

Interfacial interactions of an IL in contact with a glassy surface by classical and first-principles molecular dynamics

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ILs

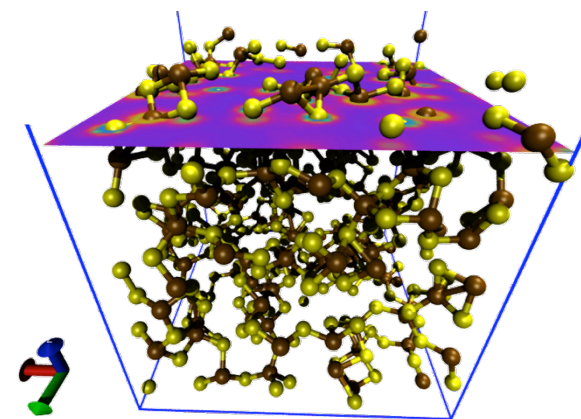
- low volatility
- low flammability
- high ionic conductivity
- high thermal stability

Applications as Hybrid Materials

- energy-storage devices
(batteries / supercapacitors)
- lubricant agents

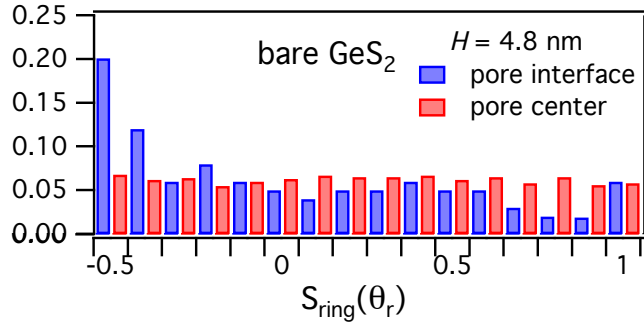
Langmuir 28, 5513 **2012**.

Eur. J. Inorg. Chem. 112, 1350 **2014**.



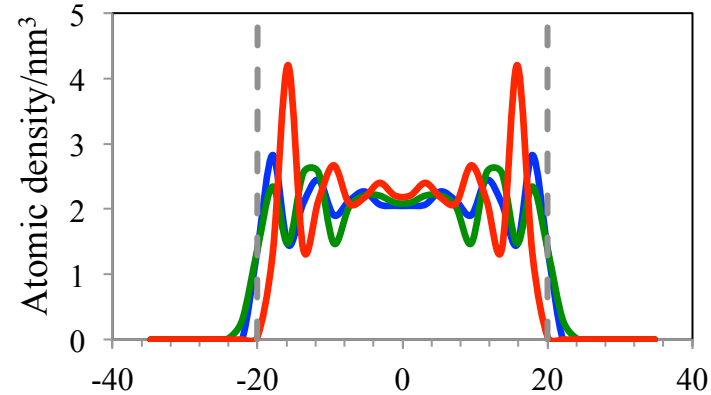
TPMN objectives: properties

Orientalional parameters

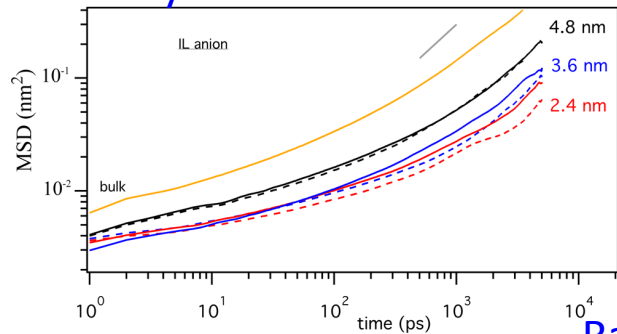


$$S_{\text{ring}}(\theta_a): \langle 3/2\cos^2(\theta_a) - 1/2 \rangle$$

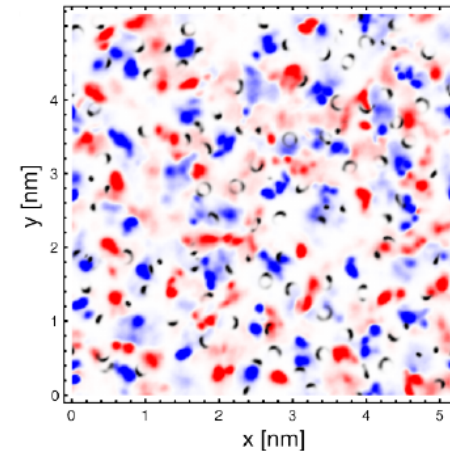
Density Profiles



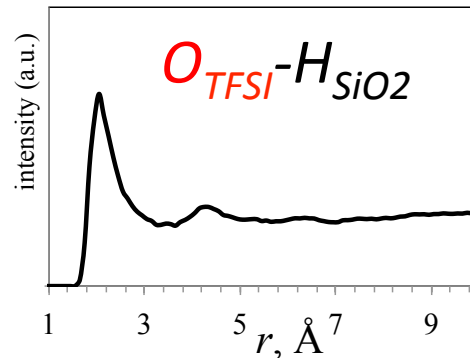
IL dynamics



Electronic structure & charge density



Radial distribution functions g(r)



Methods:

- Classical MD
- FPMD

Codes:

- DLPOLY/LAMMPS/GULP
- CPMD