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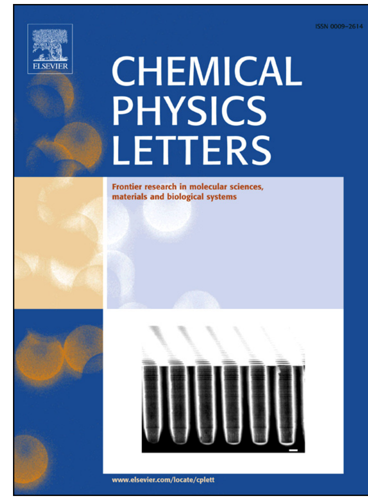

Research paper

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ACCEPTED MANUSCRIPT

Microscopic Diffusion of CO_2 in Clay Nanopores

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Abstract:

Natural gas production from shale in recent years has made a significant impact on the energy sector. It also presents potential opportunities to mitigate global warming by using shale reservoirs for CO_2 sequestration. We attempt to understand the microscopic impact of shale on CO_2 transport. We utilize equilibrium molecular dynamics (MD) to study the diffusion behavior of CO_2 in the clay part of shales. Such microscopic examination can connect micro-scale calculations to macro-scale measurements. Results show that confinement has profound effects on CO_2 diffusion. The diffusion coefficient was found to be slightly anisotropic due to the nature of the clay surface.

Introduction:

Transport and fluids flow in conventional rocks are considered mature subjects. They have been heavily studied over the past few decades. A great body of the literature was dedicated to examine conventional oil reserves, mostly composed of sedimentary rocks. However, the recent discovery of shale gas has challenged the conventional understanding of oil and gas transport and interaction with rocks. Darcy's Law, for example, which is considered a bedrock of conventional oil and gas studies, does not capture fluid behavior in shales due to the heterogeneous nanostructure of shales. Shale has unique nanoporous network that is distinct from conventional rock, which has a much higher pore size [1]. The small scale of shale pores results in unusual behavior of fluid. Similar deviation due to confinement in nanopores was observed in the case of methane and nitrogen behavior, for example, in activated carbon, where the interaction with activated carbon nanopores significantly enhanced gas density storage [2]. Furthermore, in order to make use of shale reserves for enhanced gas recovery using CO_2, or use shales for CO_2 sequestration purposes, further fundamental understanding of CO_2 interaction with shales is needed.

Shale is composed of two main media, organic and inorganic. In the past few years, many studies have been dedicated to investigating the organic part of coals as part of enhanced coal bed methane recovery [3], which has some resemblance to the organic part of shale. These studies were used as a basis to further study and elucidate the role of the organic matter in shale. However, there is still distinction between coal and shale and much remains not understood. Another major difference is that shales have a significant clay content; a material not present in

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