

Supplementary Information

Designing bioinspired green nanosilicas using statistical and machine learning approaches

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Table S1. Design and results for the pre-screening experiments.

Samples	Si:N <i>mol/mol</i>		[Si] <i>mM</i>		Yield <i>mol%</i>	Surface area <i>m²/g</i>
	Design	Actual	Design	Actual		
PEI						
1	0.0884	0.0822	30	27.89	0	n/a*
2	0.0884	0.0876	30	29.73	0	n/a
3	11.3137	11.3706	30	30.15	38	135
4	11.3137	11.4725	30	30.42	6	222
5	0.0884	0.0637	165	118.94	0	n/a
6	0.0884	0.0631	165	117.86	0	n/a
7	11.3137	12.0005	165	175.02	46	268
8	11.3137	11.7695	165	171.65	68	313
9	0.0625	0.0455	97.5	70.91	0	n/a
10	0.0625	0.0452	97.5	70.58	0	n/a
11	16	16.3344	97.5	99.54	22	235
12	16	16.4055	97.5	99.97	7	443
13	1	0.9941	2.04	2.03	0	n/a
14	1	1.1191	2.04	2.28	0	n/a
15	1	1.0202	193	196.9	95	120
16	1	0.9662	193	186.47	128**	162
17	1	0.9902	97.5	96.54	100	214
18	1	1	97.5	97.5	96	94
19	1	1	97.5	97.5	92	107
20	1	1.0203	97.5	99.48	93	73
21	1	1.0192	97.5	99.37	93	197
22	1	0.9961	97.5	97.12	89	264
23	1	1.0146	97.5	98.93	88	178
24	1	1.0025	97.5	97.74	92	181
25	1	1.0044	97.5	97.93	88	214
26	1	1.005	97.5	97.99	100	133
27	1	1.0172	97.5	99.17	96	122
28	1	1.017	97.5	99.16	94	121

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....continued Table S1

Samples	Si:N mol/mol		[Si] mM		Yield mol%	Surface area m ² /g
	Design	Actual	Design	Actual		
TEPA						
29	0.0884	0.0768	30	26.06	62	45
30	0.0884	0.0761	30	25.83	72	35
31	11.3137	11.428	30	30.3	87	256
32	11.3137	11.6075	30	30.78	1	165
33	0.0884	0.0544	165	101.56	79	70
34	0.0884	0.0556	165	103.71	86	82
35	11.3137	11.3137	165	165	10	256
36	11.3137	12.3184	165	179.65	77	256
37	0.0625	0.0347	97.5	54.17	78	40
38	0.0625	0.0356	97.5	55.59	55	55
39	16	16.8422	97.5	102.63	0	n/a
40	16	16.7363	97.5	101.99	0	n/a
41	1	0.9804	2.04	2	0	n/a
42	1	0.9804	2.04	2	0	n/a
43	1	1	193	193	84	53
44	1	1	193	193	90	56
45	1	1	97.5	97.5	84	34
46	1	1	97.5	97.5	62	37
47	1	1	97.5	97.5	82	33
48	1	1.0217	97.5	99.61	80	34
49	1	1.0242	97.5	99.86	76	27
50	1	0.9839	97.5	95.93	79	38
51	1	1.005	97.5	97.99	82	39
52	1	1.0363	97.5	101.04	83	32
53	1	1.0095	97.5	98.43	86	34
54	1	1.0461	97.5	102	82	39
55	1	1.0328	97.5	100.7	84	37
56	1	1.0095	97.5	98.43	78	37

* As no precipitate was obtained, the surface area was not available.

** A yield of $\geq 100\%$ suggests incomplete drying. Inferior gravimetric yield determination was only used for the pre-screening experiments. The superior silicomolybdic acid spectrophotometric method, which is independent of the moisture content of the silica product, was used throughout all further experiments (section 2.2.2).

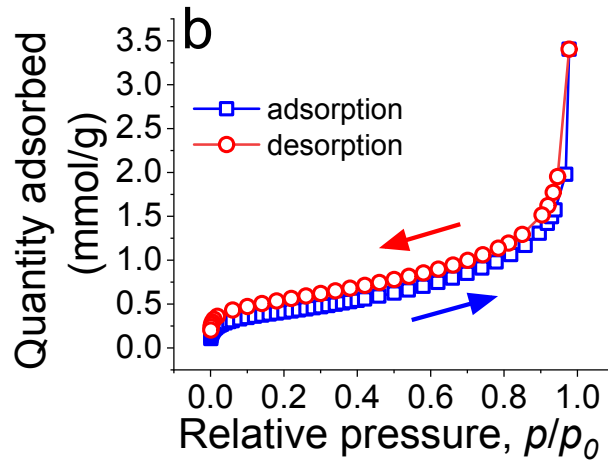


Figure S1. A representative N₂ adsorption-desorption isotherm.

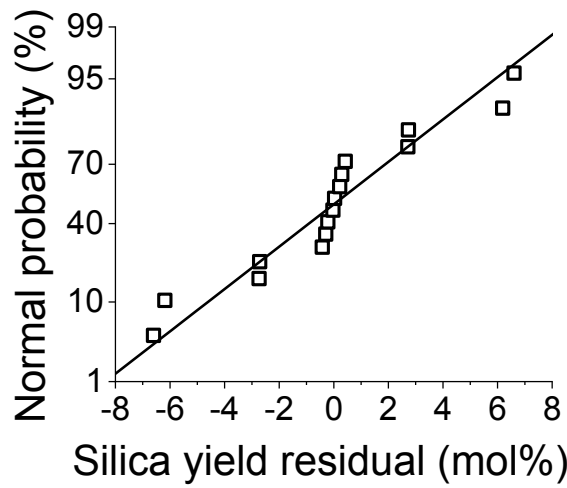


Fig. S2. Residual plot of the silica yield response. The close proximity of the experimental observations to the normal line shows that the data is normally distributed.

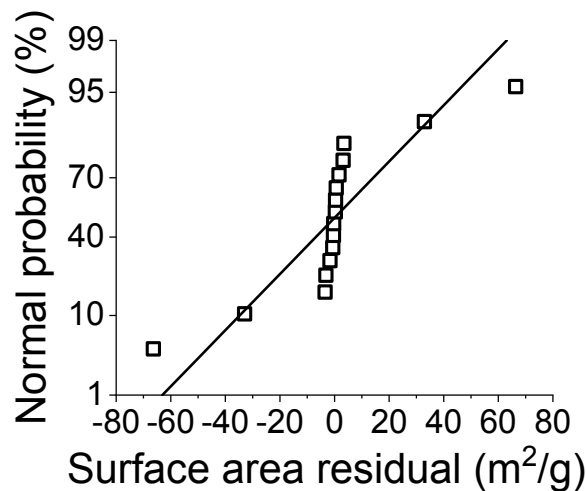


Fig. S3. Residual plot of the silica BET surface area response. The reasonably close proximity of the experimental observations to the normal line shows that the data is generally normally distributed.