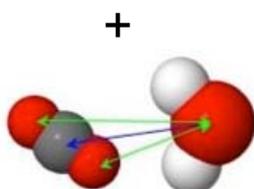
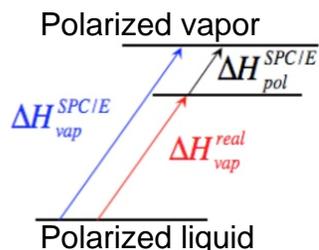
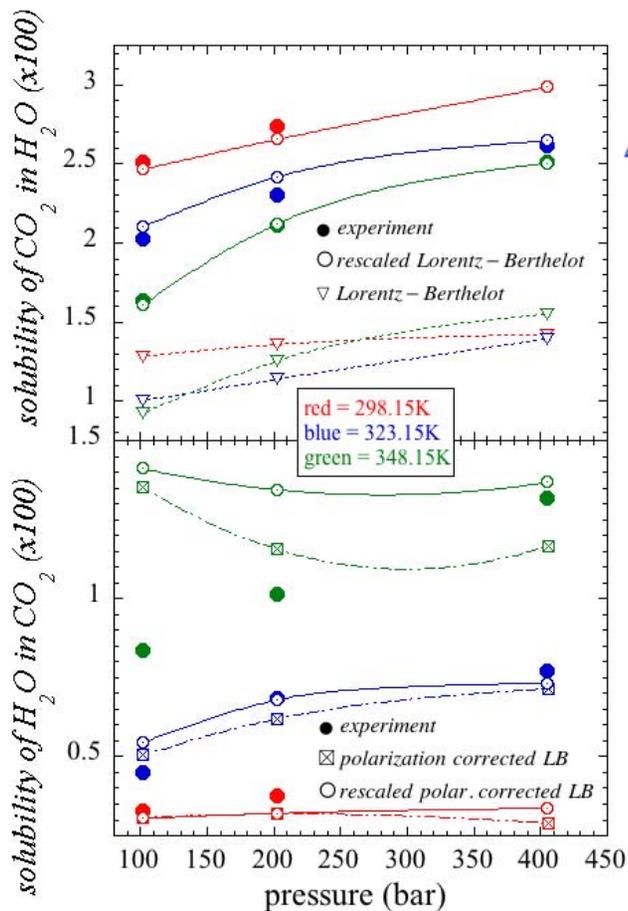


Optimized unlike-pair interactions for water-carbon dioxide mixtures

Vlcek, L., Chialvo A.A., and Cole D.R.
 EFRC: Nano-scale Control of Geologic CO₂



$$\eta = 2\sigma_{ij} / (\sigma_{ii} + \sigma_{jj})$$

$$\xi = \epsilon_{ij} / \sqrt{\epsilon_{ii}\epsilon_{jj}}$$

- Understanding dynamic and thermodynamic processes influencing carbon sequestration requires accurate predictions of H₂O-CO₂ phase equilibria at appropriate conditions (T ~ 288-348 K; P ~ 75-400 bar).
- Mixtures described by the most popular simple models of water (SPC/E) and carbon dioxide (EPM2) using traditional combining rules significantly underestimate mutual solubility of the two components, which may lead to incorrect predictions about their competitive adsorption at mineral surfaces and in pores
- To determine the optimal parameters of the SPC/E-EPM2 interactions, we used a polarization correction for the permanent dipole moment of the SPC/E water and developed an efficient global optimization methodology based on the coupling parameter approach applied to the Gibbs ensemble.
- The resulting model successfully predicts mutual solubilities and diffusivities. The solubility of CO₂ in H₂O is in a quantitative agreement with experiment. The solubility of H₂O in CO₂ is also in a good agreement, but quantitative predictions require the use of polarizable models

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