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Competitive Adsorption of Carbon Dioxide/Methane in Coal: First-Principles Quantum Mechanical Investigations[1] YINGDI LIU, SANWU WANG, Univ of Tulsa — Sequestration of CO_2 into geological formations has been suggested to mitigate the effect of the increasing of the atmospheric CO_2 concentration on global warming. Coalbeds are investigated as one of the attractive storage sites since the cost of CO_2 sequestration can be offset by the enhanced coalbed methane (ECBM) recovery. Extensive experimental studies have been performed for the competitive adsorption of CO_2/CH_4 into coalbeds. However, the atomic-level understanding for the interaction between the adsorbate (CO_2/CH_4) and the adsorbent (coal) has not been fully explored. We report first-principles density-functional calculations for the competitive adsorption between CO_2/CH_4 in the coal network. In particular, we report results of atomic structures, bonding characteristics, energetics, as well as electronic structures of the CO_2/CH_4-coal systems.

[1]This research used the supercomputer resources at NERSC, of XSEDE, at TACC, and at the Tandy Supercomputing Center.

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