Supporting Information for MoSDeF, a Python Framework Enabling Large-Scale Computational Screening of Soft Matter: Application to Chemistry-Property Relationships in Lubricating Monolayer Films

Andrew Z. Summers,[†,‡] Justin B. Gilmer,[¶,‡] Christopher R. Iacovella,[†,‡] Peter T. Cummings,[†,‡] and Clare McCabe[*,†,‡,§]

†*Department of Chemical and Biomolecular Engineering, Vanderbilt University, Nashville, TN*

‡*Center for Multiscale Modeling and Simulation, Vanderbilt University, Nashville, TN*

¶*Interdisciplinary Program for Materials Science, Vanderbilt University, Nashville, TN*

§*Department of Chemistry, Vanderbilt University, Nashville, TN*

E-mail: c.mccabe@vanderbilt.edu

Details on construction of silica surfaces

Silica surfaces are carved from an amorphous silica bulk, as in our previous work.[1] Bulk silica was generated by putting a stoichiometric ratio of Si and O into a 5nm x 5nm x 5nm box at a density of 2.2g/mL. The procedure of Litton and Garofalini[2] was then followed, whereby the system was heated to 10000K, followed by a step-wise annealing through intermediate temperatures of 8000, 6000, 4000, 3000, 2000, and 1000K before ending at 300K. The ReaxFF force field[3] was used to model silicaon and oxygen bonding, and parameters from Fogarty et al. were used.[4] Surfaces were then carved from the amorphous silica bulk using an analytical approach to achieve a hydroxyl density of 5 OH/nm^2 by bridging neighboring surface oxygens,[5,6] using the mBuild library;[7,8] the source code is available online: `https://github.com/PTC-CMC/atools/blob/master/atools/recipes/silica_interface_carve.py`. This approach yields amorphous silica surfaces that lack in-plane attachment site order (which is not the case for crystalline surface models) and feature an

atomic scale surface roughness of roughly 0.11nm, similar to values obtained in previous work using synthesis mimetic simulations to mimic the "piranha" treatment of surfaces typical in experiment.[9]

Summary of uniform films as a function of backbone length

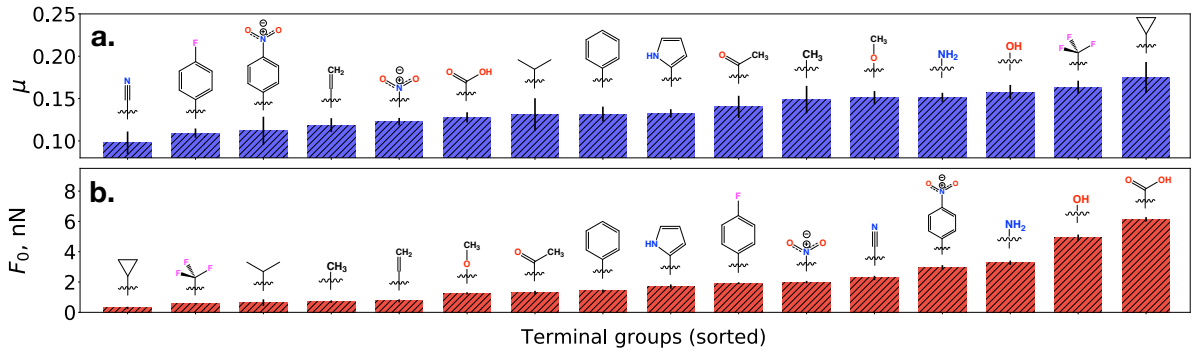

Figure S1: Bar graphs displaying a.) coefficient of friction and b.) adhesive force as a function of terminal group chemistry for chemically-identical monolayer systems with a backbone chain length of 17 carbons.

Table S1: Mean and standard deviation of the coefficient of friction (COF) of uniform monolayer films at various backbone chain lengths.

System	**c5**	**c8**	**c11**	**c14**	**c17**
acetyl - acetyl	0.162 ± 0.008	0.159 ± 0.013	0.138 ± 0.007	0.138 ± 0.010	0.140 ± 0.013
amino - amino	0.194 ± 0.019	0.180 ± 0.004	0.152 ± 0.012	0.148 ± 0.010	0.151 ± 0.005
carboxyl - carboxyl	0.164 ± 0.012	0.162 ± 0.018	0.142 ± 0.012	0.139 ± 0.010	0.128 ± 0.006
cyano - cyano	0.140 ± 0.009	0.128 ± 0.010	0.098 ± 0.017	0.099 ± 0.018	0.098 ± 0.014
cyclopropyl - cyclopropyl	0.179 ± 0.017	0.178 ± 0.015	0.171 ± 0.006	0.165 ± 0.008	0.175 ± 0.018
ethylene - ethylene	0.172 ± 0.023	0.135 ± 0.009	0.129 ± 0.011	0.122 ± 0.006	0.119 ± 0.008
fluorophenyl - fluorophenyl	0.137 ± 0.007	0.130 ± 0.007	0.117 ± 0.008	0.112 ± 0.008	0.109 ± 0.005
hydroxyl - hydroxyl	0.208 ± 0.014	0.186 ± 0.018	0.174 ± 0.012	0.174 ± 0.006	0.158 ± 0.008
isopropyl - isopropyl	0.171 ± 0.017	0.152 ± 0.009	0.139 ± 0.013	0.141 ± 0.011	0.131 ± 0.019
methoxy - methoxy	0.173 ± 0.016	0.159 ± 0.007	0.158 ± 0.008	0.154 ± 0.008	0.151 ± 0.008
methyl - methyl	0.198 ± 0.018	0.178 ± 0.011	0.165 ± 0.011	0.154 ± 0.015	0.149 ± 0.016
nitro - nitro	0.153 ± 0.013	0.142 ± 0.010	0.129 ± 0.011	0.130 ± 0.009	0.123 ± 0.004
nitrophenyl - nitrophenyl	0.129 ± 0.013	0.133 ± 0.017	0.126 ± 0.010	0.134 ± 0.018	0.112 ± 0.017
perfluoromethyl - perfluoromethyl	0.169 ± 0.014	0.177 ± 0.006	0.167 ± 0.005	0.170 ± 0.012	0.163 ± 0.008
phenyl - phenyl	0.154 ± 0.010	0.132 ± 0.002	0.129 ± 0.009	0.131 ± 0.012	0.132 ± 0.009
pyrrole - pyrrole	0.170 ± 0.020	0.150 ± 0.007	0.146 ± 0.009	0.130 ± 0.011	0.133 ± 0.005

Table S2: Mean and standard deviation of the adhesive force (F_0, nN) of uniform monolayer films at various backbone chain lengths.

System	**c5**	**c8**	**c11**	**c14**	**c17**
acetyl - acetyl	1.423 ± 0.215	1.609 ± 0.212	1.566 ± 0.097	1.443 ± 0.128	1.292 ± 0.129
amino - amino	3.071 ± 0.240	3.238 ± 0.118	3.704 ± 0.124	3.328 ± 0.050	3.274 ± 0.142
carboxyl - carboxyl	5.221 ± 0.210	6.342 ± 0.163	6.387 ± 0.237	6.189 ± 0.189	6.139 ± 0.146
cyano - cyano	3.214 ± 0.124	3.195 ± 0.179	3.063 ± 0.188	2.362 ± 0.229	2.266 ± 0.141
cyclopropyl - cyclopropyl	0.907 ± 0.163	0.824 ± 0.072	0.694 ± 0.192	0.530 ± 0.091	0.294 ± 0.075
ethylene - ethylene	0.741 ± 0.549	1.050 ± 0.132	1.012 ± 0.071	0.739 ± 0.085	0.755 ± 0.099
fluorophenyl - fluorophenyl	2.410 ± 0.130	1.857 ± 0.107	2.034 ± 0.101	1.751 ± 0.117	1.925 ± 0.061
hydroxyl - hydroxyl	3.950 ± 0.443	5.201 ± 0.093	5.325 ± 0.191	5.068 ± 0.149	4.911 ± 0.219
isopropyl - isopropyl	0.443 ± 0.544	0.712 ± 0.232	0.819 ± 0.123	0.728 ± 0.040	0.638 ± 0.221
methoxy - methoxy	1.288 ± 0.286	1.507 ± 0.065	1.380 ± 0.081	1.238 ± 0.058	1.248 ± 0.074
methyl - methyl	0.527 ± 0.428	0.956 ± 0.146	0.974 ± 0.094	0.848 ± 0.106	0.702 ± 0.084
nitro - nitro	2.383 ± 0.107	2.533 ± 0.105	2.355 ± 0.233	2.147 ± 0.108	1.995 ± 0.080
nitrophenyl - nitrophenyl	3.833 ± 0.122	3.087 ± 0.233	3.116 ± 0.172	2.732 ± 0.237	2.962 ± 0.149
perfluoromethyl - perfluoromethyl	0.780 ± 0.108	0.915 ± 0.065	0.837 ± 0.135	0.760 ± 0.104	0.566 ± 0.043
phenyl - phenyl	1.591 ± 0.136	1.479 ± 0.072	1.560 ± 0.116	1.321 ± 0.107	1.412 ± 0.091
pyrrole - pyrrole	2.033 ± 0.185	2.150 ± 0.182	2.050 ± 0.079	1.990 ± 0.121	1.700 ± 0.140

Table S3: Mean and standard deviation of the nematic order parameter($S2$) of uniform monolayer films at various backbone chain lengths and normal force 5 nN.

System	**c5**	**c8**	**c11**	**c14**	**c17**
acetyl - acetyl	0.713 ± 0.024	0.810 ± 0.033	0.902 ± 0.022	0.939 ± 0.015	0.959 ± 0.014
amino - amino	0.654 ± 0.033	0.816 ± 0.027	0.904 ± 0.029	0.943 ± 0.012	0.961 ± 0.011
carboxyl - carboxyl	0.742 ± 0.025	0.863 ± 0.031	0.923 ± 0.018	0.958 ± 0.010	0.971 ± 0.009
cyano - cyano	0.699 ± 0.036	0.825 ± 0.030	0.889 ± 0.025	0.936 ± 0.015	0.959 ± 0.009
cyclopropyl - cyclopropyl	0.743 ± 0.027	0.812 ± 0.018	0.893 ± 0.022	0.933 ± 0.024	0.955 ± 0.014
ethylene - ethylene	0.702 ± 0.029	0.819 ± 0.020	0.901 ± 0.023	0.933 ± 0.014	0.955 ± 0.011
fluorophenyl - fluorophenyl	0.782 ± 0.031	0.823 ± 0.019	0.891 ± 0.013	0.907 ± 0.015	0.942 ± 0.013
hydroxyl - hydroxyl	0.656 ± 0.013	0.842 ± 0.029	0.911 ± 0.014	0.949 ± 0.009	0.966 ± 0.007
isopropyl - isopropyl	0.751 ± 0.018	0.810 ± 0.021	0.862 ± 0.024	0.914 ± 0.019	0.951 ± 0.024
methoxy - methoxy	0.681 ± 0.027	0.815 ± 0.028	0.897 ± 0.030	0.938 ± 0.012	0.963 ± 0.011
methyl - methyl	0.695 ± 0.020	0.796 ± 0.033	0.892 ± 0.022	0.935 ± 0.017	0.955 ± 0.015
nitro - nitro	0.679 ± 0.034	0.800 ± 0.035	0.890 ± 0.024	0.931 ± 0.018	0.960 ± 0.012
nitrophenyl - nitrophenyl	0.814 ± 0.026	0.860 ± 0.020	0.895 ± 0.016	0.914 ± 0.006	0.932 ± 0.009
perfluoromethyl - perfluoromethyl	0.714 ± 0.027	0.801 ± 0.023	0.878 ± 0.029	0.930 ± 0.014	0.958 ± 0.013
phenyl - phenyl	0.778 ± 0.035	0.828 ± 0.015	0.881 ± 0.021	0.931 ± 0.012	0.946 ± 0.011
pyrrole - pyrrole	0.758 ± 0.029	0.868 ± 0.027	0.921 ± 0.012	0.949 ± 0.014	0.972 ± 0.006

Table S4: Mean and standard deviation of the nematic order parameter($S2$) of uniform monolayer films at various backbone chain lengths and normal force 15 nN.

System	**c5**	**c8**	**c11**	**c14**	**c17**
acetyl - acetyl	0.701 ± 0.034	0.800 ± 0.035	0.889 ± 0.029	0.938 ± 0.013	0.959 ± 0.011
amino - amino	0.643 ± 0.025	0.814 ± 0.028	0.894 ± 0.037	0.937 ± 0.010	0.961 ± 0.011
carboxyl - carboxyl	0.721 ± 0.031	0.854 ± 0.025	0.915 ± 0.024	0.951 ± 0.011	0.968 ± 0.009
cyano - cyano	0.686 ± 0.032	0.819 ± 0.024	0.887 ± 0.022	0.926 ± 0.019	0.950 ± 0.014
cyclopropyl - cyclopropyl	0.736 ± 0.030	0.811 ± 0.018	0.893 ± 0.031	0.933 ± 0.021	0.955 ± 0.012
ethylene - ethylene	0.711 ± 0.033	0.818 ± 0.029	0.892 ± 0.030	0.918 ± 0.018	0.946 ± 0.015
fluorophenyl - fluorophenyl	0.793 ± 0.032	0.829 ± 0.027	0.900 ± 0.016	0.894 ± 0.005	0.932 ± 0.017
hydroxyl - hydroxyl	0.645 ± 0.018	0.837 ± 0.026	0.905 ± 0.015	0.943 ± 0.010	0.962 ± 0.009
isopropyl - isopropyl	0.727 ± 0.030	0.809 ± 0.015	0.867 ± 0.024	0.909 ± 0.017	0.945 ± 0.021
methoxy - methoxy	0.684 ± 0.025	0.817 ± 0.032	0.891 ± 0.031	0.936 ± 0.012	0.957 ± 0.010
methyl - methyl	0.677 ± 0.032	0.807 ± 0.038	0.887 ± 0.017	0.934 ± 0.015	0.950 ± 0.015
nitro - nitro	0.670 ± 0.038	0.797 ± 0.036	0.894 ± 0.023	0.936 ± 0.015	0.960 ± 0.013
nitrophenyl - nitrophenyl	0.824 ± 0.022	0.861 ± 0.014	0.885 ± 0.015	0.916 ± 0.011	0.933 ± 0.011
perfluoromethyl - perfluoromethyl	0.698 ± 0.031	0.815 ± 0.030	0.869 ± 0.025	0.914 ± 0.027	0.950 ± 0.013
phenyl - phenyl	0.779 ± 0.034	0.827 ± 0.021	0.894 ± 0.023	0.917 ± 0.017	0.946 ± 0.011
pyrrole - pyrrole	0.758 ± 0.036	0.870 ± 0.030	0.912 ± 0.016	0.946 ± 0.016	0.967 ± 0.009

Table S5: Mean and standard deviation of the nematic order parameter($S2$) of uniform monolayer films at various backbone chain lengths and normal force 25 nN.

System	**c5**	**c8**	**c11**	**c14**	**c17**
acetyl - acetyl	0.700 ± 0.035	0.803 ± 0.030	0.887 ± 0.022	0.933 ± 0.021	0.952 ± 0.020
amino - amino	0.635 ± 0.032	0.807 ± 0.030	0.888 ± 0.026	0.933 ± 0.010	0.954 ± 0.011
carboxyl - carboxyl	0.722 ± 0.026	0.847 ± 0.030	0.922 ± 0.020	0.953 ± 0.011	0.964 ± 0.010
cyano - cyano	0.682 ± 0.036	0.819 ± 0.035	0.880 ± 0.023	0.920 ± 0.020	0.946 ± 0.018
cyclopropyl - cyclopropyl	0.732 ± 0.031	0.819 ± 0.019	0.886 ± 0.032	0.917 ± 0.022	0.945 ± 0.019
ethylene - ethylene	0.704 ± 0.039	0.817 ± 0.036	0.890 ± 0.026	0.909 ± 0.026	0.942 ± 0.015
fluorophenyl - fluorophenyl	0.793 ± 0.037	0.828 ± 0.026	0.896 ± 0.016	0.902 ± 0.015	0.922 ± 0.022
hydroxyl - hydroxyl	0.640 ± 0.019	0.830 ± 0.033	0.908 ± 0.020	0.944 ± 0.014	0.959 ± 0.010
isopropyl - isopropyl	0.713 ± 0.036	0.814 ± 0.023	0.867 ± 0.021	0.911 ± 0.028	0.939 ± 0.033
methoxy - methoxy	0.688 ± 0.039	0.811 ± 0.034	0.884 ± 0.027	0.926 ± 0.008	0.957 ± 0.012
methyl - methyl	0.669 ± 0.034	0.812 ± 0.033	0.884 ± 0.024	0.932 ± 0.023	0.946 ± 0.015
nitro - nitro	0.673 ± 0.037	0.796 ± 0.030	0.888 ± 0.019	0.926 ± 0.019	0.958 ± 0.012
nitrophenyl - nitrophenyl	0.825 ± 0.018	0.863 ± 0.014	0.885 ± 0.015	0.913 ± 0.016	0.930 ± 0.014
perfluoromethyl - perfluoromethyl	0.695 ± 0.033	0.814 ± 0.027	0.879 ± 0.024	0.911 ± 0.018	0.942 ± 0.013
phenyl - phenyl	0.786 ± 0.036	0.827 ± 0.023	0.882 ± 0.025	0.916 ± 0.017	0.943 ± 0.016
pyrrole - pyrrole	0.770 ± 0.043	0.866 ± 0.034	0.913 ± 0.012	0.941 ± 0.019	0.962 ± 0.013

Summary of chemically dissimilar films and model predictions

Table S6: Mean and standard deviation of the coefficient of friction (COF) and adhesive force (F_0, nN) of chemically dissimilar films with c17 backbone length. Predictions from the models are also provided, representing the mean and standard deviation of the 5 models.

System	COF Calc.	COF Pred.	F_o Calc. (nN)	F_o Pred. (nN)
acetyl-acetyl	0.147 ± 0.015	0.137 ± 0.003	1.467 ± 0.188	1.642 ± 0.307
acetyl-carboxyl	0.145 ± 0.005	0.137 ± 0.003	3.382 ± 0.150	3.070 ± 0.254
acetyl-fluorophenyl	0.121 ± 0.011	0.125 ± 0.002	1.448 ± 0.202	1.587 ± 0.102
acetyl-hydroxyl	0.150 ± 0.010	0.147 ± 0.001	2.171 ± 0.176	2.562 ± 0.332
acetyl-isopropyl	0.132 ± 0.008	0.132 ± 0.001	0.749 ± 0.141	0.743 ± 0.015
acetyl-methyl	0.137 ± 0.010	0.137 ± 0.001	0.819 ± 0.106	0.772 ± 0.038
acetyl-nitro	0.137 ± 0.005	0.134 ± 0.004	1.683 ± 0.124	1.892 ± 0.146
acetyl-perfluoromethyl	0.150 ± 0.005	0.143 ± 0.003	0.677 ± 0.045	0.695 ± 0.029
amino-amino	0.165 ± 0.022	0.151 ± 0.001	3.323 ± 0.252	3.631 ± 0.348
amino-carboxyl	0.139 ± 0.012	0.139 ± 0.001	7.942 ± 0.140	5.360 ± 1.361
amino-fluorophenyl	0.131 ± 0.005	0.133 ± 0.001	1.978 ± 0.118	1.696 ± 0.208
amino-hydroxyl	0.154 ± 0.012	0.154 ± 0.001	4.300 ± 0.111	3.664 ± 0.313
amino-isopropyl	0.136 ± 0.010	0.140 ± 0.001	0.758 ± 0.105	0.745 ± 0.012
amino-methyl	0.152 ± 0.011	0.149 ± 0.002	0.732 ± 0.144	0.773 ± 0.020
amino-nitro	0.137 ± 0.005	0.137 ± 0.001	2.629 ± 0.132	3.160 ± 0.435
amino-perfluoromethyl	0.157 ± 0.016	0.152 ± 0.003	0.832 ± 0.169	0.751 ± 0.050
carboxyl-carboxyl	0.147 ± 0.018	0.136 ± 0.005	6.055 ± 0.470	5.594 ± 0.239
carboxyl-cyano	0.112 ± 0.010	0.115 ± 0.003	6.251 ± 0.159	3.965 ± 0.928
carboxyl-cyclopropyl	0.136 ± 0.030	0.135 ± 0.001	0.471 ± 0.148	0.580 ± 0.012
carboxyl-ethylene	0.106 ± 0.011	0.115 ± 0.002	0.993 ± 0.102	1.032 ± 0.013
carboxyl-fluorophenyl	0.124 ± 0.012	0.123 ± 0.001	2.005 ± 0.127	1.880 ± 0.075
carboxyl-hydroxyl	0.147 ± 0.014	0.147 ± 0.001	7.335 ± 0.060	5.952 ± 0.647
carboxyl-isopropyl	0.111 ± 0.009	0.125 ± 0.006	0.834 ± 0.110	0.742 ± 0.033
carboxyl-methoxy	0.137 ± 0.014	0.138 ± 0.003	2.718 ± 0.219	2.859 ± 0.245
carboxyl-methyl	0.134 ± 0.013	0.134 ± 0.001	0.689 ± 0.118	0.743 ± 0.030
carboxyl-nitro	0.151 ± 0.015	0.136 ± 0.007	3.002 ± 0.172	3.702 ± 0.280
carboxyl-nitrophenyl	0.133 ± 0.006	0.131 ± 0.002	2.998 ± 0.142	3.257 ± 0.109
carboxyl-perfluoromethyl	0.141 ± 0.014	0.139 ± 0.001	0.558 ± 0.212	0.768 ± 0.042
carboxyl-phenyl	0.118 ± 0.010	0.125 ± 0.003	1.623 ± 0.086	1.478 ± 0.081
carboxyl-pyrrole	0.123 ± 0.004	0.128 ± 0.002	2.395 ± 0.113	2.706 ± 0.309
cyano-cyano	0.112 ± 0.022	0.109 ± 0.006	2.820 ± 0.455	2.477 ± 0.410
cyano-fluorophenyl	0.099 ± 0.012	0.110 ± 0.006	1.717 ± 0.183	1.660 ± 0.075
cyano-hydroxyl	0.144 ± 0.016	0.135 ± 0.004	3.394 ± 0.131	3.295 ± 0.655
cyano-isopropyl	0.103 ± 0.007	0.114 ± 0.006	0.477 ± 0.120	0.613 ± 0.054
cyano-methyl	0.116 ± 0.013	0.125 ± 0.005	0.475 ± 0.114	0.682 ± 0.099
cyano-nitro	0.104 ± 0.023	0.112 ± 0.006	2.063 ± 0.343	2.254 ± 0.298
cyano-perfluoromethyl	0.114 ± 0.010	0.126 ± 0.007	0.610 ± 0.099	0.721 ± 0.071
cyclopropyl-cyclopropyl	0.173 ± 0.014	0.165 ± 0.001	0.650 ± 0.252	0.382 ± 0.007
cyclopropyl-fluorophenyl	0.128 ± 0.013	0.132 ± 0.003	0.711 ± 0.163	0.793 ± 0.042
cyclopropyl-hydroxyl	0.150 ± 0.013	0.153 ± 0.002	0.675 ± 0.153	0.690 ± 0.018
cyclopropyl-isopropyl	0.152 ± 0.015	0.148 ± 0.001	0.561 ± 0.185	0.529 ± 0.010
cyclopropyl-methyl	0.148 ± 0.019	0.151 ± 0.001	0.539 ± 0.151	0.539 ± 0.021
cyclopropyl-nitro	0.131 ± 0.012	0.132 ± 0.001	0.629 ± 0.203	0.648 ± 0.018
cyclopropyl-perfluoromethyl	0.162 ± 0.016	0.160 ± 0.001	0.335 ± 0.123	0.411 ± 0.019

System	COF Calc.	COF Pred.	F_o Calc. (nN)	F_o Pred. (nN)
ethylene-ethylene	0.135 ± 0.023	0.120 ± 0.002	0.859 ± 0.278	0.858 ± 0.033
ethylene-fluorophenyl	0.112 ± 0.011	0.118 ± 0.002	0.908 ± 0.111	1.136 ± 0.183
ethylene-hydroxyl	0.132 ± 0.006	0.138 ± 0.001	0.891 ± 0.039	0.975 ± 0.023
ethylene-isopropyl	0.130 ± 0.010	0.130 ± 0.001	0.587 ± 0.076	0.635 ± 0.010
ethylene-methyl	0.128 ± 0.014	0.132 ± 0.000	0.812 ± 0.188	0.787 ± 0.025
ethylene-nitro	0.111 ± 0.013	0.114 ± 0.001	0.960 ± 0.183	1.050 ± 0.024
ethylene-perfluoromethyl	0.133 ± 0.007	0.137 ± 0.002	0.583 ± 0.135	0.662 ± 0.024
fluorophenyl-fluorophenyl	0.121 ± 0.013	0.117 ± 0.002	1.996 ± 0.251	1.731 ± 0.141
fluorophenyl-hydroxyl	0.148 ± 0.012	0.145 ± 0.002	1.738 ± 0.119	1.723 ± 0.104
fluorophenyl-isopropyl	0.131 ± 0.007	0.129 ± 0.001	0.778 ± 0.045	0.840 ± 0.020
fluorophenyl-methoxy	0.140 ± 0.007	0.135 ± 0.003	1.360 ± 0.103	1.479 ± 0.066
fluorophenyl-methyl	0.122 ± 0.008	0.131 ± 0.004	1.098 ± 0.076	0.968 ± 0.063
fluorophenyl-nitro	0.116 ± 0.009	0.119 ± 0.002	1.748 ± 0.138	1.838 ± 0.069
fluorophenyl-nitrophenyl	0.117 ± 0.006	0.117 ± 0.001	2.292 ± 0.132	1.927 ± 0.152
fluorophenyl-perfluoromethyl	0.142 ± 0.005	0.137 ± 0.003	1.031 ± 0.051	0.972 ± 0.049
fluorophenyl-phenyl	0.125 ± 0.011	0.125 ± 0.002	1.175 ± 0.138	1.319 ± 0.109
fluorophenyl-pyrrole	0.115 ± 0.009	0.121 ± 0.002	1.532 ± 0.169	1.640 ± 0.061
hydroxyl-hydroxyl	0.180 ± 0.020	0.156 ± 0.001	4.891 ± 0.550	4.288 ± 0.390
hydroxyl-isopropyl	0.150 ± 0.018	0.148 ± 0.001	0.721 ± 0.133	0.740 ± 0.010
hydroxyl-methoxy	0.167 ± 0.006	0.160 ± 0.001	2.128 ± 0.073	2.414 ± 0.121
hydroxyl-methyl	0.153 ± 0.011	0.152 ± 0.001	0.765 ± 0.151	0.822 ± 0.054
hydroxyl-nitro	0.151 ± 0.012	0.147 ± 0.003	2.588 ± 0.128	3.201 ± 0.283
hydroxyl-nitrophenyl	0.146 ± 0.014	0.143 ± 0.001	2.646 ± 0.220	2.759 ± 0.026
hydroxyl-perfluoromethyl	0.152 ± 0.006	0.154 ± 0.001	0.807 ± 0.144	0.833 ± 0.032
hydroxyl-phenyl	0.154 ± 0.005	0.145 ± 0.003	1.524 ± 0.066	1.329 ± 0.048
hydroxyl-pyrrole	0.147 ± 0.016	0.147 ± 0.001	2.636 ± 0.168	2.521 ± 0.259
isopropyl-isopropyl	0.147 ± 0.019	0.137 ± 0.001	0.668 ± 0.293	0.626 ± 0.020
isopropyl-methoxy	0.145 ± 0.008	0.143 ± 0.002	0.873 ± 0.180	0.766 ± 0.040
isopropyl-methyl	0.140 ± 0.015	0.141 ± 0.001	0.598 ± 0.177	0.607 ± 0.015
isopropyl-nitro	0.123 ± 0.013	0.124 ± 0.003	0.774 ± 0.080	0.759 ± 0.030
isopropyl-nitrophenyl	0.120 ± 0.014	0.123 ± 0.001	1.082 ± 0.148	1.134 ± 0.028
isopropyl-perfluoromethyl	0.150 ± 0.012	0.147 ± 0.002	0.429 ± 0.096	0.547 ± 0.058
isopropyl-phenyl	0.132 ± 0.013	0.131 ± 0.001	0.910 ± 0.141	0.839 ± 0.049
isopropyl-pyrrole	0.131 ± 0.007	0.130 ± 0.001	0.797 ± 0.085	0.801 ± 0.034
methoxy-methoxy	0.159 ± 0.012	0.151 ± 0.002	1.332 ± 0.166	1.440 ± 0.066
methoxy-methyl	0.157 ± 0.014	0.151 ± 0.003	0.813 ± 0.152	0.781 ± 0.021
methoxy-nitro	0.151 ± 0.013	0.137 ± 0.007	1.540 ± 0.163	1.683 ± 0.249
methoxy-perfluoromethyl	0.167 ± 0.006	0.157 ± 0.003	0.599 ± 0.113	0.692 ± 0.045
methyl-methyl	0.169 ± 0.023	0.148 ± 0.001	0.801 ± 0.261	0.668 ± 0.016
methyl-nitro	0.125 ± 0.010	0.130 ± 0.002	0.822 ± 0.082	0.805 ± 0.056
methyl-nitrophenyl	0.133 ± 0.013	0.131 ± 0.002	1.255 ± 0.063	1.175 ± 0.032
methyl-perfluoromethyl	0.148 ± 0.019	0.150 ± 0.001	0.630 ± 0.178	0.598 ± 0.030
methyl-phenyl	0.142 ± 0.015	0.138 ± 0.002	1.080 ± 0.167	0.944 ± 0.021
methyl-pyrrole	0.140 ± 0.011	0.138 ± 0.000	0.972 ± 0.141	0.917 ± 0.048
nitro-nitro	0.135 ± 0.014	0.123 ± 0.001	2.283 ± 0.231	2.276 ± 0.091
nitro-nitrophenyl	0.119 ± 0.010	0.122 ± 0.001	2.326 ± 0.134	2.329 ± 0.089
nitro-perfluoromethyl	0.129 ± 0.015	0.134 ± 0.001	0.957 ± 0.132	0.912 ± 0.032
nitro-phenyl	0.133 ± 0.009	0.126 ± 0.003	1.416 ± 0.109	1.449 ± 0.049
nitro-pyrrole	0.127 ± 0.012	0.127 ± 0.002	1.928 ± 0.072	2.475 ± 0.351
nitrophenyl-nitrophenyl	0.127 ± 0.016	0.121 ± 0.004	3.146 ± 0.414	2.378 ± 0.251
nitrophenyl-perfluoromethyl	0.133 ± 0.006	0.133 ± 0.001	1.347 ± 0.062	1.224 ± 0.022
perfluoromethyl-perfluoromethyl	0.169 ± 0.010	0.150 ± 0.007	0.772 ± 0.148	0.586 ± 0.059
perfluoromethyl-phenyl	0.154 ± 0.010	0.143 ± 0.005	0.712 ± 0.189	0.872 ± 0.128
perfluoromethyl-pyrrole	0.134 ± 0.015	0.137 ± 0.001	0.791 ± 0.121	0.925 ± 0.094
phenyl-phenyl	0.136 ± 0.013	0.129 ± 0.002	1.473 ± 0.140	1.385 ± 0.062
pyrrole-pyrrole	0.146 ± 0.018	0.129 ± 0.001	1.985 ± 0.205	1.891 ± 0.208

Additional details on molecular descriptors

Table S7: Overview of molecular descriptors.

Molecular descriptor	**Description**	**Category**
Approximate Surface Area	Approximation of molecular surface area using the approach defined by Labute [10]	Size
Asphericity	Measure of molecular shape (from Baumgartner [11]); $A = 0$ for spherical shape, $A = 1$ for highly prolate shapes, and $A = 0.25$ for oblate shapes	Shape
Balaban J	Related to connectivity, degree of branching [12]	Complexity
Bertz C_T	Measure of molecular complexity through connectivity [13]	Complexity
Chi0, Chi1	Connectivity indices [14]	Complexity
Chi0n - Chi4n	Connectivity indices over various molecular fragments (0=atoms, 1=one bond fragments, 2=two bond fragments, etc.) [14]	Complexity
Chi0v - Chi4v	Valence connectivity indices (0=atoms, 1=one bond fragments, 2=two bond fragments, etc.) [14]	Complexity
Eccentricity	Shape descriptor calculated from the inertia matrix (0=spherical, 1=linear), from Arteca [15]	Shape
Hall-Kier alpha	Modifying term for kappa descriptors, related to shape/flexibility [16]	Shape
Hall-Kier kappa1	Alpha-modified topological shape descriptor; related to complexity/number of cycles (rings) in the bond graph [16]	Shape
Hall-Kier kappa2	Alpha-modified topological shape descriptor; related to degree of star-like bond graph vs. linearity [16]	Shape
Hall-Kier kappa3	Alpha-modified topological shape descriptor; related to "centrality" of branching [16]	Shape
Hydrogen bond factor	Developed in this work; related to ability for formation of inter-monolayer hydrogen bonds	Charge distribution, Misc.
IPC	Complexity/connectivity descriptor estimated from adjacency matrix of bond graph [17]	Complexity

Molecular descriptor	Description	Category
Inertial shape factor	Characterization of molecular shape from principal moments of inertia ($pm_2/(pm_1 * pm_3)$, where pm1-3 are the three principal moments), from Todeschini and Consoni [16]	Shape
logP	Octanol - water partition coefficient estimated through the method of Wildman and Crippen; [18] measure of hydrophobicity	Charge distribution/Misc.
Molar refractivity	Estimation of molecular polarizability; calculated through the method of Wildman and Crippen [18]	Size
Molecular weight	-	Size
Molecular weight (heavy atoms)	Molecular weight excluding hydrogens	Size
Normalized principal moments ratios (NPR1, NPR2)	Used to characterize molecular shape, from Sauer and Schwarz [19]	Shape
Number of heavy atoms	Number of non-hydrogen atoms	Size
Number of rotatable bonds	-	Size/Shape
Number of valence electrons	-	Size
Plane of best fit	Measure of molecular planarity (0=planar, increasing with less planarity) [20]	Shape
Principal moments of inertia (PMI1, PMI2, PMI3)	Three principal moments of inertia for the molecule (1=smallest, 3=largest)	Shape
Radius of gyration	(From Arteca [15]) Characterizes molecular shape, specifically elongation	Shape/Size
Spherocity	Measure of molecular shape (0=spherical, 1=flat), from Robinson et al. [21]	Shape
Topological polar surface area	Estimation of surface area of only polar atoms, from Ertl et al. [22]	Charge distribution

Molecular descriptor	Description	Category
Total hydrophobic VSA	Sum of SA contributions from atoms with $-0.20 \leq q < 0.20$	Charge distribution
Total negative van der Waals surface area (VSA)	Sum of SA contributions from atoms with $q < 0.0$	Charge distribution
Total negative polar VSA	Sum of SA contributions from atoms with $q < -0.20$	Charge distribution
Total polar VSA	Sum of SA contributions from atoms with $\|q\| > 0.20$	Charge distribution
Total positive VSA	Sum of SA contributions from atoms with $q > 0.0$	Charge distribution
Total positive polar VSA	Sum of SA contributions from atoms with $q \geq 0.20$	Charge distribution
Fractional hydrophobic VSA	Total hydrophobic VSA / Total VSA	Charge distribution
Fractional negative VSA	Total negative VSA / Total VSA	Charge distribution
Fractional negative polar VSA	Total negative polar VSA / Total VSA	Charge distribution
Fractional polar VSA	Total polar VSA / Total VSA	Charge distribution
Fractional positive VSA	Total positive VSA / Total VSA	Charge distribution
Fractional positive polar VSA	Total positive polar VSA / Total VSA	Charge distribution

Summary of chemically dissimilar models

Table S8: List of systems used to develop the 5 models presented in the main text, annotating for each model which systems were used for training and which for testing.

System	Model 1	Model 2	Model 3	Model 4	Model 5
acetyl - acetyl	Test	**Train**	**Train**	Test	**Train**
acetyl - carboxyl	Test	**Train**	**Train**	**Train**	**Train**
acetyl - fluorophenyl	Test	Test	**Train**	Test	**Train**
acetyl - hydroxyl	**Train**	**Train**	**Train**	Test	**Train**
acetyl - isopropyl	**Train**	**Train**	**Train**	**Train**	**Train**
acetyl - methyl	Test	**Train**	**Train**	**Train**	**Train**
acetyl - nitro	**Train**	**Train**	**Train**	**Train**	Test
acetyl - perfluoromethyl	**Train**	Test	**Train**	**Train**	**Train**
amino - amino	**Train**	Test	**Train**	**Train**	**Train**
amino - carboxyl	Test	**Train**	**Train**	**Train**	Test
amino - fluorophenyl	**Train**	**Train**	Test	**Train**	**Train**
amino - hydroxyl	Test	**Train**	**Train**	**Train**	**Train**
amino - isopropyl	**Train**	**Train**	**Train**	**Train**	**Train**
amino - methyl	Test	Test	**Train**	Test	**Train**
amino - nitro	**Train**	**Train**	**Train**	Test	**Train**
amino - perfluoromethyl	Test	**Train**	**Train**	**Train**	Test
carboxyl - carboxyl	**Train**	Test	**Train**	Test	**Train**
carboxyl - cyano	**Train**	**Train**	Test	**Train**	**Train**
carboxyl - cyclopropyl	**Train**	**Train**	**Train**	**Train**	**Train**
carboxyl - ethylene	**Train**	**Train**	**Train**	**Train**	**Train**
carboxyl - fluorophenyl	Test	**Train**	**Train**	**Train**	**Train**
carboxyl - hydroxyl	**Train**	**Train**	**Train**	Test	**Train**
carboxyl - isopropyl	Test	Test	**Train**	**Train**	**Train**
carboxyl - methoxy	**Train**	**Train**	**Train**	Test	Test
carboxyl - methyl	**Train**	Test	**Train**	Test	**Train**
carboxyl - nitro	**Train**	**Train**	**Train**	**Train**	Test
carboxyl - nitrophenyl	**Train**	Test	**Train**	**Train**	**Train**
carboxyl - perfluoromethyl	**Train**	**Train**	**Train**	Test	**Train**
carboxyl - phenyl	**Train**	**Train**	**Train**	Test	**Train**
carboxyl - pyrrole	**Train**	**Train**	**Train**	Test	**Train**
cyano - cyano	**Train**	Test	**Train**	Test	**Train**
cyano - fluorophenyl	**Train**	**Train**	Test	**Train**	**Train**
cyano - hydroxyl	**Train**	**Train**	Test	**Train**	**Train**
cyano - isopropyl	**Train**	Test	Test	**Train**	**Train**
cyano - methyl	**Train**	**Train**	**Train**	**Train**	Test
cyano - nitro	**Train**	**Train**	**Train**	**Train**	**Train**
cyano - perfluoromethyl	**Train**	**Train**	Test	**Train**	**Train**
cyclopropyl - cyclopropyl	**Train**	**Train**	**Train**	**Train**	**Train**
cyclopropyl - fluorophenyl	Test	**Train**	**Train**	**Train**	**Train**
cyclopropyl - hydroxyl	**Train**	**Train**	Test	**Train**	**Train**
cyclopropyl - isopropyl	**Train**	**Train**	**Train**	**Train**	**Train**
cyclopropyl - methyl	**Train**	**Train**	**Train**	**Train**	**Train**
cyclopropyl - nitro	**Train**	**Train**	**Train**	**Train**	Test
cyclopropyl - perfluoromethyl	**Train**	**Train**	**Train**	**Train**	**Train**
ethylene - ethylene	**Train**	**Train**	Test	**Train**	**Train**
ethylene - fluorophenyl	**Train**	**Train**	**Train**	**Train**	Test
ethylene - hydroxyl	**Train**	**Train**	**Train**	**Train**	**Train**
ethylene - isopropyl	**Train**	**Train**	**Train**	**Train**	**Train**

System	Model 1	Model 2	Model 3	Model 4	Model 5
ethylene - methyl	**Train**	**Train**	**Train**	**Train**	**Train**
ethylene - nitro	**Train**	**Train**	**Train**	**Train**	**Train**
ethylene - perfluoromethyl	**Train**	**Train**	**Train**	**Train**	**Train**
fluorophenyl - fluorophenyl	**Train**	**Train**	Test	**Train**	**Train**
fluorophenyl - hydroxyl	**Train**	**Train**	Test	**Train**	**Train**
fluorophenyl - isopropyl	**Train**	Test	**Train**	**Train**	**Train**
fluorophenyl - methoxy	**Train**	Test	**Train**	**Train**	**Train**
fluorophenyl - methyl	Test	Test	**Train**	**Train**	**Train**
fluorophenyl - nitro	**Train**	**Train**	Test	Test	**Train**
fluorophenyl - nitrophenyl	Test	**Train**	**Train**	**Train**	**Train**
fluorophenyl - perfluoromethyl	**Train**	**Train**	**Train**	**Train**	**Train**
fluorophenyl - phenyl	**Train**	**Train**	**Train**	**Train**	Test
fluorophenyl - pyrrole	**Train**	**Train**	**Train**	**Train**	**Train**
hydroxyl - hydroxyl	**Train**	**Train**	**Train**	Test	**Train**
hydroxyl - isopropyl	**Train**	**Train**	**Train**	**Train**	**Train**
hydroxyl - methoxy	**Train**	**Train**	**Train**	**Train**	**Train**
hydroxyl - methyl	**Train**	**Train**	**Train**	**Train**	Test
hydroxyl - nitro	**Train**	**Train**	Test	**Train**	**Train**
hydroxyl - nitrophenyl	**Train**	**Train**	**Train**	**Train**	**Train**
hydroxyl - perfluoromethyl	**Train**	**Train**	**Train**	**Train**	Test
hydroxyl - phenyl	**Train**	**Train**	**Train**	**Train**	**Train**
hydroxyl - pyrrole	Test	**Train**	Test	**Train**	**Train**
isopropyl - isopropyl	**Train**	**Train**	**Train**	**Train**	**Train**
isopropyl - methoxy	**Train**	**Train**	**Train**	**Train**	Test
isopropyl - methyl	**Train**	**Train**	**Train**	**Train**	**Train**
isopropyl - nitro	**Train**	Test	**Train**	**Train**	**Train**
isopropyl - nitrophenyl	**Train**	**Train**	**Train**	**Train**	**Train**
isopropyl - perfluoromethyl	**Train**	Test	**Train**	**Train**	Test
isopropyl - phenyl	**Train**	**Train**	**Train**	Test	**Train**
isopropyl - pyrrole	**Train**	**Train**	**Train**	**Train**	Test
methoxy - methoxy	**Train**	Test	Test	**Train**	**Train**
methoxy - methyl	Test	**Train**	**Train**	Test	**Train**
methoxy - nitro	**Train**	**Train**	Test	**Train**	**Train**
methoxy - perfluoromethyl	**Train**	**Train**	Test	**Train**	**Train**
methyl - methyl	**Train**	**Train**	Test	**Train**	Test
methyl - nitro	Test	**Train**	**Train**	Test	Test
methyl - nitrophenyl	**Train**	**Train**	Test	**Train**	**Train**
methyl - perfluoromethyl	Test	**Train**	**Train**	**Train**	**Train**
methyl - phenyl	**Train**	Test	**Train**	**Train**	**Train**
methyl - pyrrole	**Train**	**Train**	**Train**	**Train**	**Train**
nitro - nitro	**Train**	**Train**	**Train**	**Train**	**Train**
nitro - nitrophenyl	Test	**Train**	**Train**	**Train**	**Train**
nitro - perfluoromethyl	**Train**	**Train**	**Train**	**Train**	**Train**
nitro - phenyl	Test	**Train**	**Train**	**Train**	**Train**
nitro - pyrrole	**Train**	Test	Test	Test	**Train**
nitrophenyl - nitrophenyl	**Train**	Test	Test	**Train**	Test
nitrophenyl - perfluoromethyl	**Train**	**Train**	**Train**	**Train**	**Train**
perfluoromethyl - perfluoromethyl	Test	Test	**Train**	**Train**	**Train**
perfluoromethyl - phenyl	**Train**	**Train**	**Train**	**Train**	Test
perfluoromethyl - pyrrole	**Train**	**Train**	**Train**	**Train**	Test
phenyl - phenyl	**Train**	**Train**	**Train**	**Train**	Test
pyrrole - pyrrole	**Train**	**Train**	**Train**	Test	**Train**

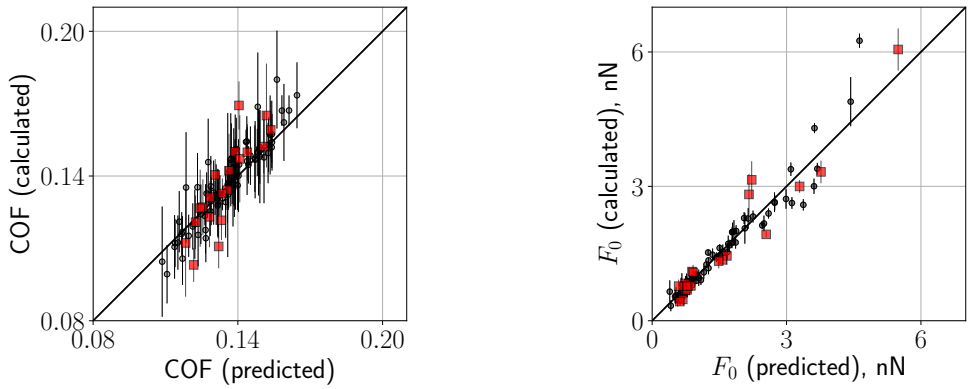

Figure S2: Plots of the predicted values vs. values calculated from simulation for COF and F_0 for model 2; red data points represent those reserved for testing. Data points represent the mean and error bars represent the standard deviation of the calculated values (see Table S6).

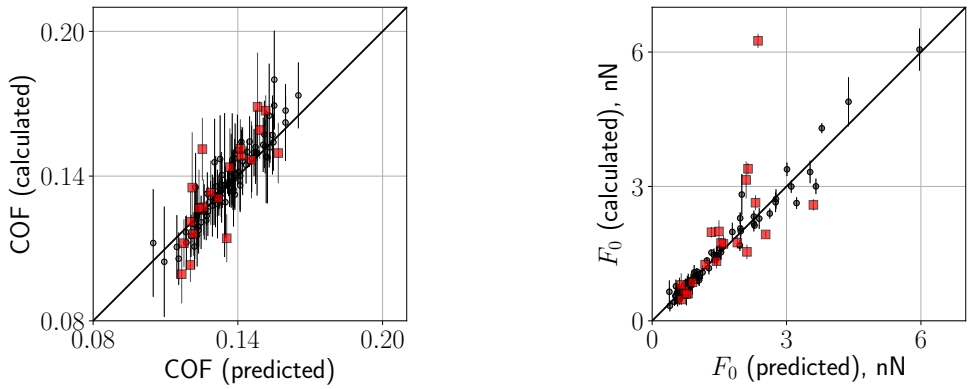

Figure S3: Plots of the predicted values vs. values calculated from simulation for COF and F_0 for for model 3; red data points represent those reserved for testing. Data points represent the mean and error bars represent the standard deviation of the calculated values (see Table S6).

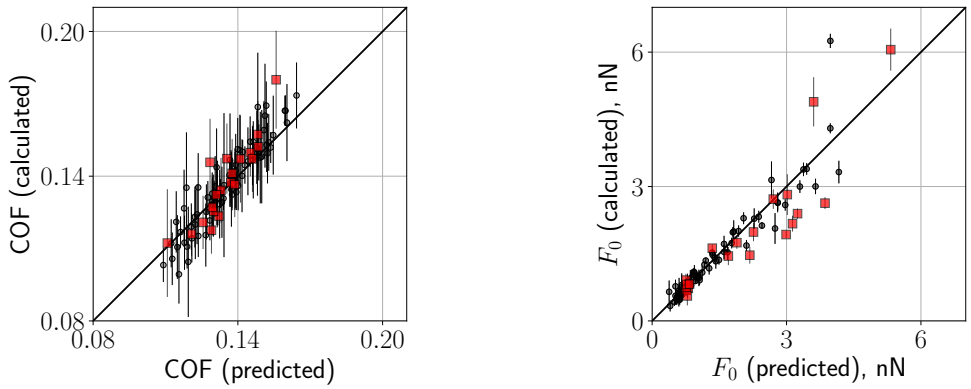

Figure S4: Plots of the predicted values vs. values calculated from simulation for COF and F_0 for model 4; red data points represent those reserved for testing. Data points represent the mean and error bars represent the standard deviation of the calculated values (see Table S6).

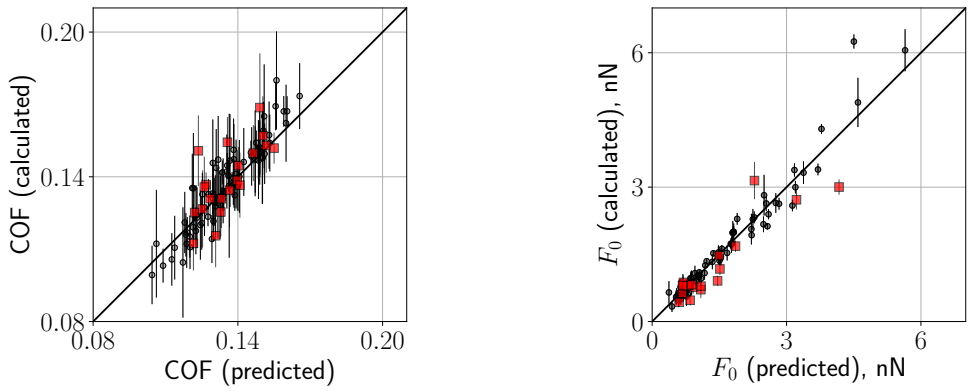

Figure S5: Plots of the predicted values vs. values calculated from simulation for COF and F_0 for model 5; red data points represent those reserved for testing. Data points represent the mean and error bars represent the standard deviation of the calculated values (see Table S6).

Summary of properties of toluene and phenol containing films

Table S9: Mean and standard deviation of the COF and F_0 for chemically dissimilar films containing toluene and phenol, comparing the calculated values from simulation to those predicted by the models. Values represents the mean and standard deviation.

System	**COF Calc.**	**COF Pred.**	**F_o Calc. (nN)**	**F_o Pred. (nN)**
acetyl-toluene	0.140 ± 0.007	0.127 ± 0.001	1.305 ± 0.161	1.095 ± 0.090
acetyl-phenol	0.128 ± 0.006	0.133 ± 0.002	3.627 ± 0.403	2.474 ± 0.491
fluorophenyl-toluene	0.140 ± 0.013	0.123 ± 0.003	0.958 ± 0.302	1.352 ± 0.111
fluorophenyl-phenol	0.134 ± 0.006	0.119 ± 0.001	2.766 ± 0.013	1.734 ± 0.115
nitro-toluene	0.133 ± 0.009	0.123 ± 0.002	1.280 ± 1.054	1.460 ± 0.083
nitro-phenol	0.148 ± 0.012	0.124 ± 0.002	3.408 ± 0.137	2.698 ± 0.295
amino-toluene	0.143 ± 0.004	0.137 ± 0.001	1.559 ± 0.071	1.155 ± 0.063
amino-phenol	0.130 ± 0.009	0.136 ± 0.002	6.656 ± 0.333	3.068 ± 0.532
methyl-toluene	0.146 ± 0.007	0.135 ± 0.002	0.700 ± 0.374	0.840 ± 0.043
methyl-phenol	0.130 ± 0.014	0.134 ± 0.002	1.180 ± 0.189	0.980 ± 0.075
phenyl-toluene	0.139 ± 0.011	0.129 ± 0.002	0.903 ± 0.617	1.338 ± 0.085
ethylene-toluene	0.129 ± 0.013	0.125 ± 0.001	0.847 ± 0.336	1.109 ± 0.141
ethylene-phenol	0.117 ± 0.005	0.118 ± 0.002	1.345 ± 0.110	1.250 ± 0.142
isopropyl-toluene	0.141 ± 0.009	0.130 ± 0.001	1.041 ± 0.091	0.818 ± 0.036
isopropyl-phenol	0.117 ± 0.010	0.128 ± 0.002	1.234 ± 0.069	0.925 ± 0.089
nitrophenyl-toluene	0.136 ± 0.006	0.121 ± 0.001	1.668 ± 0.339	1.421 ± 0.105
nitrophenyl-phenol	0.134 ± 0.009	0.126 ± 0.004	3.477 ± 0.092	2.700 ± 0.257
carboxyl-toluene	0.136 ± 0.005	0.126 ± 0.001	1.468 ± 0.098	1.459 ± 0.070
carboxyl-phenol	0.121 ± 0.002	0.133 ± 0.003	6.476 ± 0.532	4.170 ± 0.616
perfluoromethyl-toluene	0.151 ± 0.018	0.141 ± 0.003	0.419 ± 0.558	0.855 ± 0.080
perfluoromethyl-phenol	0.140 ± 0.013	0.138 ± 0.003	1.152 ± 0.064	1.038 ± 0.079
hydroxyl-toluene	0.164 ± 0.010	0.142 ± 0.004	1.219 ± 0.601	1.299 ± 0.051
hydroxyl-phenol	0.138 ± 0.012	0.145 ± 0.001	6.372 ± 0.349	2.808 ± 0.251
cyclopropyl-toluene	0.152 ± 0.008	0.136 ± 0.002	0.709 ± 0.097	0.768 ± 0.046
cyclopropyl-phenol	0.147 ± 0.004	0.134 ± 0.003	0.899 ± 0.068	0.902 ± 0.104
pyrrole-toluene	0.132 ± 0.002	0.126 ± 0.002	1.351 ± 0.245	1.401 ± 0.066
methoxy-toluene	0.146 ± 0.018	0.134 ± 0.002	1.406 ± 0.567	1.005 ± 0.038
methoxy-phenol	0.139 ± 0.006	0.134 ± 0.002	3.337 ± 0.122	2.195 ± 0.291
cyano-toluene	0.128 ± 0.012	0.111 ± 0.006	0.773 ± 0.235	1.483 ± 0.075
cyano-phenol	0.113 ± 0.016	0.112 ± 0.006	5.346 ± 0.096	3.024 ± 0.592

Mean-based estimation of chemically-dissimilar tribology

As an initial attempt at exploring how the mixing of monolayer chemistries alters tribological response, the COF and adhesion of chemically-dissimilar monolayers was predicted from the results calculated for chemically-identical systems using a simple arithmetic mean. For example, the COF and adhesion of a "hydroxyl-methyl" system is estimated by taking the average of the COF and adhesion calculated for the "hydroxyl-hydroxyl" and "methyl-methyl" systems. If the estimation over-predicts the actual value, that would suggest that the mixing of monolayer chemistries provides an advantageous route to improving monolayer tribological performance. The actual vs. expected values for both COF and adhesion using this ap-

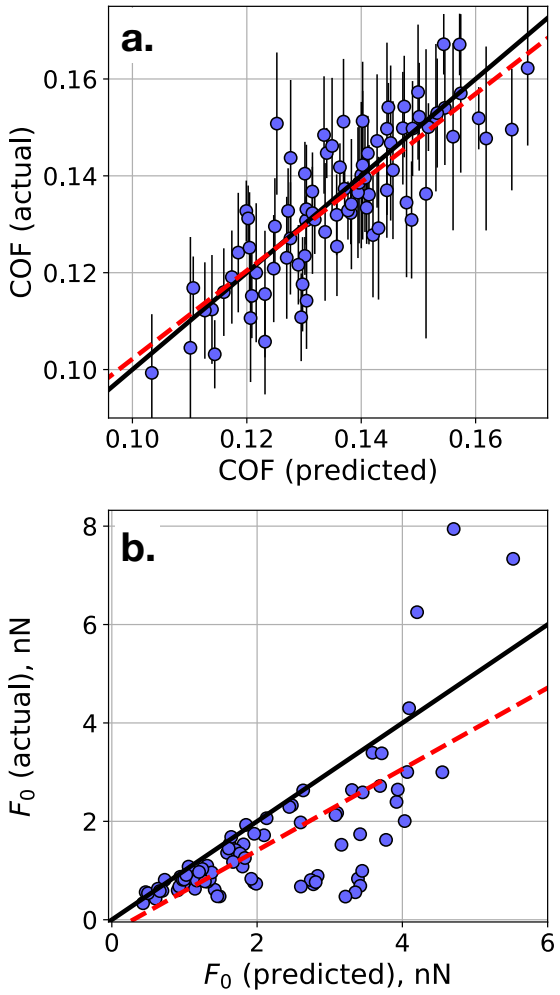

Figure S6: Predicted values of a. COF and b. adhesive force for chemically-dissimilar monolayer systems, as calculated by the mean of the values obtained for chemically identical systems, compared to the actual values. The y=x line is drawn in black for reference, while the dashed red line represents a linear regression of the data. Each unique surface chemistry (averaged over five monolayer surface configurations) is represented by a single point, and errors bars represent a single standard deviation calculated from the estimation of these five configurations.

proach are shown in Fig. S6. Interestingly, from Fig. S6a it is observed that the COF of chemically-dissimilar systems is reasonably-approximated by the averaging of values from the chemically-identical systems, as the COF of nearly all chemically-dissimilar systems is predicted correctly within error of the measurement.

Conversely, Fig. S6b shows that the force of adhesion is not well predicted by this approach. It appears that if one monolayer in a system is terminated by a polar functional group and the other is terminated by a nonpolar functional group, the adhesive force will be most similar to that of the pure nonpolar system, rather than an average of the two. As a result, when predicting the adhesive force for chemically-dissimilar systems featuring a mixture of polar and nonpolar groups using mean data from chemically-identical systems, adhesion values are over-estimated, as evidenced by the high concentration of points below the y=x line in Fig. S6b.

Additional force field details

The OPLS force field uses the following contributions to the total potential:[23]

$$E_{\text{non-bonded}} = \sum_i \sum_{j>i} \left[\frac{q_i q_j e^2}{r_{ij}} + 4\epsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^{6} \right] \right] \tag{1}$$

$$E_{\text{bond}} = \sum_{\text{bonds}} K_r (r - r_0)^2 \tag{2}$$

$$E_{\text{angle}} = \sum_{\text{angles}} K_\theta (\theta - \theta_0)^2 \tag{3}$$

$$E_{\text{torsion}} = \sum_{\text{torsions}} \frac{1}{2} \left[K_1(1 + \cos\phi) + K_2(1 - \cos 2\phi) + K_3(1 + \cos 3\phi) - K_4(1 - \cos 4\phi) \right] \tag{4}$$

where q_i and q_j are the partial charges on particles i and j, e is Coulomb's constant, r_{ij} is the inter-particle separation, ϵ and σ are interaction-specific Lennard-Jones parameters, K_r, K_θ, and $K_{1,2,3,4}$ are force constants, r_0 is the equilibrium bond distance, θ_0 is the equilibrium angle, and ϕ is the torsion angle.

For certain molecules, such as aromatics and alkenes, improper torsions are necessary to enforce planarity. The OPLS force field primarily utilizes improper parameters from the AMBER family of force fields, where impropers have the following potential form:

$$E_{\text{impropers}} = \sum_{\text{impropers}} \frac{1}{2} K_\phi [1 + \cos(n\phi - \gamma)] \tag{5}$$

where ϕ is the torsion angle, K_ϕ is the force constant, n is the multiplicity, and γ is the phase angle.

OPLS uses geometric mixing rules for cross-interactions:

$$\sigma_{ij} = (\sigma_{ii}\sigma_{jj})^{\frac{1}{2}} \tag{6}$$

$$\epsilon_{ij} = (\epsilon_{ii}\epsilon_{jj})^{\frac{1}{2}} \tag{7}$$

Additionally, non-bonded interactions are excluded for particles separated by one or two bonds. For particles separated by three bonds, non-bonded interactions are scaled by 0.5.

Detailed below are the OPLS parameters utilized in this work. Parameters used for silica surfaces, silane headgroups, and alkane backbones are provided first. Parameters used for each of the sixteen terminal groups are provided next, where they have been separated by terminal group chemistry.

Silica Surfaces and Alkane Backbones

Nonbonded parameters						
Atom type	Element	Charge	Sigma, nm	Epsilon, kcal/mol	Reference	Notes
opls_135	C	-0.18	0.35	0.066	23	-
opls_136	C	-0.12	0.35	0.066	23	-
opls_140	H	0.06	0.25	0.03	23	-
opls_1001	O	-0.43	0.3	0.17	24	-
opls_1002	Si	0.86	0.4	0.1	24	-
opls_1003	Si	0.745	0.4	0.1	24	-
opls_1004	C	-0.12	0.35	0.066	23	-
opls_1005	O	-0.683	0.312	0.17	23	-
opls_1006	H	0.418	0	0	23	-
opls_1007	O	-0.215	0.3	0.17	24	-
opls_1008	O	-0.215	0.3	0.17	24	-
opls_1009	H	0.215	0.0	0	n/a	1

[1] Parameters for hydroxyl surface caps on silica surfaces are not available in the OPLS force field. We have used the same σ and ϵ values as the standard OPLS hydroxyl parameters and use a charge of 0.215 to maintain charge neutrality in the system.

Bond parameters					
Bond	Elements	k, kcal/mol^{-1} Å^2	r_0, nm	Reference	Notes
opls_135-opls_136	C-C	268	0.1529	23	-
opls_135-opls_140	C-H	340	0.109	23	-
opls_136-opls_140	C-H	340	0.109	23	-
opls_136-opls_1004	C-C	268	0.1529	23	-
opls_1004-opls_140	C-H	340	0.109	23	-
opls_1004-opls_1003	C-Si	200	1.85	24	-
opls_1003-opls_1005	Si-O	300	1.65	24	-
opls_1005-opls_1006	O-H	553	0.945	23	-
opls_1003-opls_1007	Si-O	300	1.65	24	-
opls_1007-opls_1002	O-Si	300	1.65	24	-
opls_1001-opls_1002	O-Si	300	1.65	24	-
opls_1002-opls_1008	Si-O	300	1.65	24	-
opls_1008-opls_1009	O-H	553	0.945	23	-

Angle parameters					
Angle	Elements	k, kcal/mol^{-1} deg^2	θ_0, deg	Reference	Notes
opls_135-opls_136-opls_136	C-C-C	58.35	112.7	23	-
opls_136-opls_136-opls_136	C-C-C	58.35	112.7	23	-
opls_136-opls_136-opls_1004	C-C-C	58.35	112.7	23	-
opls_140-opls_135-opls_140	H-C-H	33	107.8	23	-
opls_140-opls_136-opls_140	H-C-H	33	107.8	23	-
opls_140-opls_1004-opls_140	H-C-H	33	107.8	23	-
opls_140-opls_135-opls_136	H-C-C	37.5	110.7	23	-
opls_140-opls_136-opls_136	H-C-C	37.5	110.7	23	-
opls_140-opls_136-opls_1004	H-C-C	37.5	110.7	23	-
opls_136-opls_1004-opls_1003	C-C-Si	30.47	120	24	-
opls_140-opls_1004-opls_1003	H-C-Si	37.5	110.7	n/a	1
opls_1004-opls_1003-opls_1005	C-Si-O	60	100	24	-
opls_1004-opls_1003-opls_1007	C-Si-O	60	100	24	-
opls_1005-opls_1003-opls_1005	O-Si-O	60	110	24	-
opls_1005-opls_1003-opls_1007	O-Si-O	60	110	24	-
opls_1003-opls_1005-opls_1006	Si-O-H	23.7764	122.888	24	-
opls_1003-opls_1007-opls_1002	Si-O-Si	20	145	24	-
opls_1007-opls_1002-opls_1001	O-Si-O	60	110	24	-
opls_1002-opls_1001-opls_1002	Si-O-Si	20	145	24	-
opls_1001-opls_1002-opls_1001	O-Si-O	60	110	24	-
opls_1001-opls_1002-opls_1008	O-Si-O	60	110	24	-
opls_1002-opls_1008-opls_1009	Si-O-H	23.7764	122.888	24	-

[1] H-C-Si parameters do not exist in OPLS. In the work of Lorenz et al.[24] F-C-C angle parameters were also used for F-C-Si angles. Following this approach, H-C-C angle parameters have been used for H-C-Si angles.

Dihedral parameters							
Dihedral	Elements	k1, kcal/mol	k2, kcal/mol	k3, kcal/mol	k4, kcal/mol	Reference	Notes
opls_135-opls_136-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	25	-
opls_136-opls_136-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	25	-
opls_136-opls_136-opls_136-opls_1004	C-C-C-C	1.3	-0.05	0.2	0.0	25	-
opls_140-opls_135-opls_136-opls_136	H-C-C-C	0.0	0.0	0.3	0.0	25	-
opls_140-opls_136-opls_136-opls_136	H-C-C-C	0.0	0.0	0.3	0.0	25	-
opls_140-opls_136-opls_136-opls_135	H-C-C-C	0.0	0.0	0.3	0.0	25	-
opls_140-opls_136-opls_136-opls_1004	H-C-C-C	0.0	0.0	0.3	0.0	25	-
opls_140-opls_1004-opls_136-opls_136	H-C-C-C	0.0	0.0	0.3	0.0	25	-
opls_140-opls_135-opls_136-opls_140	H-C-C-H	0.0	0.0	0.3	0.0	25	-
opls_140-opls_136-opls_136-opls_140	H-C-C-H	0.0	0.0	0.3	0.0	25	-
opls_140-opls_136-opls_1004-opls_140	H-C-C-H	0.0	0.0	0.3	0.0	25	-
All torsions containing silicon	X-Si-X-X, Si-X-X-X	0	0	0	0	24	1

[1] Any torsion containing a silicon atom is treated as a null torsion.

Methyl

Nonbonded parameters						
Atom type	Element	Charge	Sigma, nm	Epsilon, kcal/mol	Reference	Notes
opls_135	C	-0.18	0.35	0.066	23	-
opls_140	H	0.06	0.25	0.03	23	-

Bond parameters					
Bond	Elements	k, kcal/mol^{-1} Å^2	r_0, nm	Reference	Notes
opls_135-opls_136	C-C	268	0.1529	23	-
opls_135-opls_140	C-H	340	0.109	23	-

Angle parameters					
Angle	Elements	k, kcal/mol^{-1} deg^2	θ_0, deg	Reference	Notes
opls_136-opls_136-opls_135	C-C-C	58.35	112.7	23	-
opls_136-opls_135-opls_140	C-C-H	37.5	110.7	23	-
opls_140-opls_135-opls_140	H-C-H	33	107.8	23	-

Dihedral parameters							
Dihedral	Elements	k1, kcal/mol	k2, kcal/mol	k3, kcal/mol	k4, kcal/mol	Reference	Notes
opls_136-opls_136-opls_136-opls_135	C-C-C-C	1.3	-0.05	0.2	0.0	25	-
opls_136-opls_136-opls_135-opls_140	C-C-C-H	0.0	0.0	0.3	0.0	25	-
opls_140-opls_136-opls_135-opls_140	H-C-C-H	0.0	0.0	0.3	0.0	25	-

Acetyl

Nonbonded parameters						
Atom type	Element	Charge	Sigma, nm	Epsilon, kcal/mol	Reference	Notes
opls_135	C	-0.18	0.35	0.066	23	-
opls_282	H	0.06	0.242	0.015	23	-
opls_280	C	0.47	0.375	0.105	23	-
opls_281	O	-0.47	0.296	0.21	23	-

Bond parameters					
Bond	Elements	k, kcal/mol^{-1} Å^2	r_0, nm	Reference	Notes
opls_135-opls_282	C-H	340	0.109	23	-
opls_135-opls_280	C-C	317	0.1522	26	-
opls_280-opls_281	C-O	570	0.1229	26	-
opls_280-opls_136	C-C	317	0.1522	26	-

Angle parameters					
Angle	Elements	k, kcal/mol^{-1} deg^2	θ_0, deg	Reference	Notes
opls_282-opls_135-opls-282	H-C-H	33	107.8	23	-
opls_282-opls_135-opls_280	H-C-C	35	109.5	26	-
opls_135-opls_280-opls_281	C-C-O	80	120.4	26	-
opls_135-opls_280-opls_136	C-C-C	70	116.0	N/A	[1]
opls_281-opls_280-opls_136	O-C-C	80	120.4	26	-
opls_280-opls_136-opls_282	C-C-H	35	109.5	26	-
opls_280-opls_136-opls_136	C-C-C	63	111.1	26	-
opls_282-opls_136-opls_136	H-C-C	37.5	110.7	23	-
opls_136-opls_136-opls_140	C-C-H	37.5	110.7	23	-
opls_136-opls_136-opls_136	C-C-C	58.35	112.7	23	-

[1] No reference found. Parameters used from GROMACS *as is*.

Dihedral parameters							
Dihedral	Elements	k1, kcal/mol	k2, kcal/mol	k3, kcal/mol	k4, kcal/mol	Reference	Notes
opls_282-opls_135-opls_280-opls_281	H-C-C-O	0.0	0.0	0.0	0.0	23	-
opls_282-opls_135-opls_280-opls_136	H-C-C-C	0.0	0.0	0.275	0.0	23	-
opls_135-opls_280-opls_136-opls_136	C-C-C-C	1.454	-0.144	-0.775	0.0	23	-
opls_135-opls_280-opls_136-opls_282	C-C-C-H	0.0	0.0	0.275	0.0	23	-
opls_281-opls_280-opls_136-opls_136	O-C-C-C	-0.277	1.228	-0.694	0.0	23	-
opls_281-opls_280-opls_136-opls_282	O-C-C-H	0.0	0.0	0.0	0.0	23	-
opls_280-opls_136-opls_136-opls_136	C-C-C-C	-1.697	-0.456	0.585	0.0	23	-
opls_280-opls_136-opls_136-opls_140	C-C-C-H	0.0	0.0	-0.076	0.0	23	-
opls_282-opls_136-opls_136-opls_136	H-C-C-C	0.0	0.0	0.3	0.0	25	-
opls_282-opls_136-opls_136-opls_140	H-C-C-H	0.0	0.0	0.3	0.0	25	-

Improper parameters						
Improper	Elements	γ, degrees	K_ϕ, kcal/mol	n	Reference	Notes
opls_281-opls_280-opls_135-opls_136	O-C-C-C	180	21.0	2	26	-

Amino

Nonbonded parameters						
Atom type	Element	Charge	Sigma, nm	Epsilon, kcal/mol	Reference	Notes
opls_909	H	0.36	0	0	27	-
opls_900	N	-0.9	0.33	0.17	27	-
opls_906	C	0.06	0.35	0.066	27	-
opls_911	H	0.06	0.25	0.015	27	-

Bond parameters					
Bond	Elements	k, kcal/mol^{-1} Å^2	r_0, nm	Reference	Notes
opls_909-opls_900	H-N	434	0.101	27	-
opls_900-opls_906	N-C	382	0.1448	27	-
opls_906-opls_911	C-H	340	0.109	27	-
opls_906-opls_136	C-C	268	0.1529	27	-

Angle parameters					
Angle	Elements	k, kcal/mol^{-1} deg^2	θ_0, deg	Reference	Notes
opls_909-opls_900-opls_909	H-N-H	43.6	106.4	27	-
opls_909-opls_900-opls_906	H-N-C	35	109.5	27	-
opls_900-opls_906-opls_911	N-C-H	35	109.5	27	-
opls_900-opls_906-opls_136	N-C-C	56.2	109.47	27	-
opls_911-opls_906-opls-911	H-C-H	33	107.8	23	-
opls_911-opls_906-opls_136	H-C-C	37.5	110.7	23	-
opls_906-opls_136-opls_140	C-C-H	37.5	110.7	23	-
opls_906-opls_136-opls_136	C-C-C	58.35	112.7	23	-

Dihedral parameters							
Dihedral	Elements	k1, kcal/mol	k2, kcal/mol	k3, kcal/mol	k4, kcal/mol	Reference	Notes
opls_909-opls_900-opls_906-opls_911	H-N-C-H	0.0	0.0	0.4	0.0	27	-
opls_909-opls_900-opls_906-opls_136	H-N-C-C	-0.19	-0.417	0.418	0.0	27	-
opls_900-opls_906-opls_136-opls_136	N-C-C-C	2.392	-0.674	0.55	0.0	27	-
opls_900-opls_906-opls_136-opls_140	N-C-C-H	-1.013	-0.709	0.473	0.0	27	-
opls_911-opls_906-opls_136-opls_136	H-C-C-C	0.0	0.0	0.3	0.0	25	-
opls_911-opls_906-opls_136-opls_140	H-C-C-H	0.0	0.0	0.3	0.0	25	-
opls_906-opls_136-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	25	-
opls_906-opls_136-opls_136-opls_140	C-C-C-H	0.0	0.0	0.3	0.0	25	-

Carboxyl

Nonbonded parameters						
Atom type	Element	Charge	Sigma, nm	Epsilon, kcal/mol	Reference	Notes
opls_270	H	0.45	0	0	23	-
opls_268	O	-0.53	0.3	0.17	23	-
opls_267	C	0.52	0.375	0.105	23	-
opls_269	O	-0.44	0.296	0.21	23	-

Bond parameters					
Bond	Elements	k, kcal/mol^{-1} Å^2	r_0, nm	Reference	Notes
opls_270-opls_268	H-O	553	0.0945	26	-
opls_268-opls_267	O-C	450	0.1364	26	-
opls_267-opls_269	C-O	570	0.1229	26	-
opls_267-opls_136	C-C	317	0.1522	26	-

Angle parameters					
Angle	Elements	k, kcal/mol^{-1} deg^2	θ_0, deg	Reference	Notes
opls_270-opls_268-opls_267	H-O-C	35	113	26	-
opls_268-opls_267-opls_269	O-C-O	80	121	28	-
opls_268-opls_267-opls_136	O-C-C	70	108	28	-
opls_269-opls_267-opls_136	O-C-C	80	120.4	26	-
opls_267-opls_136-opls_140	C-C-H	35	109.5	26	-
opls_267-opls_136-opls_136	C-C-C	63	111.1	26	-

Dihedral parameters							
Dihedral	Elements	k1, kcal/mol	k2, kcal/mol	k3, kcal/mol	k4, kcal/mol	Reference	Notes
opls_270-opls_268-opls_267-opls_269	H-O-C-O	0.0	5.5	0.0	0.0	N/A	1
opls_270-opls_268-opls_267-opls_136	H-O-C-C	1.5	5.5	0.0	0.0	N/A	1
opls_268-opls_267-opls_136-opls_136	O-C-C-C	1.0	0.546	0.45	0.0	28	-
opls_268-opls_267-opls_136-opls_140	O-C-C-H	0.0	0.0	0.0	0.0	28	-
opls_269-opls_267-opls_136-opls_140	O-C-C-H	0.0	0.0	0.0	0.0	28	-
opls_269-opls_267-opls_136-opls_136	O-C-C-C	0.0	0.546	0.0	0.0	28	-
opls_269-opls_267-opls_136-opls_136	C-C-C-C	-2.06	-0.313	0.315	0.0	23	-
opls_267-opls_136-opls_136-opls_140	C-C-C-H	0.0	0.0	-0.1	0.0	23	-

[1] No reference found. Parameters used from GROMACS *as is*.

Improper parameters						
Improper	Elements	γ, degrees	K_ϕ, kcal/mol	n	Reference	Notes
opls_269-opls_267-opls_268-opls_136	O-C-O-C	180	21.0	2	26	-

Nitrile

Nonbonded parameters						
Atom type	Element	Charge	Sigma, nm	Epsilon, kcal/mol	Reference	Notes
opls_753	N	-0.56	0.32	0.17	25	-
opls_754	C	0.46	0.33	0.066	25	-
opls_756	C	-0.02	0.33	0.066	25	-
opls_759	H	0.06	0.25	0.15	25	-

Bond parameters					
Bond	Elements	k, kcal/mol^{-1} Å^2	r_0, nm	Reference	Notes
opls_753-opls_754	N-C	650	0.1157	25	-
opls_754-opls_756	C-C	385	0.1458	25	1
opls_756-opls_759	C-H	340	0.109	23	-
opls_756-opls_136	C-C	268	0.1529	23	-

[1] GROMACS parameters differ from the literature. Parameters from Ref. 25 have been used.

Angle parameters					
Angle	Elements	k, kcal/mol^{-1} deg^2	θ_0, deg	Reference	Notes
opls_753-opls_754-opls_756	N-C-C	150	180	25	-
opls_754-opls_756-opls_759	C-C-H	35	108.5	25	-
opls_754-opls_756-opls_136	C-C-C	58.35	112.7	25	-
opls_759-opls_756-opls_759	H-C-H	33	107.8	23	-
opls_759-opls_756-opls_136	H-C-C	37.5	110.7	23	-
opls_756-opls_136-opls_140	C-C-H	37.5	110.7	23	-
opls_756-opls_136-opls_136	C-C-C	58.35	112.7	23	-

Dihedral parameters							
Dihedral	Elements	k1, kcal/mol	k2, kcal/mol	k3, kcal/mol	k4, kcal/mol	Reference	Notes
opls_753-opls_754-opls_756-opls_136	N-C-C-C	0.0	0.0	0.0	0.0	25	-
opls_753-opls_754-opls_756-opls_759	N-C-C-H	0.0	0.0	0.0	0.0	25	-
opls_754-opls_756-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	N/A	1
opls_754-opls_756-opls_136-opls_140	C-C-C-H	0.0	0.0	0.366	0.0	25	-
opls_759-opls_756-opls_136-opls_136	H-C-C-C	0.0	0.0	0.3	0.0	25	-
opls_759-opls_756-opls_136-opls_140	H-C-C-H	0.0	0.0	0.3	0.0	25	-
opls_756-opls_136-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	25	-
opls_756-opls_136-opls_136-opls_140	C-C-C-H	0.0	0.0	0.3	0.0	25	-

[1] Parameters don't exist in GROMACS or the literature. Parameters for alkane C-C-C-C dihedrals have been used.

Cyclopropyl

Nonbonded parameters						
Atom type	Element	Charge	Sigma, nm	Epsilon, kcal/mol	Reference	Notes
opls_140	H	0.06	0.25	0.03	N/A	1
opls_711	C	-0.12	0.35	0.066	N/A	1
opls_712	C	-0.06	0.35	0.066	N/A	1

[1] No reference found. Parameters used from GROMACS *as is*.

Bond parameters					
Bond	Elements	k, kcal/mol^{-1} Å^2	r_0, nm	Reference	Notes
opls_711-opls_140	C-H	340	0.1088	N/A	1
opls_711-opls_712	C-C	260	0.1509	N/A	1
opls_712-opls_140	C-H	340	0.1088	N/A	1
opls_712-opls_136	C-C	280	0.151	N/A	1

[1] No reference found. Parameters used from GROMACS *as is*.

Angle parameters					
Angle	Elements	k, kcal/mol^{-1} deg^2	θ_0, deg	Reference	Notes
opls_140-opls_711-opls_140	H-C-H	35	114.3	N/A	1
opls_140-opls_711-opls_711	H-C-C	37.5	117.2	N/A	1
opls_140-opls_711-opls_712	H-C-C	37.5	117.2	N/A	1
opls_711-opls_711-opls_712	C-C-C	30	60	N/A	1
opls_711-opls_712-opls_711	C-C-C	30	60	N/A	1
opls_711-opls_711-opls_140	C-C-H	37.5	117.2	N/A	1
opls_711-opls_712-opls_140	C-C-H	37.5	117.2	N/A	1
opls_711-opls_712-opls_136	C-C-C	37.5	117.2	N/A	1
opls_140-opls_712-opls_136	H-C-C	35	114.3	N/A	1
opls_712-opls_136-opls_136	C-C-C	58.35	112.7	N/A	2
opls_712-opls_136-opls_140	C-C-H	37.5	110.7	N/A	1

[1] No reference found. Parameters used from GROMACS *as is*.
[2] Parameters not found in GROMACS or the literature. Alkane C-C-C parameters have been used.

Dihedral parameters							
Dihedral	Elements	k1, kcal/mol	k2, kcal/mol	k3, kcal/mol	k4, kcal/mol	Reference	Notes
opls_140-opls_711-opls_711-opls_140	H-C-C-H	0.0	0.0	0.3	0.0	N/A	1
opls_140-opls_711-opls_711-opls_712	H-C-C-C	0.0	0.0	0.3	0.0	N/A	1
opls_140-opls_711-opls_712-opls_711	H-C-C-C	0.0	0.0	0.3	0.0	N/A	1
opls_140-opls_711-opls_712-opls_140	H-C-C-H	0.0	0.0	0.3	0.0	N/A	1
opls_140-opls_711-opls_712-opls_136	H-C-C-C	0.0	0.0	0.3	0.0	N/A	1
opls_711-opls_711-opls_712-opls_140	C-C-C-H	0.0	0.0	0.3	0.0	N/A	1
opls_711-opls_711-opls_712-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	N/A	1
opls_711-opls_712-opls_711-opls_140	C-C-C-H	0.0	0.0	0.3	0.0	N/A	1
opls_711-opls_712-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	N/A	2
opls_711-opls_712-opls_136-opls_140	C-C-C-H	0.0	0.0	0.3	0.0	N/A	1
opls_140-opls_712-opls_136-opls_136	H-C-C-C	0.0	0.0	0.3	0.0	N/A	3
opls_140-opls_712-opls_136-opls_140	H-C-C-H	0.0	0.0	0.3	0.0	N/A	4
opls_712-opls_136-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	N/A	2
opls_712-opls_136-opls_136-opls_140	C-C-C-H	0.0	0.0	0.3	0.0	N/A	3

[1] No reference found. Parameters used from GROMACS *as is*.
[2] Parameters not found in GROMACS or the literature. Parameters for alkane C-C-C-C dihedrals have been used.
[3] Parameters not found in GROMACS or the literature. Parameters for alkane C-C-C-H dihedrals have been used.
[4] Parameters not found in GROMACS or the literature. Parameters for alkane H-C-C-H dihedrals have been used.

Vinyl

Nonbonded parameters						
Atom type	Element	Charge	Sigma, nm	Epsilon, kcal/mol	Reference	Notes
opls_144	H	0.115	0.242	0.03	23	-
opls_143	C	-0.23	0.355	0.076	23	-
opls_142	C	-0.115	0.355	0.076	23	-

Bond parameters					
Bond	Elements	k, kcal/mol^{-1} Å^2	r_0, nm	Reference	Notes
opls_144-opls_143	C-H	340	0.108	26	-
opls_143-opls_142	C-C	549	0.134	26	-
opls_142-opls_144	C-H	340	0.108	26	-
opls_142-opls_136	C-C	317	0.151	26	-

Angle parameters					
Angle	Elements	k, kcal/mol^{-1} deg^2	θ_0, deg	Reference	Notes
opls_144-opls_143-opls_144	H-C-H	35	117	N/A	1
opls_144-opls_143-opls_142	H-C-C	35	120	29	
opls_143-opls_142-opls_136	C-C-C	70	124	N/A	1
opls_143-opls_142-opls_144	C-C-H	35	120	29	
opls_144-opls_142-opls_136	H-C-C	35	117	N/A	1
opls_142-opls_136-opls_136	C-C-C	63	111.1	26	
opls_142-opls_136-opls_140	C-C-H	35	109.5	26	

[1] No reference found. Parameters used from GROMACS *as is*.

Dihedral parameters							
Dihedral	Elements	k1, kcal/mol	k2, kcal/mol	k3, kcal/mol	k4, kcal/mol	Reference	Notes
opls_144-opls_143-opls_142-opls_136	H-C-C-C	0.0	14.0	0.0	0.0	N/A	1
opls_144-opls_143-opls_142-opls_144	H-C-C-H	0.0	14.0	0.0	0.0	N/A	1
opls_143-opls_142-opls_136-opls_136	C-C-C-C	0.346	0.405	-0.904	0.0	N/A	1
opls_143-opls_142-opls_136-opls_140	C-C-C-H	0.0	0.0	-0.372	0.0	23	-
opls_144-opls_142-opls_136-opls_136	H-C-C-C	0.0	0.0	0.3	0.0	N/A	2
opls_144-opls_142-opls_136-opls_140	H-C-C-H	0.0	0.0	0.318	0.0	N/A	1
opls_142-opls_136-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	N/A	1
opls_142-opls_136-opls_136-opls_140	C-C-C-H	0.0	0.0	0.366	0.0	N/A	1

[1] No reference found. Parameters used from GROMACS *as is*.
[2] Parameters not found in GROMACS or the literature. Parameters for alkane C-C-C-H dihedrals have been used.

Improper parameters						
Improper	Elements	γ, degrees	K_ϕ, kcal/mol	n	Reference	Notes
opls_142-opls_143-opls_144-opls_144	C-C-H-H	180	21.0	2	N/A	1
opls_143-opls_142-opls_144-opls_136	C-C-H-C	180	30.0	2	N/A	1

[1] No reference found. Parameters used from GROMACS *as is*.

Fluorophenyl

Nonbonded parameters						
Atom type	Element	Charge	Sigma, nm	Epsilon, kcal/mol	Reference	Notes
opls_719	F	-0.22	0.285	0.061	30	-
opls_718	C	0.22	0.355	0.07	30	-
opls_145	C	-0.115	0.355	0.07	23	-
opls_146	H	0.115	0.242	0.03	23	-
opls_149	C	-0.005	0.35	0.066	23	-
opls_140	H	0.06	0.25	0.03	23	-

Bond parameters					
Bond	Elements	k, kcal/mol^{-1} Å^2	r_0, nm	Reference	Notes
opls_719-opls_718	F-C	420	0.1354	31	-
opls_718-opls_145	C-C	469	0.14	26	-
opls_145-opls_146	C-H	367	0.108	32	-
opls_145-opls_145	C-C	469	0.14	26	-
opls_145-opls_149	C-C	317	0.151	26	-
opls_149-opls_140	C-H	340	0.109	23	-
opls_149-opls_136	C-C	268	0.1529	23	-

Angle parameters					
Angle	Elements	k, kcal/mol^{-1} deg^2	θ_0, deg	Reference	Notes
opls_719-opls_718-opls_145	F-C-C	80	120	31	-
opls_718-opls_145-opls_146	C-C-H	35	120	26	-
opls_718-opls_145-opls_145	C-C-C	63	120	27	-
opls_146-opls_145-opls_145	H-C-C	35	120	26	-
opls_145-opls_718-opls_145	C-C-C	63	120	27	-
opls_145-opls_145-opls_145	C-C-C	63	120	27	-
opls_145-opls_145-opls_149	C-C-C	70	120	26	-
opls_145-opls_149-opls_136	C-C-C	63	114	26	-
opls_145-opls_149-opls_140	C-C-H	35	109.5	26	-
opls_149-opls_136-opls_136	C-C-C	58.35	112.7	23	-
opls_149-opls_136-opls_140	C-C-H	37.5	110.7	23	-
opls_140-opls_149-opls_140	H-C-H	33	107.8	23	-

Dihedral parameters							
Dihedral	Elements	k1, kcal/mol	k2, kcal/mol	k3, kcal/mol	k4, kcal/mol	Reference	Notes
opls_719-opls_718-opls_145-opls_145	F-C-C-C	0.0	7.25	0.0	0.0	27	-
opls_719-opls_718-opls_145-opls_146	F-C-C-H	0.0	7.25	0.0	0.0	27	-
opls_718-opls_145-opls_145-opls_145	C-C-C-C	0.0	7.25	0.0	0.0	27	-
opls_718-opls_145-opls_145-opls_146	C-C-C-H	0.0	7.25	0.0	0.0	27	-
opls_146-opls_145-opls_718-opls_145	H-C-C-C	0.0	7.25	0.0	0.0	27	-
opls_146-opls_145-opls_145-opls_146	H-C-C-H	0.0	7.25	0.0	0.0	27	-
opls_146-opls_145-opls_145-opls_145	H-C-C-C	0.0	7.25	0.0	0.0	27	-
opls_146-opls_145-opls_145-opls_149	H-C-C-C	0.0	7.25	0.0	0.0	27	-
opls_145-opls_145-opls_145-opls_145	C-C-C-C	0.0	7.25	0.0	0.0	27	-
opls_145-opls_145-opls_145-opls_149	C-C-C-C	0.0	7.25	0.0	0.0	27	-
opls_145-opls_718-opls_145-opls_145	C-C-C-C	0.0	7.25	0.0	0.0	27	-
opls_145-opls_145-opls_149-opls_136	C-C-C-C	0.0	0.0	0.0	0.0	23	-
opls_145-opls_145-opls_149-opls_140	C-C-C-H	0.0	0.0	0.0	0.0	23	-
opls_145-opls_149-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	N/A	1
opls_145-opls_149-opls_136-opls_140	C-C-C-H	0.0	0.0	0.462	0.0	23	-

[1] No reference found. Parameters used from GROMACS *as is*. GROMACS uses same parameters as alkane C-C-C-C.

Improper parameters						
Improper	Elements	γ, degrees	K_ϕ, kcal/mol	n	Reference	Notes
opls_719-opls_718-opls_145-opls_145	F-C-C-C	180	2.2	2	27	-
opls_146-opls_145-opls_718-opls_145	H-C-C-C	180	2.2	2	27	-
opls_146-opls_145-opls_145-opls_145	H-C-C-C	180	2.2	2	27	-
opls_149-opls_145-opls_145-opls_145	C-C-C-C	180	2.2	2	27	-

Hydroxyl

Nonbonded parameters						
Atom type	Element	Charge	Sigma, nm	Epsilon, kcal/mol	Reference	Notes
opls_155	H	0.418	0	0	23	-
opls_154	O	-0.683	0.312	0.17	23	-
opls_157	C	0.145	0.35	0.066	23	-
opls_140	H	0.06	0.25	0.03	23	-

Bond parameters					
Bond	Elements	k, kcal/mol^{-1} Å^2	r_0, nm	Reference	Notes
opls_155-opls_154	H-O	553	0.0945	26	-
opls_154-opls_157	O-C	320	0.141	26	-
opls_157-opls_140	C-H	340	0.109	23	-
opls_157-opls_136	C-C	268	0.1529	23	-

Angle parameters					
Angle	Elements	k, kcal/mol^{-1} deg^2	θ_0, deg	Reference	Notes
opls_155-opls_154-opls_157	H-O-C	55	108.5	26	-
opls_154-opls_157-opls_136	O-C-C	50	109.5	26	-
opls_154-opls_157-opls_140	O-C-H	35	109.5	26	-
opls_140-opls_157-opls_140	H-C-H	33	107.8	23	-
opls_140-opls_157-opls_136	H-C-C	37.5	110.7	23	-
opls_157-opls_136-opls_136	C-C-C	58.35	112.7	23	-
opls_157-opls_136-opls_140	C-C-H	37.5	110.7	23	-

Dihedral parameters							
Dihedral	Elements	k1, kcal/mol	k2, kcal/mol	k3, kcal/mol	k4, kcal/mol	Reference	Notes
opls_155-opls_154-opls_157-opls_136	H-O-C-C	-0.356	-0.174	0.492	0.0	23	-
opls_155-opls_154-opls_157-opls_140	H-O-C-H	0.0	0.0	0.45	0.0	23	-
opls_154-opls_157-opls_136-opls_136	O-C-C-C	1.711	-0.5	0.663	0.0	23	-
opls_154-opls_157-opls_136-opls_140	O-C-C-H	0.0	0.0	0.468	0.0	23	-
opls_140-opls_157-opls_136-opls_136	H-C-C-C	0.0	0.0	0.3	0.0	25	-
opls_140-opls_157-opls_136-opls_140	H-C-C-H	0.0	0.0	0.3	0.0	25	-
opls_157-opls_136-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	25	-
opls_157-opls_136-opls_136-opls_140	C-C-C-H	0.0	0.0	0.3	0.0	25	-

Isopropyl

Nonbonded parameters						
Atom type	Element	Charge	Sigma, nm	Epsilon, kcal/mol	Reference	Notes
opls_140	H	0.06	0.25	0.03	23	-
opls_135	C	-0.18	0.35	0.066	23	-
opls_137	C	-0.06	0.35	0.066	23	-

Bond parameters					
Bond	Elements	k, kcal/mol^{-1} Å^2	r_0, nm	Reference	Notes
opls_140-opls_135	H-C	340	0.109	23	-
opls_135-opls_137	C-C	268	0.1529	23	-
opls_137-opls_140	C-H	340	0.109	23	-
opls_137-opls_136	C-C	268	0.1529	23	-

Angle parameters					
Angle	Elements	k, kcal/mol^{-1} deg^2	θ_0, deg	Reference	Notes
opls_140-opls_135-opls_140	H-C-H	33	107.8	23	-
opls_140-opls_135-opls_137	H-C-C	37.5	110.7	23	-
opls_135-opls_137-opls_135	C-C-C	58.35	112.7	23	-
opls_135-opls_137-opls_140	C-C-H	37.5	110.7	23	-
opls_135-opls_137-opls_136	C-C-C	58.35	112.7	23	-
opls_140-opls_137-opls_136	H-C-C	37.5	110.7	23	-
opls_137-opls_136-opls_136	C-C-C	58.35	112.7	23	-
opls_137-opls_136-opls_140	C-C-H	37.5	110.7	23	-

Dihedral parameters							
Dihedral	Elements	k1, kcal/mol	k2, kcal/mol	k3, kcal/mol	k4, kcal/mol	Reference	Notes
opls_140-opls_135-opls_137-opls_140	H-C-C-H	0.0	0.0	0.3	0.0	25	-
opls_140-opls_135-opls_137-opls_135	H-C-C-C	0.0	0.0	0.3	0.0	25	-
opls_140-opls_135-opls_137-opls_136	H-C-C-C	0.0	0.0	0.3	0.0	25	-
opls_140-opls_137-opls_136-opls_136	H-C-C-C	0.0	0.0	0.3	0.0	25	-
opls_140-opls_137-opls_136-opls_140	H-C-C-H	0.0	0.0	0.3	0.0	25	-
opls_135-opls_137-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	25	-
opls_135-opls_137-opls_136-opls_140	C-C-C-H	0.0	0.0	0.3	0.0	25	-
opls_137-opls_136-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	25	-
opls_137-opls_136-opls_136-opls_140	C-C-C-H	0.0	0.0	0.3	0.0	25	-

Methoxy

Nonbonded parameters						
Atom type	Element	Charge	Sigma, nm	Epsilon, kcal/mol	Reference	Notes
opls_185	H	0.03	0.25	0.03	23	-
opls_181	C	0.11	0.35	0.066	23	-
opls_180	O	-0.4	0.29	0.14	23	-
opls_182	C	0.14	0.35	0.066	23	-

Bond parameters					
Bond	Elements	k, kcal/mol^{-1} Å^2	r_0, nm	Reference	Notes
opls_185-opls_181	H-C	340	0.109	23	-
opls_181-opls_180	C-O	320	0.141	26	-
opls_180-opls_182	O-C	320	0.141	26	-
opls_182-opls_185	C-H	340	0.109	23	-
opls_182-opls_136	C-C	268	0.1529	23	-

Angle parameters					
Angle	Elements	k, kcal/mol^{-1} deg^2	θ_0, deg	Reference	Notes
opls_185-opls_181-opls_185	H-C-H	33	107.8	23	-
opls_185-opls_181-opls_180	H-C-O	35	109.5	26	-
opls_181-opls_180-opls_182	C-O-C	60	109.5	26	-
opls_180-opls_182-opls_136	O-C-C	50	109.5	26	-
opls_180-opls_182-opls_185	O-C-H	35	109.5	26	-
opls_185-opls_182-opls_185	H-C-H	33	107.8	23	-
opls_185-opls_182-opls_136	H-C-C	37.5	110.7	23	-
opls_182-opls_136-opls_136	C-C-C	58.35	112.7	23	-
opls_182-opls_136-opls_140	C-C-H	37.5	110.7	23	-

Dihedral parameters							
Dihedral	Elements	k1, kcal/mol	k2, kcal/mol	k3, kcal/mol	k4, kcal/mol	Reference	Notes
opls_185-opls_181-opls_180-opls_182	H-C-O-C	0.0	0.0	0.76	0.0	23	-
opls_181-opls_180-opls_182-opls_136	C-O-C-C	0.65	-0.25	0.67	0.0	23	-
opls_181-opls_180-opls_182-opls_185	C-O-C-H	0.0	0.0	0.76	0.0	23	-
opls_180-opls_182-opls_136-opls_136	O-C-C-C	1.711	-0.5	0.663	0.0	23	-
opls_180-opls_182-opls_136-opls_140	O-C-C-H	0.0	0.0	0.468	0.0	23	-
opls_185-opls_182-opls_136-opls_136	H-C-C-C	0.0	0.0	0.3	0.0	25	-
opls_185-opls_182-opls_136-opls_140	H-C-C-H	0.0	0.0	0.3	0.0	25	-
opls_182-opls_136-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	25	-
opls_182-opls_136-opls_136-opls_140	C-C-C-H	0.0	0.0	0.3	0.0	25	-

Nitro

Nonbonded parameters						
Atom type	Element	Charge	Sigma, nm	Epsilon, kcal/mol	Reference	Notes
opls_761	O	-0.37	0.296	0.17	25	-
opls_760	N	0.54	0.325	0.12	25	-
opls_764	C	0.08	0.35	0.066	25	-
opls_763	H	0.06	0.25	0.015	25	-

Bond parameters					
Bond	Elements	k, kcal/mol^{-1} Å^2	r_0, nm	Reference	Notes
opls_761-opls_760	O-N	550	0.1225	25	-
opls_760-opls_764	N-C	375	0.149	25	-
opls_764-opls_763	C-H	340	0.109	23	-
opls_764-opls_136	C-C	268	0.1529	23	-

Angle parameters					
Angle	Elements	k, kcal/mol^{-1} deg^2	θ_0, deg	Reference	Notes
opls_761-opls_760-opls_761	O-N-O	80	125	25	-
opls_761-opls_760-opls_764	O-N-C	80	117.5	25	-
opls_760-opls_764-opls_763	N-C-H	35	105	25	-
opls_760-opls_764-opls_136	N-C-C	63	111.1	25	-
opls_763-opls_764-opls_763	H-C-H	33	107.8	23	-
opls_763-opls_764-opls_136	H-C-C	37.5	110.7	23	-
opls_764-opls_136-opls_136	C-C-C	58.35	112.7	23	-
opls_764-opls_136-opls_140	C-C-H	37.5	110.7	23	-

Dihedral parameters							
Dihedral	Elements	k1, kcal/mol	k2, kcal/mol	k3, kcal/mol	k4, kcal/mol	Reference	Notes
opls_761-opls_760-opls_764-opls_136	O-N-C-C	0.0	0.4	0.0	0.0	25	-
opls_761-opls_760-opls_764-opls_763	O-N-C-H	0.0	0.0	0.0	0.0	25	-
opls_760-opls_764-opls_136-opls_136	N-C-C-C	-1.54	-0.214	0.0	0.0	25	1
opls_760-opls_764-opls_136-opls_140	N-C-C-H	0.0	0.0	-0.225	0.0	25	-
opls_763-opls_764-opls_136-opls_136	H-C-C-C	0.0	0.0	0.3	0.0	25	-
opls_763-opls_764-opls_136-opls_140	H-C-C-H	0.0	0.0	0.3	0.0	25	-
opls_764-opls_136-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	25	-
opls_764-opls_136-opls_136-opls_140	C-C-C-H	0.0	0.0	0.3	0.0	25	-

[1] Parameters did not exist in GROMACS. Parameters from Ref. 25 have been used.

Nitrophenyl

Nonbonded parameters						
Atom type	Element	Charge	Sigma, nm	Epsilon, kcal/mol	Reference	Notes
opls_761	O	-0.37	0.296	0.17	25	-
opls_767	N	0.65	0.325	0.12	25	-
opls_768	C	0.09	0.355	0.07	25	-
opls_145	C	-0.115	0.355	0.07	23	-
opls_146	H	0.115	0.242	0.03	23	-
opls_149	C	-0.005	0.35	0.066	23	-
opls_140	H	0.06	0.25	0.03	23	-

Bond parameters					
Bond	Elements	k, kcal/mol^{-1} Å^2	r_0, nm	Reference	Notes
opls_761-opls_767	O-N	550	0.1225	25	-
opls_767-opls_768	N-C	400	0.146	25	-
opls_768-opls_145	C-C	469	0.14	27	-
opls_145-opls_146	C-H	367	0.108	32	-
opls_145-opls_149	C-C	317	0.151	26	-
opls_149-opls_140	C-H	340	0.109	23	-
opls_149-opls_136	C-C	268	0.1529	23	-

Angle parameters					
Angle	Elements	k, kcal/mol^{-1} deg^2	θ_0, deg	Reference	Notes
opls_761-opls_767-opls_761	O-N-O	80	125	25	-
opls_761-opls_767-opls_768	O-N-C	80	117.5	25	-
opls_767-opls_768-opls_145	N-C-C	85	120	25	-
opls_768-opls_145-opls_145	C-C-C	63	120	27	-
opls_768-opls_145-opls_146	C-C-H	35	120	26	-
opls_145-opls_768-opls_145	C-C-C	63	120	26	-
opls_146-opls_145-opls_768	H-C-C	35	120	26	-
opls_146-opls_145-opls_145	H-C-C	35	120	26	-
opls_145-opls_145-opls_145	C-C-C	63	120	27	-
opls_145-opls_145-opls_149	C-C-C	70	120	26	-
opls_145-opls_149-opls_136	C-C-C	63	114	26	-
opls_145-opls_149-opls_140	C-C-H	35	109.5	26	-
opls_140-opls_149-opls_140	H-C-H	33	107.8	23	-
opls_140-opls_149-opls_136	H-C-C	37.5	110.7	23	-
opls_149-opls_136-opls_136	C-C-C	58.35	112.7	23	-
opls_149-opls_136-opls_140	C-C-H	37.5	110.7	23	-

Dihedral parameters							
Dihedral	Elements	k1, kcal/mol	k2, kcal/mol	k3, kcal/mol	k4, kcal/mol	Reference	Notes
opls_761-opls_767-opls_768-opls_145	O-N-C-C	0.0	1.15	0.0	0.0	25	-
opls_767-opls_768-opls_145-opls_145	N-C-C-C	0.0	7.25	0.0	0.0	27	-
opls_767-opls_768-opls_145-opls_146	N-C-C-H	0.0	7.25	0.0	0.0	27	-
opls_768-opls_145-opls_145-opls_145	C-C-C-C	0.0	7.25	0.0	0.0	27	-
opls_768-opls_145-opls_145-opls_146	C-C-C-H	0.0	7.25	0.0	0.0	27	-
opls_146-opls_145-opls_768-opls_145	H-C-C-C	0.0	7.25	0.0	0.0	27	-
opls_146-opls_145-opls_145-opls_146	H-C-C-H	0.0	7.25	0.0	0.0	27	-
opls_146-opls_145-opls_145-opls_145	H-C-C-C	0.0	7.25	0.0	0.0	27	-
opls_146-opls_145-opls_145-opls_149	H-C-C-C	0.0	7.25	0.0	0.0	27	-
opls_145-opls_145-opls_145-opls_145	C-C-C-C	0.0	7.25	0.0	0.0	27	-
opls_145-opls_145-opls_145-opls_149	C-C-C-C	0.0	7.25	0.0	0.0	27	-
opls_145-opls_768-opls_145-opls_145	C-C-C-C	0.0	7.25	0.0	0.0	27	-
opls_145-opls_145-opls_149-opls_136	C-C-C-C	0.0	0.0	0.0	0.0	23	-
opls_145-opls_145-opls_149-opls_140	C-C-C-H	0.0	0.0	0.0	0.0	23	-
opls_145-opls_149-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	N/A	1
opls_145-opls_149-opls_136-opls_140	C-C-C-H	0.0	0.0	0.462	0.0	23	-

[1] No reference found. Parameters used from GROMACS *as is*. GROMACS uses same parameters as alkane C-C-C-C.

Improper parameters						
Improper	Elements	γ, degrees	K_ϕ, kcal/mol	n	Reference	Notes
opls_767-opls_768-opls_145-opls_145	N-C-C-C	180	2.2	2	27	-
opls_146-opls_145-opls_768-opls_145	H-C-C-C	180	2.2	2	27	-
opls_146-opls_145-opls_145-opls_145	H-C-C-C	180	2.2	2	27	-
opls_149-opls_145-opls_145-opls_145	C-C-C-C	180	2.2	2	27	-

Perfluoromethyl

Nonbonded parameters						
Atom type	Element	Charge	Sigma, nm	Epsilon, kcal/mol	Reference	Notes
opls_965	F	-0.12	0.295	0.053	33	-
opls_961	C	0.36	0.35	0.066	33	-

Bond parameters					
Bond	Elements	k, kcal/mol^{-1} Å^2	r_0, nm	Reference	Notes
opls_965-opls_961	F-C	367	0.1332	33	-
opls_961-opls_136	C-C	268	0.1529	33	-

Angle parameters					
Angle	Elements	k, kcal/mol^{-1} deg^2	θ_0, deg	Reference	Notes
opls_965-opls_961-opls_965	F-C-F	77	109.1	33	-
opls_965-opls_961-opls_136	F-C-C	50	109.5	33	-
opls_961-opls_136-opls_136	C-C-C	58.35	112.7	23	-
opls_961-opls_136-opls_140	C-C-H	37.5	110.7	23	-

Dihedral parameters							
Dihedral	Elements	k1, kcal/mol	k2, kcal/mol	k3, kcal/mol	k4, kcal/mol	Reference	Notes
opls_965-opls_961-opls_136-opls_136	F-C-C-C	0.0	0.0	0.463	0.0	34	1
opls_965-opls_961-opls_136-opls_140	F-C-C-H	0.0	0.0	0.29	0.0	34	1
opls_961-opls_136-opls_136-opls_136	C-C-C-C	0.104	-0.312	0.048	-0.083	34	1
opls_961-opls_136-opls_136-opls_140	C-C-C-H	0.0	0.0	0.133	0.0	34	1

[1] These parameters are not in GROMACS, as the GROMACS parameters do not distinguish between dihedrals for fluorinated and hydrogenated carbons.

Phenyl

Nonbonded parameters						
Atom type	Element	Charge	Sigma, nm	Epsilon, kcal/mol	Reference	Notes
opls_145	C	-0.115	0.355	0.07	23	-
opls_146	H	0.115	0.242	0.03	23	-
opls_149	C	-0.005	0.35	0.066	23	-
opls_140	H	0.06	0.25	0.03	23	-

Bond parameters					
Bond	Elements	k, kcal/mol^{-1} Å^2	r_0, nm	Reference	Notes
opls_146-opls_145	H-C	367	0.108	32	-
opls_145-opls_149	C-C	317	0.151	26	-
opls_149-opls_140	C-H	340	0.109	23	-
opls_149-opls_136	C-C	268	0.1529	23	-
opls_145-opls_145	C-C	469	0.14	26	-

Angle parameters					
Angle	Elements	k, kcal/mol^{-1} deg^2	θ_0, deg	Reference	Notes
opls_146-opls_145-opls_145	H-C-C	35	120	26	-
opls_145-opls_145-opls_145	C-C-C	63	120	27	-
opls_145-opls_145-opls_149	C-C-C	70	120	26	-
opls_145-opls_149-opls_136	C-C-C	63	114	26	-
opls_145-opls_149-opls_140	C-C-H	35	109.5	26	-
opls_140-opls_149-opls_140	H-C-H	33	107.8	23	-
opls_140-opls_149-opls_136	H-C-C	37.5	110.7	23	-
opls_149-opls_136-opls_136	C-C-C	58.35	112.7	23	-
opls_149-opls_136-opls_140	C-C-H	37.5	110.7	23	-

Dihedral parameters							
Dihedral	Elements	k1, kcal/mol	k2, kcal/mol	k3, kcal/mol	k4, kcal/mol	Reference	Notes
opls_146-opls_145-opls_145-opls_146	H-C-C-H	0.0	7.25	0.0	0.0	27	-
opls_146-opls_145-opls_145-opls_145	H-C-C-C	0.0	7.25	0.0	0.0	27	-
opls_146-opls_145-opls_145-opls_149	H-C-C-C	0.0	7.25	0.0	0.0	27	-
opls_145-opls_145-opls_145-opls_145	C-C-C-C	0.0	7.25	0.0	0.0	27	-
opls_145-opls_145-opls_145-opls_149	C-C-C-C	0.0	7.25	0.0	0.0	27	-
opls_145-opls_145-opls_149-opls_136	C-C-C-C	0.0	0.0	0.0	0.0	23	-
opls_145-opls_145-opls_149-opls_140	C-C-C-H	0.0	0.0	0.0	0.0	23	-
opls_145-opls_149-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	N/A	1
opls_145-opls_149-opls_136-opls_140	C-C-C-H	0.0	0.0	0.462	0.0	23	-

[1] No reference found. Parameters used from GROMACS *as is*. GROMACS uses same parameters as alkane C-C-C-C.

Improper parameters						
Improper	Elements	γ, degrees	K_ϕ, kcal/mol	n	Reference	Notes
opls_146-opls_145-opls_145-opls_145	H-C-C-C	180	2.2	2	27	-
opls_149-opls_145-opls_145-opls_145	C-C-C-C	180	2.2	2	27	-

Pyrrole

Nonbonded parameters						
Atom type	Element	Charge	Sigma, nm	Epsilon, kcal/mol	Reference	Notes
opls_547	H	0.118	0.242	0.03	32	-
opls_546	H	0.155	0.242	0.03	32	-
opls_544	C	-0.149	0.355	0.07	32	-
opls_543	C	-0.163	0.355	0.07	32	-
opls_542	N	-0.239	0.325	0.17	32	-
opls_545	H	0.317	0	0	32	-
opls_679	C	0.035	0.35	0.066	N/A	1
opls_140	H	0.06	0.25	0.03	23	-

[1] No reference found. Parameters used from GROMACS *as is*.

Bond parameters					
Bond	Elements	k, kcal/mol^{-1} Å^2	r_0, nm	Reference	Notes
opls_547-opls_544	H-C	367	0.108	32	-
opls_544-opls_543	C-C	546	0.1367	32	-
opls_546-opls_543	H-C	367	0.108	32	-
opls_543-opls_542	C-N	427	0.1381	32	-
opls_542-opls_545	N-H	434	0.101	32	-
opls_544-opls_544	C-C	469	0.1424	32	-
opls_543-opls_679	C-C	317	0.1504	N/A	1
opls_679-opls_140	C-H	340	0.109	23	-
opls_679-opls_136	C-C	268	0.1529	23	-

[1] No reference found. Parameters used from GROMACS *as is*.

Angle parameters					
Angle	Elements	k, kcal/mol^{-1} deg^2	θ_0, deg	Reference	Notes
opls_546-opls_543-opls_544	H-C-C	35	132.1	32	-
opls_546-opls_543-opls_542	H-C-N	35	121.6	32	-
opls_543-opls_544-opls_547	C-C-H	35	125.7	32	-
opls_543-opls_544-opls_544	C-C-C	70	107.3	32	-
opls_543-opls_542-opls_545	C-N-H	35	120	32	-
opls_543-opls_542-opls_543	C-N-C	70	109.8	32	-
opls_547-opls_544-opls_544	H-C-C	35	127.5	32	-
opls_545-opls_542-opls_543	H-N-C	35	120	32	-
opls_542-opls_543-opls_544	N-C-C	70	107.7	32	-
opls_542-opls_543-opls_679	N-C-C	70	121.6	N/A	1
opls_544-opls_543-opls_679	C-C-C	70	132.1	N/A	1
opls_543-opls_679-opls_136	C-C-C	63	114	N/A	1
opls_543-opls_679-opls_140	C-C-H	35	109.5	N/A	1
opls_140-opls_679-opls_140	H-C-H	33	107.8	23	-
opls_140-opls_679-opls_136	H-C-C	37.5	110.7	23	-
opls_679-opls_136-opls_136	C-C-C	58.35	112.7	23	-
opls_679-opls_136-opls_140	C-C-H	37.5	110.7	23	-

[1] No reference found. Parameters used from GROMACS *as is*.

Dihedral parameters							
Dihedral	Elements	k1, kcal/mol	k2, kcal/mol	k3, kcal/mol	k4, kcal/mol	Reference	Notes
opls_546-opls_543-opls_544-opls_547	H-C-C-H	0.0	7.25	0.0	0.0	N/A	1
opls_546-opls_543-opls_544-opls_544	H-C-C-C	0.0	7.25	0.0	0.0	N/A	1
opls_546-opls_543-opls_542-opls_545	H-C-N-H	0.0	3.0	0.0	0.0	N/A	1
opls_546-opls_543-opls_542-opls_543	H-C-N-C	0.0	3.2	0.0	0.0	N/A	1
opls_543-opls_544-opls_544-opls_543	C-C-C-C	0.0	7.25	0.0	0.0	N/A	1
opls_543-opls_544-opls_544-opls_547	C-C-C-H	0.0	7.25	0.0	0.0	N/A	1
opls_543-opls_542-opls_543-opls_544	C-N-C-C	0.0	3.2	0.0	0.0	N/A	1
opls_543-opls_542-opls_543-opls_679	C-N-C-C	0.0	3.2	0.0	0.0	N/A	1
opls_544-opls_543-opls_542-opls_543	C-C-N-C	0.0	3.2	0.0	0.0	N/A	1
opls_544-opls_543-opls_542-opls_545	C-C-N-H	0.0	3.2	0.0	0.0	N/A	1
opls_544-opls_544-opls_543-opls_542	C-C-C-N	0.0	7.25	0.0	0.0	N/A	1
opls_544-opls_544-opls_543-opls_679	C-C-C-C	0.0	7.25	0.0	0.0	N/A	1
opls_547-opls_544-opls_543-opls_542	H-C-C-N	0.0	7.25	0.0	0.0	N/A	1
opls_545-opls_542-opls_543-opls_679	H-N-C-C	0.0	3.2	0.0	0.0	N/A	1
opls_542-opls_543-opls_679-opls_136	N-C-C-C	1.7	-0.6	0.0	0.0	N/A	1
opls_542-opls_543-opls_679-opls_140	N-C-C-H	0.0	0.0	0.42	0.0	N/A	1
opls_547-opls_544-opls_543-opls_679	H-C-C-C	0.0	7.25	0.0	0.0	N/A	1
opls_544-opls_543-opls_679-opls_136	C-C-C-C	0.0	0.0	0.0	0.0	N/A	1
opls_544-opls_543-opls_679-opls_140	C-C-C-H	0.0	0.0	0.0	0.0	N/A	1
opls_543-opls_679-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	N/A	2
opls_543-opls_679-opls_136-opls_140	C-C-C-H	0.0	0.0	0.462	0.0	N/A	1
opls_140-opls_679-opls_136-opls_136	H-C-C-C	0.0	0.0	0.3	0.0	N/A	1
opls_140-opls_679-opls_136-opls_140	H-C-C-H	0.0	0.0	0.3	0.0	N/A	1
opls_679-opls_136-opls_136-opls_136	C-C-C-C	1.3	-0.05	0.2	0.0	N/A	1
opls_679-opls_136-opls_136-opls_140	C-C-C-H	0.0	0.0	0.3	0.0	N/A	1

[1] No reference found. Parameters used from GROMACS *as is*.
[2] Parameters don't exist in GROMACS or the literature. Parameters for C(aromatic)-C-C-C dihedrals have been used.

Improper parameters						
Improper	Elements	γ, degrees	K_ϕ, kcal/mol	n	Reference	Notes
opls_546-opls_543-opls_542-opls_544	H-C-N-C	180	2.2	2	27	-
opls_547-opls_544-opls_543-opls_544	H-C-C-C	180	2.2	2	27	-
opls_679-opls_543-opls_542-opls_544	C-C-N-C	180	2.2	2	27	-
opls_545-opls_542-opls_543-opls_543	H-N-C-C	180	2.0	2	26	-

References

(1) Summers, A. Z.; Iacovella, C. R.; Cummings, P. T.; M^{c}Cabe, C. *Langmuir* **2017**, *33*, 11270–11280.

(2) Litton, D. A.; Garofalini, S. H. *Journal of Applied Physics* **2001**, *89*, 6013–6023.

(3) van Duin, A. C. T.; Strachan, A.; Stewman, S.; Zhang, Q.; Xu, X.; Goddard, W. A. *The Journal of Physical Chemistry A* **2003**, *107*, 3803–3811.

(4) Fogarty, J. C.; Aktulga, H. M.; Grama, A. Y.; van Duin, A. C. T.; Pandit, S. A. *The Journal of Chemical Physics* **2010**, *132*, 174704.

(5) Zhuravlev, L. *Colloids and Surfaces A: Physicochemical and Engineering Aspects* **2000**, *173*, 1–38.

(6) Hartkamp, R.; Siboulet, B.; Dufrêche, J.-F.; Coasne, B. *Physical Chemistry Chemical Physics* **2015**, *17*, 24683–24695.

(7) mBuild amorphous silica recipe. `https://github.com/mosdef-hub/mbuild/blob/master/mbuild/recipes/silica_interface.py`.

(8) Klein, C.; Sallai, J.; Jones, T. J.; Iacovella, C. R.; M^{c}Cabe, C.; Cummings, P. T. *Molecular Modeling and Simulation* **2016**, 79–92.

(9) Black, J. E.; Iacovella, C. R.; Cummings, P. T.; M^{c}Cabe, C. *Langmuir* **2015**, *31*, 3086–3093.

(10) Labute, P. *Journal of Molecular Graphics and Modelling* **2000**, *18*, 464–477.

(11) Baumgärtner, A. *The Journal of Chemical Physics* **1993**, *98*, 7496–7501.

(12) Balaban, A. T. *Chemical Physics Letters* **1982**, *89*, 399–404.

(13) Bertz, S. H. *Journal of the American Chemical Society* **1981**, *103*, 3599–3601.

(14) Hall, L. H.; Kier, L. B. *Reviews in Computational Chemistry* **2007**, 367–422.

(15) Arteca, G. A. *Reviews in Computational Chemistry* **2007**, 191–253.

(16) Todeschini, R.; Consonni, V. *Methods and Principles in Medicinal Chemistry* **2000**,

(17) Bonchev, D.; Trinajstić, N. *The Journal of Chemical Physics* **1977**, *67*, 4517–4533.

(18) Wildman, S. A.; Crippen, G. M. *Journal of Chemical Information and Computer Sciences* **1999**, *39*, 868–873.

(19) Sauer, W. H. B.; Schwarz, M. K. *Journal of Chemical Information and Computer Sciences* **2003**, *43*, 987–1003.

(20) Firth, N. C.; Brown, N.; Blagg, J. *Journal of Chemical Information and Modeling* **2012**, *52*, 2516–2525.

(21) Robinson, D. D.; Barlow, T. W.; Richards, W. G. *Journal of Chemical Information and Computer Sciences* **1997**, *37*, 939–942.

(22) Ertl, P.; Rohde, B.; Selzer, P. *Journal of Medicinal Chemistry* **2000**, *43*, 3714–3717.

(23) Jorgensen, W. L.; Maxwell, D. S.; Tirado-Rives, J. *Journal of the American Chemical Society* **1996**, *118*, 11225–11236.

(24) Lorenz, C.; Webb, E.; Stevens, M.; Chandross, M.; Grest, G. *Tribology Letters* **2005**, *19*, 93–98.

(25) Price, M. L. P.; Ostrovsky, D.; Jorgensen, W. L. *Journal of Computational Chemistry* **2001**, *22*, 1340–1352.

(26) Weiner, S. J.; Kollman, P. A.; Nguyen, D. T.; Case, D. A. *Journal of Computational Chemistry* **1986**, *7*, 230–252.

(27) Rizzo, R. C.; Jorgensen, W. L. *Journal of the American Chemical Society* **1999**, *121*, 4827–4836.

(28) Price, D. J.; Roberts, J. D.; Jorgensen, W. L. *Journal of the American Chemical Society* **1998**, *120*, 9672–9679.

(29) Cornell, W. D.; Cieplak, P.; Bayly, C. I.; Gould, I. R.; Merz, K. M.; Ferguson, D. M.; Spellmeyer, D. C.; Fox, T.; Caldwell, J. W.; Kollman, P. A. *Journal of the American Chemical Society* **1995**, *117*, 5179–5197.

(30) Jorgensen, W. L.; Ulmschneider, J. P.; Tirado-Rives, J. *The Journal of Physical Chemistry B* **2004**, *108*, 16264–16270.

(31) Jorgensen, W. L.; Schyman, P. *Journal of Chemical Theory and Computation* **2012**, *8*, 3895–3901.

(32) McDonald, N. A.; Jorgensen, W. L. *The Journal of Physical Chemistry B* **1998**, *102*, 8049–8059.

(33) Watkins, E. K.; Jorgensen, W. L. *The Journal of Physical Chemistry A* **2001**, *105*, 4118–4125.

(34) Pádua, A. A. H. *The Journal of Physical Chemistry A* **2002**, *106*, 10116–10123.