Electronic Supplementary Information

Polar soft-SAFT: Theory and Comparison with Molecular Simulations and Experimental Data of Pure Polar Fluids.

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Fig. S1. Coexisting curves for the monomeric density vs. reduced temperature from soft-SAFT (solid lines) compared to molecular simulations1 (symbols) for LJ fluids with different chain lengths, m = 1, m = 2, and m = 4.
**Fig. S2.** VLE coexistence curves for tangent-sphere LJ dimer fluid ($m = 2$) from soft-SAFT (solid lines) compared to molecular simulations for non-polar LJ dimer fluid ($\circ$), and for non-polar 2CLJ fluid with $L^* = 1.0$ ($\bigodot$), $1.2$ ($\boxdot$), $1.4$ ($\bigoplus$) and ($\Delta$).

**Fig. S3.** Surface tension vs. temperature for non-polar LJ spheres, $m = 1$ (black) and LJ dimer, $m = 2$ (red) fluids from soft-SAFT + DGT model (solid lines) compared to results from molecular simulations for tangent-sphere LJs ($\circ$), and 2CLJ fluids ($\Delta$) (converted to the tangent-sphere model). See text for details.
References


