

Supporting Information

Fluorination Strategies for Mn₃O₄ Nanoparticles: Enhancing Reversibility and Capacity in Li-Ion Batteries

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Figure S1. Adsorption isotherms of Mn₃O₄ oxide nanoparticles (non fluorinated, fluorinated with XeF₂ and fluorinated with F₂)

Figure S2. Full-pattern matching of Mn₃O₄ X-ray diffractograms of a) pristine Mn₃O₄, b) Mn₃O₄ fluorinated with XeF₂ and c) Mn₃O₄ fluorinated with F₂

Figure S3. Galvanostatic profiles of Mn₃O₄ (XeF₂) sample at D/20 (46.85 mA g⁻¹) current density for cycles 1; 10; 20; 40 and 160 highlighted in dotted red line

Figure S4. (a) GITT curves for the discharge and charge of the three Mn₃O₄ samples, with or without fluorination (b) Voltage versus time curve of a single discharge/relaxation GITT step; (c) evolution of the Li⁺ diffusion coefficient in potential vs. Li⁺/Li calculated by Fick's second law with the discharge GITT results of the three samples

Figure S5. Relative evolution of the mean capacity at each current density step of the C-rate experiments for the non-fluorinated and fluorinated Mn₃O₄ materials. The reference initial capacity was obtained by averaging the stabilized cycles 6 to 10, without taking into account the initial 1 to 5 cycles where large irreversibility of the conversion material is observed.

Table S1. Fitting parameters for the EIS equivalent circuit of No F, F₂ and XeF₂ samples before discharge.

Table S2. Fitting parameters for the EIS equivalent circuit of No F, F₂ and XeF₂ samples after discharge.

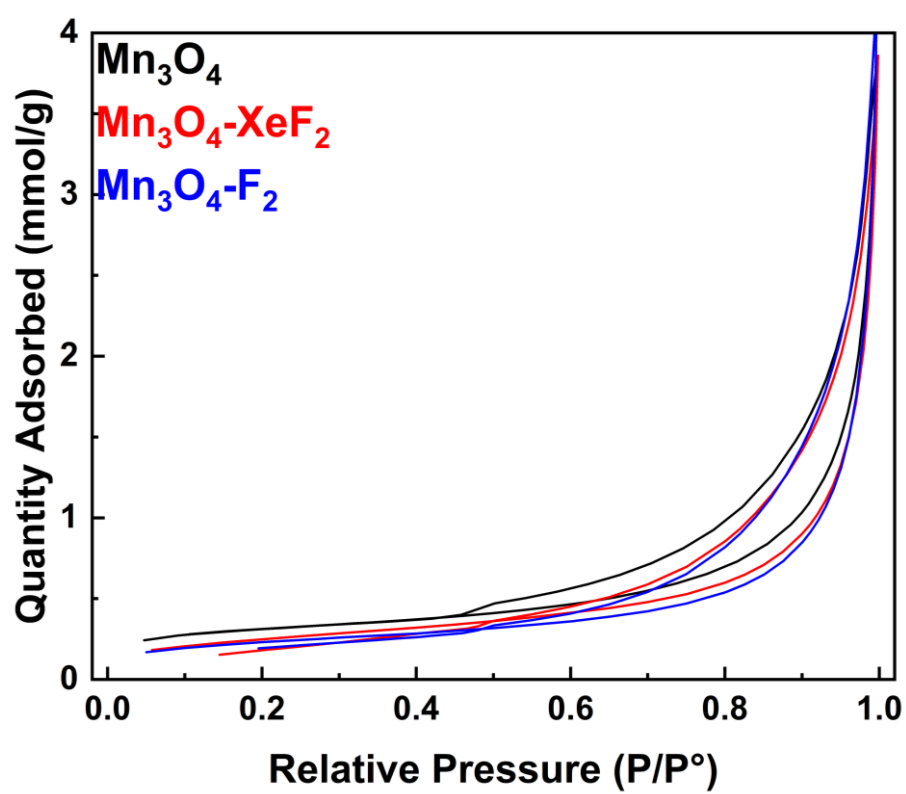


Figure S1. Adsorption isotherms of Mn_3O_4 oxide nanoparticles (non fluorinated, fluorinated with XeF_2 and fluorinated with F_2)

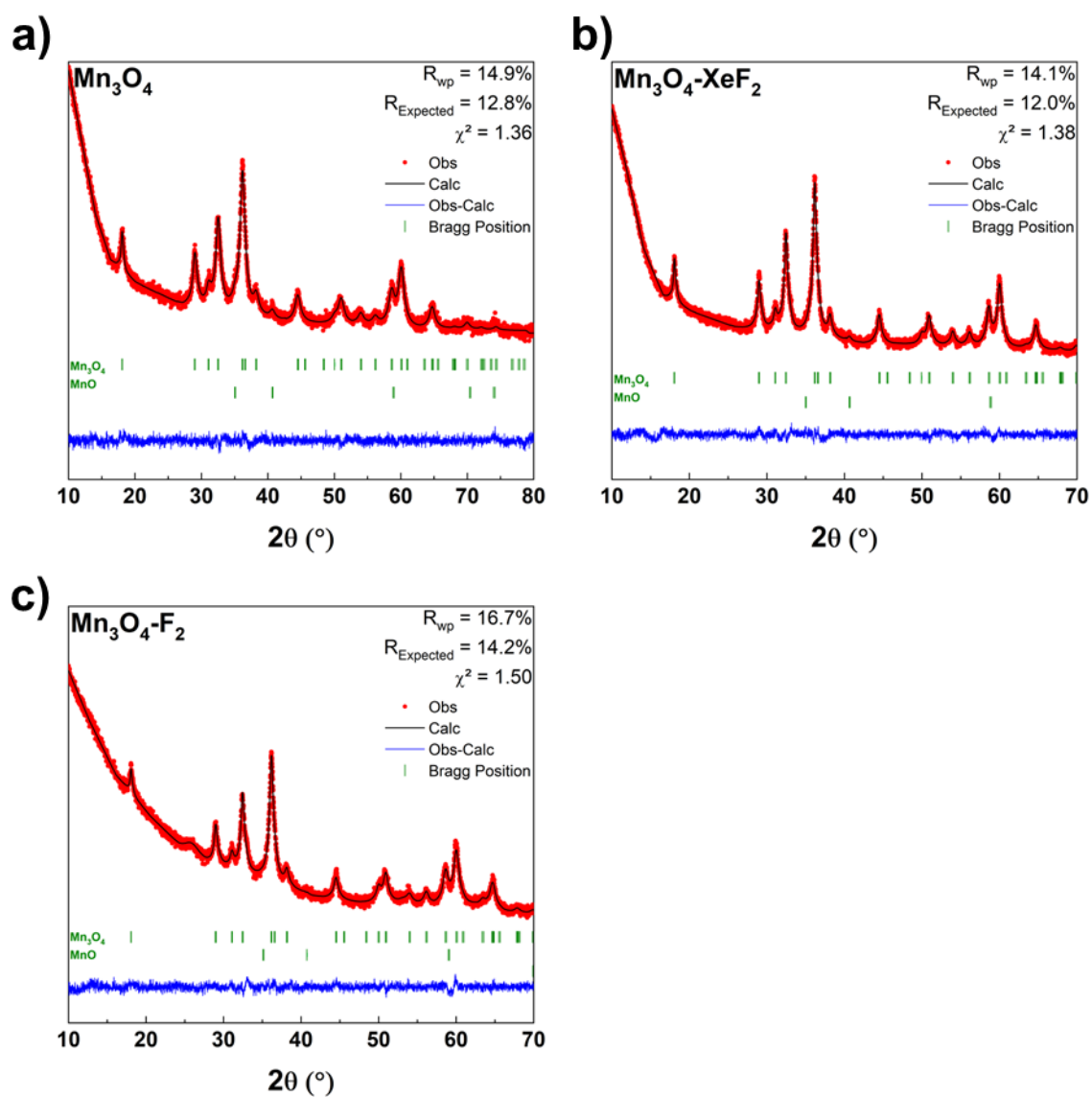


Figure S2. Full-pattern matching of Mn_3O_4 X-ray diffractograms of a) pristine Mn_3O_4 , b) Mn_3O_4 fluorinated with XeF_2 and c) Mn_3O_4 fluorinated with F_2

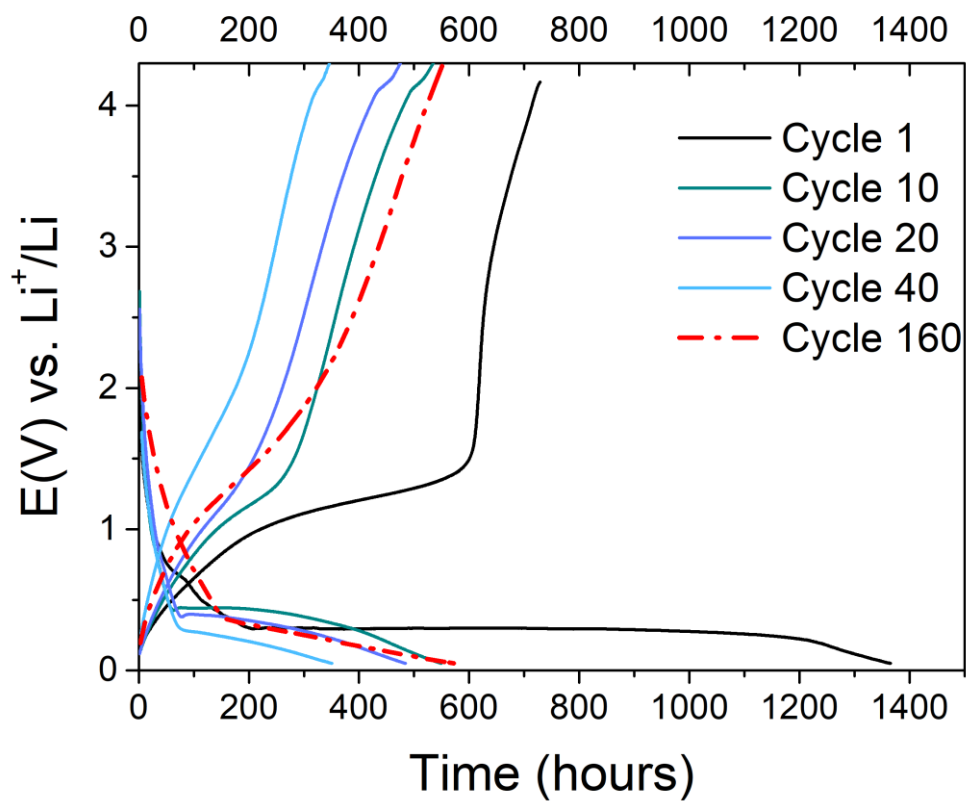


Figure S3. Galvanostatic profiles of Mn₃O₄ (XeF₂) sample at D/20 (46.85 mA g⁻¹) current density for cycles 1; 10; 20; 40 and 160 highlighted in dotted red line

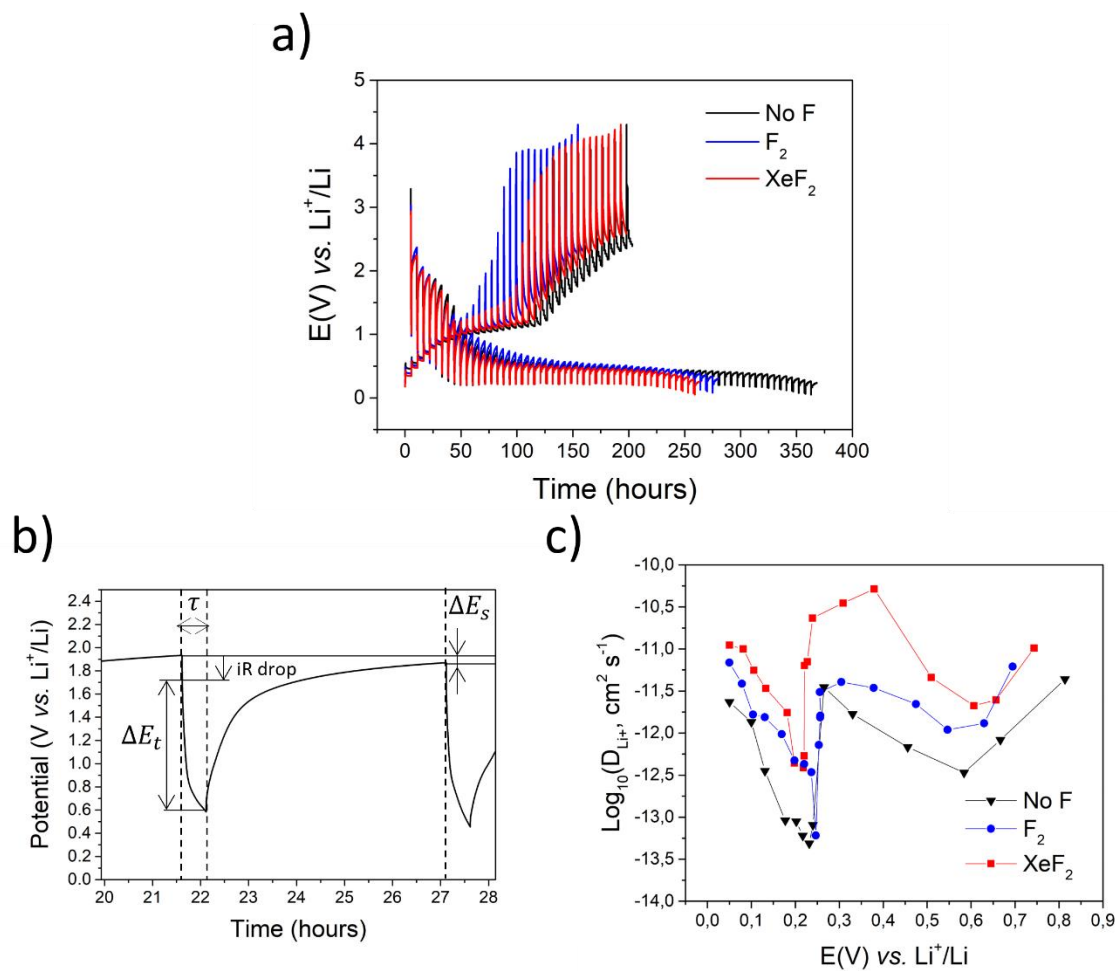


Figure S4. (a) GITT curves for the discharge and charge of the three Mn_3O_4 samples, with or without fluorination (b) Voltage versus time curve of a single discharge/relaxation GITT step; (c) evolution of the Li^+ diffusion coefficient in potential vs. Li^+/Li calculated by Fick's second law with the discharge GITT results of the three samples

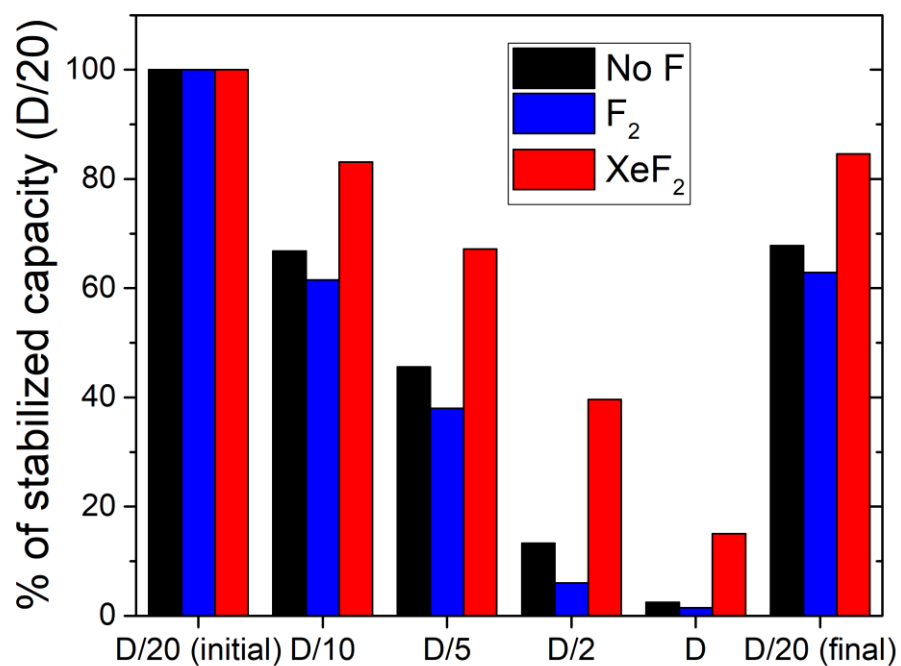


Figure S5. Relative evolution of the mean capacity at each current density step of the C-rate experiments for the non-fluorinated and fluorinated Mn₃O₄ materials. The reference initial capacity was obtained by averaging the stabilized cycles 6 to 10, without taking into account the initial 1 to 5 cycles where large irreversibility of the conversion material is observed.

Table S1. Fitting parameters for the EIS equivalent circuit of No F, F₂ and XeF₂ samples
before discharge.

Sample	R1 (Rs) (Ω)	Q2 (CPE1) ($F \cdot s^{(a-1)}$)	a2 (CPE1)	R2 (Rct+R1) (Ω)	Q3 (CPE2) ($F \cdot s^{(a-1)}$)	a3 (CPE2)	$\chi^2/ N $
No F	21.74	25.5 10 ⁻⁶	0.8102	311.5	8.58 10 ⁻⁴	0.8846	9.7 10 ⁻³
F ₂	25.87	17.79 10 ⁻⁶	0.8314	279.4	5.59 10 ⁻⁴	0.8468	1.54 10 ⁻³
XeF ₂	20.36	21.55 10 ⁻⁶	0.7944	380.6	1.37 10 ⁻³	0.8213	4.83 10 ⁻³

Table S2. Fitting parameters for the EIS equivalent circuit of No F, F₂ and XeF₂ samples after
discharge.

Sample	R1 (Rs) (Ω)	Q1 (CPE2) ($F \cdot s^{(a-1)}$)	a1 (CPE2)	R2 (Ω)	Q3 (CPE2) ($F \cdot s^{(a-1)}$)	a3 (CPE2)	R3 (Ω)	S4 (Wo)	$\chi^2/ N $
No F	25.11	38.74 10 ⁻⁶	0.7015	356.7	4.569 10 ⁻³	0.6786	136.6	35.55	7.06 10 ⁻³
F ₂	29.12	32.46 10 ⁻⁶	0.6798	475.2	2.236 10 ⁻³	0.8416	160.4	43.46	4.24 10 ⁻³
XeF ₂	24.75	10.13 10 ⁻⁶	0.7903	309.2	20.91 10 ⁻⁶	0.6332	43.08	32.18	5.91 10 ⁻³