Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Atomic-scale mechanism of incorporation of carbon dioxide in coal[1] YINGDI LIU, HONGLI DANG, The University of Tulsa, PONGTORN CHAROENSUPPANIMIT, SAYEED MOHAMMAD, Oklahoma State University, KHALED GASEM, University of Wyoming, SANWU WANG, The University of Tulsa — Global warming is attributed to the rise of CO_2 concentration in the atmosphere. Sequestration of CO_2 into geological formations has been suggested for mitigating this phenomenon. Coalbeds are investigated as potential storage sites. Numerous experimental studies have demonstrated that coal swelling occurs after the injection of CO_2 into coal seams. However, the atomic-scale mechanism of such a phenomenon has not been well established. We report first-principles density-functional-theory calculations for the interaction between CO_2 and the coal network. The calculations show that the activation energies for incorporation of CO_2 into the coal bonding network are low at $\sim$ 0.9-1.3 eV depending on the bonding sites. We have found that the incorporated configurations are stable at low temperatures. However, high temperatures could stimulate the dissociation of CO_2 from such configurations as the activation energies are low at $\sim$ 0.5-0.9 eV, suggesting that coal swelling is reversible at high temperatures.

[1]Supported by Oklahoma State University. This research also used the supercomputer resources of the XSEDE, the NERSC center, and the Tandy Supercomputing Center.

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Date submitted: 15 Nov 2013 Electronic form version 1.4