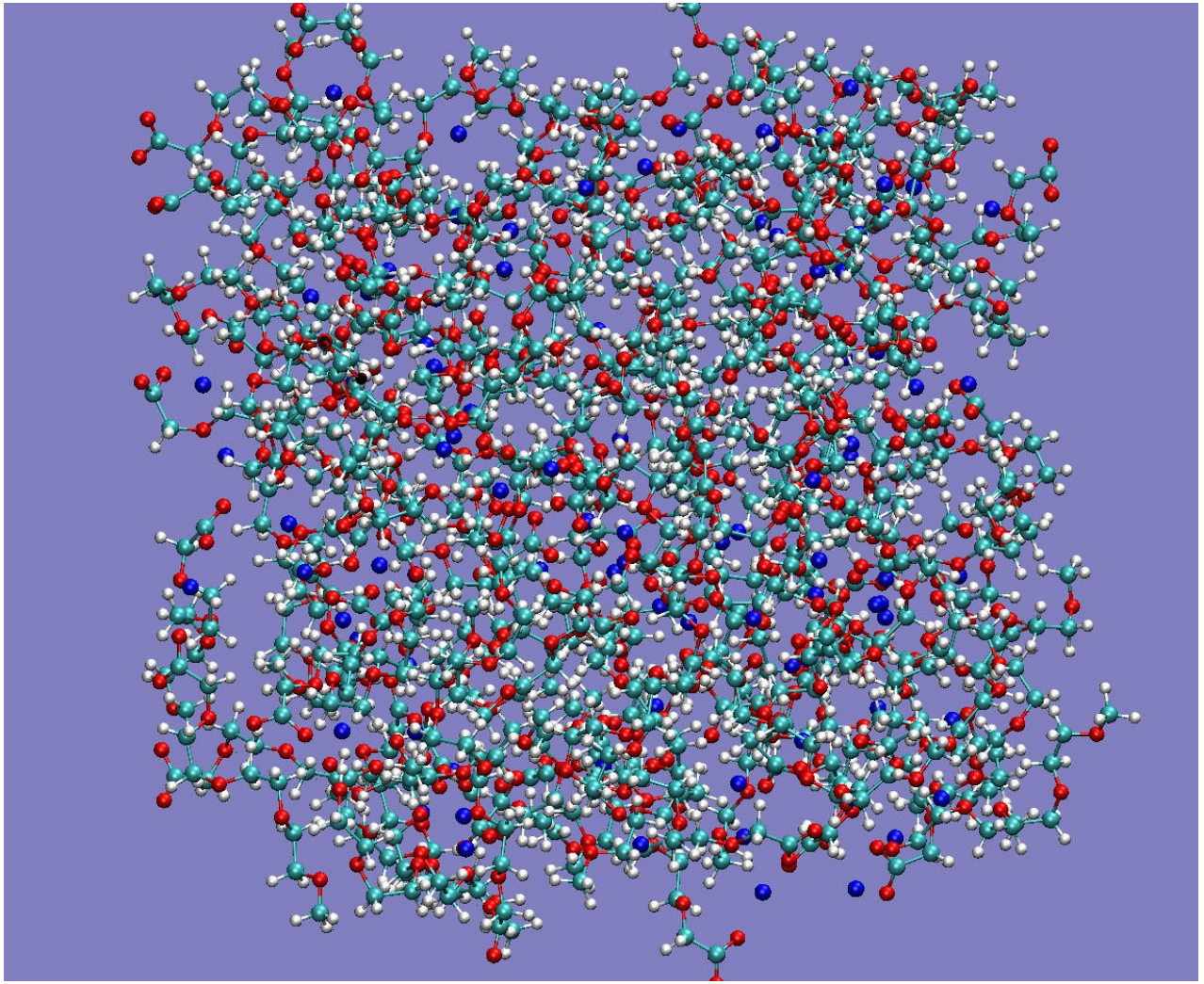
GPGPU accelerated Molecular Dynamics investigation of the structure and interionic interactions in ionic liquids

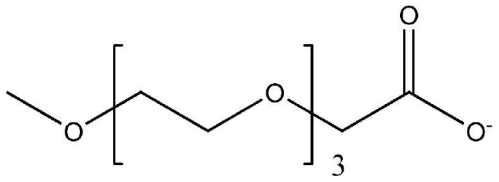
Piotr Kubisiak, Andrzej Eilmes



Cation coordination

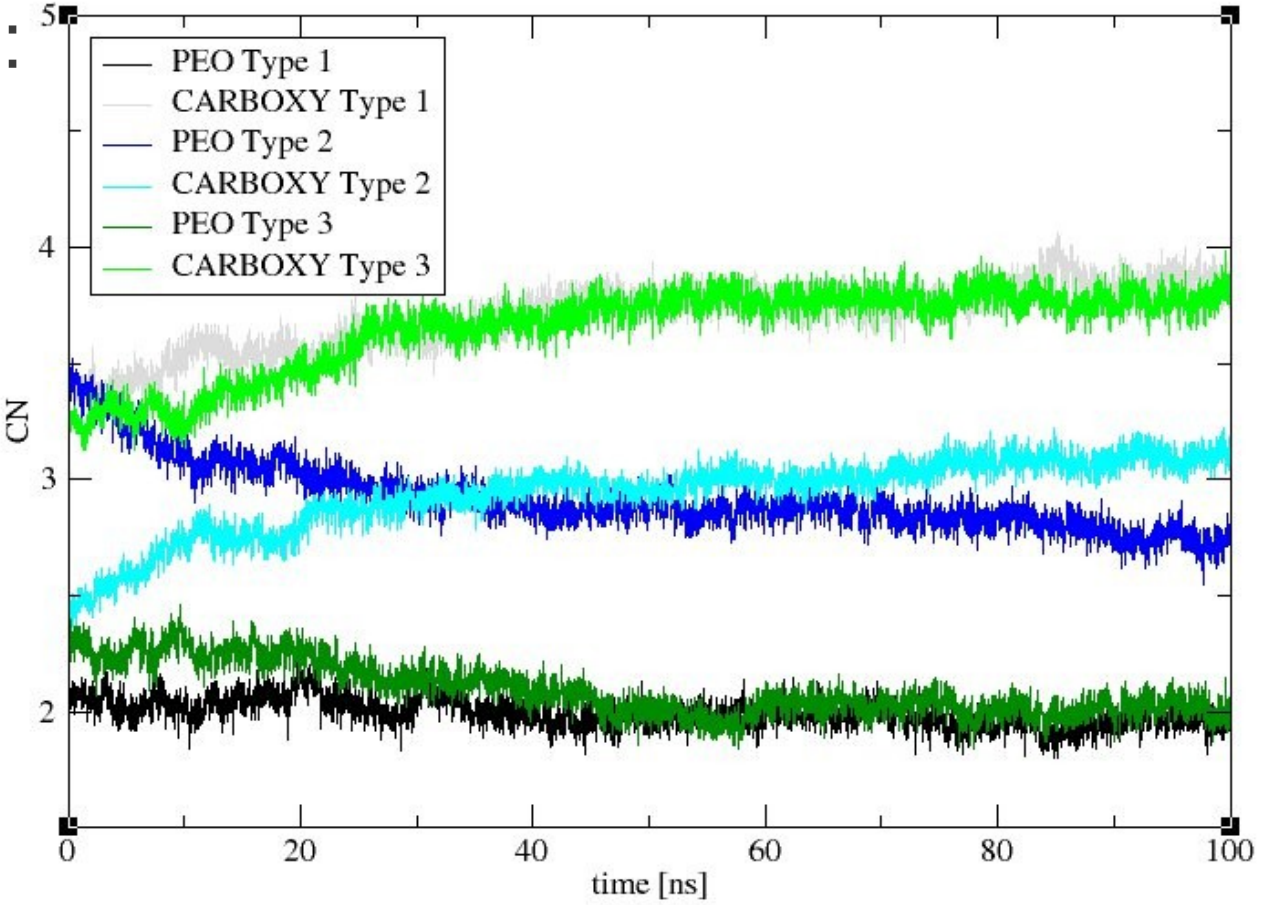
Investigated systems:

$[TOTO]^-Me^+$, Me = Li, Na, K

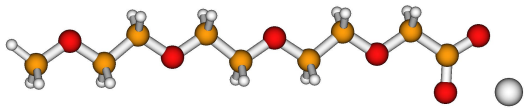


2,5,8,11-tetraoxatridecan-13-oate anion $[TOTO]^-$

100 ion pairs
NPT ensemble (T=400K)
timestep=1fs
simulation time > 100ns
GPGPU acceleration



Type 1:



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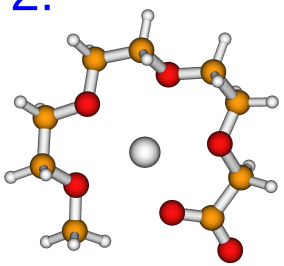
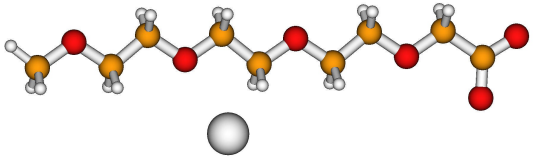


Type 3:

Random positions



Collective diffusion and conductivity

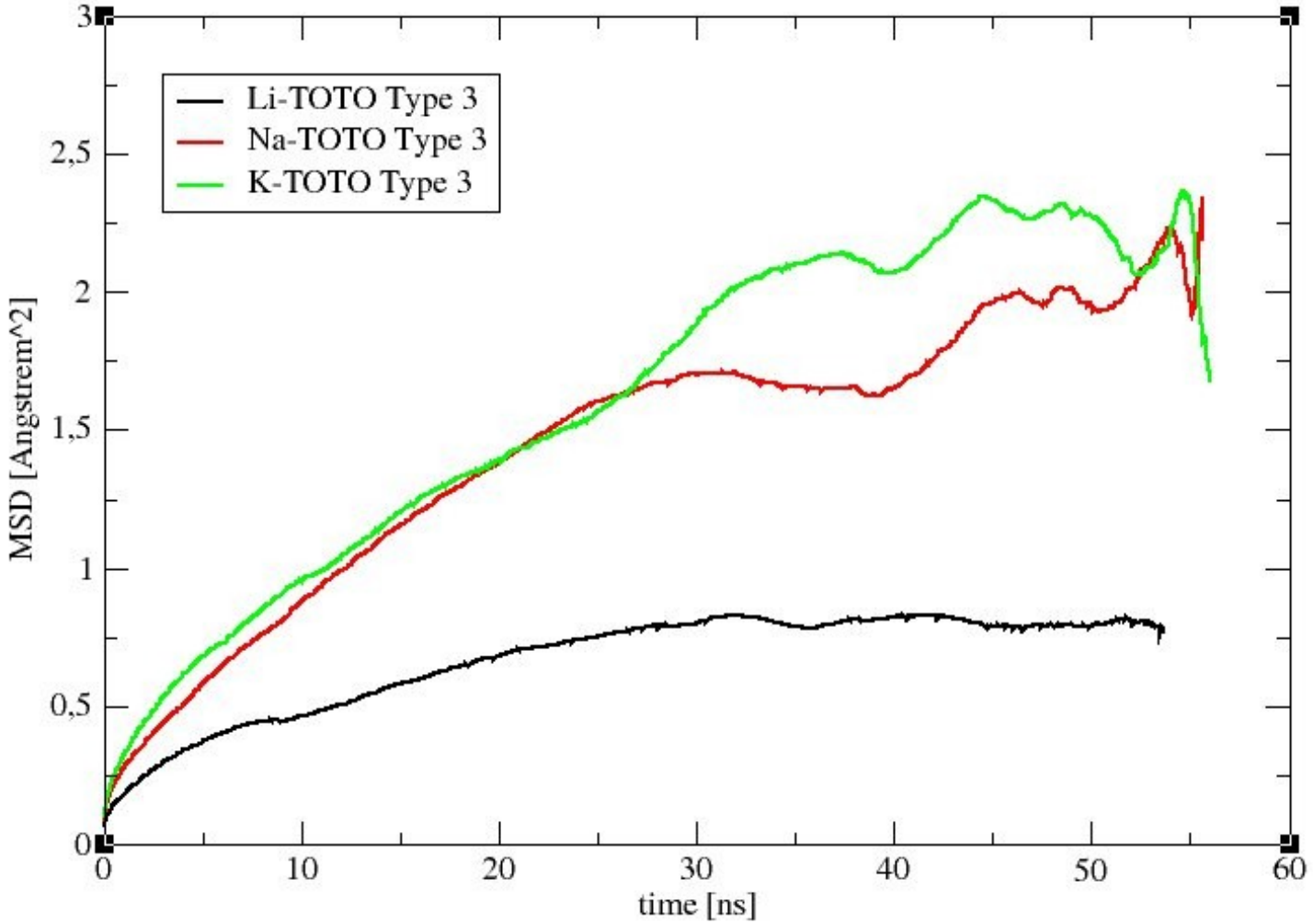
The mean square displacement of the ions taking into account correlations between their movements

<u>Calculated conductivities</u>

Li-TOTO type 3:
4.0×10^{-3} [S/m]

Na-TOTO type 3:
11.5×10^{-3} [S/m]
(25.0×10^{-3} [S/m])*

K-TOTO type 3:
11.5×10^{-3} [S/m]



*O. Zech, M. Kellermeier, S. Thomaier, E. Maurer, R. Klein, C. Schreiner, W. Kunz, *Chem. Eur. J.* **2009**, *15*, 1341