

Electronic supplementary information for

Theoretical perspectives on the structure, electronic, and optical properties of titanosilicates $\text{Li}_2\text{M}_4[(\text{TiO})\text{Si}_4\text{O}_{12}]$ ($\text{M} = \text{K}^+, \text{Rb}^+$)

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Figure S1 Band gap values predicted for $\text{Li}_2\text{K}_4[(\text{TiO})\text{Si}_4\text{O}_{12}]$ through variation of the parameter U.

Table S1 Selected bond lengths (Si-O, and Ti-O), angles (O-Si-O, and O-Ti-O), and lattice constants of titanosilicates compared with available experimental values.

Table S2 Comparisons of the calculated band gaps using different methods with the experimental values (eV).

Figure S1 Band gap values predicted for $\text{Li}_2\text{K}_4[(\text{TiO})\text{Si}_4\text{O}_{12}]$ through variation of the parameter U . The dashed black lines indicate the point at which the U tuning theoretically agrees well with the experimental band gap 4.11 eV.

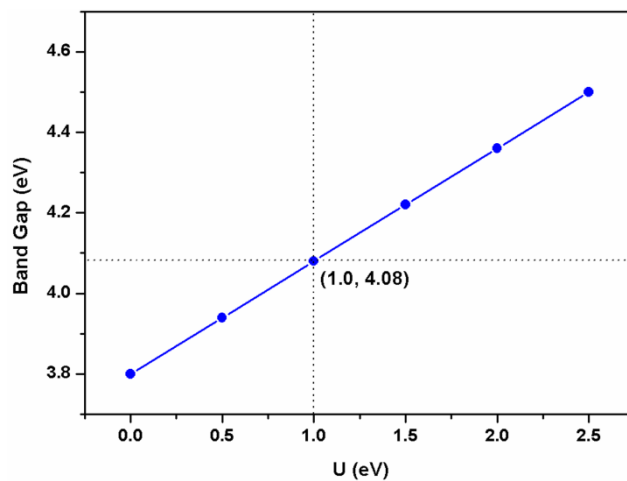


Table S1 Selected bond lengths (Si-O, and Ti-O), angles (O-Si-O, and O-Ti-O), and lattice constants of titanosilicates obtained with PBE functional compared with available experimental values.

		Li ₂ K ₄ [(TiO)Si ₄ O ₁₂]		Li ₂ Rb ₄ [(TiO)Si ₄ O ₁₂]	
		exp. ¹	cal.	exp. ¹	cal.
<i>a</i>	(Å)	11.33	11.48	11.50	11.65
<i>c</i>	(Å)	5.00	5.08	5.14	5.20
Si-O (SiO ₄ , Å)	Si-O1	1.59	1.61	1.60	1.61
	Si-O2	1.60	1.62	1.61	1.63
	Si-O3	1.65	1.68	1.65	1.68
	Si-O4	1.66	1.69	1.67	1.68
Ti-O (TiO ₅ , Å)	Ti-O1	1.98	2.00	1.97	2.00
	Ti-O5	1.68	1.71	1.67	1.71
O-Si-O (SiO ₄ , °)	O1-Si-O2	115.26	115.21	115.59	115.71
	O1-Si-O3	111.02	111.40	111.14	111.28
	O1-Si-O4	110.66	111.07	110.73	111.19
	O2-Si-O3	108.30	108.03	108.01	107.80
	O2-Si-O4	107.32	106.93	107.08	106.70
O-Ti-O (TiO ₅ , °)	O3-Si-O4	103.56	103.45	103.50	103.33
	O1-Ti-O2	86.72	86.66	87.10	87.16
	O1-Ti-O5	103.84	103.96	103.00	102.85

Table S2 Comparisons of the calculated band gaps using different methods with the experimental values (eV).

	$\text{Li}_2\text{K}_4[(\text{TiO})\text{Si}_4\text{O}_{12}]$	$\text{Li}_2\text{Rb}_4[(\text{TiO})\text{Si}_4\text{O}_{12}]$
Exp. ¹	4.11	4.13
PBE	3.80	3.68
HSE03	5.49	/
HSE06	5.67	/
PBE+U (U=1eV)	4.08	4.10

1 T. L. Chao, W. J. Chang, S. H. Wen, Y. Q. Lin, B. C. Chang and K. H. Lii, *J. Am. Chem. Soc.*, 2016, **138**, 9061-9064.