Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporing Information

First-principles study on properties of Sn-doped $LiCoO_2$ for Li-ion batteries

Ruhan Yang[a], Mengke Guan[a], Ruirui Zhao*[a] and Qiong Luo*[a]

[a]Key Laboratory of Theoretical Chemistry of Environment, Ministry of Education; Center for Computational Quantum Chemistry, School of Chemistry, South China Normal University, Guangzhou, 510006, P. R. China.

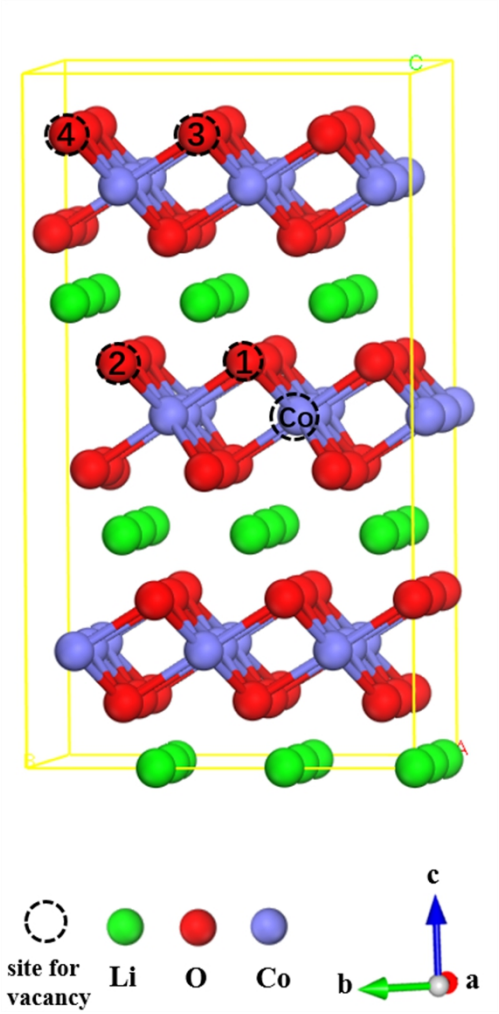

Fig. S1. Possible relative positions between Co vacancy and O vacancy of the pair of Co-O vacancies in LCO.

Table. S1. Lattice parameters, volume and energy of LCO containing a pair of Co-O vacancies.

Structure[a]	a/ Å	b/ Å	c/ Å	α/°	β/°	γ/°	V/ Å^3	E/eV
LCO_1	8.455	8.455	13.685	90.075	89.925	119.964	847.419	-607.404
LCO_2	8.471	8.460	13.668	89.917	90.026	120.046	847.906	-607.025
LCO_3	8.446	8.445	13.689	90.013	90.001	120.005	845.543	-605.566
LCO_4	8.456	8.449	13.675	90.067	90.021	120.034	854.808	-606.081

[a]The four structures have the same Co vacancy site as shown in Fig. S1. The subscript number (1, 2, 3, or 4) refers to the position of O vacancy in LCO marked in Fig. S1.

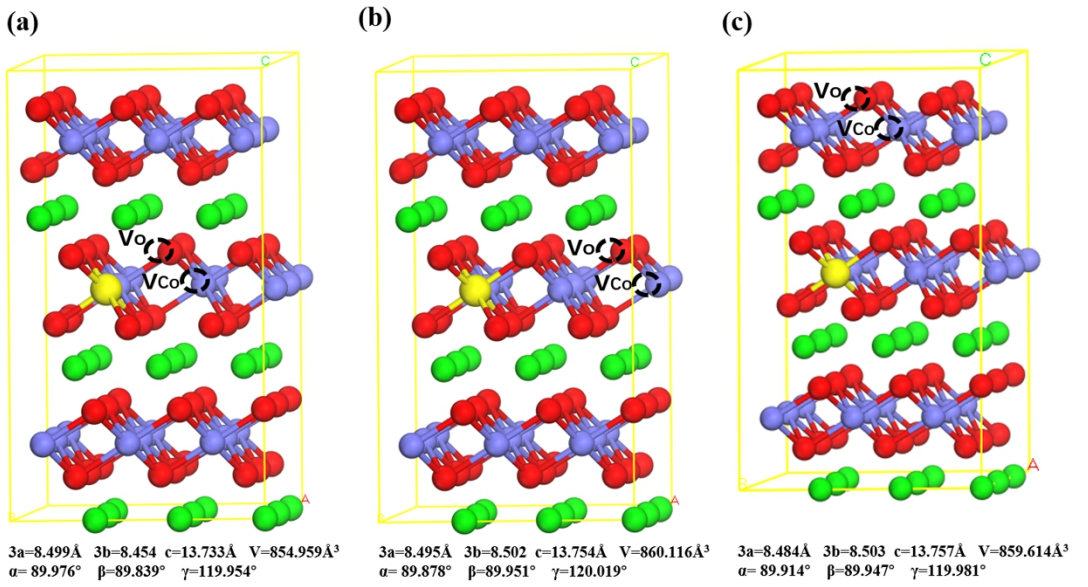

Fig. S2. Atomic configurations for the structure (a) where the doped Sn atom directly neighbors to the pair of Co-O vacancies, (b) where the doped Sn atom and the Co-O vacancies are in the same layer but not neighbor to each other, and (c) where the doped Sn atom and the Co-O vacancies are positioned in different layers.

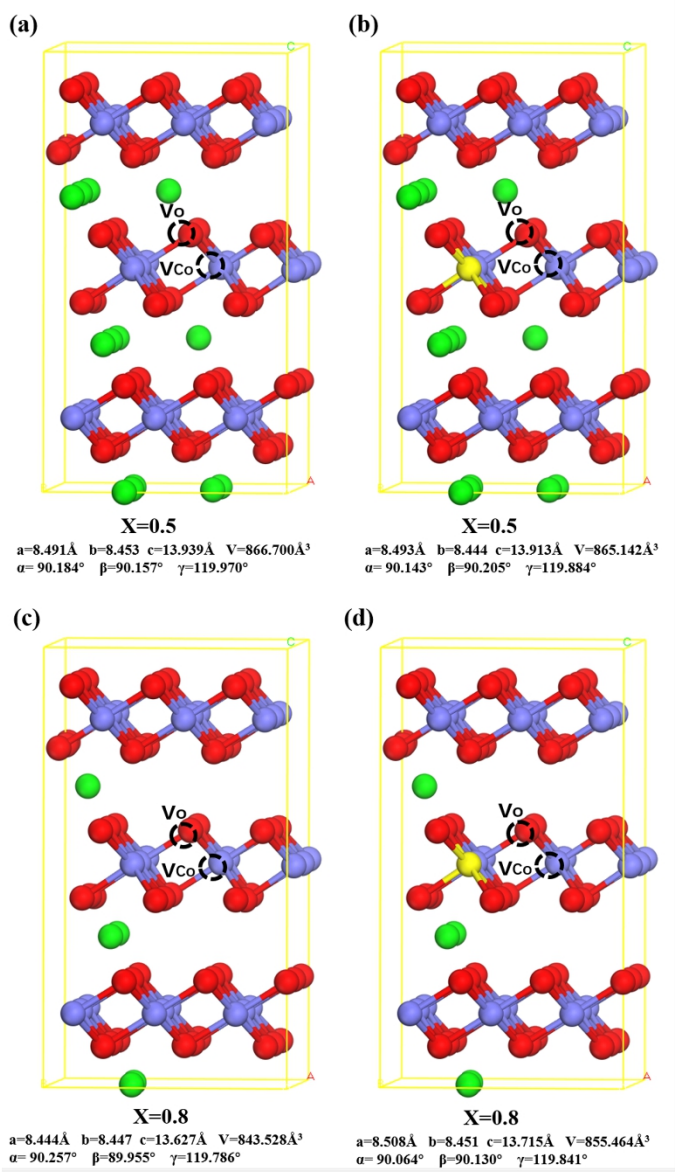

Fig. S3. The structures for vLCO with the degrees of delithiation at 50% (a) and 80% (c), respectively, along with the structures for vSLCO with the degrees of delithiation at 50% (b) and 80% (d), respectively.

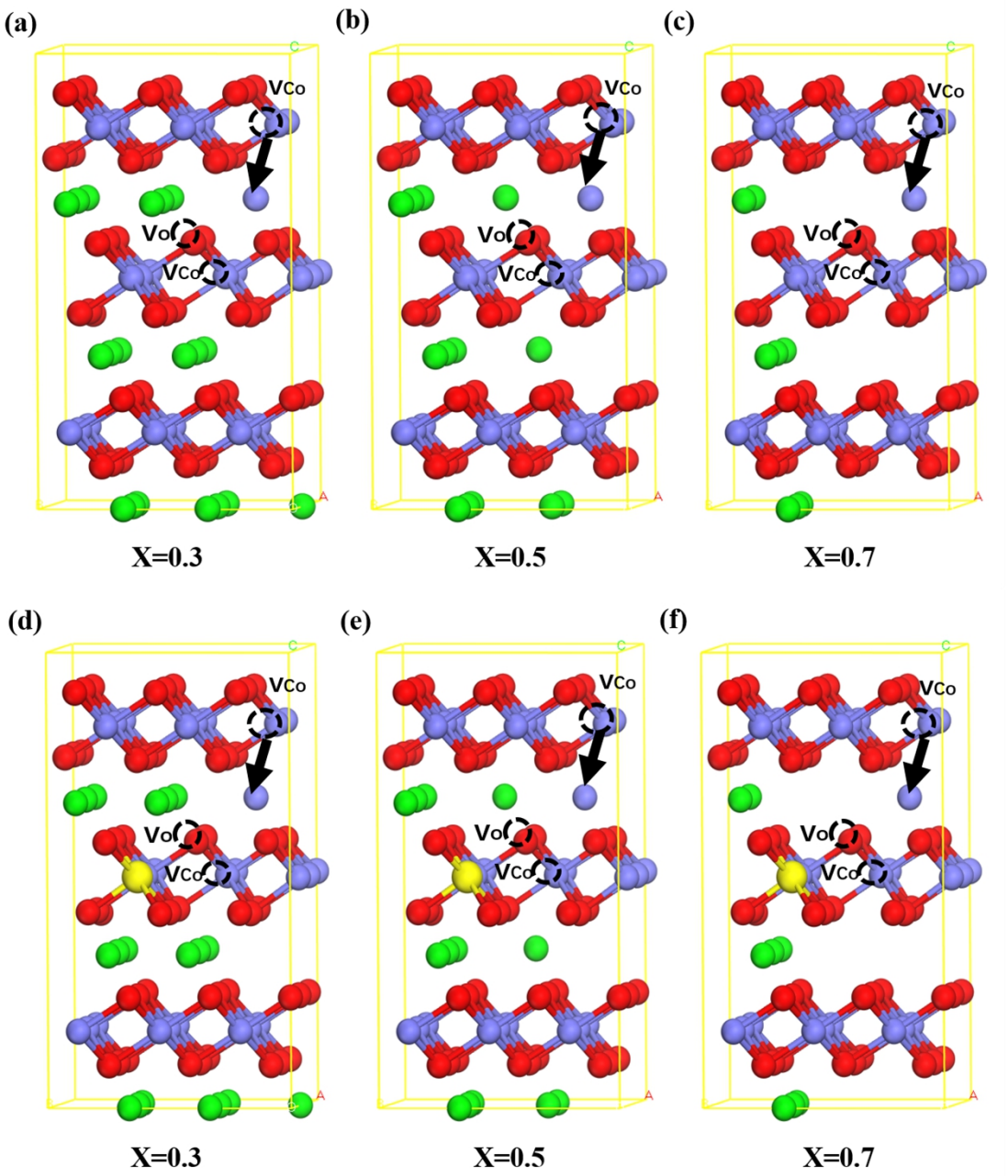

Fig. S4. The structures of vLCO containing cationic disorder with the degrees of delithiation at 30% (a), 50% (b), and 70% (c), along with the structures of vSLCO containing cationic disorder with the degrees of delithiation at at 30% (d), 50% (e) and 70% (f), respectively.

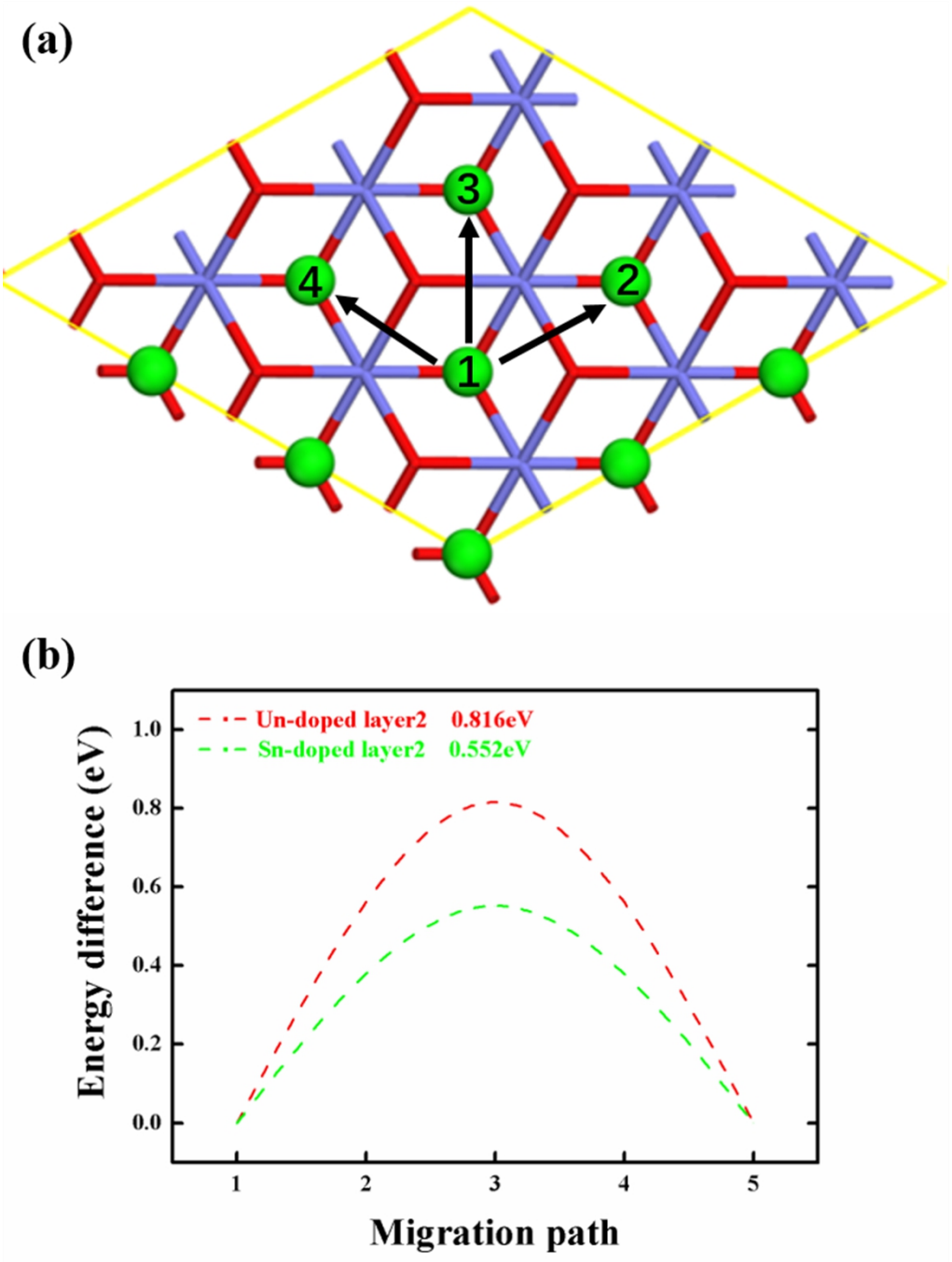

Fig. S5 (a) Three paths for Li migrating within the Li layer that is not adjacent to the Co-O layer containing the Co-O vacancies. (b) Energy profile of the Li ion migration which is the average energy profile across the three paths shown in Fig. S5 (a).