Supporting Information for

"Chemically Inspired Convolutional Neural Network using Electronic Structure Representation"

Dong Hyeon Mok[1†], Daeun Shin[2,3 †], Jonggeol Na[2,3] and Seoin Back[1]**

[1]Department of Chemical and Biomolecular Engineering, Institute of Emergent Materials, Sogang University, Seoul 04107, Republic of Korea

[2]Department of Chemical Engineering and Materials Science, Ewha Womans University, Seoul 03760, Republic of Korea

[3]Graduate Program in System Health Science and Engineering, Ewha Womans University, Seoul 03760, Republic of Korea

AUTHOR INFORMATION

Corresponding author(s)

E-mail: sback@sogang.ac.kr; jgna@ewha.ac.kr;

Appendix A. Supplementary Information

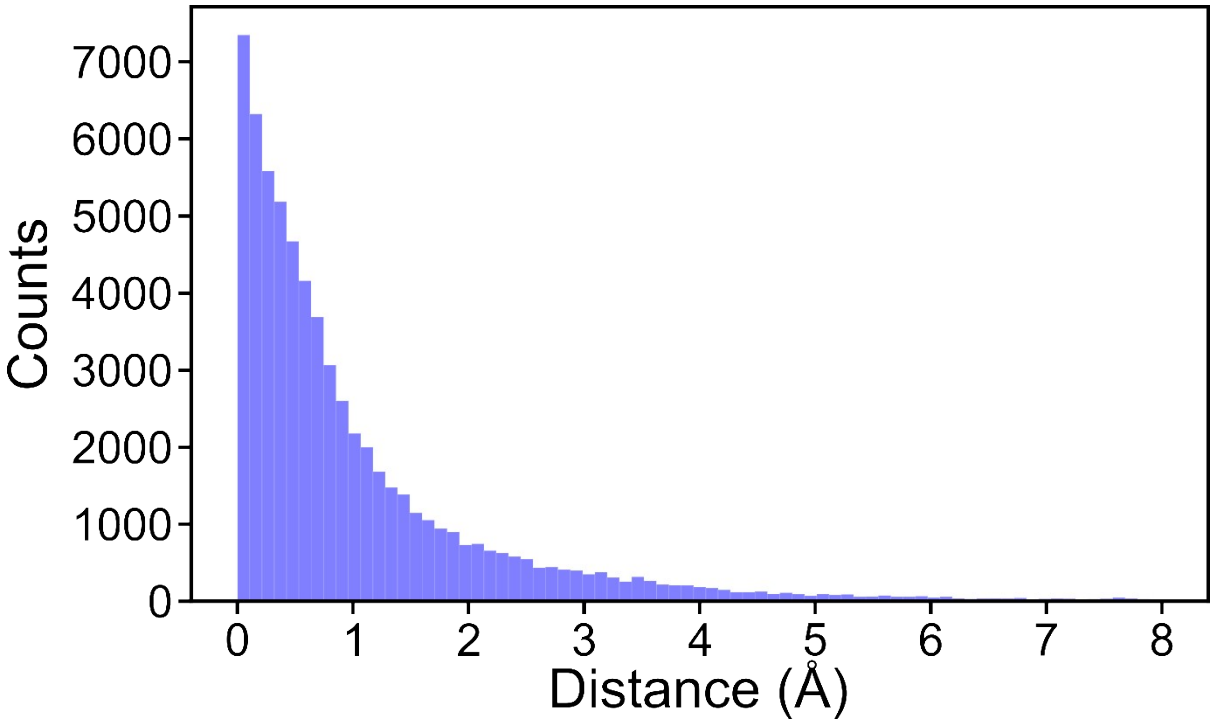

Figure A1 Histogram of distance changes between two atoms during geometry optimizations.

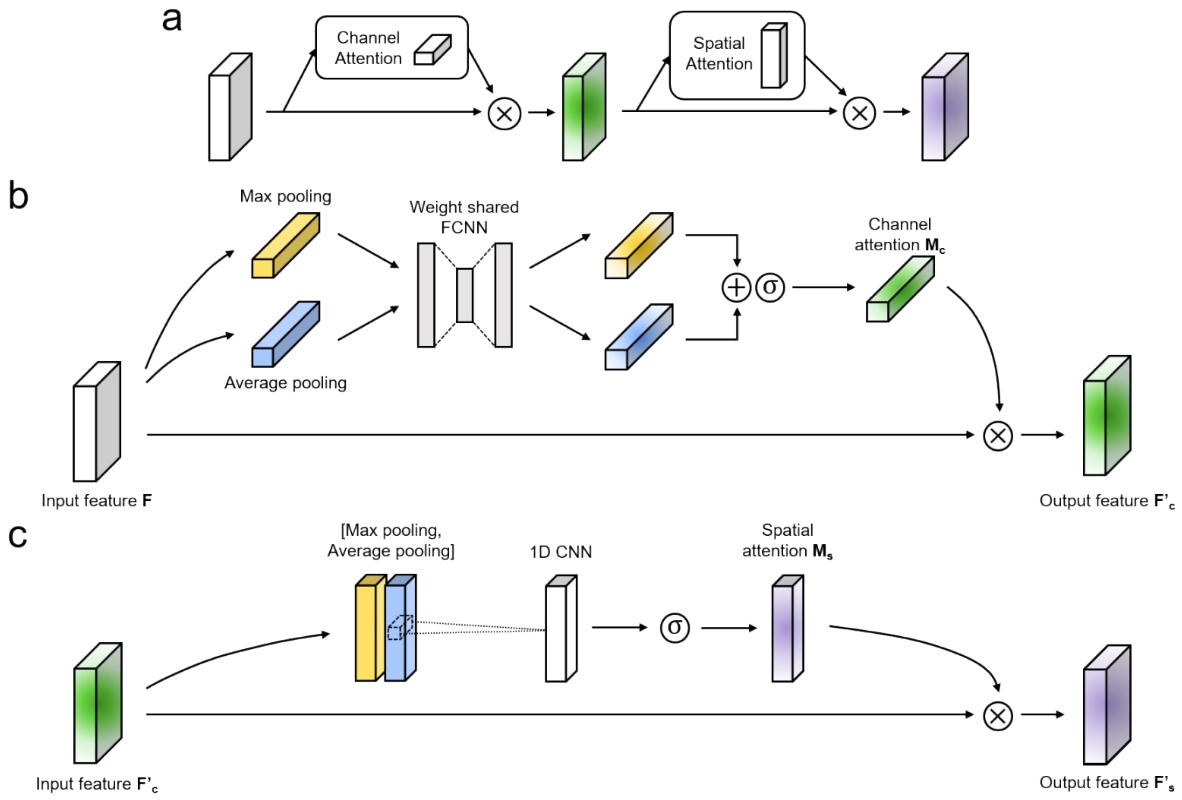

Figure A2 Detailed structure of CBAM. a) Overall scheme of CBAM which perform channel attention and spatial attention in sequence. b) Channel attention starting with global max pooling and global average pooling in channel dimension outputs weighted feature maps for channel dimension. c) Spatial attention starting with global max pooling and global average pooling in spatial dimension outputs weighted feature maps for spatial dimension.

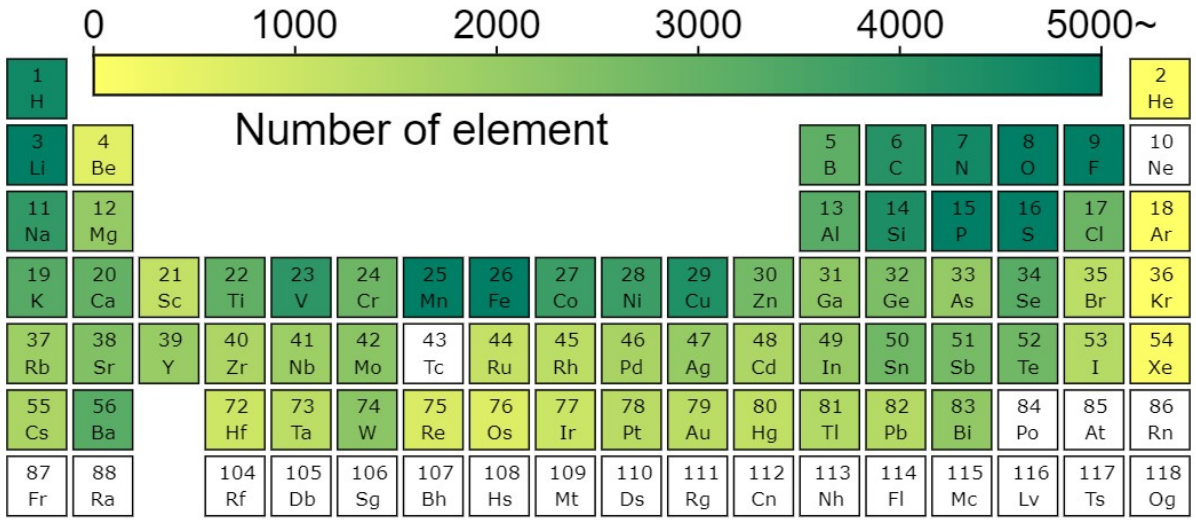

Figure A3 Periodic table displaying the number of each element in MP training dataset.

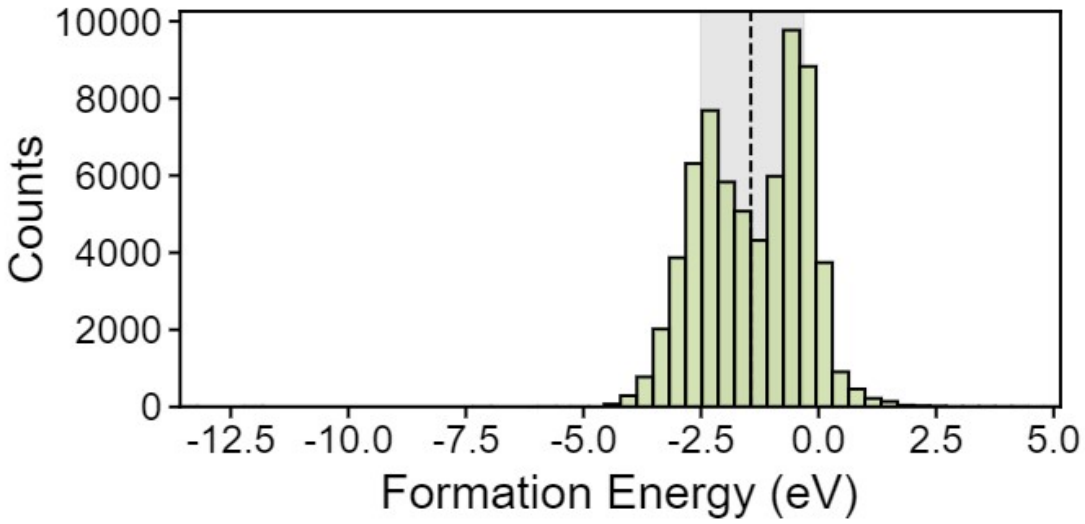

Figure A4 Histogram of formation energy distribution of MP training dataset. Black dashed line and gray area indicate average and standard deviation, respectively**.**

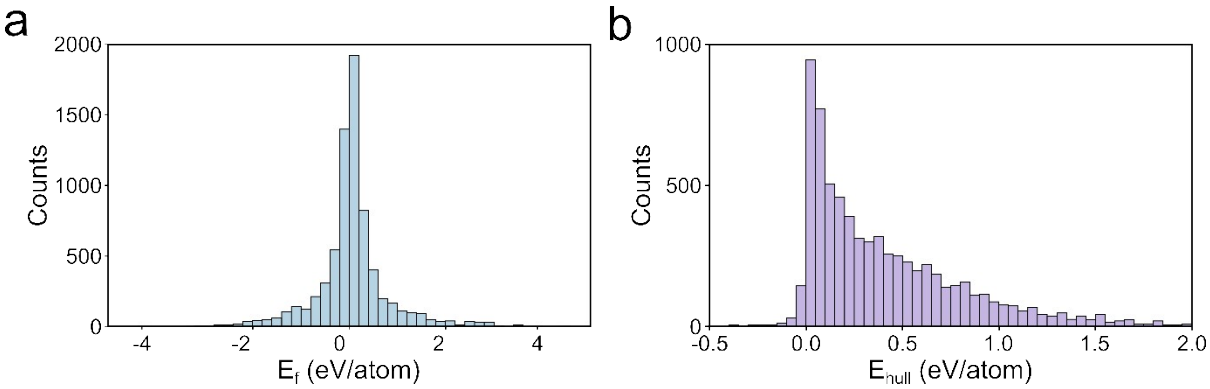

Figure A5. Histogram of DFT-calculated a) E_f and b) E_{hull} of 2e-ORR validation set.

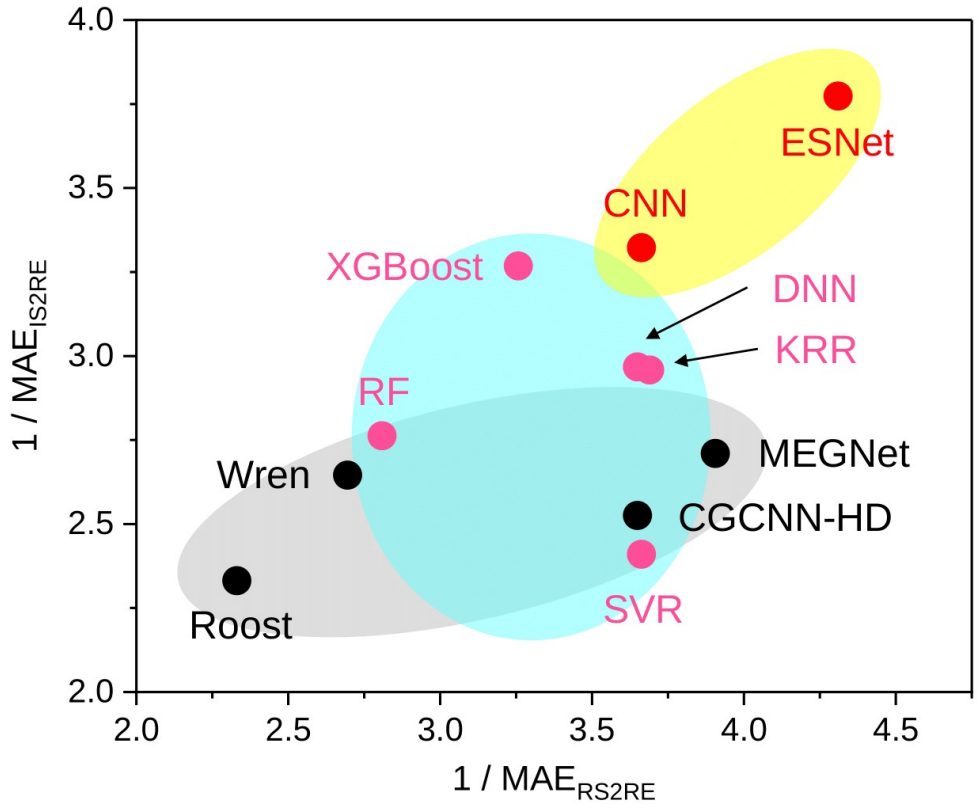

Figure A6 Comparison of RS2RE and IS2RE performances for various models with different input descriptors and algorithms (**Table 1**). A reciprocal of MAE was used as a performance metric. Yellow, blue, and gray-colored areas correspond to DOS signal-based, DOS features-based and other descriptors, respectively. ESNet achieved the best accuracy for both tasks.

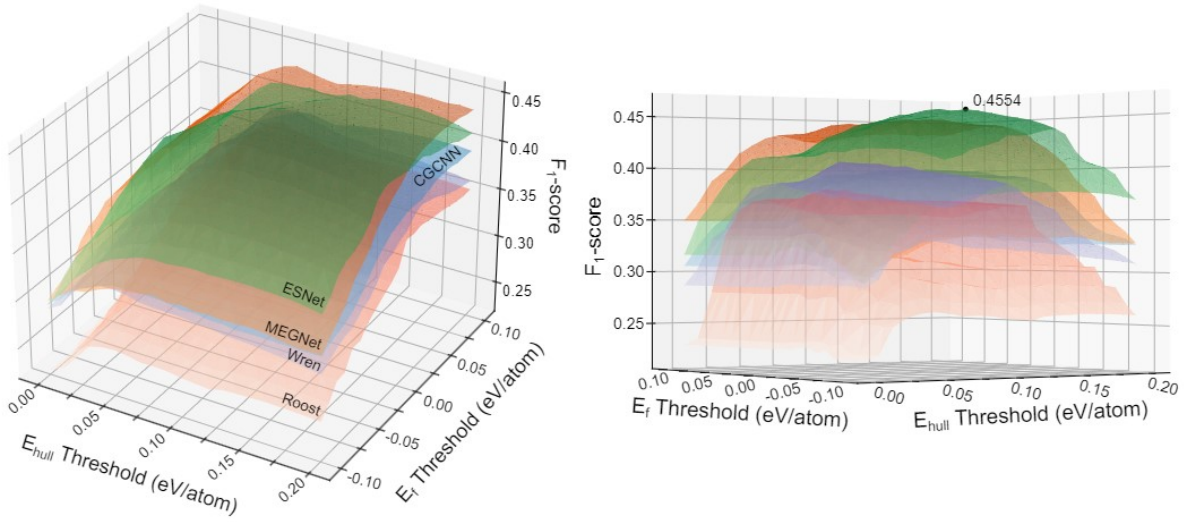

Figure A7 3D surfaces visualizing F_1-score of various models with respect to E_f^{ML} and E_{hull}^{ML} thresholds. ESNet with thresholds of $E_f^{ML} \leq$ -0.02 eV/atom and $E_{hull}^{ML} \leq$ 0.13 eV/atom achieved the highest F_1-score, 0.4554.

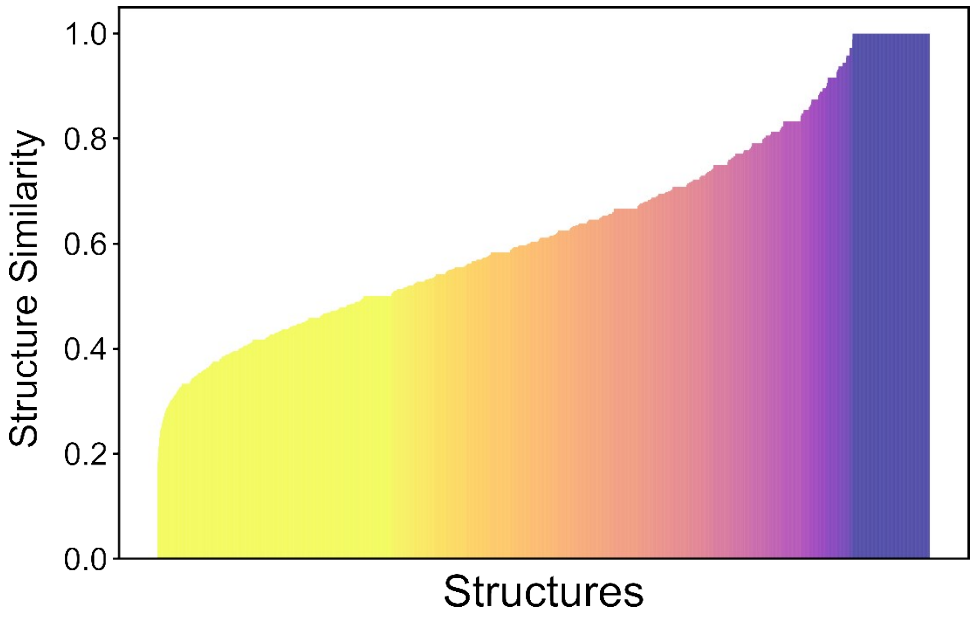

Figure A8 Structure similarities in the 2e-ORR validation dataset: Crystal structures were converted into graph representations using CGCNN, and a graph edit distance − the minimum number of operations (e.g., deletion, substitution, and insertion) required for two graphs to be identical − was defined to measure the quantitative similarity between two graph structures. The similarity was evaluated by normalizing the graph edit distances between crystal graphs of the initial and relaxed structures. The similarity value of 1 indicates the identical graph structures.

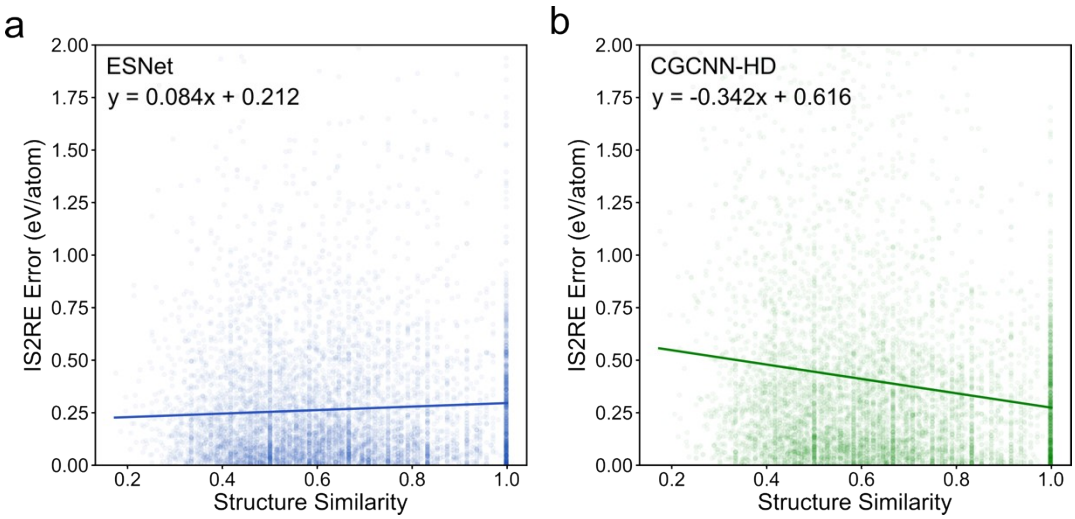

Figure A9 IS2RE errors plotted with respect to the structure similarity for (a) ESNet and (B) CGCNN-HD. ESNet is much less sensitive to structural differences between IS and RS compared to CGCNN-HD

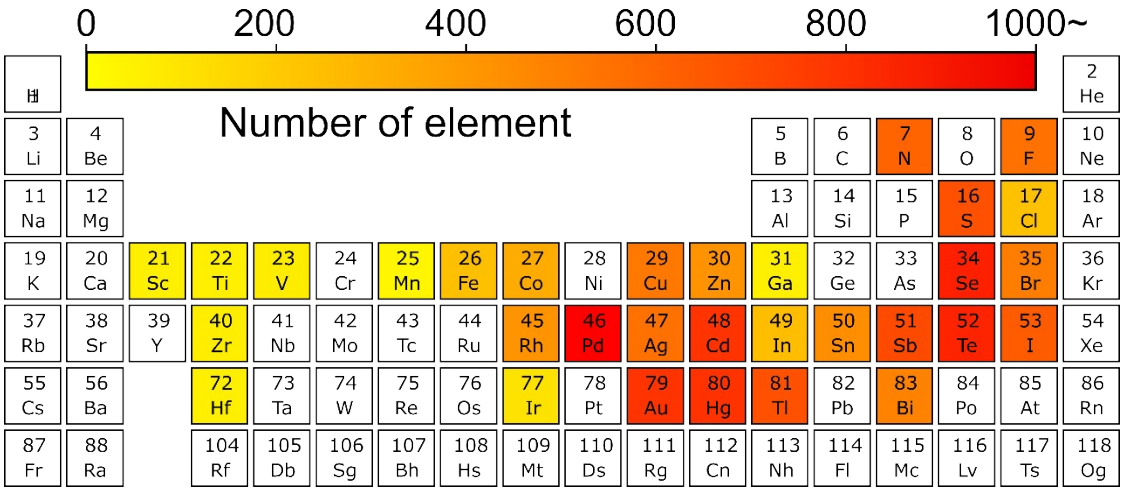

Figure A10 Periodic table displaying the number of each element in 2eORR test dataset.

Table A1 All features used in feature-based models.

Spin	Orbital	Feature name	Number of features
Up	s, p_x, p_y, p_z, d_{xy}, d_{yz}, $d_{z^2-x^2}$, d_{xz}, $d_{x^2-y^2}$	d-band center, width, skewness, kurtosis, number of fillings	45
Down	s, p_x, p_y, p_z, d_{xy}, d_{yz}, $d_{z^2-x^2}$, d_{xz}, $d_{x^2-y^2}$	d-band center, width, skewness, kurtosis, number of fillings	45
		One-hot encoded composition	111
		Total	201

Table A2. ML model prediction performance evaluated on the Materials Project dataset split into 8:2 train-test ratio. The MAEs above 0.2 eV/atom of ESNet and benchmark models for formation energy prediction in **Table 1** seem to be high compared to the MAE below 0.1 eV/atom reported in the original papers. However, in this result, most of models achieved MAE smaller than 0.1 eV/atom in agreement with the previous papers. This demonstrates that relatively high MAE in **Table 1** is due to the use of a different test set (**Supplementary Fig.A10**).

	RS2RE	
Model	MAE (eV/atom)	RMSE (eV/atom)
DOS-free feature-based		
CGCNN-HD	0.051	0.138
MEGNet	0.061	0.135
Wren	0.072	0.193
Roost	0.073	0.203
DOS feature-based		
KRR	0.142	0.253.
SVR	0.142	0.231
RF	0.170	0.281
XGBoost	0.182	0.279
DNN	0.107	0.192
DOS signal-based		
CNN	0.118	0.210
ESNet (This work)	0.085	0.182

Table A3 The optimal E_f^{ML} and E_{hull}^{ML} thresholds of various models for maximum F_1-score.

Model	E_f^{ML} Threshold (eV/atom)	E_{hull}^{ML} Threshold (eV/atom)	F_1-score
ESNet	-0.02	0.13	0.4554
CGCNN-HD	0.05	0.15	0.3999
MEGNet	0.04	0.14	0.4481
Wren	0.03	0.06	0.3793
Roost	0.03	0.07	0.4054