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

Supplementary Information

for

Characterizing structure and properties of dry and wet polyethylene glycol using multi-scale simulations

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The functional forms in order to compute the DPD interaction parameters are given in the main manuscript. In Table S1, we tabulate the Flory-Huggins parameters, dimensionless number densities and the computed DPD interaction parameters. These values, together with the physical length scale of DPD are used to compute the pair-wise interaction parameters. The physical DPD length scales correspond to 6.62 Å and 5.75 Å, respectively for dry and wet PEG, which are computed by employing the average volume computation as detailed in reference [1]. Therefore, there are two sets of DPD interaction parameters (dry PEG in Table S1 and wet PEG in Table S2) as a result of the different physical length scales of DPD for the dry and wet conditions. In DPD, the magnitude of the repulsion is dependent on the value of the χ_{ij} parameter rather than the DPD parameter itself. For a more detailed information, the reader is referred to our previous work on the DPD parameterization [2].

A harmonic bond potential is set for the bonded interactions of H-L, L-L and L-K. The spring constant is set as 50 kT/r_{DPD}^2 and the bond lengths are set to 0.50 r_{DPD}. Angle potential contribution is neglected in the DPD simulations.

Table S1. Computed Flory-Huggins parameters χ_{ij} and the pairwise DPD interaction parameters a_{ij} of the coarse-grained beads of dry PEG. Values in parentheses indicate the solubility parameters δ_i in dimensions $(\mathrm{J/cm^3})^{0.5}$ and the dimensionless number densities of beads ρ_i obtained by $\rho_i = \rho_{i,\mathrm{liquid}}/M_{\mathrm{W},i}$, in rows and columns, respectively.

χ_{ij}	**L (or H) (δ_i = 25.09)**	**K (δ_i = 31.86)**
a_{ij}		
L (or H) (ρ_i = 0.0103)	0.00	1.12
K (ρ_i = 0.0112)	25.10 27.14	0.00 20.89

Table S2. Computed Flory-Huggins parameters χ_{ij} and the pairwise DPD interaction parameters a_{ij} of the coarse-grained beads of wet PEG. Values in parentheses indicate the solubility parameters δ_i in dimensions $(J/cm^3)^{0.5}$ and the dimensionless number densities of beads ρ_i obtained by $\rho_i = \rho_{i,\text{liquid}}/M_{W,i}$, in rows and columns, respectively.

χ_{ij} / a_{ij}	**L (or H) (δ_i = 25.09)**	**K (δ_i = 31.86)**	**W (δ_i = 47.00)**
L (or H) (ρ_i = 0.0103)	0.00 61.21	1.12	11.79
K (ρ_i = 0.0112)	57.69	0.00 51.15	5.63
W (ρ_i = 0.0334)	44.91	29.93	0.00 4.76

The hydrogen bonds are modeled between PEG beads and water bead with the Morse potential. The Morse potential parameters used in the simulations are taken from a previous work for the corresponding molar fraction of PEG beads [3] (x_{PEG} = 0.50) and tabulated in Table S3.

Table S3. Hydrogen bond interaction D_0 and the hydrogen bond equilibrium distance r_0 values used in the DPD simulations.

Morse parameters	**L**	**H**	**K**
$\boldsymbol{D_0}$ **[$\boldsymbol{k_BT}$]**	10.91	7.76	8.82
$\boldsymbol{r_0}$ **[$\boldsymbol{r_{DPD}}$]**	0.84	0.84	0.84

References

1. G. Kacar, E. A. J. F. Peters and G. de With, *Soft Matter*, 2013, **9**, 5785-5793.
2. G. Kacar, E. A. J. F. Peters and G. de With, *Epl-Europhys Lett*, 2013, **102**.
3. G. Kacar, *Chemical Physics Letters*, 2017, **690**, 133-139.