Molecular simulations of ionic liquids confined inside nanoporous carbon CMK-3

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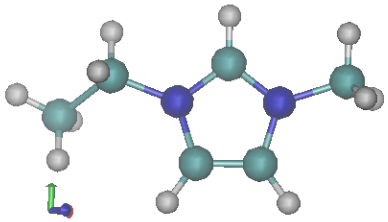
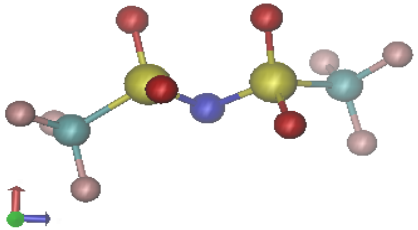
Goal

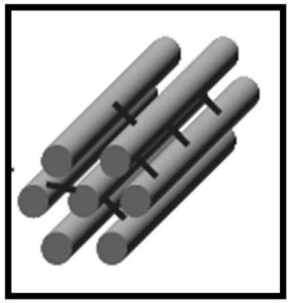
- Investigate structure, dynamics of the ionic liquid (IL) [$emim^+$][NTf_2^-] inside CMK-3 nanoporous carbon



1-ethyl-3-methylimidazolium, [$emim^+$]



bis-(trifloromethylsulfonyl) imide, [NTf_2^-]

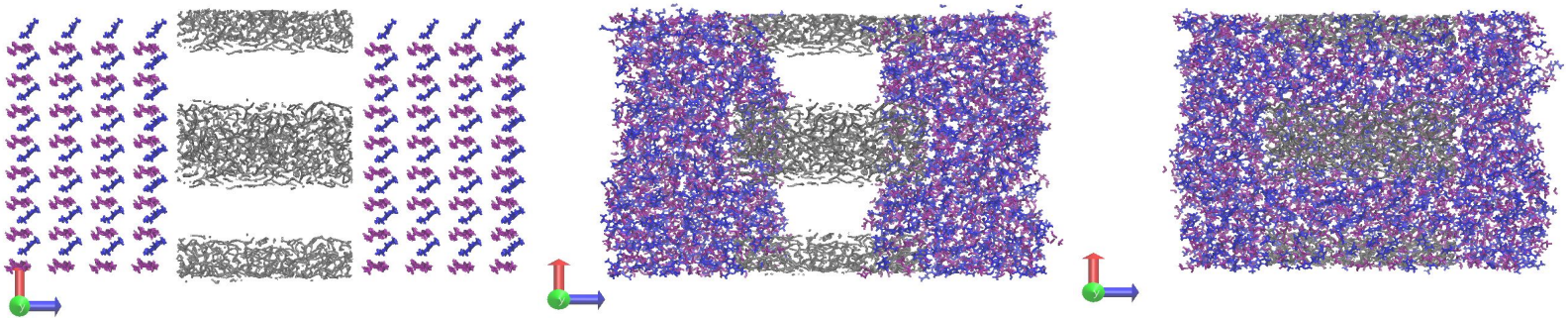


Scheme of CMK-3

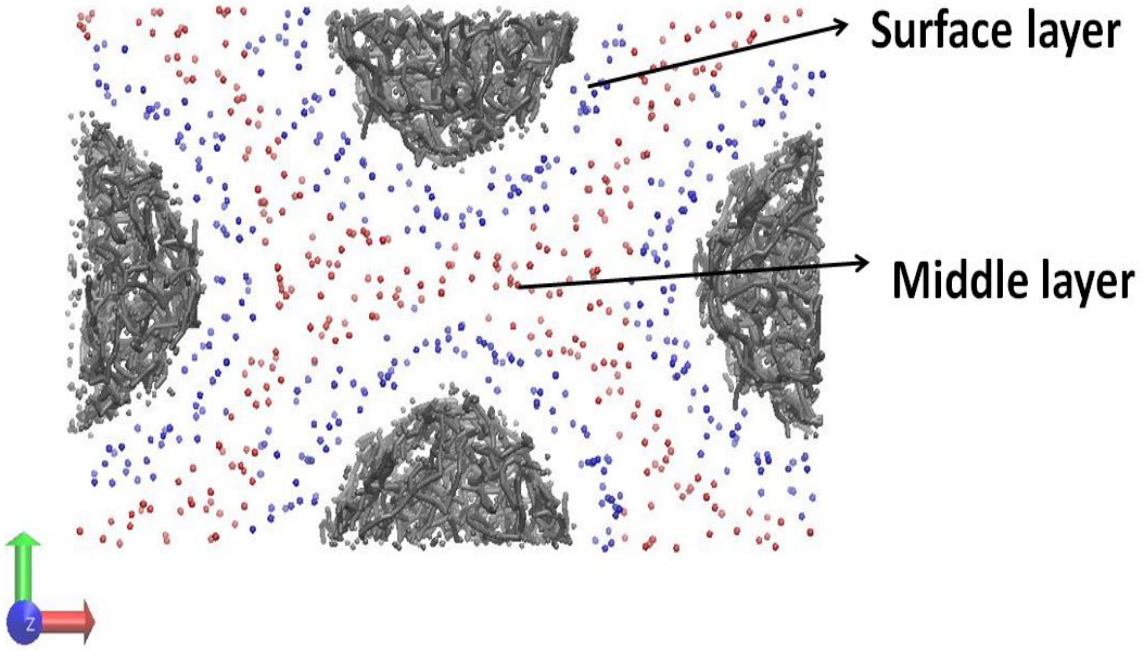
- Relevant to applications in electrochemical double layer capacitors (EDLCs), batteries, solar cells

Procedure

- Initially place ions in lattice, outside of pores
- Minimize energy of the system
- Melt IL at T = 500 K
- Reduce T gradually to 333 K, allow IL to enter pores
- Equilibrate, measure properties



Results

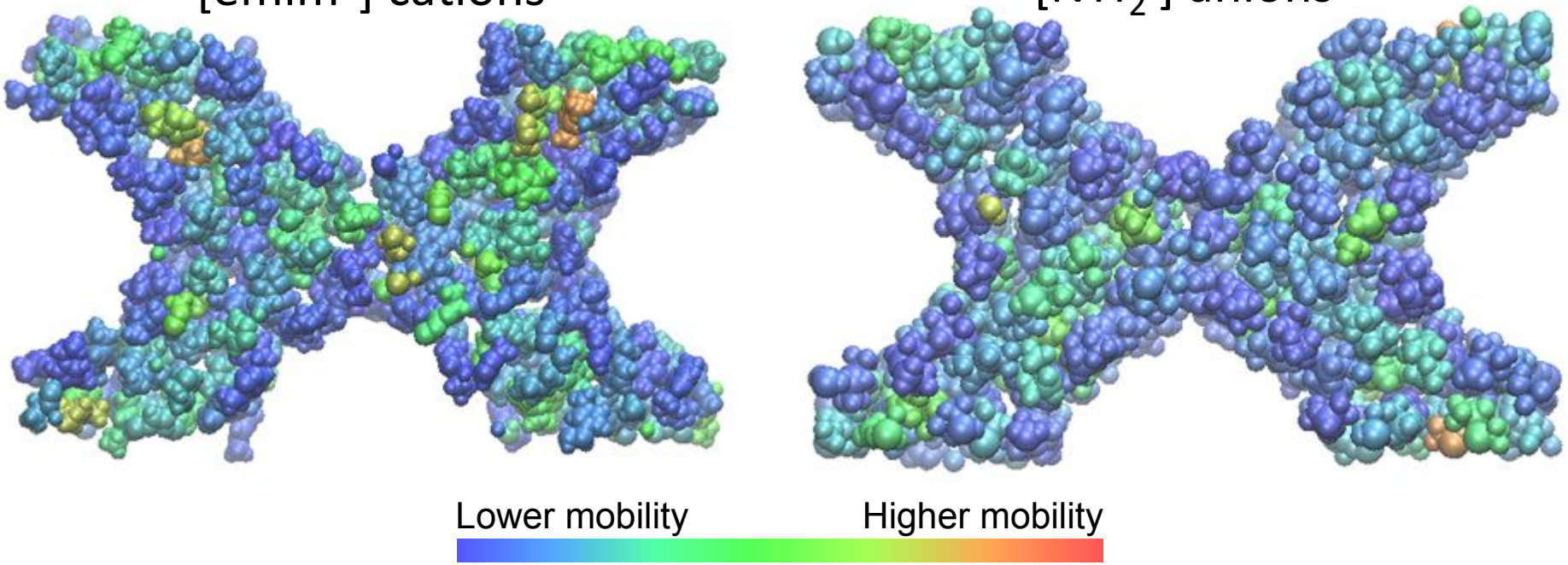


- IL forms layers of fluid around the surface of CMK-3

Results

[emim$^+$] cations

[NTf_2^-] anions



- Layers of ions have different mobilities

Challenges

Acknowledgements

- National Science Foundation
- Francisco Hung + Xioaxia He
- HPC@LSU
- LA-SiGMA faculty

Questions, Comments, or Concerns