

Supplementary documents

Supplementary table 1

Performance of different hidden neurons in the prediction of thermal conductivity

No. of hidden neurons	5	6	7	10	11	12	13
Training Results							
MSE	7.7e-32	3.7e-04	3.2e-31	7.8e-05	7.1e-05	2.8e-04	2.4e-27
R	1	0.82	1	0.96	0.97	0.86	1
Testing Results							
MSE	7.3e-04	2.3e-04	9.4e-05	3.3e-04	2.1e-04	2.7e-04	3.1e-04
R	0.98	0.98	0.99	0.92	0.98	0.99	0.93

Supplementary table 2

Performance of different hidden neurons in the prediction of crystallization temperature

No. of hidden neurons	4	5	6	7	8	9	10
Training Results							
MSE	5.67e-4	.0958	.9059	.0088	.1467	.0333	7.34e-7
R	.99	.99	.81	.99	.98	.99	1
Testing Results							
MSE	.0180	.9545	1.1364	.4585	2.5932	1.8180	.6214
R	.99	.95	.84	.97	.81	.92	.96
No. of hidden neurons	4	5	6	7	8	9	10
Training Results							

MSE	5.67e-4	.0958	.9059	.0088	.1467	.0333	7.34e-7
R	.99	.99	.81	.99	.98	.99	1
Testing Results							
MSE	.0180	.9545	1.1364	.4585	2.5932	1.8180	.6214
R	.99	.95	.84	.97	.81	.92	.96
MSE	.1175	.4427	2.2391	.5465	2.5598	1.4334	.2301
R	.99	.95	.71	.95	.62	.88	.97
Error	.0966	.7009	.6678	.4564	1.0118	1.0913	.6261
MSE	.1175	.4427	2.2391	.5465	2.5598	1.4334	.2301
R	.99	.95	.71	.95	.62	.88	.97
Error	.0966	.7009	.6678	.4564	1.0118	1.0913	.6261

Supplementary table 3

Performance of different hidden neurons in the prediction of degradation temperature

No. of hidden neurons	2	3	4	5	7	8	10
Training Results							
MSE	1.4656	.8420	.0468	.0222	1.28e-6	5.78e-4	.2174
R	.89	.94	.99	.99	1	.99	.99
Testing Results							
MSE	.2300	2.8703	1.4484	.8712	1.2145	.9213	6.5410
R	.99	.93	.97	.99	.99	.99	.88
MSE	2.4024	4.3940	5.4968	.7731	4.0496	2.1786	5.5315
R	.98	.92	.96	.99	.94	.96	.89
Error	.0842	.2896	.2435	.1643	.1919	.1753	.4016

Supplementary table 4

Performance of different hidden neurons in the prediction of tensile strength

No. of hidden neurons	5	6	7	10	11	12	13
Training Results							
MSE	6.09	.138	20.87	5.49	2.39	.45	3.13
R	.68	.99	.35	.81	.90	.98	.87
Testing Results							
MSE	1.57	.989	7.64	.95	1.07	1.99	9.83
R	.92	.91	.70	.94	.82	.94	.56