Spin-orbitronic materials with record spin-charge conversion from high-throughput ab initio calculations

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Abstract

Today’s limitations of charge-based electronics in terms of power consumption motivates the field of spintronics 1. The spin Hall effect (SHE) 2 is an important spintronics phenomenon, which allows transforming a charge current into a spin current and vice versa 5 without the use of magnetic materials or magnetic fields. To gain new insight into the physics of the SHE and to identify materials with a substantial spin Hall conductivities (SHC), we performed high-precision, high-throughput ab initio electronic structure calculations of the intrinsic SHC for over 20,000 non-magnetic crystals. The calculations reveal a strong and unexpected relation of the magnitude of the SHC with the crystalline symmetry, which we show exists because large SHC is typically associated with mirror symmetry protected nodal lines in the band structure. From the new developed database, we identify new promising materials. This includes eleven materials with a SHC comparable or even larger than that the up to now record Pt as well as materials with different types of spin currents, which could allow for new types of spin-obitronics devices.

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Even if the extrinsic spin Hall effect (SHE) was predicted almost 50 years ago [2, 3], the SHE did not receive extensive attention until last decade, after theoretical studies of its intrinsic mechanism [8, 9] and its experimental observation [10–12]. The SHE causes an electrical current to generate a transverse spin current [2–4]. Vice versa, a spin current can also generate a transverse voltage drop by the inverse SHE [5–7]. Strong SHE materials being of central importance for the detection, generation and manipulation of spin currents suggests performing a large-scale screening to identify the most suitable materials for spintronics devices. Experimentally, however such a large-scale screening is very impractical, as quantitative determination of the spin Hall conductivity (SHC) by electrical measurement requires integrating each material separately into a complex multicomponent microscopic transport device [5–7]. Furthermore, different experiments often give very different results for the SHC since the spin current cannot be measured directly and other effects such as the inverse spin-galvanic effect complicate the interpretation of experiments. Theoretically and computationally the situation is in principle much more straight-forward. An additional advantage of high-throughput calculations is that they can reveal further insight into the physics of the SHE and suggest general guidelines for designing new SHE materials.

In general, the SHE has two origins: an extrinsic contribution from scattering and an intrinsic contribution from the electronic band structure. In this work we focus only on the intrinsic contribution for two reasons. First, the intrinsic contribution is typically the dominant one in systems with strong spin-orbit coupling [4]. Second, it can be accurately predicted theoretically as long as the electronic structure calculation is precise enough [4, 8, 9, 13, 14] whereas the extrinsic contributions are much harder to calculate and strongly depend on the type of scattering and other parameters such as temperature. In many cases, the calculated intrinsic SHE yields good qualitative agreement with experimental measurements [4, 15]. For example, the large intrinsic SHC of Pt [16–18] or the predicted sign change of SHC from Pt to Ta were experimentally observed [19, 20]. Therefore, this database can be helpful for selecting new spin-to-charge conversion materials even if it cannot be expected that the predicted values will be precisely reproduced in experiments. Apart from the SHC, there are other parameters that determine the usefulness of a material for spin-to-charge conversion. This is in particular the ratio of spin and charge conductivities, known as the spin Hall angle but also other parameters such as the spin diffusion length. We do not attempt to evaluate these parameters here, however we note that the charge
conductivity is straightforward to measure experimentally and thus the spin Hall angles can be easily obtained from our calculations for materials in which the conductivity is experimentally known.

To perform the high-throughput simulations, we developed the automatic Wannier function generating code, which enables us to do high-throughput calculations of the intrinsic SHE for over 20,000 different known non-magnetic materials with a workflow that is shown in Fig. 1. We first consider all lattice structures from the ICSD database \cite{21} and Materials Project \cite{22, 23}. Most of the studied materials are in the ICSD database (17,682 in total), which contains real, experimentally characterized materials. In addition we also consider computational materials (i.e., materials that have not been experimentally synthesized, but have been predicted to be stable by \textit{ab-initio} calculations) from the Materials Project \cite{22, 23} since they are extracted from alloys or similar structures on the basis of experimentally known materials and can thus be possibly synthesized. Considering the limited accuracy of the density functional theory (DFT) for the strongly correlated systems, we leave them out of consideration (see Fig. 1). In total we considered 17,682 real materials from the ICSD database and 2,486 calculational materials from the Materials Project.

These lattice structures are loaded into the full-potential local-orbital minimum-basis DFT code of FPLO for the DFT calculations \cite{24, 25}. After excluding the magnetic materials, self-consistent nonmagnetic DFT calculations were performed. We then project the Bloch wavefunctions into highly symmetric atomic-orbital-like Wannier functions, and generate the corresponding tight binding model Hamiltonians. We note that the commonly used approach based on maximally localized Wannier functions cannot easily be used for the high-throughput calculations since it is not easily automatized and the resulting tight binding Hamiltonians often contain spurious symmetry breaking. In our approach, we make use of the fact that FPLO code uses a local basis set, which makes it straightforward to generate a very high precision tight-binding Hamiltonian. Based on the tight binding model Hamiltonian that fulfills all symmetries, the intrinsic spin Hall conductivities (SHCs) are computed by the Kubo formula approach in the clean limit \cite{9, 13, 14}. To confirm the \textit{k}-point convergence, a dense \textit{k}-grid of 250 × 250 × 250 was applied in the SHC calculations. The accuracy of calculated SHC was double checked by the symmetry analysis \cite{26, 27}. All of the SHC calculations are based on nonmagnetic DFT calculations. Some of the considered materials may be magnetic, however, and for these the SHC calculation would not
be accurate (though it could in some cases correspond to temperatures above the Curie
temperature). We thus checked the magnetic states of materials with large SHC (>500
\((h/e)(S/cm)\)) and left the magnetic materials out of consideration. For materials that are
in the Materials Project we have utilized the information on the magnetic state from the
Materials Project. For materials that are only in the ICSD database, we have performed a
collinear spin polarized DFT calculation, and classified systems with a total moment larger
than 0.05 \(\mu_B\) per unit cell as magnetic.

The distribution of calculated SHC for the full set of materials is shown in Fig. 2 (details
for each separate compound are listed in the Supplementary material). From the more than
20,000 materials we find only 1048 with a SHC larger than 500 \((h/e)(S/cm)\), and only 169
above 1000 \((h/e)(S/cm)\). From the distribution of SHC in the space groups (Fig. 2(a)),
one sees that the large value (>500 \((h/e)(S/cm)\)) is mainly contained in six blocks, which
are No. 61-63, No. 138-140, No. 160-164, No. 186-187, No. 191-194, and No. 221-229.
To identify the common characteristics of these space groups in the six blocks, one can
directly check their common symmetry operations. It turns out that all these space groups
contain more than one mirror plane. Further statistical analysis finds that materials with
much larger SHC than the average have significantly more mirrors than materials with much
smaller SHC than the average, see Fig. 2(b). This shows that surprisingly there is a strong
connection between the magnitude of the SHE and crystalline symmetry. As we discuss
below, this connection exists because of special features in the band structure, which are
protected by mirror symmetry.

Chemical element analysis of the materials with a value of the SHC larger than 500
\((h/e)(S/cm)\) shows that the 5\(d\) transition metals Pt, Ir, Hf, and Ta are the most common
elements (see Supplementary material). This is in accordance with the general intuition
that to achieve a large SHC, on one hand, a large spin orbit coupling is required and, on the
other hand, rather extended electronic orbitals should contribute to the electron transport.
In these two respects the 5\(d\) transition metal compounds are better than 4\(d\) and 3\(d\) ones.
Indeed previous SHE studies confirm that materials with large SHC are 5\(d\) transition metal
related compounds [4, 5, 16, 19, 28, 29].

As highlighted in Fig. 2(a) we identify eleven materials with a SHC comparable or even
larger than Pt: IrN, Bi\(_2\)In\(_5\), Tl\(_3\)Ru, Pt\(_3\)Rh, CuPt\(_7\), LiPt\(_7\), Bi\(_2\)OsAu, Bi\(_3\)In\(_4\)Pb, HgOsPb\(_2\),
LiIr, and PtRh\(_3\). The compound with the largest SHC is IrN, which has SHC over 2900
(ℏ/e)(S/cm), however, we note that this is for a theoretically proposed phase of IrN.\textsuperscript{30, 31}

The next largest is the In\textsubscript{5}Bi\textsubscript{3}, which, unlike the other record compounds that all contain 5d elements, is a pure p-orbital metal with a SHC above 2500 (ℏ/e)(S/cm). As we show in the following, the giant SHC in In\textsubscript{5}Bi\textsubscript{3} originates not only from its large spin orbit coupling but also from a set of special features in its band structure. The fact that out of the 20,000 studied crystals, only a handful has SHC larger than Pt and none has a significantly higher value suggests that we may have approached the realistic limit of the intrinsic SHC in our calculations.

To analyse the origin of large SHC we consider the spin Berry curvature distribution in the Brillouin zone (in analogy to the ordinary Berry curvature in the anomalous Hall effect \textsuperscript{14}) of three selected materials with different point groups: YIr, In\textsubscript{5}Bi\textsubscript{3}, and Pt. Fig. 3(a-c) show the example of YIr with space group $Pm\bar{3}m$ (No. 221) and point group $m\bar{3}m$ \textsuperscript{32}. This material has a simple electronic structure and it is, therefore, useful for illustrating the origin of the SHC. The large intrinsic SHC in this material is associated with nodal lines in the band structure as illustrated in Fig. 2(c). The nodal lines are one dimensional band crossings, which are in absence of the spin-orbit coupling protected by mirror symmetry. With spin-orbit coupling, the nodal lines are split, which gives rise to a large spin Berry curvature. It can be seen in Fig. 3(a) that the main contribution to the SHC in YIr is indeed around the nodal lines. The band structure forms an independent nodal ring in the $k_z=\pi$ plane, centered at the $(\pi, 0, \pi)$ point, which is protected by the mirror symmetry $M_z$.

In combination with $c_4$ rotation symmetry with respect to the $x$, $y$, and $z$ axes, there are 24 nodal rings in total in the cubic Brillouin zone (Fig. 3(a)). Because of the large spin Berry curvature from the 24 nodal rings, the SHC of YIr reaches $\sim 1600 (ℏ/e)(S/cm)$, see Fig. 3(c).

Apart from the record breaking In\textsubscript{5}Bi\textsubscript{3}, the high-throughput calculations identify four other non-transition metal compounds (InBi, In\textsubscript{2}Bi, In\textsubscript{5}Bi\textsubscript{2}Pb, and element Tl) with a large SHE. The giant SHC in In\textsubscript{5}Bi\textsubscript{3} is related to the mirror planes $m_{100}$ and $m_{110}$ which cause two independent nodal lines in $k_x=0$ and $k_x + k_y=0$ planes, respectively. In combination with the $m_{001}$ and $c_4^2$ rotation symmetry, there are 16 nodal lines in total. In addition to these mirror symmetry protected nodal lines, In\textsubscript{5}Bi\textsubscript{3} also contains special $PT$ symmetry protected nodal rings out of high symmetry planes. It is clear from Fig. 3(d) that the hot lines of spin Berry curvatures are dominated by these nodal lines.
Performing a similar symmetry analysis on the electronic structure of Pt indicates that also in this well-known SHE material the large SHC originates from mirror symmetry: it protects nodal rings whose spin Berry curvature distribution is shown in Fig. 3(g). Interestingly, the contribution to the spin Berry curvature of the high symmetry points of $L$ and $X$ are less than 15% of the contribution from the nodal lines. Even if the Berry curvatures themselves are very large around the two high symmetry points of $L$ and $X$, their volumes are much smaller compared to the nodal lines. This brings to an important advantage of nodal rings in the context of the SHE: their significant dispersion in energy space offers a large possibility to cross the Fermi level and contribute strongly to the SHC.

In all of the materials where we have explored the origin of large SHE in depth, we have found that the SHE mainly originates from symmetry protected nodal lines. This is the likely explanation for the strong statistical relation of large SHE to symmetry shown in Fig. 2c. Importantly, similar relation to symmetry will likely exist also in other effects that have similar origin to the intrinsic SHE, such as the anomalous Hall effect or the anti-damping spin-orbit torque. Our result thus has quite fundamental significance: it shows that the symmetry determines not only the presence or absence of the transport phenomena as has been previously thought, but can also have a strong influence on their magnitude.

In most materials, the symmetry of the SHE is such that the spin-polarization of the spin current is perpendicular to both the spin current and the charge current. This is not a general rule, however. In materials with low crystalline symmetry, other types of spin current are allowed. This includes a spin current which flows in the transverse direction to the charge current like normal SHE but has spin-polarization along the spin current flow direction or longitudinal spin currents: Spin currents which flow in the same direction as the charge current (which can then have either spin-polarization parallel with the flow direction or perpendicular to it), as illustrated in Fig. 4. These types of spin currents could allow for new functionalities in spintronic devices, however they have not received much experimental attention since materials where they are allowed are quite rare. A theoretical screening to identify promising materials is thus essential. We note that the SHE normally refers to a spin current flowing in transverse direction to the charge current and thus it is not clear whether the longitudinal spin currents should be referred to as the SHE. Nevertheless, we stress, that the longitudinal spin currents have the same origin as the conventional SHE.

SHE which flows in the transverse direction to the charge current and has a spin-
polarization along the spin current flow direction is of great interest for spin-orbit torques in heavy metal / ferromagnet bilayer systems (or other similar systems) [34] (see Fig. 4b). In these structures, the SHE from the heavy metal layer flows into the ferromagnetic layer and thus exerts a torque on the magnetization [35]. For scalability, it is preferential to utilize ferromagnet with a perpendicular magnetic anisotropy (PMA). However, for deterministic field-free switching of the PMA systems, it is necessary to have a spin current with spin-polarization perpendicular to the interface (and thus parallel to the spin current flow direction). This is not allowed by symmetry in materials commonly used in these systems such as Pt and thus materials with lower symmetry are needed. Our calculations reveal that a large SHC with spin-polarization along spin current can occur, but is relatively rare. Out of the 1048 materials with SHC larger than 500 \( \frac{\hbar}{e} \frac{(S/cm)}{S/cm} \), only 2 have spin-polarization along the spin current: \( \text{Ni}_2\text{P}_6\text{W}_4 \) and \( \text{Ba}_2\text{C}_4\text{S}_4\text{N}_4 \). We have identified 32 other materials with SHC larger than 250 \( \frac{\hbar}{e} \frac{(S/cm)}{S/cm} \), which are listed in the Supplementary material.

The longitudinal spin currents have been experimentally studied in ferromagnetic systems, where the origin of such currents lie in the ferromagnetic order. It has been, however, predicted earlier that the same mechanism generating the SHE can also generate such spin currents [33]. In our database we identify a number of materials which exhibit large longitudinal spin currents, with spin-polarization parallel or perpendicular to the spin-current flow, see Fig. 4 (c, d). The largest longitudinal spin current can reach \( \sim 610 \frac{\hbar}{e} \frac{(S/cm)}{S/cm} \) at \( \sigma_{zz}^z \) in \( \text{P}_7\text{Ru}_{12}\text{Sc}_2 \). We list all the materials with longitudinal SHC larger than 250\( \frac{\hbar}{e} \frac{(S/cm)}{S/cm} \) in the supplementary material. The longitudinal spin current in non-magnetic crystals may offer a new platform for the study and utilization of the spin current in non-magnetic materials.

Our calculations reveal that the origin of large SHC is usually associated with mirror-symmetry protected nodal lines in the band structure, which results in a strong correlation between the crystalline symmetry and the SHC magnitude. This suggests that for the design of new SHC materials it is beneficial to consider high-symmetry materials with a large number of mirror planes. In addition we find that, apart from the obvious requirement of the presence of heavy elements with a strong spin-orbit coupling, the presence of 5d transition metal elements is advantageous, but not decisive. We identify a number of promising spin-to-charge conversion materials, including 169 materials with SHC above 1000 \( \frac{\hbar}{e} \frac{(S/cm)}{S/cm} \), 11 materials with SHC comparable or even larger than the up to now record Pt and materials in
which the symmetry of SHE is lower thus allowing for different types of spin currents. With these general design principles on one hand, and the specific information on each separate compound on the other hand, our high-throughput database can provide a powerful tool for the experimental design of spintronic devices.

**Method:** The *ab initio* calculations were performed based on density functional theory (DFT) by using the FPLO code [21]. The exchange and correlation energies were considered in the generalized gradient approximation (GGA) [25]. The *k*-point grid in DFT calculation is set as $12 \times 12 \times 12$, and the criterion of total energy convergency is below $10^{-6}$ eV. To perform the SHC, we have projected the Bloch wavefunctions to atomic-orbital-like Wannier functions by an automatically procedure. To make the Wannier projection automatically and accurately, we set the constraint of the mean error between DFT and tight binding below 0.02 eV in the energy window of $E_f - 2.0$ eV to $E_f + 2.0$ eV. The symmetry of the Wannier functions is well restored from the FPLO DFT code, where the Wannier functions are directly mapped from the atomic orbitals without maximum localization process. Starting from the tight binding model Hamiltonian, the SHC was calculated by the linear response Kubo formula approach in the clean limit [4, 14]:

$$
\sigma_{ij}^k = e \int_{BZ} \frac{d\vec{k}}{(2\pi)^3} \sum_n f_{nk} \Omega_{n,ij}^{S,k}(\vec{k}),
$$

$$
\Omega_{n,ij}^{S,k}(\vec{k}) = -2i \text{Im} \sum_{n' \neq n} \frac{\langle n\vec{k} | J^k_i | n'\vec{k} \rangle \langle n'\vec{k} | v_j | n\vec{k} \rangle}{(E_{n\vec{k}} - E_{n'\vec{k}})^2}
$$

where $f_{nk}$ is the Fermi–Dirac distribution for the $n$-th band. $J^k_i = \frac{1}{2} \left\{ v_i, s_k \right\}$ is the spin current operator with spin operator $s$, velocity operator $v_i$, and $i, j, k = x, y, z$. $| n\vec{k} \rangle$ is the eigenvector for the Hamiltonian $H$ at eigenvalue $E_{n\vec{k}}$. $\Omega_{n,ij}^{S,k}(\vec{k})$ is referred to as the spin Berry curvature for the $n$-th band at point $\vec{k}$ as an analogy to the ordinary Berry curvature.

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FIG. 1. Workflow of the high-throughput calculations for intrinsic SHC. The lattice structures are loaded from the Materials Project and ICSD database. Since the DFT is not accurate for the strong correlated system, all the compounds consisted from magnetic atoms V, Mn, Fe, Co, Ni or elements of N, O, F, and Cl are removed for Materials Project structures. All the f-electron related materials of both databases are excluded. The known Mott insulators to our knowledge are also removed. For the repeated lattice structures from the International Crystal Structure Database (ICSD) [21] and Materials Project, we only calculate one single structure. With this input list we performed self-consistent calculations with inclusion of spin orbit coupling for all compounds. The Bloch wavefunctions were automatically projected into highly symmetric atomic-orbital-like Wannier functions and the corresponding tight bonding model Hamiltonian was constructed. Based on the highly symmetric tight binding model Hamiltonians, the intrinsic SHC are computed automatically based on Kubo formula at the clean limit.
FIG. 2. Calculated intrinsic SHC. (a) SHC distribution for compounds as a function of space group. The SHC below 500, between 500-1000, between 1000-2000, between 2000-2500, and above 2500 \((\hbar/e)(S/cm)\) are labeled by black, blue, green, orange, and grey dots, respectively. (b) The average number of mirror symmetry operations in the space groups for materials with maximum value of SHC larger than threshold (black line) and smaller than threshold (red line) as a function of the threshold. To determine the relation between symmetry and SHC, we only choose the maximum tensor element for each compound in the \(3 \times 3 \times 3\) SHC tensor. We note that for the statistical analysis we have also included the calculations for materials that are likely to be magnetic. (c) The illustration of the nodal line mechanism. Left figure shows the nodal line, which is present without spin-orbit coupling. The right figure shows the splitting of the bands due to spin-orbit coupling, which results in a large spin Berry curvature along the original nodal line, as illustrated by the red circle.
FIG. 3. Three typical examples with large SHC with different spaces. Spin Berry curvature and nodal line distributions for (a) YIr with point group $m\overline{3}m$, (d) In$_5$Bi$_3$ with point group 4/mmm, and (g) Pt with point group $m\overline{3}m$, respectively. The green lines represent nodal lines. The color bar is in arbitrary unit. Energy dispersion for (b) YIr, (e) In$_5$Bi$_3$, and (h) Pt, respectively. The position of nodal lines are labeled using green rectangles. Fermi level dependent SHC for (c) YIr, (f) In$_5$Bi$_3$, and (i) Pt, respectively.
FIG. 4. The heterojunction of ferromagnet and non-magnets with four types of spin current obtained in this database. The top layer is ferromagnet and the bottom layer is non-magnet (a) Traditional SHE with spin-polarization of the spin current perpendicular to both the spin current and the charge current. (b) Spin-polarization of the spin current along the direction of the spin-current flow. (c) Longitudinal spin current with spin-current flow along the electric field and perpendicular to spin-polarization. (d) Longitudinal spin current with both of spin-polarization and spin-current flow along the electric field.