Supporting Information

Structural Stability and Stabilization of Li_2MoO_3

Meng Tian[a, b], Yurui Gao[c], Ruijuan Xiao[a, b], Zhaoxiang Wang[a, b] *, Liquan Chen[a, b]

[a] Key Laboratory for Renewable Energy, Beijing Key Laboratory for New Energy Materials and Devices, National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

[b] School of Physical Sciences, University of Chinese Academy of Sciences, Beijing 100049, China

[c] Department of Physics and Astronomy, California State University Northridge, Northridge, California 91330-8268, USA

*E-mail: zxwang@iphy.ac.cn

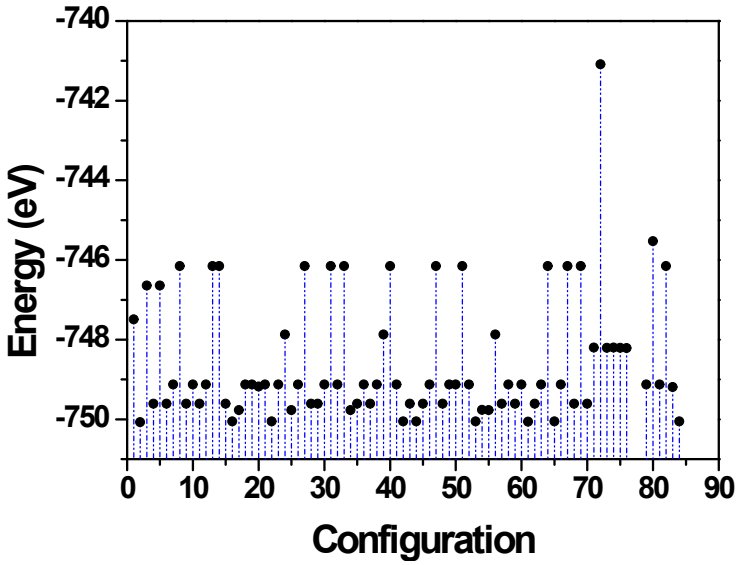

Fig. S1 Total energies of different configurations.

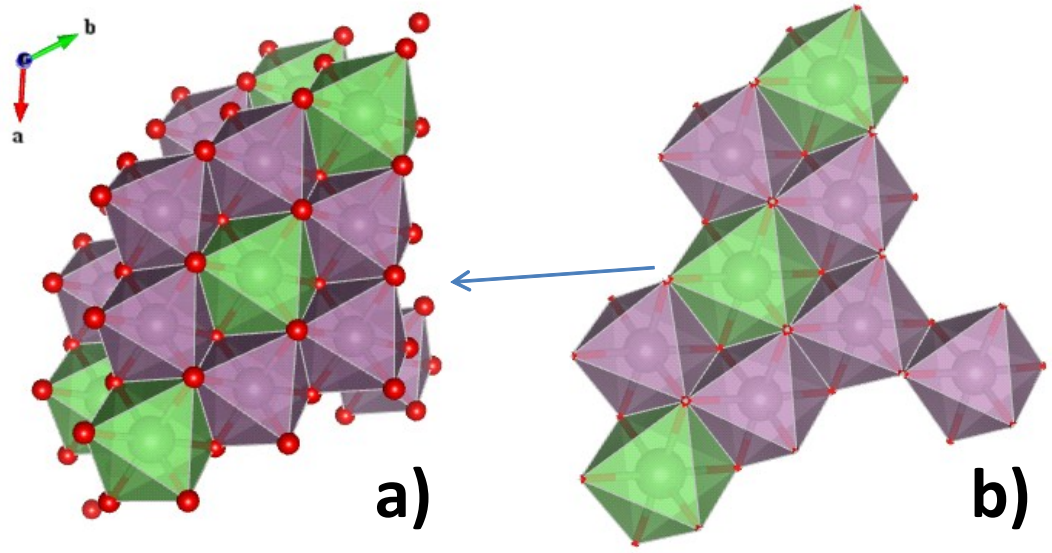

Fig. S2 The schematic diagram of the $LiMo_2$ of Li_2MoO_3 in a top view a) all the three $LiMo_2$ layer, b) the second $LiMo_2$ layer with some displacement of Mo-ion.

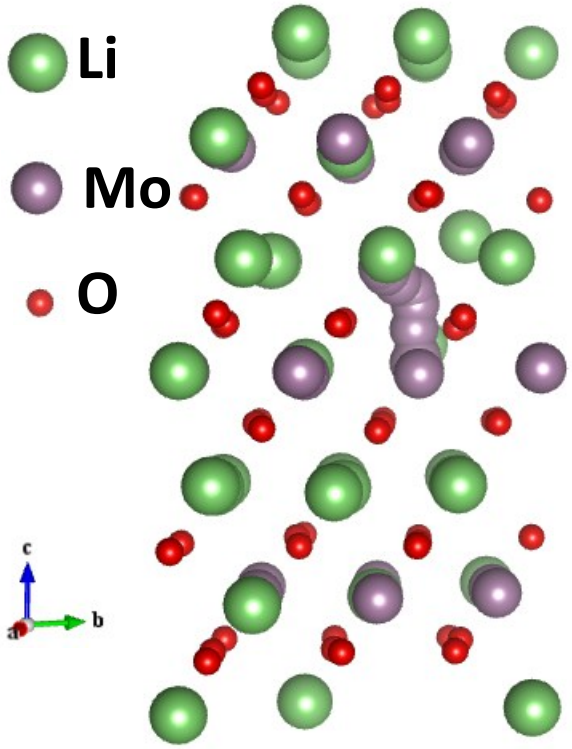

Fig. S3 The migration pathway of the Mo-ion associated to Fig. 2a.

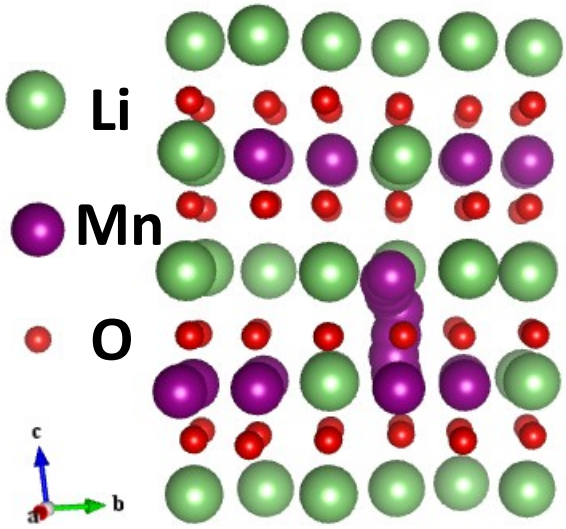

Fig. S4 The migration pathway of the Mn-ion associated to Fig. 2b.

Table S1 The distortion of MoO_6 octahedron before and after Li-vacancy conducted.

Six MoO_6 octahedra	Distortion index (before)	Distortion index (after)
Mo1	0.00805	0.06861
Mo2	0.00393	0.04342
Mo3	0.00393	0.03784
Mo4	0.00805	0.05976
Mo5	0.00805	0.03365
Mo6	0.00393	0.06283

Table S2 The calculated length of the M-O bonds in Li_2MoO_3.

octahedron	bond	d(Å)	octahedron	Bond	d(Å)	octahedron	bond	d(Å)
MoO_6	Mo6-O23	2.0938	TcO_6	Tc1-O23	2.0570	NbO_6	Nb1-O23	2.0455
	Mo6-O24	2.0674		Tc1-O24	2.0561		Nb1-O24	2.0480
	Mo6-O27	2.0782		Tc1-O27	2.0557		Nb1-O27	2.0220
	Mo6-O50	2.0938		Tc1-O50	2.0570		Nb1-O50	2.0455
	Mo6-O53	2.0674		Tc1-O53	2.0561		Nb1-O53	2.0480
	Mo6-O54	2.0782		Tc1-O54	2.0557		Nb1-O54	2.0220
SbO_6	Sb1-O23	2.0350	PdO_6	Pd1-O23	2.1763	RuO_6	Ru1-O23	2.0605
	Sb1-O24	2.0385		Pd1-O24	2.1752		Ru1-O24	2.1451
	Sb1-O27	2.0253		Pd1-O27	2.1803		Ru1-O27	2.0961
	Sb1-O50	2.0350		Pd1-O50	2.1763		Ru1-O50	2.0605
	Sb1-O53	2.0385		Pd1-O53	2.1752		Ru1-O53	2.1451
	Sb1-O54	2.0253		Pd1-O54	2.1803		Ru1-O54	2.0961
SnO_6	Sn1-O23	2.0471	TiO_6	Ti1-O23	1.9893			
	Sn1-O24	2.0574		Ti1-O24	2.0188			
	Sn1-O27	2.0515		Ti1-O27	2.0118			
	Sn1-O50	2.0471		Ti1-O50	1.9893			
	Sn1-O53	2.0574		Ti1-O53	2.0188			
	Sn1-O54	2.0515		Ti1-O54	2.0118			

Table S3 The length of Mo-O bond before and after transition metal doped.

Configurations	Origin	Tc_doped	Nb_doped	Sb_doped	Pd_doped	Ru_doped	Sn_doped	Ti_doped
Average bond length (Å)	2.0824	2.0812	2.0874	2.0841	2.0815	2.0859	2.0813	2.0818
Mo5-O49 (Å)	2.07086	2.07907	2.05091	2.05188	2.08674	2.08900	2.07196	2.08302
Mo5-O22 (Å)	2.07086	2.05870	2.05782	2.05206	2.05644	2.07924	2.06924	2.06850
Mo5-O23 (Å)	2.10757	2.13105	2.16786	2.15765	2.13256	2.12193	2.13704	2.12702
Mo5-O52 (Å)	2.10757	2.13283	2.12079	2.11251	2.13129	2.15897	2.13046	2.14208
Mo5-O26 (Å)	2.06889	2.04070	2.05126	2.05032	2.04186	2.04189	2.03872	2.03436
Mo5-O53 (Å)	2.06889	2.04480	2.07565	2.07988	2.04034	2.02465	2.04055	2.03573