Theoretical study of the electronic structure of $\text{Sn}_4\text{Ge}$ using first-principles

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Background

- The first-principle calculations are a powerful tool to predict the electronic properties of solids.
- It was recently predicted\(^1\) that the tetragonal structure of $\text{Ge}_5$ and $\text{Sn}_5$, as topological semi-metal and topological insulators, respectively, using first-principles calculations.
- As $\text{Ge}$ and $\text{Sn}$ both have the same valency, it is likely to have similar (topological) properties in the tetragonal allotropes of compounds made up of $\text{Ge}$ and $\text{Sn}$. Subsequently, we studied the electronic properties of the new $\text{Sn}_4\text{Ge}$.

AIM

- The main aim of this work is to study the electronic properties of $\text{Sn}_4\text{Ge}$.
- The stability of the system is confirmed by calculating the formation energy of $\text{Sn}_4\text{Ge}$.
- Spin-orbit interaction (SOI) plays a significant role in heavy elements. Therefore we also consider SOI while performing the electronic structure calculations.

Methodology

- Geometry optimization and self-consistent calculations are performed using density functional theory as implemented in Quantum Espresso\(^2\).
- The Projector Augmented Wave (PAW) pseudopotential: Scalar relativistic (without SOI) and fully relativistic (with SOI) with PBE exchange-correlation functional.
- We used 80 Rydberg kinetic energy cut off with Monkhorst Pack $k$-point mesh of $18 \times 18 \times 18$.

Results & discussion

Optimized Structure

- Tetragonal crystal structure with space group $P\overline{4}M2$ (No. 115).
- Primitive unit cell contains four $\text{Sn}$ atoms and one $\text{Ge}$ atom with Wyckoff positions $4j$ (0.0000, 0.2731, 0.3190) and $1a$ (0.0, 0.0, 0.0), respectively.
- Formation energy of $\text{Sn}_4\text{Ge}$ is calculated to be $-4.17$ eV.

Electronic Properties

- Band structure of $\text{Sn}_4\text{Ge}$ with and without spin-orbit interaction (SOI).
- $\text{Sn}_4\text{Ge}$ is metallic, and significant band splitting due to SOI is observed along $M-\Gamma$ path.

TABLE 1. Bond lengths and lattice parameters comparison in the unit of Å

<table>
<thead>
<tr>
<th>Structure</th>
<th>a</th>
<th>c</th>
<th>$d_1$</th>
<th>$d_2$</th>
<th>$d_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\text{Ge}_5$</td>
<td>5.63</td>
<td>5.23</td>
<td>2.53</td>
<td>2.50</td>
<td>2.54</td>
</tr>
<tr>
<td>$\text{Sn}_5$</td>
<td>6.49</td>
<td>5.99</td>
<td>2.91</td>
<td>2.89</td>
<td>2.93</td>
</tr>
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<td>$\text{Sn}_4\text{Ge}$</td>
<td>6.42</td>
<td>5.63</td>
<td>2.51</td>
<td>2.92</td>
<td>3.21</td>
</tr>
</tbody>
</table>

- $\text{Ge}_5$ and $\text{Sn}_5$ data taken from Ref. 1

Summary

- The ground state of newly predicted $\text{Sn}_4\text{Ge}$ was found to be metallic and non-magnetic in nature.
- The inclusion of spin-orbit interaction leads to a significant band-splitting along $M-\Gamma$.
- The Fermi surface plot of one of the bands shows the typical Dirac cone with a gap at the $\Gamma$ point.

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References