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Supplementary Information

Bayesian optimisation with transfer learning for NASICON-type

solid electrolytes for all-solid-state Li metal batteries

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(b)







20 µm -

- 20 μm

= 20 μm



Fig. S1 EDX elemental maps of calcium (red) and silicon (green) in the fracture surfaces of (a) $Si_{0.1}/Ca_{0.05},$ (b) $Si_{0.1}/Ca_{0.1},$ (c) $Si_{0.1}/Ca_{0.3},$ (d) $Si_{0.2}/Ca_{0.1},$ and (e) $Si_{0.3}/Ca_{0.1}.$



Fig. S2 (a) Arrhenius plot of the Li-ion conductivity of $Si_{0.1}/Ca_{0.05}$. (b) Composition dependence of the activation energy for the as-synthesised Si_x/Ca_y pellets.



Fig. S3 Galvanostatic cycle measurement of the Li | $Li_{1.2}Ca_{0.05}Zr_{1.95}Si_{0.1}P_{2.9}O_{12}$ | Li symmetric cell over a period of 110 h at a current density of 50 μ A cm⁻².