Supporting Information: Predictive Machine Learning Models Trained on Experimental Datasets for Electrochemical Nitrogen Reduction

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1.1 Partial Decision Trees

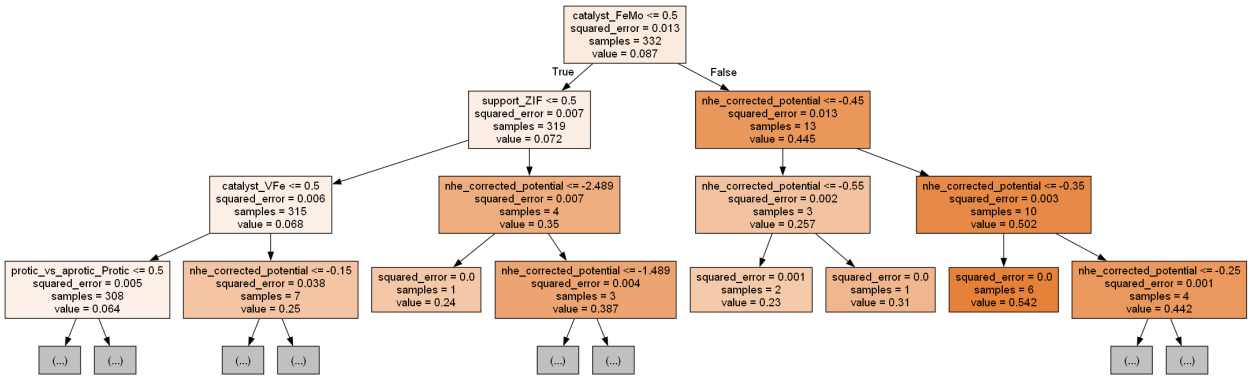

Figure S1a. Efficiency regression decision tree shown with a depth of 3

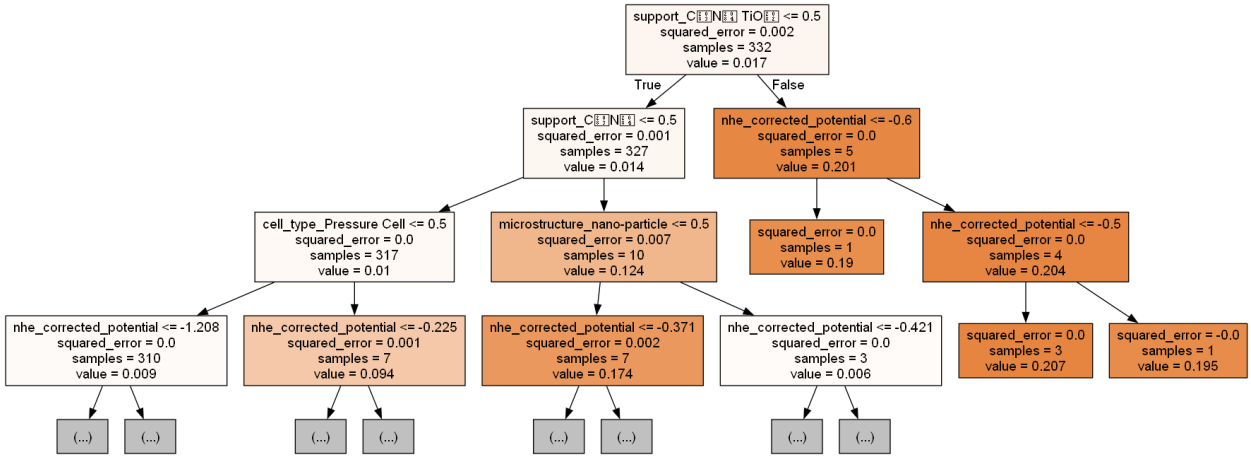

Figure S1b. Rate regression decision tree shown with a depth of 3

1.2 Feature Classifications

Table S1. Unique Categorical Features

Category	Features
Catalyst	C_3N_4, Au, Nb_2O_5, Ru, Ag/Pd, Pt, Fe_2O_3, MoS_2, Co, VN/CC, B_4C, WS_2WO_2, Rh, CoP-MoP, Fe_3O_4, $K_3Ti_8O_{17}$, VFe, Bi, Mo_2C, FeMo, Fe_3O_4/Bi, Fe, Pd, Zn, VS_2, $MOSe_2$, Cu, Mn, CrN, C, Ir
Atomic Number	6, 79, 41, 44, 47, 78, 26, 42, 27, 23, 5, 22, 83, 45, 46, 30, 29, 25, 74, 24, 77
Electrode	Carbon Paper, carbon membrane, TiO2, BCY, Carbon Cloth, Glassy Carbon, Catalyst, Au
Support	unsupported, carbon nanotube, Carbon, C3N4, TiO_2, rGO, NC, FeS_2/C, BiClO, MnO_2, Graphdiyne, Carbon Fiber, TCPP, $MoSe_2$, TPP, C_3N_4/TiO_2, Mxene, RGO, ZIF
Dopant	Yes, No
Micro-Structure	Nanorod, Agglomerated, Nanoparticle, Nanosheet, Nanocage, Nanofiber, Heterostructured, Single Atom, Nanosphere, Amorphous, Microsphere, Polycrystalline
Cell Type	Traditional, Solid State, Pressure Cell
Electrolyte	$NaClO_4$, $LiClO_4$, HCl, Na_2SO_4, H_2SO_4, KOH, BCY, $KClO_4$,CsH_2PO_4, K_2SO_4, lithium trifluoromethanesulfonate
Protic vs Aprotic	Protic, Aprotic

1.3 Max Depth Determination

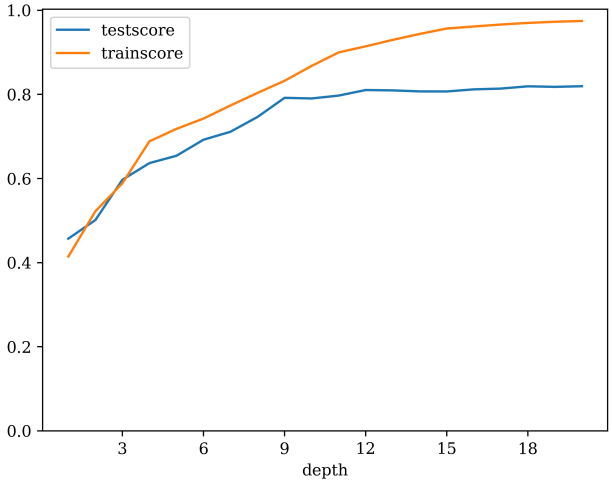

Figure S2a. Max depth vs the Accuracy for the decision tree Efficiency Regression

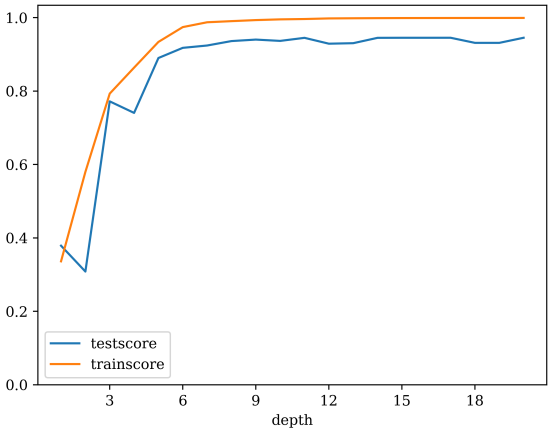

Figure S2b. Max depth vs the Accuracy for the decision tree Rate Regression

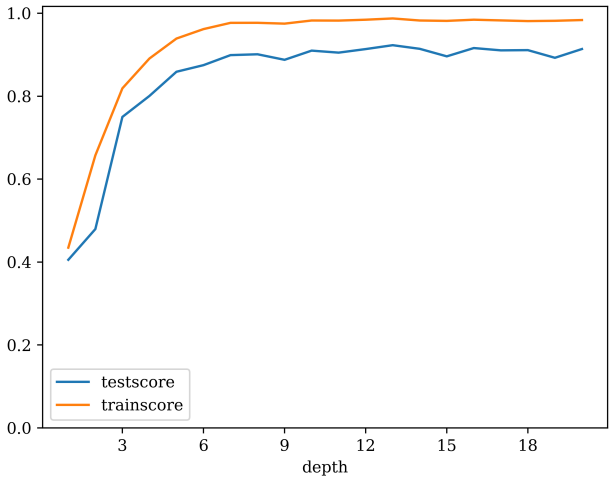

Figure S2c. Max depth vs the Accuracy for the random forest Efficiency Regression

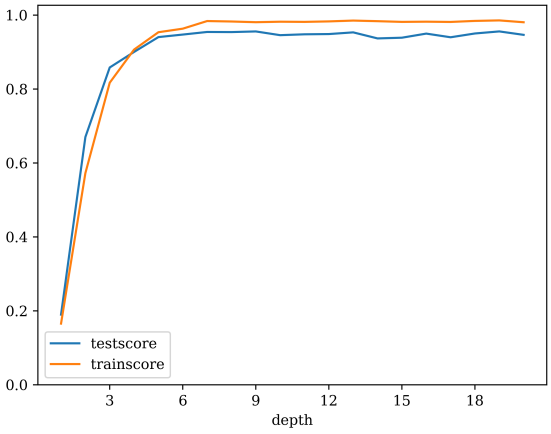

Figure S2d. Max depth vs the Accuracy for the random forest Rate Regression

1.4 Random Seed Testing

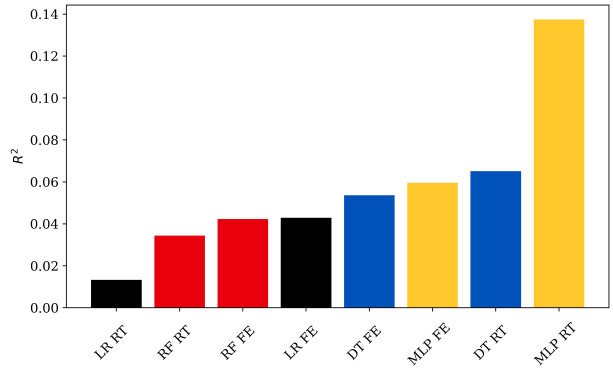

Figure S3a. Variance in cross validated standard deviation detected using 10 random seeds.

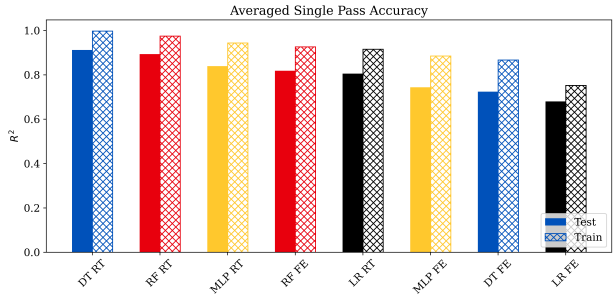

Figure S3b. Averaged single pass accuracy showing testing vs training using 10 random seeds.

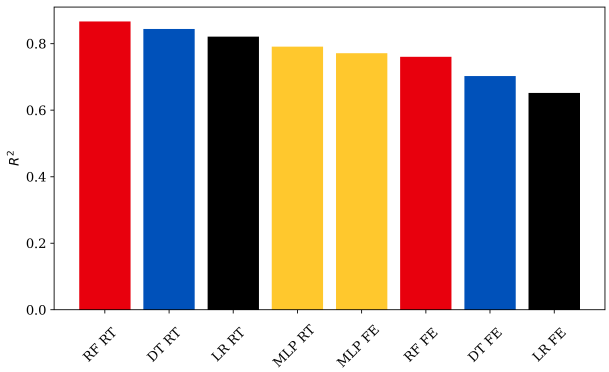

Figure S3c. Averaged cross validated accuracy using 10 random seeds.

1.5 Label Encoded Results

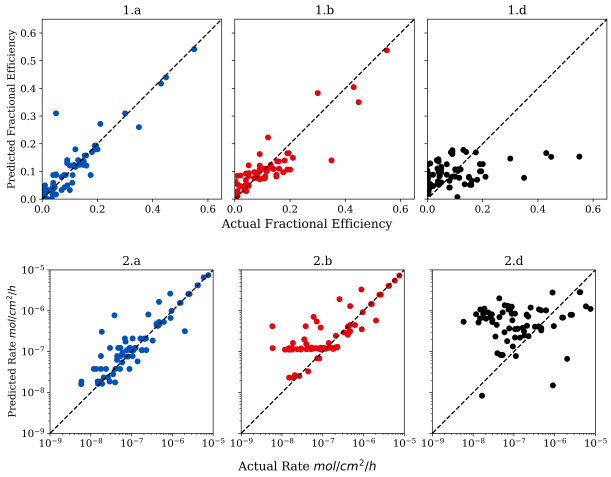

Figure S4a. Diagonal plots showing results for label encoded Decision Trees, Random Forests and Linear Regressions

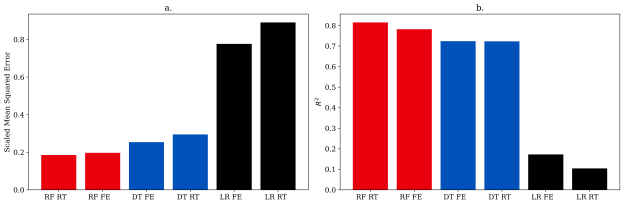

Figure S4b. Scoring for label encoded Decison Trees, Random Forests and Linear Regressions

1.6 Machine Learning Methods

This section will review the procedure for using the attached machine learning models for analyzing electrochemical Nitrogen Reduction Reactions. All software, functions and programming used for this analysis are attached and open for public use and study. Run the IPYNB files in this order: DataProcessing, All Models Exporting Data and Discussion. The first file, Data Processing, is used to condition the data-set for machine learning. The second file does the bulk of the machine learning work. When running the second file we strongly recommend attempting to use our data-set first. If the data-set is altered then the Keras Tuners attached to the MLP neural networks will need to be re-run by setting their "Overwrite" parameter to "True". Tuning neural networks is a time intensive process which can be expedited by applying GPU instead of CPU - however GPU may have lower physical memory than CPU which leads to smaller neural nets. Thus the tuning parameters may need to be altered depending on hardware and time constraints. Finally, the Discussion file will provide useful graphics to understand the outputs of each machine learning model.

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