

Insights on the Rate Performance of Polyaniline Supercapacitors by Integrated Mathematical Modeling and Machine Learning

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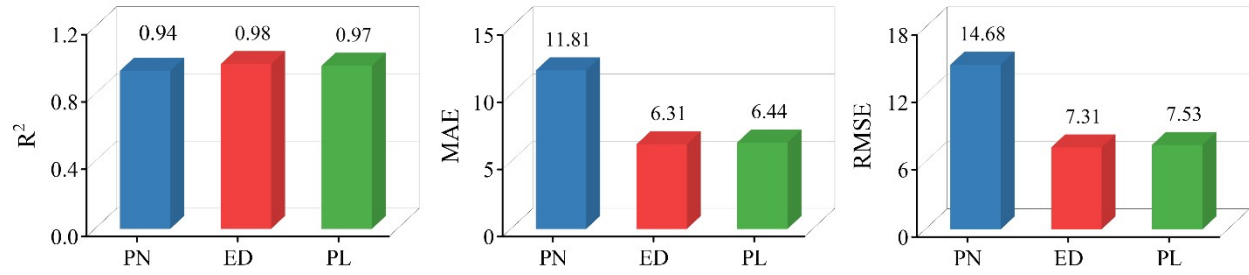


Figure S1. Comparison of R^2 , MAE, and RMSE fit metrics for mathematical models of rate performance. The exponential decay model performs best, followed by the power law, with both outperforming the polynomial model.

Table S1. Collected data for modeling rate performance of PANI-based SCs. “a”, “b”, and “c” are the rate performance parameters obtained by fitting an exponential decay function.

Dopant	SSA	AMR	BR	CR	CC	Electrolyte	PW	Start CD	End CD	a	b	c	DOI
H ₂ SO ₄	179	85	5	10	FTO	H ₂ SO ₄	1	0.1	2	147.732	1.395	127.830	10.1016/j.electacta.2017.09.109
H ₂ SO ₄	267	85	5	10	FTO	H ₂ SO ₄	1	0.1	2	243.304	2.255	240.702	
H ₂ SO ₄	256	85	5	10	FTO	H ₂ SO ₄	1	0.1	2	234.857	2.043	212.146	
H ₂ SO ₄	99.7	80	5	15	Carbon	H ₂ SO ₄	1	0.5	10	139.970	0.506	226.392	10.1016/j.est.2023.107764 10.1038/srep21002
HCl	3	85	5	15	Carbon	H ₂ SO ₄	0.7	0.5	40	172.591	0.0844	170.583	
PA	45	85	5	15	Carbon	H ₂ SO ₄	0.7	5	40	326.202	0.0346	0	
HCl+PA	32	85	5	15	Carbon	H ₂ SO ₄	0.7	0.5	40	155.886	0.6375	343.661	
HCl+PA	15	85	5	15	Carbon	H ₂ SO ₄	0.7	0.5	40	250.497	0.0133	0	
PA	60	100	0	0	Carbon	PVA-H ₂ SO ₄	0.8	1	20	301.221	0.3254	278.006	10.1021/acsami.5b00504
HCl	12.63	100	0	0	ITO	LiClO ₄	0.8	1	10	76.890	0.122	19.571	10.1039/d0ta08263e
HCl	16.18	80	5	15	Steel	H ₂ SO ₄	1.2	0.75	15	207.540	0.196	61.285	10.1021/ef301795g
HCl	26.62	80	10	10	Free	H ₂ SO ₄	0.8	1	5	214.695	0.816	118.218	10.1002/pat.5670
H ₂ SO ₄	22.1	100	0	0	Platinum	BQHQ-H ₂ SO ₄ -AcOH	0.65	4	240	3620.362	0.150	603.158	10.1002/adma.201400966
H ₂ SO ₄	22.1	100	0	0	Platinum	BQHQ-H ₂ SO ₄ -AcOH	0.65	0.5	30	494.222	0.551	464.136	
H ₂ SO ₄	22.1	100	0	0	Platinum	H ₂ SO ₄ -AcOH	0.65	4	240	466.997	0.001	0	
H ₂ SO ₄	22.1	100	0	0	Platinum	H ₂ SO ₄ -AcOH	0.65	0.5	30	253.537	0.035	157.084	
PA	48	95	5	0	Carbon	He-Ao-H ₃ PO ₄	0.8	0.25	20	208.297	0.516	188.362	10.1021/acssuschemeng.8b01175
PA	48	95	5	0	Carbon	He-Ao-H ₃ PO ₄	0.8	0.05	4	94.710	1.587	162.779	
HCl	29	100	0	0	Carbon	H ₂ SO ₄	0.8	1	5	646.625	0.291	0	10.1007/s00289-021-03971-9
HCl	12.13	80	0	20	Carbon	H ₂ SO ₄	1.2	1	3.5	128.706	0.832	84.157	10.1039/d1nj05380a
HCl	27.05	80	10	10	Carbon	H ₂ SO ₄	0.8	1	5	44.102	0.556	62.486	10.1016/j.jallcom.2022.163733
HCl	57.8	100	0	0	Carbon	H ₂ SO ₄	0.8	0.5	25	339.564	1.065	458.219	10.1016/j.polymer.2016.01.049
H ₂ SO ₄	68.9	100	0	0	Carbon	H ₂ SO ₄	0.8	0.5	25	256.696	0.950	332.749	
HNO ₃	66.8	100	0	0	Carbon	H ₂ SO ₄	0.8	0.5	25	228.228	0.490	318.459	
HCl	31.1	100	0	0	Carbon	H ₂ SO ₄	0.8	0.5	25	85.128	0.211	139.567	
H ₂ SO ₄	27.6	70	10	20	Nickel	HClO ₄ -NaClO ₄	0.75	0.3	6	388.285	0.255	23.221	10.1007/s10008-016-3464-4
HClO ₄	361	80	10	10	Carbon	H ₂ SO ₄	0.6	0.5	10	143.541	0.167	237.007	10.1016/j.apsusc.2017.10.010
PA	25.3	100	0	0	Carbon	H ₂ SO ₄	0.8	0.2	30	336.428	0.018	0	10.1002/mame.202200180
HCl	17.89	80	10	10	Nickel	KOH	0.65	1	10	131.829	1.313	91.377	10.1016/j.est.2023.108825
H ₂ SO ₄	30.8	80	10	10	Nickel	KOH	0.45	2	10	712.964	0.201	625.313	10.1007/s10854-020-03297-8
Pzdc	14.08	100	0	0	Carbon	KCl	1	0.2	50	273.219	3.063	45.121	10.1016/j.est.2022.105740
H ₂ SO ₄	137.5	100	0	0	Carbon	H ₂ SO ₄	1	1	10	84.941	0.215	152.608	10.1016/j.electacta.2018.07.098
H ₂ SO ₄	35.36	100	0	0	Carbon	H ₂ SO ₄	1	1	32	273.349	0.0390	50.522	10.1016/j.est.2021.102738
H ₂ SO ₄	137.5	100	0	0	Carbon	H ₂ SO ₄	0.6	1	10	460.733	0.055	0	10.1016/j.jpowsour.2016.10.110
HCl	35	80	10	10	Steel	H ₂ SO ₄	0.68	1	8	117.910	0.271	179.227	10.1016/j.cej.2016.01.069
Acid free	315	85	5	10	FTO	H ₂ SO ₄	0.7	0.1	2	505.284	3.644	232.939	10.1016/j.jpowsour.2016.04.113
Acid free	234	85	5	10	FTO	H ₂ SO ₄	0.7	0.1	2	192.459	1.702	154.258	
Acid free	154	85	5	10	FTO	H ₂ SO ₄	0.7	0.1	2	114.346	1.527	37.326	
Sodium Phytate	230	100	0	0	FTO	H ₂ SO ₄	0.8	1	40	212.860	0.320	374.955	10.3390/polym13142329
HCl	21	85	5	10	Carbon	H ₂ SO ₄	1	1	10	218.131	0.212	24.387	10.1016/j.jallcom.2020.156602
HCl	62.2	80	10	10	Carbon	H ₂ SO ₄	0.8	0.14	0.56	163.087	6.981	108.393	10.1016/j.est.2023.107328
HCl	61.5	80	5	15	Carbon	H ₂ SO ₄	1	0.5	50	120.872	0.086	147.212	10.1016/j.matdes.2017.04.053
HCl	17.85	80	5	15	Carbon	H ₂ SO ₄	0.8	1	10	164.526	0.211	180.165	10.1016/j.mseb.2017.05.001
HCl	36.3	70	10	20	Steel	Na ₂ SO ₄	2	0.5	10	172.258	0.467	112.479	10.1016/j.polymer.2022.125235

HCl	24.48	70	10	20	Carbon	H ₂ SO ₄	0.7	0.5	20	470.203	1.297	563.572	10.1016/j.polymer.2018.12.037
HCl	30.2	70	10	20	Carbon	H ₂ SO ₄	0.7	0.5	20	77.066	0.254	376.862	
HClO ₄	17.6	75	5	20	Nickel	Na ₂ SO ₄	1	0.1	2	57.964	2.539	77.384	10.1007/s10854-017-6961-z
HCl	53.1	85	5	10	Nickel	TEABF ₄ -PC	0.8	0.5	4	219.860	0.340	0	10.1016/j.carbon.2012.09.055
HCl	17.87	100	0	0	Carbon	H ₂ SO ₄	0.6	0.5	10	185.757	0.313	21.823	10.1016/j.electacta.2022.140740
HCl	17.87	100	0	0	Carbon	H ₂ SO ₄ -HQ	0.6	0.5	10	507.018	0.877	98.728	
HCl	17.87	100	0	0	Carbon	H ₂ SO ₄	1	2	10	225.247	0.123	0	
HCl	17.87	100	0	0	Carbon	H ₂ SO ₄ -HQ	1	2	10	249.644	0.037	0	
CSA+H ₂ SO ₄	45.2	70	10	20	Carbon	Et ₄ NBF ₄ -AN	1.4	1	100	79.135	0.059	107.036	10.1016/j.ccej.2017.05.094
HCl	16.81	80	5	15	Nickel	KOH	0.5	1	10	83.444	0.059	0	10.1016/j.est.2021.102303
HCl	35	95	0	5	Gold	H ₂ SO ₄	0.9	0.2	20	396.099	0.126	46.515	10.1016/j.compositesb.2018.09.069
HCl	31.9	80	10	10	Carbon	H ₂ SO ₄	1	0.1	5	132.299	0.474	272.088	10.1016/j.est.2022.105893
H ₂ SO ₄	41.9	80	5	15	Titanium	H ₂ SO ₄	0.8	1	50	393.646	0.142	276.285	10.1016/j.synthmet.2013.10.010
TFA	43.8	80	10	10	Carbon	H ₂ SO ₄	0.8	1	20	331.056	0.018	0	10.1021/acsam.0c01309
HCl	50.4	100	0	0	Carbon	H ₂ SO ₄	1	1	20	718.765	0.002	0.001	10.1016/j.electacta.2021.138448
HCl	36.8	100	0	0	Carbon	H ₂ SO ₄	1	1	20	129.674	0.143	413.914	
HCl	29.4	100	0	0	Carbon	H ₂ SO ₄	1	1	20	100.810	0.171	375.025	
HCl	36.3	80	10	10	Carbon	H ₂ SO ₄	1	1	10	128.995	0.273	179.194	10.1016/j.apsusc.2022.153457
HCl	24.58	80	10	10	Steel	H ₂ SO ₄	1	0.5	10	194.541	0.271	146.616	10.1021/acsam.3c00507
HCl	38	85	10	5	Steel	H ₂ SO ₄	1	0.5	10	684.227	0.856	41.710	10.1021/acsam.2c01040
H ₂ SO ₄	30.9	90	5	5	Carbon	H ₂ SO ₄	0.7	1	30	30.134	0.127	375.835	10.1021/jp405300p
H ₂ SO ₄	67.9	90	5	5	Carbon	H ₂ SO ₄	0.7	1	30	68.339	0.067	280.329	
H ₂ SO ₄	77.1	90	5	5	Carbon	H ₂ SO ₄	0.7	1	30	47.059	0.083	455.338	
H ₂ SO ₄	30.9	90	5	5	Carbon	H ₂ SO ₄ -HQ	0.5	1	30	229.110	0.289	511.605	
H ₂ SO ₄	67.9	90	5	5	Carbon	H ₂ SO ₄ -HQ	0.5	1	30	211.755	0.223	453.336	
H ₂ SO ₄	77.1	90	5	5	Carbon	H ₂ SO ₄ -HQ	0.5	1	30	255.726	0.096	669.929	
HCl	10	80	10	10	Carbon	H ₂ SO ₄	1.2	1	20	431.271	0.262	65.591	10.1002/sml.201403744
HCl	10	80	10	10	Carbon	H ₂ SO ₄	1.6	1	20	456.481	0.212	83.451	
HCl	10	80	10	10	Carbon	H ₂ SO ₄	2	1	20	403.181	0.213	97.307	
H ₂ SO ₄	22.1	80	5	15	Steel	H ₂ SO ₄	1	0.5	5	97.859	0.194	37.416	10.1016/j.jallcom.2017.06.068
HCl	42	90	5	5	Steel	H ₂ SO ₄	0.9	1	20	110.965	0.171	314.284	10.1016/j.jallcom.2022.166856
DBSA+H ₂ S O ₄	48.8	80	5	15	Steel	H ₂ SO ₄	1	5	100	196.453	0.028	112.846	10.1016/j.synthmet.2023.117451
H ₂ SO ₄	6	100	0	0	Steel	H ₂ SO ₄	1	1	3	457.746	1.052	85.721	10.1016/j.mseb.2023.116432
H ₂ SO ₄	7	100	0	0	Steel	H ₂ SO ₄	1	1	3	386.073	0.335	0	
H ₂ SO ₄	25	100	0	0	Steel	H ₂ SO ₄	1	1	3	963.924	1.193	429.351	
H ₂ SO ₄	21	100	0	0	Steel	H ₂ SO ₄	1	1	3	258.351	0.188	0	
HCl	63	90	5	5	Steel	H ₂ SO ₄	1	0.1	10	554.673	0.218	0	10.1021/am4018016
H ₂ SO ₄	21.92	80	10	10	Nickel	Na ₂ SO ₄	1	1	5	1052.311	1.141	63.552	10.1039/c7se00490g
HCl	21.9	72	5	23	Steel	H ₂ SO ₄	1	2	10	213.358	0.111	117.683	10.1021/acs.iecr.5b02507
MSA	27.6	80	10	10	Steel	PVA-H ₂ SO ₄	1	0.5	10	48.302	0.151	0.314	10.1016/j.electacta.2023.143263
MSA	38.9	80	10	10	Steel	PVA-H ₂ SO ₄	1	0.5	10	44.979	0.136	8.637	
MSA	28.6	80	10	10	Steel	PVA-H ₂ SO ₄	1	0.5	10	42.379	0.207	9.007	
HCl	94.5	70	10	20	Carbon	H ₂ SO ₄	0.9	1	20	78.357	0.072	430.662	10.1016/j.electacta.2019.135259
HCl	89.2	70	10	20	Carbon	H ₂ SO ₄	0.9	1	20	136.481	0.069	353.003	
H ₂ SO ₄	29.26	80	10	10	Nickel	KOH	0.45	2	10	737.250	0.230	643.273	10.1016/j.ijhydene.2020.04.093
HCl	32	80	10	10	Carbon	H ₂ SO ₄	1	0.5	20	508.955	0.218	225.643	10.1016/j.electacta.2018.09.178
HCl	22.58	80	5	15	Nickel	Na ₂ SO ₄	1	0.5	5	402.770	0.8774	78.867	10.1016/j.jelechem.2017.08.014
HCl	237	85	5	10	Carbon	H ₂ SO ₄	0.8	1	20	176.218	0.158	121.933	10.1016/j.carbon.2019.05.043
HCl	40.5	90	0	10	Titanium	H ₂ SO ₄	1	0.4	2	345.494	1.748	78.425	10.1039/c3ra00151b
H ₂ SO ₄	32.3	80	10	10	Steel	H ₂ SO ₄	1	0.2	5	170.951	0.501	218.828	10.1007/s00339-019-2883-3
H ₂ SO ₄	14.6	80	10	10	Steel	H ₂ SO ₄	1	0.2	5	105.982	0.333	151.525	
H ₂ SO ₄	55	80	10	10	Steel	H ₂ SO ₄	1	0.2	5	210.963	0.630	280.770	
HClO ₄	34.4	100	0	0	Platinum	H ₂ SO ₄	0.8	0.3	6	44.267	0.770	176.520	10.1021/nn1000035
HCl	53.44	75	5	20	Carbon	H ₂ SO ₄	0.8	0.5	3	349.820	1.480	323.941	10.1016/j.jallcom.2018.05.108
HCl	29.68	75	10	15	Steel	H ₂ SO ₄	0.8	0.5	10	237.898	0.270	100.644	10.1007/s11051-022-05418-2
HCl	215.3	80	5	15	Steel	H ₂ SO ₄	1.2	0.25	2.5	241.955	1.392	323.733	10.1016/j.jpowsour.2014.09.013
HCl	21.9	72	5	23	Steel	H ₂ SO ₄	1	2	10	205.237	0.118	126.725	10.1039/c5ra01949d

HCl	10.3	85	10	5	Platinum	H ₂ SO ₄	0.8	1	10	128.252	0.164	196.821	10.1039/d1qm01059j
HCl	84.6	100	0	0	Carbon	H ₂ SO ₄	1	1	10	74.310	0.279	447.660	10.1021/acsanm.3c02021
H ₃ PO ₄	68.3	100	0	0	Carbon	H ₂ SO ₄	1	1	10	18.415	0.231	427.683	
H ₂ SO ₄	75.5	100	0	0	Carbon	H ₂ SO ₄	1	1	10	21.259	0.525	411.107	
HCl	84.6	85	10	5	Steel	H ₂ SO ₄	1	1	10	107.376	0.273	117.086	
H ₃ PO ₄	68.3	85	10	5	Steel	H ₂ SO ₄	1	1	10	112.002	0.352	109.970	
H ₂ SO ₄	75.5	85	10	5	Steel	H ₂ SO ₄	1	1	10	118.681	0.274	60.624	