

## SUPPLEMENTARY FILE

### **A machine learning approach for estimating supercapacitor performance of graphene oxide nano-rings based electrode materials**

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**Table S1. Electrochemical predictor and response variable for ML training.**

	<b>ELEC</b>	<b>CNC</b>	<b>CD</b>	<b>PW</b>	<b>SCAP</b>
<b>1</b>	'KOH'	2	2	1	236
<b>2</b>	'NaClO4'	1	0.5000	3	117
<b>3</b>	'KOH'	6	0.2000	0.8000	207
<b>4</b>	'KOH'	6	0.2000	0.8000	193
<b>5</b>	'H2SO4'	1	1	1	253
<b>6</b>	'KOH'	6	1	1	170
<b>7</b>	'KOH'	6	0.5000	1	176
<b>8</b>	'H2SO4'	2	0.5000	0.7000	208
<b>9</b>	'H2SO4'	1	1	0.8000	240
<b>10</b>	'KOH'	6	0.2000	1	225
<b>11</b>	'KOH'	6	1	1	159
<b>12</b>	'KOH'	6	0.5000	2	210
<b>13</b>	'KOH'	6	0.5000	1	269
<b>14</b>	'KOH'	6	0.2000	1	288

	<b>ELEC</b>	<b>CNC</b>	<b>CD</b>	<b>PW</b>	<b>SCAP</b>
15	'KOH'	6	0.5000	0.8000	239
16	'KOH'	6	0.2000	0.9000	227
17	'H2SO4'	1	0.2000	0.9000	262
18	'HCl'	1	1	2	275
19	'H2SO4'	1	1	1.2000	111
20	'H2SO4'	1	0.1000	1.2000	240
21	'KOH'	6	1	1	210
22	'KOH'	1	0.5000	1.5000	150
23	'Na2SO4'	1	3	1	186
24	'KOH'	6	0.5000	1	266
25	'KOH'	1	1	1.1000	165
26	'H2SO4'	1	1	1.1000	283
27	'KOH'	6	1	1	214
28	'KOH'	6	0.5000	1	160
29	'H2SO4'	1	1	0.8000	225
30	'KOH'	6	0.5000	1.2000	275
31	'H2SO4'	1	0.5000	0.5000	132
32	'KOH'	6	0.5000	3	185
33	'KOH'	6	1	1	271
34	'KOH'	6	1	1	285
35	'H2SO4'	1	1	0.8000	206
36	'KOH'	3	0.1000	1	205
37	'H2SO4'	1	50	0.8000	273
38	'Na2SO4'	0.1000	1	1	128
39	'Na2SO4'	0.1000	5	1	74
40	'Na2SO4'	0.1000	7	1	62
41	'KCl'	0.1000	1	1	85.3000
42	'NaCl'	0.1000	0.2000	0.8000	75
43	'KOH'	0.3000	1	1	225
44	'KOH'	0.3000	1	1	230
45	'HOH'	0.3000	1	1	185
46	'H3PO4'	1	1	0.8000	14
47	'H2SO4'	1	0.2000	0.8000	180
48	'H2SO4'	0.1000	1.5000	2.5000	170
49	'H2SO4'	2	1	1	194
50	'LiTFSI'	0.1000	0.5000	3.5000	99
51	'KOH'	6	0.1000	1	97
52	'Na2SO4'	0.5000	1.0400	0.8000	141
53	'KOH'	6	0.2000	0.7000	300
54	'Na2SO4'	1	1	0.8000	128
55	'KOH'	5	0.7500	1	182

	ELEC	CNC	CD	PW	SCAP
56	'KOH'	6	0.4000	0.8000	260
57	'KOH'	6	1	1	236
58	'KOH'	5	0	3	97
59	'KOH'	6	0.1000	1	244
60	'KOH'	1	2	2.5000	120
61	'H2SO4'	1	0.1000	0.8000	238
62	'H2SO4'	1	5	0.8000	140
63	'KOH'	6	0.1000	2	80.4000
64	'KOH'	6	0.1000	1	41.5000

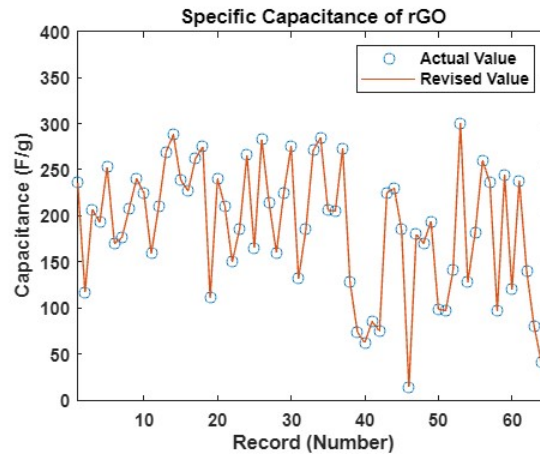


Fig. S1. The actual capacitance and revised outlier capacitance of GO-based electrode materials.

## 1. Neural Network

Table S2. Hyperparameter optimization observation table for ANN training.

```

=====
| Iter | Eval | Objective: | Objective | BestSoFar | BestSoFar | Activations | Standardize |
| Lambda | result | LayerSizes | log(1+loss) | runtime | (observed) | (estim.) | |
|=====
| 1 | Best | 8.53 | 2.7022 | 8.53 | 8.53 | sigmoid | false |
2.3991e-06 | [ 2 1] |
| 2 | Accept | 12.198 | 8.512 | 8.53 | 8.6758 | relu | true |
6.4779e-05 | [230 22] |
| 3 | Best | 8.3912 | 2.4262 | 8.3912 | 8.5276 | relu | false |
0.070108 | [ 3 1 2] |
| 4 | Accept | 8.9911 | 0.34152 | 8.3912 | 8.4936 | none | true |
30.764 | 37 |
| 5 | Accept | 8.5461 | 3.0176 | 8.3912 | 8.3913 | sigmoid | false |
0.004881 | [ 2 1] |
| 6 | Accept | 8.8727 | 3.079 | 8.3912 | 8.3916 | relu | false |
2.6967 | [ 3 2 13] |
| 7 | Accept | 9.2455 | 0.17246 | 8.3912 | 8.3916 | sigmoid | false |
20.886 | [ 2 16] |
| 8 | Accept | 8.5868 | 0.79519 | 8.3912 | 8.392 | relu | false |
5.474e-07 | [ 5 2 2] |
| 9 | Accept | 9.2564 | 0.96273 | 8.3912 | 8.3919 | relu | true |
113.1 | [ 6 1 1] |
=====

```

```

| 10 | Accept | 8.53 | 0.15916 | 8.3912 | 8.3918 | tanh | false |
6.0806e-07 | [ 2 1 1] |
| 11 | Accept | 8.4139 | 14.205 | 8.3912 | 8.392 | tanh | false |
7.0058e-07 | [ 37 281 35] |
| 12 | Accept | 9.0035 | 7.2386 | 8.3912 | 8.3921 | tanh | false |
0.0062681 | [ 21 5 289] |
| 13 | Accept | 8.6055 | 1.2125 | 8.3912 | 8.3918 | tanh | false |
4.5312e-06 | [ 2 294 1] |
| 14 | Accept | 8.53 | 0.11548 | 8.3912 | 8.3917 | tanh | true |
5.8047e-07 | [ 17 22 1] |
| 15 | Accept | 8.6963 | 2.5619 | 8.3912 | 8.3918 | tanh | true |
1.6748e-06 | [151 1 294] |
| 16 | Accept | 8.5624 | 25.081 | 8.3912 | 8.3921 | tanh | true |
1.1696 | [ 1 260 290] |
| 17 | Accept | 10.277 | 0.38827 | 8.3912 | 8.3918 | sigmoid | false |
19.438 | [150 51 1] |
| 18 | Accept | 8.9011 | 0.22659 | 8.3912 | 8.3918 | none | false |
1.7565e-07 | [ 13 1] |
| 19 | Accept | 8.53 | 0.094858 | 8.3912 | 8.3918 | sigmoid | true |
1.5779e-07 | [ 2 1] |
| 20 | Accept | 8.4792 | 0.19636 | 8.3912 | 8.3919 | sigmoid | true |
16.75 | [ 1 300] |

```

```

=====
| Iter | Eval | Objective: | Objective | BestSoFar | BestSoFar | Activations | Standardize |
Lambda | LayerSizes |
| result | log(1+loss) | runtime | (observed) | (estim.) |
=====
| 21 | Accept | 8.9011 | 1.2148 | 8.3912 | 8.3918 | none | true |
7.2905e-06 | [ 1 10] |
| 22 | Accept | 8.525 | 0.10199 | 8.3912 | 8.3922 | tanh | false |
1.7368e-07 | [ 71 1] |
| 23 | Accept | 8.9739 | 16.85 | 8.3912 | 8.3924 | tanh | false |
2.2711 | [ 91 300] |
| 24 | Accept | 8.5062 | 1.4397 | 8.3912 | 8.3917 | sigmoid | true |
0.088287 | 37 |
| 25 | Accept | 9.2784 | 1.2318 | 8.3912 | 8.3923 | relu | false |
39.434 | [ 10 1] |
| 26 | Accept | 8.4956 | 1.153 | 8.3912 | 8.3921 | sigmoid | true |
4.7795e-06 | [ 85 39 1] |
| 27 | Accept | 8.53 | 0.069716 | 8.3912 | 8.3915 | sigmoid | false |
3.6875e-07 | 1 |
| 28 | Accept | 10.585 | 0.088884 | 8.3912 | 8.3915 | sigmoid | true |
1016 | [ 17 9] |
| 29 | Accept | 8.8048 | 7.1948 | 8.3912 | 8.3914 | sigmoid | true |
0.00017906 | [ 80 78 2] |
| 30 | Accept | 8.6623 | 24.618 | 8.3912 | 8.3914 | tanh | false |
8.1101e-06 | [ 39 155 287] |

```

Optimization completed.  
MaxObjectiveEvaluations of 30 reached.  
Total function evaluations: 30  
Total elapsed time: 153.3897 seconds  
Total objective function evaluation time: 127.4503

Best observed feasible point:

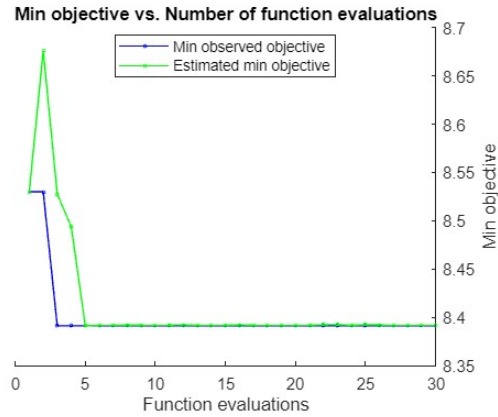
Activations	Standardize	Lambda	LayerSizes
relu	false	0.070108	3 1 2

Observed objective function value = 8.3912  
Estimated objective function value = 8.3914  
Function evaluation time = 2.4262

Best estimated feasible point (according to models):

Activations	Standardize	Lambda	LayerSizes
relu	false	0.070108	3 1 2

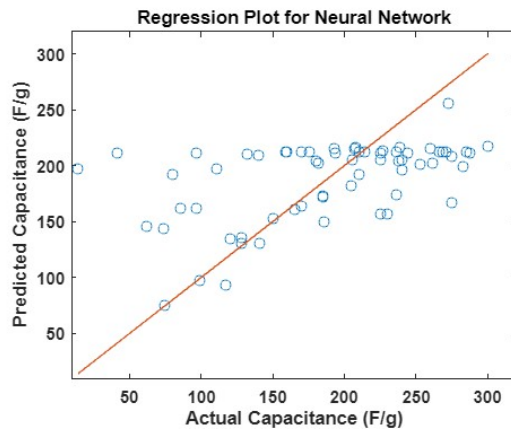
Estimated objective function value = 8.3914  
Estimated function evaluation time = 2.4259



**Fig. S2. Comparison plot for minimum observed and estimated objective values during ANN model.**

```
mdl =
  RegressionNeuralNetwork
    ResponseName: 'Y'
    CategoricalPredictors: []
    ResponseTransform: 'none'
    NumObservations: 64
    HyperparameterOptimizationResults: [1x1 BayesianOptimization]
    LayerSizes: [3 1 2]
    Activations: 'relu'
    OutputLayerActivation: 'none'
    Solver: 'LBFGS'
    ConvergenceInfo: [1x1 struct]
    TrainingHistory: [1000x7 table]
```

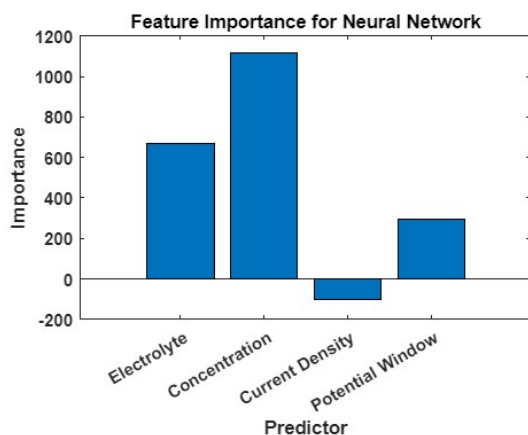
```
Properties, Methods
yNet = 64x1
174.1323
92.9361
215.5875
215.5875
201.3410
212.4765
211.9619
216.5713
205.2754
211.6531
```



**Fig. S3. Predicted vs Actual capacitance of ANN model.**

```
yNet2 = 212.4765
MSE = 3.4842e+03
```

**testMSE = 3.4842e+03**  
**RMSE = 59.0275**  
**R2 = 0.2602**  
**R = 0.5101**  
**MAE = 44.5477**



**Fig. S4. Predictor estimate of ANN model.**

## 2. Regression Tree

**Table S3. Hyperparameter optimization observation table for RT model.**

Iter	Eval result	Objective: log(1+loss)	Objective runtime	BestSoFar (observed)	BestSoFar (estim.)	MinLeafSize
1	Best	8.3909	0.94647	8.3909	8.3909	7
2	Accept	8.5521	0.12766	8.3909	8.4246	3
3	Accept	8.6091	0.061359	8.3909	8.4093	1
4	Accept	8.4965	0.083907	8.3909	8.4382	17
5	Accept	8.3909	0.094932	8.3909	8.391	7
6	Accept	8.4881	0.036855	8.3909	8.391	12
7	Accept	8.5302	0.034922	8.3909	8.391	6
8	Accept	8.4965	0.03585	8.3909	8.391	18
9	Accept	8.4574	0.039428	8.3909	8.391	8
10	Accept	8.5209	0.034828	8.3909	8.391	10
11	Accept	8.5689	0.03855	8.3909	8.391	14
12	Accept	8.4693	0.03404	8.3909	8.391	23
13	Accept	8.5422	0.061848	8.3909	8.391	26
14	Accept	8.4887	0.036786	8.3909	8.391	21
15	Accept	8.3909	0.038442	8.3909	8.391	7
16	Accept	8.4693	0.036064	8.3909	8.391	24
17	Accept	8.4396	0.04027	8.3909	8.391	2
18	Accept	8.5227	0.035928	8.3909	8.391	4
19	Accept	8.53	0.042154	8.3909	8.391	32
20	Accept	8.3909	0.041007	8.3909	8.391	7
21	Accept	8.5713	0.043355	8.3909	8.391	5
22	Accept	8.4785	0.033942	8.3909	8.391	9
23	Accept	8.53	0.036874	8.3909	8.391	29
24	Accept	8.5124	0.037725	8.3909	8.391	11
25	Accept	8.4909	0.038175	8.3909	8.391	15
26	Accept	8.5369	0.03586	8.3909	8.391	13
27	Accept	8.4965	0.03876	8.3909	8.391	19
28	Accept	8.4961	0.036615	8.3909	8.391	16
29	Accept	8.4861	0.03545	8.3909	8.391	20
30	Accept	8.53	0.035184	8.3909	8.391	28

Optimization completed.

MaxObjectiveEvaluations of 30 reached.  
 Total function evaluations: 30  
 Total elapsed time: 19.8992 seconds  
 Total objective function evaluation time: 2.2732

Best observed feasible point:

**MinLeafSize**

7

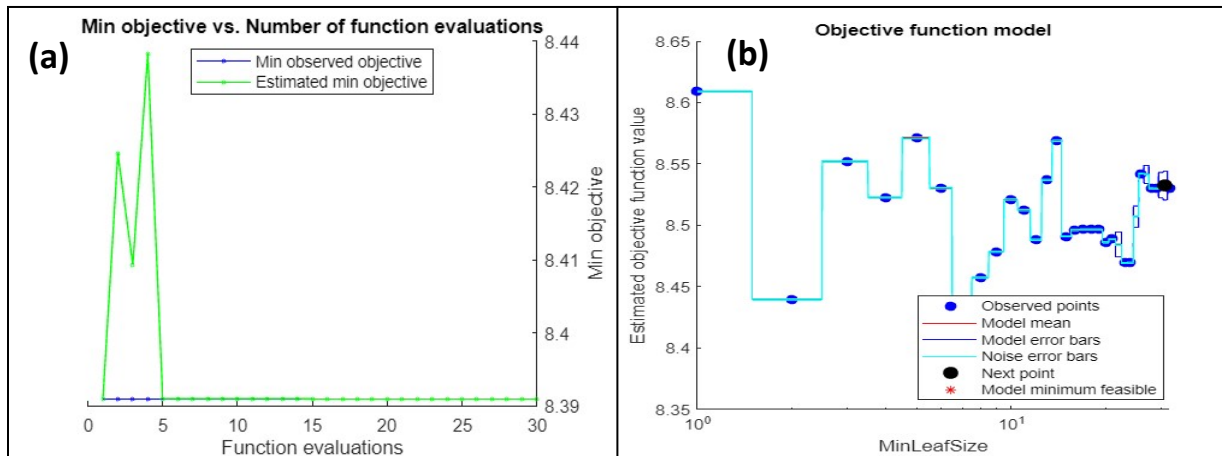
Observed objective function value = 8.3909  
 Estimated objective function value = 8.391  
 Function evaluation time = 0.94647

Best estimated feasible point (according to models):

**MinLeafSize**

7

Estimated objective function value = 8.391  
 Estimated function evaluation time = 0.052774



**Fig. S5. (a) Comparison plot for minimum observed and estimated objective values during RT model and (b) illustration of estimated objective function value against MinLeafSize.**

```
mdl2 =
  RegressionTree
    PredictorNames: {'Electrolyte' 'Concentration' 'Current Density'
'Potential Window'}
    ResponseName: 'Y'
    CategoricalPredictors: []
    ResponseTransform: 'none'
    NumObservations: 64
    HyperparameterOptimizationResults: [1x1 BayesianOptimization]
```

```
Properties, Methods
yTree = 64x1
172.4545
154.3000
202.5000
202.5000
212.3333
220.7143
235.0000
212.3333
212.3333
```

202.5000

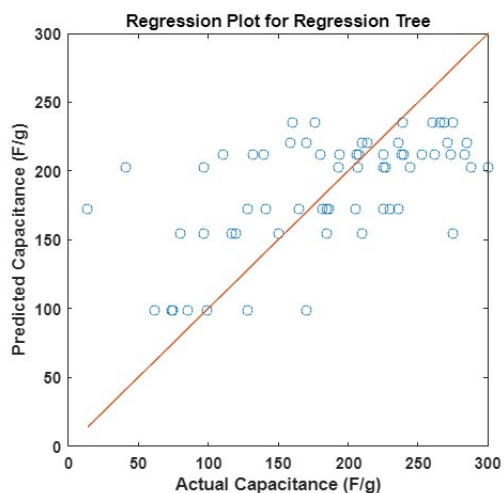


Fig. S6. Predicted vs Actual capacitance of RT model.

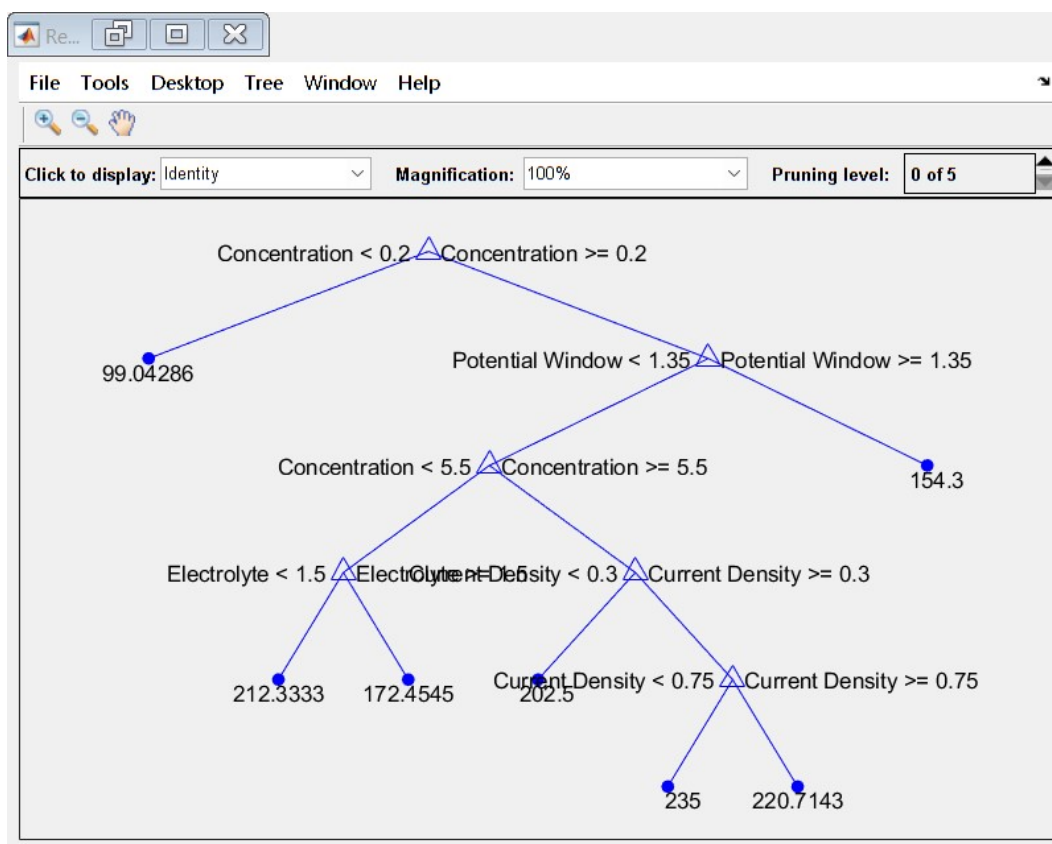
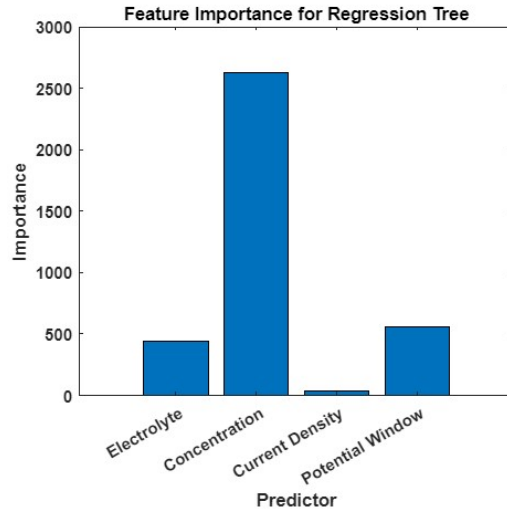


Fig. S7. Visualization of decision obtained from regression tree.

yTree2 = 220.7143  
MSE = 3.1338e+03  
testMSE = 3.4842e+03  
RMSE = 55.9800  
R2 = 0.3346  
R = 0.5785  
MAE = 43.8757





**Fig. S8. Predictor estimate of RT model.**

### 3. Support Vector Machine

```
mdl3 =
  RegressionSVM
    ResponseName: 'Y'
    CategoricalPredictors: []
    ResponseTransform: 'none'
        Alpha: [61x1 double]
        Bias: 163.0130
    KernelParameters: [1x1 struct]
        Mu: [4.9062 3.0953 1.7139 1.1797]
        Sigma: [2.5306 2.5678 6.2472 0.6315]
    NumObservations: 64
    BoxConstraints: [64x1 double]
    ConvergenceInfo: [1x1 struct]
    IsSupportVector: [64x1 logical]
    Solver: 'SMO'
```

#### Properties, Methods

```
ySVM = 64x1
207.9692
124.7281
224.0109
224.0109
228.5079
221.6664
221.7180
200.2549
213.8801
221.3860
```

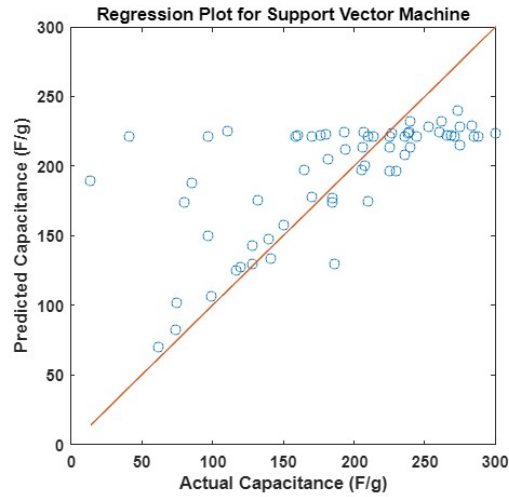


Fig. S9. Predicted vs Actual capacitance of SVM model.

$y_{SVM2} = 221.6664$   
 $MSE = 2.7789e+03$   
 $testMSE = 2.7789e+03$   
 $RMSE = 52.7155$   
 $R^2 = 0.4100$   
 $R = 0.6501$   
 $MAE = 37.1678$

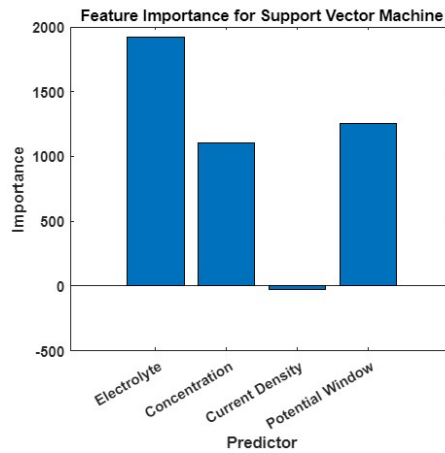


Fig. S10. Predictor estimate of SVM model.

#### 4. Linear Regression

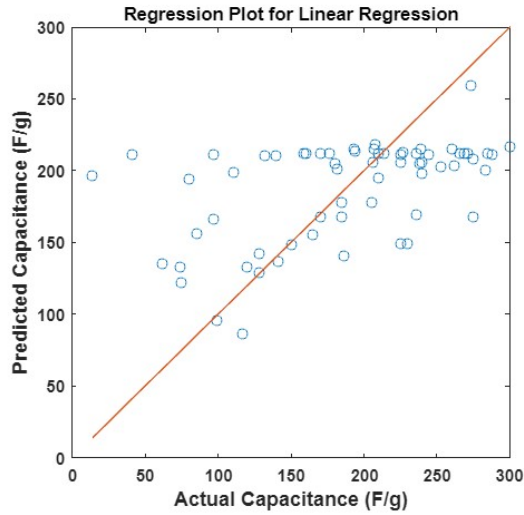
$mdl4 =$   
 Linear regression model:  
 $y \sim 1 + x1 + x2 + x3 + x4$

Table S4. Coefficient estimate for linear regression model.

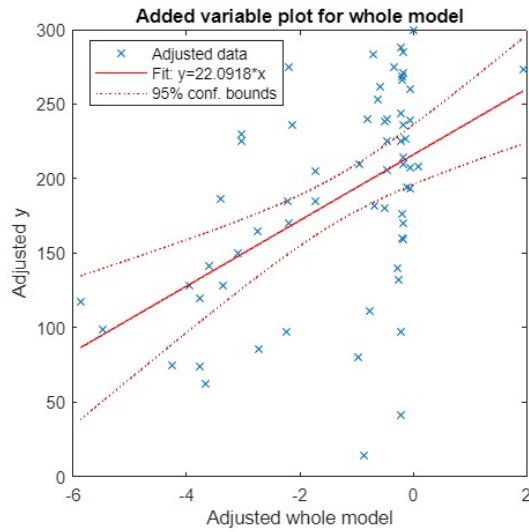
Estimated Coefficients:

	Estimate	SE	tStat	pValue
(Intercept)	216.12	22.453	9.6257	1.0523e-13
x1	-9.0825	3.3747	-2.6914	0.0092437
x2	11.06	3.2651	3.3873	0.0012619
x3	1.0868	1.2811	0.84833	0.39968
x4	-16.794	12.751	-1.3171	0.19291

Number of observations: 64, Error degrees of freedom: 59  
 Root Mean Squared Error: 61.9  
 R-squared: 0.25, Adjusted R-Squared: 0.2  
 F-statistic vs. constant model: 4.93, p-value = 0.0017  
 yLR = 64x1  
 169.1275  
 86.5184  
 214.7697  
 214.7697  
 202.3935  
 212.2803  
 211.7369  
 217.9484  
 205.7524  
 211.4108



**Fig. S11. Predicted vs Actual capacitance of LR model.**



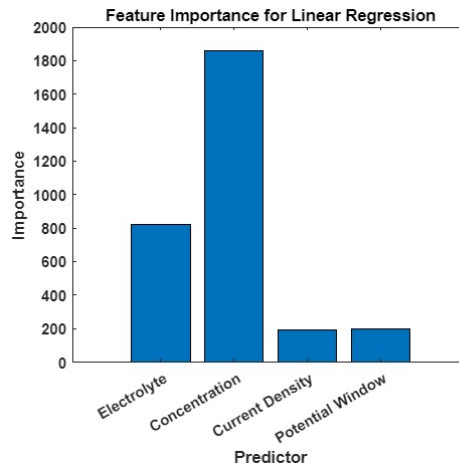
**Fig. S12. Plot for adjusted whole model vs. adjusted y, with a fitted linear regression line (red) and 95% confidence bounds (dotted red lines), illustrating the model's fit and prediction confidence.**

ans = 5x5 table

	SumSq	DF	MeanSq	F	pValue
1 x1	2.7739e+04	1	2.7739e+04	7.2435	0.0092
2 x2	4.3939e+04	1	4.3939e+04	11.4739	0.0013

	SumSq	DF	MeanSq	F	pValue
<b>3 x3</b>	2.7559e+03	1	2.7559e+03	0.7197	0.3997
<b>4 x4</b>	6.6429e+03	1	6.6429e+03	1.7347	0.1929
<b>5 Error</b>	2.2594e+05	59	3.8295e+03	1	0.5000

$y_{SVM2} = 212.2803$   
 $MSE = 3.5303e+03$   
 $RMSE = 59.4162$   
 $R^2 = 0.2504$   
 $R = 0.5004$   
 $MAE = 45.4212$



**Fig. S13. Predictor estimate of LR model.**