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Supporting information

Process Optimization for NASICON type solid electrolyte synthesis using combination of experiments and Bayesian optimization

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Keywords : Battery, NASICON, $LiZr_2(PO_4)_3$, Solid State Electrolyte, Bayesian Optimization, Process optimization

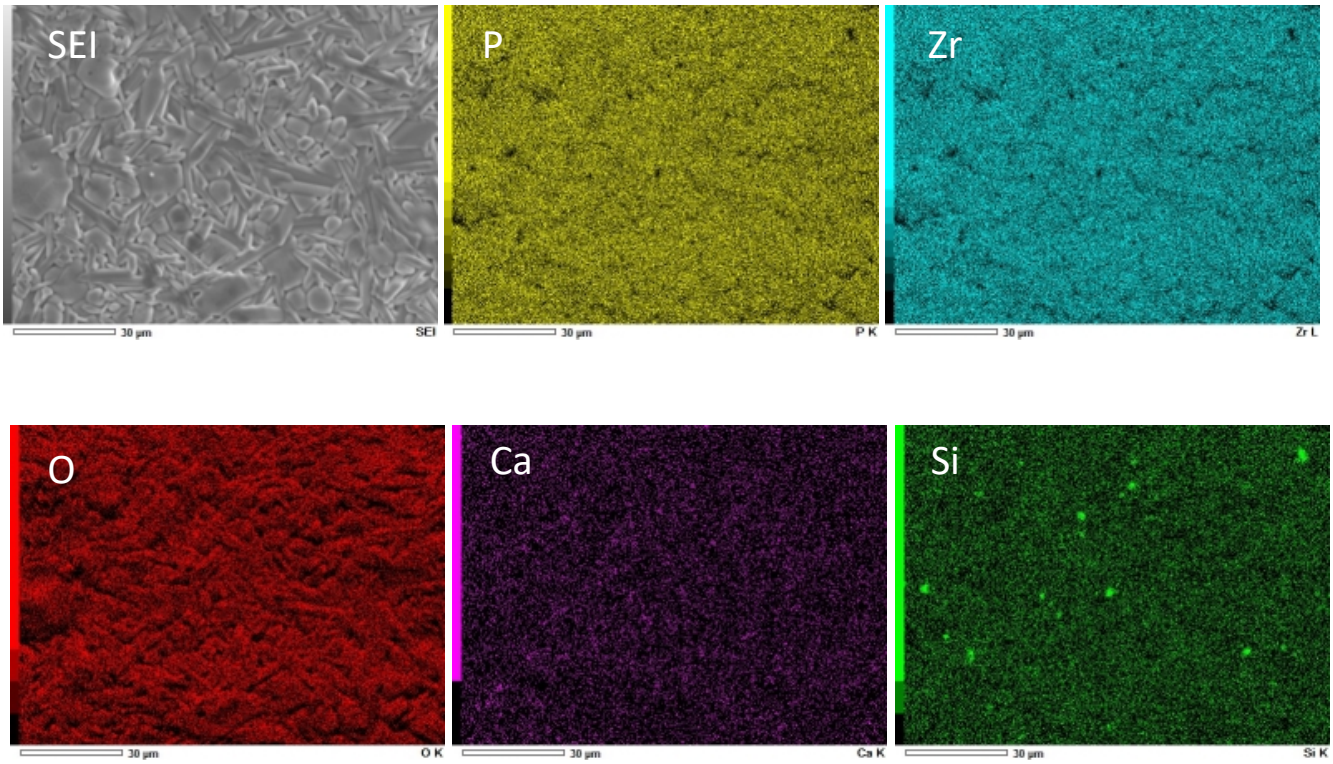

Figure S1. the mapping image of the elemental analysis of HC -1050-1100 obtained EDS. phosphate(yellow), zirconium(blue), oxygen(red), calcium(pink), silicon(green)

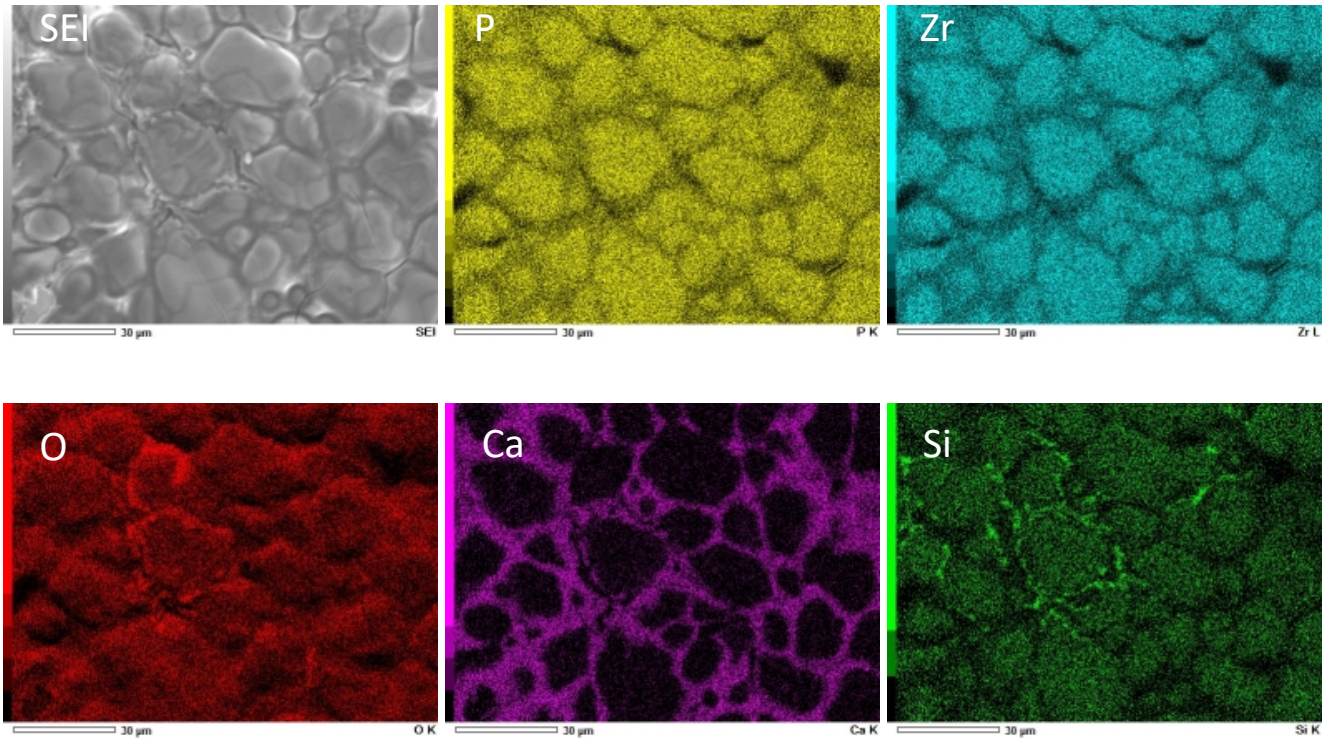

Figure S2. the mapping image of the elemental analysis of HC -1050-1250 obtained EDS. phosphate(yellow), zirconium(blue), oxygen(red), calcium(pink), silicon(green)

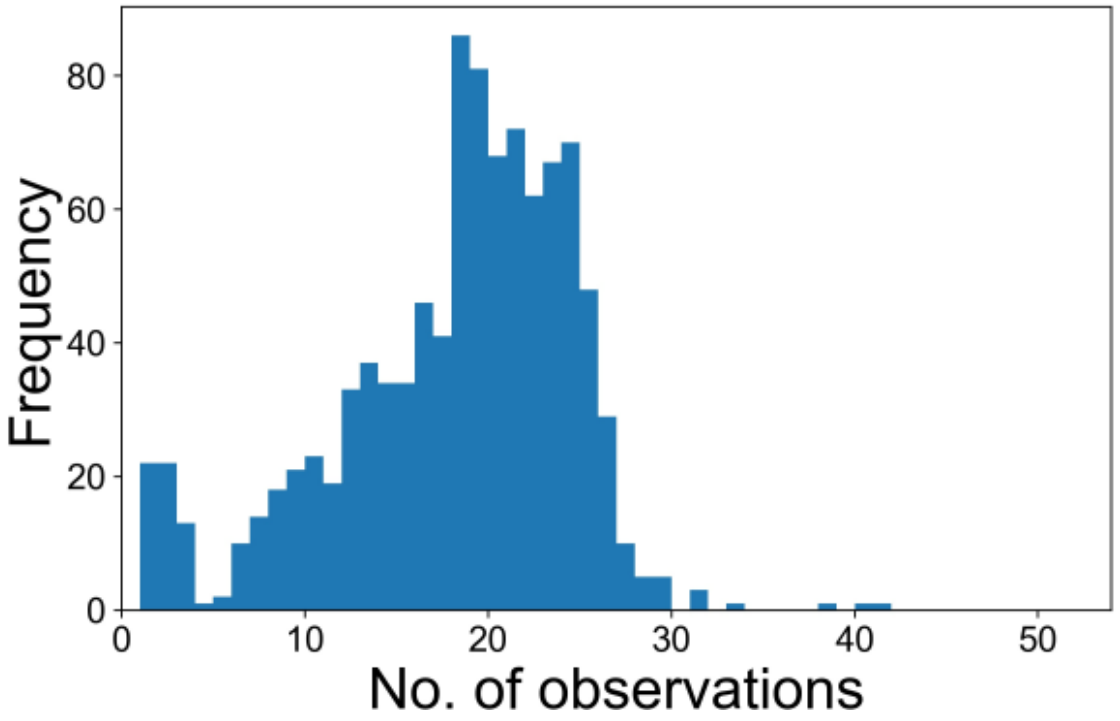

Figure S3. Histogram of the number of observations required to determine the heating conditions affording the highest ionic conductivity

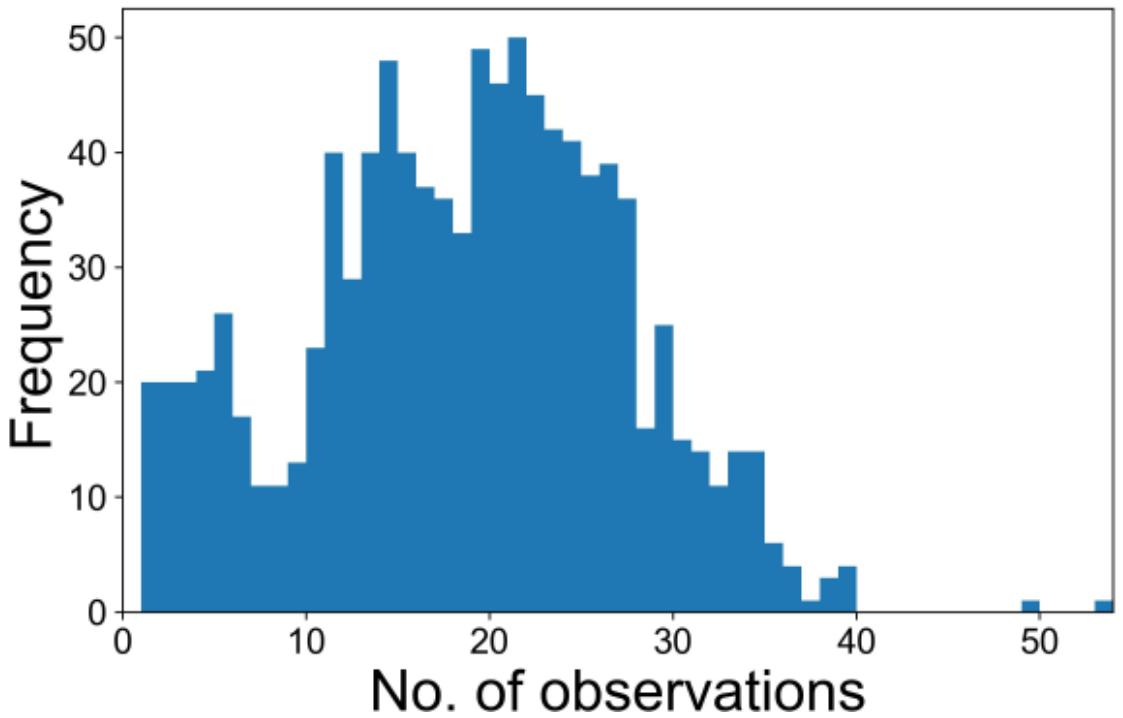

Figure S4. Histogram of the number of observations required to determine the heating conditions affording the lowest activation energy.

Table S1. Bulk densities, ionic conductivities at 30, 60, and 90 °C, and activation energies experimentally determined for all 54 samples.

1st heating (°C)	2nd heating (°C)	Bulk density (g/cm 3)	Ion conductivity @ 30°C (S/cm)	Ion conductivity @ 60°C (S/cm)	Ion conductivity @ 90°C (S/cm)	Activation energy (eV)
900	1100	2.845	1.72E-06	1.01E-05	4.28E-05	0.51
900	1150	2.714	1.81E-05	7.98E-05	1.77E-04	0.36
900	1200	2.836	2.06E-05	7.92E-05	2.35E-04	0.39
900	1250	2.74	1.52E-05	5.73E-05	1.58E-04	0.37
900	1300	2.612	2.26E-05	8.56E-05	2.49E-04	0.38
900	1350	2.6	1.19E-05	4.15E-05	1.13E-04	0.36
950	1100	2.825	1.50E-06	8.23E-06	3.46E-05	0.5
950	1150	2.744	3.36E-06	1.79E-05	6.05E-05	0.46
950	1200	2.764	1.73E-05	6.39E-05	1.75E-04	0.37
950	1250	2.769	2.38E-05	8.72E-05	2.33E-04	0.36
950	1300	2.689	1.91E-05	6.81E-05	1.79E-04	0.36
950	1350	2.686	1.21E-05	4.08E-05	1.11E-04	0.35
1000	1100	2.957	1.32E-06	7.61E-06	3.32E-05	0.51
1000	1150	2.81	5.43E-06	2.12E-05	6.88E-05	0.4
1000	1200	2.785	1.36E-05	4.94E-05	1.36E-04	0.36
1000	1250	2.779	2.68E-05	6.88E-05	2.12E-04	0.33
1000	1300	2.71	1.91E-05	5.61E-05	1.80E-04	0.35
1000	1350	2.463	1.22E-05	4.55E-05	1.30E-04	0.37
1050	1100	2.837	1.43E-06	8.46E-06	3.66E-05	0.51
1050	1150	2.819	2.07E-06	1.06E-05	4.47E-05	0.49
1050	1200	2.827	5.61E-06	2.13E-05	8.56E-05	0.43
1050	1250	2.768	3.32E-05	9.30E-05	2.62E-04	0.33
1050	1300	2.815	2.46E-05	7.26E-05	2.00E-04	0.33
1050	1350	2.822	2.60E-05	9.84E-05	2.20E-04	0.34
1100	1100	2.923	1.49E-06	8.37E-06	3.56E-05	0.5
1100	1150	2.808	3.75E-06	2.04E-05	7.56E-05	0.48
1100	1200	2.825	2.23E-05	7.29E-05	2.11E-04	0.35
1100	1250	2.736	2.15E-05	7.37E-05	2.09E-04	0.36
1100	1300	2.795	1.42E-05	4.11E-05	1.27E-04	0.34
1100	1350	2.767	1.75E-05	5.21E-05	1.41E-04	0.33
1150	1100	2.917	6.48E-07	4.30E-06	1.94E-05	0.54
1150	1150	2.803	3.73E-06	2.26E-05	8.60E-05	0.5
1150	1200	2.89	1.48E-05	5.64E-05	1.67E-04	0.38
1150	1250	2.779	2.00E-05	7.56E-05	2.12E-04	0.37
1150	1300	2.766	1.69E-05	5.71E-05	1.68E-04	0.36
1150	1350	2.706	1.94E-05	6.49E-05	1.68E-04	0.34
1200	1100	2.94	6.36E-07	4.28E-06	1.93E-05	0.54
1200	1150	2.833	6.84E-06	3.11E-05	9.73E-05	0.42
1200	1200	2.868	1.26E-05	5.09E-05	1.46E-04	0.39
1200	1250	2.779	2.43E-05	6.42E-05	1.78E-04	0.31
1200	1300	2.844	1.64E-05	4.88E-05	1.42E-04	0.34
1200	1350	2.676	1.37E-05	4.86E-05	1.24E-04	0.35
1250	1100	2.997	8.00E-07	4.96E-06	2.17E-05	0.52
1250	1150	2.904	1.27E-05	5.16E-05	1.48E-04	0.39
1250	1200	2.835	1.42E-05	5.16E-05	1.51E-04	0.37
1250	1250	2.824	2.06E-05	6.01E-05	1.48E-04	0.31
1250	1300	2.804	1.69E-05	6.45E-05	1.76E-04	0.37
1250	1350	2.699	1.53E-05	5.80E-05	1.45E-04	0.36
1300	1100	2.968	7.73E-07	4.96E-06	2.10E-05	0.52
1300	1150	2.939	1.01E-05	3.90E-05	1.15E-04	0.38
1300	1200	2.817	8.12E-06	3.23E-05	9.99E-05	0.4
1300	1250	2.786	1.92E-05	6.14E-05	1.57E-04	0.33
1300	1300	2.798	1.70E-05	6.33E-05	1.62E-04	0.36
1300	1350	2.728	1.48E-05	5.12E-05	1.35E-04	0.35