SUPPORTING INFORMATION

LGB-Stack: Stacked Generalization with *LightGBM* for Highly Accurate Predictions of Polymer Bandgap

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A. Tables of accuracy scores for the weak models molecular fingerprints

All Fingerprints here are generated by RDKit.[1] All R^2 and RMSE scores were computed using the *scikit-learn* package.[2] Group (A) fingerprints refer to those that were 4096 bits in size when generated by RDKit. Using, recursive feature elimination (RFE), the group (A) fingerprints were reduced to 256 and 512 bits and labelled groups (B) and (C) respectively.

Table S1. Best accuracy scores for the Avalon fingerprint (A-FP), with highest scores for R^2 and lowest scores for RMSE.

Fingerprint	R^2		RMSE (eV)	
	Train	Test	Train	Test
A-FP (A)	0.9404	0.8981	0.3544	0.4580
A-FP (B)	0.9372	0.9008	0.3623	0.4522
A-FP (C)	0.9399	0.8971	0.3563	0.4601

Table S2. Mean accuracy scores for A-FP.

Fingerprint	R^2		RMSE (eV)	
	Train	Test	Train	Test
A-FP (A)	0.9359	0.8693	0.3657	0.5232
A-FP (B)	0.9332	0.8750	0.3734	0.5115
A-FP (C)	0.9351	0.8722	0.3680	0.5173

Table S3. Best accuracy scores for the Avalon Count fingerprint (AC-FP), with highest scores for R^2 and lowest scores for RMSE.

Fingerprint	R^2		RMSE (eV)	
	Train	Test	Train	Test
AC-FP (A)	0.9481	0.9030	0.3312	0.4467
AC-FP (B)	0.9470	0.9032	0.3347	0.4463
AC-FP (C)	0.9480	0.9031	0.3316	0.4465

Table S4. Mean accuracy scores for AC-FP.

Fingerprint	R^2		RMSE (eV)	
	Train	Test	Train	Test
AC-FP (A)	0.9420	0.8737	0.3478	0.5143
AC-FP (B)	0.9407	0.8782	0.3519	0.5050
AC-FP (C)	0.9420	0.8755	0.3478	0.5107

Table S5. Best accuracy scores for the Layered fingerprint (L-FP), with highest scores for R^2 and lowest scores for RMSE.

Fingerprint	R^2		RMSE (eV)	
	Train	Test	Train	Test
L-FP (A)	0.9591	0.9058	0.2919	0.4401
L-FP (B)	0.9543	0.9071	0.3110	0.4370
L-FP (C)	0.9568	0.9124	0.3013	0.4243

Table S6. Mean accuracy scores for L-FP.

Fingerprint	R^2		RMSE (eV)	
	Train	Test	Train	Test
L-FP (A)	0.9570	0.8779	0.2996	0.5056
L-FP (B)	0.9510	0.8876	0.3198	0.4851
L-FP (C)	0.9543	0.8852	0.3089	0.4901

Table S7. Best accuracy scores for the *RDKit* fingerprint (R-FP), with highest scores for R^2 and lowest scores for RMSE.

Fingerprint	R^2		RMSE (eV)	
	Train	Test	Train	Test
R-FP (A)	0.9656	0.9009	0.2689	0.4515
R-FP (B)	0.9580	0.9073	0.2958	0.4365
R-FP (C)	0.9617	0.9082	0.2825	0.4346

Table S8. Mean accuracy scores for R-FP.

Fingerprint	R^2		RMSE (eV)	
	Train	Test	Train	Test
R-FP (A)	0.9626	0.8752	0.2792	0.5112
R-FP (B)	0.9543	0.8871	0.3086	0.4863
R-FP (C)	0.9585	0.8867	0.2943	0.4870

B. Tables of accuracy scores for LGB-Stack

LGB-Stack uses the group "B" fingerprints for its first level of weak model training.

Table S9. Best accuracy scores for *LGB-Stack*.

Model	R^2		RMSE (eV)		Train/Test split ratio
	Train	Test	Train	Test	
LGB-Stack	0.9874	0.8091	0.1627	0.6305	10/90
	0.9915	0.8497	0.1357	0.5537	20/80
	0.9885	0.8744	0.1570	0.5110	30/70
	0.9860	0.8826	0.1683	0.4947	40/60
	0.9821	0.8941	0.1911	0.4665	50/50
	0.9810	0.9078	0.2001	0.4354	60/40
	0.9783	0.9147	0.2115	0.4149	70/30
	0.9760	0.9197	0.2226	0.4081	80/20
	0.9746	0.9214	0.2295	0.4026	90/10
	0.9735	0.9420	0.2355	0.3410	95/5

Table S10. Mean accuracy scores for *LGB-Stack*.

Model	R^2		RMSE (eV)		Train/Test split ratio
	Train	Test	Train	Test	
LGB-Stack	0.9788	0.7911	0.2088	0.6607	10/90
	0.9865	0.8347	0.1674	0.5878	20/80
	0.9850	0.8557	0.1762	0.5495	30/70
	0.9827	0.8700	0.1895	0.5218	40/60
	0.9802	0.8785	0.2027	0.5049	50/50
	0.9784	0.8870	0.2119	0.4869	60/40
	0.9763	0.8915	0.2221	0.4769	70/30
	0.9747	0.8958	0.2296	0.4669	80/20
	0.9732	0.9008	0.2367	0.4541	90/10
	0.9727	0.9027	0.2391	0.4458	95/5

References

(1) Landrum, G. RDKit: Open-Source Cheminformatics Software. https://www.rdkit.org (accessed Jan 11, 2022).

(2) Pedregosa, F.; Varoquaux, G.; Gramfort, A.; Michel, V.; Thirion, B.; Grisel, O.; Blondel, M.; Prettenhofer, P.; Weiss, R.; Dubourg, V.; Vanderplas, J.; Passos, A.; Cournapeau, D.; Brucher, M.; Perrot, M.; Duchesnay, E. Scikit-learn: Machine Learning in Python. *J. Mach. Learn. Res.* **2011**, *12(85)*, 2825−2830.