

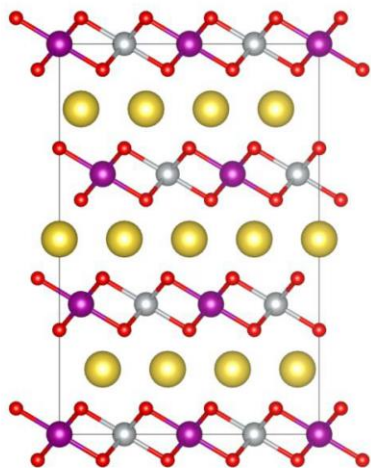
## Supporting Information

### Dual Doping with Cation and Anion for Enhancing the Structural Stability of Sodium-Ion Layered Cathode

Kyoungmin Min\*

School of Mechanical Engineering, Soongsil University, 369 Sangdo-ro, Dongjak-gu, Seoul  
06978, Republic of Korea

(a)



(b)



**Figure S1.** (a) Atomic structure of undoped  $\text{NaNi}_{0.5}\text{Mn}_{0.5}\text{O}_2$ . (b) Schematic view of cation and F dopant in a different (middle) and the same (right) transition metal (TM)-layer.

Cation Dopant	Cation-F doped			Change		
	Lattice $a$ (Å)	Lattice $c$ (Å)	Volume (Å <sup>3</sup> )	Lattice $a$ (Å)	Lattice $c$ (Å)	Volume (Å <sup>3</sup> )
Ga	3.037	16.107	259.82	0.0107	0.0746	4.600
Ge	3.059	16.088	262.48	0.0289	0.0859	4.590
Hf	3.106	16.101	269.28	0.0191	0.0312	2.730
In	3.101	16.163	269.88	0.0187	0.0660	4.570
Pt	3.092	16.065	267.18	0.0322	0.0639	4.710
Rh	3.060	16.049	261.81	0.0486	0.0673	4.670
Ru	3.065	16.094	263.60	0.0277	0.0669	4.180
Sb	3.139	16.234	277.63	0.0316	0.0721	4.960
Te	3.135	16.230	277.48	0.0398	0.0711	5.840
Ti	3.066	16.096	263.68	0.0295	0.0877	4.750
Y	3.128	16.162	274.39	0.0294	0.0603	5.310
Zr	3.117	16.156	272.71	0.0333	0.0868	5.290

**Table S1.** Lattice parameters and volume change (positive number indicates an increase) before and after doping with additional F for each cation-doped structure.

Final Rank	Element	O3-P3	O3-P3 (50%)	Volume (50%)	Sum
		(Pristine)			
		Rank	Rank	Rank	
1	Te	3	3	1	8
2	Sb	4	2	9	11.5
3	Hf	11	1	3	14
4	Y	1	6	8	14
5	Ti	2	7	5	15
6	Rh	8	4	7	17.5
7	Pt	6	5	11	19
8	Zr	5	9	10	23.5
9	Ge	7	8	12	25
10	In	9	11	4	27.5
11	Ga	10	12	2	29
12	Ru	12	10	6	30

**Table S2.** Criteria for ranking in the final list of proposed dopants. Sum =  $1.0 \times (\text{O3-P3, pristine}) + 1.5 \times (\text{O3-P3, 50\%}) + 0.5 \times (\text{volume, 50\%})$