Supporting Materials

Enhancement of Visible Light Photocatalytic Activity of SrTiO\textsubscript{3}: A Hybrid Density Functional Study

Brindaban Modak and Swapan K. Ghosh*

Theoretical Chemistry Section, Bhabha Atomic Research Centre
and Homi Bhabha National Institute, Mumbai – 400 085, India

Email: skghosh@barc.gov.in
Phone: 91-22-25595092
Fax: 91-22-25505151
**Figure S1:** Band structure plot for (a) undoped SrTiO$_3$, (b) V-doped SrTiO$_3$, (c) Nb-doped SrTiO$_3$, and (d) Ta-doped SrTiO$_3$.

**Figure S2:** Band structure plot for (a) N-doped SrTiO$_3$, (b) Na-doped SrTiO$_3$, (c) K-doped SrTiO$_3$, and (d) Rh-doped SrTiO$_3$. 
**Figure S3:** Band structure plot for (a) (V, N)-codoped SrTiO$_3$, (b) (Nb, N)-codoped SrTiO$_3$, and (c) (Ta, N)-codoped SrTiO$_3$.

**Figure S4:** Band structure plot for (a) (V, Na)-codoped SrTiO$_3$, (b) (Nb, Na)-codoped SrTiO$_3$, and (c) (Ta, Na)-codoped SrTiO$_3$. 
**Figure S5:** Band structure plot for (a) (V, K)-codoped SrTiO$_3$, (b) (Nb, K)-codoped SrTiO$_3$, and (c) (Ta, K)-codoped SrTiO$_3$.

**Figure S6:** Band structure plot for (a) (V, Rh)-codoped SrTiO$_3$, (b) (Nb, Rh)-codoped SrTiO$_3$, and (c) (Ta, Rh)-codoped SrTiO$_3$. 
Figure S7: Density of states of (a) (V, Rh)-codoped SrTiO$_3$, (b) (Nb, Rh)-codoped SrTiO$_3$, (c) (Ta, Rh)-codoped SrTiO$_3$ calculated using $2 \times 3 \times 3$ supercell. (a'), (b'), and (c') represent the same in the respective order calculated using $3 \times 3 \times 3$ supercell. Vertical dashed line indicates Fermi Level.
Table S1: Variation of calculated band gap for (V/Nb/Ta, Rh)-codoped SrTiO₃ with the dopant concentration

<table>
<thead>
<tr>
<th>Dopant Concentration</th>
<th>(V, Rh)-SrTiO₃ Band Gap (eV)</th>
<th>(Nb, Rh)-SrTiO₃ Band Gap (eV)</th>
<th>(Ta, Rh)-SrTiO₃ Band Gap (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>12.5%</td>
<td>1.66</td>
<td>2.40</td>
<td>2.53</td>
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<tr>
<td>8.33%</td>
<td>1.68</td>
<td>2.44</td>
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<td>5.55%</td>
<td>1.91</td>
<td>2.48</td>
<td>2.60</td>
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<td>3.7%</td>
<td>2.12</td>
<td>2.63</td>
<td>2.67</td>
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