Supplementary Information (SI) for Polymer Chemistry.

Supporting Information: Polymer Composites Informatics for Flammability, Thermal, Mechanical and Electrical Property Predictions

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Polymer matricies and their abbreviations, used in developing the models

Table 1: Polymer matricies and their abbreviations, used in developing the models

Abbreviation	Full name/ Description
ABS	Acrylonitrile butadiene styrene
ASA	Acrylonitrile styrene acrylate
BMI	Bismaleimide
DRK411	Derakane 411
DRK8084	Derakane 8084
HDPE	High-density polyethylene
LCP	Liquid crystal polymers
LDPE	Low-density polyethylene
MABS	Methylmethacrylate acrylonitrile butadiene styrene
MBS	Methylmethacrylate butadiene styrene
PA	Polyamide
PA1010	Polyamide 1010, Nylon 1010
PA11	Polyamide 11, Nylon 11
PA12	Polyamide 11, Nylon 12
PA410	Polyamide 410, Nylon 410
PA46	Polyamide 46, Nylon 46
PA6	Polyamide 6, Nylon 6
PA610	Polyamide 610, Nylon 610
PA612	Polyamide 612, Nylon 612
PA66	Polyamide 66, Nylon 66
PA666	Polyamide 666
PA6I	Polyamide 6I
PA6T	Polyamide 6T
PA9T	Polyamide 9T
PAXT	Polyamide XT
PAEK	Polyaryletherketone
PAMACM12	Polyamide with Macromolecule Chain Modifications and Methyl Groups (M12)
PAPACM12	Poly(4,4'-aminocyclohexyl methylene dodecanedicarboxylamide)
PBT	Polybutylene terephthalate
PC	Polycarbonate
PCT	Polycyclohexylenedimethylene terephthalate
PCTFE	Polychlorotrifluoroethylene
PE	Polyethylene
PEEK	Polyether ether ketone
PEI	Polyethylenimine

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Abbreviation	Full name/ Description
PESU	Polyethersulfone
PET	Polyethylene terephthalate
PHN1579	Phenolic Resinox CL1579
PHN1723	Phenolic Resinox CL1723
PI	Polyimide
PMMA	Poly(methyl methacrylate)
PMMI	Polymethyl methacrylimide
POM	Polyoxymethylene
PP	Polypropylene
PPA	Polyphthalamide
PPE	Polyphenylene ether
PPS	Polyphenylene sulfide
PPSU	Polyphenylsulfone
PS	Polystyrene
PSU	Polysulfones
PTFE	Tetrafluoroethylene
PVDF	Polyvinylidene fluoride
SAN	Styrene acrylonitrile
SMMA	Styrene methyl methacrylate
TPA	Thermoplastic polyamide elastomers
TPC	Thermoplastic polyester elastomers, block copolymers of polyester and polyether
TPU	Thermoplastic polyurethane
TPV	Thermoplastic vulcanizates

Flame retardants

Table 2: Flame retardants

Abbreviation	Full name/ Description
ADP	Aluminum diethylphosphinate
AHO	Aluminum hydroxide oxide
AHP	Aluminum hypophosphite
anhZB	Anhydrous zinc borate, see 10.1016/j.compositesa.2007.09.009
AO	Antimony (tri)oxide Sb_2O_3
AP422	Ammonium polyphosphate available from Clariant under the name EXOLIT AP422
AP760	Ammonium polyphosphate modified with tris 2-hydroxyethylisocyanurate available from Clariant under the name EXOLIT AP 760
APP	Ammonium polyphosphate
ATH	Aluminum trihydroxide
BA	Boric acid
BM	Boehmite
BR	Decabromodiphenyl oxide, see 10.1016/j.polymdegradstab.2009.12.011
BX	Borax
Cloisite15A	Organically modified montmorillonite clay (cation is dimethyldihydrogenated tallow ammonium), see 10.1016/j.polymdegradstab.2009.12.011
Cloisite30B	Natural montmorillonite (MMT) modified by methyl tallow bis-2-hydroxyethyl ammonium cation. See 10.1016/j.polymdegradstab.2012.03.043
CSM	Chopped strand mat (E-glass fiber)
DAP	Diammonium phosphate
DPER	Dipentaerythritol
DOPO	9,10-dihydro-9-oxa-10-phosphaphenanthrene-10-oxide-phosphonamidate, see 10.1016/j.commatsci.2023.112479
HPPA	3-(hydroxyphenyl phosphinyl) propanoic acid, see 10.1016/j.polymdegradstab.2020.109310
KLN	Calcined Kaolin
MAP	Monoammonium phosphate
MAPP	Maleated polypropylene
M-APP	Modified ammonium polyphosphate
MCA	Melamine cyanurate
MH	(ordinary) Magnesium hydroxide
U-MH	Ultrafine magnesium hydroxide
MMP	Montmorillonite phosphate
MMT	Montmorillonite
MP	Melamine phosphate
MPP	Melamine polyphosphate
MWNT	Multi-wall carbon nanotubes, see 10.1016/j.polymdegradstab.2009.12.011
mTiO2	Micrometric TiO2, see 10.1016/j.polymdegradstab.2020.109310, 10.1016/B978-0-12-815067-2.00011-1, 10.1016/j.polymdegradstab.2005.01.019
mFe2O3	Micrometric Fe2O3, see 10.1016/j.polymdegradstab.2005.01.019
nFe2O3	Nanometric Fe2O3, see 10.1016/S0141-3910(02)00185-4, 10.1016/j.polymdegradstab.2005.01.019
OP1311	OP1311, non-halogenated flame retardant based on organic phosphinates, see 10.1016/j.polymdegradstab.2006.09.011
OP930	Exolit OP 930 is a white, fine-grained powder based on an organic phosphinate, see 10.1016/j.polymdegradstab.2006.09.011
O-MMTPFS1	Organo-modified clay 1, see 10.1007/s13369-016-2111-9
O-MMTPFS2	Organo-modified clay 2, see 10.1007/s13369-016-2111-9
SiO2	Silicon dioxide
TBP	Tris(tribromoneopentyl) phosphate
TCP	Phosphorus containing tricresylphosphate
RDP	Resorcinol di-phosphate, see 10.1533/9781845694701.3.527
RP	Red phosphorus
ZB	Zinc borate
ZHS	Zinc hydroxystannate
ZS	Zinc stannate
WR	Woven roving (glass fiber)

Model evaluations: GPR, DL, single-task, and Pi/multi-task algorithms

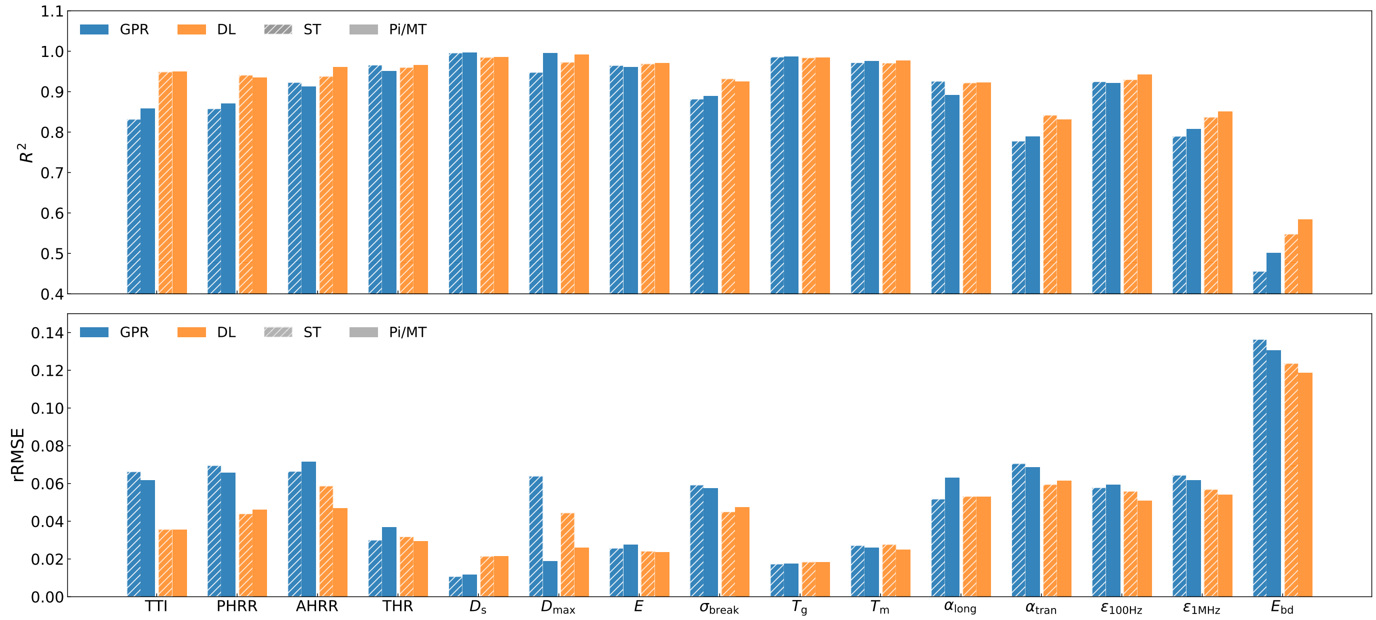

Figure 1: Coefficient of determination R^2 and relative RMSE of the models trained for the time to ignition TTI, the peak heat release rate PHRR, the averaged heat release rate AHRR, and the total heat release THR. For both GPR and DT, ST and physics-informed MT models are indicated by crossed and solid patterns, respectively.

Model evaluations: cross-validation R^2 and RMSE

Table 3: Cross-validation R^2 and RMSE during the training process of models for 15 examined properties, including time to ignition TTI (s), peak heat release rate PHRR (kW/m$_2$), averaged heat release rate AHRR (kW/m^2), total heat release THR (MJ/m^2), optical smoke density D_s (dimensionless), maximum optical smoke density D_{max} (dimensionless), tensile modulus E (MPa), stress at break σ_{break} (MPa), glass transition temperature T_g (C), melting temperature T_m (C), longitudinal coefficient of thermal expansion α_{long} (10^{-6}/K), transverse coefficient of thermal expansion α_{tran} (10^{-6}/K), relative permittivity at 1 MHz ϵ_{1MHz} (dimensionless), relative permittivity at 100 Hz ϵ_{100Hz} (dimensionless), and breakdown electric strength E_{bd} (kV/mm). For MT models, the training involve merging and transforming data of different related properties, which are usually in different scales, thus the cross-validation RMSE of transformed data typically has no meagning, and ultimately are noted as "N/A" in this Table.

	GPR								DL							
	ST				MT				ST				MT			
	train		test		train		test		train		test		train		test	
model	R2	RMSE	R2	RMSE	R2	RMSE	R2	RMSE	R2	RMSE	R2	RMSE	R2	RMSE	R2	RMSE
TTI	0.85	17.56	0.65	25.82	0.89	N/A	0.71	N/A	0.87	15.54	0.79	19.6	0.9	N/A	0.79	N/A
PHRR	0.86	129.85	0.67	193.74	0.89	N/A	0.71	N/A	0.89	0.11	0.78	0.15	0.9	N/A	0.79	N/A
AHRR	0.94	38.87	0.78	75.97	0.89	N/A	0.71	N/A	0.79	73.93	0.84	58.75	0.9	N/A	0.79	N/A
THR	0.97	15.79	0.82	40.75	0.89	N/A	0.71	N/A	0.9	29.42	0.86	35.74	0.9	N/A	0.79	N/A
D_s	1	9.13	0.94	33.87	1	N/A	0.89	N/A	0.87	55.11	0.96	26.48	0.92	N/A	0.97	N/A
D_{max}	0.95	56.92	0.81	121.5	1	N/A	0.89	N/A	0.81	110.78	0.92	71.3	0.92	N/A	0.97	N/A
E	0.97	968.35	0.94	1262.41	0.95	N/A	0.93	N/A	0.95	1131.56	0.95	1208.03	0.95	N/A	0.94	N/A
σ_{break}	0.89	18.55	0.85	21.14	0.95	N/A	0.93	N/A	0.91	16.86	0.89	18.39	0.95	N/A	0.94	N/A
T_g	0.99	7.73	0.93	16.65	0.91	N/A	0.87	N/A	0.95	15.11	0.94	15.28	0.9	N/A	0.91	N/A
T_m	0.97	7.08	0.95	9.3	0.91	N/A	0.87	N/A	0.93	11.63	0.96	8.82	0.9	N/A	0.91	N/A
α_{long}	0.93	13.07	0.88	17.02	0.91	N/A	0.87	N/A	0.9	15.54	0.9	14.9	0.9	N/A	0.91	N/A
α_{tran}	0.78	16.39	0.74	17.77	0.91	N/A	0.87	N/A	0.81	15.13	0.79	15.7	0.9	N/A	0.91	N/A
ϵ_{100Hz}	0.93	0.72	0.89	0.87	0.85	N/A	0.8	N/A	0.88	0.92	0.91	0.77	0.85	N/A	0.81	N/A
ϵ_{1MHz}	0.79	0.29	0.62	0.39	0.85	N/A	0.8	N/A	0.73	0.33	0.74	0.32	0.85	N/A	0.81	N/A
E_{bd}.	0.46	4.76	0.32	5.4	0.85	N/A	0.8	N/A	0.39	5	0.37	5.08	0.85	N/A	0.81	N/A