

Supplementary Figures:

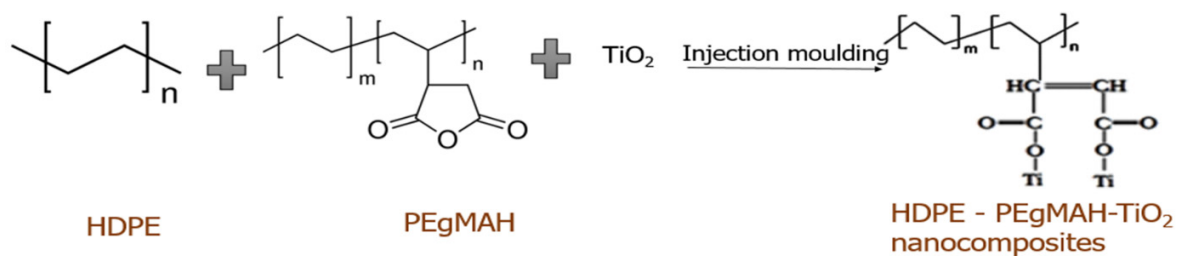


Figure S1. Schematic illustration of HDPE- TiO_2 grafting with maleic anhydride

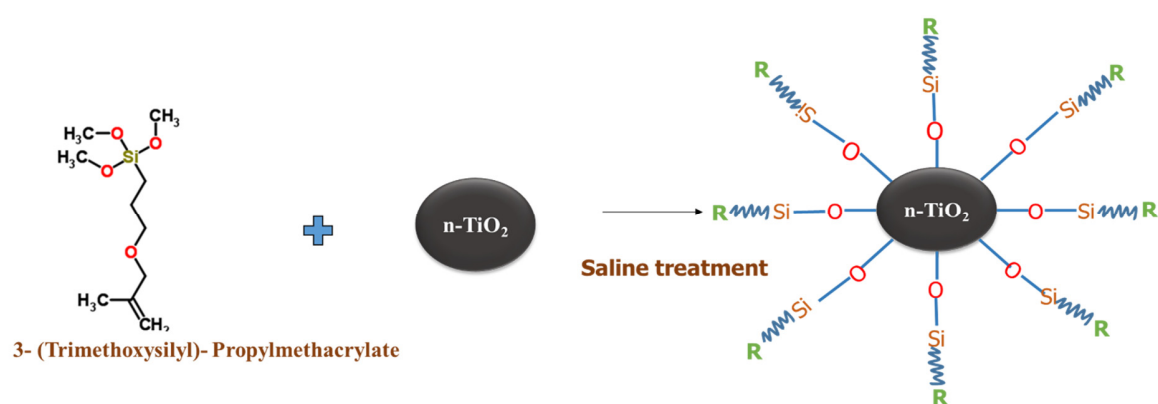


Figure S2: Schematic representation of the binding mechanism of TiO_2 to saline coupling agent (MPS).

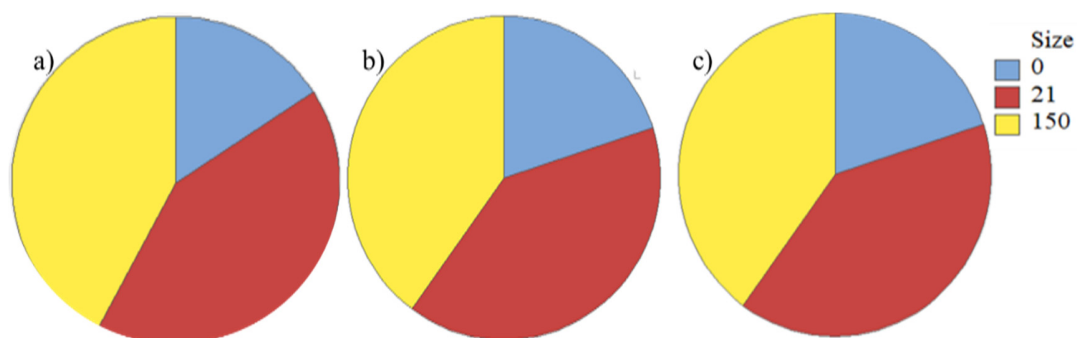


Figure S3. Pie chart showing the influence of the factor (nanoparticles' size) on: a) fracture strength b) yield strength and c) Young's modulus.

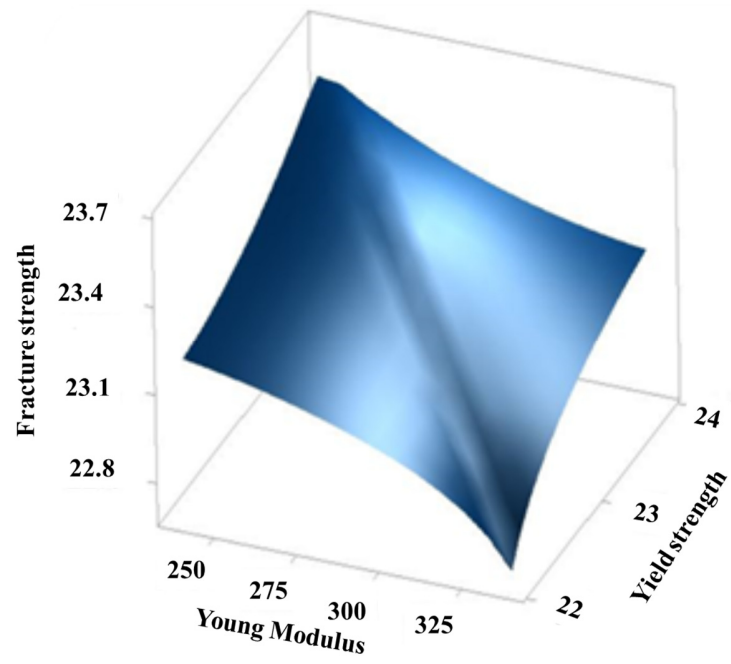


Figure S4. Surface plot comparison between the responses using RSM-GA.

Supplementary Tables:

Table S1. Factors and levels used for ANOVA analysis.

Samples	Factors	Abbreviation	Number of levels	Level 1	Level 2
A	Titanium dioxide nanofillers (%)	n-TiO ₂	2	0	5
B	Modified titanium dioxide (%)	M-(TiO ₂)	2	0	5
C	Size of the nanoparticles (nm)	Nm	2	21	150
D	Polyethylene grafted maleic anhydride (%)	PEgMAH	2	0	3
E	Cellulose nanocrystals (%)	n-CNC	2	0	5

Table S2. Working parameters for ANN model.

Variables	Parameter
Hidden Layer	1- 20 neurons
Method	Feed forward back propagation
Function	Tansig
Adaption learning function	Levenberg-Marquardt backpropagation
Performance function	Mean square error
Maximum number of epochs	1000-2000
Mu	0.01
Mu (max)	10000000000
Gradient	1e-05-1e-07

Table S3. Working parameters for GA-ANN model.

Variables	Parameter
Hidden Neurons	1- 20 neurons
Hidden neurons	2
Function	Tansig
Adaption learning function	Levenberg-Marquardt
	backpropagation
Performance function	Mean square error
Order of selection	Simulated annealing
Maximum number of epochs	1000-2000
Mu	0.01
Populations	150
Learning rate	Medium
Mutation rate	Medium
Trail No	1-10
Maximum generation	150

Table S4. Summary of ANOVA results for yield strength.

Analysis of Variance of Yeild strength							
Source	DF	Seq SS	Contribution	Adj SS	Adj MS	F-Value	P-Value
TiO2	1	4.055	1.81%	15.243	15.243	18.77	0.000
m-TiO2	1	12.995	5.79%	12.995	12.995	16.00	0.000
PEgMAH	1	0.174	0.08%	0.845	0.845	1.04	0.313
NCC	1	134.976	60.11%	105.536	105.536	129.95	0.000
TiO2*PEgMAH	1	1.601	0.71%	0.107	0.107	0.13	0.719
TiO2*NCC	1	3.577	1.59%	0.426	0.426	0.52	0.472
m-TiO2*PEgMAH	1	3.627	1.62%	3.627	3.627	4.47	0.040
m-TiO2*NCC	1	1.290	0.57%	1.290	1.290	1.59	0.214
PEgMAH*NCC	1	17.429	7.76%	7.508	7.508	9.24	0.004
TiO2*PEgMAH*NCC	1	0.002	0.00%	2.704	2.704	3.33	0.074
m-TiO2*PEgMAH*NCC	1	5.825	2.59%	5.825	5.825	7.17	0.010
Error	48	38.983	17.36%	38.983	0.812		
Total	59	224.535	100.00%				
Model Summary							
S	R-sq	R-sq(adj)	PRESS	R-sq(pred)			
0.901196	82.64%	78.66%	62.0051	72.39%			

Table S5. Summary of ANOVA results for fracture strength.

Analysis of Variance							
Source	DF	Seq SS	Contribution	Adj SS	Adj MS	F-Value	P-Value
Model	11	122.662	83.08%	122.662	11.1511	20.09	0.000
Linear	5	93.872	63.58%	88.096	17.6193	31.74	0.000
TIO2	1	1.204	0.82%	12.163	12.1634	21.91	0.000
M-TiO2	1	1.229	0.83%	6.560	6.5600	11.82	0.001
SIZE	1	11.117	7.53%	9.813	9.8133	17.68	0.000
PEGMAH	1	6.103	4.13%	0.578	0.5779	1.04	0.313
NCC	1	74.219	50.27%	66.247	66.2470	119.36	0.000
2-Way Interactions	6	28.791	19.50%	28.791	4.7984	8.65	0.000
TIO2*SIZE	1	3.497	2.37%	2.115	2.1154	3.81	0.057
TIO2*PEGMAH	1	2.409	1.63%	17.113	17.1131	30.83	0.000
TIO2*NCC	1	4.244	2.87%	6.735	6.7345	12.13	0.001
M-TiO2*PEGMAH	1	15.746	10.67%	18.123	18.1233	32.65	0.000
M-TiO2*NCC	1	0.901	0.61%	1.822	1.8220	3.28	0.077
PEGMAH*NCC	1	1.993	1.35%	1.993	1.9933	3.59	0.065
Error	45	24.977	16.92%	24.977	0.5550		
Lack-of-Fit	6	12.790	8.66%	12.790	2.1317	6.82	0.000
Pure Error	39	12.187	8.25%	12.187	0.3125		
Total	56	147.639	100.00%				
Model Summary							
S	R-sq	R-sq(adj)	PRESS	R-sq(pred)			
0.745008	83.08%	78.95%	38.7158	73.78%			

TableS6. Summary of ANOVA results for Young's modulus.

Analysis of Variance of Young's Modulus							
Source	DF	Seq SS	Contribution	Adj SS	Adj MS	F-Value	P-Value
Tio2	1	2029	0.15%	22611	22611	4.27	0.044
m-tio2	1	76133	5.49%	76133	76133	14.36	0.000
PEgMAH	1	19110	1.38%	10385	10385	1.96	0.168
NCC	1	698212	50.37%	475922	475922	89.77	0.000
Tio2*PEgMAH	1	3534	0.25%	3855	3855	0.73	0.398
Tio2*NCC	1	153575	11.08%	72447	72447	13.67	0.001
m-tio2*PEgMAH	1	711	0.05%	711	711	0.13	0.716
m-tio2*NCC	1	1184	0.09%	1184	1184	0.22	0.639
PEgMAH*NCC	1	25027	1.81%	85148	85148	16.06	0.000
Tio2*PEgMAH*NCC	1	101163	7.30%	150302	150302	28.35	0.000
m-tio2*PEgMAH*NCC	1	51044	3.68%	51044	51044	9.63	0.003
Error	48	254471	18.36%	254471	5301		
Lack-of-Fit	8	154426	11.14%	154426	19303	7.72	0.000
Pure Error	40	100045	7.22%	100045	2501		
Total	59	1386192	100.00%				
Model Summary							
S	R-sq	R-sq(adj)	PRESS	R-sq(pred)			
72.8112	81.64%	77.44%	395858	71.44%			

Table S7. Summarized data containing weights and biases of the neural networks.

Neural network weight and bias for Fracture strength				
IW	LW	B1	B2	
1.3208	-4.3184	0.29061	-4.3173	-0.57446
-1.2033	3.9163	0.74794	3.7739	
0.26228	4.4169	0.40458	-2.4685	
-4.2226	-0.59281	-0.15949	1.6306	
-4.4142	0.22458	-0.59125	-0.02313	
-3.7963	-2.3729	0.77764	-0.748	
-2.9371	3.2325	0.22993	-1.5984	
-4.152	-1.5608	-0.93387	-2.3719	
-2.7258	-3.1213	0.0074522	-3.6727	
-1.2148	4.0949	0.13766	-4.5888	

Neural network weight and bias for Yield strength

IW		LW	B1	B2
-1.526	4.023	2.1164	4.553	-1.1197
-0.22131	4.5498	-0.38493	-3.5078	
0.28086	4.3132	-0.05222	-2.3219	
4.1682	-0.2297	1.7839	-2.5589	
4.2438	0.42192	-1.1408	-0.13543	
1.9429	-3.9596	0.12785	0.80051	
-2.4126	-3.3307	0.4491	-2.5417	
4.7969	0.31626	1.3294	1.873	
0.71493	-4.7666	-0.44633	2.8774	
-1.9091	4.2094	0.96401	-4.2162	

Neural network's weight and bias for Young Modulus

IW		LW	B1	B2
2.8004	-3.1176	0.36823	-4.6656	-0.71739
3.1357	3.0576	0.56977	-3.4973	
-3.0049	3.3767	1.0615	2.32	
4.4383	-0.22631	0.7899	-1.3553	
1.7816	4.0579	0.47505	-0.39927	
-3.3798	-2.8729	0.8244	-0.50857	
-4.0678	-1.7276	0.17344	-1.4977	
0.61389	4.3956	-0.54349	2.4711	
3.7662	2.0965	0.42818	3.5398	

3.8071

3.4052

0.82552

3.5591
