SPMS08: Laptop-based First principles calculation of oxide electronic structure

Trinh Weng Yan Amber
Yao Xiaotong
Dunman High School

Expert mentor:
Wang Xiao, Renshaw
Order of presentation

◎ Aims
◎ Background information
◎ Methodology
◎ Results & Analysis
◎ Conclusion
1. Aims
Aims

◎ To calculate and compare the band gap of $SrTiO_3$ using First principles calculation

◎ To find out the effects of various structures on the band gap and electrical conductivity

◎ To explore the limitations of first principles calculations on laptops
2. Background Information
Background information on $SrTiO_3$

- Perovskite crystal structure
- Good insulating properties
- Chemical stability
Background information on $SrTiO_3$

- Computational value of the band gap = 1.7 eV
- Experimental value of band gap = 3.4 eV
Methodology
Methodology

Burai 3.1

- a GUI system for Quantum ESPRESSO
- Calculation of band gap, density of state, SCF
**Methodology**

- **Burai on Windows**
- **Burai on Virtual machine**
Methodology

Shared folders

Email
Methodology

Standard $SrTiO_3$ CIF file
**Methodology**

**Variable 1**  
Distance between atoms

**Variable 2**  
Lattice constant

**Variable 3**  
Lattice structure

**Variable 4**  
Size of structure

**Variable 5**  
Number of oxygen deficiency
4. Results & Analysis
Control

Band gap = 1.7 eV
## Control

<table>
<thead>
<tr>
<th>Methods</th>
<th>Band Gap / eV</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1.767</td>
</tr>
<tr>
<td>B1</td>
<td>1.7</td>
</tr>
<tr>
<td></td>
<td>3.25</td>
</tr>
</tbody>
</table>
Coordination of Sr Atom
# Lattice Constant

<table>
<thead>
<tr>
<th>Lattice constant</th>
<th>3.5</th>
<th>3.6</th>
<th>3.7</th>
<th>3.8</th>
<th>3.9</th>
<th>4.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>Band gap / eV</td>
<td>1.7</td>
<td>1.7</td>
<td>1.7</td>
<td>1.7</td>
<td>1.7</td>
<td>1.7</td>
</tr>
</tbody>
</table>

No change in band gap
Lattice Structure

Trigonal R structure

Density of states

Energy / eV

DOS / (states/eV)
Size of Lattice Structure

2 x 1 x 1

2 x 2 x 2
Number of Deficient Oxygen Atoms

No band gap
5. Conclusion
Conclusion

◎ Oxygen deficiency
➢ Conductivity

◎ Methodology

<table>
<thead>
<tr>
<th>Positive</th>
<th>Negative</th>
</tr>
</thead>
<tbody>
<tr>
<td>First principles calculation</td>
<td>Long calculation time for multiple cells</td>
</tr>
<tr>
<td>Stable structure</td>
<td>Error in running lattice structures</td>
</tr>
<tr>
<td>Accuracy and consistency</td>
<td></td>
</tr>
</tbody>
</table>
Thank you!