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

Supporting Information

A synergetic promotion of surface stability for high-voltage $LiCoO_2$ by multi-element surface doping: a first-principles study

Hongbin Lin,[a] Xiumei Kang,[a] Guigui Xu,[*ab] Yue Chen,[a]
Kehua Zhong,[a] Jian-Min Zhang[a] and Zhigao Huang[*a]

[a]*Fujian Provincial Key Laboratory of Quantum Manipulation and New Energy Materials, College of Physics and Energy, Fujian Normal University, Fuzhou 350117, China*

[b]*Concord University College Fujian Normal University, Fuzhou 350117, China*

[*]Author to whom correspondence should be addressed.

E-mail: xuguigui082@126.com (G. Xu); zghuang@fjnu.edu.cn (Z. Huang).

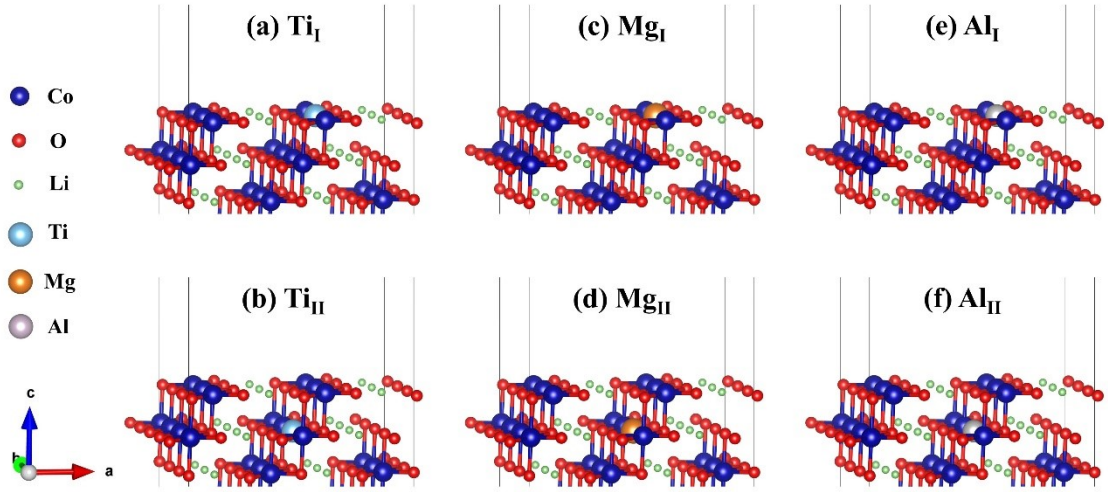

Fig. S1 Schematic illustrations of (a, b) two types of doping configurations for Ti-doped $LiCoO_2$ (104) surface, (c, d) two types of doping configurations for Mg-doped $LiCoO_2$ (104) surface and (e, f) two types of doping configurations for Al-doped $LiCoO_2$ (104) surface.

Table S1 Calculated formation energies (E_{form}) and energy differences (ΔE_{form}, relative to the surface layer doping configurations) of various doping configurations for Ti-doped, Mg-doped and Al-doped $LiCoO_2$ (104) surfaces.

System	Doping configurations	Formation energy E_{form} (eV)	Energy difference ΔE_{form} (eV)
Ti-doped $LiCoO_2$ (104)	**Ti_I**	-2.50	0
	Ti_{II}	-2.02	0.48
Mg-doped $LiCoO_2$ (104)	**Mg_I**	-3.65	0
	Mg_{II}	-4.43	-0.78
Al-doped $LiCoO_2$ (104)	**Al_I**	-5.75	0
	Al_{II}	-7.99	-2.24

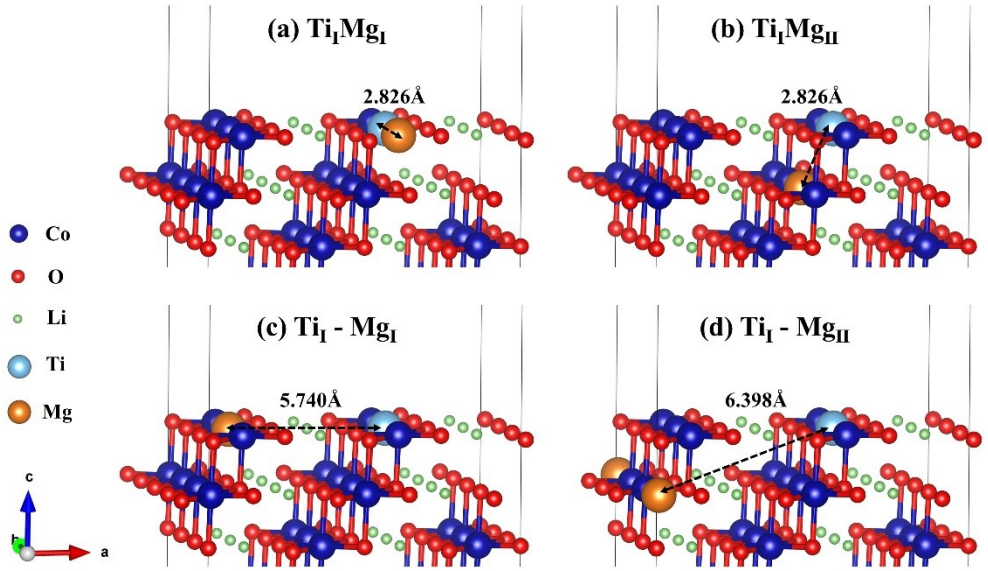

Fig. S2 Schematic illustrations of four types of doping configurations for Ti-Mg co-doped $LiCoO_2$ (104) surface. The distances between nearest doping Ti and Mg at (104) surface are 2.826 Å, 2.826 Å, 5.740 Å and 6.398 Å in these four doping configurations respectively.

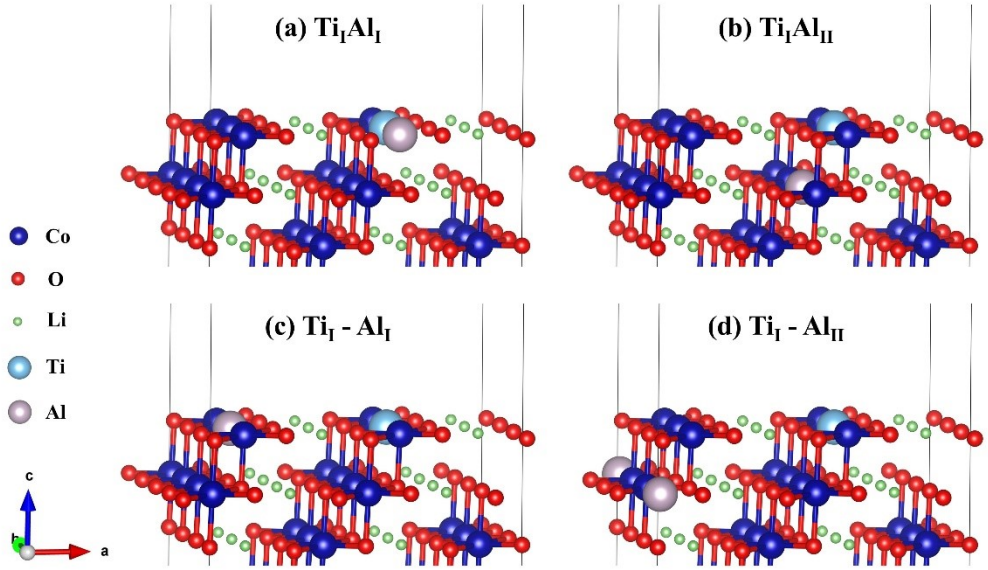

Fig. S3 Schematic illustrations of four types of doping configurations for Ti-Al co-doped $LiCoO_2$ (104) surface.

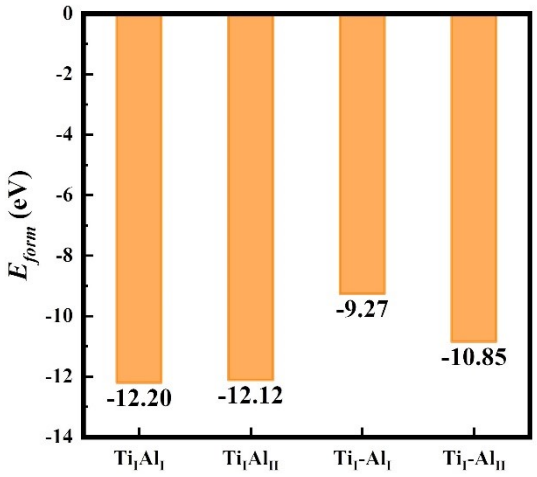

Fig.S4 Calculated formation energies (E_{form}) of various doping configurations for Ti-Al co-doped $LiCoO_2$ (104) surface.

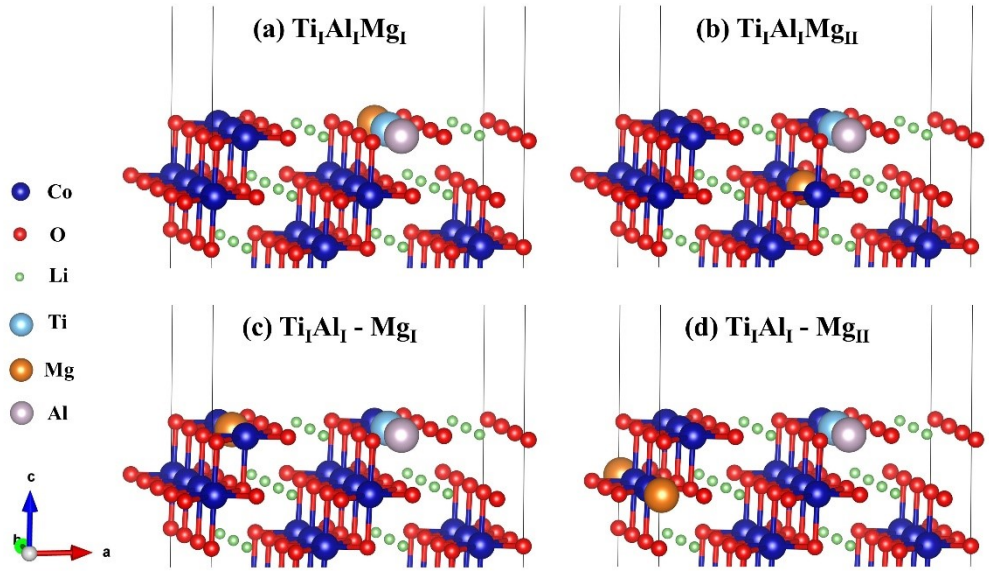

Fig. S5 Schematic illustrations of four types of doping configurations for Ti-Al-Mg co-doped $LiCoO_2$ (104) surface.

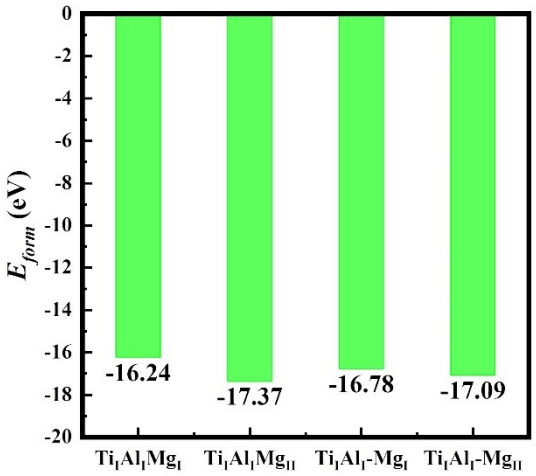

Fig. S6 Calculated formation energies (E_{form}) of various doping configurations for Ti-Al-Mg co-doped $LiCoO_2$ (104) surface.