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

SUPPORTING INFORMATION

for

Hierarchical multi-scale simulations of adhesion at polymer-metal interfaces: Dry and wet conditions

by

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The input parameters for the DPD simulations, such as the number density of beads $\rho_{i,pure}$ in a liquid made up only of beads of type *i*, the solubility parameters δ and the pair-wise interactions a_{ij} are presented in this Supporting Information. We obtained the solubility parameter δ for each bead type by taking molar group contributions into consideration as given for the van Krevelen-Hoftyzer approach [1], calculated by the Molecular Modeling Pro software [2].

Table S1. The non-bonded DPD interaction parameters used in simulations. Dashes indicate no interaction computed between the aromatic (bead B) and aliphatic (bead L) rings while W indicates the water beads.

a_{ij}/k_BT	A	B	L	C	D	J	A′	D′	D″	W	Al
A	27.8	49.8	50.1	33.2	23.3	33.9	28.6	20.2	32.8	166.9	6.2
B	49.8	62.0	–	63.0	19.3	64.3	39.2	36.0	59.8	61.3	13.2
L	50.1	–	88.5	59.4	25.9	60.5	45.5	35.5	59.4	92.2	35.2
C	33.2	63.0	59.4	35.5	36.3	35.9	38.4	26.7	37.0	195.3	82.1
D	23.3	19.3	25.9	36.3	5.8	37.4	12.8	17.4	29.6	158.7	8.7
J	33.9	64.3	60.5	35.9	37.4	36.4	39.4	27.4	37.6	196.5	23.0
A′	28.6	39.2	45.5	38.4	12.8	39.4	22.7	19.8	35.3	122.7	7.0
D′	20.2	36.0	35.5	26.7	17.4	27.4	19.8	14.2	24.8	192.9	9.2
D″	32.8	59.8	59.4	37.0	29.6	37.6	35.3	24.8	37.7	168.5	85.0
W	166.9	61.3	92.2	195.3	158.7	196.5	122.7	192.9	168.5	1.8	4.1
Al	6.2	13.2	35.2	82.1	8.7	23.0	7.0	9.2	85.0	4.1	0.0

Table S2. Liquid mass densities ($\rho_{m,i}$), molecular weights (M_W), pure component number densities ($\rho_{i,\text{pure}}$), and solubility parameters (δ_i).

Type of Bead	$\rho_{m,i}$ (g/cm^3)	M_W (g/mol)	$\rho_{i,\text{pure}} = \rho_{m,i}/M_W$ (Å^{-3})	δ_i ((J/cm^3)$^{0.5}$)
A	0.938	58.07	0.0097	20.02
B	1.034	94.11	0.0066	29.08
C	0.634	44.09	0.0087	16.11
L	0.926	100.16	0.0056	22.41
D	1.034	31.05	0.0200	27.74
J	0.654	46.07	0.0085	15.83
A′	0.821	46.07	0.0107	25.09
D′	1.001	45.08	0.0133	21.64
D″	0.825	59.11	0.0084	18.07
W	1.000	18.00	0.0334	47.70

Table S3. Bond potential parameters of the equation $V_{B,ij}(r) = k_{ij}(r - r_{0,ij})^2$ used in the simulations.

Bond type	$k_{ij}\,[kT/r_{DPD}^2]$	$r_{0,ij}$ $[r_{\text{DPD}}]$	Bond type	$k_{ij}\,[kT/r_{DPD}^2]$	$r_{0,ij}$ $[r_{\text{DPD}}]$
A-B	500.0	0.65	A'-D'	500.0	0.44
A-L	500.0	0.70	A'-D"	500.0	0.44
B-C	500.0	0.54	A'-B	500.0	0.65
L-C	500.0	0.56	A'-L	500.0	0.70
D-J	500.0	0.45	D'-J	500.0	0.45
A'-D	500.0	0.44	D"-J	500.0	0.45

Table S4. Angle potential parameters of the equation $V_{A,ijk}(\theta) = k_{ijk}(\theta - \theta_{0,ijk})^2$ used in the simulations.

Angle type	k_{ijk} [kT/rad^2]	$\theta_{0,ijk}$ [deg]
A-B-C	50.0	170.6
B-C-B	50.0	94.7
D-J-J	50.0	106.7
A-L-C	50.0	94.6
L-C-L	50.0	75.5
A'-B-C	50.0	170.6
D'-J-J	50.0	106.7
A'-L-C	50.0	94.6
D''-J-J	50.0	106.7

References

1. D. W. van Krevelen, *Properties of Polymers*, Elsevier, Amsterdam, 1990.
2. *Molecular Modeling Pro*, (1992) Norgwyn Montgomery Software Inc.