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Multiscale Modeling of Solutions OLAYINKA OLATUNJI-OJO, SANDRA BOETCHER, THOMAS CUNDARI, Center for Advanced Scientific and Computer Modeling, University of North Texas, Denton Tx 76203 — The sequestration of carbon dioxide is one proposed solution to alleviate the growing problem of increased atmospheric CO_2 concentration, and its resulting effect on global climate. However, the efficacy of such methods has yet to be demonstrated. Improved CO_2 sequestration methods are needed and this can be achieved through a better understanding of the chemical and physical consequences of CO_2 encapsulation through multiscale modeling. Multiscale modeling is an effective tool for combining different methods thereby creating an efficient way of modeling diverse chemical and physical phenomena. The goal of this research is to model carbon dioxide interactions in solutions from the quantum to continuum level. This is achieved through a combination of DFT calculations, molecular modeling (mesoscale) and computational fluid dynamics (continuum) simulations on CO_2 + H_2O. Interaction energies and interatomic distances are obtained from DFT calculations, which are used to derive a Lennard-Jones potential, from which one may obtain continuum properties such as viscosity via reverse non-equilibrium molecular dynamics (RNEMD) simulations.

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