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Supplemental information

Polymer informatics with multi-task learning

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Table S1: **Description of the 15 most important fingerprint components.**

Component	Description
e,main,chain,ring	Ratio of non-H atoms in atomic rings vs. total number of atoms
e,fam,acrylate	1 if the acrylate group is present, 0 otherwise
b,289	Number of methylene groups (R-CH2)
e,fam,polyamides	1 if the polyamide group is present, 0 otherwise
m,MQNs29	Number of cyclic divalent nodes; normalized to the number of atoms
e,ring,dist,shortest	Shortest distance between two atomic rings
a,C3,C3,C3	Atomic triple C3-C3-C3
b,267	Number of methyl groups (R-CH3)
e,side,chain,large,abs	Length of the longest side chain
m,MQNs13	Number of acyclic double bonds in repeat unit; normalized to number of atoms
b,239	Number of ethene groups (R-C2H4)
b,145	Number of phenylenes rings (R-C6H4-R ring)
b,197	Number of C3H6 groups
e,multi,ring,dimer	1 if two overlapping rings are present, 0 otherwise
b,349	Number of H atoms

Table S2: **Compendium of RMSE and R^2 values.** The RMSE and R^2 values are fold averages of the five cross-validation models. The units of the RMSE values are specified in Table 1 of the publication. R^2 values smaller than 0 are omitted.

	RMSE					R^2				
	GP-ST	ST	MT1	MT2-all	MT2-sub	GP-ST	ST	MT1	MT2-all	MT2-sub
T_m	50.35	49.48	50.77	50.45	49.95	0.75	0.76	0.68	0.70	0.72
T_g	33.56	33.76	37.24	36.88	36.19	0.90	0.89	0.85	0.86	0.87
T_d	60.91	60.00	64.33	62.49	60.16	0.63	0.64	0.52	0.58	0.60
λ	0.07	0.08	0.07	0.07	0.07					
c_p	0.19	0.17	0.20	0.22	0.25	0.60	0.57	0.54	0.19	
E_at	0.04	0.05	0.05	0.06	0.11	0.98	0.98	0.94	0.81	0.87
O_i	9.85	7.78	7.37	8.64	7.56		0.26	0.31		0.26
X_c	24.42	20.74	19.08	18.02	18.32					
X_e	17.99	14.71	17.45	14.21	12.56					
ρ	0.07	0.07	0.09	0.08	0.09	0.83	0.83	0.68	0.68	0.77
V_ff	0.03	0.03	0.04	0.03	0.03					
E_gc	0.48	0.49	0.53	0.54	0.48	0.90	0.89	0.85	0.86	0.90
E_gb	0.55	0.57	0.58	0.54	0.43	0.91	0.89	0.89	0.91	0.95
E_ea	0.32	0.32	0.39	0.43	0.33	0.90	0.87	0.81	0.76	0.88
E_i	0.42	0.45	0.45	0.41	0.36	0.77	0.74	0.70	0.71	0.83
n_c	0.10	0.10	0.10	0.09	0.07	0.79	0.78	0.79	0.79	0.91
n_e	0.09	0.06	0.06	0.04	0.03		0.63	0.66	0.78	0.90
ε_0	0.53	0.54	0.54	0.47	0.39	0.68	0.71	0.67	0.71	0.86
$\varepsilon_{1.78}$	1.05	1.02	0.92	0.75	0.50				0.43	0.72
ε_2	1.10	1.05	0.97	0.76	0.44				0.20	0.83
ε_3	1.12	1.13	0.99	0.72	0.63				0.29	0.64
ε_4	0.71	0.65	0.59	0.52	0.27		0.28	0.09	0.32	0.88
ε_5	0.93	1.11	0.79	0.44	0.31				0.15	0.78
ε_6	0.86	0.77	0.77	0.56	0.40					0.59
ε_7	0.48	0.42	0.36	0.41	0.22					0.26
ε_9	0.63	0.70	0.67	0.62	0.32					
ε_{15}	0.33	0.20	0.19	0.14	0.12		0.62	0.60	0.78	0.87
σ_ts	28.09	26.67	26.76	26.25	23.45	0.11	0.38	0.22	0.22	0.50
Y	0.98	0.93	0.90	0.83	0.80		0.38	0.13	0.35	0.49
δ_s	1.50	1.34	1.55	2.02	1.81	0.32	0.59	0.23		0.01
μ_H2	0.36	0.33	0.34	0.23	0.12	0.84	0.84	0.79	0.93	0.98
μ_He	0.26	0.30	0.30	0.21	0.13	0.86	0.82	0.77	0.91	0.97
μ_N2	0.33	0.34	0.32	0.22	0.12	0.85	0.85	0.82	0.93	0.98
μ_O2	0.37	0.36	0.34	0.22	0.13	0.84	0.84	0.82	0.94	0.98
μ_CH4	0.34	0.35	0.32	0.25	0.13	0.87	0.86	0.84	0.92	0.98
μ_CO2	0.39	0.43	0.40	0.28	0.19	0.88	0.84	0.81	0.93	0.97