Interaction between carbon dioxide and coal: atomic-scale characteristics and electronic structures\textsuperscript{1} YINGDI LIU, SANWU WANG, Department of Physics and Engineering Physics, The University of Tulsa — Geologic sequestration of CO\textsubscript{2} in unmineable coal seams has been suggested to mitigate the effect of the increasing of the atmospheric CO\textsubscript{2} concentration on global warming. Extensive experimental studies have been performed for the injection of CO\textsubscript{2} into coalbeds. However, the atomic-level mechanism for the interaction between CO\textsubscript{2} and coal has not been fully explored. We report first-principles density-functional calculations and \textit{ab initio} molecular dynamics simulations for the interaction between CO\textsubscript{2} and the coal network. In particular, we report results about atomic-scale and electronic properties of the interaction. We also report a comparison with the interaction between CH\textsubscript{4} and coal.

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