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Supplementary Materials

for

Accentuating the Ambient Curing Behavior of Geopolymers: Metamodel-Guided Optimization for Fast-Curing Geopolymers with High Flexural Strength

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Supplementary Information Text

Table S1 summarizes the molar ratios of raw materials and curing conditions presented in the geopolymer literatures. While various studies exist, it is noteworthy that geopolymers do not have a consistency in the formulation nor the process. As shown, the molar ratio is distributed for a wide range, and the curing condition varies from one study to another.

Table S2 – S4 show the weight of raw materials, molar ratio, and measured flexural strength and curing time for *D1-D3*.

Table S5 contains the raw XRD data for Kaolin, Metakaolin, and Geopolymer as shown in Figure 2 (a) of the manuscript.

Table S6 A table has been prepared to organize the abbreviations used throughout the manuscript. This provides clarity and ensures consistency for readers as they navigate the document.

Figure S1 presents (a) XRF component analysis table of metakaolin, showing a distribution of SiO_2 and Al_2O_3 of 97% or more, and (b) images of silicone mold (specifications according to ASTM D 790) and fabricated specimens for flexural strength.

Figure S2 shows the initial assessment of the effect of $Ca(OH)_2$ contents on the flexural strength. It is discovered that the strength tends to increase with $Ca(OH)_2$ contents up to 2.5 g, but beyond that amount, the formability of GP becomes poor; it cannot be stirred nor consolidated.

Figure S3 is an index that measures the average difference between the value predicted by the prediction model and the actual value, and is a graph that estimates how well the prediction model can predict accurately. The lower the error value, the more reliable the modeling.

Figure S4 shows the correlation matrix plot for variables in geopolymer fabrication.

Figure S5 illustrates elemental analysis other than Ca presented in the maintext (Si, Al, O and K). The Si, Al, and K are depleted in the regions where Ca compounds were found in Figure 7 of maintext, indicating the Ca compounds are formed first and

geopolymer hardly co-exist with Ca compounds.

Figure S6 presents the results of thermogravimetry analysis (TGA) was used to evaluate high temperature performance.

Table S1. Summary of molar ratios and test preparation (curing time and curing conditions) of high strength samples in the geopolymer literature.

Author (First only)	Year	SiO_2/Al_2O_3	M_2O/Al_2O_3	M_2O/SiO_2	H_2O/M_2O	Curing time (day)	Curing condition
Peigang He	2016	2.5	1	0.4	11	3	Sealed at 70°C, for 24h
Kalaiyarrasi	2018	2.89	0.11	0.04	17	28	Room temperature for 48h
Rodrigue Cyriaque Kaze	2018	8.89	4.14	0.47	4.66	28	Chamber at 23°C, for 3h room temperature and oven at 90°C, for 24h
Ali Nazari	2015	4.16	0.89	0.21	21.5	27	Plastic bag for 24h, at 70°C
Pavel Rovnaník	2010	4.11	0.62	0.15	8.84	28	In the first experiment: 10, oven at 40, 60, 80°C for 4h In second experiment : Oven at 40,60,80°C, for 1,2,3,4h after 20°C and humidity above 45%
Rashidah Mohamed Hamidi	2016	3.68	1.96	0.53	14.34	1	Oven at 60°C, for 24h
Peng Zhang	2020	4.29	1.3	0.3	1.82	28	Demolded at room temperature, for 24h The temperature of 20°C and humidity above 95%
Huang Ji Zhuang	2017	3.23	1.92	0.6	2.46	35	The temperature of 20°C and humidity above 95% after 6days follow-up curing
Pradip Nath	2017	4.51	1.41	0.31	2.7	90	18-23°C and relative 70% for 24h
Harun Tanyildizi	2016	7.07	1.69	0.24	6.95	28	Oven at 60, 80, 100 60,80,100°C for 24h and cured at 20°C room temperature
Shilang Xu	2018	5.23	4.78	0.91	2.42	28	At room temperature (25°C) until the tested
A.Natali	2011	3.24	1.45	0.45	5.24	7	Humidity above 90% in chamber and room temperature for 7days
F.N. Okoye	2016	3.67	0.8	0.22	2.36	28	Oven at 100°C for 72h and room temperature until the tested
M. Sofi	2007	6.13	5.38	0.88	4.19	28	Approximately 24h in a steam room (30-35°C, humidity above 80%)
C.D. Atisß	2015	5.37	0.34	0.06	28.67	0.5	Heat curing temperature 45 to 115°C, with 10°C curing durations 24,48 and 72h
Xueying Li	2013	7.72	0.85	0.11	14.61	28	Sealed with a film 1day And oven at 70°C for 24h
Yao Jun Zhang	2009	3.75	2	0.53	13.38	28	Humidity above 99% at 20°C in the chamber
Hafez E. Elyamany	2018	3.75	0.44	0.12	10.19	7	Demolded after 24h from casting and oven at 30, 60, 90°C for 48h
A.Aboulayt	2017	2.27	0.3	0.13	17.76	0.5	Oven at 40°C for 12h

Tanakorn Phoo-ngernkham	2014	4.69	1.54	0.33	11.8	90	Wrapped with vinyl sheet 23℃ controlled room
Piotr Prochon	2020	3.55	0.59	0.17	23.08	3	Laboratory conditions for 4h and cured in a dryer at a temperature of 65℃ for 4h

Table S2. The weight of raw materials, molar ratio, and measured flexural strength for *D1*. In *D1*, f-SiO_2 is mainly optimized.

Sample No.	Molar ratio				Weight of input materials (g)							Measured
	SiO_2/Al_2O_3	$Ca(OH)_2/Al_2O_3$	K_2O/SiO_2	H_2O/K_2O	MK	Ca	C_f	f-SiO_2	KOH	K_2SiO_3	H_2O	σ_f (MPa) (stdev)
D_1-1	2.4	0.4	0.2	8.1	20	2.5	0.1	0	12	6	6.2	5.14 (0.50)
D_1-2	2.4	0.4	0.3	5.9	20	2.5	0.1	0	18	6	3.8	4.22 (0.68)
D_1-3	2.4	0.4	0.4	4.7	20	2.5	0.1	0	24	6	1.4	4.13 (1.00)
D_1-4	2.5	0.4	0.2	9.2	20	2.5	0.1	0	12	9	3.2	9.65 (2.08)
D_1-5	2.5	0.4	0.3	6.6	20	2.5	0.1	0	18	9	0	10.64 (0.91)
D_1-6	2.5	0.4	0.4	5.6	20	2.5	0.1	0	24	9	0	8.53 (1.16)
D_1-7	2.7	0.4	0.2	10.1	20	2.5	0.1	0	12	12	0	9.58 (2.03)
D_1-8	2.7	0.4	0.3	7.9	20	2.5	0.1	0	18	12	0	7.14 (1.07)
D_1-9	2.7	0.4	0.4	6.6	20	2.5	0.1	0	24	12	0	5.13 (1.41)
D_1-10	2.4	0.4	0.2	8.1	20	2.5	0.1	0.3	12	6	6.2	2.71 (1.38)
D_1-11	2.4	0.4	0.3	5.9	20	2.5	0.1	0.3	18	6	3.8	1.94 (0.63)
D_1-12	2.4	0.4	0.4	4.7	20	2.5	0.1	0.3	24	6	1.4	2.53 (1.48)
D_1-13	2.6	0.4	0.2	9.2	20	2.5	0.1	0.3	12	9	3.2	6.30 (1.72)
D_1-14	2.6	0.4	0.3	6.6	20	2.5	0.1	0.3	18	9	0	10.07 (2.45)

D_1 – 15	2.6	0.4	0.4	5.6	20	2.5	0.1	0.3	24	9	0	7.71 (1.04)
D_1 – 16	2.8	0.4	0.2	10.1	20	2.5	0.1	0.3	12	12	0	7.83 (2.17)
D_1 – 17	2.8	0.4	0.3	7.9	20	2.5	0.1	0.3	18	12	0	5.97 (1.57)
D_1 – 18	2.8	0.4	0.4	6.6	20	2.5	0.1	0.3	24	12	0	3.13 (0.64)
D_1 – 19	2.5	0.4	0.2	8.1	20	2.5	0.1	0.6	12	6	6.2	4.13 (0.50)
D_1 – 20	2.5	0.4	0.3	5.9	20	2.5	0.1	0.6	18	6	3.8	3.55 (1.00)
D_1 – 21	2.5	0.4	0.4	4.7	20	2.5	0.1	0.6	24	6	1.4	8.60 (3.15)
D_1 – 22	2.7	0.4	0.2	9.2	20	2.5	0.1	0.6	12	9	3.2	8.71 (3.57)
D_1 – 23	2.7	0.4	0.4	5.6	20	2.5	0.1	0.6	24	9	0	8.10 (1.63)
D_1 – 24	2.8	0.4	0.2	10.1	20	2.5	0.1	0.6	12	12	0	7.87 (1.50)
D_1 – 25	2.8	0.4	0.3	7.9	20	2.5	0.1	0.6	18	12	0	14.49 (3.52)
D_1 – 26	2.8	0.4	0.3	6.6	20	2.5	0.1	0.6	24	12	0	10.48 (3.12)

Table S3. The weight of raw materials, molar ratio, and measured flexural strength and curing time for *D2*.

Sample No.	Molar ratio				Weight of input materials (g)							Measured	
	SiO_2/Al_2O_3	$Ca(OH)_2/Al_2O_3$	K_2O/SiO_2	H_2O/K_2O	MK	Ca	C_f	f-SiO_2	KOH	K_2SiO_3	H_2O	σ_f(MPa) (stdev)	Curing time (m)
D_2-1	2.7	0.4	0.2	11.7	20	2.5	0.1	0.6	9	9	5.6	9.77 (2.91)	21
D_2-2	2.8	0.4	0.2	12.9	20	2.5	0.1	0.6	9	12	3.8	8.24 (2.38)	40
D_2-3	3.0	0.4	0.2	14.1	20	2.5	0.1	0.6	9	15	2	8.63 (1.03)	-
D_2-4	2.7	0.4	0.2	9.1	20	2.5	0.1	0.6	12	9	2.6	13.72 (3.01)	19
D_2-5	2.8	0.4	0.2	10.3	20	2.5	0.1	0.6	12	12	0.8	12.28 (2.48)	32
D_2-6	3.0	0.4	0.2	11.5	20	2.5	0.1	0.6	12	15	0	12.42 (1.63)	-
D_2-7	2.8	0.4	0.2	8.8	20	2.5	0.1	0.6	15	12	0	11.3 (2.46)	44
D_2-8	3.0	0.4	0.2	10.1	20	2.5	0.1	0.6	15	15	0	8.53 (2.46)	50

Table S4. The weight of raw materials, molar ratio, and measured flexural strength and curing time for *D3*.

Sample No.	Molar ratio				Weight of input materials (g)							Measured	
	SiO_2/Al_2O_3	$Ca(OH)_2/Al_2O_3$	K_2O/SiO_2	H_2O/K_2O	MK	Ca	C_f	f-SiO_2	KOH	K_2SiO_3	H_2O	σ_f (MPa) (stdev)	Curing time (m)
D_3 – 1	2.4	0.4	0.2	7.3	20	2.5	0.1	0.6	12	5	5.6	14.03 (2.79)	12
D_3 – 2	2.4	0.4	0.2	6.0	20	2.5	0.1	0.6	15	5	3.8	13.33 (2.25)	24
D_3 – 3	2.4	0.4	0.3	5.1	20	2.5	0.1	0.6	18	5	2	10.93 (6.83)	60
D_3 – 4	2.6	0.4	0.2	7.9	20	2.5	0.1	0.6	12	7	2.6	18.76 (6.07)	9
D_3 – 5	2.6	0.4	0.2	6.5	20	2.5	0.1	0.6	15	7	0.8	17.67 (6.43)	20
D_3 – 6	2.6	0.4	0.3	5.7	20	2.5	0.1	0.6	18	7	0	16.95 (5.21)	45
D_3 – 7	2.7	0.4	0.2	8.5	20	2.5	0.1	0.6	12	9	0	27.83 (2.59)	7
D_3 – 8	2.7	0.4	0.2	7.4	20	2.5	0.1	0.6	15	9	0	19.85 (4.90)	19
D_3 – 9	2.7	0.4	0.3	6.6	20	2.5	0.1	0.6	18	9	0	17.73 (7.35)	43
D_3 – 10	2.6	0.4	0.2	7.6	20	2.5	0.1	0.6	12	7	0	11.71 (0.60)	52
D_3 – 11	2.4	0.4	0.2	9.9	20	2.5	0.1	0.6	9	5	9	6.1 (0.79)	47

Table S5. Raw XRD data of Kaolin, Metakaolin, and Geopolymer. (It has been attached as a separate Excel file)

Table S6. List of Abbreviations also used in the manuscript text and figures.

Abbreviations	Definitions
GP	Geopolymer
MK	Metakaolin
KOH	Potassium hydroxide
K_2SiO_3	Potassium silicate
$Ca(OH)_2$	Calcium hydroxide
C_f	Carbon fiber
f-SiO_2	Fumed silica
σ_f	Flexural strength
σ_c	Compressive strength
DOE	Design of experiment
W_{KOH}	Weight of KOH / Weight of MK
W_{c_f}	Weight of KOH / Weight of C_f
$W_{K_2SiO_3}$	Weight of KOH / Weight of K_2SiO_3
$W_{Ca(OH)_2}$	Weight of KOH / Weight of $Ca(OH)_2$
W_{f-SiO_2}	Weight of KOH / Weight of f-SiO_2
t_{sc}	The surface curing time
GP_{OFC}	Optimized composition with C_f, f-SiO_2
GP_{OF}	Optimized composition without C_f
GP_{OC}	Optimized composition without f-SiO_2
GP_O	Optimized composition without C_f, f-SiO_2

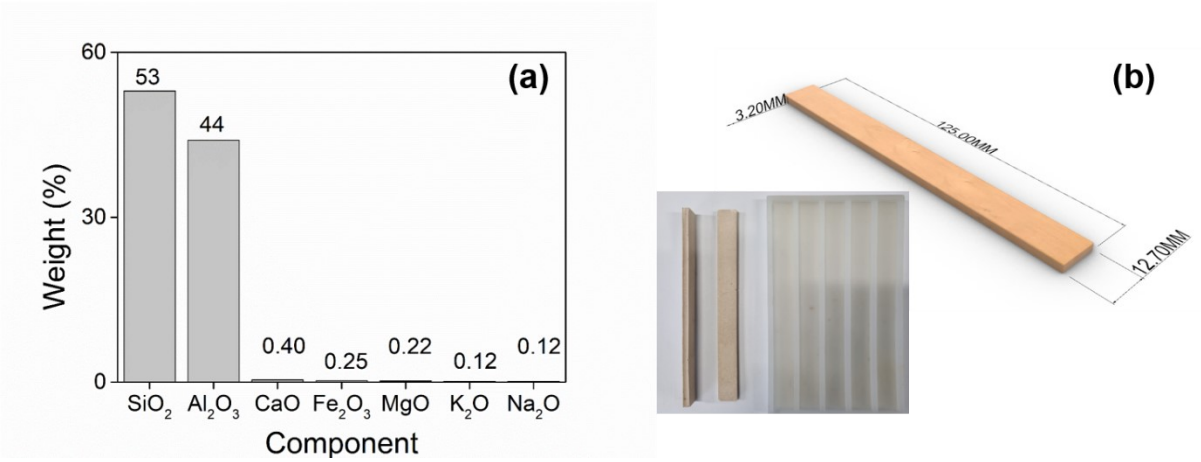


Figure S1. (a) Compositional analysis by XRF, and (b) the dimensions of specimen for flexural strength measurement, and the picture of casted sample in a silicone mold.

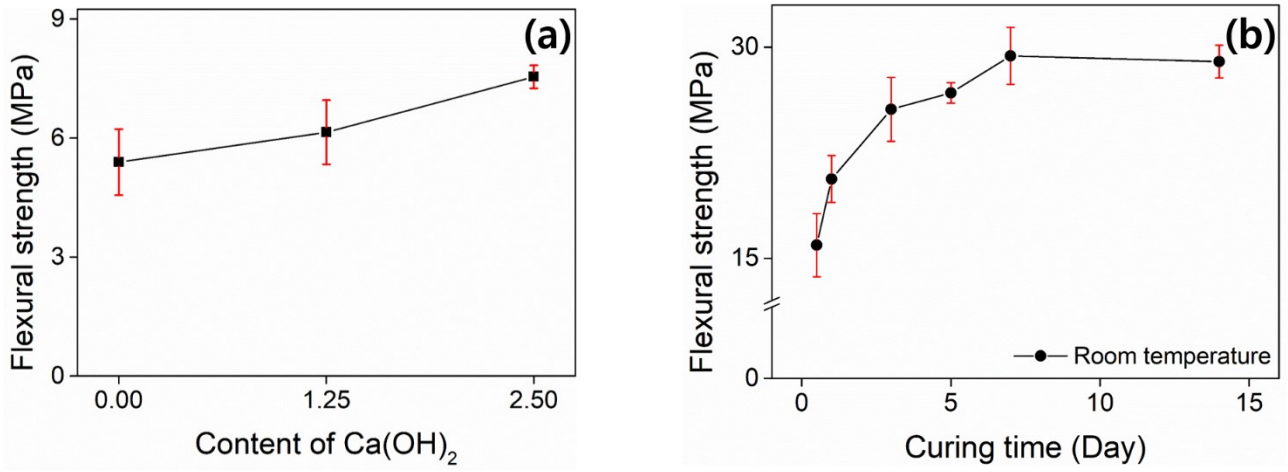
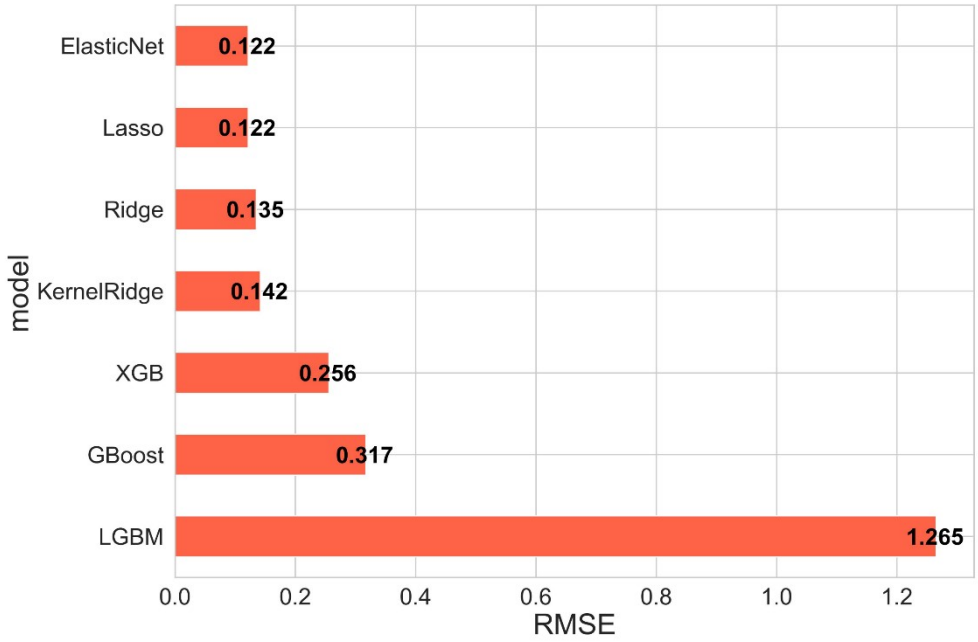


Figure S2. (a) The effect of $Ca(OH)_2$ content (g) on the flexural stress of initial GP formulation of D_1-26, and (b) the flexural stress development as the curing time increases for D_3-7 at room temperature.



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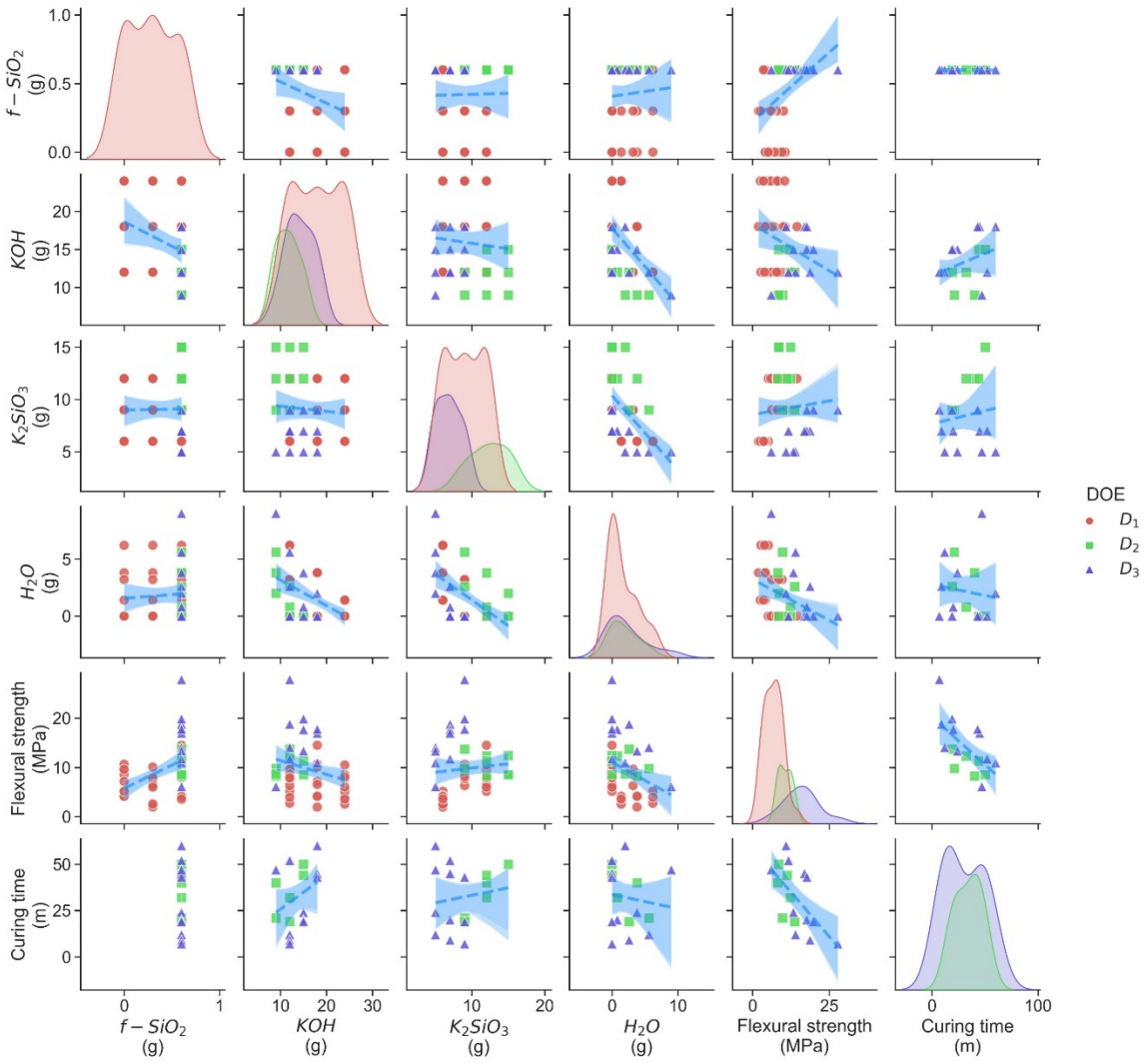
61 Figure S3. Types of linear modeling that are effective when using limited data.



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63 Figure S4. The correlation matrix plot for variables in geopolymer fabrication.

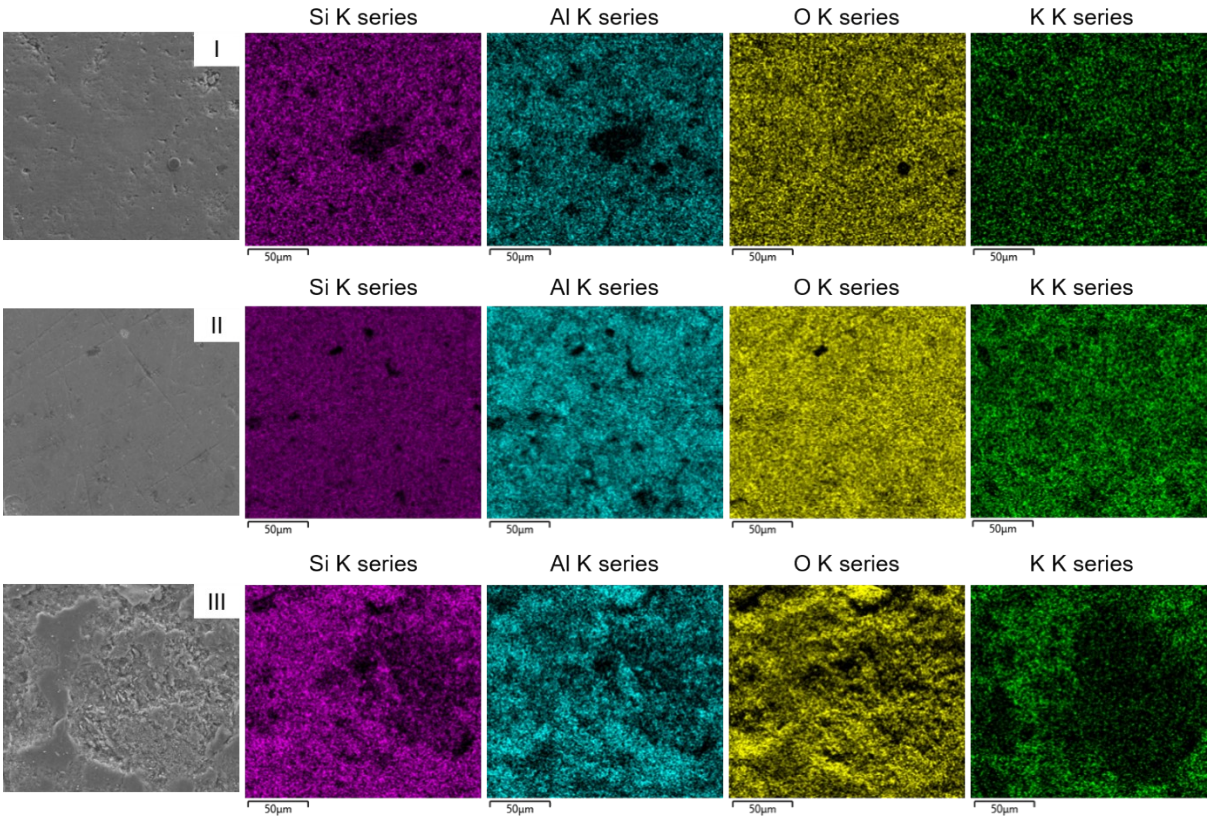
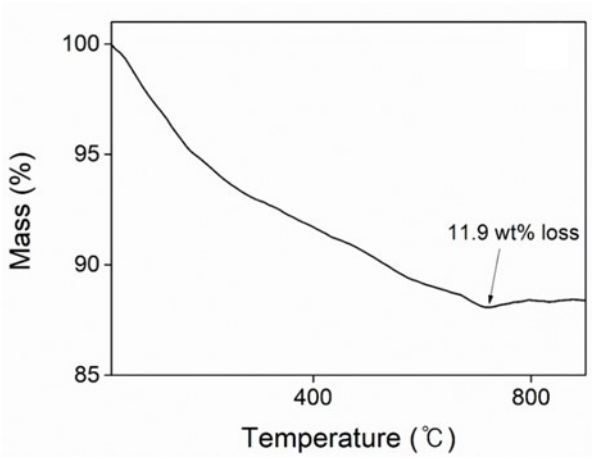


Figure S5. EDS analysis of other key elements (Si, Al, O, and K) for (I) GP_{IFC}, (II) GP_{OFC} and (III) GP_{OC}.



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68 Figure S6. The weight loss of *D_3-7* measured by TGA for temperature change from ambient to 900°C.