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Coarse-grained potential models for structural prediction of carbon dioxide in confined environments TARUN SANGHI, NARAYANA ALURU, University of Illinois at Urbana-Champaign — Geological storage of carbon dioxide is a promising option to reduce the level of carbon dioxide in the atmosphere and mitigate its effect on climate change. In geological storage, high-pressure carbon dioxide is injected into the underground porous rock formations, where it gets trapped inside the tiny nanometer size pores of the rocks. Thus, a good understanding of the microstructure of carbon dioxide inside nanoscale confinements is of great practical importance in developing an efficient technology for carbon dioxide storage. In this work, we discuss the systematic development of coarse-grained single-site (CGSS) potential models to study the structure of carbon dioxide in confined environments. These single-site potentials allow computationally efficient simulations, which are several orders of magnitude faster than all-atom MD (AAMD) simulations. The potential models are used in our earlier proposed multi-scale quasi-continuum theory, called EQT, and in coarse-grained MD (CGMD) to predict the equilibrium structure of carbon dioxide confined inside graphite slit pores. The results obtained from both EQT and CGMD are found be in good agreement with those obtained from computationally expensive AAMD simulations.

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