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

Supplementary Information

Enhancing pressure consistency and transferability of structure-based coarse-graining

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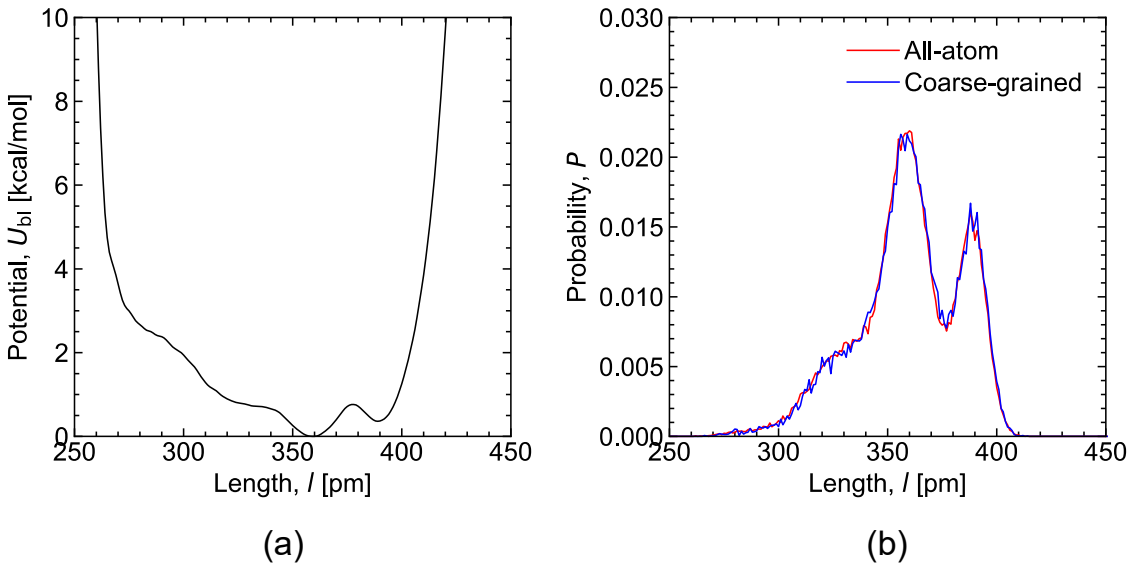

Fig. S1 (a) Coarse-grained bond-length potential. (b) Distribution functions of bond length calculated from simulations of bulk *n*-dodecane systems with the all-atom and our coarse-grained model.

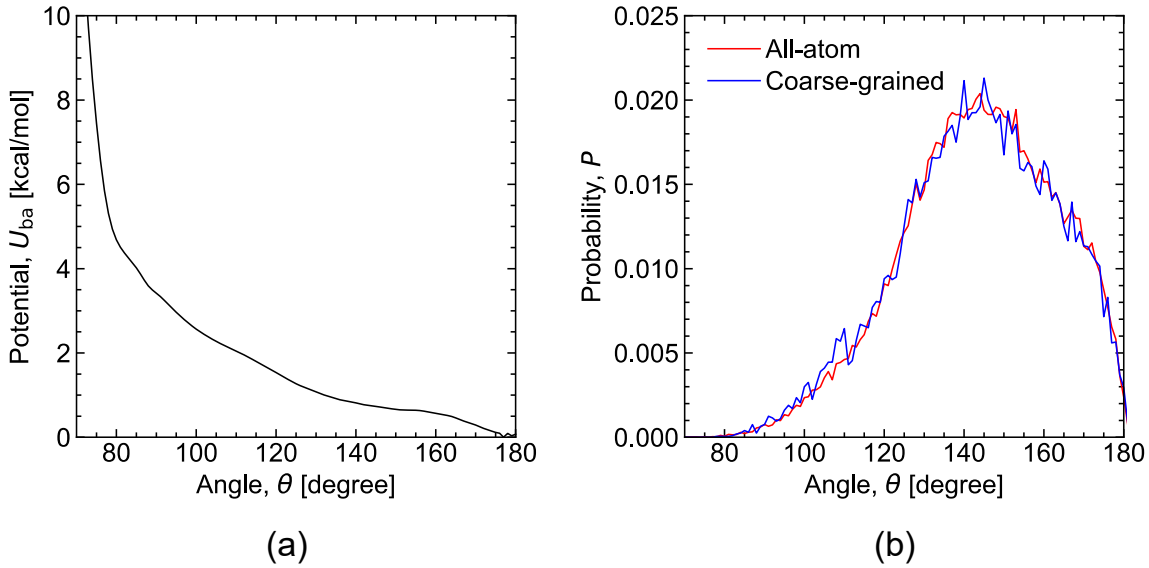

Fig. S2 (a) Coarse-grained bond-angle potential. (b) Distribution functions of bond angle calculated from simulations of bulk *n*-dodecane systems with the all-atom and our coarse-grained model.

Table. S1 Values of parameters *A, B, C*, *a, b, c,* and *d* in eqn (18) for the two initial potentials n-mRDF and n-uRDF, which used the modified and unmodified reference RDFs at 0.1 MPa. Note that the units of *r* and U_{nb}^{0} in eqn (18) are Å and kcal/mol, respectively.

	A	*B*	*a*	*b*	*c*	*d*	*C* (J ·m^6)
n-mRDF	1.05×10^5	7.25	−0.031	0.63	−4.20	8.79	5.7×10^{-77}
n-uRDF	8.49×10^5	9.50	−0.024	0.48	−3.03	5.98	