Supporting Information: Bioplastic Design using Multitask Deep Neural Networks

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Table S1: Optimized hyperparameters of the five cross-validation (CV) models and meta learner (Meta). N_{layers} stands for the number of layers, and S_{con} for the layer after which the property selector vector is concatenated. N_x, D_x, and A_x indicate the number of neurons, dropout rates, and activation functions of the x^{th} dense layer. LR shows the learning rate used by the Adam optimizer.

	Cat.	LR	N_{layers}	S_{con}	N_0	D_0	A_0	N_1	D_1	A_1	N_2	D_2	A_2
CV1	therm	0.001	3	0	550	0.10	relu	450	0.65	relu	450	0.4	gelu
	mech	0.005	2	1	200	0.10	relu	100	0.15	prelu			
	perm	0.001	3	1	400	0.20	relu	450	0.15	gelu	150	0.15	prelu
CV2	therm	0.001	2	1	250	0.20	relu	300	0.00	relu			
	mech	0.001	3	1	250	0.30	prelu	400	0.25	prelu	500	0.4	gelu
	perm	0.001	3	1	500	0.25	prelu	200	0.15	gelu	100	0.1	gelu
CV3	therm	0.001	3	1	550	0.20	relu	300	0.50	relu	250	0.45	gelu
	mech	0.001	3	1	150	0.20	prelu	550	0.10	prelu	300	0.1	gelu
	perm	0.005	3	1	450	0.00	prelu	150	0.10	prelu	300	0.25	relu
CV4	therm	0.001	2	0	450	0.30	prelu	550	0.30	relu			
	mech	0.005	2	1	150	0.35	relu	350	0.35	prelu			
	perm	0.005	3	1	150	0.20	prelu	300	0.00	gelu	200	0.4	prelu
CV5	therm	0.001	2	1	450	0.25	prelu	350	0.05	relu			
	mech	0.001	3	1	400	0.55	relu	250	0.20	gelu	500	0.55	prelu
	perm	0.001	3	1	400	0.25	prelu	150	0.05	tanh	300	0.05	relu
Meta	therm	0.005	2		350	0.10	gelu	150	0.25	relu			
	mech	0.005	3		200	0.35	tanh	300	0.10	prelu	150	0.45	tanh
	mech	0.005	3		200	0.35	tanh	300	0.10	prelu	150	0.45	tanh
	perm	0.001	2		250	0.60	tanh	200	0.35	tanh			

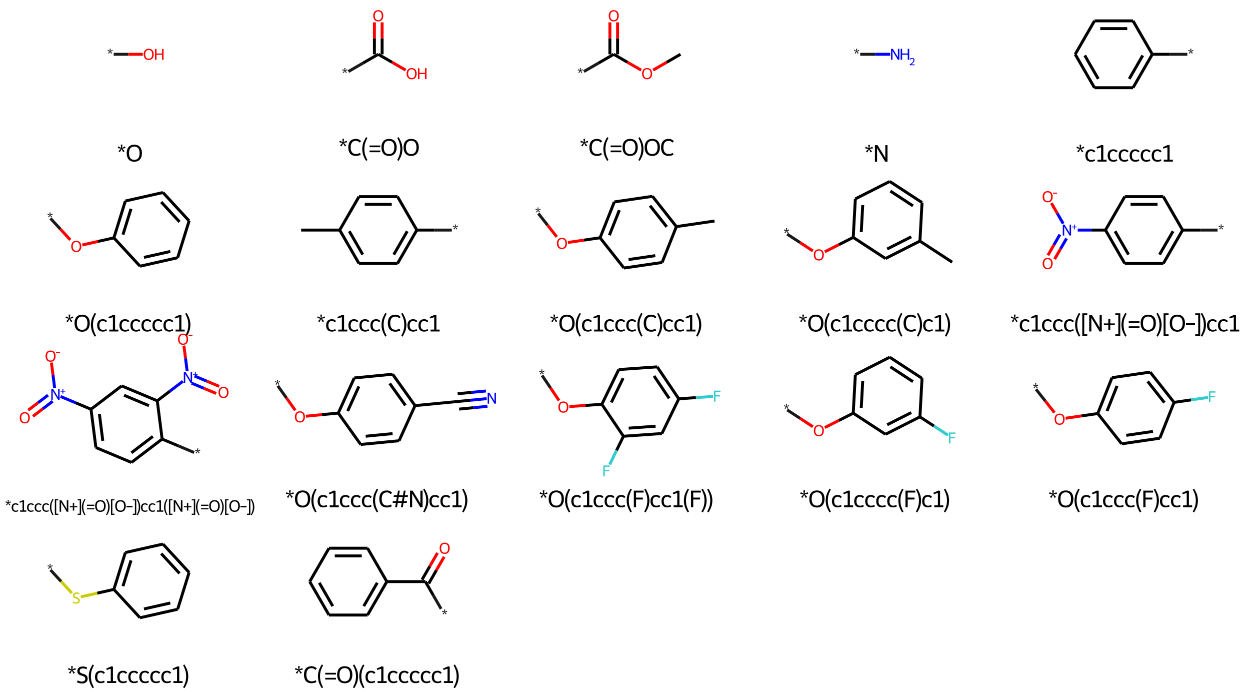

Figure S1: Chemical drawings of the 17 functional groups (R) and SMILES strings. The star ("∗") indicates the connection point to the side-chain of the PHAs.

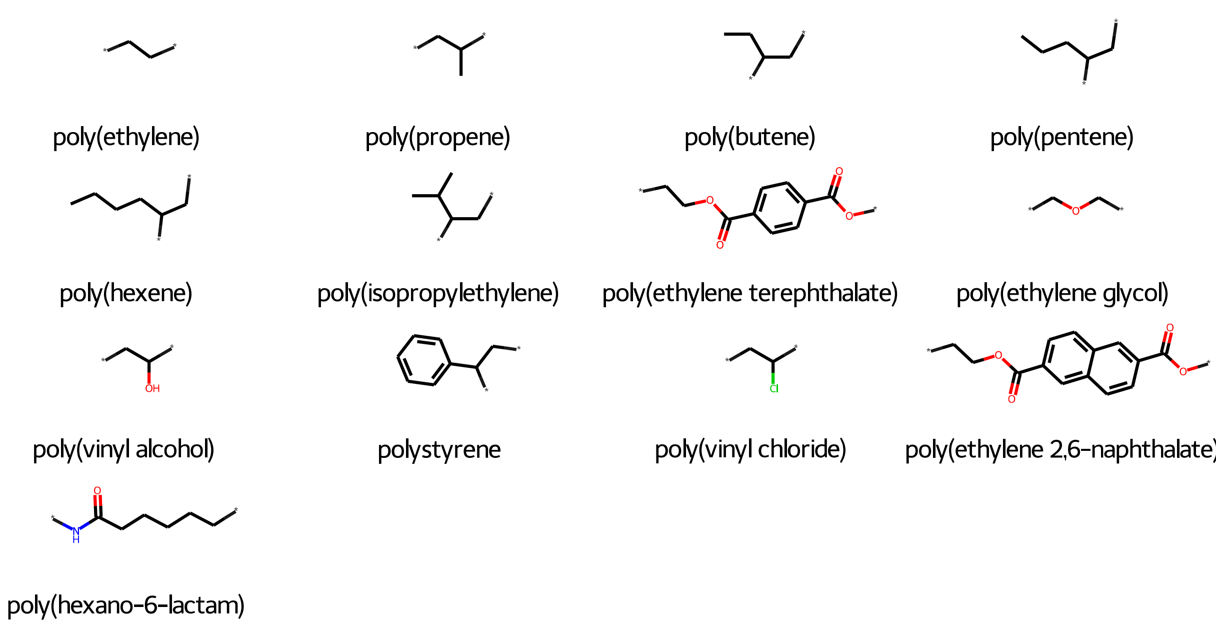

Figure S2: Chemical drawings of the 13 conventional polymers and names. The two stars ("∗") indicate the endpoints of the polymer repeat unit.

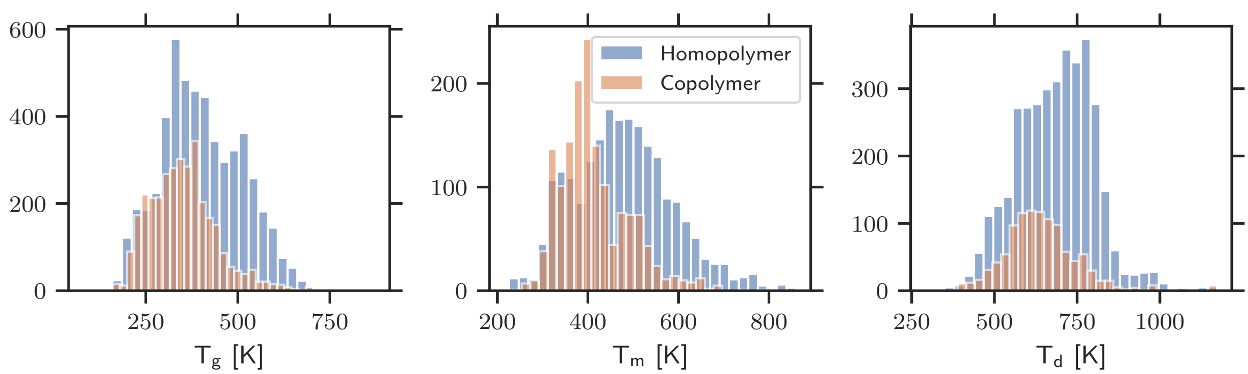

Figure S3: Histograms of the data points of the thermal properties.

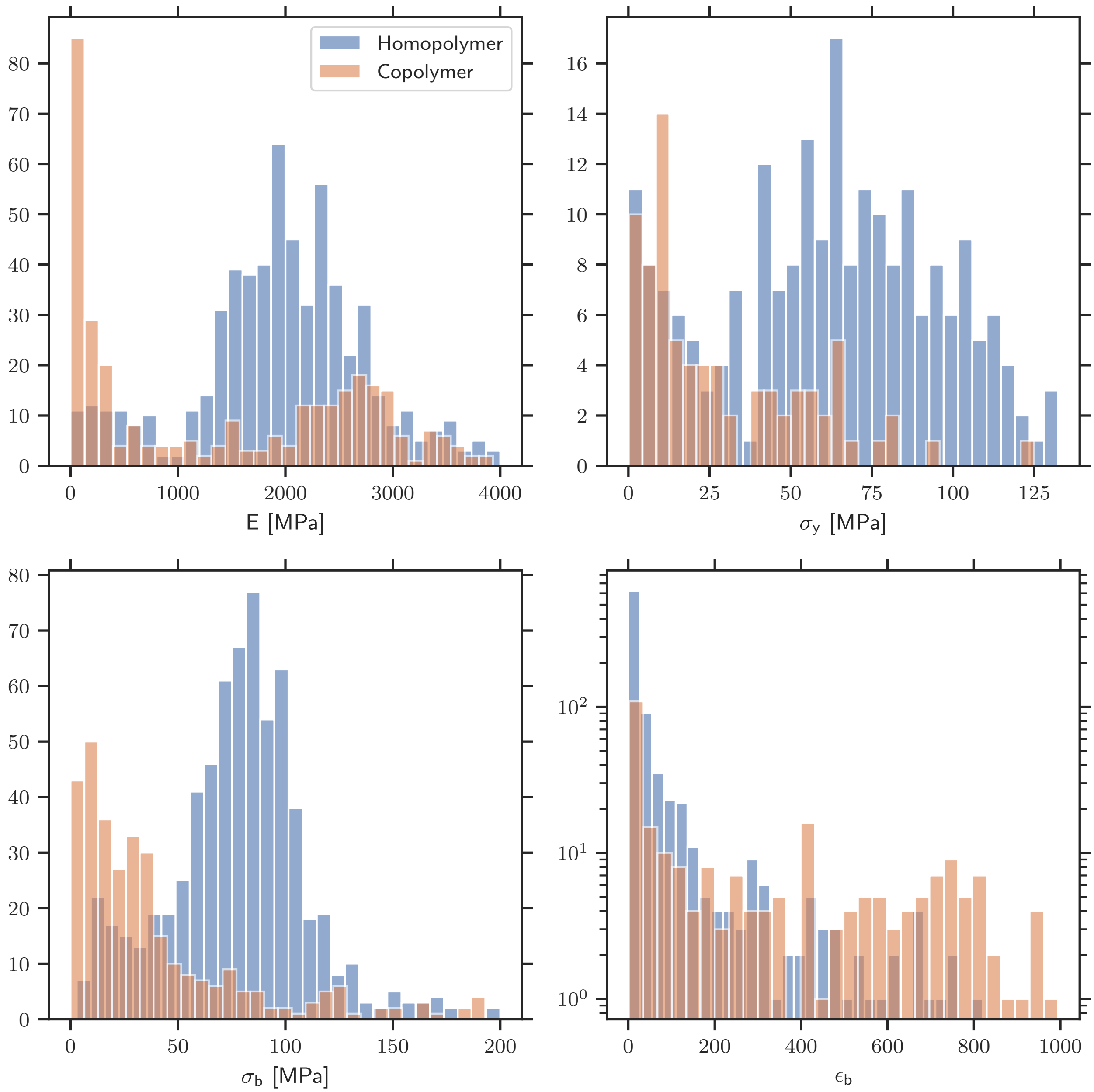

Figure S4: Histograms of the data points of the mechanical properties.

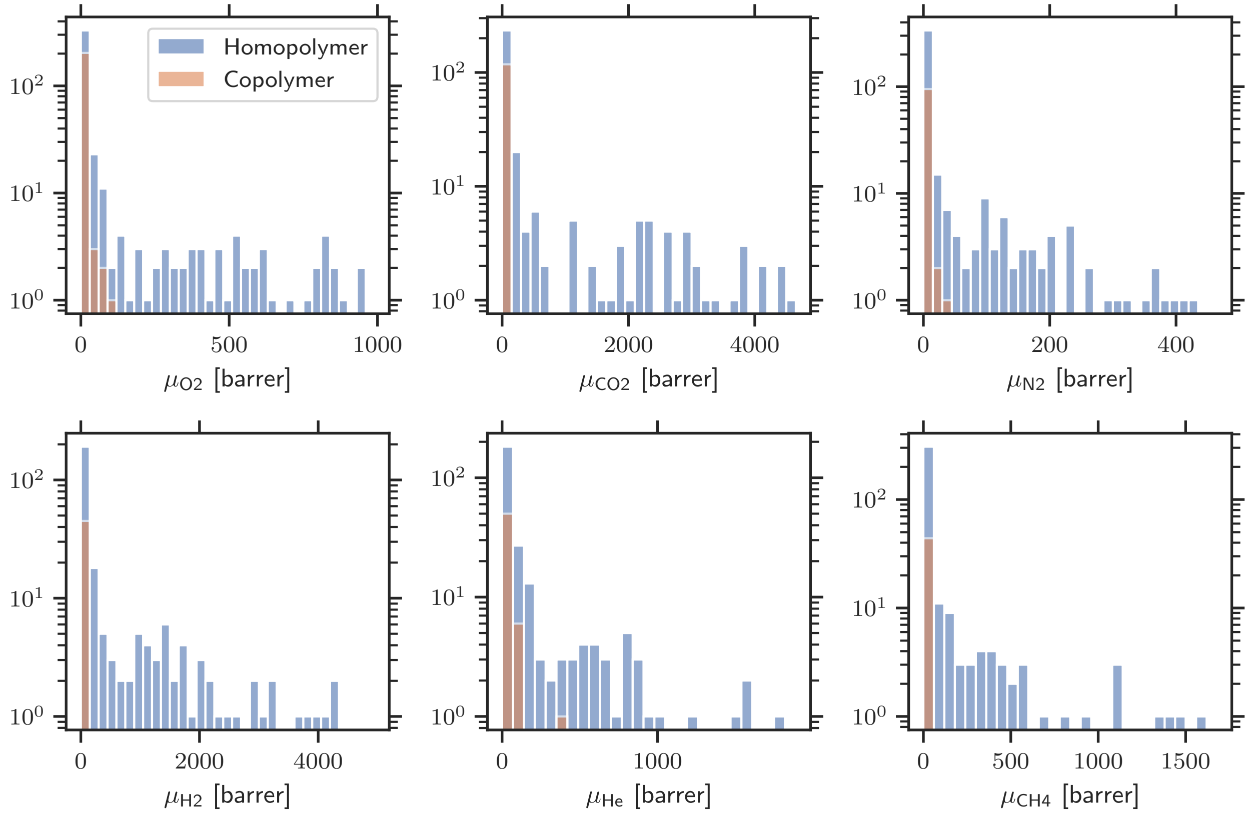

Figure S5: Histograms of the data points of the gas permeabilities.

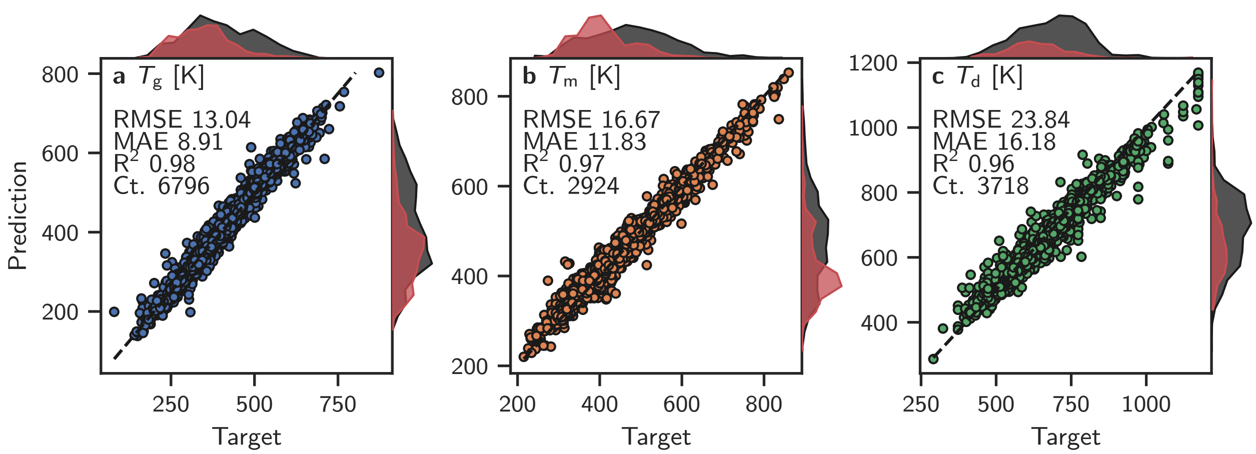

Figure S6: Meta learner parity plots of the three thermal properties. The frequencies of the homopolymer and copolymer data points are indicated in black and red in the margins of the plots.

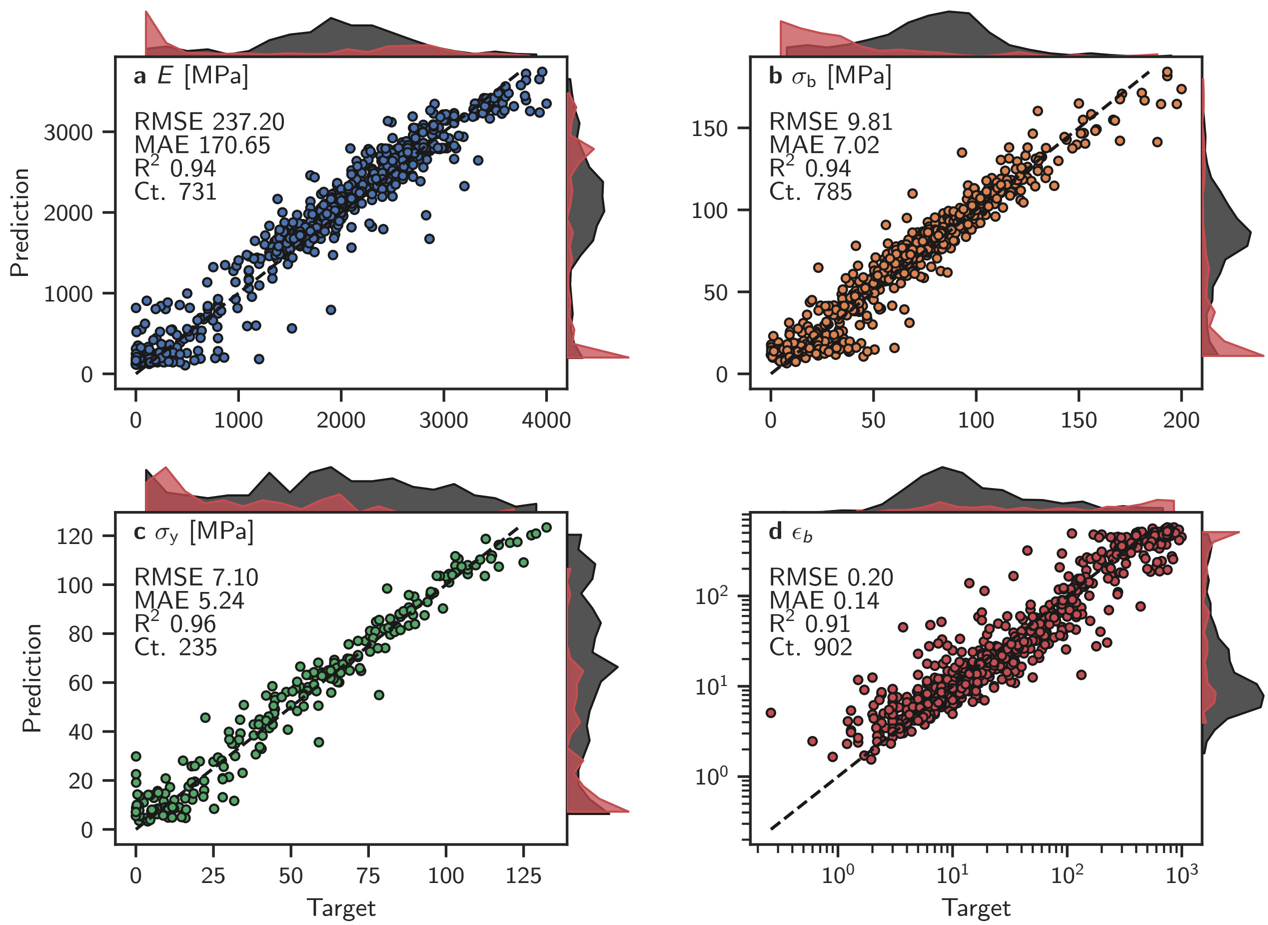

Figure S7: Meta learner parity plots of the four mechanical properties. The frequencies of the homopolymer and copolymer data points are indicated in black and red in the margins of the plots.

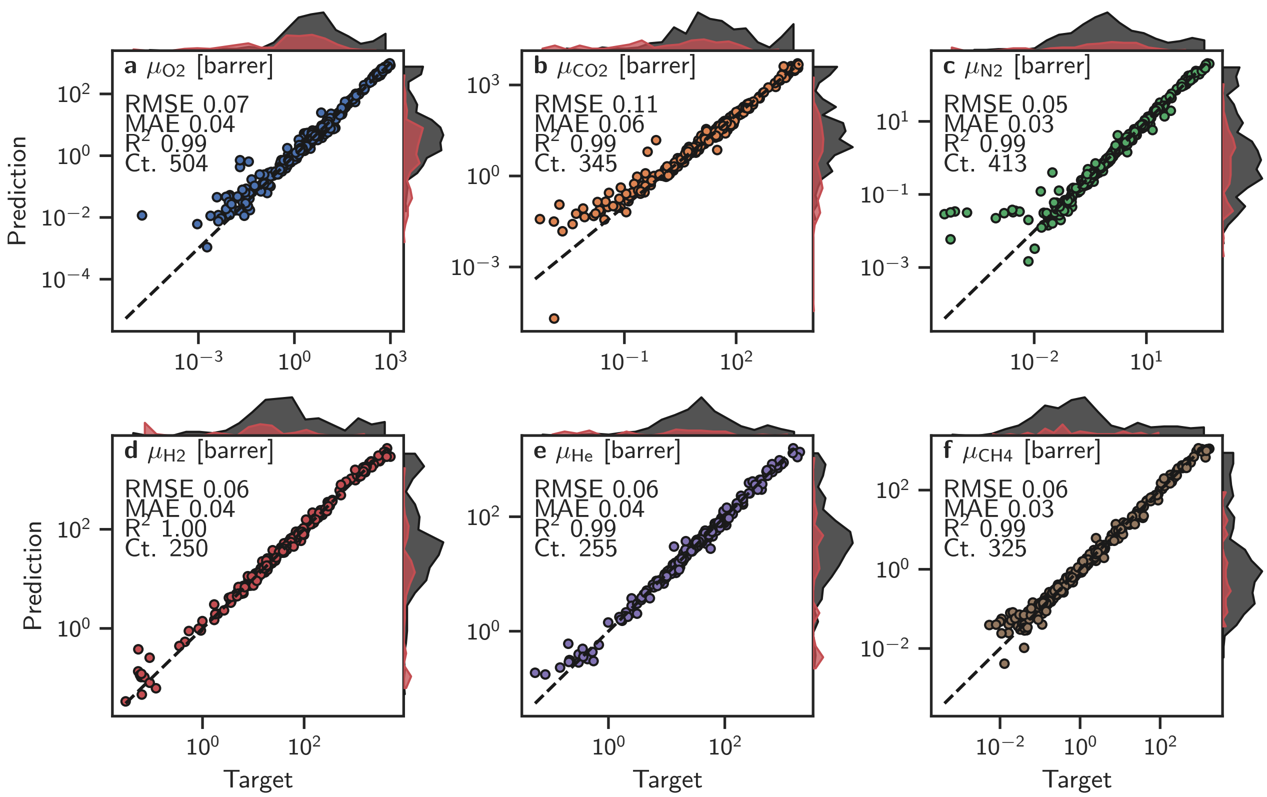

Figure S8: Meta learner parity plots of the six gas permeabilities. The frequencies of the homopolymer and copolymer data points are indicated in black and red in the margins of the plots.

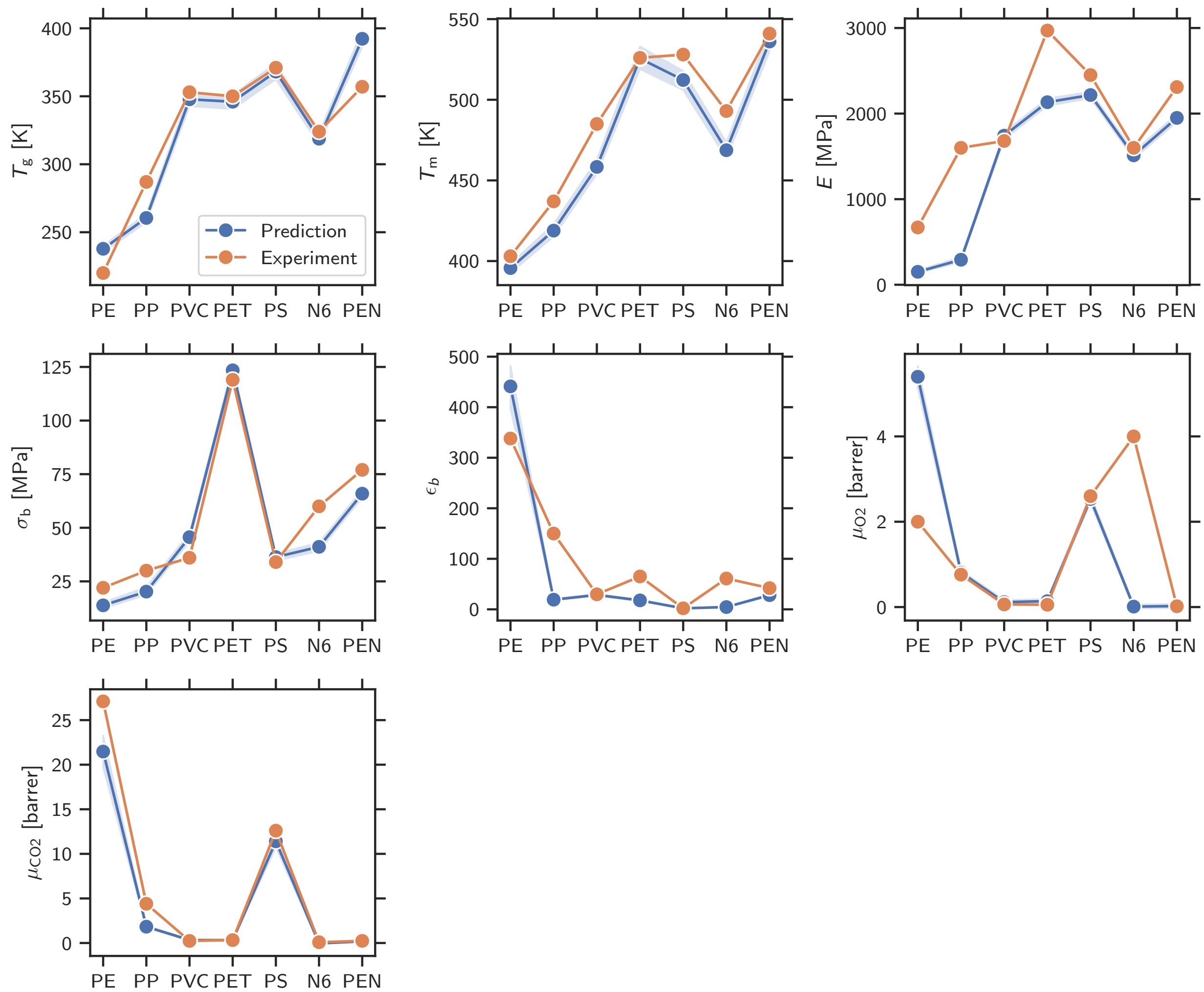

Figure S9: Predicted and experimental values for the seven common plastics defined in Table 3 of the main manuscript.