Electronic supplementary information for

A promising lead-free fluoride carbonates SHG material designed in a theoretical perspective

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Table S1 The comparison between experimental lattice parameters (Å), volume (Å^3), and band gap (eV) for $CsPbCO_3F$ and those calculated values using various exchange and correlation functions. Percentage changes from experiments are given in units of % in parentheses. And the band gap calculated with nonlocal potentials PBE0 is 5.04 eV based on the PBE optimized structure of $CsPbCO_3F$.

	a	*c*	Volume	Band gap
LDA	5.312(-1.5)	4.874(-4.7)	119.11(-7.6)	3.252
PBE	5.509 (2.1)	5.049 (-1.3)	132.71 (2.9)	3.54
RPBE	5.609 (4.0)	5.150 (0.7)	140.29 (8.9)	3.42
PBESOL	5.411 (0.3)	4.961 (-3.1)	125.83 (-2.4)	3.35
Exp.	5.393[1]	5.116[1]	128.861[1]	4.15[2]

[1] Ref.1 [2] Ref.2

Figure S1 Optimized ball-and-stick model of $RbSnCO_3F$ from different perspectives: in the *ab*-plane (a) and *bc*-plane (b).

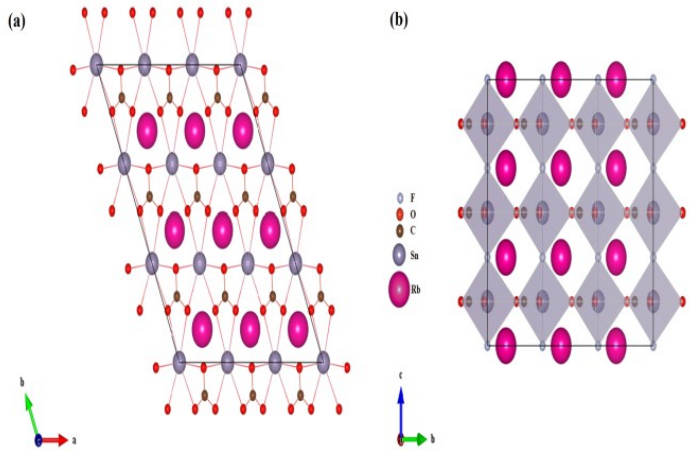


Figure S2 Calculated band structure of $RbPbCO_3F$, $CsPbCO_3F$, and $RbSnCO_3F$. The dispersion curves are shown along the directions G→A→H→K→G→M→L→H, where G = (0, 0, 0), A = (0, 0, 1/2), H = (-1/3, 2/3, 1/2), K = (-1/3, 2/3, 0), M = (0, 1/2, 0) and L = (0, 1/2, 1/2). The dashed line is the Fermi level.

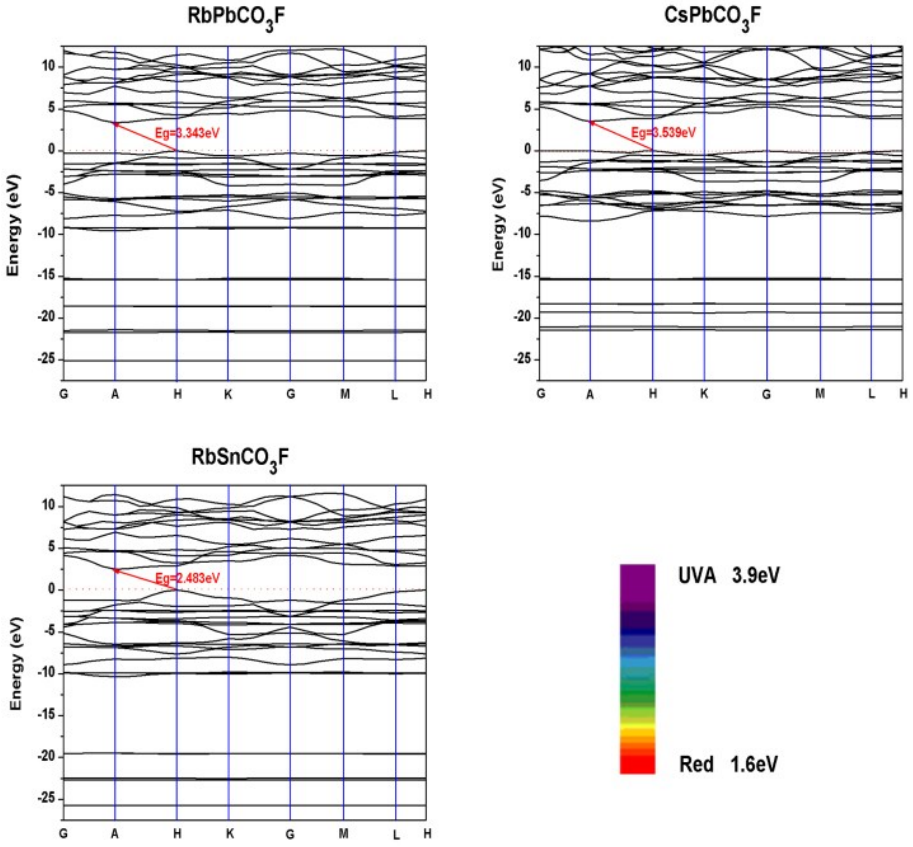


Figure S3 Calculated Loss Function of $CsPbCO_3F$, $RbPbCO_3F$, and $RbSnCO_3F$. Dark yellow and blue represent the [100] and [001] direction of $CsPbCO_3F$. Pink and wine represent the [100] and [001] direction of $RbPbCO_3F$. Besides, Cyan and green represent the [100] and [001] direction of $RbSnCO_3F$.

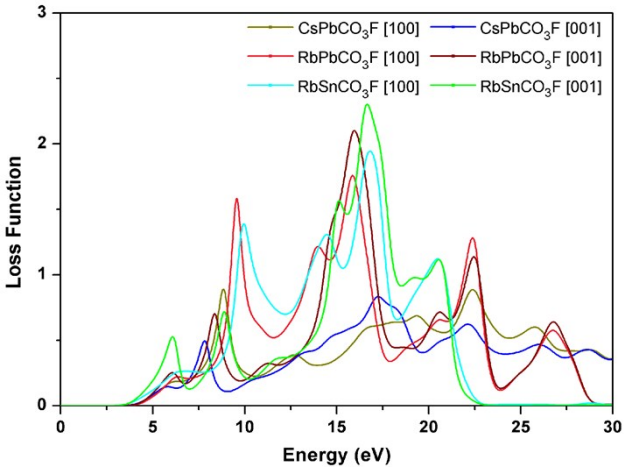


Figure S4 Calculated conductivities of $CsPbCO_3F$ (a), $RbPbCO_3F$ (b), and $RbSnCO_3F$ (c).

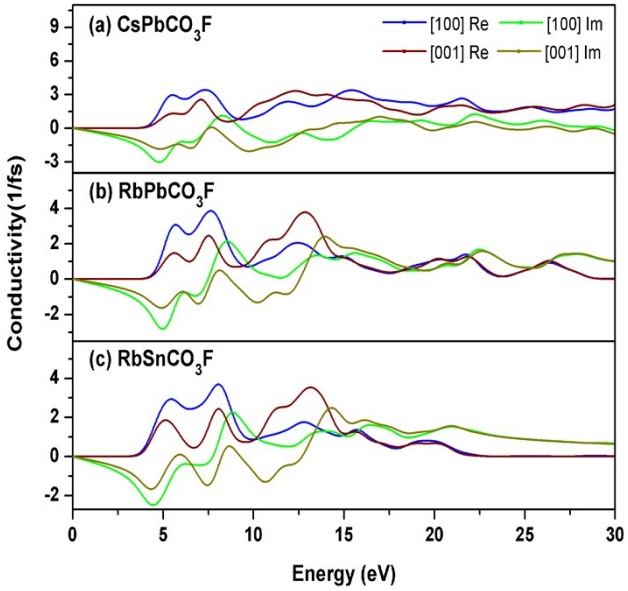
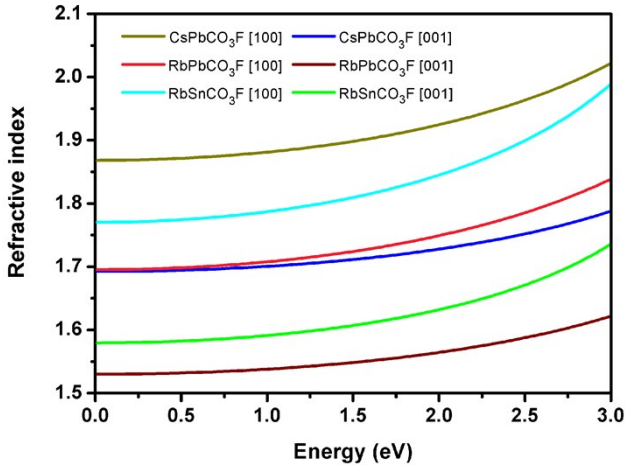


Figure S5 Dispersion curves of refractive index of $RbSnCO_3F$.



Reference

1 T. T. Tran, P. S. Halasyamani and J. M. Rondinelli, *Inorg. Chem.*, 2014, **53**, 6241-6251.

2 G. Zou, L. Huang, N. Ye, C. Lin, W. Cheng and H. Huang, *J. Am. Chem. Soc.*, 2013, **135**, 18560-18566.