Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

A first-principles study of the preventive effects of Al and Mg doping on the degradation in $LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$ cathode materials

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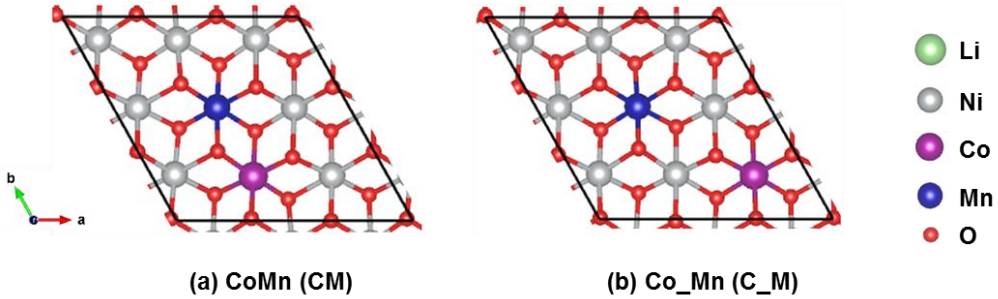
S.1. Initial structural properties

Property	Un-doped	Al-doped	Mg-doped
Lattice parameter *a* (Å)	2.895	2.882	2.887
Lattice parameter *c* (Å)	14.304	14.283	14.298
Volume (Å^3/unit-cell)	103.964	103.196	103.757
Thickness of TM-layer (Å)	2.154	2.138	2.154
Thickness of Li-layer (Å)	2.619	2.624	2.609

Table S1. Initial structural properties for un-doped, Al-doped, and Mg-doped structures.

S.2. Co and Mn clustering



(a) CoMn (CM) (b) Co_Mn (C_M)

Figure S1. Atomic configuration of NCM structure a) with and b) without Co and Mn neighboring.

The atomic snapshot of structures (a) with and (b) without Co and Mn neighboring is shown in Figure S1. The total energy of the structure with clustered (CM) and not clustered (C_M) CoMn is -23.4163 eV/f.u. and -23.4059 eV/f.u., respectively.

S.3. Delithiation process

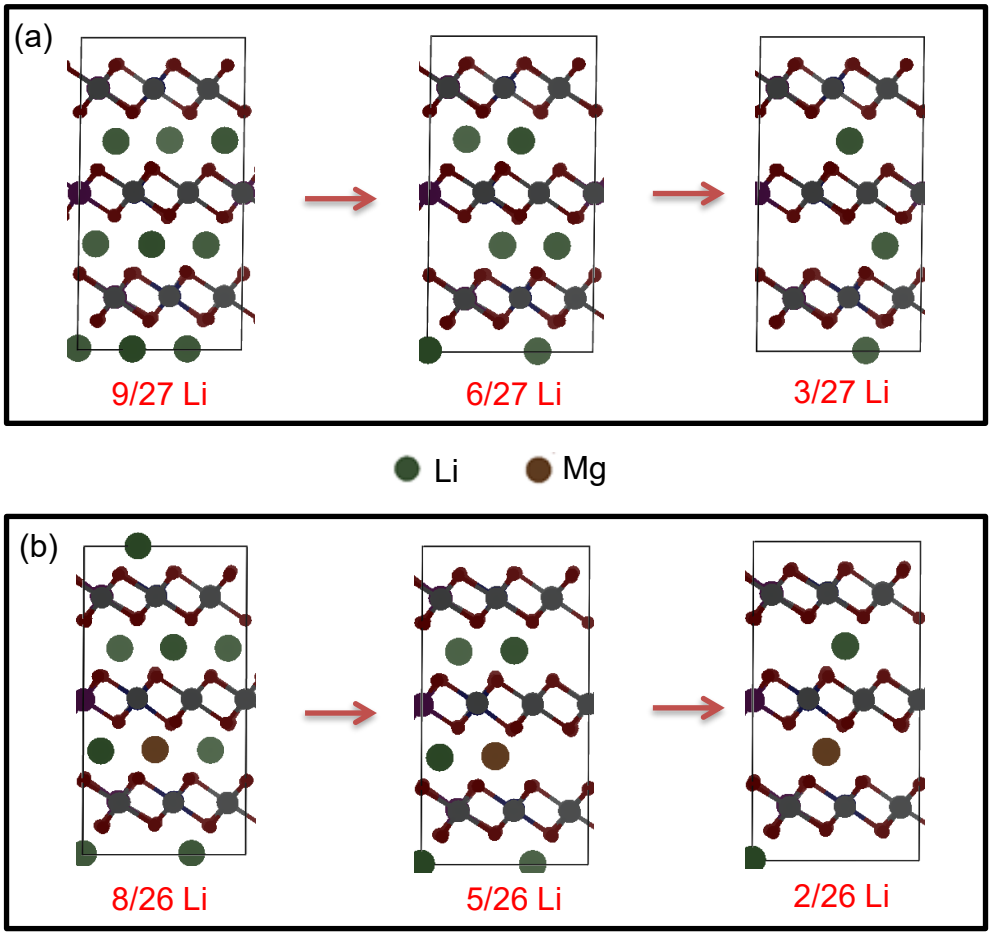


Figure S2. Delithiation process of (a) un-doped, Al-doped, and (b) Mg-doped structure. A number at the bottom indicates the number of delithiated Li out of a total number of Li for each structure.

S.4. TM- and Li-layer thickness variations during delithiation

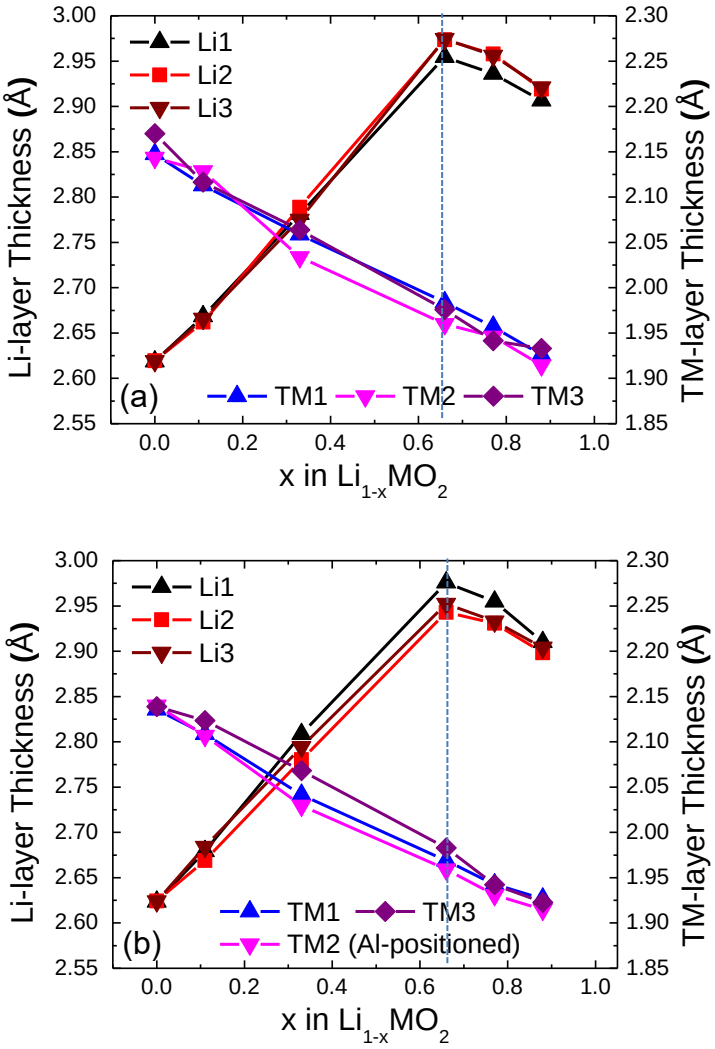


Figure S3. The variation in the thickness of TM- and Li-layer during delithiation for (a) un-doped and (b) Al-doped structure. ($Li_{1-x}MO_2$ where $0 \leq x \leq 0.9$) The vertical dashed line represents the practical usage of Li extraction.