A highly fluorinated lithium iron phosphate with interpenetrating lattices:

Electrochemistry and Ionic conductivity

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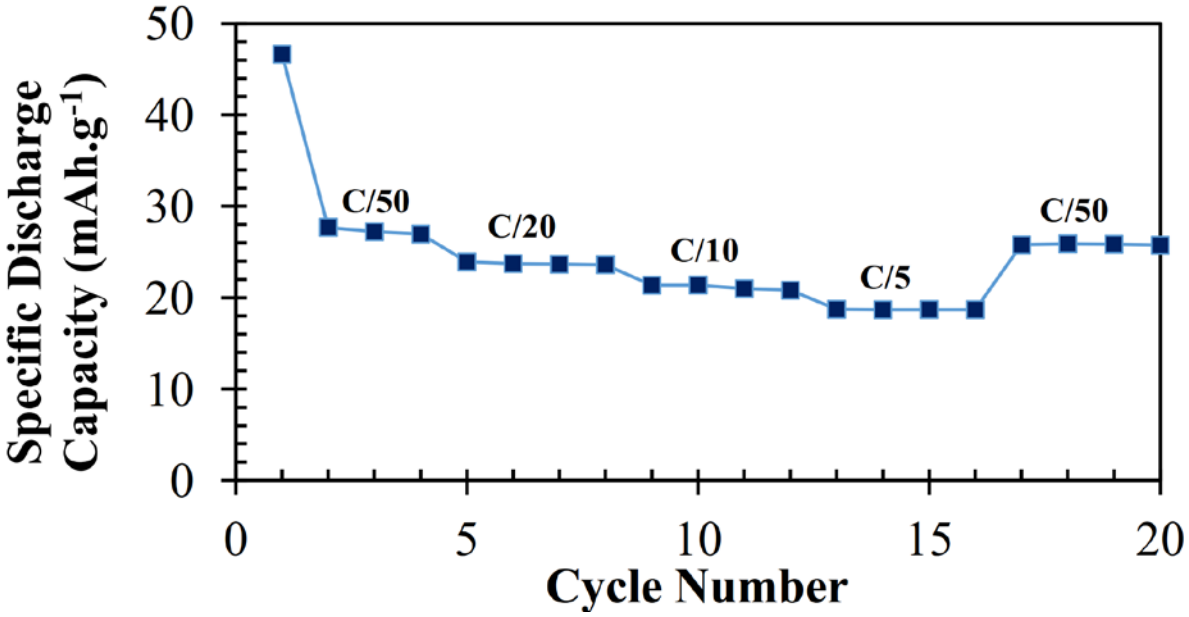

Figure S1: Test of cycle life showing capacity retention at various C-rates for $Li_5Fe_2(PO_4)F_8$ cathode.

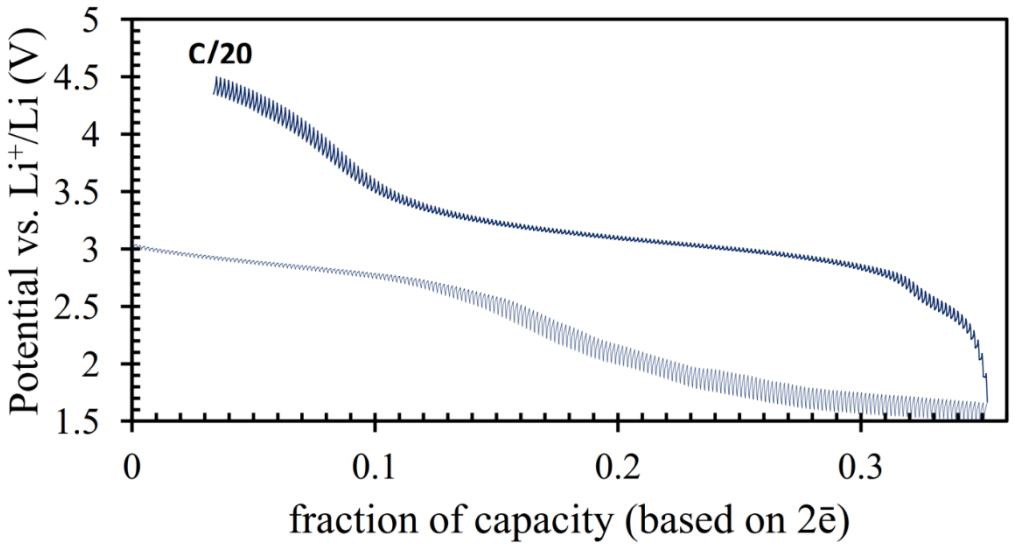

Figure S2. Charge-discharge GITT curves for $Li_5Fe_2(PO_4)F_8$

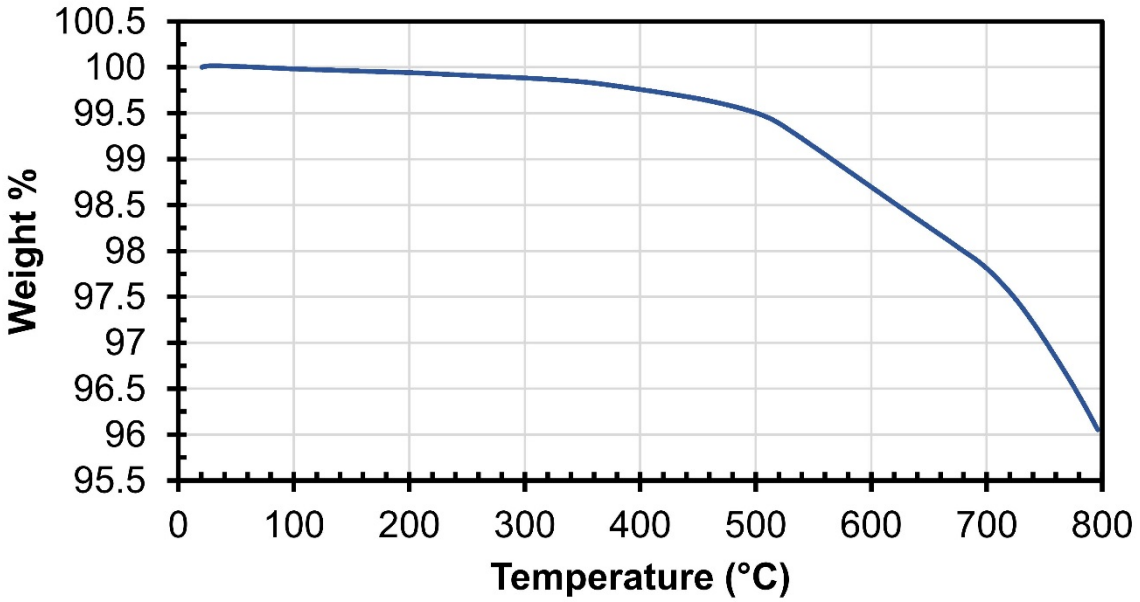

Figure S3. TGA curve of $Li_5Fe_2PO_4F_8$ under N_2 flow at 10 °C.min^{-1} heating rate.

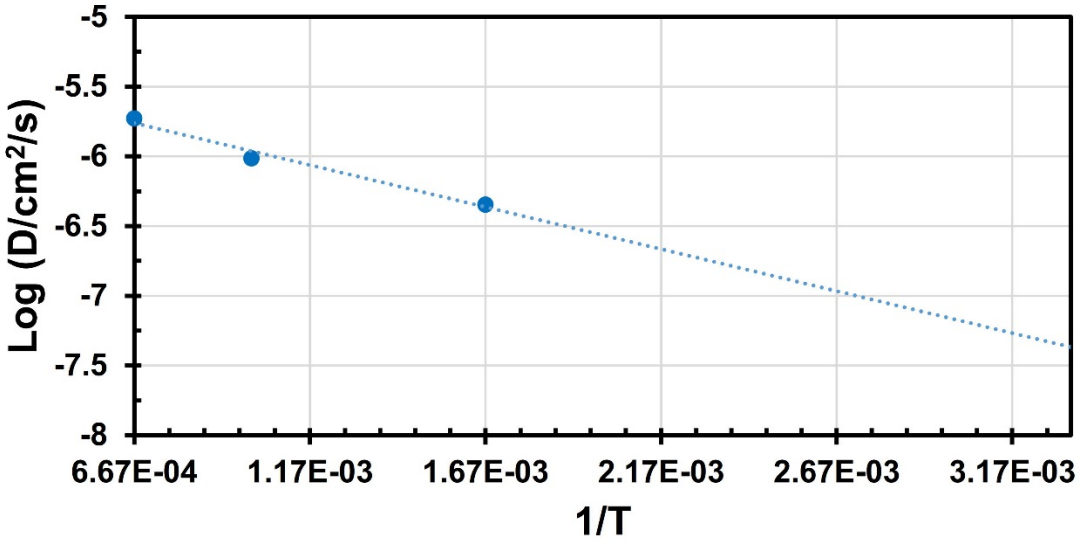

Figure S4. Arrhenius plot of Li^+ diffusivity vs. temperature as obtained from ab initio molecular dynamic (AIMD) simulations.

Table S1. Atom list, fractional coordinates and isotropic thermal displacement parameters for $Li_5Fe_2PO_4F_8$. Ueq = 1/3rd of the trace of the orthogonalized U tensor.

Atom	**Wyck.**	**Occ.**	**x/a**	**y/b**	**z/c**	**U [Å^2]**
Fe1	8f	1.00	0.37601(2)	0.51532(4)	0.27215(4)	0.0083(1)
Fe2	4d	1.00	0.25	1.00	-0.04605(5)	0.0087(1)
Fe3	4a	1.00	0.25	1.00	0.00	0.0083(1)
P1	8f	1.00	0.37435(3)	0.74656(7)	0.00677(6)	0.0071(1)
O1	8f	1.00	0.31682(9)	0.83157(8)	-0.07309(7)	0.0120(3)
O2	8f	1.00	0.33937(8)	0.65843(7)	0.12638(7)	0.0104(3)
O3	8f	1.00	0.42926(8)	0.85150(8)	0.07129(7)	0.0100(3)
O4	8f	1.00	0.41226(8)	0.64232(8)	-0.09649(6)	0.0094(3)
F1	8f	1.00	0.44384(7)	0.64609(1)	0.35583(3)	0.0140(3)
F2	8f	1.00	0.44287(7)	0.43440(6)	0.14193(4)	0.0136(3)
F3	8f	1.00	0.54925(7)	0.85730(1)	-0.12015(6)	0.0131(3)
F4	8f	1.00	0.30643(7)	0.38820(3)	0.19217(4)	0.0143(3)
F5	8f	1.00	0.30977(7)	0.59885(2)	0.40567(7)	0.0141(3)
F6	8f	1.00	0.55805(7)	0.94338(6)	0.15107(4)	0.0143(3)
F7	8f	1.00	0.30736(7)	1.10281(8)	0.09011(6)	0.0158(3)
F8	8f	1.00	0.30515(7)	1.09828(7)	-0.18947(6)	0.0145(3)
Li1	4e	1.00	0.25	0.50	0.5506(7)	0.0201(4)
Li2	4b	1.00	0.50	0.50	0.00	0.0291(8)
Li3	8f	1.00	0.6239(2)	1.0111(6)	0.2834(5)	0.0218(1)
Li4	4c	1.00	0.50	0.7893(7)	0.25	0.0181(3)
Li5	4c	1.00	0.50	0.7160(8)	-0.25	0.0231(3)
Li6	8f	1.00	0.2460(3)	0.2546(7)	0.2584(7)	0.0367(6)
Li7	8f	1.00	0.3765(3)	0.7436(9)	0.5112(9)	0.060(3)

Table S2. Polyhedral details and distortion analysis for the three crystallographically unique iron sites in $Li_5Fe_2PO_4F_8$.

	Fe1	Fe2	Fe3
Average bond length (Å)	1.9570	1.9584	1.9558
Polyhedral volume ($Å^3$)	9.8999	9.8986	9.9272
Distortion index (bond length)	0.02412	0.01769	0.02716
Quadratic elongation	1.0070	1.0081	1.0042
Bond angle variance ($°^2$)	19.4884	25.3239	8.0046
Effective C.N.	5.8539	5.9258	5.7554