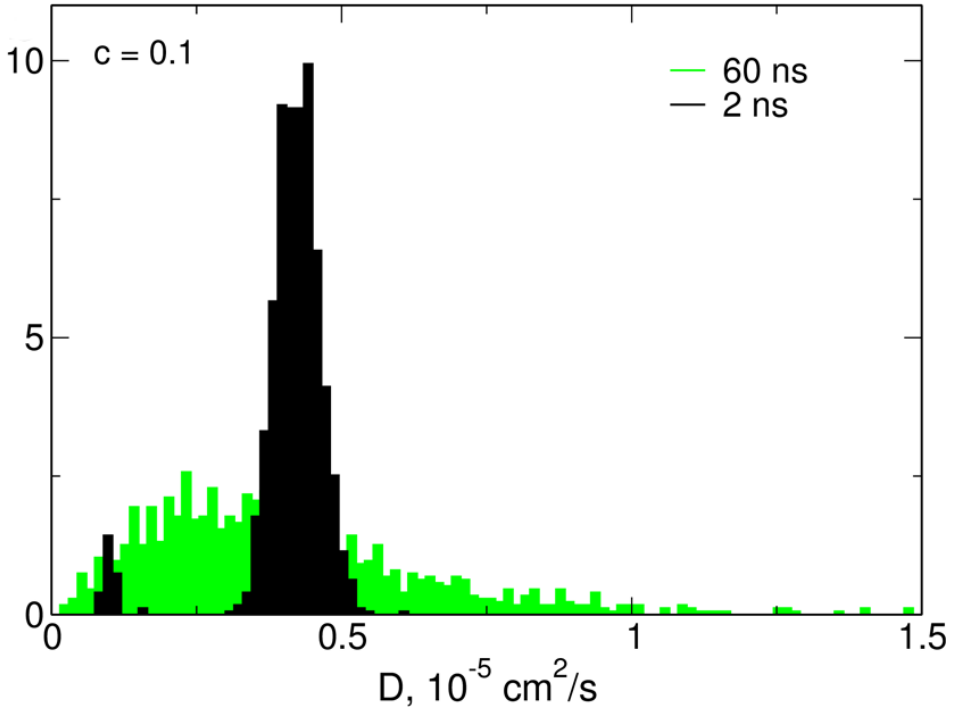
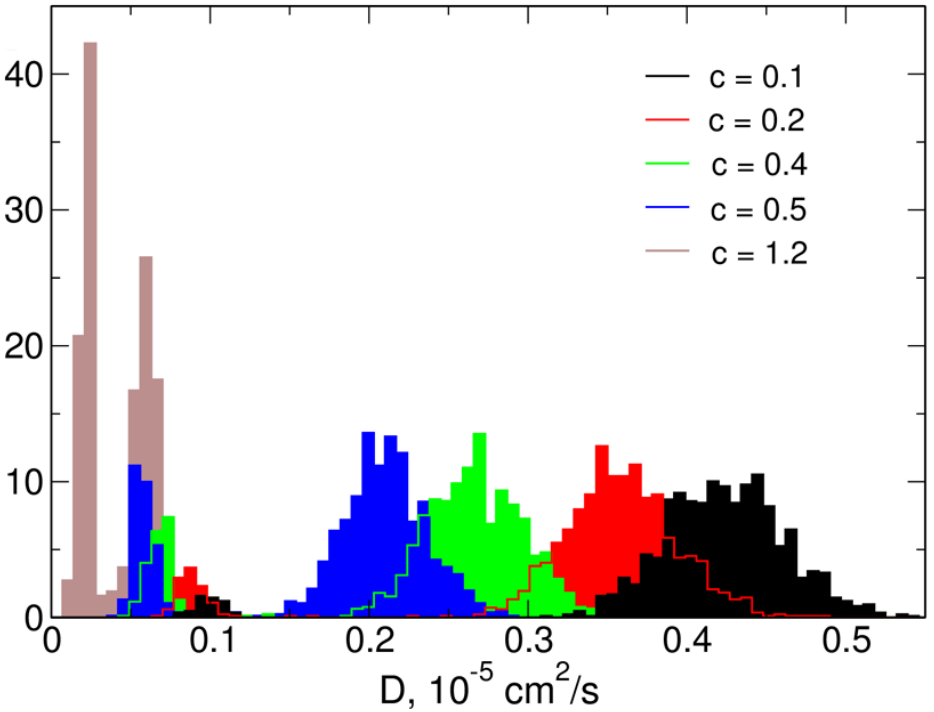
# Results



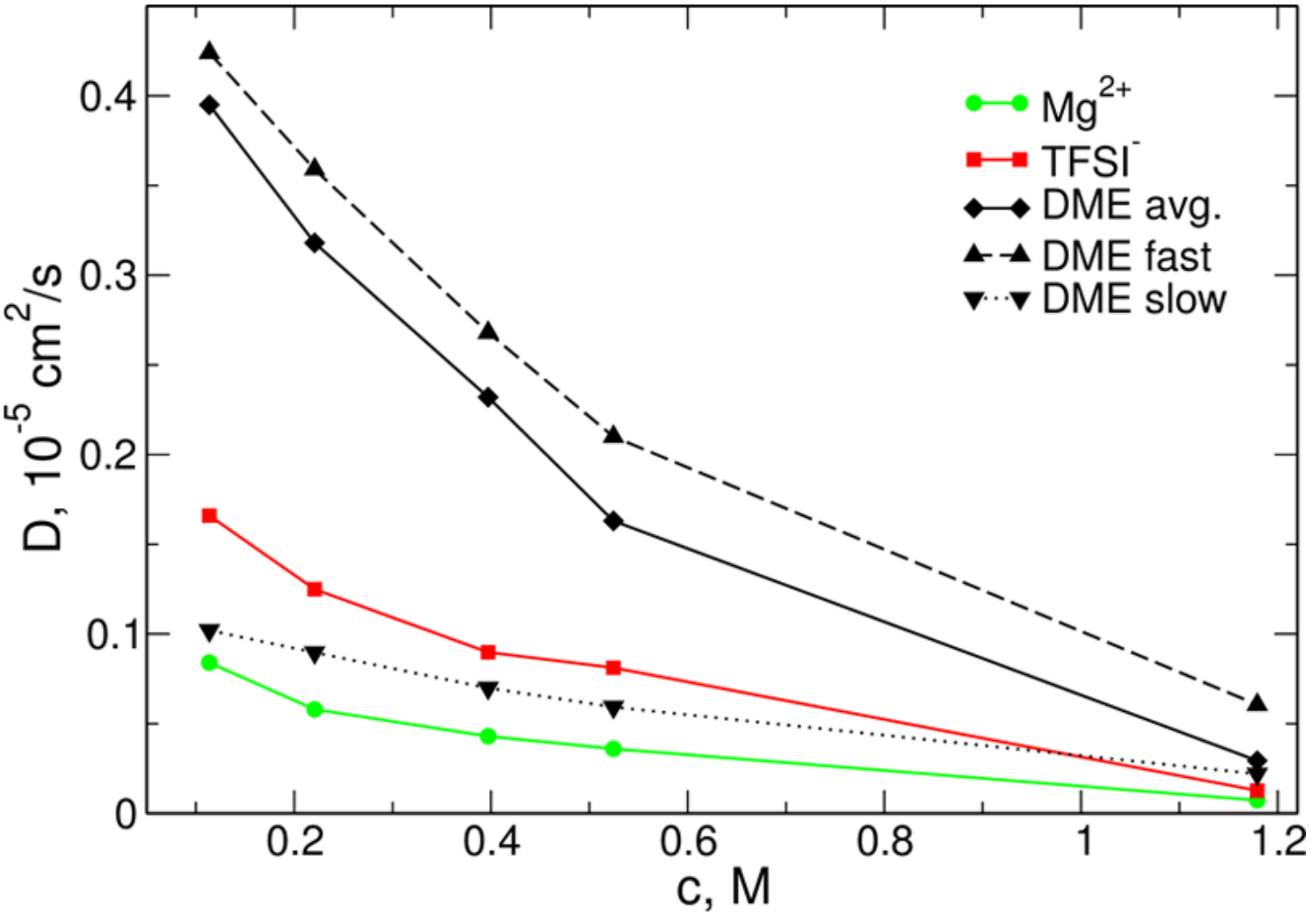

distributions of DME diffusion coefficients estimated in different time intervals for the c = 0.1 M electrolyte




distributions of DME diffusion coefficients estimated for 2 ns intervals in electrolytes with increasing salt concentration

Kubisiak, P.; Eilmes, A. Solvation of $Mg^{2+}$ Ions in $Mg(TFSI)_2$−Dimethoxyethane Electrolytes-A View from Molecular Dynamics Simulations. *J. Phys. Chem. C* **2016**, *122*, 12615-12622

# Results




diffusion coefficients estimated from MD simulations for electrolytes with increasing salt concentration

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