For the oxides, we include the single-metal bulk and the most stable single-metal oxides and compare them with the DFT energy of the combination in the perovskite structure. We consider a compound non-stable when the ABO$_3$ energy is 0.2 eV/atom greater than the best outcome from the LP:

$$\Delta E = ABO_3(s) + \min_{c_i}(c_1A(s) + c_2B(s)) + c_3A_xO_y(s) + c_4B_xO_y(s) + c_5O),$$

(1)

where A and B are the bulk metals, A$_x$O$_y$ and B$_x$O$_y$ are the single metal oxides included in the references and O is simply obtained from H$_2$O $\rightarrow$ H$_2$. The problem is solved with the constraints:

$$c_1 + c_3 = 1,$$
$$c_2 + c_4 = 1,$$
$$c_3 + c_4 + c_5 = 3,$$

(2)

for the A, B metals and oxygen, respectively, to obtain the perovskite stoichiometry. A similar analysis has been performed for the oxynitrides with the most stable single- and bi-metal nitrides and single-metal oxynitrides in the pool of reference system and with the constraints that the sum of the oxygen and nitrogen atoms must be equal to 2 and 1, respectively.

**Bandgaps of Single-Metal Oxides**

In Table 1 we report the comparison between the theoretical gaps evaluated using the GLLB-SC functional with the experimental values in the most stable single-metal oxide structure obtained from the ICSD database. Those values have been used for Fig. 1 in the manuscript. For each structure, we use the same procedure used for the screening: i.e. starting from the experimental data, we find the lattice parameters and we completely relax the internal degrees of freedom using an RPBE functional and afterward we evaluate the gaps using the GLLB-SC functional.

**Cubic Perovskite Oxides**

Table 2 reports the combinations that fulfill the conditions for stability and for the gap. We specify the heat of formation and the indirect (direct) bandgap. The heat of formation
is obtained using the linear programming approach with the single-metal bulks, the single- and bi-metal oxides as pool of references. We report also if the band edges match with the water redox potential and the experimental bandgap for the combinations showing a perovskite or a perovskite-like experimental structure.

† Fig 1 reports the band edge positions, evaluated using the empirical rule provided by Butler and Ginley, and using the DFT gaps calculated here, for all the combinations of Table 2. Three combinations do not match with the H⁺/H₂ po-

Table 2 Cubic Perovskite Oxides: Formation energies (ΔE) per atom and indirect (direct) bandgap for the candidates for a new solar light capture material. It is also indicated (√) if the band edges match with the water redox potential. The experimental bandgaps for the two known cubic perovskite materials, AgNbO₃ and BaSnO₃, are equal to 2.8 eV²⁹ and 3.1 eV³⁰, respectively. SrSnO₃ and CaSnO₃ suffer from a lattice distortion and they show an orthorhombic perovskite with a DFT (experimental) bandgaps equal to 4.2 (4.1) eV³⁰ and 3.8 (4.4) eV³⁰, respectively.

Table 1 bandgaps: theoretical and experimental bandgap evaluated for the metal oxides included in Fig. 1 of the manuscript. The type of the experimental gap is reported, when available, in the method column.
Table 3 Cubic perovskite oxynitrides: Formation energies (ΔE) per atom and indirect (direct) bandgap for the candidates for a new solar light capture material. It is also indicated (✓) if the position of the band edges matches with the water redox potential and the experimental bandgap for the cubic perovskites known structures.

<table>
<thead>
<tr>
<th>Oxynitride</th>
<th>ΔE [eV/atom]</th>
<th>DFT Gap [eV]</th>
<th>Band Edges</th>
<th>Experimental Gap [eV]</th>
</tr>
</thead>
<tbody>
<tr>
<td>BaTaO$_2$N</td>
<td>−0.01</td>
<td>2.0</td>
<td>✓</td>
<td>2.0$^{32}$</td>
</tr>
<tr>
<td>SrTaO$_2$N</td>
<td>0.00</td>
<td>2.1</td>
<td>✓</td>
<td>2.1$^{32}$</td>
</tr>
<tr>
<td>CaTaO$_2$N</td>
<td>0.09</td>
<td>2.2</td>
<td>✓</td>
<td>2.5$^{32}$</td>
</tr>
<tr>
<td>MgTaO$_2$N</td>
<td>0.19</td>
<td>2.1 (2.8)</td>
<td>✓</td>
<td>2.5$^{33}$</td>
</tr>
<tr>
<td>PbTaO$_2$N</td>
<td>0.19</td>
<td>1.9 (2.1)</td>
<td>✓</td>
<td>2.1$^{33}$</td>
</tr>
<tr>
<td>LaTiO$_2$N</td>
<td>0.05</td>
<td>2.5</td>
<td>✓</td>
<td>2.1$^{33}$</td>
</tr>
</tbody>
</table>

Fig. 2 Band edge position evaluated for the oxynitride combinations of † Table 3.

Cubic Perovskite Oxynitrides

As in † Table 2 for the oxides, in † Table 3 we list the combinations that come out after the screening on the stability and on the bandgap. In addition we report if the position of band edges matches with the water redox potential. The experimental values for the gaps are in a good agreement with the DFT values.

† Fig 2 shows the bands position of all the combinations of † Table 3.

References