# Intercalcation of $CO_2$ in Clay Layers for Additional Storage Capacity

## Scientific Achievement

**Our molecular simulations have provided a model confirming the intercalation of $CO_2$ into a montmorillonite clay interlayer based on the red-shift in the vibrational energy of the asymmetrical stretch of $CO_2$. This research provides an accurate molecular description of $CO_2$ for evaluating surface tension, contact angles, capillary flow, snap-off, and related phenomena associated with $CO_2$ trapping.**

## Significance and Impact

**Continuation of this research could demonstrate additional storage capacity for $CO_2$ in clay layers on reservoir rock coatings and in the caprock. Intercalcation could also be a mechanism for controlling potential leakage.**

## Publications


Myshakin, E. M., W. A. Saidi, V. N. Romanov, R. T. Cygan, and K. D. Jordan (2013), Molecular Dynamics Simulations of Carbon Dioxide Intercalation in Hydrated Na-montmorillonite, *The Journal of Physical Chemistry C*, *117*, 11028−11039.

Cygan, R. T., V. N. Romanov, and E. M. Myshakin (2012), Molecular Simulation of Carbon Dioxide Capture by Montmorillonite Using an Accurate and Flexible Force Field, *Journal of Physical Chemistry C*, *116*(24), 13079-13091.


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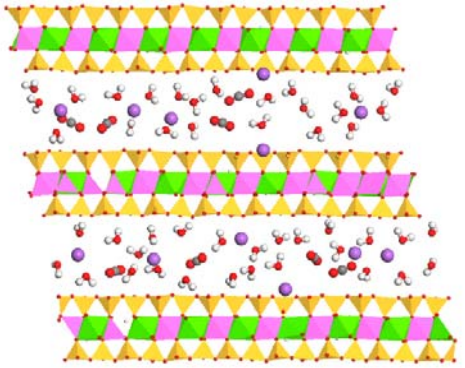

Intercalation of $CO_2$ and $H_2O$ molecules in in a montmorillonite clay interlayer. Color designation: red balls − oxygens; purple − sodium ions; white − hydrogens; gray − carbon.


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