Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Molecular Dynamics Simulations of Aggregation and Viscosity Properties of Model Asphaltene Molecules Containing Polycyclic Hydrocarbon Nucleus with Toluene Additive under Shear Interactions

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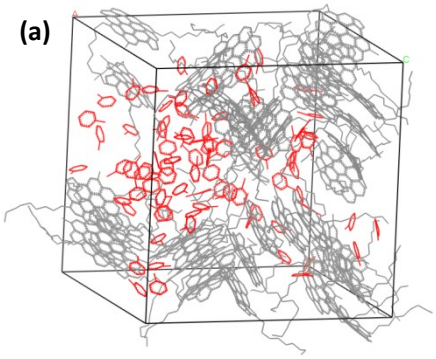
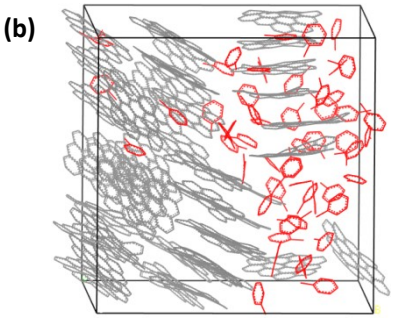
Table S1 Calculated dipole moment (in unit of Debye) of three types of asphaltene molecules. [a]Calculated by Gaussian 09 package; [b]Calculated based on PCFF force field parameters.

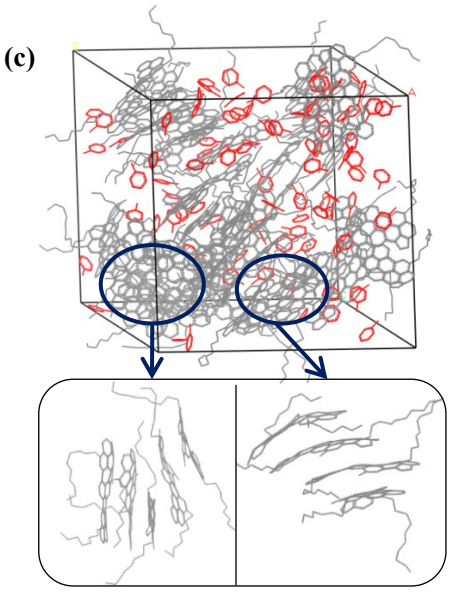
	PAHs-I	PAHs-L	PAHs-O	PAHs-T	PAHs-Y
Type-0	0.03[a] / 0.05[b]	1.37[a] / 0.30[b]	0.10[a] /0.02[b]	0.22[a] / 0.03[b]	0.10[a] / 0.17[b]
Type-1	2.94[a] / 2.55[b]	0.77[a] / 0.20[b]	1.53[a] /0.03[b]	4.17[a] / 0.02[b]	3.30[a] / 0.36[b]
Type-2	8.67[a] / 6.51[b]	11.22[a] / 3.46[b]	10.99[a] /1.77[b]	6.46[a] / 9.55[b]	7.25[a] / 8.06[b]



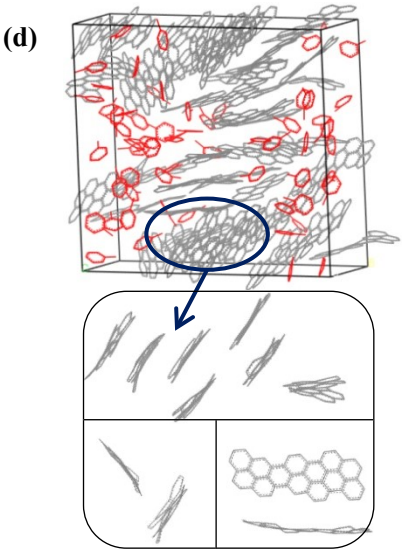
O1, 20Wt% toluene



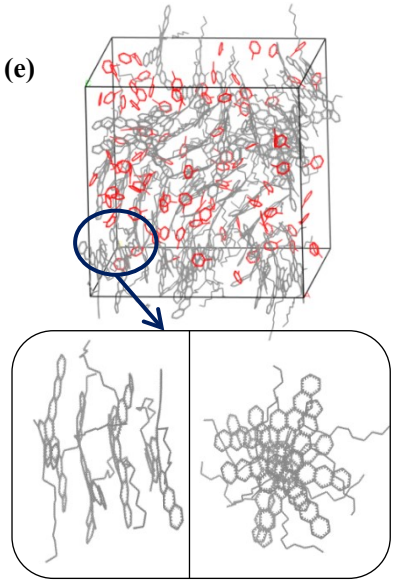
O0, 20Wt% toluene

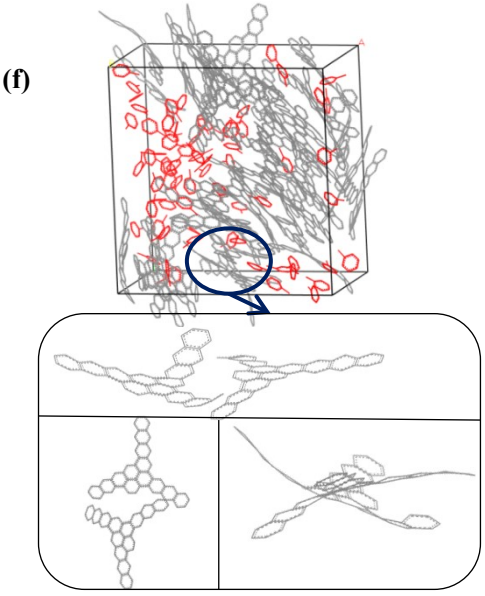


I1, 20Wt% toluene



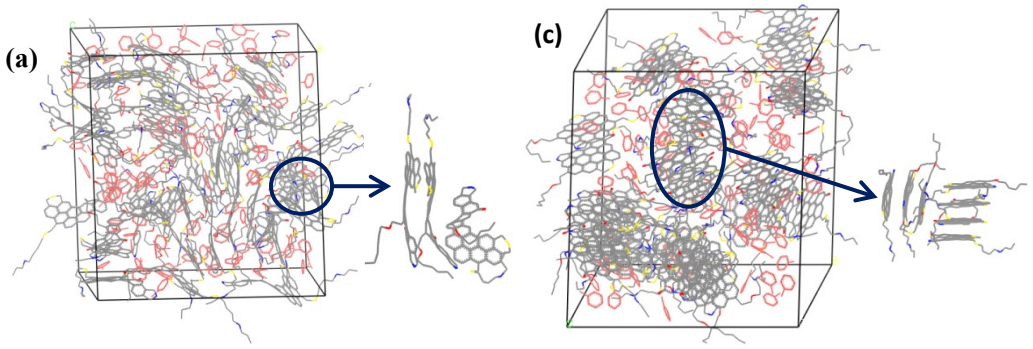
I0, 20Wt% toluene



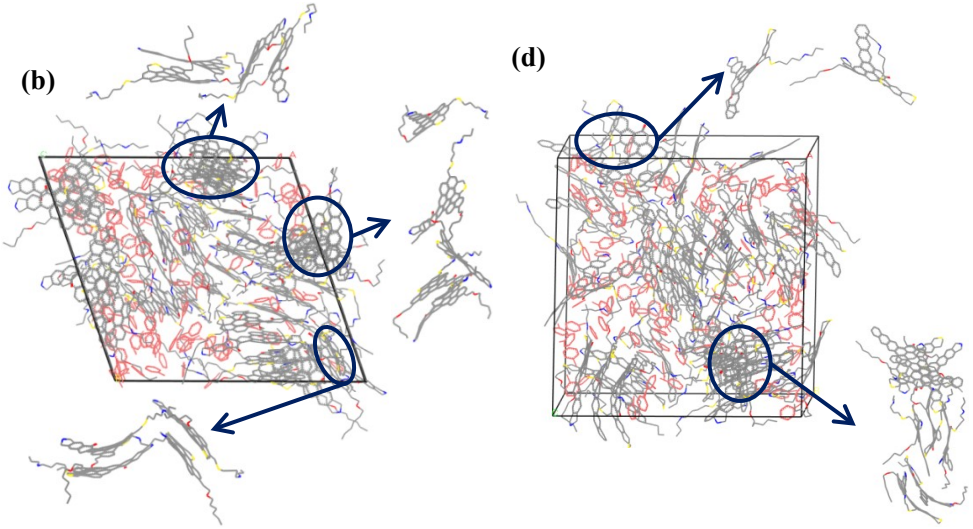


Y1, 20Wt% toluene Y0, 20Wt% toluene

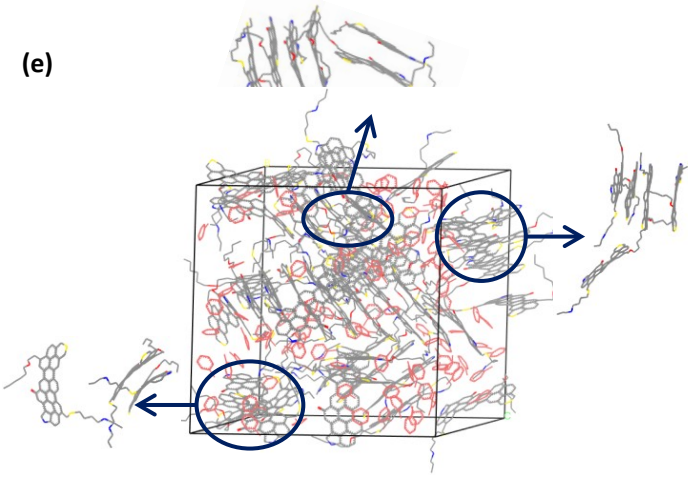
Figure S1 Snapshot structures of (a) PAHs-O1, (b) PAHs-O0, (c) PAHs-L1, (d) PAHs-L0, (e) PAHs-L1, and (y) PAHs-L0 type asphaltene molecular aggregates in the presence of 20 wt% toluene additive. Red lines shows the toluene molecules, grey lines represent the carbon atom skeletons. H atoms are omitted.



L2, 20Wt% toluene O2, 20Wt% toluene



T2, 20Wt% toluene Y2, 20Wt% toluene



I2, 20Wt% toluene

Figure S2 Snapshot structures of (a) PAHs-L2, (b) PAHs-O2, (c) PAHs-T2, (d) PAHs-Y2, and (e)

PAHs-I2 asphaltene molecular aggregates in the presence of 20 wt% toluene additive. Red lines shows the toluene molecules, grey lines represent the carbon atom skeletons. H atoms are omitted.