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 (Å³), and band gap (eV) for CsPbCO₃F 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 CsPbCO₃F.

<table>
<thead>
<tr>
<th></th>
<th>$a$</th>
<th>$c$</th>
<th>Volume</th>
<th>Band gap</th>
</tr>
</thead>
<tbody>
<tr>
<td>LDA</td>
<td>5.312 (−1.5)</td>
<td>4.874 (−4.7)</td>
<td>119.11 (−7.6)</td>
<td>3.252</td>
</tr>
<tr>
<td>PBE</td>
<td>5.509 (2.1)</td>
<td>5.049 (−1.3)</td>
<td>132.71 (2.9)</td>
<td>3.54</td>
</tr>
<tr>
<td>RPBE</td>
<td>5.609 (4.0)</td>
<td>5.150 (0.7)</td>
<td>140.29 (8.9)</td>
<td>3.42</td>
</tr>
<tr>
<td>PBESOL</td>
<td>5.411 (0.3)</td>
<td>4.961 (−3.1)</td>
<td>125.83 (−2.4)</td>
<td>3.35</td>
</tr>
<tr>
<td>Exp.</td>
<td>5.393¹</td>
<td>5.116¹</td>
<td>128.861¹</td>
<td>4.15²</td>
</tr>
</tbody>
</table>

¹ Ref.1  ² Ref.2
**Figure S1** Optimized ball-and-stick model of RbSnCO$_3$F from different perspectives: in the *ab*-plane (a) and *bc*-plane (b).
**Figure S2** Calculated band structure of RbPbCO$_3$F, CsPbCO$_3$F, and RbSnCO$_3$F. The dispersion curves are shown along the directions $G \rightarrow A \rightarrow H \rightarrow K \rightarrow G \rightarrow M \rightarrow L \rightarrow H$, 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$_3$F, RbPbCO$_3$F, and RbSnCO$_3$F. Dark yellow and blue represent the [100] and [001] direction of CsPbCO$_3$F. Pink and wine represent the [100] and [001] direction of RbPbCO$_3$F. Besides, Cyan and green represent the [100] and [001] direction of RbSnCO$_3$F.
**Figure S4** Calculated conductivities of CsPbCO$_3$F (a), RbPbCO$_3$F (b), and RbSnCO$_3$F (c).

**Figure S5** Dispersion curves of refractive index of RbSnCO$_3$F.
Reference
