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Supplementary Information

Optimisation of the GAFF Force Field to Describe Liquid Crystal Molecules: The Path to a Dramatic Improvement in Transition Temperature Predictions

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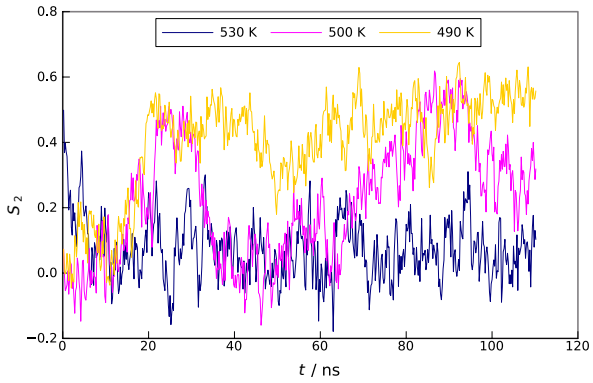

Fig. 1 The time dependence of the orientational order parameter at different temperatures for the GAFF force field using the original GAFF Lennard-Jones potentials and the new torsional parameters from this study.

References

1 C. Caleman, P. J. van Maaren, M. Hong, J. S. Hub, L. T. Costa and D. van der Spoel, *J. Chem. Theory Comp.*, 2012, **8**, 61–74.

2 J. Wang and T. Hou, *J. Chem. Theory Comp.*, 2011, **7**, 2151–2165.

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Table 1 List of the experimental densities and heats of vaporization used to assess GAFF for liquid crystal fragment molecules. (Data taken from Caleman et al.[1] and [a] from Wang & Hou.[2].)

Molecule	Property	T(K)	Experiment	GAFF	% Diff.
Methanoic acid	Density (g/cm^3)	293.15	1.2200	1.3971± 0.0005	+14.5
	Heat of Vaporization (kJ/mol)	293.15	19.82	68.74 ± 0.06	+246.8
Acetic acid[a]	Density (g/cm^3)	298	1.0446	1.1200	+7.2
	Heat of Vaporization (kJ/mol)	298	51.59	56.00	+8.6
Propanoic acid[a]	Density (g/cm^3)	298	0.9882	1.026	+3.8
	Heat of Vaporization (kJ/mol)	298	55.02	60.34	+9.7
Methyl formate	Density (g/cm^3)	293.15	0.9713	1.0512 ± 0.0002	+8.0
	Heat of Vaporization (kJ/mol)	293.15	28.85	38.68 ± 0.03	+34.1
Methylacetate	Density (g/cm^3)	293.15	0.9342	0.9714 ± 0.0002	+4.0
	Heat of Vaporization (kJ/mol)	293.15	32.67	41.57± 0.07	+27.2
Ethenyl acetate	Density (g/cm^3)	298.15	0.9256	0.9790 ± 0.0001	+5.3
	Heat of Vaporization (kJ/mol)	298.15	34.58	43.40 ± 0.02	+25.5
Diethyl carbonate	Density (g/cm^3)	298.15	0.9691	1.0209 ± 0.0002	+5.3
	Heat of Vaporization (kJ/mol)	298.15	41.1	60.79 ± 0.09	+47.9
Methyl benzoate	Density (g/cm^3)	298.15	1.0840	1.1113 ± 0.0002	+2.5
	Heat of Vaporization (kJ/mol)	298.15	55.57	64.21 ± 0.03	+15.6
Heterocyclic compounds					
1-H -pyrrole	Density (g/cm^3)	293.15	0.9698	1.0201± 0.0003	+ 5.2
	Heat of Vaporization (kJ/mol)	293.15	45.7	52.93 ± 0.05	+15.8
1,3-dioxolane	Density (g/cm^3)	293.15	1.0600	1.1223 ± 0.0002	+5.9
	Heat of Vaporization (kJ/mol)	293.15	35.80	43.45 ± 0.02	+21.4
Morpholine	Density (g/cm^3)	293.15	1.0005	1.0880 ± 0.0003	+ 8.8
	Heat of Vaporization (kJ/mol)	293.15	45.32	59.56 ± 0.40	+31.4
Pyrimidine	Density (g/cm^3)	298.15	1.0164	1.1160 ± 0.0003	+ 9.8
	Heat of Vaporization (kJ/mol)	298.15	49.81	50.47± 0.03	+1.3
Furan	Density (g/cm^3)	298.15	0.9313	0.9660 ± 0.0002	+3.7
	Heat of Vaporization (kJ/mol)	298.15	27.46	30.33 ± 0.03	+10.5

Table 2 Comparison of ACD Labs calculated densities and experimental values for small aromatic compounds.

Molecule	ACD(Labs-software) / g cm^{-3} (293 K)	Exp. / g cm^{-3} (293 K)	% error
Phenylacetate	1.071 ± 0.06	1.0739	-0.27
Butylbenzene	0.864 ± 0.06	0.8670	-0.34
Furan	0.942 ± 0.06	0.9403	+0.18
Benzene	0.873 ± 0.06	0.8790	-0.68
m-cresol	1.038 ± 0.06	1.0338	+0.41