Supplementary information

Table S 1 Formulation for the test/train model.

ID	PA	PEGDA	PEDOT:PSS	HEC	ID	PA	PEGDA	PEDOT:PSS	HEC
Ink1	2.5	2.5	0	0	Ink18	7.5	7.5	1	0
Ink2	2.5	2.5	0.5	0	Ink19	9	6	1	0
Ink3	3	2	0	0	Ink20	12	3	1	0
Ink4	3	2	0.5	0	Ink21	12	8	1	0
Ink5	4	1	0	0	Ink22	16	4	1	0
Ink6	4	1	0.5	0	Ink23	16	4	1	2
Ink7	7.5	7.5	0.5	0	Ink24	0	2	0.1	0
Ink8	9	6	0	0	Ink25	0	2	0.3	0
Ink9	9	6	0.5	0	Ink26	0	2	0.5	0
Ink10	10	10	0	0	Ink27	1	10	2	2
Ink11	10	10	0.5	0	Ink28	16	4	2	1
Ink12	12	3	0	0	Ink29	1	10	0	0
Ink13	12	3	0.5	0	Ink30	7.5	7.5	0	0
Ink14	12	8	0	0					
Ink15	12	8	0.5	0	Ink31	6.8	6.7	2	1.1
Ink16	16	4	0	0	Ink32	6.6	17.2	2	1.9
Ink17	16	4	0.5	0	Ink33	4.2	8.9	2	0.9

PA and PEGDA were first prepared as stock solutions of 32%w/v and 40%w/v, respectively. The powder was dissolved in deionised water and stirred until it was homogeneous. Inks 1 – 30 were experimental setup defined by user that span across 8 levels of PA concentration, 10 levels of PEGDA concentration, 6 levels of PEDOT:PSS concentration, and 3 levels of HEC concentration. Inks 31 – 33 are combinations suggested by the ML prediction models for formulations with high conductivity values.

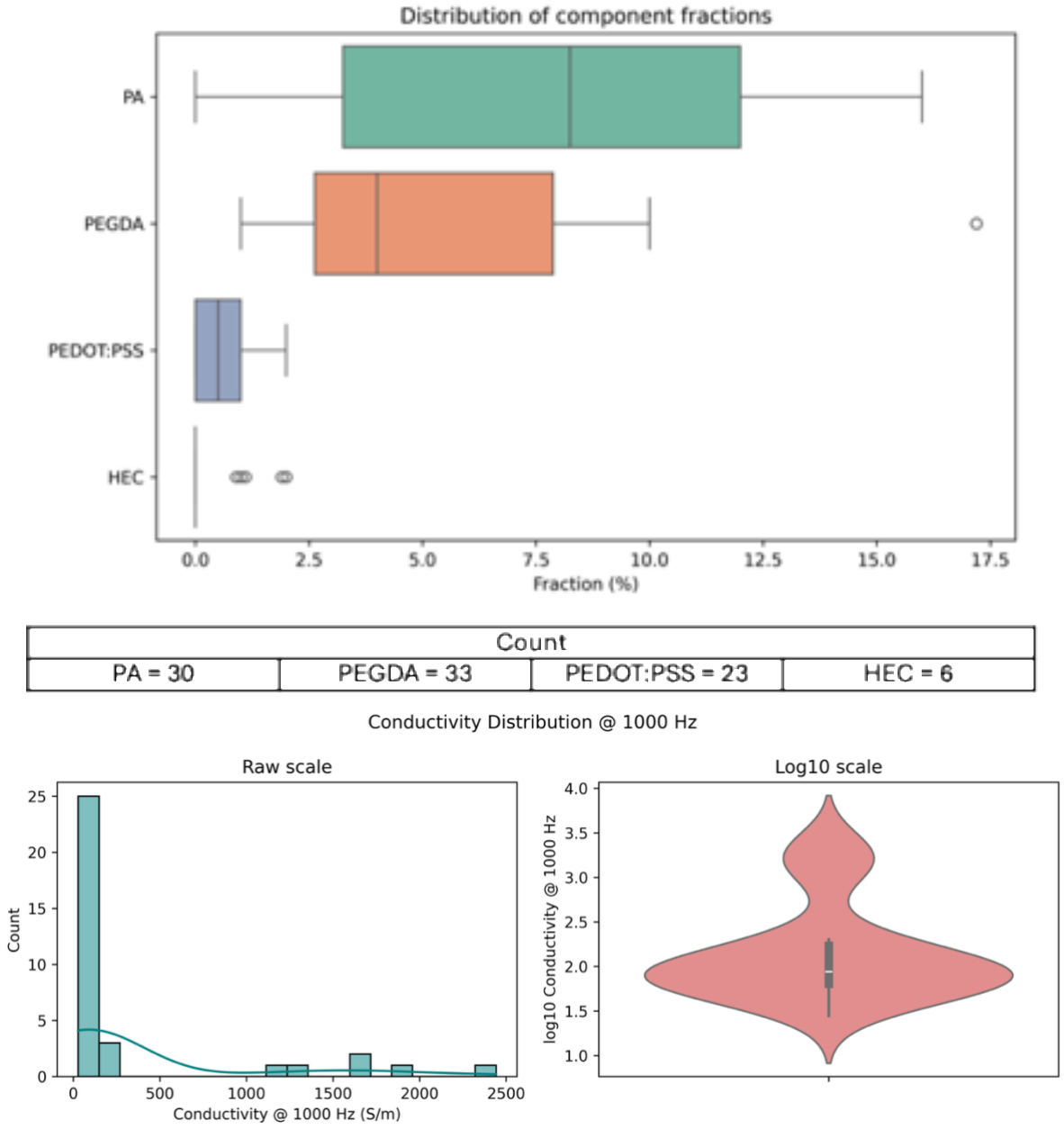


Figure S 1 Distribution of raw conductivity of the dataset for model training

Table S 2 Categorical labelling of polymer backbone corresponding to the polymers used in current study

Polymer	Backbone Type
PA	Vinyl
PEGDA	Polyether
PEDOT:PSS	Conjugated
HEC	Polysaccharide

Table S 3 SMILES for respective polymer used for physicochemical descriptors are obtained through pubchem database

Polymer	**SMILES**
Acrylamide	C=CC(=O)N
PEGDA	C=CC(=O)OCCOC(=O)C=C
PEDOT:PSS	C1COC2=CSC=C2O1.C1=CC=C(C=C1)/C=C/S(=O)(=O)O
HEC	CC(COCC1C(C(C(C(O1)OC2C(OC(C(C2OCC(C)O)OCC (C)O)OCC(C)O)COCC(C)O)OCC(C)O)OCC(C)O)OCC(C)O)O

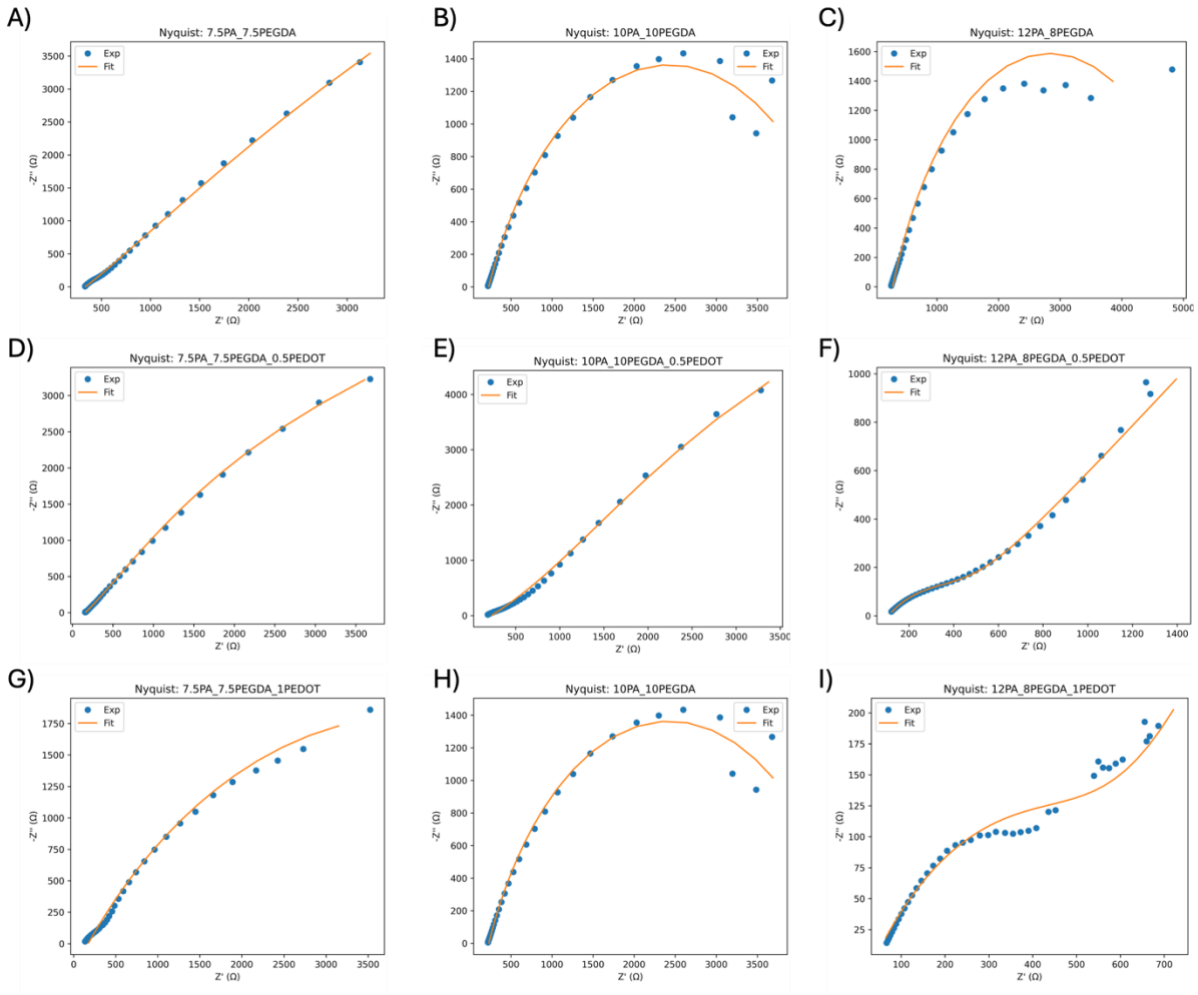


Figure S 2 Representative Nyquist plots of the small dataset group showing 3 main variations in polymer matrix % (A, D, G: 7.5PA_7.5PEGDA; B, E, H: 10PA_10PEGDA; C, F, I: 12PA_8PEGDA) with the addition of conductive PEDOT:PSS fillers (A, B, C: 0PEDOT; D, E, F: 0.5PEDOT; G, H, I: 1PEDOT)

Table S 4 Final model parameters used in training

Model	Key parameters, hyperparameters and values
Ridge Regression	α = 1.0; solver = auto; tol = 1e−4; fit_intercept = True
Random Forest Regressor	n_estimators = 100; criterion = *squared_error*; bootstrap = True; max_features = 1.0; random_state = 42
XGBoost Regressor	objective = *reg:squarederror*; learning_rate = 0.3; max_depth = 3; n_estimators = 579; subsample = 0.968; colsample_bytree = 0.999; random_state = 42
Ridge + XGB	Base: Ridge (α = 1.0); XGBoost (as above); Final estimator = RandomForestRegressor (n_estimators = 100, bootstrap = True)
RF + XGB	Base: RandomForestRegressor (as above); XGBoost (as above); Final estimator = Ridge (α = 1.0)RF + XGB; Final: Ridge (α=1.0)
Kernel Ridge Regression	kernel = *rbf*; α = 0.0027; γ = 0.0016; degree = 3
Gaussian Process Regressor	kernel = (1^2 × RBF(length_scale=1)) + WhiteKernel(noise_level=1); α = 7.45×10^{-5}; n_restarts_optimizer = 5; random_state = 42
LightGBM Regressor	boosting_type = *gbdt*; learning_rate = 0.; max_depth = 5; num_leaves = 96; n_estimators = 224; subsample = 0.818; colsample_bytree = 0.919; reg_alpha = 0; reg_lambda = 0; random_state = 42

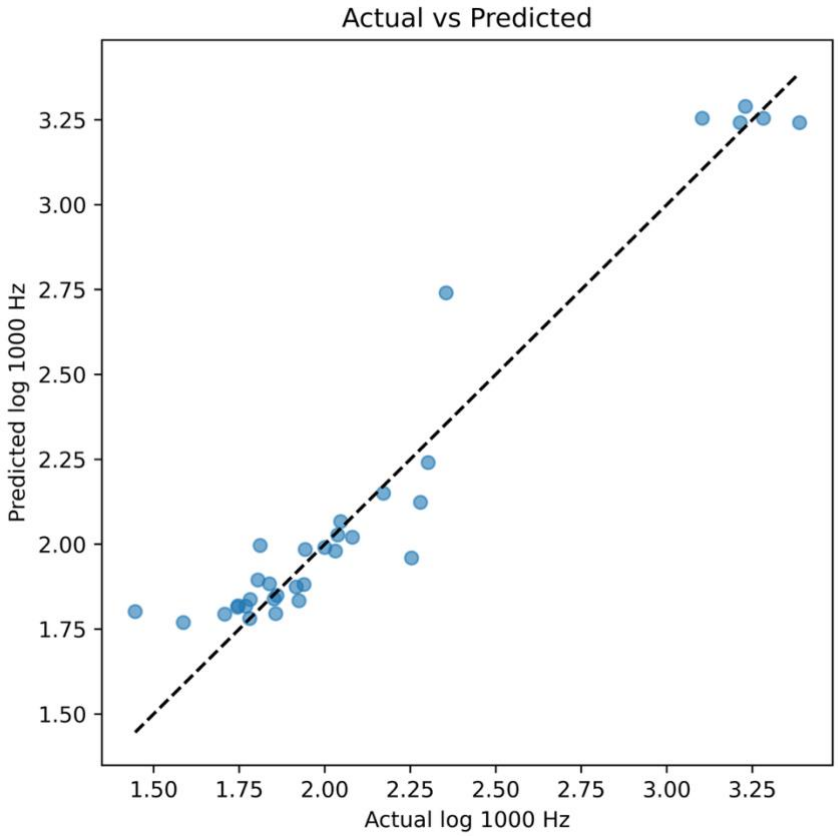


Figure S 3 Scatterplot of predicted vs measured value of dataset based on stacked ensemble (Ridge + XGBoost) model

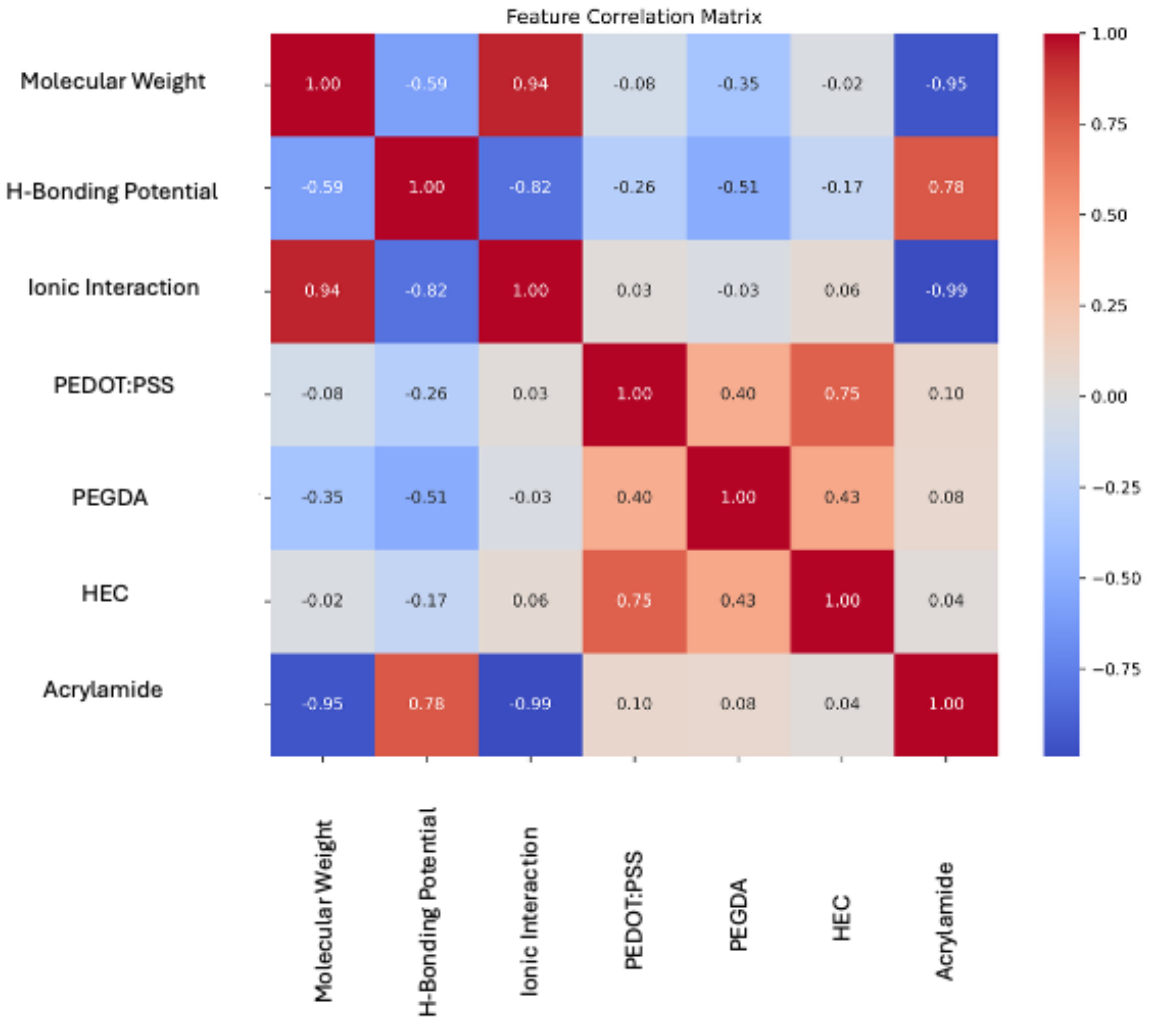
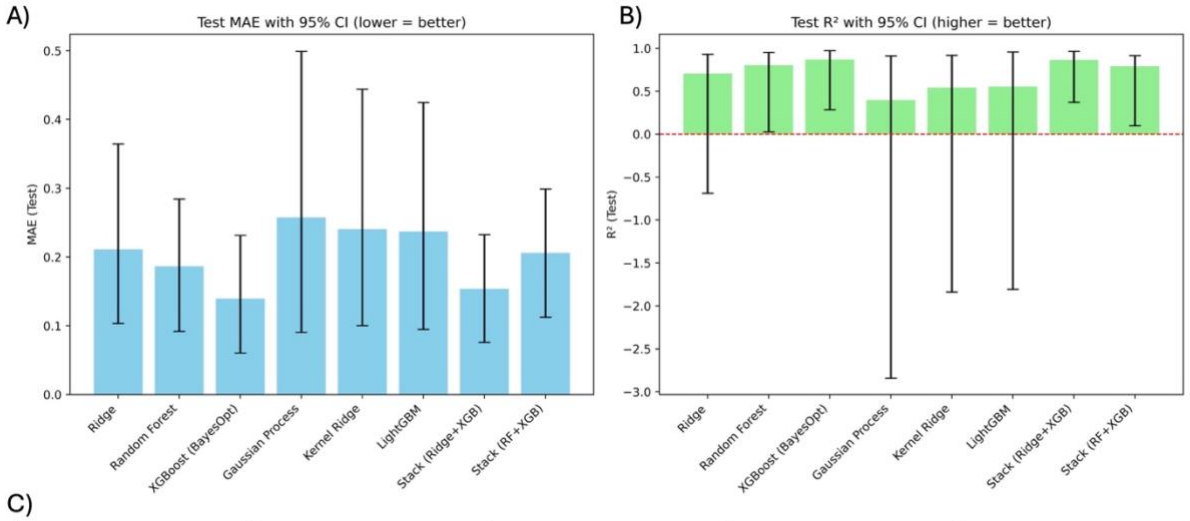


Figure S 4 Feature correlation map summarises the statistical distribution of key physicochemical and categorical descriptors for the polymer formulations, including Molecular Weight (MW), Hydrogen Bonding Potential (HBP), Ionic Interaction (II), and categorical backbone types.

Table S 5 Principal component loadings for PC1, PC2, and PC3 derived from the physicochemical descriptors of the polymer formulations.

Feature	PC1	PC2	PC3
Conjugated (PEDOT:PSS)	0.613	-0.059	-0.374
Polysaccharide (HEC)	0.618	-0.140	-0.294
Polyether (PEGDA)	0.480	0.024	0.875
Vinyl (PA)	0.113	0.988	-0.085

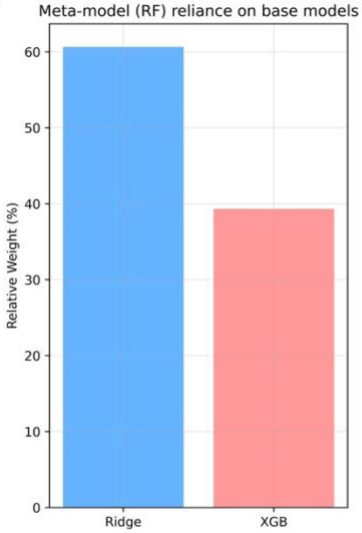


C)

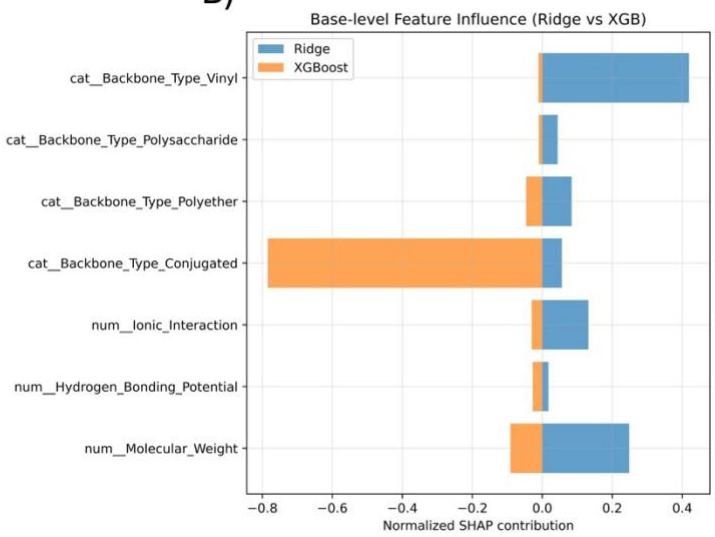
Model	MAE_Train	MAE_Test	R2_Train	R2_Test
Ridge	0.083 [0.059, 0.110]	0.211 [0.103, 0.364]	0.952 [0.689, 0.974]	0.706 [-0.687, 0.931]
Random Forest	0.051 [0.039, 0.064]	0.186 [0.092, 0.284]	0.985 [0.878, 0.992]	0.803 [0.026, 0.952]
XGBoost (BayesOpt)	0.001 [0.000, 0.001]	0.139 [0.060, 0.232]	1.000 [1.000, 1.000]	0.870 [0.285, 0.974]
Gaussian Process	0.058 [0.044, 0.075]	0.257 [0.090, 0.499]	0.980 [0.801, 0.992]	0.396 [-2.842, 0.913]
Kernel Ridge	0.070 [0.051, 0.090]	0.241 [0.100, 0.444]	0.970 [0.750, 0.986]	0.542 [-1.836, 0.918]
LightGBM	0.000 [0.000, 0.000]	0.237 [0.095, 0.425]	1.000 [1.000, 1.000]	0.555 [-1.806, 0.958]
Stack (Ridge+XGB)	0.063 [0.046, 0.085]	0.154 [0.076, 0.233]	0.974 [0.782, 0.988]	0.865 [0.371, 0.965]
Stack (RF+XGB)	0.046 [0.027, 0.067]	0.206 [0.112, 0.299]	0.981 [0.962, 0.985]	0.792 [0.098, 0.915]

Figure S 5 Bootstrapping-based secondary validation assessing model robustness and prediction stability. Distribution of bootstrapped A) MAE and B) R^2 values based on resampling. The narrow spread of resampled metrics supports model generalisability and confirms the reliability of the stacked ensemble model for extrapolative conductivity prediction. C) Table showing the values in the format (average)[0.25 percentile | 0.75 percentile].

A)



B)



C)

Feature	Ridge	XGB	Weighted Total
Backbone Type Conjugated	0.056057	0.784292	0.342556
Backbone Type Vinyl	0.418990	0.011005	0.258483
Molecular Weight	0.247969	0.091029	0.186226
Ionic Interaction	0.131514	0.030337	0.091710
Backbone Type Polyether	0.083966	0.046310	0.069151
Backbone Type Polysaccharide	0.043988	0.009658	0.030482
Hydrogen Bonding Potential	0.017515	0.027369	0.021392

Figure S 6 Meta-model and hierarchical SHAP analysis of the stacked ensemble (Ridge + XGBoost). A) Meta-model (Random Forest) reliance on the two base learners quantified by relative weight contribution, highlighting Ridge (≈60%) and XGBoost (≈40%) influence in the final prediction. B) Base-level feature influence of Ridge (positive direction) and XGBoost (negative direction) models showing complementary feature sensitivities. C) Table showing the respective SHAP values.