

Supporting Information

Revealing the Role of Dopants in Mitigating Degradation Phenomena in Sodium-Ion Layered Cathodes

Kyoungmin Min^{1,*} and Young-Han Shin^{2,*}

¹School of Mechanical Engineering, Soongsil University, 369 Sangdo-ro, Dongjak-gu, Seoul 06978,
Republic of Korea

²Department of Physics, University of Ulsan, 93 Daehak-ro, Nam-gu, Ulsan 44610, Republic of
Korea

O3-type	Lattice a (Å)	Lattice c (Å)	Volume (Å³/f.u.)
Pristine	3.01	15.95	124.86
Mg-doped	3.01	16.01	125.35
Ti-doped	2.99	15.94	124.49

Table S.1. The initial lattice parameters and volume for pristine and doped structures.

Structure	Atomic charge variation (Δe)				
	Ni	Co	Mn	O	Dopant
Pristine	0.1013	0.0538	0.0190	0.3984	n/a
Mg-doped	0.0895	0.0634	0.0150	0.3927	0.0069
Ti-doped	0.1029	0.0693	0.0180	0.3636	0.0155

Table S.2. Atomic charge variation for each element after full desodiation in pristine and doped structures.