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Ab initio study of doping effects in $LiMnO_2$ and Li_2MnO_3 cathode materials for Li-ion batteries

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Support information

Tables

Table S1. Formation energy of Fe, Nb, Cu doped Li_2MnO_3, $LiMnO_2$ and $LiMn_2O_4$.

	Formation energy (eV/atom)		
	Fe	Nb	Cu
Li_2MnO_3	-2.037	-2.132	-2.006
$LiMnO_2$	-2.143	-2.199	-2.100
$LiMn_2O_4$	-1.934	-2.127	-1.904

Table S2 (a). Redox potential of doped $LiMnO_2$.

	Dopants				
	Mg	Ti	V	Nb	F
8.33% Li	3.22 V	2.57 V	2.90 V	2.70 V	2.84 V
16.67% Li	3.41 V	3.62 V	3.66 V	3.03 V	3.69 V
25% Li	3.40 V	3.50 V	3.39 V	3.45 V	-

Table S2 (b). Redox potential of doped Li_2MnO_3.

	Dopants				
	V	Nb	Fe	Ru	F
6.25% Li	3.35 V	2.18 V	3.85 V	3.38 V	3.65 V
12.5% Li	4.60 V	4.57 V	4.68 V	4.30 V	4.54 V

Figures

Figure S1. (a) Observed Mn-O distortion during the migration of Lithium along TSH-V_{Li} path and (b) the ODH diffusion path, doping site and nearest neighboring Mn of the dopant (Mn_{NN}) in doped $LiMnO_2$.

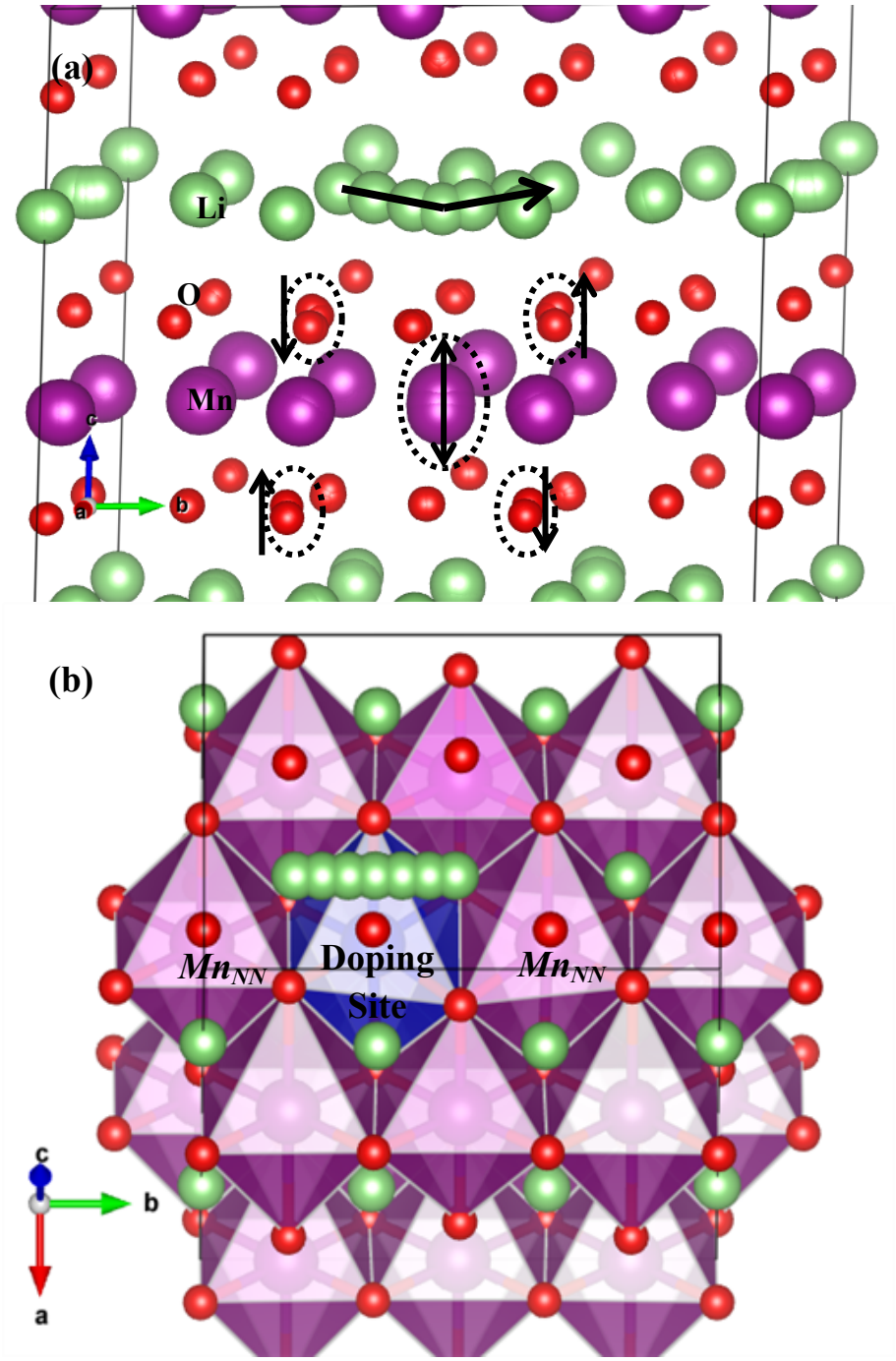
Figure S2. Mn and O atomic displacements for Li diffusion from the initial to the transition state along ODH (a) and TSH-V_{Li} paths (b).

Figure S3. Band structure of $LiMnO_2$.

Figure S4. Charge density of hole in Al doped $LiMnO_2$. (a) Hole distributed through the whole structure and (b) the hole is localized on Mn.

Figure S5. Band structure of Li_2MnO_3.

Figure S6. (a) Configuration of M doped Li_2MnO_3, where M is the dopant, p1 and p2 are two polaron sites. (b) Charge density of extra electron in Al doped Li_2MnO_3.



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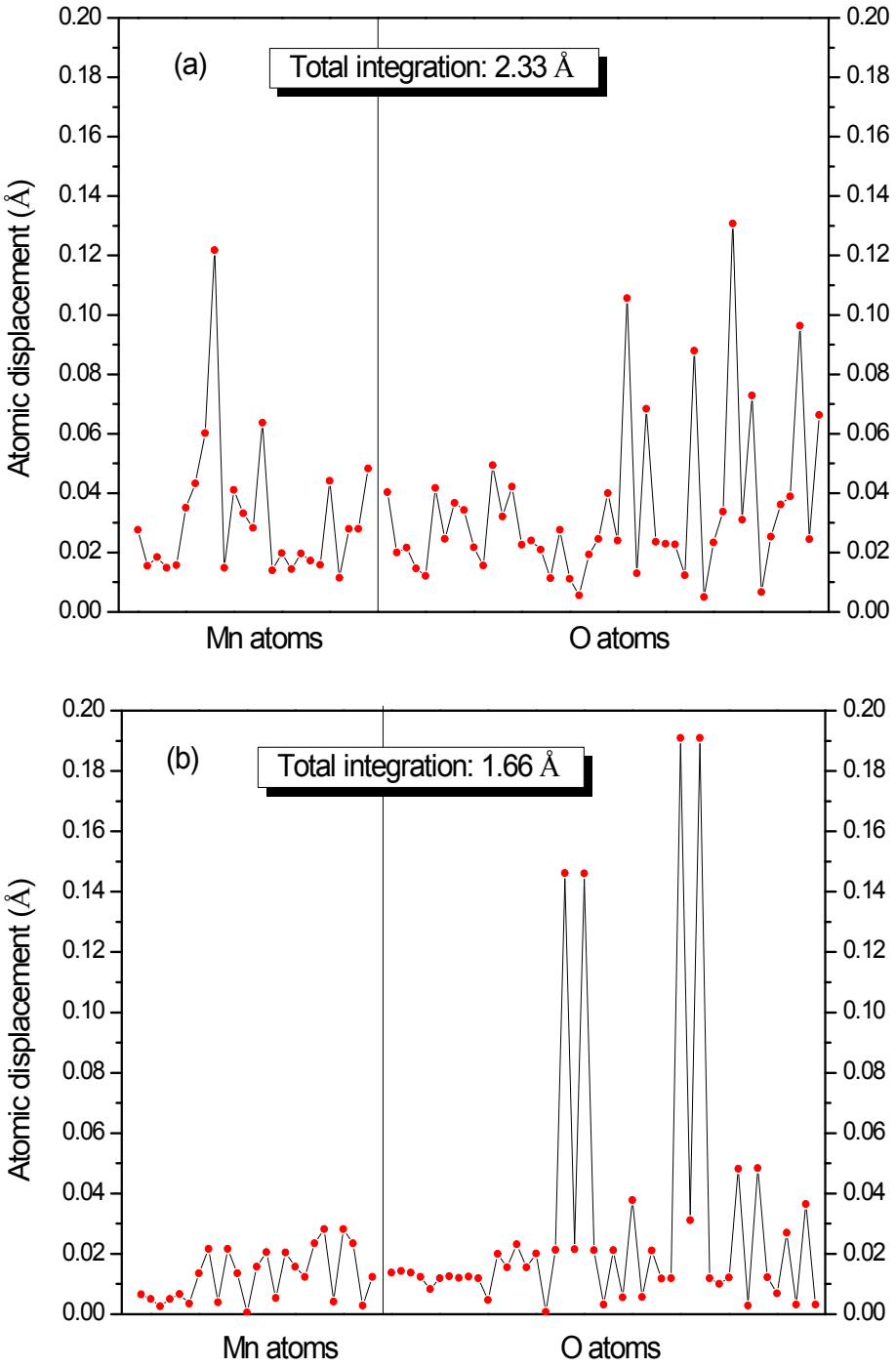

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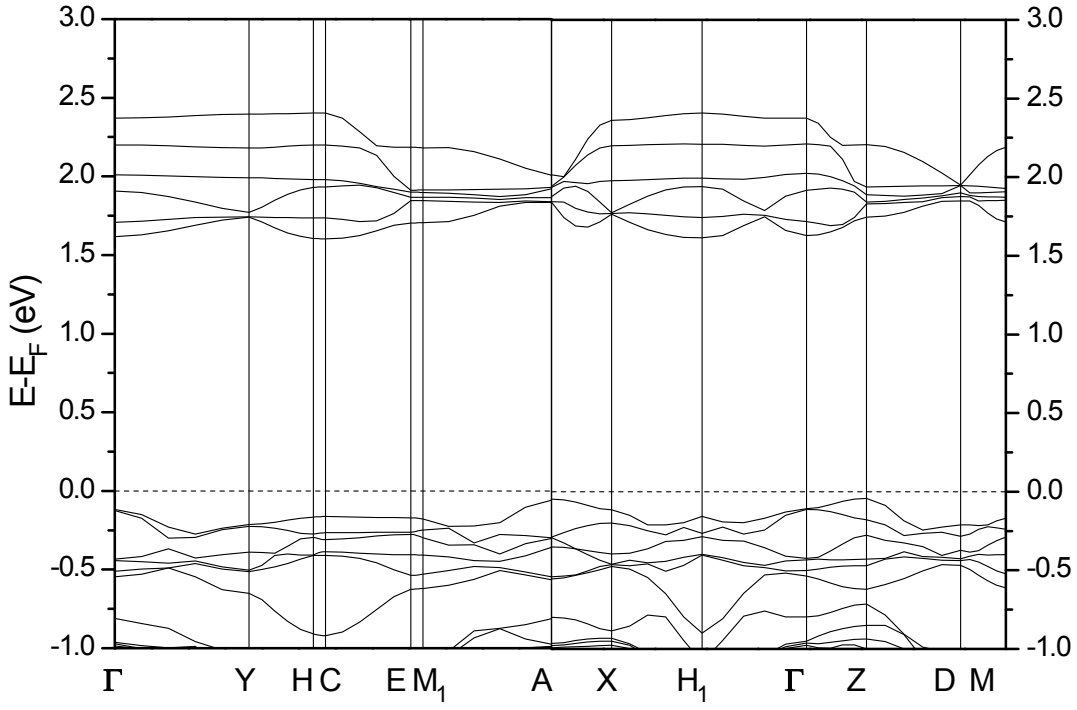

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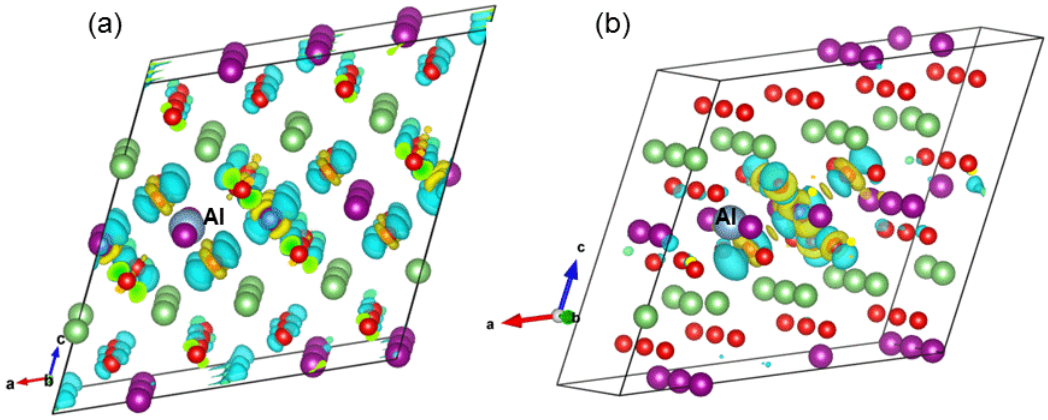

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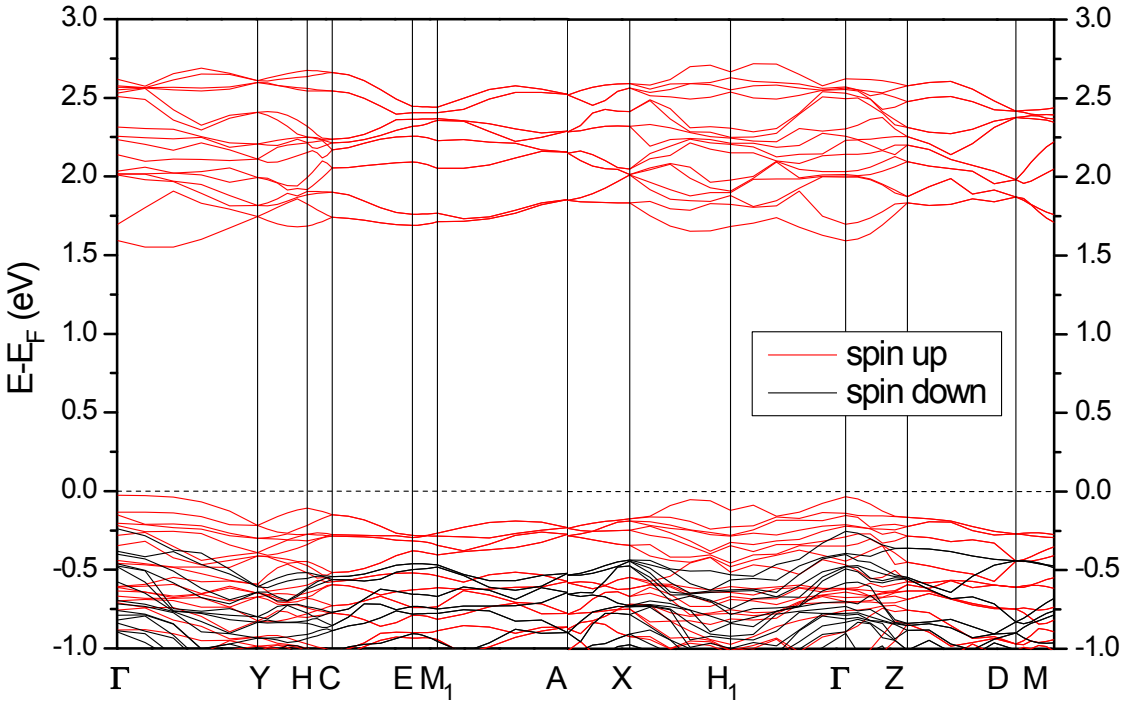
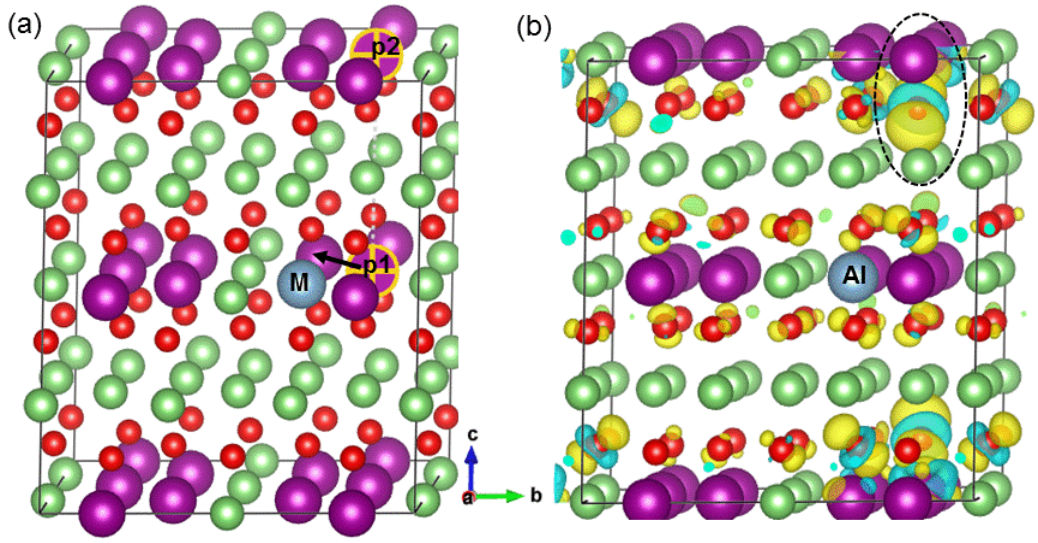


Figure S5. Band structure of Li_2MnO_3.



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