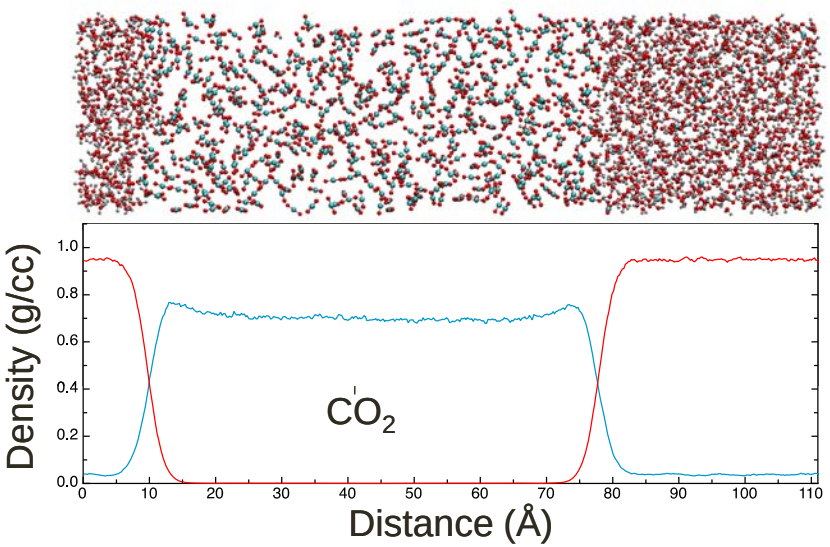
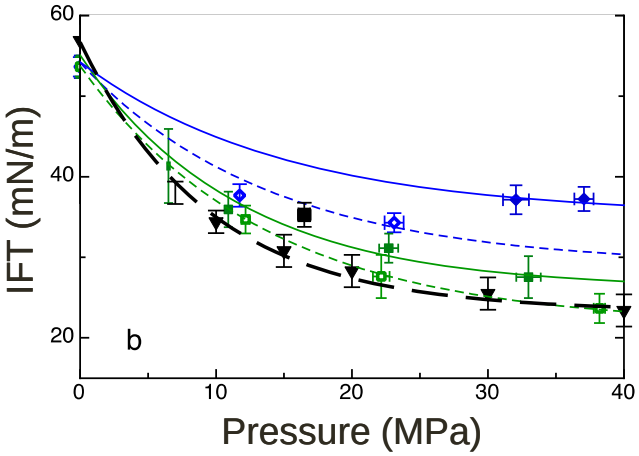
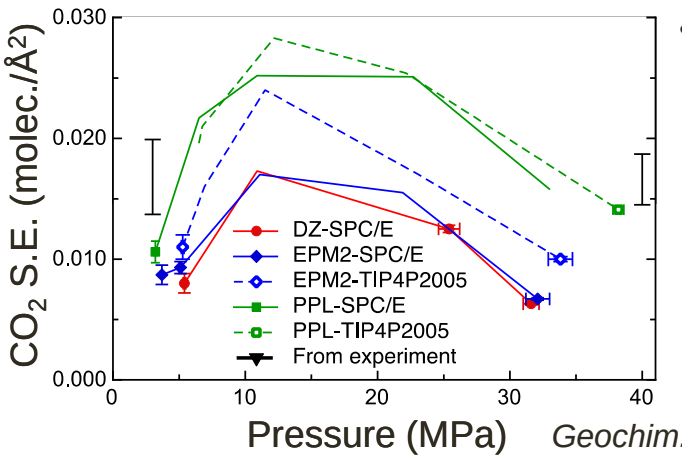
Predicting CO_2-water interfacial tension under pressure and temperature conditions of geologic CO_2 storage



- Interfacial tension (IFT) between CO_2 and reservoir brine directly controls the capillary phenomena that determine the efficacy of structural and residual capillary trapping in GCS systems.
- Molecular dynamics (MD) simulations may be used to calculate fluid-fluid interfacial tension (IFT) and to probe the link between molecular-scale interfacial structure and IFT, but predictions are sensitive to the choice of interatomic potential parameters.
- To our knowledge, this study constitutes the first comparative test of several CO_2-water interatomic potential models against the properties of CO_2-water interfaces.





- We find that CO_2-water IFT is strongly related to CO_2 adsorption on the water surface – surface excess (S.E.) – as predicted by the well-known Gibbs adsorption equation.

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