Molecular Simulation of Deep Eutectic Solvents Inside Nanoporous Materials

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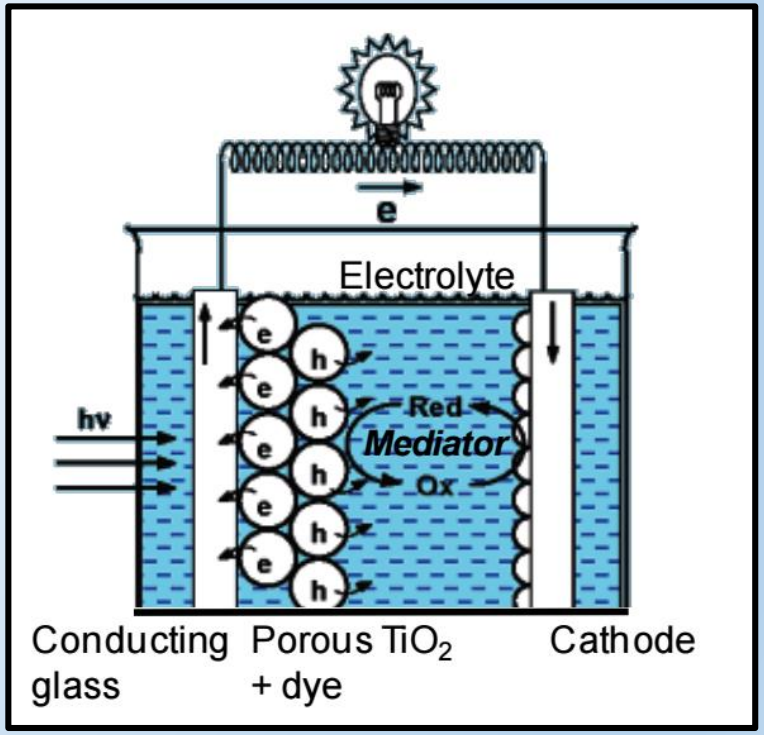
Background

- Deep Eutectic Solvent (DES)
  - mix two solids (hydrogen bond acceptor and donor) in proper ratio = resulting mixture is liquid
  - shares physical, chemical properties with ionic liquids (ILs)
  - nontoxic, biodegradable, less expensive
  - used in dye-synthesized solar cells (DSSC)
- Molecular Dynamics (MD)
  - study of molecular-level properties via simulation software

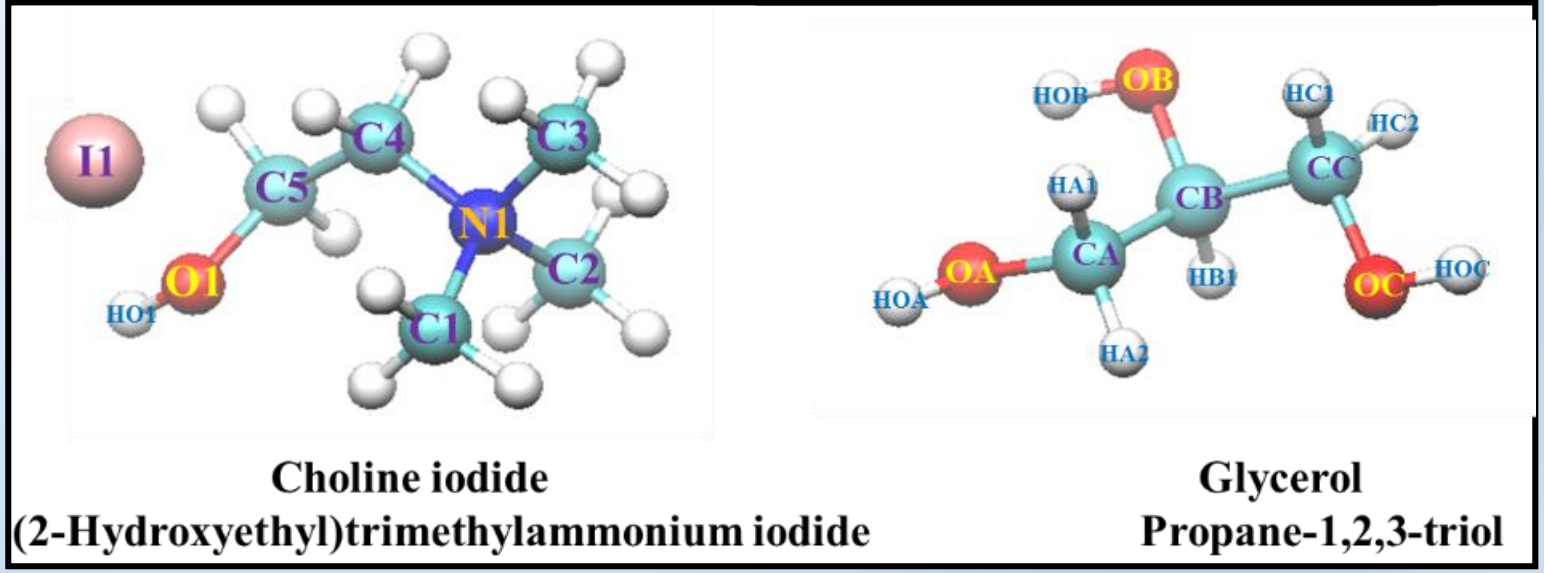


Dye-synthesized solar cell

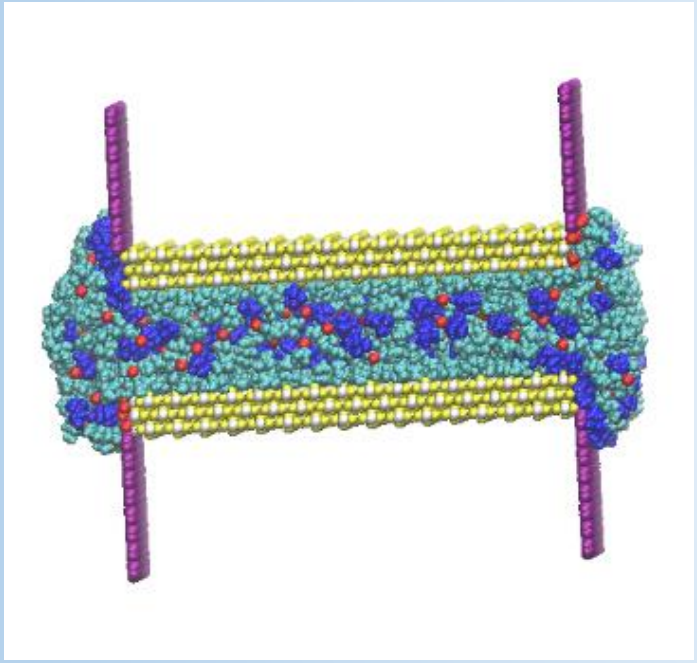
Methods & Materials

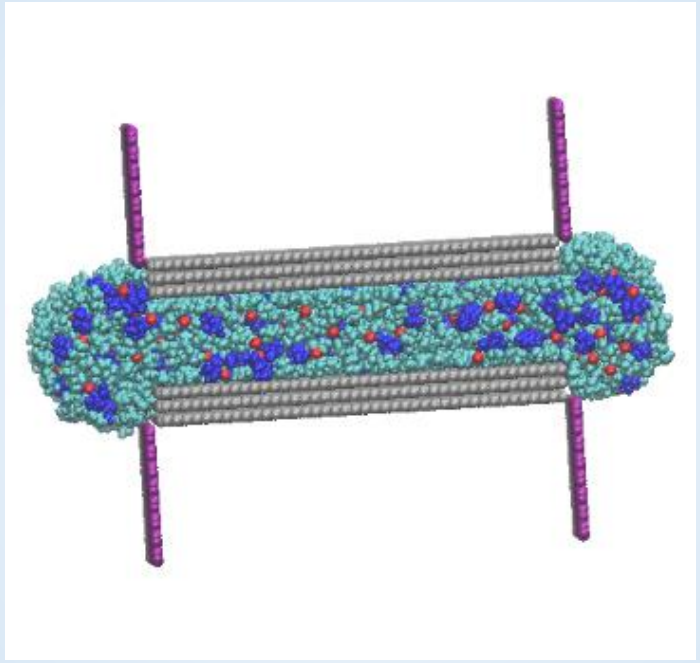
1. Prepare input files using GROMACS MD software: simulation of
   a. DES (1:3 mol ratio choline iodide and glycerol)
   b. in 2.5 nm pore of titania (TiO_2) or graphite
   c. and in bulk system (no pore walls)
   d. under general AMBER force field (GAFF)
   e. under initial temp. 333K
2. Visualize output data using Visual Molecular Dynamics (VMD)
3. Analyze output data using GROMACS and VMD

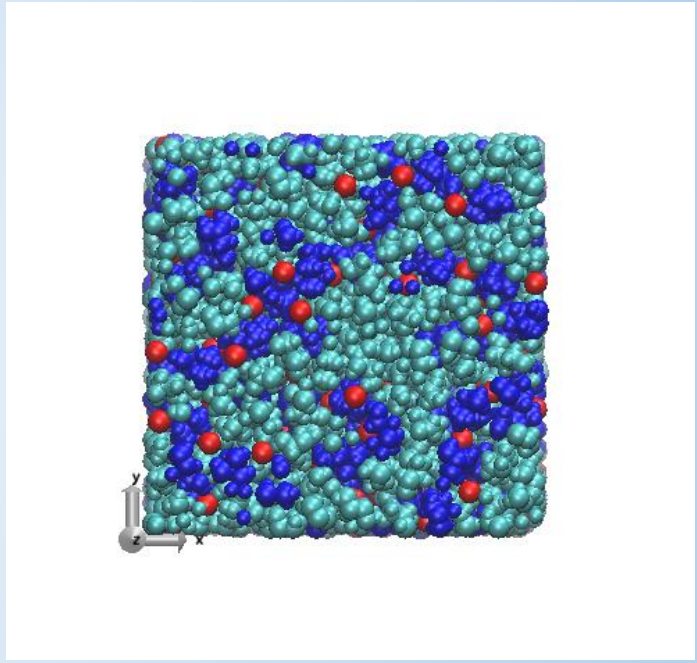
Composition of DES (in 1:3 ratio)



Results & Interpretation: Visualizations







Titania

Graphite

Glycerol

Choline

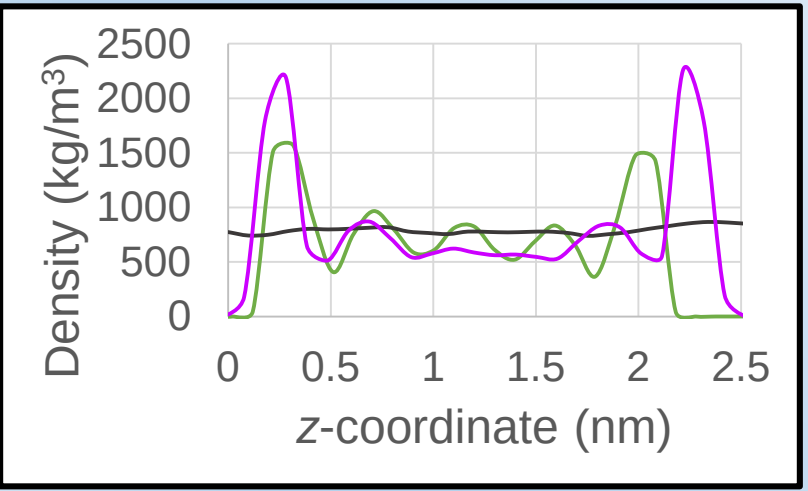
Iodide

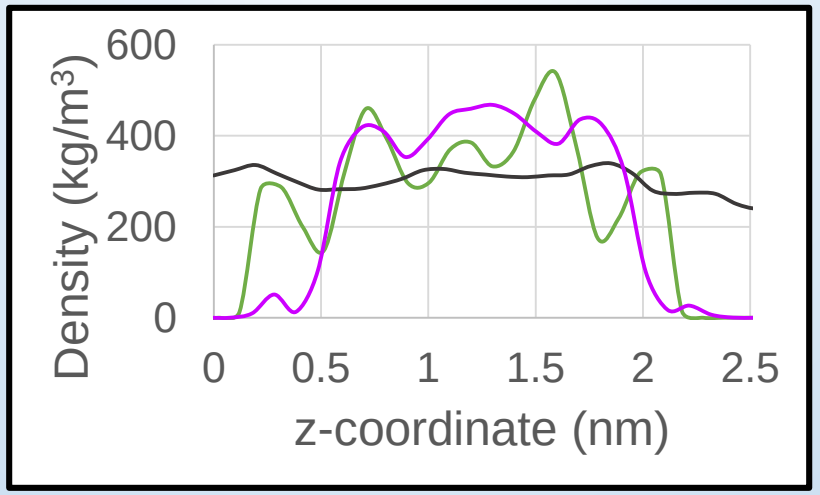
Results & Interpretation: Density Profiles

- No peaks in bulk proves chemical interactivity with pore walls.
- Density peaks represent aggregation of glycerol species near pore walls

Rutile Graphite Bulk

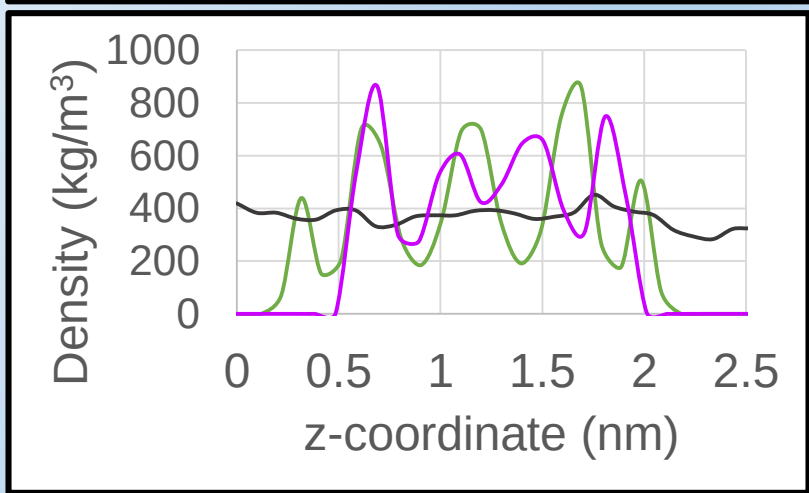
Partial Density: Glycerol





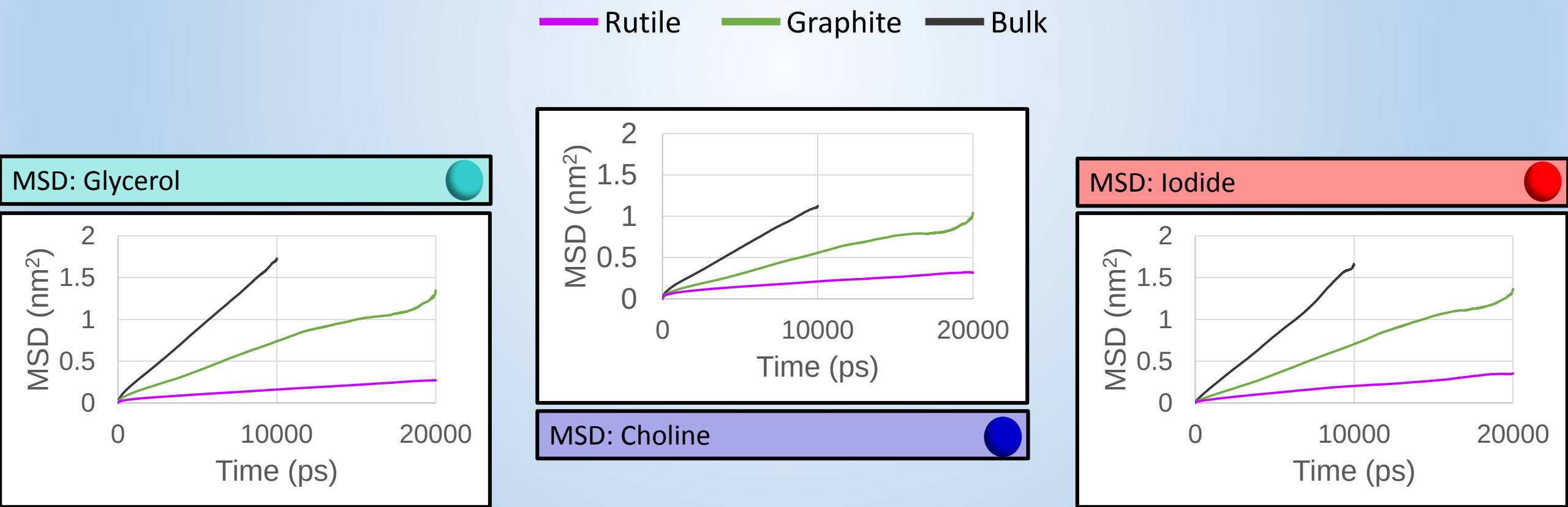
Partial Density: Choline

Partial Density: Iodide



Results & Interpretation: MSD

- Linear MSD plots reflect diffusive displacement (random).
- Exponential MSD plots indicate a directionality of movement.



Conclusions

- Dynamic properties of all three species change when in confinement; particularly the density of hydrogen bonding properties of glycerol.
- Of the confined systems, the graphite system shows behavior more similar to that of the bulk system (e.g., subtler density peaks, non-linear ends to MSD within 20 ns, displacement.

More study can be done to analyze the behavior of species among density layers.

All data can be used to further compare behavior of DESs to ILs in confinement and evaluate DESs as a substitute.