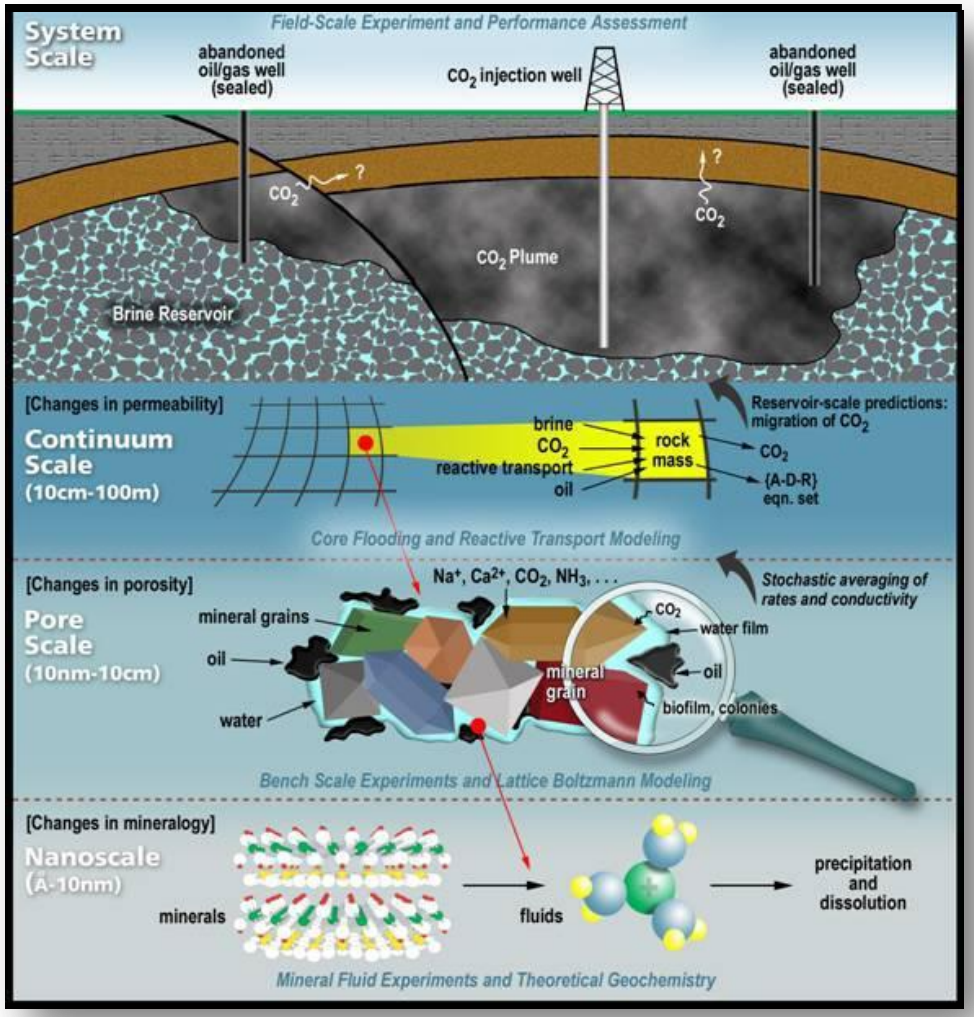
# Multi-Scale, Multi-Physics Approach for the Study of Underground $CO_2$ Storage

The **Center for Frontiers of Subsurface Energy Security** (CFSES) is pursuing scientific understanding of multi-scale, multi-physics processes to ensure safe and economically feasible storage of carbon dioxide and other byproducts of energy production without harming the environment



# Molecular Simulation of $CO_2$ Capture and Sequestration

## Scientific Achievement

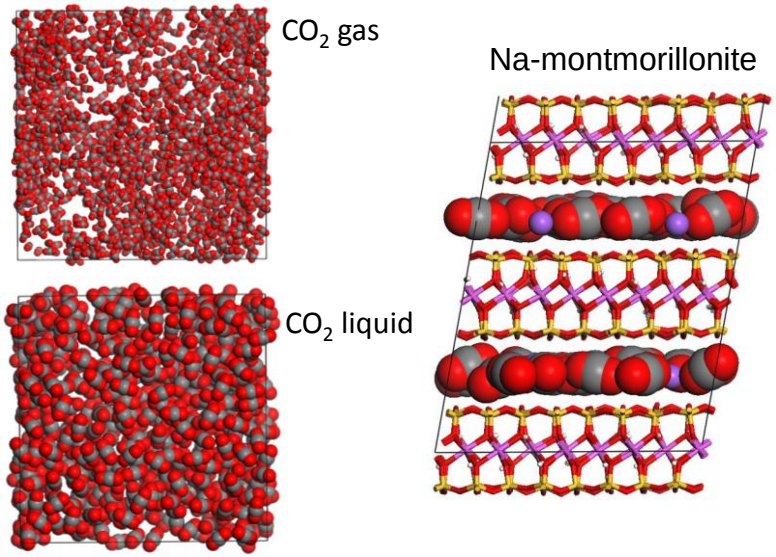
**Developed accurate molecular models of $CO_2$ for simulating carbon capture mechanisms associated with clay minerals and for evaluating $CO_2$ solubility in reservoir brines associated with $CO_2$ sequestration**

## Significance and Impact

**Provides molecular-based description of $CO_2$ effects in environments difficult to assess by experiment or in field tests**

## Research Details

- Three-point force field for $CO_2$ is fully flexible providing for accurate simulations of interfaces and brines
- Flexibility improves prediction of thermodynamic and transport properties for nonlinear $CO_2$ molecule at supercritical conditions
- Molecular dynamics simulations confirm mechanism of $CO_2$ intercalation in clay mineral




Periodic molecular models of pure $CO_2$ and intercalated $CO_2$ in clay mineral

Cygan, R.T. et al. *Journal of Physical Chemistry C*, **2012**, 116, 13079-13091

# Brine Chemistry and Cation Solvation at the Brine-$CO_2$ Interface

## Scientific Achievement

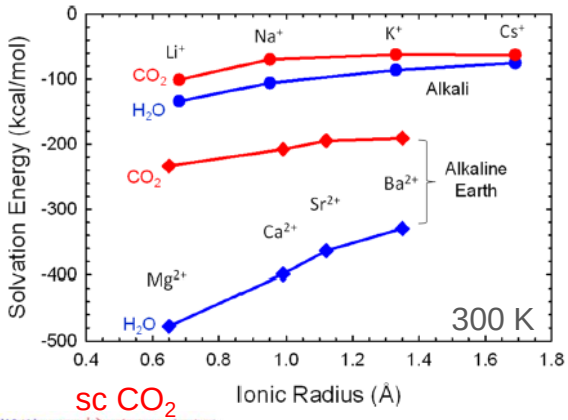
**Comparison of cation solvation by $H_2O$ and $CO_2$ by molecular simulation for evaluating solubility and density of reservoir brine and supercritical $CO_2$ fluid**

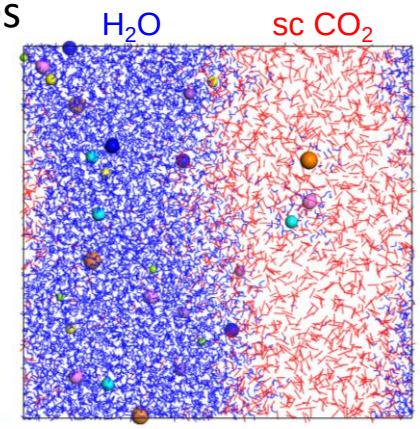
## Significance and Impact

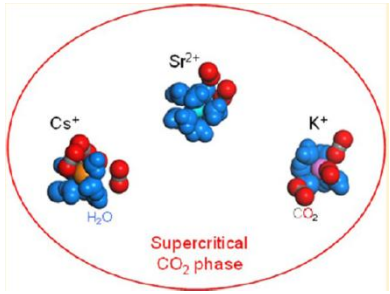
**Provides molecular-based description of $CO_2$ behavior in environments difficult to assess by experiment or in field tests**

## Research Details

- Solvation energy, derived by molecular dynamics simulation, is a function of cation charge and size; small divalent cations expected to be preferentially solvated by $H_2O$
- MD simulation of $H_2O$-$CO_2$ interface demonstrates partitioning of cations between fluids
- Some cations are co-solvated by both molecules within the supercritical $CO_2$ phase




350 K and 20 MPa

Criscenti L. J. and Cygan, R.T. *Environmental Science & Technology*, **2012**, Special issue "Environmental and Geochemical Aspects of Carbon Sequestration"