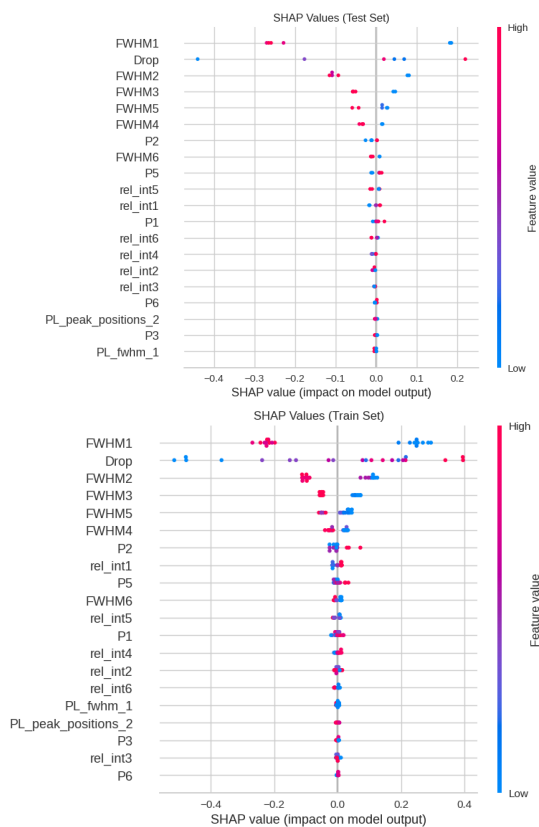


## XGBoost

Cross-Validation R2 Scores: Fold 1: 0.5068. - Fold 2: -0.1882 - Fold 3: -0.0008- Fold 4: -0.7942 - Fold 5: 0.0990

R2 (Test)	R2 (Train)	Adjusted R2 (Test)	Adjusted R2 (Train)	RMSE (Test)	RMSE (Trai)	MAE (Test)	MAE (Trai)	Explained Variance (Test)	Explained Variance (Train)	Max Error (Test)	Max Error (Trai)	CV Mean R2	CV Std R2
0.84	0.89	1.03	1.40	0.28	0.21	0.22	0.18	0.84	0.89	0.51	0.41	-0.075	0.425

Feature	Importance
FWHM3	0.17
rel_int5	0.09
FWHM6	0.08
FWHM1	0.076
FWHM2	0.074
FWHM5	0.068
rel_int1	0.064
FWHM4	0.046
PL_fwhm_1	0.037
Drop	0.029
rel_int3	0.027
PL_intensity_1	0.025
P2	0.025
PL_peak_positions_2	0.023
rel_int6	0.022
P5	0.021
rel_int2	0.020
P1	0.019
P3	0.016
rel_int4	0.013
P4	0.0126
P6	0.011
PL_intensity_2	0.0098
PL_fwhm_2	0.0
PL_peak_positions_1	0.0

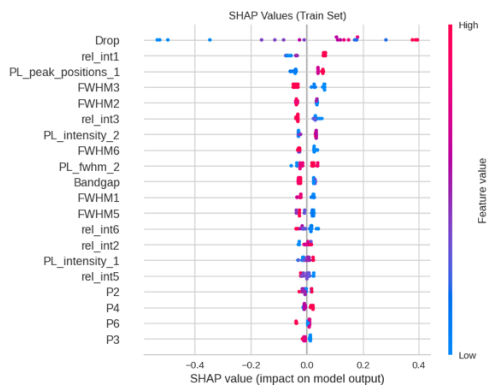
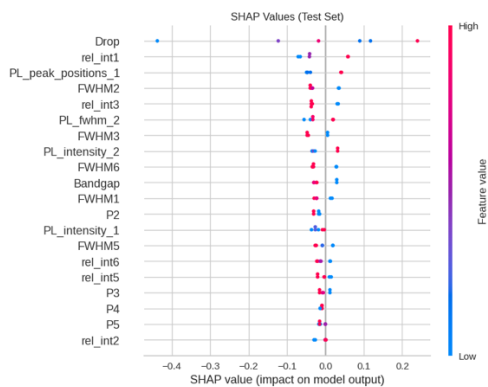


## Catboost

Cross-Validation R2 Scores: Fold 1: 0.4501 Fold 2: -0.0288 Fold 3: 0.0013 Fold 4: -0.6253 Fold 5: 0.0321

R2 (Test)	R2 (Train)	RMSE (Test)	RMSE (Trai)	MAE (Test)	MAE (Trai)	Explained Variance (Test)	Explained Variance (Train)	Max Error (Test)	Max Error (Trai)	CV Mean R2	CV Std R2
0.83	0.87	0.28	0.24	0.23	0.20	0.837	0.874	0.549	0.456	-0.03	0.34

Feature	Importance
Drop	33.24
rel_int1	12.68
PL_peak_positions_1	6.01
PL_intensity_2	5.60
rel_int3	4.41
PL_fwhm_2	4.24
FWHM3	4.169
Bandgap	3.90
FWHM1	3.317
FWHM2	3.193
rel_int2	3.031
FWHM6	2.89
FWHM5	2.179
P2	1.95
rel_int6	1.560
PL_intensity_1	1.27
P5	1.188
P6	1.032
rel_int5	0.922
PL_fwhm_1	0.83
rel_int4	0.49
PL_peak_positions_2	0.47
P3	0.44
P1	0.373
FWHM4	0.274



## GBR

Cross-Validation R2 Scores: Fold 1: 0.4881 Fold 2: -0.432 Fold 3: -0.3356 Fold 4: -5.2584 Fold 5: 0.1354

R2 (Test)	R2 (Train)	RMSE (Test)	RMSE (Train)	MAE (Test)	MAE (Train)	Explained Variance Score (Test)	Explained Variance Score (Train)	Max Error (Test)	Max Error (Train)	Cross-Validation Mean R2	Cross-Validation Std R2
0.92	0.99	0.19	0.056	0.16	0.04	0.93	0.99	0.32	0.10	-1.08	2.115

Feature	Importance
Drop	0.41
PL_fwhm_2	0.085
FWHM1	0.0675
PL_intensity_2	0.052
FWHM6	0.0481
PL_peak_positions_1	0.042
FWHM4	0.0412
FWHM5	0.0397
FWHM2	0.0349
rel_int1	0.0338
Bandgap	0.0331
rel_int5	0.0218
FWHM3	0.0211
rel_int6	0.0145
rel_int3	0.0122
PL_peak_positions_2	0.00544
rel_int2	0.00494
PL_fwhm_1	0.00472
rel_int4	0.00426
P3	0.00398
P1	0.00394
P4	0.00393
P5	0.00389
PL_intensity_1	0.0035
P2	0.000498

