

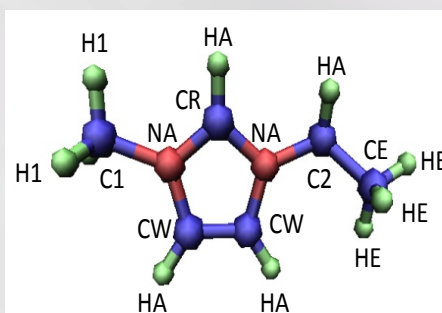
MOLECULAR SIMULATION OF IONIC LIQUIDS INSIDE NANOPORES

Jermain Franklin

Xiaoxia He, Francisco Hung

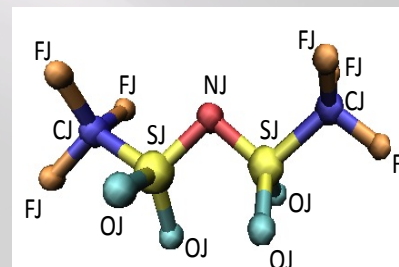
What is an Ionic Liquid (IL)?

- Organic salts that are in a liquid state at room temperature
 - Melting point is below boiling point of water (100 °C)



[EMIM⁺]

1-ethyl-3-methylimidazolium

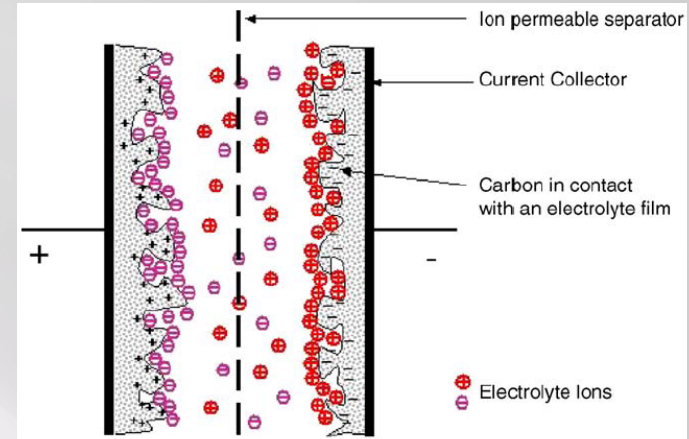
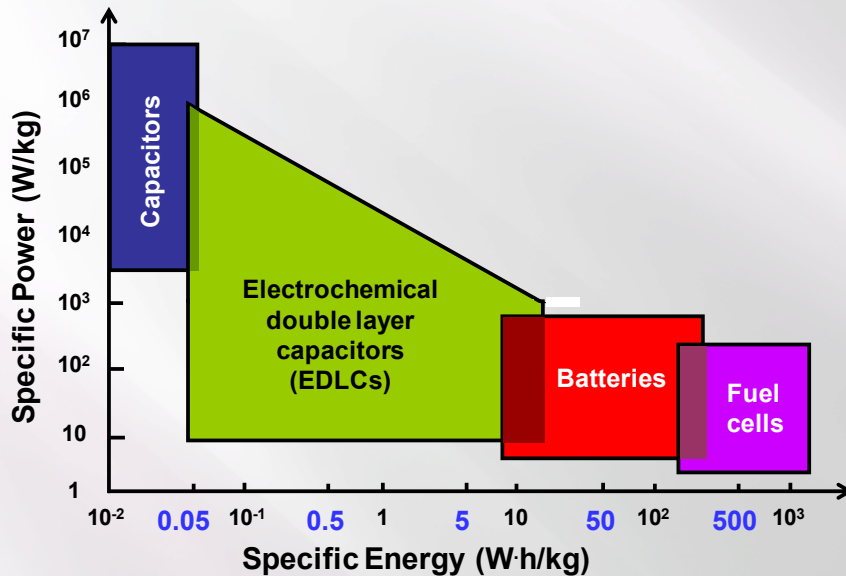


[TFMS⁻]

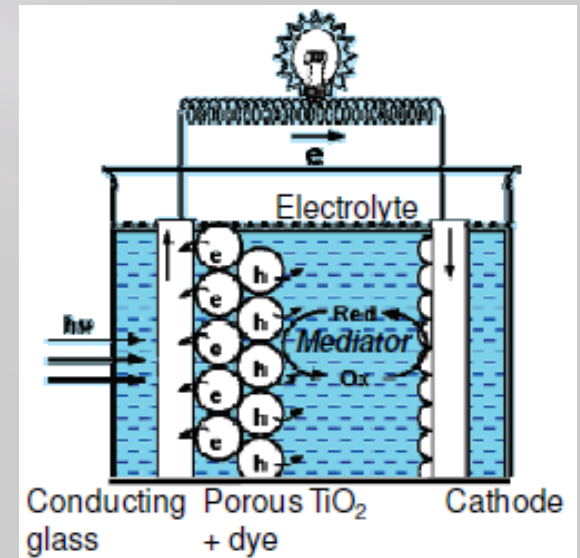
Bis-(trifluoromethanesulfonyl)imide

Applications of ionic liquids

Alternative electrolytes in electrochemical double-layer capacitors



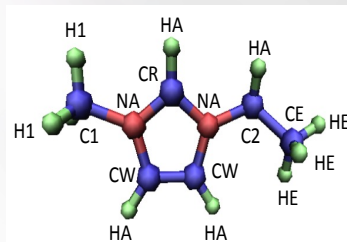
Pandolfo and Hollekamp,
J. Power Sources 2006, 157, 11



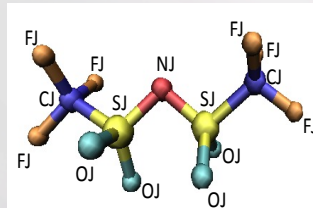
Dye-sensitized solar cells

Proposed tasks

- MD simulations of the IL [EMIM⁺][TFMSI⁻] confined inside titania nanopores
 - In contact with two bulk-like regions of IL

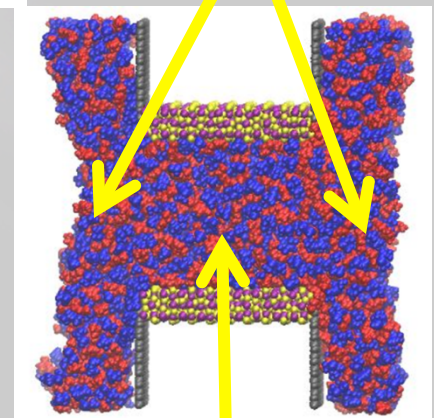
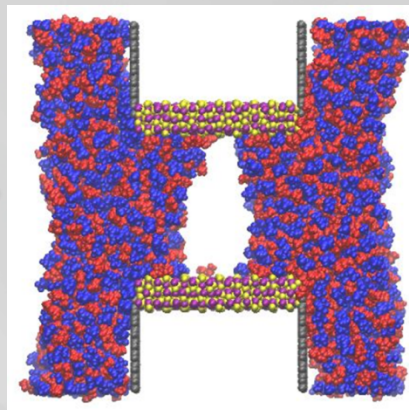
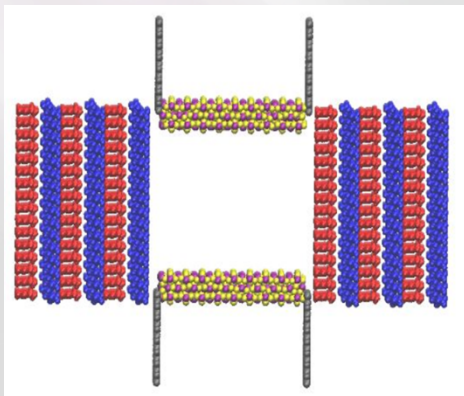


[EMIM⁺]
1-ethyl-3-methylimidazolium



[TFMSI⁻]
Bis-(trifluoromethanesulfonyl)imide

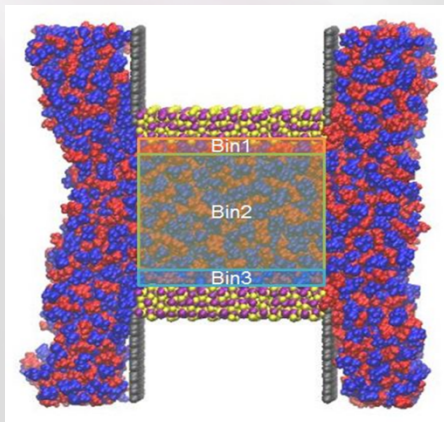
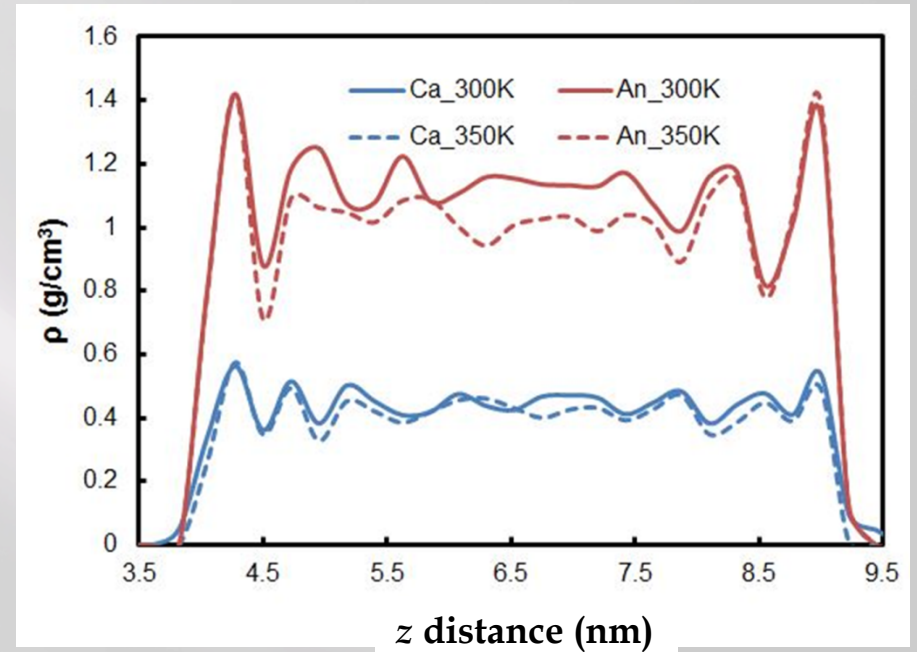
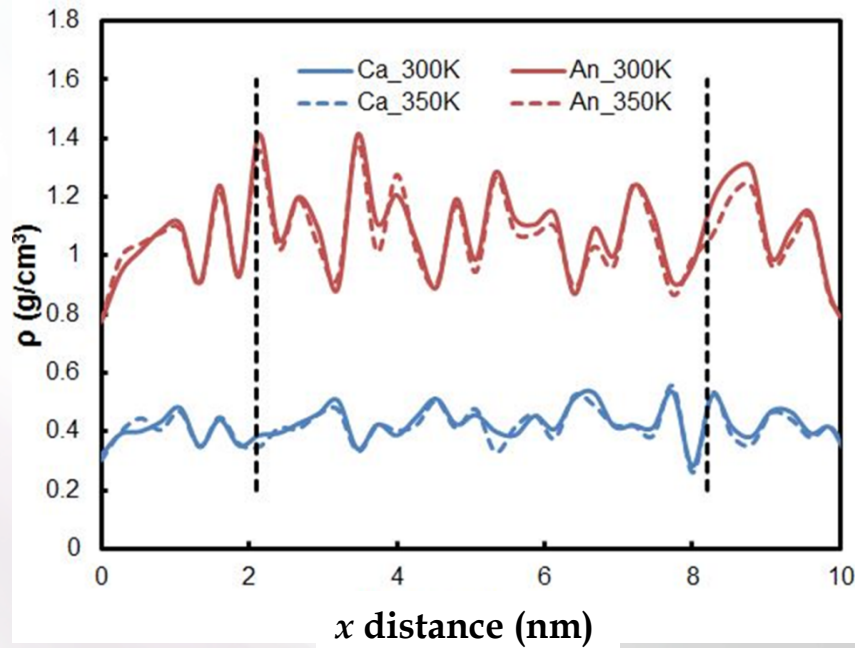
Red = [EMIM⁺]
Blue = [TFMSI⁻]



IL inside TiO₂ nanopore

Structural Properties

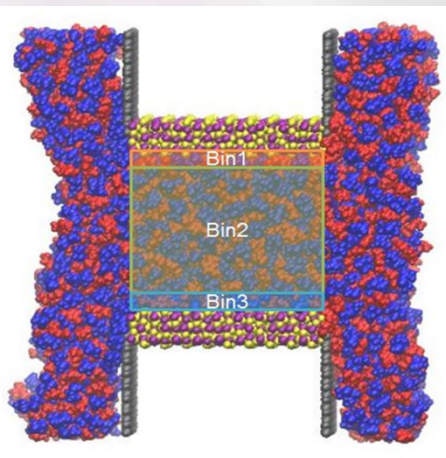
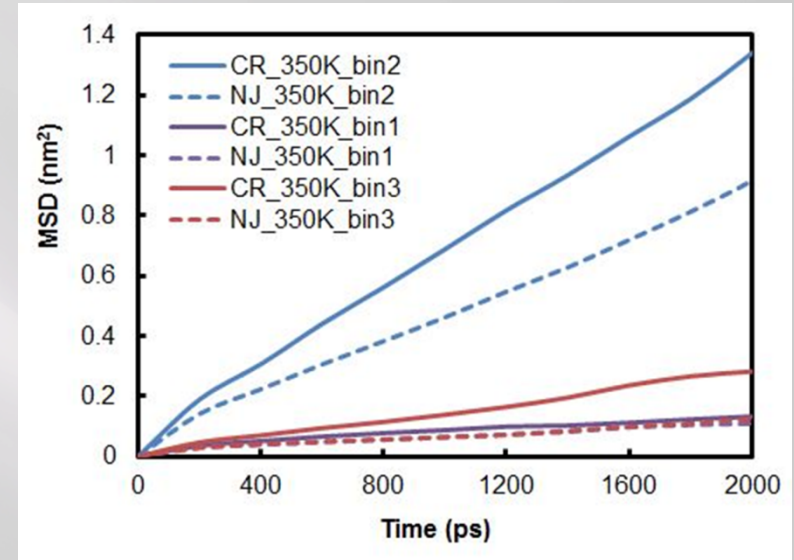
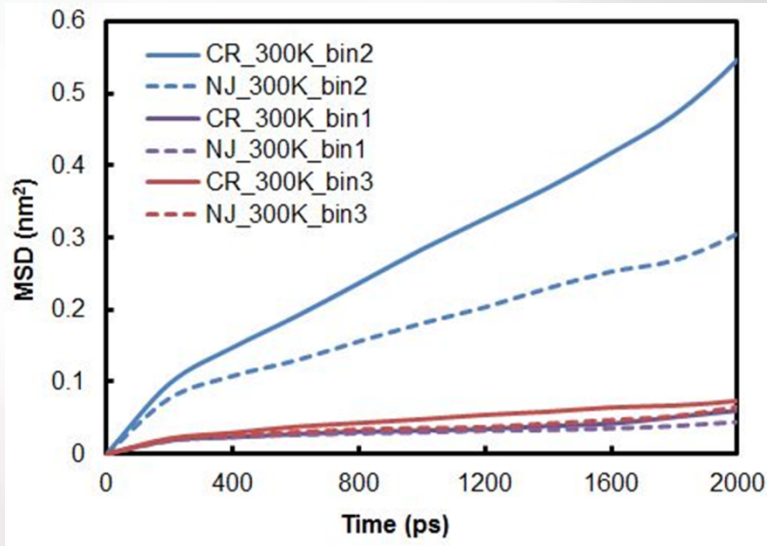
Density of cations and anions, 300 K and 350 K



- Higher densities at lower temperatures
- Larger density of ions near pore walls

Dynamical Properties

Mean Square Displacement of IL in different layers



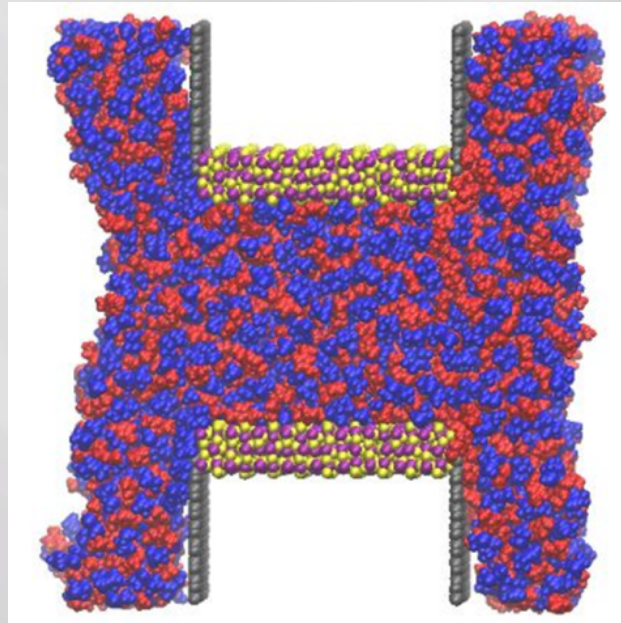
- Dynamics faster at higher temperature
- Cations move faster than anions
- Ions in center of pore move faster than those near walls

Resources

GROMACS software (MD simulations)

VMD (visualize molecules from MD simulations)

HPC@LSU, LONI (running simulations)



MOLECULAR SIMULATION OF IONIC LIQUIDS INSIDE NANOPORES

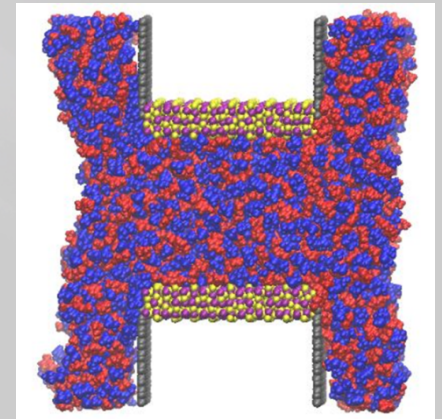
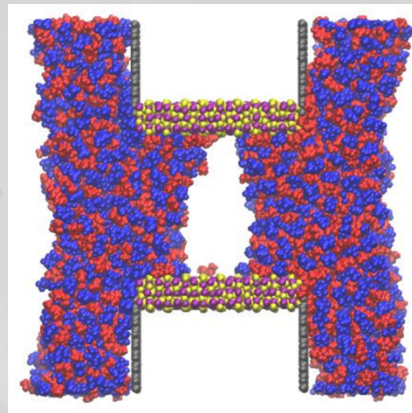
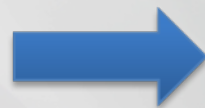
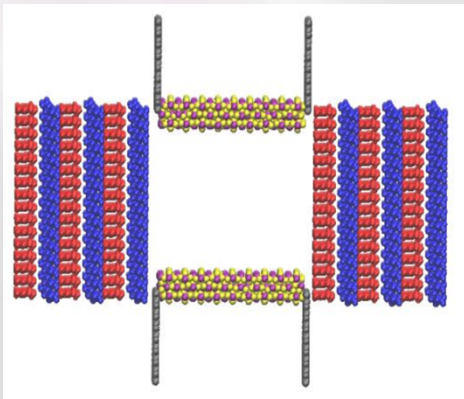
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Objective

Perform classical molecular dynamics (MD) simulations, investigate behavior of ionic liquids (ILs) confined in titania nanopores

- Complement experimental studies

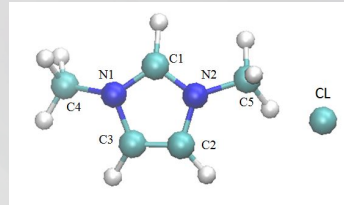
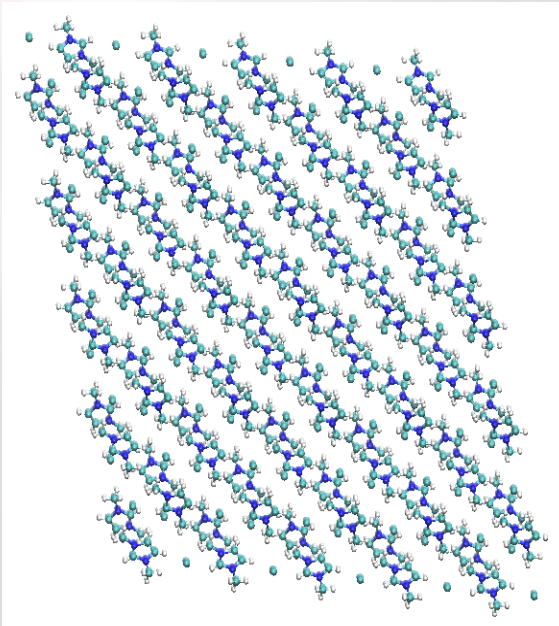


Ionic liquids vs. common salts

IL: [dmim⁺][Cl⁻]

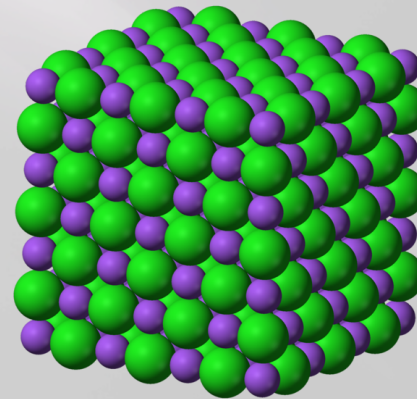
Melting point: 126.3 °C
(259.3 °F)

Packing ions is more
difficult (complex
shape)



Common salt (NaCl)

- ❑ Melting point: 801 °C
(1,474 °F)
- ❑ Packing ions is easier
(spherical shape)

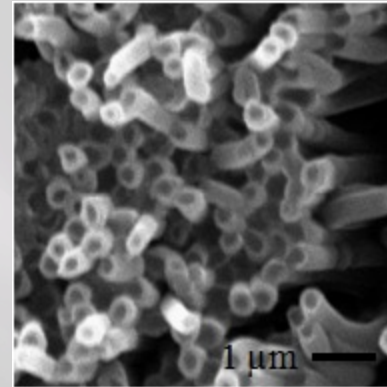


NaCl

<http://en.wikipedia.org>

Biomedical Research

- Magnetic hyperthermia cancer treatment (delivered to cancerous tumors and heated to destroy cancer cells)
- Medical Imaging



de Rooy *et al.*, *Chem. Commun.* 2011

Outcomes

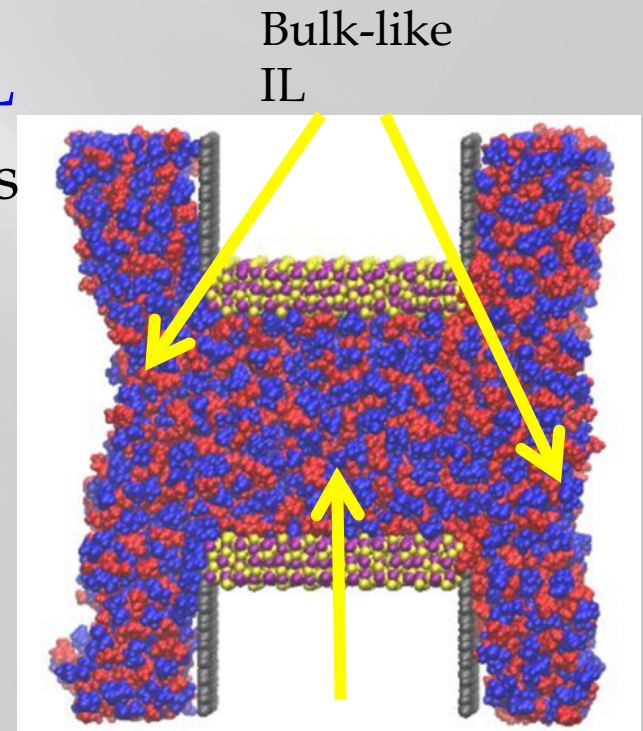
Structural properties of IL:

- Local density profiles

Dynamical properties of IL

- Mean squared displacements

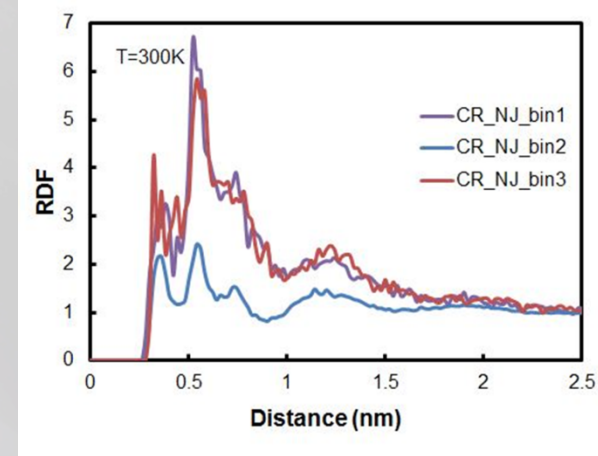
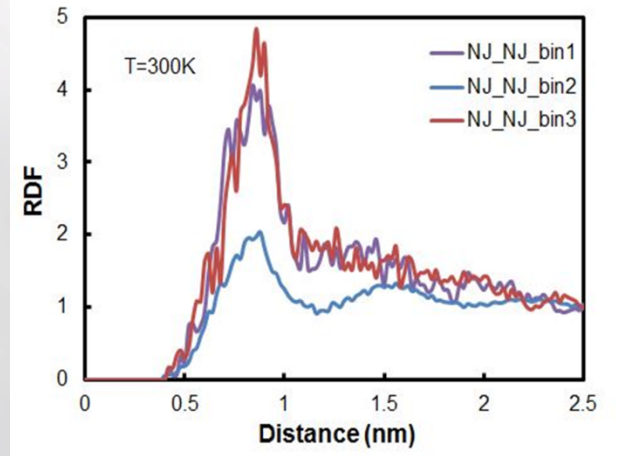
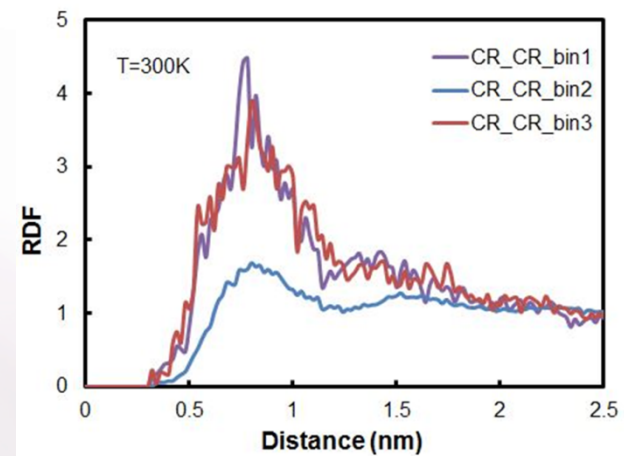
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IL inside TiO₂ nanopore

Structural Properties

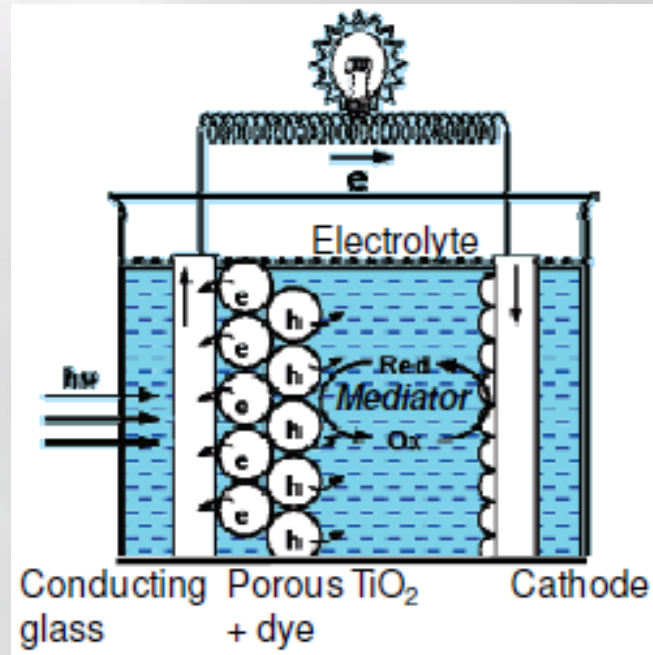
Radial distribution of IL in different layers



The height of the peaks of RDF is higher for the ions near the surface.

Dye-sensitized solar cells

Alternative electrolyte for conversion of solar energy



What is our planned approach?

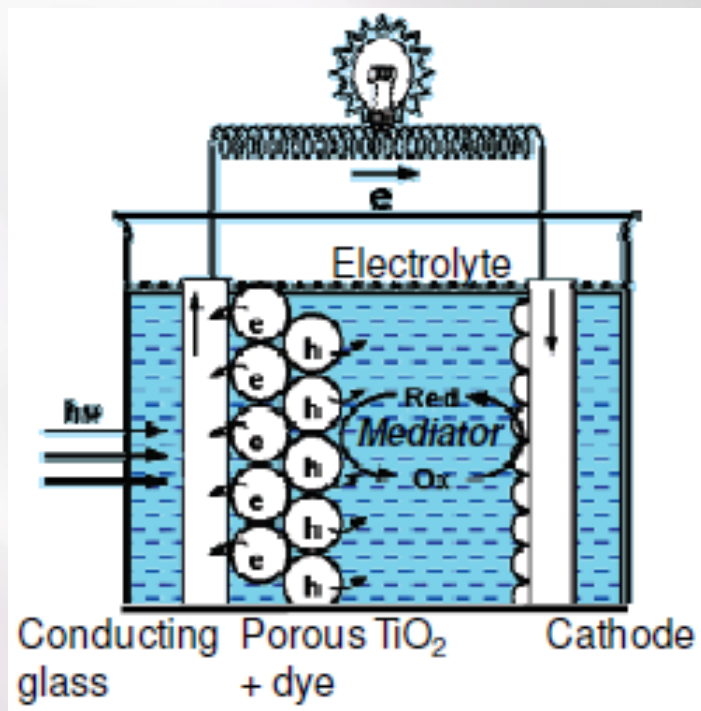
① - manipulate temperature

② - force fields

③ - pressures

Applications of ionic liquids

Alternative electrolytes in dye-sensitized solar cells



Kamat, J. *Phys. Chem. C* 2007, 111, 2834-2860