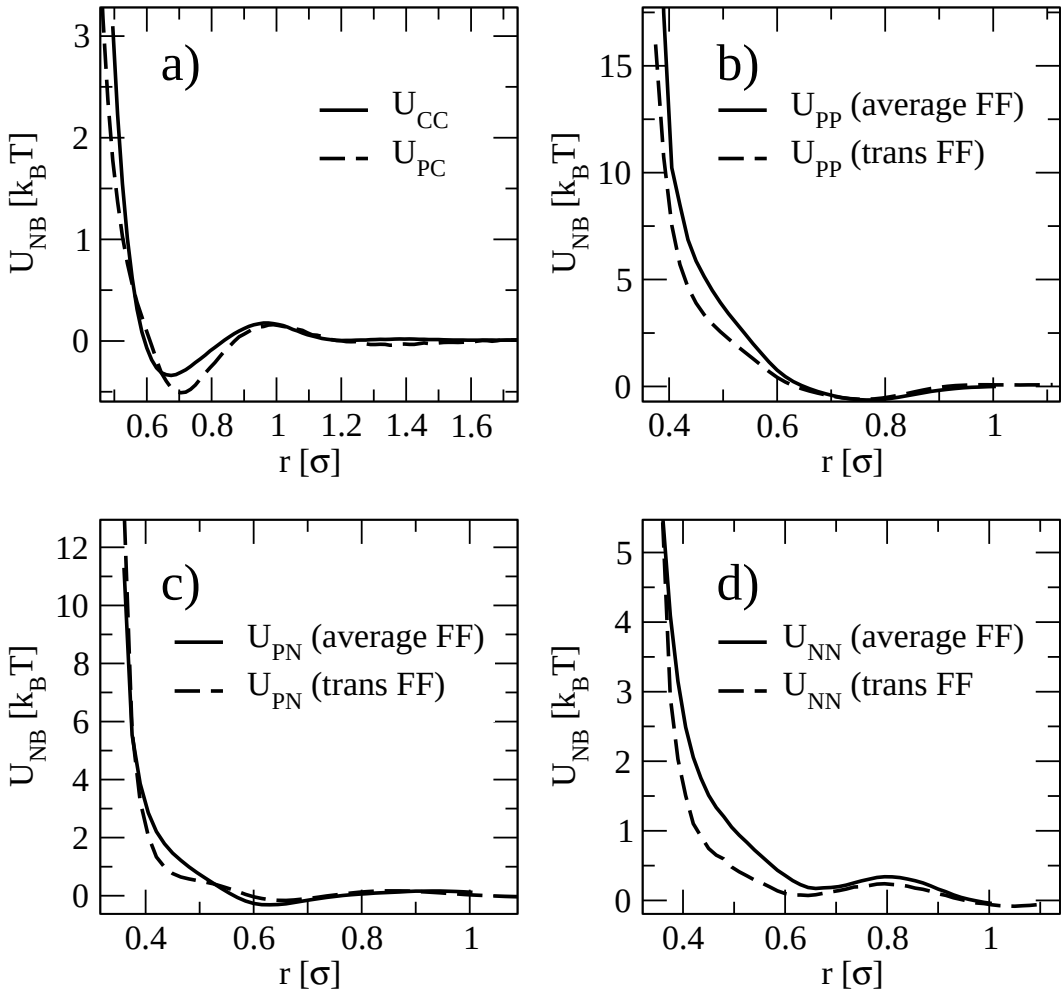
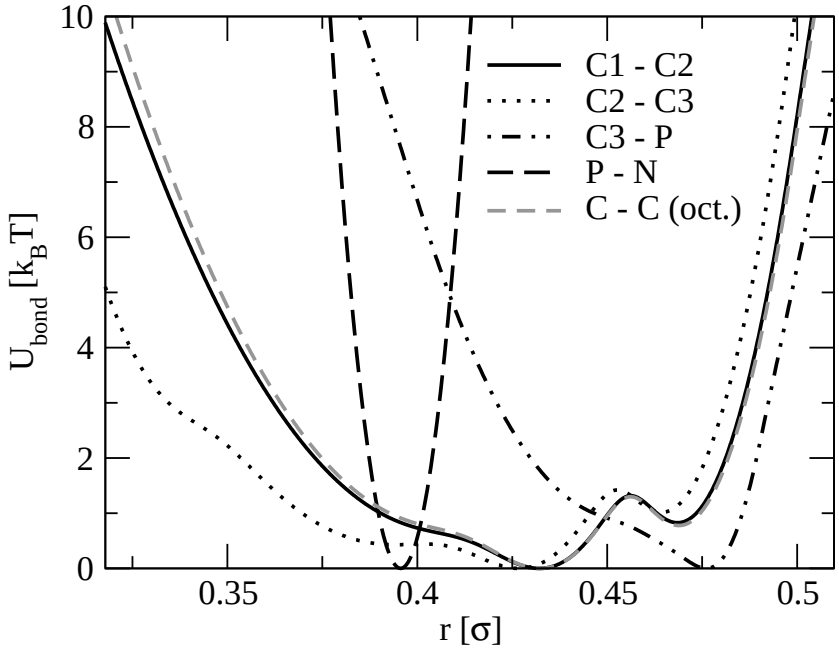
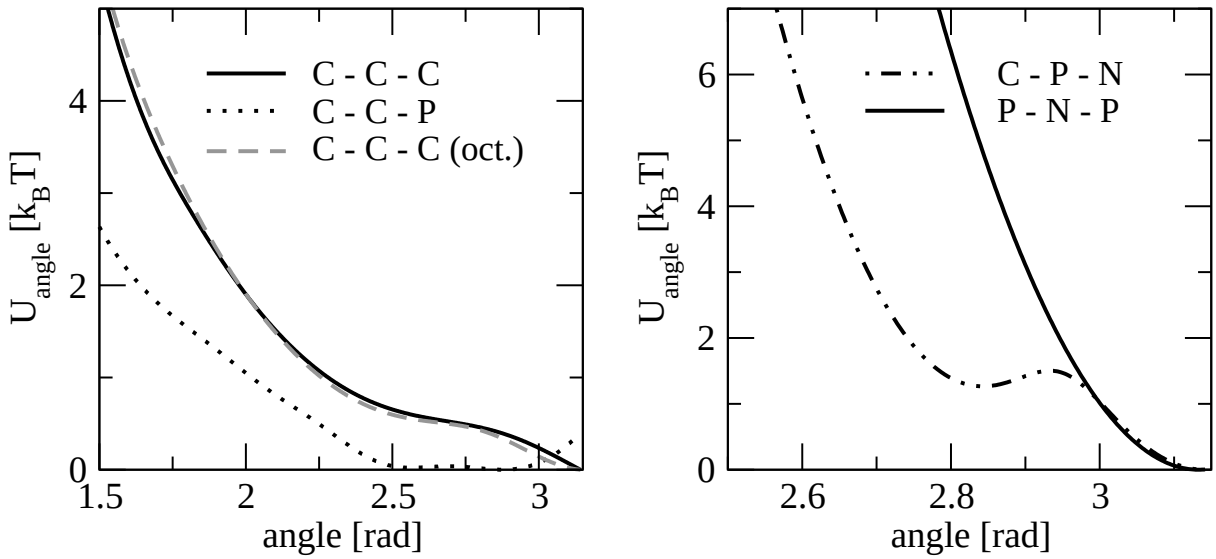
Supplementary material for ”Peter et al.: Classical simulations from the atomistic to the mesoscale and back: coarse graining an azobenzene liquid crystal”



Suppl. Mat. Fig. 1: Tabulated potentials for nonbonded interactions between CG beads determined by iterative Boltzmann inversion (at 400 K). Bead types labeled according to Fig. 1 in paper. Panel a: solid line – C-C interaction parametrized on octadecane melt; dashed line – P-C interactions parametrized on bezene in octadecane mixture. Panels b, c, and d: P-P, P-N and N-N interactions parametrized on azobenzene; solid lines – average-8AB8 FF (see text); dashed lines *trans*-8AB8 FF. Reduced unit length conversion: 1 σ = 8 Å.



Suppl. Mat. Fig. 2: Bond potentials between CG beads in *trans* 8AB8 (black lines) and octadecane (gray dashed line). Bead types are labeled according to Fig. 1 in paper, for 8AB8 C1, C2, and C3 refer to the consecutive beads in the alkoxy tail with C3 being the alkoxy bead adjacent to the P bead. Reduced unit conversion: 1 σ = 8 Å, T = 1.0 corresponds to 400 K.



Suppl. Mat. Fig. 3: Angle potentials between CG beads in *trans* 8AB8 (black lines) and octadecane (gray dashed line). Bead types are labeled according to Fig. 1 in paper. Reduced unit conversion: T = 1.0 corresponds to 400 K.

interaction	K [k$_B$T]	n	p
C-C-C-P (8AB8)	0.4	1	-1
C-C-P-N (8AB8)	0.6	1	-1
C-P-N-P (8AB8)	0.1	1	-1
C-C-C-C (oct.)	0.35	1	-1

Suppl. Mat. Tab. I: Force constant for dihedral potentials between CG beads in *trans* 8AB8 and octadecane (C-C-C-C). Functional form of the (cosine) potential: $U^{CG}(\phi) = K(1+p\cos(n\phi))$. Bead types are labeled according to Fig. 1 in paper. Reduced unit conversion: T = 1.0 corresponds to 400 K.

interaction	ϵ [k$_B$T]	σ_M	α
N - N	0.226	0.618	5.686
P - P	0.2	1.122	3.0
N - P	0.137	0.721	6.468
C - C	0.207	0.704	8.563
P - C	0.096	0.92	4.658
N - C	0.226	0.618	5.686

Suppl. Mat. Tab. II: Parameters for repulsive morse potentials (Equation 6 in paper) used in repulsive-Morse 8AB8 FF. Bead types are labeled according to Fig. 1 in paper. Reduced unit conversion: 1 σ = 8 Å, T = 1.0 corresponds to 400 K.