Development of new coarse-grained models for chromonic liquid crystals: insights from top-down approaches

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Supplementary Information

1. GROMACS topology file containing force field information for the MARTINI TP6EO2M model.

; TP6EO2M_GMX.top

[ defaults ]
; nhbfunc comb-rule gen-pairs fudgeLJ fudgeQQ
1 2 yes 0.5 0.8333
1 1

[ atomtypes ]
; name bond_type mass charge type sigma epsilon Amb
CC CC 24.00000 0.00000 A 0.0 0.0
CO CO 25.00000 0.00000 A 0.0 0.0
AI AI 44.00000 0.00000 A 0.0 0.0
AG AG 31.00000 0.00000 A 0.0 0.0
P4 P4 72.00000 0.00000 A 0.0 0.0
BP4 BP4 72.00000 0.00000 A 0.0 0.0
POL POL 24.0 0.000 A 0.0 0.0
D D 24.0 0.000 A 0.0 0.0

[ nonbond_params ]
; name name fubct 4*e*(s^6) 4*e*(s^12)
P4 P4 1 0.21558E-00 0.23238E-02 ; attractive
BP4 BP4 1 0.21558E-00 0.23238E-02 ; attractive
CC CC 1 0.66375E-01 0.41957E-03 ; 75intermediate, s=0.43
CO CO 1 0.66375E-01 0.41957E-03 ; 75intermediate, s=0.43
AI AI 1 0.85338E-01 0.53946E-03 ; 75almost attractive, s=0.43
AO AO 1 0.85338E-01 0.53946E-03 ; 75almost attractive, s=0.43
P4 BP4 1 0.76824E-00 0.26348E-01 ; supra attractive, s=0.57
P4 CC 1 0.11642E-00 0.12549E-02 ; semi repulsive
P4 CO 1 0.11642E-00 0.12549E-02 ; semi repulsive
P4 AI 1 0.17246E-00 0.18590E-02 ; semi attractive
P4 AO 1 0.17246E-00 0.18590E-02 ; semi attractive
P4 CC 1 0.11642E-00 0.12549E-02 ; semi repulsive
P4 CO 1 0.11642E-00 0.12549E-02 ; semi repulsive
P4 AI 1 0.17246E-00 0.18590E-02 ; semi attractive
P4 AO 1 0.17246E-00 0.18590E-02 ; semi attractive

[ moleculetype ]
; name nrexcl
TP6EO2M 2

[ atoms ]
; resi res atom cgnr charge mass ; qtot bond_type
1 CC 1 MOL CC 1 ; -0.02
2 CC 1 MOL CC 2 ; -0.02
3 CC 1 MOL CC 3 ; -0.02
4 CO 1 MOL CO 4 ; 0.0801
5 CO 1 MOL CO 5 ; 0.0801
6 CO 1 MOL CO 6 ; 0.0801
7 CO 1 MOL CO 7 ; 0.0801
8 CO 1 MOL CO 8 ; 0.0801
9 CO 1 MOL CO 9 ; 0.0801
10 AI 1 MOL AI 10 ; 0.1407
11 AI 1 MOL AI 11 ; -0.007
12 AO 1 MOL AO 12 ; -0.2038
13 AI 1 MOL AI 13 ; 0.1407
14 AI 1 MOL AI 14 ; -0.007
15 AO 1 MOL AO 15 ; -0.2038
16 AI 1 MOL AI 16 ; 0.1407
17 AI 1 MOL AI 17 ; -0.007
[bonds]
1 2 1 0.212 15000 ;core-core
1 3 1 0.212 15000 ;core-core
2 3 1 0.212 15000 ;core-core
2 4 1 0.212 15000 ;core-core
2 5 1 0.212 15000 ;core-core
3 4 1 0.212 15000 ;core-core
3 5 1 0.212 15000 ;core-core
4 5 1 0.212 15000 ;core-core
5 6 1 0.424 15000 ;core-adjcore
6 7 1 0.424 15000 ;core-adjcore
5 9 1 0.424 15000 ;core-adjcore
8 9 1 0.424 15000 ;core-adjcore
7 6 1 0.424 15000 ;core-adjcore
4 6 1 0.424 15000 ;core-adjcore
4 10 1 0.276 10000 ;core-arm
10 11 1 0.328 10000 ;arm-arm
11 12 1 0.282 10000 ;arm-arm
5 13 1 0.276 10000 ;arm-arm
13 14 1 0.328 10000 ;arm-arm
14 15 1 0.282 10000 ;arm-arm
6 25 1 0.276 10000
25 26 1 0.282 10000
26 27 1 0.282 10000
7 22 1 0.276 10000
22 23 1 0.328 10000
23 24 1 0.282 10000
8 19 1 0.276 10000
19 20 1 0.328 10000
20 21 1 0.282 10000
9 16 1 0.276 10000
16 17 1 0.328 10000
17 18 1 0.282 10000
[angles]
14 1 2 180.0 50 ;4 1 2 180.0 50
14 1 3 120.0 50 ;4 1 3 120.0 50
7 1 2 120.0 50 ;7 1 2 120.0 50
7 1 3 120.0 50 ;7 1 3 120.0 50
6 3 1 180.0 50 ;6 3 1 180.0 50
6 2 1 120.0 50 ;6 2 1 120.0 50
8 2 1 120.0 50 ;8 2 1 120.0 50
9 2 1 120.0 50 ;9 2 1 120.0 50
9 2 3 180.0 50 ;9 2 3 180.0 50
3 7 2 180.0 85 ;3 7 2 180.0 85
7 2 2 180.0 85 ;7 2 2 180.0 85
22 23 2 180.0 85 ;22 23 2 180.0 85
22 24 2 180.0 85 ;22 24 2 180.0 85
3 6 2 180.0 85 ;3 6 2 180.0 85
6 25 2 180.0 85 ;6 25 2 180.0 85
6 26 2 180.0 85 ;6 26 2 180.0 85
26 27 2 180.0 85 ;26 27 2 180.0 85
1 4 1 180.0 85 ;1 4 1 180.0 85
4 10 1 180.0 85 ;4 10 1 180.0 85
10 11 2 180.0 85 ;10 11 2 180.0 85
11 12 2 180.0 85 ;11 12 2 180.0 85
1 5 1 180.0 85 ;1 5 1 180.0 85
5 13 1 180.0 85 ;5 13 1 180.0 85
13 14 2 180.0 85 ;13 14 2 180.0 85
14 15 2 180.0 85 ;14 15 2 180.0 85
2 8 19 1 180.0 85 ;2 8 19 1 180.0 85
8 19 20 1 180.0 85 ;8 19 20 1 180.0 85
19 20 1 180.0 85 ;19 20 1 180.0 85
2 9 16 2 180.0 85 ;2 9 16 2 180.0 85
9 16 17 2 180.0 85 ;9 16 17 2 180.0 85
16 17 18 2 180.0 85 ;16 17 18 2 180.0 85
[dihedrals]
15 1 2 9 2 0.0 20.0 ;15 1 2 9 2 0.0 20.0
15 2 3 7 2 0.0 20.0 ;15 2 3 7 2 0.0 20.0
16 3 4 2 0.0 20.0 ;16 3 4 2 0.0 20.0
13 7 22 3 2 180.0 5.0 ;13 7 22 3 2 180.0 5.0
17 22 23 4 2 180.0 2.5 ;17 22 23 4 2 180.0 2.5
13 6 25 6 2 180.0 5.0 ;13 6 25 6 2 180.0 5.0
14 25 26 2 180.0 2.5 ;14 25 26 2 180.0 2.5
14 10 11 2 180.0 5.0 ;14 10 11 2 180.0 5.0
10 11 12 2 180.0 2.5 ;10 11 12 2 180.0 2.5
11 13 14 2 180.0 5.0 ;11 13 14 2 180.0 5.0
13 14 15 2 180.0 2.5 ;13 14 15 2 180.0 2.5
12 19 20 2 180.0 5.0 ;12 19 20 2 180.0 5.0
19 20 21 2 180.0 2.5 ;19 20 21 2 180.0 2.5
19 16 17 2 180.0 5.0 ;19 16 17 2 180.0 5.0

;; 9 16 17 18 2 180.0 2.5
[ dihedrals ]: impropers
; 1 2 3 5 2 0.00 8.0
; 1 2 3 4 2 0.00 8.0
; 2 1 3 9 2 0.00 8.0
; 2 3 1 8 2 0.00 8.0
; 3 2 1 7 2 0.00 8.0
; 3 2 1 6 2 0.00 8.0
; 4 5 3 1 2 0.00 8.0
; 4 5 2 1 2 0.00 8.0
; 8 9 1 2 2 0.00 8.0
; 8 9 3 2 2 0.00 8.0
; 6 7 1 3 2 0.00 8.0
; 6 7 2 3 2 0.00 8.0
[ dihedrals ]: mark
; 4 1 3 6 2 0.00 30.0
; 5 1 2 9 2 0.00 30.0
; 7 3 2 8 2 0.00 30.0
; 1 2 3 4 2 0.00 30.0
; 2 1 3 9 2 0.00 30.0
; 3 1 6 7 2 0.00 30.0
; 3 2 6 7 2 0.00 30.0
; 5 1 2 9 2 0.00 30.0
; 7 3 2 8 2 0.00 30.0
; 1 2 5 4 2 0.00 30.0
; 1 3 4 5 2 0.00 30.0
; 2 1 3 9 2 0.00 30.0
; 2 3 8 9 2 0.00 30.0
[ molecules ]
W 3917
AW 435

;;;;; POLARIZABLE WATER
[ moleculetype ]
; molname nrexcl
W 1
[ atoms ]
; id type resnr residu atom cgnr charge
1 P4 1 W W 1 0
[ moleculetype ]
; molname nrexcl
AW 1
[ atoms ]
; id type resnr residu atom cgnr charge
1 BP4 1 AW AW 1 0
[ system ]
TP6EO2M in water
[ molecules ]
; Compound nmoles
TP6EO2M 10
W 3917
AW 435
2. SAFT fits to thermodynamic data

Figure 1. Enthalpies of mixing (excess enthalpies) of 1,2-dimethoxyethane (EO2) and benzene at 298.15 K. The SAFT model (lines) with fitted interaction of $\epsilon_{EO,Ar} = 323.4$ K to the experimental data (symbols)[1, 2]. Benzene is modelled in the SAFT calculations as a chain, the EO2 model is made of 2 beads fitted to properties of EO4 by Lobanova[3].
Figure 2. Enthalpies of mixing (excess enthalpies) of 2,5,8,11-tetraoxadodecane (EO4) and water at 298.15 K. The SAFT model (lines) with fitted interaction of $\epsilon_{\text{EO,W}} = 465$ K to the experimental data (symbols)[4, 5].
Figure 3. Solubility limit of water in benzene. The experimental data was measured at 1 bar, the SAFT calculations were performed at 5 bar to keep the water model from boiling, which does not significantly influence the solubility. The SAFT model (lines) are with a fitted interaction of $\epsilon_{Ar,W} = 195$ K to the experimental data (symbols)[6–8].
Figure 4. The influence of unfavourable cross-interactions on chromonic stacking. Results are shown for the final revised SAFT model with the same bond lengths as used in the MARTINI model. Up arrows indicate interactions that are less favourable than mixing rules with $k_{ij} = 0$. Equals signs indicate $k_{ij} = 0$. For the case where pure combining rules are used ($k_{ij} = 0$ for all cross-interactions), only monomers and transient self-assembled dimers are seen.

### References

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