Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

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

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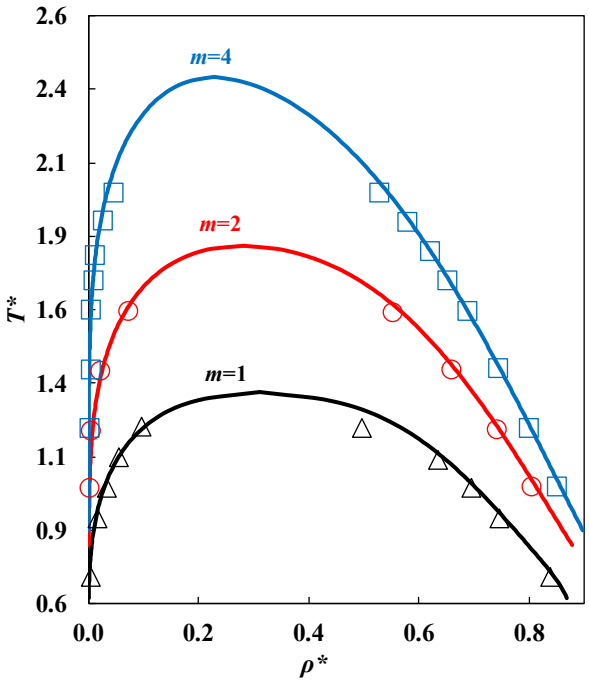

Fig. S1. Coexisting curves for the monomeric density vs. reduced temperature from soft-SAFT (solid lines) compared to molecular simulations[1] (symbols) for LJ fluids with different chain lengths, $m = 1$, $m = 2$, and $m = 4$.

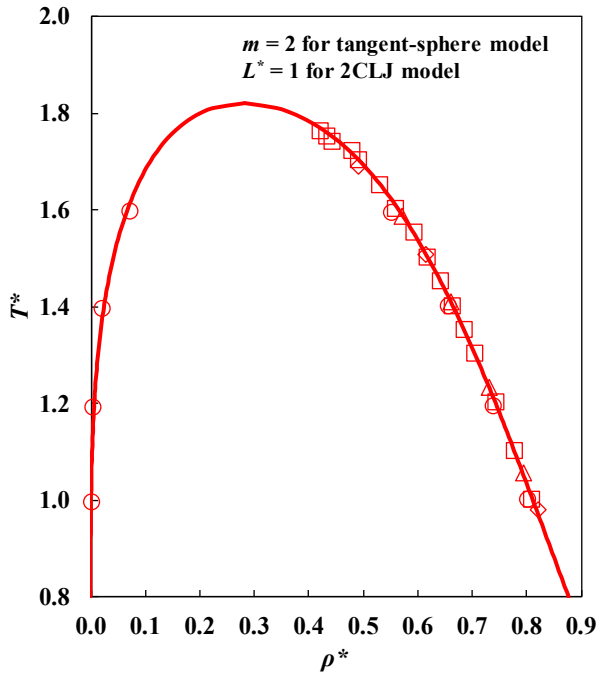

Fig. S2. VLE coexistence curves for tangent-sphere LJ dimer fluid ($m = 2$) from soft-SAFT (solid lines) compared to molecular simulations for non-polar LJ dimer fluid[1] (○), and for non-polar 2CLJ fluid with $L^* = 1.0$ (◊),[2] (□),[3] and (Δ).[4]

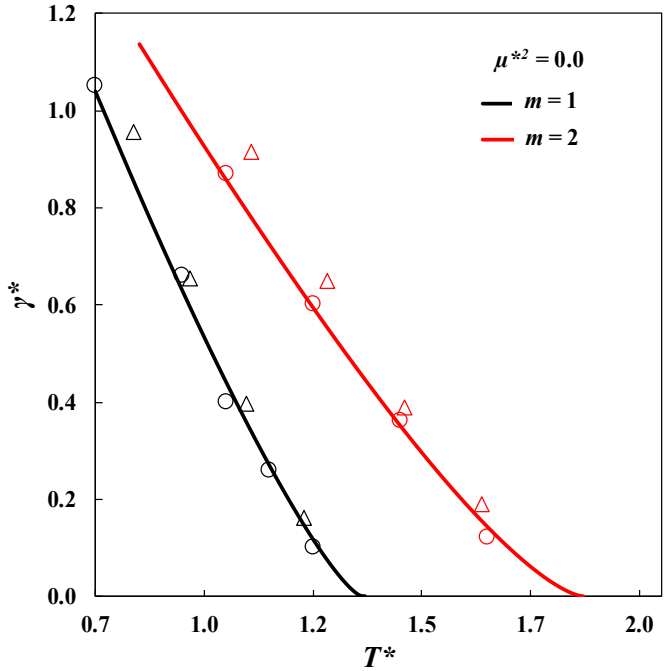

Fig. S3. Surface tension vs. temperature for non-polar LJ spheres, $m = 1$ (black) and LJ dimer, $m = 2$ (red) fluids from soft-SAFT + DGT model (solid lines) compared to results from molecular simulations for tangent-sphere LJs[1] (○),and 2CLJ fluids[4] (Δ)(converted to the tangent-sphere model). See text for details.

References

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