Supporting Information

Analysis and prediction of hydrothermally synthesized ZnO based dye-sensitized solar cells properties using statistical and machine learning techniques

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Table S1: Dataset used in the present investigation

Structure	Precursor	Dye	Synthesis temperature (°c)	Synthesis time (h)	Seed layer	Electrical parameter (Efficiency or PCE)	Reference
Microrod	1	1	150	18	0	0.22	1
Nanosheet		1	150	18	0	1.47	
Nanorod	1	1	95	12	0	1.29	2
Nanosphere		1	120	12	0	1.94	
Nanorod		1	180	12	0	1.27	
Nanoflower		1	120	12	0	1.68	
Nanorod		1	120	12	0	1.31	
Nanosphere		1	120	12	0	1.94	
Nanorod		1	120	6	0	1.29	
Nanosphere		1	120	12	0	1.94	
Nanorod			120	18	0	2.41	
Nanoflower	2	1	160	12	0	0.3	3
Nanosphere		1	160	12	0	2.6	
Nanoplates		1	160	12	0	1.9	
Nanowire	1	1	60	24	1	0.09	4
Nanowire		1	70	24	1	0.17	
Nanowire		1	80	24	1	0.22	
Nanowire		1	90	24	1	0.26	
Nanorod	3	1	95	40	1	1.0	5
Nanoflower	2	1	95	30	1	1.9	
Nanoforest	1	1	95	7	1	0.85	6
Nanoforest		1	95	7	1	2.63	
Nanoparticles	3	2	160	8	0	0.75	7
Nanosheets		2	160	3	0	1.55	
Nanowire	2	1	85	12	1	0.42	8
Nanoparticles		1	85	12	1	0.90	
Nanowire	1	1	90	10	1	0.22	9
Nanorod	2	2	40	4	1	0.50	10
Nanorod		2	60	4	1	1.1	
Nanorod		2	80	4	1	1.8	
Nanorod		2	95	4	1	2.4	
Microsphere	1	1	80	12	1	3.7	11
Nanorod	1	2	95	16	1	2.1	12
Nanowire	1	3	92	2	1	0.093	13
Nanowire		4	92	2	1	0.088	
Nanorod	2	1	60	6	1	1.34	14
Nanobelts	1	1	60	24	0	1.28	15
Nanoplates		1	100	24	0	1.58	

Nanoplates		1	140	24	0	1.75	
Nanorods		1	180	24	0	2.00	
Nanocrystal	2	4	160	1	0	4.56	16
Nanorods	1	1	96	6	1	0.56	17
Nanorods		1	96	12	1	0.76	
Nanorods		1	96	22	1	0.92	
Nanorods		1	96	28	1	0.89	
Nanorods		1	150	6	1	0.51	
Nanorods		1	150	12	1	0.63	
Nanorods		1	150	22	1	1.08	
Nanorods		1	150	28	1	1.32	
Nanorods	3	1	95	48	1	0.62	18
Nanowire	3	1	95	16	1	1.70	
Nanorod	2	1	180	10	1	2.81	20
Nanorod		1	180	10	1	2.21	
Nanorod		1	180	10	1	2.07	
Nanomushrooms	1	2	150	3	0	2.38	21
Nanorod		2	85	3	0	1.41	
Nanorod	2	3	65	2	1	0.42	22
Nanorod		3	70	2	1	0.33	
Nanorod		3	80	2	1	0.25	
Microsphere	1	2	100	10	0	0.34	23
Nanoplates	2	1	130	10	0	5.05	24
Nanoflower	1	1	120	24	0	1.37	25
Nanorod		1	120	24	0	0.19	
Nanorod	1	1	60	4	1	0.005	26
Nanorod		1	70	4	1	0.04	
Nanorod		1	90	4	1	0.12	
Nanorod		1	100	4	1	0.31	
Nanograss	1	1	90	48	1	0.40	27
Nanorod	1	1	90	6	1	0.52	28
Nanorod		1	90	6	1	0.91	
Nanorod	1	1	60	24	1	0.70	29
Nanowire	1	1	92	30	1	0.69	30
Nanoparticles	3	1	160	3	0	3.13	31
Nano Flake	3	1	160	6	0	5.72	
Nanotubes	2	2	120	16	0	1.10	32
Nanowires	3	2	150	24	0	0.99	
Microrod	1	5	97	2	0	0.021	33
Nanorod	1	5	97	2	0	0.022	
Nanoplates	1	5	97	2	0	0.049	
Nanoplates	1	5	97	2	0	0.100	
Nanoparticles	1	5	97	2	0	0.160	
Nanoparticles	1	5	97	2	0	0.180	
Nanorod	1	5	90	15	1	1.1	34

Nanostar	1	1	160	6	0	1.13	35
Nanorod	2	5	200	4	0	4.12	36
Nanorod	2	5	200	4	0	4.62	
Nanorod	2	5	200	4	0	2.47	
Nanorod	2	5	200	4	0	2.76	
Nanowire	2	1	200	1.5	1	1.55	37
Nanoparticles	2	5	160	3	0	0.58	38
Nanoflakes	3	1	130	12	0	3.39	39
Nanoparticles	3	5	150	4	0	1.1	40
Nanowire	2	1	90	2.5	1	1	41
Microrod	2	1	90	6	1	0.03	42
Nanorod	2	5	200	7	0	3.93	43
Nanorod	2	5	200	7	0	4.53	
Nanorod	2	5	200	7	0	5.32	
Nanorod	2	5	200	7	0	6.07	
Nanorod	1	1	90	26.5	1	1.65	44
Nanorod	2	1	90	1	1	0.16	45
Nano Bead	2	1	120	24	0	3.56	46
Microrod	1	4	90	12	1	2.21	47
Microrod	1	1	160	24	0	0.86	48
Nanoflower	1	1	95	8	1	1.08	49
Nanoflower	1	1	95	8	1	2.23	
Nanorod	1	1	90	2	1	0.25	50
Nanocrystal	2	4	150	0.5	0	3.92	51
Nanopyramid	2	4	100	0.5	0	2.82	
Nanosheet	2	4	180	0.5	0	2.80	
Nanocrystal	2	5	150	0.5	0	1.38	
Nanopyramid	2	5	100	0.5	0	1.33	
Nanosheet	2	5	180	0.5	0	0.39	
Nanoparticles	2	5	160	3	0	0.94	52
Nanosheet	2	1	120	3	1	3.23	53
Nanowires	1	1	80	1	1	0.82	54
Nanodisk	3	1	75	3	0	1.94	55
Nanorod	1	1	100	5	0	2.4	56
Nanorod	1	1	100	5	0	0.39	
Nanoparticles	1	1	100	5	0	3.51	
Nanorod	2	1	180	10	0	2.81	57
Nanoparticles	2	1	100	10	0	2.07	
Nanowires	1	1	92	2.5	1	1	58
Microspheres	1	1	105	1	0	5.78	59
Microspheres	1	1	105	2	0	7.66	
Nanorod	1	1	95	2	1	0.22	60
Nanorod	1	1	95	10	1	0.10	
Nanosheet	1	1	130	2	0	1.57	61
Nanotube	1	1	90	8	1	0.37	62

Nanorod	1	1	90	8	1	0.34	
Nanorod	1	1	150	4	0	1.90	63
Nanoparticles	1	1	70	0.5	0	1.25	64
Nanosheet	1	1	150	8	0	3.39	65
Nanorod	2	1	95	8	1	1.23	66
Nanorod	2	1	92	5	1	1.8	67
Nanorod	1	1	90	9	1	0.28	68
Nanorod	1	1	90	18	1	0.42	
Nanorod	1	1	90	27	1	0.64	
Microflower	2	1	150	10	0	4.52	69
Microflower	2	1	150	10	0	4.13	
Microflower	2	1	150	10	0	4.23	
Nanowires	1	1	95	3	1	0.49	70
Microorod	1	1	95	8	1	0.20	71
Microorod	1	1	95	12	1	0.26	
Microorod	1	1	95	24	1	0.12	
Nanoflower	1	1	175	24	0	5.11	72
Nanowires	1	1	175	24	0	2.1	73
Nanowires	1	2	175	24	0	1.4	
Microrods	1	1	90	3	0	0.41	74
Microspheres	1	1	90	3	0	1.42	
Microspheres	1	1	90	3	0	0.79	
Nanowires	1	1	150	5	1	1.25	75
Nanomushrooms	1	1	150	3	1	2.38	76
Nanorod	1	1	85	3	1	1.41	
Nanourchin	1	5	91.5	3	1	6.40	77
Nanorod	1	5	85	4	1	0.22	78
Nanorod	1	5	85	4	1	0.08	
Nanorod	1	5	85	4	1	0.12	
Nanoneedles	1	1	100	5	0	0.24	79
Nanoflower	1	1	100	5	0	0.85	
Nanocluster	1	1	100	5	0	2.22	
Nanowires	1	5	200	1.5	1	0.79	80
Nanorod	2	1	100	12	0	4.7	81
Nanowires	1	1	95	3	1	0.78	82
Nanowires	1	1	95	3	1	1.78	
Nanorod	1	1	96	6	1	0.53	83
Nanorod	1	1	96	4	1	0.33	
Nanorod	1	1	96	2	1	0.21	
Nanorod	1	1	80	4	1	0.065	84
Nanorod	1	1	80	8	1	0.133	
Nanorod	1	1	80	12	1	0.186	
Nanorod	1	1	80	24	1	0.221	
Nanosheet	1	1	90	10	1	2.51	85
Nanorod	1	1	95	2	1	0.08	86

Nanorod	1	1	95	4	1	0.27	
Nanorod	1	1	95	8	1	1.27	
Nanorod	1	1	95	4	1	0.04	87
Nanorod	1	1	95	6	1	0.09	
Nanorod	1	1	95	72	1	0.47	
Microarchitecture	1	1	90	3	0	0.54	88
Microflowers	1	1	100	3	0	3.98	89
Microsheet	1	1	120	3	0	5.16	
Nanosheet	1	1	180	3	0	3.11	
Nanotubes	1	1	95	3	1	1.44	90
Nanowires	2	1	90	9	1	0.98	91
Nanowires	2	1	99	9	1	0.45	
Microflower	2	1	90	9	1	0.70	
Microurchin	2	1	90	9	1	1.21	
Microurchin	2	1	90	9	1	1.92	
Nanobelt	1	1	120	1	1	1.36	92
Nanobelt	1	1	120	2	1	2.09	
Nanobelt	1	1	120	3	1	3.28	
Nanoparticles	2	1	150	4	0	4.45	93
Microsphere	1	1	160	2	0	2.34	94
Nanoflower	1	1	70	4	0	3.6	95
Nanotree	1	1	90	9	1	0.23	96
Nanorod	1	1	90	9	1	0.20	
Nanorod	1	1	100	24	0	0.35	97
Nanorod	1	1	70	6	1	0.67	
Nanowire	1	1	95	2	1	0.18	98
Nanowire	1	1	95	4	1	0.25	
Nanowire	1	1	95	8	1	0.34	
Nanowire	1	1	95	16	1	0.52	
Nanowire	1	1	95	20	1	0.70	
Microsphere	1	1	120	12	0	1.76	99
Microsphere	1	1	120	12	0	1.48	
Nanoparticle	1	1	75	24	0	1.12	100
Nanoparticle	1	1	75	24	0	0.77	
Nanowire	1	1	100	3	0	0.30	101
Nanowire	1	1	150	3	0	0.70	
Nanorod	1	1	80	4	1	0.06	102
Nanorod	1	1	80	8	1	0.13	
Nanorod	1	1	80	12	1	0.18	
Nanorod	1	1	80	24	1	0.22	
Nanosheet	1	1	180	6	0	1.82	103
Microflower	1	1	70	4	0	3.59	104
Microflower	1	1	80	8	0	0.23	105
Nanorod	2	1	90	10	1	1.25	106
Nanorod	1	1	90	9	1	0.056	107

Nanorod	1	1	90	18	1	0.078	
Nanorod	1	1	90	27	1	0.11	
Microflower	1	1	120	10	0	1.2	108
Nanorod	1	1	70	4	1	2.32	109
Nanorod	1	1	80	4	1	2.99	
Nanorod	1	1	90	4	1	2.55	
Nanorod	1	1	100	4	1	1.98	
Nanowire	1	1	88	6	1	1.62	110
Nanorod	1	5	70	4	1	0.33	111
Nanorod	1	5	70	4	1	0.41	
Nanorod	1	5	70	4	1	0.28	
Nanorod	2	1	95	4	1	1.18	112
Nanowire	1	2	95	3	1	0.9	113
Nanorod	2	3	65	2	1	0.42	114
Nanorod	2	3	70	2	1	0.33	
Nanorod	2	3	80	2	1	0.25	
Nanorod	1	1	85	4	1	3.25	115
Nanograss	1	1	92	32	1	0.73	116
Nanorod	1	2	83	0.5	1	0.58	117
Nanorod	1	2	83	1	1	0.62	
Nanorod	1	2	83	1.5	1	0.79	
Nanorod	1	2	83	3	1	1.04	
Nanorod	1	1	95	24	1	0.54	118
Nanosheet	1	1	95	24	1	0.82	119
Nanowire	1	1	92.5	5	1	0.41	120
Nanowire	1	1	92.5	10	1	0.46	
Nanowire	1	1	92.5	18	1	0.61	
Nanowire	1	1	92.5	24	1	0.63	
Nanowire	1	1	92.5	30	1	0.72	
Nanowire	1	1	92.5	40	1	0.80	
Nanowire	1	1	92.5	50	1	0.87	
Nanorod	1	1	90	6	1	0.52	121
Nanoflower	2	2	180	2	0	1.6	122
Nanorod	1	5	92	1	1	0.73	123
Nanorod	1	2	140	10	1	0.08	124
Nanorod	1	2	140	48	1	0.32	
Nanodisk	3	1	95	10	0	2.15	125
Nanoparticle	1	1	220	18	0	0.02	126
Nanorod	1	1	90	24	1	1.93	127
Nanorod	1	1	60	4	1	0.005	128
Nanorod	1	1	70	4	1	0.04	
Nanorod	1	1	90	4	1	0.12	
Nanorod	1	1	100	4	1	0.31	
Nanodisk	3	1	95	10	0	2.15	129
Nanorod	1	1	60	6	1	0.71	130

Nanowire	1	1	95	24	1	0.73	131
Nanowire	1	1	95	48	1	0.97	
Nanowire	1	1	95	96	1	1.13	
Nanowire	1	1	95	144	1	1.31	
Nanorod	1	1	120	24	0	0.15	132
Nanoflower	1	1	120	24	0	1.37	
Nanowire	3	4	150	12	1	0.66	133
Nanoplates	2	1	130	10	0	5.05	134
Nanowire	1	1	92.5	2.5	1	0.73	135
Nanorod	1	1	80	4	1	0.065	136
Nanorod	1	1	80	8	1	0.133	
Nanorod	1	1	80	12	1	0.186	
Nanorod	1	1	80	24	1	0.221	
Nanorod	1	1	90	24	1	0.84	137
Nanowire	1	5	88	3	1	1.62	138
Nanoflower	1	1	90	5	1	2.3	139
Nanocone	1	5	80	3	1	1.58	140
Nanobullets	2	1	150	10	0	1.93	141
Nanoflakes	2	1	130	10	0	3.64	
Nanocubes	1	1	110	1	0	4.28	142
Nanocaterpillar	1	1	90	5	1	5.20	143
Nanocrystal	2	1	100	48	0	1.04	144
Nanocrystal	2	1	100	48	0	2.05	
Nanoflower	1	5	145	3	0	1.38	145
Nanotubes	1	1	85	3	1	2.2	146
Nanowire	1	1	92	3	1	0.70	147
Nanorods	2	5	200	36	0	1.66	148
Nanorods	1	1	92	2.5	1	2.17	149
Nanorods	1	5	70	5	1	0.67	150
Nanorods	1	5	70	4	1	0.29	151
Nanorods	1	5	70	6	1	0.37	
Nanorods	1	5	70	8	1	0.53	
Nanorods	1	5	70	10	1	0.76	
Nanorods	1	3	90	5	1	1.06	152
Nanorods	1	4	90	5	1	0.95	

Precursors: Zinc Nitrate- 1; Zinc Acetate- 2; Zinc Chloride- 3
Dyes: Dye 1: N719; Dye 2: N3; Dye 3: D102; Dye 4: D149; Dye 5: Natural Dye, Rodhamine B, Eosin-Y, D205, Mercurochrome, Z907, LEG-4, and C-218
Seed Layer: 0- Absent; 1: Present

In some instances, the authors' domain knowledge was applied to complete missing information.

Details of the decision tree, random forest, and artificial neural network algorithms

Classification and clustering are two basic data analysis tools. Classification is a procedure to build a model that describes and distinguishes data labels. Whereas clustering analyzes data objects without consulting class labels and is used to generate class labels for group data [153]. In general, the data is partitioned into two subsets namely training data and test data. The training data are used to build the model and test data can be used to test the accuracy of the proposed model. In short, it is a two-step procedure, where learning from the model (building a model from training data) is the first step and classification/clustering step (prediction of class labels). In the case of classification, the model is used to class labels of the objects. Whereas in the case of clustering, the group of objects is taken together to form a cluster in such a way that the similarities with the cluster are maximum and among the clusters is minimum. Clustering can be used to generate the class labels for a group of data points.

Decision tree and neural network are two effective tools of classification. The decision tree is used to identify possible rules and heuristics. We have used this technique to identify the factors and conditions leading to different classes and develop some heuristics. In the case of supervised learning, i.e. when efficiency class labels are known we can get four classes. In unsupervised learning, the Classification and Regression Tree (CART) model has split into four clusters viz. very high efficiency, high efficiency, low efficiency, and very low efficiency. The classification rules can be extracted through a decision tree. The structure of a decision is shown the Figure S1.

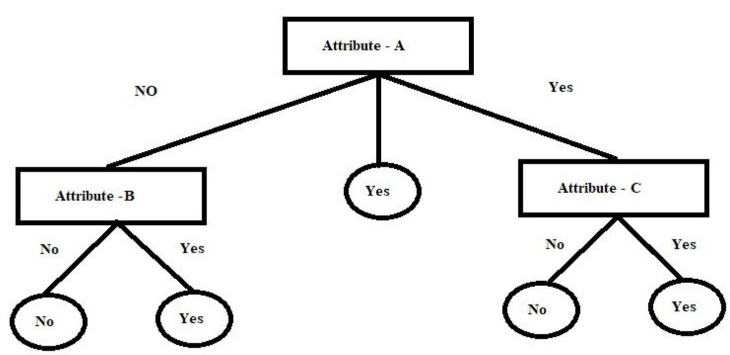

Figure S1. Structure of Decision Tree

Random Forest is the collection of decision tree classifiers [153-154]. It is an ensemble method used to increase overall accuracy by learning and combination of a series of individual tree classifier models. In the case of machine learning methodology, the variables are always termed as attributes. Thus, the selection of the attributes and the splitting rules are the two main concerned of this case. The ranking for each attribute is provided by the selection measures such as Information Gain, Gain Ratio, and Gini Index. Based on the value of these measures the splitting rule, also known as a classifier is constructed.

There are few metrics available for the performance evaluation of classifiers. The metrics or measures are defined in the following terms. For a given classifier, True Positive (TP) number denotes the true classes correctly classified as true. True Negative (TN) number is the number of wrong classes correctly classified as wrong. Whereas False Positive (FP) number denotes the wrong classes classified as true and that of False Negative (FN) number is the number of positive classes classified as wrong ones. Based on the term the confusion matrix is constructed, as shown in Table S2.

Table S2: Confusion Matrix

	Predicted Class		
Actual Class		True	Wrong
	True	TP	FN
	Wrong	FP	TN

The evaluation measures such as accuracy (equation 1) and error (misclassification) rate (equation 2) are defined as,

$$Accuracy = \frac{TP + TN}{Total\ Number\ of\ Classes} \quad (1)$$

$$Error\ Rate = \frac{FP + FN}{Total\ Number\ of\ Classes} \quad (2)$$

The accuracy measures the proportion of correctly classified classes by the classifier and the proportion of wrongly classified classes as error rate or rate of misclassification. The sensitivity is referred to the proportion of true classes that are correctly classified and the proportion of wrong classes that are correctly classified as specificity.

The Artificial Neural Network (ANN) is used for both classification (to predict the class label of a given tuple) and numeric prediction (to predict a continuous-value output). It is a tool for analyzing big data. The more complex model can be build and used for prediction and pattern recognition. ANN mimics the behavior of the human brain to solve complex data-driven problems. It behaves similarly to the neural networks in the human brain and it functions when input data is fed to it and then this data is processed via layers of perceptrons to produce the desired output. This model generally consists of three layers namely the input layer, the hidden layer, and the output layer. The typical structure and block diagram of ANN is as shown in Figure S2 and S3, respectively. The information is propagated through neurons from the input layer to the output layer via hidden layers.

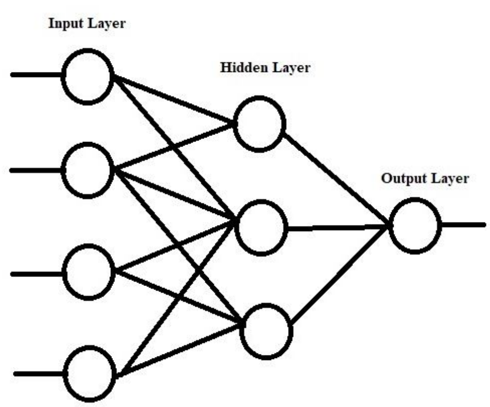

Figure S2: Structure of an artificial neural network

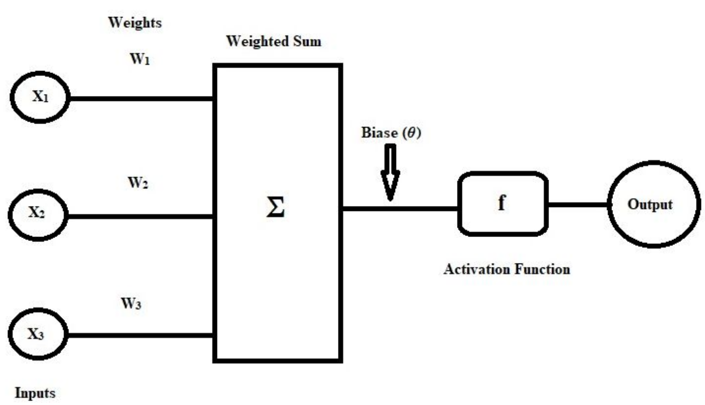

Figure S3: Block diagram of ANN

In the case of a neural network, the outputs of a hidden layer act as the inputs of the next layer. The net input of the hidden layer can be computed as the linear combination of inputs. Thus input of j^{th} element of a hidden layer in terms of weights (w_{ij}) and output of i^{th} element and Bias (θ_j) can be defined using equation 3.

$$Input\ of\ j^{th} element = \left\{ \sum_i w_{ij} \times (Output\ of\ i^{th} element) \right\} + \theta_j \qquad (3)$$

The functioning of ANN is represented in Figure S3. The logistic or sigmoid function can be used as an activation function.

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