Tunable spin Hall and spin Nernst effects in Dirac nodal line semimetals XCuYAs (X=Zr, Hf; Y=Si, Ge)

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Introduction

Recent theoretical studies have shown that 27 – 30 % of all non-magnetic crystalline materials in Inorganic Crystal Structure Database (ICSD) are topological, with roughly 12% insulators and 15-18 % semimetals\textsuperscript{1}. The studied XCuYAs (X=Zr, Hf; Y= Si, Ge) compounds belong to the vast family of the 1111-like quaternary phases, which exhibit unique physical properties ranging from p-type transparent semiconductors to Fe-based superconductors. XCuYAs compounds have the same tetragonal symmetry (space group P4mm) as ZrSiS family. Only a few studies on these XCuYAs compounds have been carried out so far, focused mainly on the structural, elastic, electronic properties as well as chemical bonding and stability of these compounds\textsuperscript{2,3}. However, SHE & SNE have not been studied yet in these compounds. So, in this work, we have studied thoroughly the electronic structure, SHE and SNE in these compounds by performing ab-initio DFT calculations. Our main findings are summarized below.

Computational Details

- VASP
- GGA-PBE
- SHC & SNC are calculated within the elegant Berry-phase formalism\textsuperscript{4}

\[ \sigma_{ij} = \frac{1}{n} \sum \frac{d k}{d \Omega_{ij}} = \frac{1}{n} \sum \frac{d k}{d (2\pi)} \mathbf{O}_{ij}(k) \]

\[ \alpha_{ij}^\alpha = \frac{1}{n} \sum \frac{d k}{d (2\pi)} \mathbf{O}_{ij}(k) \]

\[ \sum_{\alpha} \left( \left\langle \epsilon_{\alpha} - \mu \right\rangle f_{\alpha} k_B T \ln \left( 1 + e^{-\beta (\epsilon_{\alpha} - \mu)} \right) \right) \]

Results and Summary

- FIG. 1. (a) Crystal structure of the XCuYAs family, (b) illustration of its nonsymmetric glide mirror symmetry, and (c) the corresponding tetragonal Brillouin zone (BZ)
- FIG. 2. Relativistic band structures
- FIG. 3. Total and atom-decomposed density of states (DOS)
- FIG. 4. HiCuGeAs

Summary

- Dirac semimetals with non-symmetric symmetry protected Dirac line nodes along A-M & X-R.
- \textsc{SHC}$_{\text{HiCuGeAs}} = -0.514 \text{ (h/e)}$ (S/cm)
- \textsc{SNC}$_{\text{HiCuGeAs}} = -0.73 \text{ (h/e)}$ (A/m K)
- Tunability in the SHC & SNC values.
- Originate largely from the presence of a large number of spin-orbit coupling-gapped DPs near $E_F$ as well as the gapless DNLs, which give rise to large spin Berry curvatures.
- Promising applications in spintronics and spin caloritronics.

References

\textsuperscript{3}A. M. Baergen et. al, Quaternary germanide arsenides ZrCuGeAs and HfCuGeAs, Z. Anorg. Allg. Chem. 637, 2007 (2011).
\textsuperscript{5} D. Xiao et. al, Berry phase effects on electronic properties, Rev. Mod. Phys. 82, 1959 (2010).

TABLE I. Experimental lattice constants (a, c), calculated density of states at the Fermi level [N(EF)] (states/eVf.u.), spin Hall conductivity (\(\sigma_{xy}\), \(\sigma_{xz}\), and \(\sigma_{yz}\)) and spin Nernst conductivity (\(\sigma_{xy}^s\), \(\sigma_{xz}^s\), and \(\sigma_{yz}^s\)) at temperature T = 300 K. Note that the unit of the spin Hall conductivity (spin Nernst conductivity) is (h/e)(S/cm) [(h/e)(A/m K)]

<table>
<thead>
<tr>
<th>System</th>
<th>d/a</th>
<th>c/a</th>
<th>N(EF)</th>
<th>(\sigma_{xy})</th>
<th>(\sigma_{xz})</th>
<th>(\sigma_{yz})</th>
<th>(\sigma_{xy}^s)</th>
<th>(\sigma_{xz}^s)</th>
<th>(\sigma_{yz}^s)</th>
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<tr>
<td>ZrCuGeAs</td>
<td>3.8735</td>
<td>0.5712</td>
<td>0.67</td>
<td>-0.45</td>
<td>-0.100</td>
<td>-0.175</td>
<td>0.20</td>
<td>-0.17</td>
<td>-0.22</td>
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<tr>
<td>HfCuGeAs</td>
<td>3.7525</td>
<td>0.5040</td>
<td>0.65</td>
<td>-0.113</td>
<td>-0.112</td>
<td>-0.110</td>
<td>0.46</td>
<td>-0.14</td>
<td>-0.14</td>
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<tr>
<td>HfCuSiAs</td>
<td>3.8535</td>
<td>0.5530</td>
<td>0.65</td>
<td>-0.113</td>
<td>-0.112</td>
<td>-0.110</td>
<td>0.46</td>
<td>-0.14</td>
<td>-0.14</td>
</tr>
<tr>
<td>ZrCuSiAs</td>
<td>3.6036</td>
<td>0.5085</td>
<td>0.65</td>
<td>-0.113</td>
<td>-0.112</td>
<td>-0.110</td>
<td>0.46</td>
<td>-0.14</td>
<td>-0.14</td>
</tr>
</tbody>
</table>

FIG. 5. SNC as a function of temperature T

FIG. 6. Contour plot of (a) total and (b) Dirac line node only contributions to spin Berry curvature \(\Omega_{xy}^\alpha\) (k) of HiCuGeAs on the X-R-A-M plane (see Fig. 1(c))