



University of Colorado  
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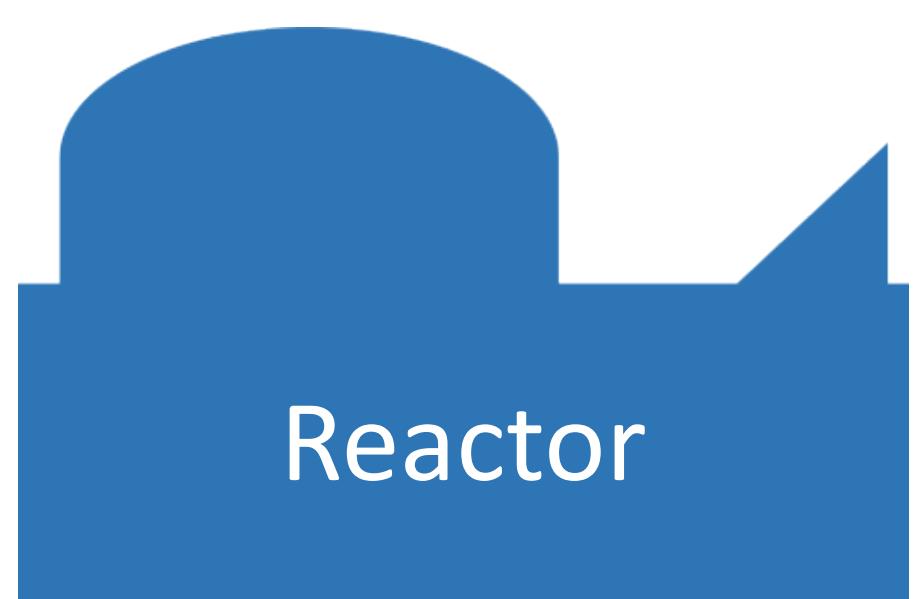
# Molecular Simulations of Engineered Barrier Systems with Enhanced Anionic Radionuclide Sorption

Jordan Winetrot

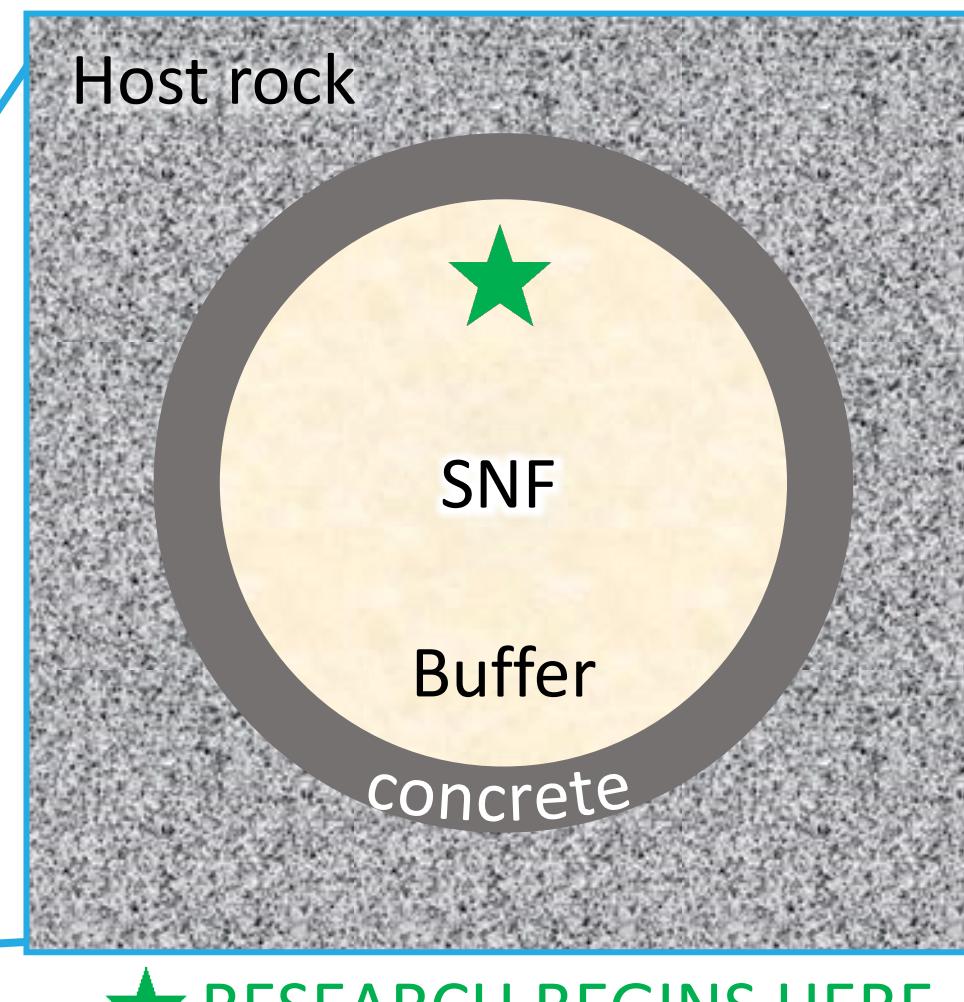
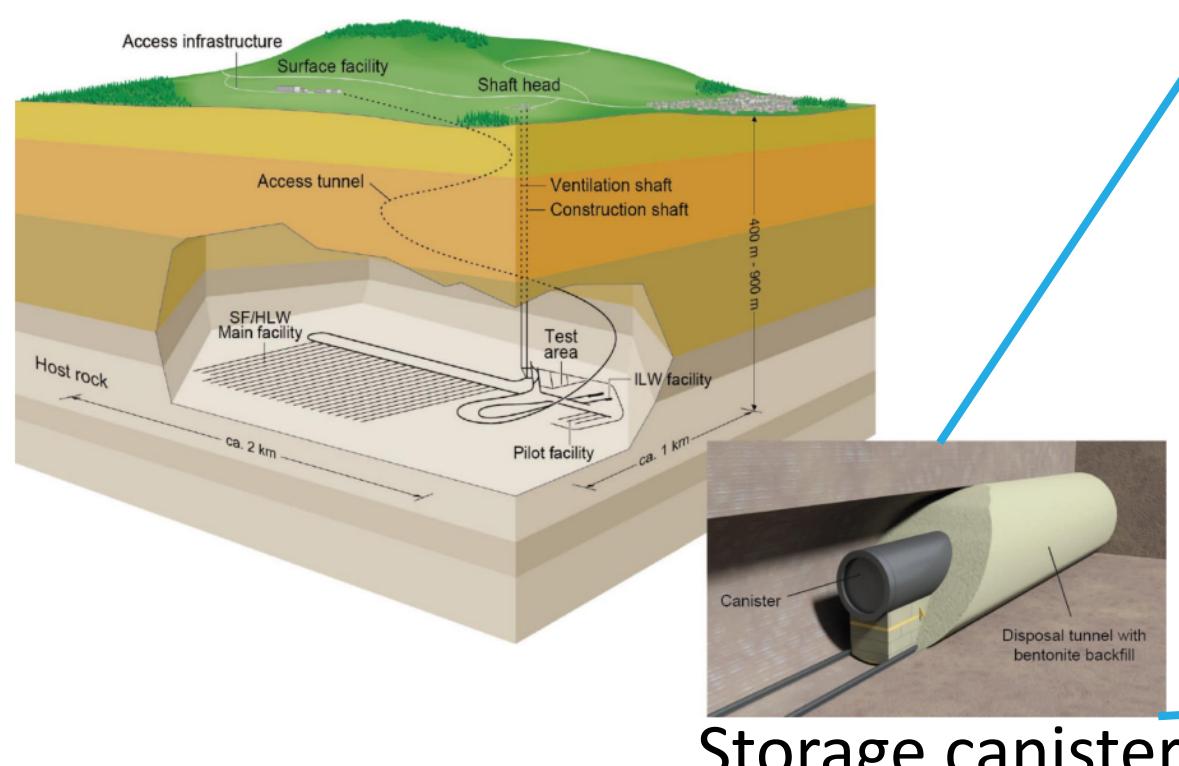
Jeffery Greathouse (8842, mentor), Chris Camphouse (8842, manager)

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## Deep geological disposal of spent nuclear fuel (SNF)

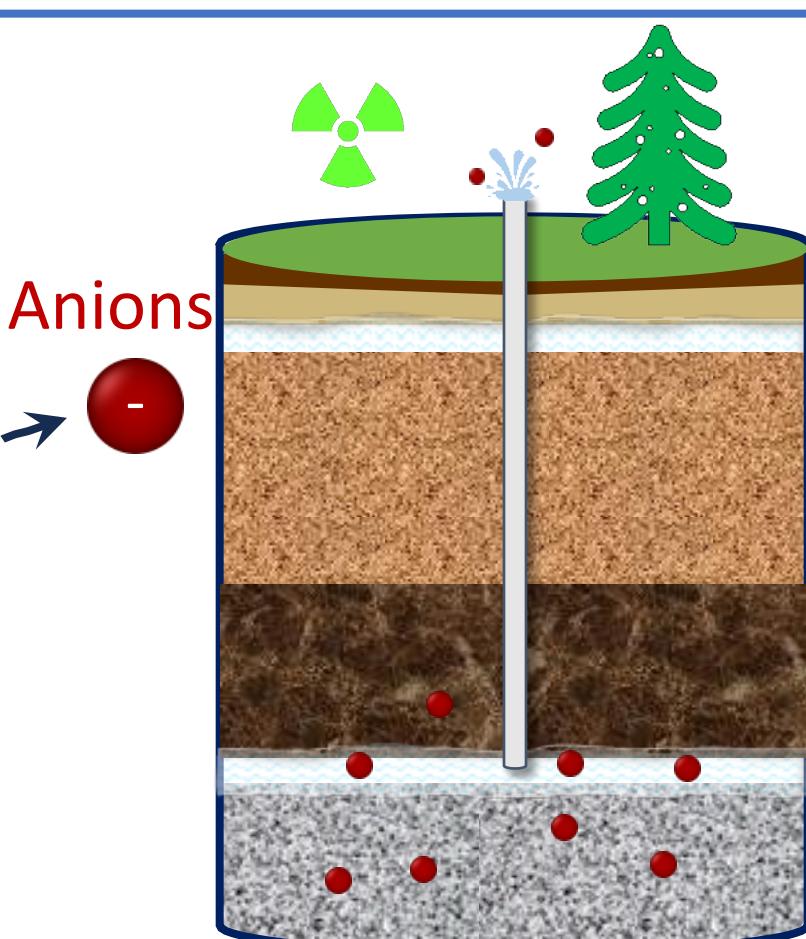
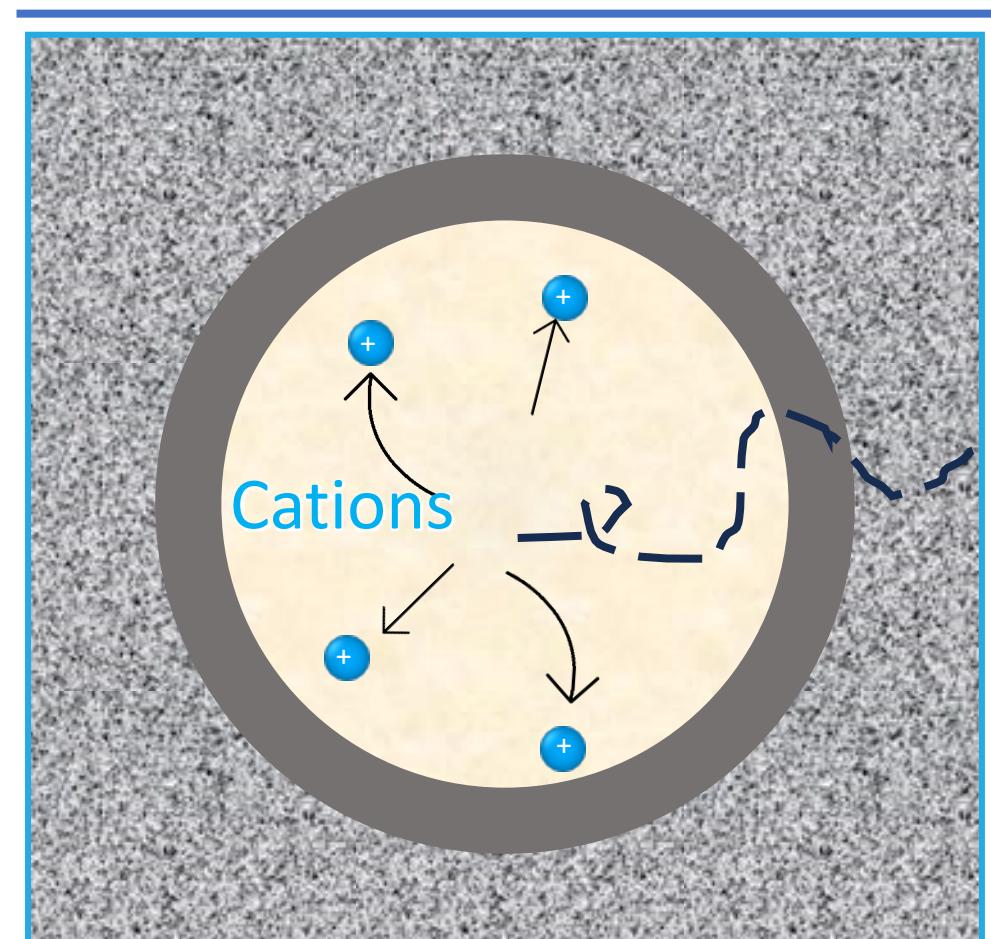


Spent fuel storage



★ RESEARCH BEGINS HERE

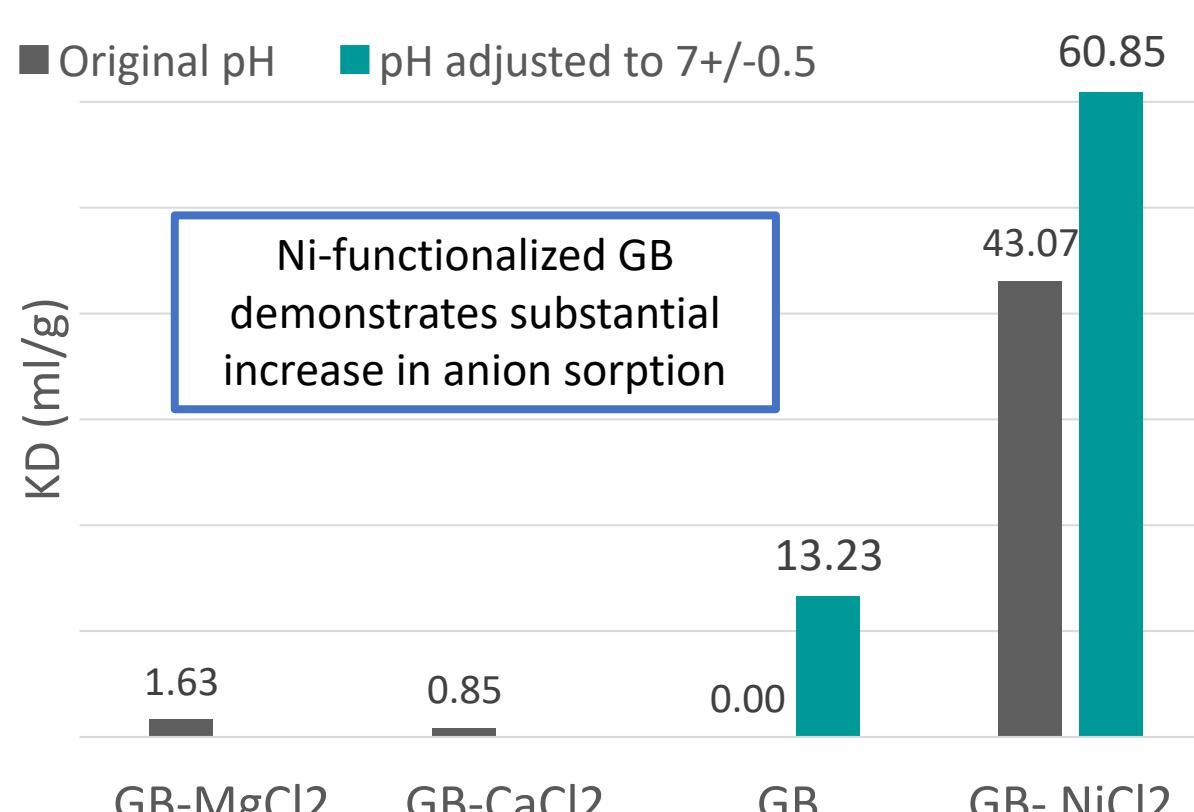
**Challenge.** Current buffer material has poor capture ability for high mobility anionic radionuclides.



Solution

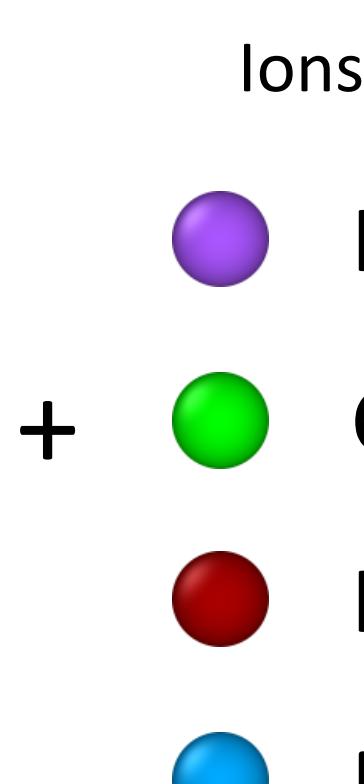
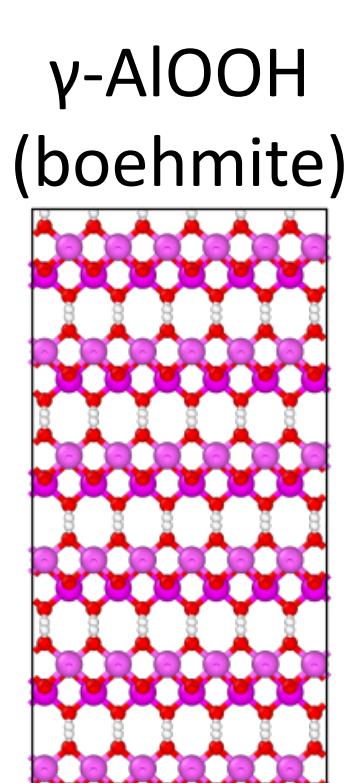
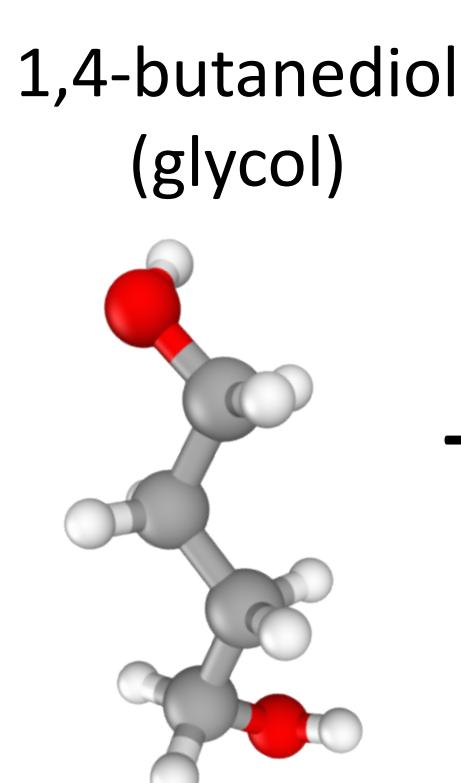
Glycoboehmite (GB) Iodide Sorption<sup>2</sup>

■ Original pH ■ pH adjusted to 7+-0.5



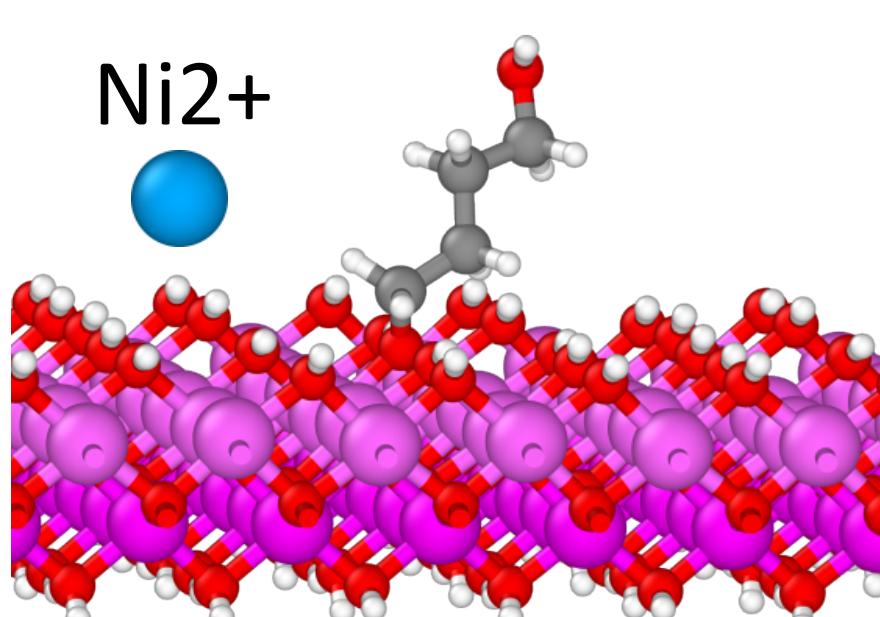
**Goal.** Design anion sorbents that are compatible with EBS seal systems and stable under repository conditions.

## Methods

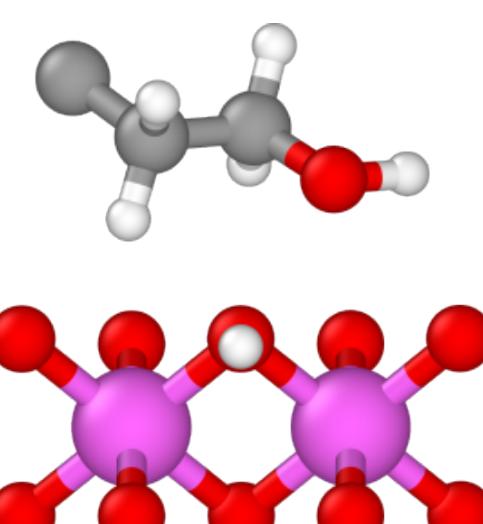


## Results

### Parameter development

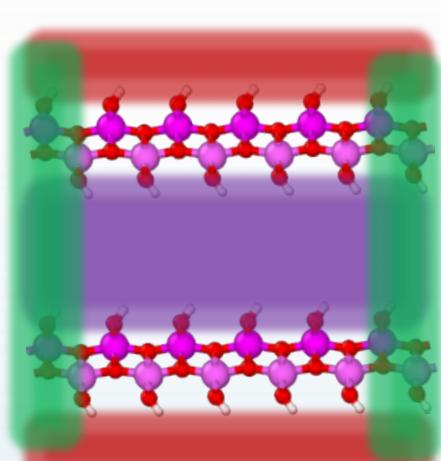


### Reactive templates

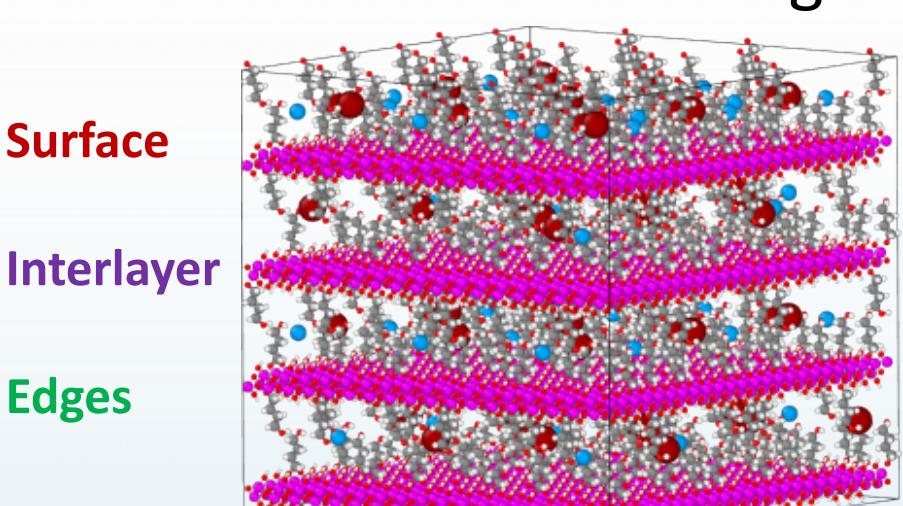


## Future Work

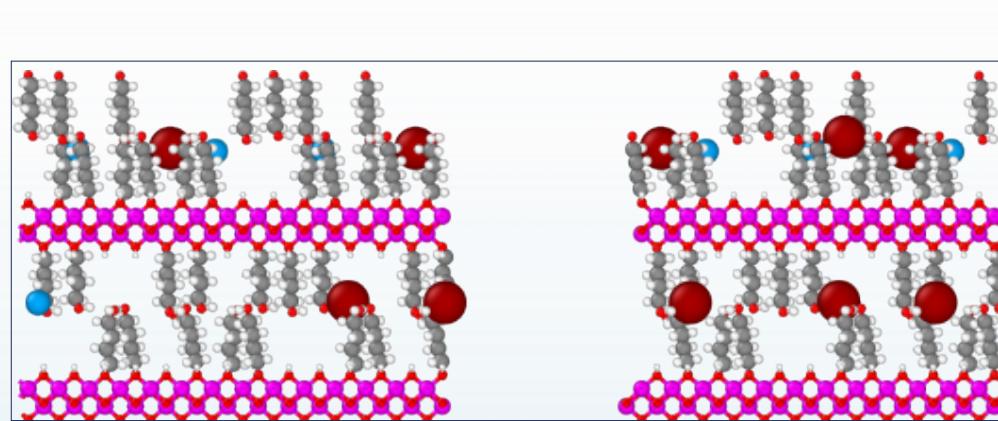
### Docking study



### Ion intercalation through NP



### Solvated slit-pore model



## Bibliography

1. Sellin, P. and Leupin, O.X. (2013) The Use of Clay as an Engineered Barrier in Radioactive-Waste Management -- A Review. *Clays Clay Miner.*, 61, 477-498.
2. Kruichak, J. et. al., Anionic Contaminant Capture using Nickel-functionalized Glycoboehmite (in prep).