

## **422c Molecular Simulation of Hydrogen Sulfide**

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A new force field for H<sub>2</sub>S is introduced that quantitatively reproduces the vapor-liquid equilibria and PVT behavior of pure H<sub>2</sub>S and its mixtures with CO<sub>2</sub> and n-pentane. The PVT and VLE calculations are performed with grand canonical histogram-reweighting Monte Carlo simulations.