Supplementary Material for

Calcium Oxalate and Gallic Acid: Structural Characterization and Process Optimization Toward Obtaining High Contents of Calcium Oxalate Monohydrate and Dihydrate

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Content of listed material

Table S1.

Simple system	*1st step*			*total 1st step*	*2nd step*			*total 2nd step*
	t_0 / °C	t_{max} / °C	t_e / °C	Δm / %	t_0 / °C	t_{max} / °C	t_e / °C	Δm / %
1	39.55	55.46	79.68	1.76	79.54	142.48	196.06	11.51
2	46.08	140.67	200.87	12.78	-	-	-	-
3	41.44	54.65	74.78	1.19	74.51	142.84	196.67	11.54
4	40.48	40.54	84.32	2.36	84.45	132.51	195.71	18.65
5	43.04	54.73	80.77	0.66	80.49	144.28	200.98	12.52
6	39.99	137.90	195.97	13.08	-	-	-	
7	65.68	146.36	196.21	12.69	-	-	-	-
8	42.74	141.38	197.12	13.47	-	-	-	-
9	39.88	68.07	92.07	6.45	92.76	138.18	196.35	11.51
10	40.42	66.88	88.57	4.70	88.71	141.63	195.35	11.12
11	39.75	62.75	87.32	4.13	87.32	143.89	195.98	11.13
12	42.98	71.10	93.03	8.80	92.75	133.87	200.89	10.41
13	42.26	79.06	97.32	12.28	97.32	135.76	200.69	8.57
14	60.22	137.25	196.17	21.35	-	-	-	
15	60.56	146.96	200.37	21.84	-	-	-	
16	40.93	55.92	79.91	1.51	79.64	142.83	195.39	12.13
17	42.98	71.10	93.03	8.80	92.75	133.87	200.89	10.41
model COM	66.58	144.08	196.95	11.77	-	-	-	-
model COD	45.58	149.08	202.95	19.87	-	-	-	-

Table S2

COM	COD	COT	Vibrational mode
3483	3469	3528	
3429		3427	ν(OH)
3336		3222	
3258			2δ(HOH)
3058			ν(OH)
1624-1622	1640 - 1638	1636	ν_a(CO)
	1470		
1384			ν_s(CO)
1368			
1320-1316	1324	1324	
958-889			L(H_2O)
	912		ν_s(CO) + L(H_2O)
782	782	783	δ(OCO)
656	630	651	L(HOH)

ν – stretching; δ – bending; *a*-antisymmetric; *s* – symmetric; L - libration.

Table S3

Source	Sum of Squares	Degree of Freedom (df)	Mean Square	F-Value	*p*-Value[a]
Model	17037.19	9	1893.02	21.12	0.0003
X_1 - Temperature	2370.85	1	2370.85	26.45	0.0013
X_2 – System pH	4876.67	1	4876.67	54.41	0.0002
X_3 – Added gallic acid	5666.01	1	5666.01	63.22	< 0.0001
X_1X_2	2154.40	1	2154.40	24.04	0.0017
X_1X_3	377.97	1	377.97	4.22	0.0791
X_2X_3	1283.61	1	1283.61	14.32	0.0069
X_1^2	72.87	1	72.87	0.8131	0.3972
X_2^2	222.41	1	222.41	2.48	0.1592
X_3^2	28.53	1	28.53	0.3183	0.5902
Residual	627.39	7	89.63		
Lack of fit	457.18	3	152.39	3.58	0.1248
Pure error	170.21	4	42.55		
Total	17664.59	16			
R^2	**0.9645**				

[a] $p < 0.01$ highly significant; $0.01 \leq p < 0.05$ significant; $p \geq 0.05$ not significant.

Table S4

Source	Sum of Squares	Degree of Freedom (df)	Mean Square	F-Value	*p*-Value[a]
Model	18316.52	9	2035.17	28.73	0.0001
X_1 - Temperature	4223.36	1	4223.36	59.61	0.0001
X_2 – System pH	5472.04	1	5472.04	77.24	< 0.0001
X_3 – Added gallic acid	3091.97	1	3091.97	43.64	0.0003
X_1X_2	1986.13	1	1986.13	28.04	0.0011
X_1X_3	1969.5	1	1969.5	27.8	0.0012
X_2X_3	1504.35	1	1504.35	21.23	0.0025
X_1^2	12.94	1	12.94	0.1826	0.682
X_2^2	3.46	1	3.46	0.0489	0.8313
X_3^2	47.45	1	47.45	0.6697	0.4401
Residual	495.91	7	70.84		
Lack of fit	1.15	3	0.3844	0.0031	0.9997
Pure error	494.76	4	123.69		
Total	18812.43	16			
R^2	**0.9736**				

[a] $p < 0.01$ highly significant; $0.01 \leq p < 0.05$ significant; $p \geq 0.05$ not significant.

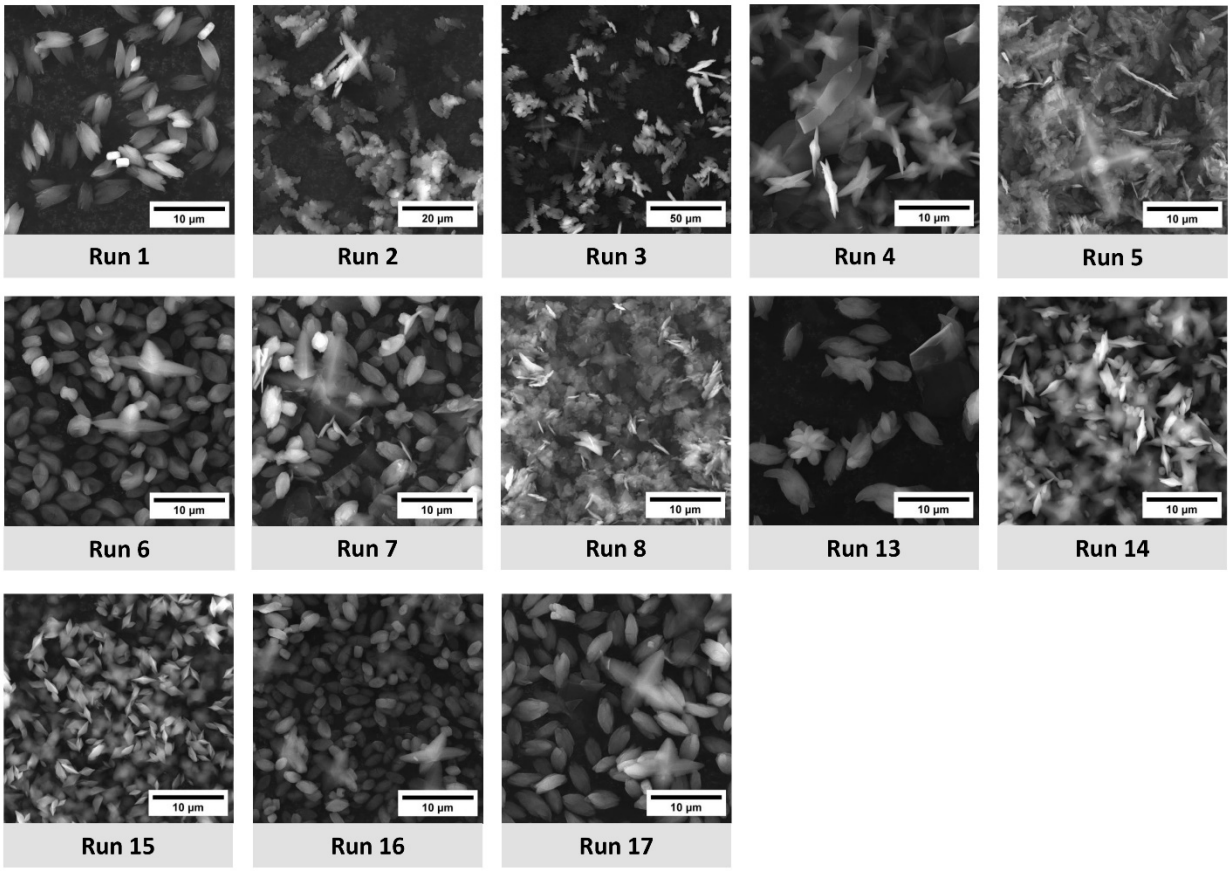
10 µm
Run 1
20 µm
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Figure S1.

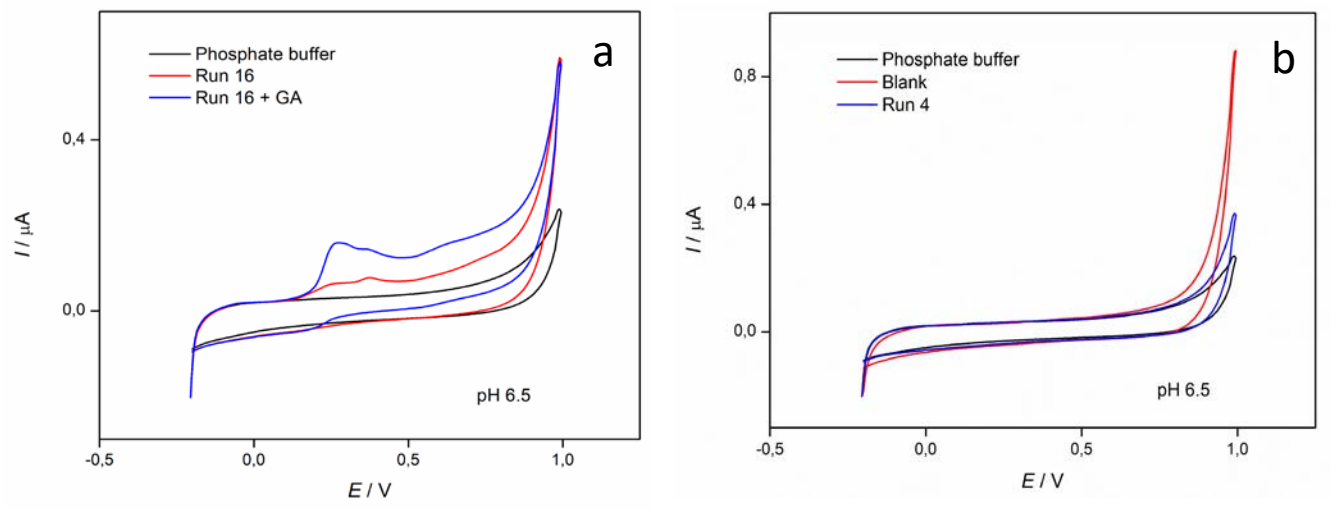
a
Phosphate buffer
Run 16
Run 16 + GA
pH 6.5
I / µA
E / V
b
Phosphate buffer
Blank
Run 4
pH 6.5
I / µA
E / V

Figure S2.