Supplementary materials for ”Chirality induced spin selectivity in chiral crystals”

Qun Yang[1,2,†], Yongkang Li[2,†], Claudia Felser[1], and Binghai Yan[2,*]

[1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany.

[2]Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot 7610001, Israel

[†]These authors contributed equally

[*]binghai.yan@weizmann.ac.il

Sec1 Supplementary Figures

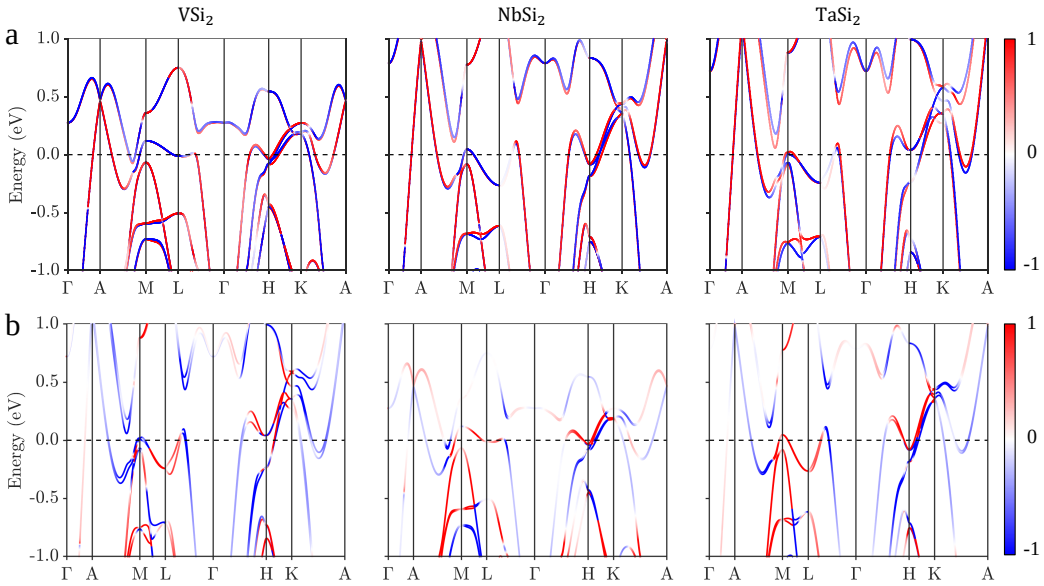

Figure S1. SAM- and OAM-resolved band structure in transition metal disilicide. Band dispersion with the z-component of **a**. SAM and **b**. OAM of the transmitted electrons in VSi_2, $NbSi_2$, and $TaSi_2$. The color red (blue) represents spin up (down) states in **a** and positive (negative) OAM in **b**.

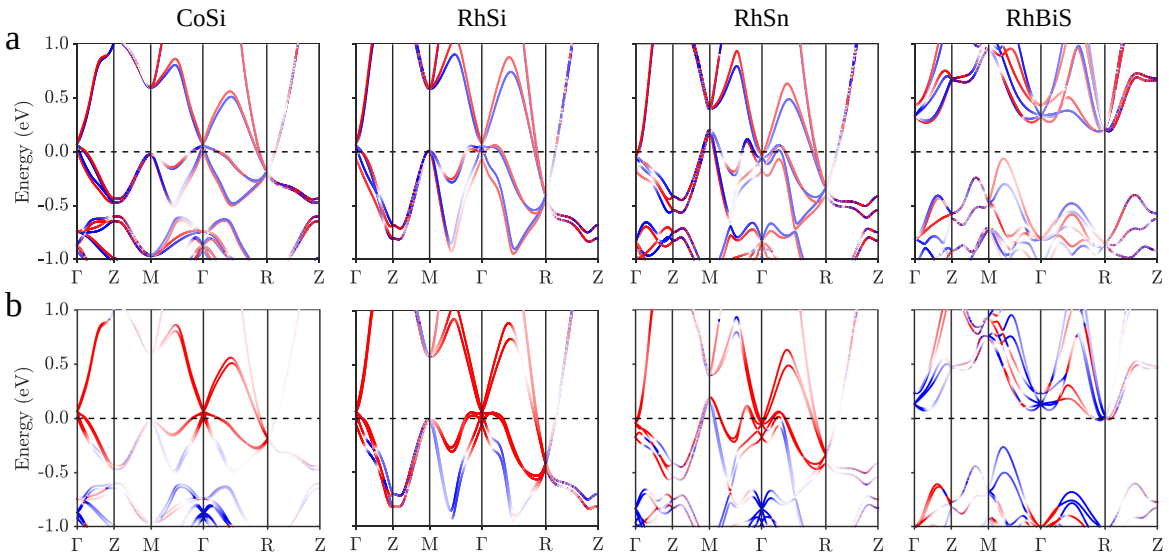

Figure S2. SAM- and OAM-resolved band structure in chiral materials with the space group $P2_13$.

Band dispersion with the z-component of **a**. SAM and **b**. OAM of the transmitted electrons in CoSi, RhSi, RhSn, and RhBiS.

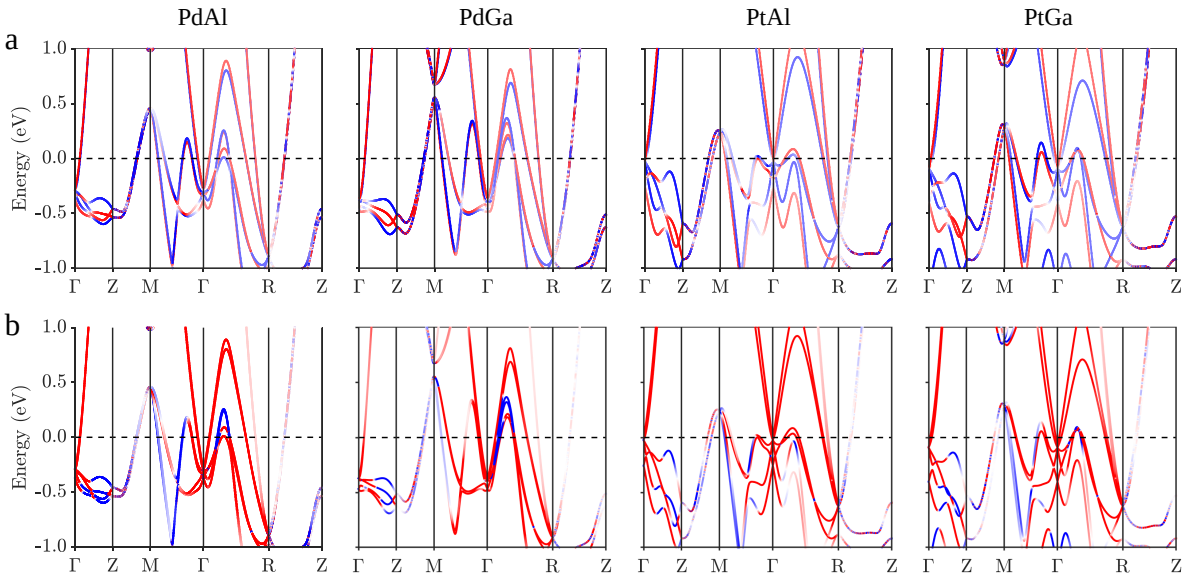

Figure S3. SAM- and OAM-resolved band structure in chiral materials with the space group $P2_13$.

Band dispersion with the z-component of **a**. SAM and **b**. OAM of the transmitted electrons in PdAl, PdGa, PtAl, and PtGa

Sec2 Methods of quantum transport calculation

Sec2.1 Device setup

We use a two-terminal device for transport calculation and only consider momentum-conserving transport. The chiral crystal is placed in the central region which is connected to two leads on the left and right side. The transverse dimension (perpendicular to the transport direction) is infinite and periodically extended. Hence, the transverse crystal momentum $k_{//}$ is a conserved quantity. All transport quantities are calculated for each $k_{//}$ and then sum over transverse momentum.

Sec2.2 Basis definitions

The quantum transport quantities including conductance and orbital/spin polarizations are calculated based on Landauer-Büttiker formalism[1,2]. All the quantities can be calculated from the scattering matrix S. The scattering matrix elements S_{mn} is defined as the transition probability amplitude from mode n to mode m. If there are N modes in each lead, then S is a $2N \times 2N$ matrix

$$S = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \tag{S1}$$

where r and t (r' and t') are $N \times N$ reflection and transmission amplitudes from left (L) to right (R) (from R to L). Here all coefficients depend on energy E and transverse momentum $k_{//}$. The probability conservation implies S is a unitary matrix: $SS^{\dagger} = S^{\dagger}S = I$, which gives constrictions on r and t (r' and t')

$$r^{\dagger}r + t^{\dagger}t = I, \qquad r'^{\dagger}r' + t'^{\dagger}t' = I \tag{S2}$$

The Landauer formula connects the total conductance G_{RL} (from L to R) and G_{LR} (from R to L) with

total transmission probability T_t for a given E and $k_{//}$[3,4]

$$\begin{aligned} G_{RL}(E,k_{//}) &= \frac{e^2}{h}T_t(E,k_{//}) = \frac{e^2}{h}\sum_{m,n}\left|t_{mn}(E,k_{//})\right|^2 = \frac{e^2}{h}\mathrm{Tr}\left[t^{\dagger}(E,k_{//})t(E,k_{//})\right] \\ G_{LR}(E,k_{//}) &= \frac{e^2}{h}T_t'(E,k_{//}) = \frac{e^2}{h}\sum_{m,n}\left|t'_{nm}(E,k_{//})\right|^2 = \frac{e^2}{h}\mathrm{Tr}\left[t'^{\dagger}(E,k_{//})t'(E,k_{//})\right] \end{aligned} \tag{S3}$$

Inspired by the Landauer formula, one can also define reflection conductance according to the total reflection probability R_t

$$\begin{aligned} G_{LL}(E,k_{//}) &= \frac{e^2}{h}R_t(E,k_{//}) = \frac{e^2}{h}\sum_{n',n}\left|r_{n'n}(E,k_{//})\right|^2 = \frac{e^2}{h}\mathrm{Tr}\left[r^{\dagger}(E,k_{//})r(E,k_{//})\right] \\ G_{RR}(E,k_{//}) &= \frac{e^2}{h}R_t'(E,k_{//}) = \frac{e^2}{h}\sum_{m',m}\left|r'_{m'm}(E,k_{//})\right|^2 = \frac{e^2}{h}\mathrm{Tr}\left[r'^{\dagger}(E,k_{//})r'(E,k_{//})\right] \end{aligned} \tag{S4}$$

In the above summation, n, n' refers to the modes in L lead, and m, m' refers to the modes in R lead. Indeed these conductances are not independent quantities, which must satisfy a sum relation due to the unitarity requirement (S2)

$$G_{RL}(E,k_{//}) + G_{LL}(E,k_{//}) = G_{LR}(E,k_{//}) + G_{RR}(E,k_{//}) = N(E,k_{//})\frac{e^2}{h} \tag{S5}$$

For a physical quantity J which is conserved in lead, its matrix representation in mode basis is diagonal: $\mathscr{J}_{mm'} = j_m\delta_{mm'}$. For example, when spin-orbital coupling (SOC) is negligible in lead, the spin angular momentum is conserved and in this case, $\mathscr{J} = \sigma_i (i = x,y,z)$ are three Pauli matrices. In this paper, we mainly focus on orbital and spin conductance so that $\mathscr{J} = L_i$ or $\mathscr{J} = \sigma_i$. The conductance associated with J can be defined similarly as (S3) and (S4)[5]

$$\begin{aligned} G_{RL,J}(E,k_{//}) &= \frac{e^2}{h}T_{t,J}(E,k_{//}) = \frac{e^2}{h}\sum_{m,n} j_m\left|t_{mn}(E,k_{//})\right|^2 = \frac{e^2}{h}\mathrm{Tr}\left[t^{\dagger}(E,k_{//})\mathscr{J}t(E,k_{//})\right] \\ G_{LL,J}(E,k_{//}) &= \frac{e^2}{h}R_{t,J}(E,k_{//}) = \frac{e^2}{h}\sum_{n',n} j_{n'}\left|r_{n'n}(E,k_{//})\right|^2 = \frac{e^2}{h}\mathrm{Tr}\left[r^{\dagger}(E,k_{//})\mathscr{J}r(E,k_{//})\right] \\ G_{RR,J}(E,k_{//}) &= \frac{e^2}{h}R'_{t,J}(E,k_{//}) = \frac{e^2}{h}\sum_{m',m} j_{m'}\left|r'_{m'm}(E,k_{//})\right|^2 = \frac{e^2}{h}\mathrm{Tr}\left[r'^{\dagger}(E,k_{//})\mathscr{J}r'(E,k_{//})\right] \end{aligned} \tag{S6}$$

As mentioned before, the final transport quantities should sum over transverse momentum

$$G(E)=\sum_{k_{//}}G(E,k_{//}),\qquad G_J(E)=\sum_{k_{//}}G_J(E,k_{//}) \tag{S7}$$

Here G and G_J refer to the various conductance in (S3), (S4) and (S6). The polarization associated with J is therefore defined by[5]

$$P_J(E)=\frac{G_J(E)}{G(E)} \tag{S8}$$

For example, the transmission spin polarization from lead L to lead R is $P_{RL,S}(E)=\frac{G_{RL,S}(E)}{G_{RL}(E)}$.

In the absence of phase incoherent scattering or magnetization M, the probability conservation or time-reversal symmetry implies $T=T'$[3,5]. Therefore, the conductance from lead L to lead R and from lead R to lead L makes no difference: $G_{RL}(E)=G_{LR}(E)$. But if both magnetization and dephasing are introduced in the central region, the current conservation and time reversal symmetry are violated and the transport becomes unidirectional: $G_{RL}(E,M)\neq G_{LR}(E,M)$. From Onsager's relation: $G_{RL}(E,-M)=G_{LR}(E,M)$, this implies the magneto-conductance $G_{RL}(E,M)\neq G_{RL}(E,-M)$ or magneto-current $I(V,M)\neq I(V,-M)$ upon integration with energy. To characterize this magneto-current, we define a ratio P_M[6] as

$$P_M(V)=\frac{I(V,M)-I(V,-M)}{I(V,M)+I(V,-M)} \tag{S9}$$

Sec2.3 Conductances from Green's function

Based on mode matching methods[7,8], the S matrix can be expressed by Green's function (below we suppress the dependence on E and $k_{//}$)

$$\begin{aligned} t_{mn}&=\sqrt{\frac{v_{Rm}(+)a_R}{v_{Ln}(+)a_L}}\langle\tilde{u}_{Rm}(+)|G^r_{RL}(G^{r(0)}_{00})^{-1}|u_{Ln}(+)\rangle \\ r_{n'n}&=\sqrt{\frac{v_{Ln'}(-)}{v_{Ln}(+)}}\left[-\langle\tilde{u}_{Ln'}(-)|u_{Ln}(+)\rangle+\langle\tilde{u}_{Ln'}(-)|G^r_{LL}(G^{r(0)}_{00})^{-1}|u_{Ln}(+)\rangle\right] \end{aligned} \tag{S10}$$

$v_{Rm}(+)$ ($v_{Ln}(\pm)$) is the velocity of m-th (n-th) mode in lead R (L) and $\pm$ represents the propagating or decaying direction (+ for right and - for left). a_R (a_L) is the spacing between principal layer in lead R (L).

$|u_{Rm}(+)\rangle$ ($|u_{Ln}(\pm)\rangle$) is the eigenstate of m-th (n-th) mode in lead R (L) and $|\tilde{u}_{Rm}(+)\rangle$ is dual states defined by $\langle\tilde{u}_{Rm'}(+)|u_{Rm}(+)\rangle = \delta_{m'm}$. G^r_{RL} (G^r_{LL}) is retarded Green's function of the full device between lead R (L) and lead L, while $G^{r(0)}_{00}$ is the retarded Green's function of the perfect lead within single principle layer. In lead L, the incoming wave is mixed with the reflected wave and must be subtracted for the calculation of reflection coefficients, which is just the first term in $r_{n'n}$. The Green's function acting on the incoming wave $|u_{Ln}(+)\rangle$ converts it to the eigenstate of full lead so the second term of $r_{n'n}$ (t_{mn}) is the $n'(m)$-th output mode component of full scattering wave. Combining these terms and normalizing the states according to the probability flux gives transmission/reflection amplitudes as in (S10).

In the S matrix method, one needs to solve a generalized eigenvalue problem[5,9,10] to get leads' eigenstate apart from Green's function. This extra step is not only time-consuming for large systems but also needs some careful treatment to distinguish propagating states from decaying states. Especially near the band edge, where the velocity of propagating states approaches to zero and non-propagating states' decaying becomes very slow, the distinction between these two kinds of states is small. Since only propagating states contribute to transport, care must be taken to distinguish and eliminate decaying states. On the other hand, Caroli[11] has shown the total transmission can be expressed solely through the Green's function and the lead's level width function which avoids solving lead's eigenstates

$$T_t = \sum_{mn} |t_{mn}|^2 = \mathrm{Tr}(\Gamma_R G^r_{RL} \Gamma_L G^a_{LR}) \tag{S11}$$

$G^a_{LR} = G^{r\dagger}_{RL}$ is advanced Green's function between lead L and lead R. The trace is taken in the lattice site base. Apparently, (S11) is more convenient for the calculation of total transmission than (S10) since lead's eigenmodes are not required. Indeed this type expression can be obtained for all quantities we considered in Sec2.2 and there is no need to solve the eigenmodes at all, as we show below.

First, we rewrite (S10) by dual states along. Define Green's function due to reflection

$$G^{r*}_{LL} = G^r_{LL} - G^{r(0)}_{00} \tag{S12}$$

then reflection amplitudes can be rewritten as a similar form to transmission amplitudes

$$r_{n'n} = \sqrt{\frac{v_{Ln'}(-)}{v_{Ln}(+)}}\left[\langle\tilde{u}_{Ln'}(-)|G^{r*}_{LL}(G^{r(0)}_{00})^{-1}|u_{Ln}(+)\rangle\right] \tag{S13}$$

Following the way of Khomyakov[8], the transmission/reflection amplitudes can be recast as

$$\begin{aligned} t_{mn} &= i\hbar\sqrt{\frac{v_{Rm}(+)v_{Ln}(+)}{a_R a_L}}\langle\tilde{u}_{Rm}(+)|G^r_{RL}|\tilde{u}^a_{Ln}(-)\rangle \\ r_{n'n} &= i\hbar\sqrt{\frac{v_{Ln'}(-)v_{Ln}(+)}{a_L a_L}}\langle\tilde{u}_{Ln'}(-)|G^{r*}_{LL}|\tilde{u}^a_{Ln}(-)\rangle \end{aligned} \tag{S14}$$

$|\tilde{u}^a_{Ln}(-)\rangle$ is the eigenstate propagating or growing to the right in lead L. (S14) is nothing but the lattice version of Fisher-Lee relation[4,12,13]. Defining velocity matrix $V_L(+)$ whose diagonal elements are $\hbar v_{Ln}(+)/a_L$ and mode matrix $U_R(+)$ whose column vectors are the eigenmodes $|u_{Rm}(+)\rangle$, etc, (S14) can be written in matrix form

$$\begin{aligned} t &= iV_R^{1/2}(+)U_R^{-1}(+)G^r_{RL}(U_L^{a\dagger}(-))^{-1}V_L^{1/2}(+) \\ r &= iV_L^{1/2}(-)U_L^{-1}(-)G^{r*}_{LL}(U_L^{a\dagger}(-))^{-1}V_L^{1/2}(+) \end{aligned} \tag{S15}$$

Next, since the transport quantities only depend on probability not amplitudes, we define probability S matrix: $(S_p)_{mn} = |S_{mn}|^2$, i.e.

$$S_p = \begin{pmatrix} R & T' \\ T & R' \end{pmatrix} \tag{S16}$$

To get the matrix elements of R and T, introduce the mode projection matrix in local orbital basis

$$\begin{aligned} &P^a_{Ln}(-) = |u^a_{Ln}(-)\rangle\langle\tilde{u}^a_{Ln}(-)| \qquad P_{Rm}(+) = |u_{Rm}(+)\rangle\langle\tilde{u}_{Rm}(+)| \qquad P_{Ln'}(-) = |u_{Ln'}(-)\rangle\langle\tilde{u}_{Ln'}(-)| \\ \text{or}\quad &P^a_{Ln}(-) = U^a_L(-)I_n(U^a_L(-))^{-1} \quad P_{Rm}(+) = U_R(+)I_m(U_R(+))^{-1} \quad P_{Ln'}(-) = U_L(-)I_{n'}(U_L(-))^{-1} \end{aligned} \tag{S17}$$

I_n is a matrix whose only non-zeros elements are the n-th diagonal elements and equals to 1. $P^a_{Ln}(-)$ is the projection onto the n-th right propagating or right growing mode $|u^a_{Ln}(-)\rangle$ in lead L, etc. The velocity

matrix can also be expressed by the level width matrix and mode matrix[8]

$$V_R(+) = U_R^{\dagger}(+)\Gamma_R U_R(+) \qquad V_L(+) = U_L^{\dagger}(-)\Gamma_L U_L(-) = U_L^{a\dagger}(-)\Gamma_L U_L^{a}(-) \tag{S18}$$

Making use of (S15), (S17), (S18), and the fact I_n commutes with all velocity matrix, R and T can be obtained as

$$\begin{aligned} T_{mn} &= |t_{mn}|^2 = Tr(t^{\dagger} I_m t I_n) \\ &= \mathrm{Tr}\left[V_L^{1/2}(+)(U_L^{a}(-))^{-1} G_{RL}^{r\dagger}(U_R^{\dagger}(+))^{-1} V_R^{1/2}(+) I_m V_R^{1/2}(+) U_R^{-1}(+) G_{RL}^{r}(U_L^{a\dagger}(-))^{-1} V_L^{1/2}(+) I_n\right] \\ &= \mathrm{Tr}\left[(U_R^{\dagger}(+))^{-1} V_R(+) I_m U_R^{-1}(+) G_{RL}^{r}(U_L^{a\dagger}(-))^{-1} V_L(+) I_n (U_L^{a}(-))^{-1} G_{RL}^{r\dagger}\right] \\ &= \mathrm{Tr}\left[\Gamma_R P_{Rm}(+) G_{RL}^{r} \Gamma_L P_{Ln}^{a}(-) G_{LR}^{a}\right] \end{aligned} \tag{S19}$$

$$\begin{aligned} R_{n'n} &= |r_{n'n}|^2 = Tr(r^{\dagger} I_{n'} r I_n) \\ &= \mathrm{Tr}\left[V_L^{1/2}(+)(U_L^{a}(-))^{-1} G_{LL}^{r*\dagger}(U_L^{\dagger}(-))^{-1} V_L^{1/2}(-) I_{n'} V_L^{1/2}(-) U_L^{-1}(-) G_{LL}^{r*}(U_L^{a\dagger}(-))^{-1} V_L^{1/2}(+) I_n\right] \\ &= \mathrm{Tr}\left[(U_L^{\dagger}(-))^{-1} V_L(-) I_{n'} U_L^{-1}(-) G_{LL}^{r*}(U_L^{a\dagger}(-))^{-1} V_L(+) I_n (U_L^{a}(-))^{-1} G_{LL}^{r*\dagger}\right] \\ &= \mathrm{Tr}\left[\Gamma_L P_{Ln'}(-) G_{LL}^{r*} \Gamma_L P_{Ln}^{a}(-) G_{LL}^{a*}\right] \end{aligned} \tag{S20}$$

R' and T' have similar expressions. In this way, the full probability S matrix is constructed from Green's function and mode projection matrix. If one uses the completeness relation $\sum_m P_{Rm}(+) = I$ and $\sum_n P_{Ln}^{a}(-) = I$, the Caroli formula (S11) is easily derived from (S19) which is a refined version for the separate transmission probability.

Finally, to get the J conductance, the matrix representation of conserved quantity J in local orbital basis is needed, which can be obtained from eigendecomposition

$$J_R = \sum_m j_m P_{Rm}(+) \qquad J_L = \sum_n j_n P_{Ln}(-) \tag{S21}$$

Hence, for example, $G_{RL,J} = \frac{e^2}{h}\mathrm{Tr}(t^\dagger J_R t) = \frac{e^2}{h}\sum_{mn} j_m T_{mn} = \frac{e^2}{h}\mathrm{Tr}\left[\Gamma_R J_R G^r_{RL}\Gamma_L G^a_{LR}\right)]$ is the transmission J conductance and the trace is taken in local orbital basis. Other conductances have similar expressions and we have successfully obtained all the quantities in Sec2.2 without referring to leads' eigenstates. For reference convenience, the expressions of full total conductance and J conductance are listed below

$$G = \begin{pmatrix} G_{LL} & G_{LR} \\ G_{RL} & G_{RR} \end{pmatrix} = \frac{e^2}{h}\begin{pmatrix} \mathrm{Tr}\left[\Gamma_L G^{r*}_{LL}\Gamma_L G^{a*}_{LL}\right] & \mathrm{Tr}\left[\Gamma_L G^{r}_{LR}\Gamma_R G^{a}_{RL}\right] \\ \mathrm{Tr}\left[\Gamma_R G^{r}_{RL}\Gamma_L G^{a}_{LR}\right] & \mathrm{Tr}\left[\Gamma_R G^{r*}_{RR}\Gamma_R G^{a*}_{RR}\right] \end{pmatrix} \tag{S22}$$

$$G_J = \begin{pmatrix} G_{LL,J} & G_{LR,J} \\ G_{RL,J} & G_{RR,J} \end{pmatrix} = \frac{e^2}{h}\begin{pmatrix} \mathrm{Tr}\left[\Gamma_L J_L G^{r*}_{LL}\Gamma_L G^{a*}_{LL}\right] & \mathrm{Tr}\left[\Gamma_L J_L G^{r}_{LR}\Gamma_R G^{a}_{RL}\right] \\ \mathrm{Tr}\left[\Gamma_R J_R G^{r}_{RL}\Gamma_L G^{a}_{LR}\right] & \mathrm{Tr}\left[\Gamma_R J_R G^{r*}_{RR}\Gamma_R G^{a*}_{RR}\right] \end{pmatrix} \tag{S23}$$

Although here we only focus on two terminal devices, the results (S22) and (S23) can be very easily generalized to multi-terminal devices. For conductance between any two terminals, one only needs to replace L and R by general terminal indices and replace Green's function $G^{r/a}$ by the reflected one (S12) $G^{r/a*}$ if two terminals are the same one. This formulation would be helpful, e.g., for the calculation of spin conductance in multi-terminal devices.

Sec2.4 Wide band approximation

The wide band approximation[4,14] (WBA) represents the lead with an energy-independent self-energy Σ. Physically, it means the lead has an infinite bandwidth and the detailed band structure is not important in the transport energy range. So the only effect of leads is to provide a mechanism for the quasi-particles in the central region to leak into leads, which can be represented by an imaginary self-energy. In our calculation, to avoid the influence of the detailed structure of leads and to manifest the magneto-resistance simply, we use WBA for all calculations. Ignoring the real part of self-energy which is just an energy shift, then

$$\Sigma = -\frac{i}{2}(\Gamma_\uparrow P_\uparrow + \Gamma_\downarrow P_\downarrow) \tag{S24}$$

$P_\uparrow$ ($P_\downarrow$) is the projection matrix onto spin up (down) states and $\Gamma_\uparrow$ ($\Gamma_\downarrow$) is the corresponding level width function or DOS. Here we associated two different Γ with spin up and down states to allow for spin-dependent DOS in leads, which mimics the effect of magnetization. For the spin polarization calculation in which leads are unmagnetized, we simply take $\Gamma_\uparrow = \Gamma_\downarrow = \Gamma$. Whereas in the magneto-current calculation, the lead is ferromagnetic and has a spin-polarized density of states (DOS), i.e. $\Gamma_\uparrow \neq \Gamma_\downarrow$. Hence, within WBA, a spin-polarized DOS ratio $\Delta\Gamma/\Gamma = (\Gamma_\uparrow - \Gamma_\downarrow)/(\Gamma_\uparrow + \Gamma_\downarrow)$ can be used to represent the sign and strength of magnetization M (it's plausible that $\Delta\Gamma$ should be proportional to M for small M).

References

1. Landauer, R. Electrical resistance of disordered one-dimensional lattices. *The Philos. Mag. A J. Theor. Exp. Appl. Phys.* **21**, 863–867, DOI: 10.1080/14786437008238472 (1970). https://doi.org/10.1080/14786437008238472.

2. Büttiker, M. Four-terminal phase-coherent conductance. *Phys. Rev. Lett.* **57**, 1761–1764, DOI: 10.1103/PhysRevLett.57.1761 (1986).

3. Datta, S. *Electronic Transport in Mesoscopic Systems*. Cambridge Studies in Semiconductor Physics and Microelectronic Engineering (Cambridge University Press, 1995).

4. Ryndyk, D. *Theory of Quantum Transport at Nanoscale: An Introduction*. Springer Series in Solid-State Sciences (Springer International Publishing, 2015).

5. Liu, Y., Xiao, J., Koo, J. & Yan, B. Chirality-driven topological electronic structure of dna-like materials. *Nat. Mater.* **20**, 638–644, DOI: 10.1038/s41563-021-00924-5 (2021).

6. Liu, T. & Weiss, P. S. Spin polarization in transport studies of chirality-induced spin selectivity. *ACS Nano* **17**, 19502–19507, DOI: 10.1021/acsnano.3c06133 (2023).

7. Ando, T. Quantum point contacts in magnetic fields. *Phys. Rev. B* **44**, 8017–8027, DOI: 10.1103/PhysRevB.44.8017 (1991).

8. Khomyakov, P. A., Brocks, G., Karpan, V., Zwierzycki, M. & Kelly, P. J. Conductance calculations for quantum wires and interfaces: Mode matching and green's functions. *Phys. Rev. B* **72**, 035450, DOI: 10.1103/PhysRevB.72.035450 (2005).

9. Sanvito, S., Lambert, C. J., Jefferson, J. H. & Bratkovsky, A. M. General green's-function formalism for transport calculations with spd hamiltonians and giant magnetoresistance in co- and ni-based

magnetic multilayers. *Phys. Rev. B* **59**, 11936–11948, DOI: 10.1103/PhysRevB.59.11936 (1999).

10. Rungger, I. & Sanvito, S. Algorithm for the construction of self-energies for electronic transport calculations based on singularity elimination and singular value decomposition. *Phys. Rev. B* **78**, 035407, DOI: 10.1103/PhysRevB.78.035407 (2008).

11. Caroli, C., Combescot, R., Lederer, D., Nozieres, P. & Saint-James, D. A direct calculation of the tunnelling current. ii. free electron description. *J. Phys. C: Solid State Phys.* **4**, 2598, DOI: 10.1088/0022-3719/4/16/025 (1971).

12. Fisher, D. S. & Lee, P. A. Relation between conductivity and transmission matrix. *Phys. Rev. B* **23**, 6851–6854, DOI: 10.1103/PhysRevB.23.6851 (1981).

13. Boumrar, H., Hamidi, M., Zenia, H. & Lounis, S. Equivalence of wave function matching and green's functions methods for quantum transport: generalized fisher–lee relation. *J. Physics: Condens. Matter* **32**, 355302, DOI: 10.1088/1361-648X/ab88f5 (2020).

14. Covito, F., Eich, F. G., Tuovinen, R., Sentef, M. A. & Rubio, A. Transient charge and energy flow in the wide-band limit. *J. Chem. Theory Comput.* **14**, 2495–2504, DOI: 10.1021/acs.jctc.8b00077 (2018). PMID: 29660278, https://doi.org/10.1021/acs.jctc.8b00077.