Electronic Supplementary Information for: Morphology and surface properties of $LiVOPO_4$: A first principles study

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Table S1. Relaxed parameters and calculated results for surface structures in all orientations.

Orientation	Slab (Å)	Relaxation Layer (Å)	Low-energy Termination	Surface Energy (J/m^2)	High-energy Termination	Surface Energy (J/m^2)
(1 0 0)	22.9	7.7	(0, 0, 0)	0.98	(0.25, 0, 0)	1.45
(0 1 0)	19.2	6.4	(0, 0, 0) and /or (0, 0.25, 0)	0.86	——	——
(0 0 1)	22.1	7.4	(0, 0, 0.25)	0.61	(0, 0, 0)	1.26
(0 1 1)	16.4	5.8	(0, 0.5, 0)	0.85	(0, 0, 0)	
(1 0 1)	15.7 Å	5.2	(0.5, 0, 0)	1.40	(0, 0, 0)	1.76
(1 1 0)	15.1	4.8	(0.5, 0, 0)	1.08	(0, 0, 0)	1.33
(1 1 1)	16.7	6.1	(0.5, 0, 0)	0.62	(0, 0, 0)	0.91
(2 0 1)	17.2	6.5	(0, 0, 0)	0.97	(0.5, 0, 0)	1.13

Table S2. Relaxed surface structures for the low energy terminations in all orientations Li atoms, V atoms, P atoms and O atoms are shown as pink, blue, green and red, respectively.

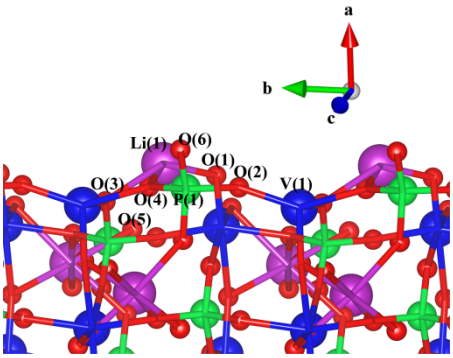
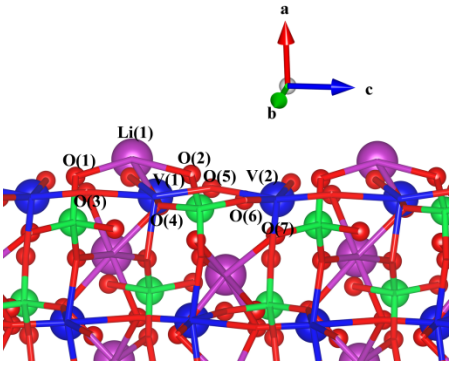
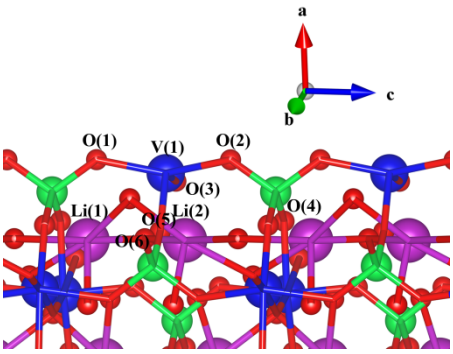
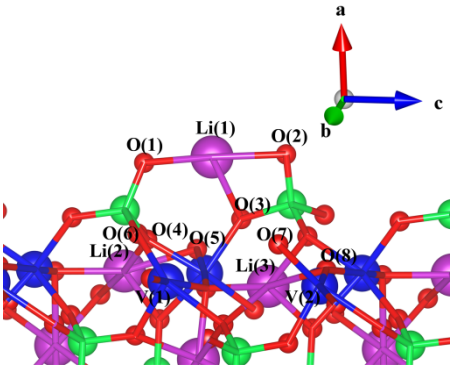
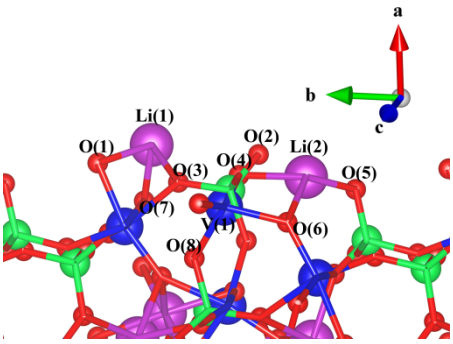
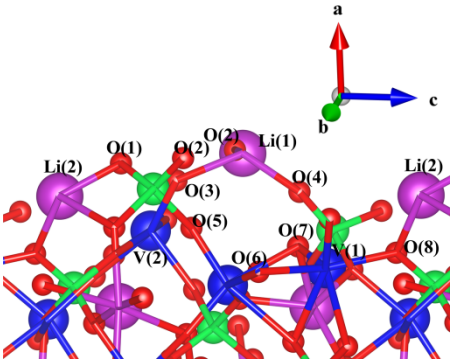
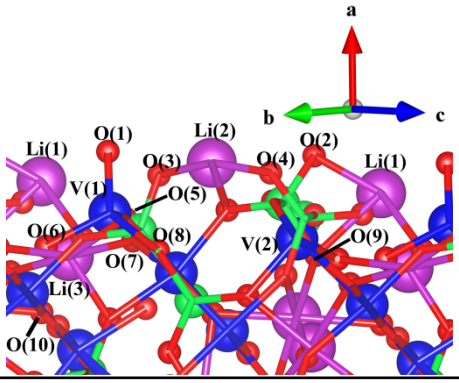
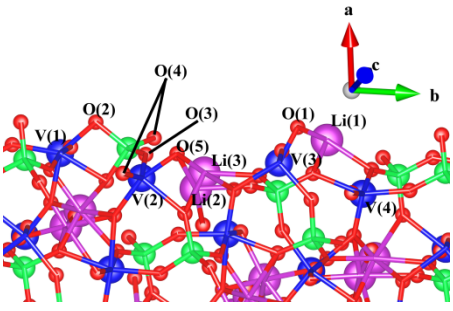
Surface	Surface Structure	Surface	Surface Structure
(1 0 0)		(0 1 0)	
(0 0 1)		(0 1 1)	
(1 0 1)		(1 1 0)	
(1 1 1)		(2 0 1)	

Table S3. Relaxations (displacements Δa, Δb, and Δc are in Å) of undercoordinated Li, V, P, and O atoms on the nine surfaces.

Surface	Label	Coord.[a]	Δa	Δb	Δc	Surface	Label	Coord.	Δa	Δb	Δc
(1 0 0)	Li(1)	3-3	-0.34	-0.25	0.08		O(7)	2-2	0.26	0.07	-0.02
	V(1)	4-4	-0.12	0.19	-0.18		O(8)	3-3	0.27	0.11	0.00
	P(1)	4-4	0.24	0.12	0.17	(1 0 1)	Li(1)	3-3	-0.22	0.11	0.19
	O(1)	2-2	0.24	0.12	0.17		Li(2)	3-3	-0.48	0.02	-0.38
	O(2)	2-2	0.20	-0.03	0.21		V(1)	4-4	-0.35	-0.41	0.04
	O(3)	3-3	0.03	-0.12	-0.02		O(1)	2-2	-0.09	-0.18	0.19
	O(4)	3-3	0.18	0.17	0.13		O(2)	2-2	0.19	0.16	-0.06
	O(5)	4-4	0.00	0.21	0.20		O(3)	3-3	0.07	0.02	-0.01
	O(6)	1-1	0.20	0.12	0.12		O(4)	3-3	0.15	0.04	0.01
(0 1 0)	Li(1)	3-3	0.12	1.20	0.66		O(5)	2-2	-0.06	-0.01	-0.04
	V(1)	5-5	-0.15	-0.06	-0.10		O(6)	3-3	-0.06	-0.05	-0.25
	V(2)	5-5	-0.10	-0.03	-0.09		O(7)	3-3	-0.02	-0.04	0.01
	P(1)	4-4	0.09	-0.02	-0.10		O(8)	2-2	-0.07	0.04	-0.11
	P(2)	4-4	0.13	-0.08	-0.10	(1 1 0)	Li(1)	5-3	1.59	-2.02	-0.47
	O(1)	2-2	0.09	0.07	-0.05		Li(2)	4-3	0.59	-1.01	0.36
	O(2)	1-2	0.13	-0.19	-0.27		V(1)	3-6	-1.75	0.84	-0.30
	O(3)	4-3	0.05	-0.27	-0.08		V(2)	5-5	-0.06	-0.02	0.00
	O(4)	4-4	0.01	-0.11	-0.10		O(1)	1-2	-0.07	0.12	-0.44
	O(5)	3-3	-0.12	-0.06	-0.07		O(2)	1-2	0.19	-0.02	-0.23
	O(6)	2-2	0.22	-0.11	-0.08		O(3)	2-2	0.15	-0.11	-0.40
	O(7)	3-3	-0.03	0.02	-0.06		O(4)	2-2	0.21	-0.01	0.13
(0 0 1)	Li(1)	5-5	-0.08	-0.08	0.21		O(5)	3-2	0.07	0.11	-0.15
	Li(2)	5-5	-0.08	-0.07	-0.20		O(6)	2-3	0.03	0.00	0.25
	V(1)	4-4	-0.14	-0.01	0.00		O(7)	4-3	-0.07	0.15	-0.09
	O(1)	2-2	0.04	0.04	0.05		O(8)	3-3	-0.06	-0.05	0.00
	O(2)	2-2	0.03	0.04	-0.05	(1 1 1)	Li(1)	6-3	1.18	0.84	0.44
	O(3)	3-3	0.08	0.02	0.08		Li(2)	3-3	-0.17	-2.16	-0.60
	O(4)	4-4	0.08	0.01	0.00		Li(3)	5-5	-0.23	-0.01	0.05
	O(5)	2-2	-0.01	0.06	-0.01		V(1)	4-4	-0.32	-0.01	0.09
	O(6)	3-3	-0.12	0.05	0.00		V(2)	4-4	-0.28	-0.17	-0.15
(0 1 1)	Li(1)	3-3	0.98	1.57	0.76		O(1)	2-1	0.73	-2.01	-1.30
	Li(2)	5-5	-0.16	0.15	-0.05		O(2)	1-2	-0.10	-0.06	0.33
	Li(3)	5-5	-0.16	-0.18	-0.02		O(3)	1-2	0.11	0.29	0.24
	V(1)	5-5	-0.03	-0.06	-0.21		O(4)	1-2	0.29	-0.13	-0.05
	V(2)	5-5	0.06	0.13	-0.25		O(5)	4-3	0.20	-0.21	-0.10
	O(1)	1-2	-0.06	-0.38	0.53		O(6)	3-2	0.14	0.01	-0.01
	O(2)	1-2	0.10	0.28	-0.33		O(7)	4-3	-0.20	0.10	-0.10
	O(3)	3-3	0.01	0.02	-0.11		O(8)	3-2	0.09	-0.11	0.10
	O(4)	4-3	-0.28	0.01	-0.15		O(9)	4-4	-0.08	0.16	0.00
	O(5)	4-3	-0.18	-0.05	0.02		O(10)	3-3	-0.16	0.16	0.08
	O(6)	2-2	0.15	-0.03	0.08	(2 0 1)	Li(1)	3-3	-0.40	-0.28	0.33

Surface	Label	Coord.	Δa	Δb	Δc	Surface	Label	Coord.	Δa	Δb	Δc
(2 0 1)	Li(2)	5-4	-0.12	0.13	0.39		O(1)	2-2	-0.06	-0.26	-0.30
	Li(3)	5-4	-0.07	-0.05	-0.18		O(2)	1-2	-0.52	-1.70	-0.07
	V(1)	5-6	-0.25	0.04	-0.02		O(3)	3-2	0.49	-0.55	0.01
	V(2)	5-5	0.14	0.00	-0.01		O(4)	3-2	0.59	-0.69	0.06
	V(3)	5-5	-0.18	-0.01	0.01		O(5)	3-3	-0.25	-0.40	0.06
	V(4)	5-5	-0.02	0.03	-0.03						

[a] Coordination of atoms in unrelaxed surface structures - Coordination of atoms in relaxed surface structures

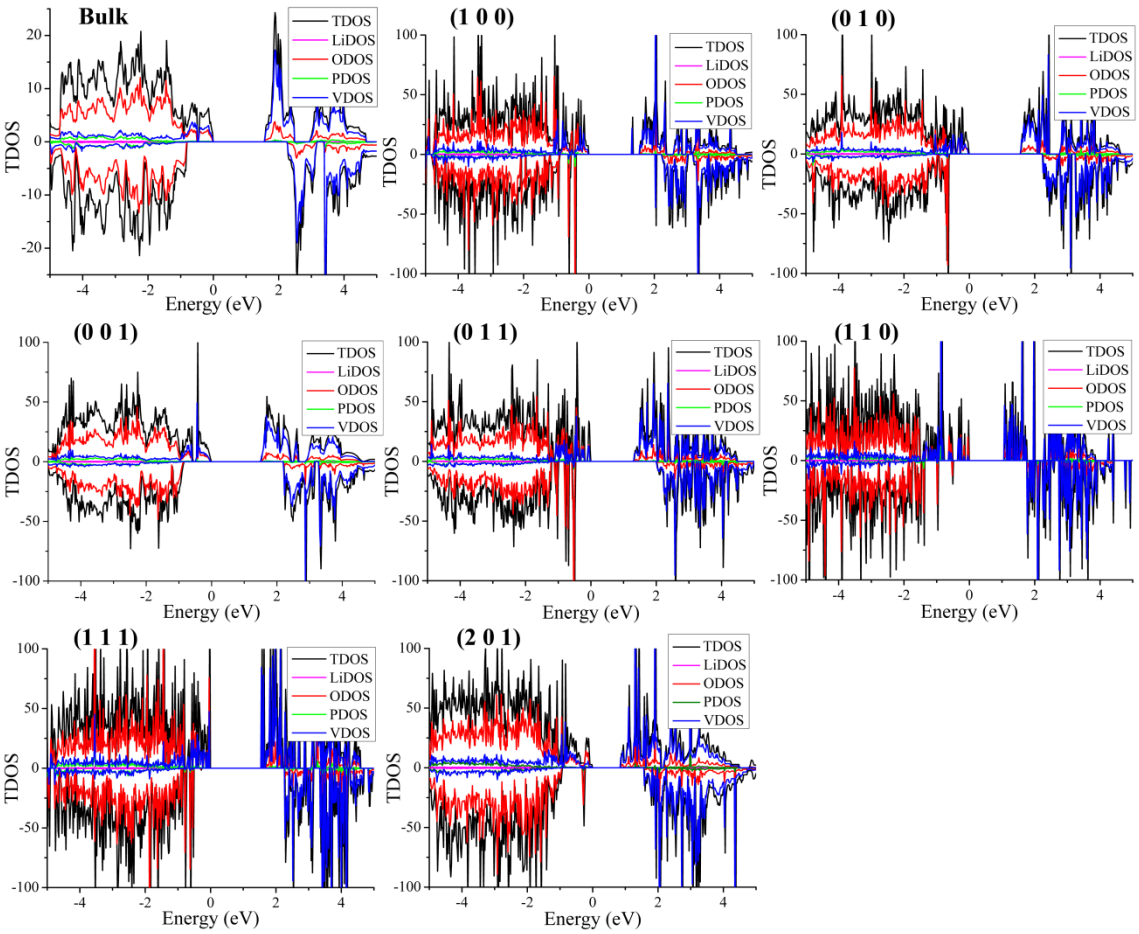


Fig. S1 Local density of states for surface and bulk structures of $LiVOPO_4$. The total density of states is illustrated by a black line, Li with pink, O with red, P with green and V with blue.