Supplementary Data for
“Symmetry Dictionary on Charge and Spin Nonlinear Responses for All Magnetic
Point Groups with Nontrivial Topological Nature”

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SI. The Second Charge and Spin Response Tensors

We suppose that there is an ac driving electric field $E_c(t) = \text{Re}\{E_c e^{i\omega t}\}$ for $c = x, y, z$ and in the relaxation-time approximation, the Boltzmann equation reads

$$-\frac{e\tau}{\hbar} \partial_c \partial_c f + \tau \partial_t f = f_0 - f,$$

where $f_0$ is the equilibrium distribution in the absence of $E_c(t)$, $\tau$ is the relaxation time of electrons, $\partial_c = \frac{\partial}{\partial k_c}$, and $\partial_t = \frac{\partial}{\partial t}$. Here we write the infinite-order distribution function like this: $f = \text{Re}\{f_0 + f_1 + f_2\}$, we have [1]

$$f_1 = \frac{e\tau E_c \partial_c f_0}{\hbar(1 + i\omega\tau)} e^{i\omega t},$$

$$f_2 = \frac{e^2\tau^2 E_c E_d \partial_c \partial_d f_0}{2\hbar(1 + i\omega\tau)(1 + 2i\omega\tau)} + \frac{e^2\tau^2 E_c^* E_d \partial_c \partial_d f_0}{2\hbar(1 + i\omega\tau)(1 + 2i\omega\tau)} e^{2i\omega t}.$$

The response charge current density is given by

$$j_a = -e \int_k v_a f,$$

where $\int_k = \frac{d^3 k}{(2\pi)^3}$, $v_a$ is the electric velocity in the $a$ direction, and we omit the band index. Gao et al. [2] proposed a modification of Berry curvature under driving electric field,

$$\dot{r} = \frac{1}{\hbar} \frac{\partial \varepsilon}{\partial k} - \dot{k} \times [\nabla \times (A + A')]$$

$$\dot{k} = -\frac{e}{\hbar} E,$$

where $A$ is the Berry curvature connection, the modification is $A'_a = eG_{ac}\varepsilon_c$. $G_{ac}(k) = 2\text{Re}\sum_{m \neq n} \frac{A_{am}^m(k)}{\varepsilon_m(k) - \varepsilon_n(k)} A_{nm}^m(k)$ is the Berry connection polarizability (BCP). Here we can directly get the electric velocity in the $a$ direction,

$$v_a = \frac{1}{\hbar} \frac{\partial \varepsilon}{\partial k_a} + \frac{e}{\hbar} \varepsilon_{a bd} \varepsilon_b \Omega_d + \frac{e^2}{\hbar} (\partial_d G_{bc} - \partial_b G_{ac}) \varepsilon_b \varepsilon_c,$$
where $\epsilon_{abc}$ is the Levi-Civita symbol and the last term is the modification. Thus, we can get the response charge current $j_a = \Re\{j^0_a + j^1_a + j^2_a\}$,

$$j^0_a = -\frac{e}{h} \int_k \frac{\partial \epsilon}{\partial k_a} f_0,$$

$$j^1_a = -\left[ \frac{e^2 \tau}{2h^2 (1 + i\omega \tau)} \int_k \frac{\partial \epsilon}{\partial k_a} \frac{\partial f_0}{\partial k_b} + \frac{e^2}{h} \epsilon_{abcd} \int_k \Omega_d f_0 \right] E_b e^{i\omega t},$$

$$j^2_a = -\frac{e^3 \tau^2}{2h^3} \left[ \frac{E_b E_c \epsilon^{2i\omega t} + E_b^* E_c}{(1 + i\omega t)} \int_k \frac{\partial \epsilon}{\partial k_a} \frac{\partial f_0}{\partial k_b} \frac{\partial f_0}{\partial k_c} \right] + \frac{e^3 \tau^2}{2h^3} (E_b E_c e^{i\omega t} + E_b^* E_c) \int_k (\partial_a G_{bc} - \partial_b G_{ac}) f_0,$$

where $j^2_a$ refers to the second-order current in the direction of $a$ in response to the driving electric field, which is the part of our work. In the low frequency limit,

$$j^2_a (\omega \to 0) = \chi_{abc} E_b E_c,$$

$$\chi^{\text{BCD}}_{abc} = -\frac{e^3 \tau}{h^2} \int_k \epsilon_{abcd} \frac{\partial f_0}{\partial k_c},$$

$$\chi^{\text{BCP}}_{abc} = -\frac{e^3}{h} \int_k \left( \partial_a G_{bc} - \partial_b G_{ac} \right) f_0,$$

$$\chi^{\text{D}}_{abc} = -\frac{e^3 \tau^2}{h^3} \int_k \frac{\partial \epsilon}{\partial k_a} \frac{\partial^2 f_0}{\partial k_b \partial k_c}.$$

Therefore, the dependence of the coefficient on $\tau$ is

$$\chi^{\text{BCD}}_{abc} \propto \tau, \quad \chi^{\text{BCP}}_{abc} \propto \tau^0, \quad \chi^{\text{D}}_{abc} \propto \tau^2.$$

Here we figure out the second-order charge response coefficient is a rank-three tensor, contributing by the three parts, BCD [1], BCP [3, 4] and the Drude [5, 6]. According to the Ref. [6], we can do some further calculations, and we have

$$\chi^{\text{D}}_{abc} = -\frac{e^3 \tau^2}{2h^3} \int_k v_a v_b v_c \frac{\partial^2 f_0}{\partial x^2}.$$

Further, if we take the electric spin into account, the second-order conductivity can be expressed as

$$j^{2(\sigma)}_a = (\chi^{\text{BCD}}_{abc})^{(\sigma)} E_b E_c,$$

$$\chi^{(\sigma)}_{abc} = \chi^{\text{BCD}(\sigma)}_{abc} + \chi^{\text{BCP}(\sigma)}_{abc} + \chi^{\text{D}(\sigma)}_{abc},$$

where the $\sigma = \uparrow$ or $\downarrow$ is spin index of electrons. Then the second-order charge current and the spin current can be expressed separately as $j_a = j_\uparrow^a + j_\downarrow^a$ and $j^{(s)}_a = (h/2e)(j_\uparrow^a - j_\downarrow^a)$ [7]. Hence, we can write the second-order charge and spin response tensors,

$$\chi_{abc} = \chi^{\text{BCD}}_{abc} + \chi^{\text{BCP}}_{abc} + \chi^{\text{D}}_{abc},$$

$$\chi^{(s)}_{abc} = \chi^{\text{BCD}(s)}_{abc} + \chi^{\text{BCP}(s)}_{abc} + \chi^{\text{D}(s)}_{abc},$$

where $\chi_{abc} = \chi^\uparrow_{abc} + \chi^\downarrow_{abc}$, $\chi^{(s)}_{abc} = \chi^\uparrow_{abc} - \chi^\downarrow_{abc}$, and we use the upper index $s$ to represent the spin response.

These three terms are the major contributions of the second-order response. Take the charge response as example, for the BCD and BCP terms they all have $a \leftrightarrow b$ anti-symmetries, which have the same 9 independent components,

$$\chi^{\text{BCD}}_{x} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \chi^{\text{BCP}}_{y} = \begin{pmatrix} -xyx & -xyy & -xyz \\ 0 & 0 & 0 \\ yzx & yzy & yzz \end{pmatrix}, \chi^{\text{BCD}}_{z} = \begin{pmatrix} -xyz & -xzy & -xzz \\ yxz & yzy & yzz \\ 0 & 0 & 0 \end{pmatrix}. \quad (S15)$$
However the Drude term have the interchangeably symmetric for any two indices, and have 10 independent com-

ponents,

\[ \chi^D_x = \begin{pmatrix} xxx & xxy & xxz \\ xxy & xyy & yyz \\ xxz & xyz & xzz \end{pmatrix}, \chi^D_y = \begin{pmatrix} xxy & xyy & xyz \\ yyy & yyy & yyz \\ yyz & yyz & yzz \end{pmatrix}, \chi^D_z = \begin{pmatrix} xxz & xyz & xzz \\ xyz & yyz & yzz \\ xzz & yzz & zzz \end{pmatrix} \]  

(S16)

We can get similar results for the second-order spin response tensors.

SII. THE INTRODUCTION OF 122 MAGNETIC POINT GROUPS

The magnetic point groups(MPGs) \( \mathcal{M} \), or we can call the Shubnikov groups can be divided into three classes, the number of which are 32, 32 and 58. In Table S1, we give the international symbols and Schoenflies symbols for the Class I, as well as the international symbols of the Class II and III. Next we figure out all the production matrices (generators) of the three classes of magnetic point groups, which are represented by the symbol \( \Gamma^i, i = 0, 1, 2, 3, ..., 9 \) and \( \Gamma^k = \Gamma^k T, k = 0, 1, 2, 3, ..., 9 \),

\[ \Gamma^1 = \mathcal{P} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad \Gamma^2 = \mathcal{C}_2^y = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad \Gamma^3 = \mathcal{C}_2^z = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \]  

(S17)

\[ \Gamma^4 = \mathcal{P}\mathcal{C}_2^y = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \Gamma^5 = \mathcal{P}\mathcal{C}_2^z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad \Gamma^6 = \mathcal{C}_3^1 = \begin{pmatrix} -1 & 0 & 0 \\ \frac{-\sqrt{3}}{2} & \frac{1}{2} & 0 \\ \frac{-\sqrt{3}}{2} & -\frac{1}{2} & 0 \end{pmatrix}, \]  

(S18)

\[ \Gamma^7 = \mathcal{C}_4^{-1z} = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \Gamma^8 = \mathcal{P}\mathcal{C}_4^{-1z} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad \Gamma^9 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \]  

(S19)

\[ \Gamma^0 = \hat{I} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \]  

(S20)

\[ \Gamma^k = \Gamma^k T : k = 0, 1, 2, 3, ..., 9, \]  

(S21)

where the \( T \) is the time-reversal operation. In this way, we can obtain the general matrices representations of physical quantities. The general matrices of the Class I and Class III can be found in Table S2.
| Schoenflies | International | Class I | Class II | Class III |
|-------------|---------------|---------|---------|---------|
| C1          | 1             | 11'     |         |         |
| S2          | I             | 11'     | 1'      |         |
| C2          | 2             | 21'     | 2'      |         |
| C1v         | m             | m1'     | m'      |         |
| C2h         | 2/m           | 2/m1'   | 2/m', 2/m', 2'/m' |         |
| D2          | 222           | 2221'   | 22'2'  |         |
| C2v         | 2mm           | 2mm1'   | 2m'm', 2'm'm' |         |
| D2h         | mmm           | mmm1'   | m'm'm', m'm'm', m'm'm' |         |
| C4          | 4             | 41'     | 4'      |         |
| S4          | 4             | 41'     | 4'      |         |
| C4h         | 4/m           | 4/m1'   | 4/m', 4'/m, 4'/m' |         |
| D4          | 422           | 4221'   | 42'2', 4'22 |         |
| C4v         | 4mm           | 4mm1'   | 4'm', 4'm'm' |         |
| D2d         | 42m           | 42m1'   | 4'2'm', 4'2'm, 42'm' | 4/m'm', 4/m'm, 4/m'mm, |         |
| D4h         | 4/mmm         | 4/mmm1' | 4'/m'mm', 4'/m'm'm' | 4/m'm'm' |         |
| C3          | 3             | 31'     |         |         |

| Schoenflies | International | Class I | Class II | Class III |
|-------------|---------------|---------|---------|---------|
| S6          | 3             | 31'     | 3'      |         |
| D3          | 32            | 321'    | 32'     |         |
| C3v         | 3m            | 3m1'    | 3m'     |         |
| D3d         | 3m            | 3m1'    | 3'm', 3'm, 3m' |         |
| C6          | 6             | 61'     | 6'      |         |
| C3h         | 6             | 61'     | 6'      |         |
| C6h         | 6/m           | 6/m1'   | 6/m', 6'/m, 6'/m' |         |
| D6          | 622           | 6221'   | 62'2', 6'22' |         |
| C6v         | 6mm           | 6mm1'   | 6m'm', 6'm'm' |         |
| D32h        | 6m2           | 6m21'   | 6m2', 6'm2', 6'm'2 | 6'/m'm', 6'/m'm'm' |         |
| D6h         | 6/mmm         | 6/mmm1' | 6/m'm', 6/m'm'm | 6/m'm' |         |
| T           | 23            | 231'    |         |         |
| Th          | m3            | m31'    | m3'     |         |
| O           | 432           | 4321'   | 4'32    |         |
| Td          | 43m           | 43m1'   | 4'3m'   |         |
| Oh          | m3m           | m3m1'   | m3'm', m3'm, m3'm' |         |
| MPG | Generation matrix | MPG | Generation matrix | MPG | Generation matrix | MPG | Generation matrix |
|-----|------------------|-----|------------------|-----|------------------|-----|------------------|
| 1   | $\Gamma^0$      | 3'  | $\Gamma^0, \Gamma^3, \Gamma^8$ | 3'  | $\Gamma^0, \Gamma^6, \Gamma^1$ | 6m2 | $\Gamma^0, \Gamma^2, \Gamma^3, \Gamma^6$ |
| 1'  | $\Gamma^0, \Gamma^1$ | 4/m | $\Gamma^0, \Gamma^1, \Gamma^7$ | 32  | $\Gamma^0, \Gamma^2, \Gamma^6$ | 6m'2' | $\Gamma^0, \Gamma^5, \Gamma^6, \Gamma^2$ |
| 1'' | $\Gamma^0, \Gamma^1$ | 4/m' | $\Gamma^0, \Gamma^7, \Gamma^1$ | 32' | $\Gamma^0, \Gamma^6, \Gamma^2$ | 6'm'2' | $\Gamma^0, \Gamma^4, \Gamma^6, \Gamma^2$ |
| 2   | $\Gamma^0, \Gamma^3$ | 4'/m | $\Gamma^0, \Gamma^3, \Gamma^3, \Gamma^7$ | 3m' | $\Gamma^0, \Gamma^4, \Gamma^6$ | 6'm'2' | $\Gamma^0, \Gamma^2, \Gamma^6, \Gamma^5$ |
| 2'  | $\Gamma^0, \Gamma^3$ | 4'/m' | $\Gamma^0, \Gamma^8, \Gamma^1$ | 3m' | $\Gamma^0, \Gamma^6, \Gamma^4$ | 6'/mmm | $\Gamma^0, \Gamma^1, \Gamma^2, \Gamma^3, \Gamma^6$ |
| m   | $\Gamma^0, \Gamma^5$ | 422  | $\Gamma^0, \Gamma^2, \Gamma^7$ | 3m' | $\Gamma^0, \Gamma^1, \Gamma^2, \Gamma^6$ | 6'/mmm' | $\Gamma^0, \Gamma^2, \Gamma^5, \Gamma^6, \Gamma^1$ |
| m'  | $\Gamma^0, \Gamma^5$ | 42'2' | $\Gamma^0, \Gamma^7, \Gamma^2$ | 3'm' | $\Gamma^0, \Gamma^2, \Gamma^6, \Gamma^1$ | 6'/mm' | $\Gamma^0, \Gamma^1, \Gamma^2, \Gamma^6, \Gamma^2$ |
| 2/m | $\Gamma^0, \Gamma^1, \Gamma^3$ | 4'/22 | $\Gamma^0, \Gamma^2, \Gamma^3, \Gamma^7$ | 3'm | $\Gamma^0, \Gamma^4, \Gamma^6, \Gamma^1$ | 6'm' | $\Gamma^0, \Gamma^2, \Gamma^3, \Gamma^6, \Gamma^1$ |
| 2'/m | $\Gamma^0, \Gamma^3, \Gamma^1$ | 4mm | $\Gamma^0, \Gamma^4, \Gamma^7$ | 3'm | $\Gamma^0, \Gamma^1, \Gamma^6, \Gamma^2$ | 6'm' | $\Gamma^0, \Gamma^3, \Gamma^4, \Gamma^6, \Gamma^1$ |
| 2'/m' | $\Gamma^0, \Gamma^5, \Gamma^1$ | 4'm'm' | $\Gamma^0, \Gamma^7, \Gamma^4$ | 6 | $\Gamma^0, \Gamma^3, \Gamma^6$ | 6'/mm'm' | $\Gamma^0, \Gamma^1, \Gamma^3, \Gamma^6, \Gamma^2$ |
| 2'/m'' | $\Gamma^0, \Gamma^1, \Gamma^3$ | 4'm'm' | $\Gamma^0, \Gamma^3, \Gamma^4, \Gamma^7$ | 6' | $\Gamma^0, \Gamma^6, \Gamma^3$ | 23 | $\Gamma^0, \Gamma^3, \Gamma^9$ |
| 222 | $\Gamma^0, \Gamma^2, \Gamma^3$ | 42m | $\Gamma^0, \Gamma^2, \Gamma^8$ | 6 | $\Gamma^0, \Gamma^5, \Gamma^6$ | 6m3 | $\Gamma^0, \Gamma^1, \Gamma^3, \Gamma^9$ |
| 22'2 | $\Gamma^0, \Gamma^3, \Gamma^2$ | 42'm' | $\Gamma^0, \Gamma^8, \Gamma^4$ | 6' | $\Gamma^0, \Gamma^6, \Gamma^3$ | 6m'3 | $\Gamma^0, \Gamma^3, \Gamma^9, \Gamma^1$ |
| 2mm | $\Gamma^0, \Gamma^3, \Gamma^4$ | 4'/2m' | $\Gamma^0, \Gamma^2, \Gamma^3, \Gamma^3$ | 6/m | $\Gamma^0, \Gamma^1, \Gamma^3, \Gamma^6$ | 432 | $\Gamma^0, \Gamma^7, \Gamma^9$ |
| 2'm'm | $\Gamma^0, \Gamma^3, \Gamma^4$ | 4'/2m | $\Gamma^0, \Gamma^3, \Gamma^4, \Gamma^8$ | 6/m' | $\Gamma^0, \Gamma^3, \Gamma^6, \Gamma^1$ | 4'32 | $\Gamma^0, \Gamma^3, \Gamma^9, \Gamma^7$ |
| 2'm'm' | $\Gamma^0, \Gamma^4, \Gamma^3$ | 4/m'mm | $\Gamma^0, \Gamma^3, \Gamma^2, \Gamma^7$ | 6'/m | $\Gamma^0, \Gamma^5, \Gamma^6, \Gamma^1$ | 43'm | $\Gamma^0, \Gamma^8, \Gamma^9$ |
| mmm | $\Gamma^0, \Gamma^2, \Gamma^3, \Gamma^3$ | 4'/m'm'm | $\Gamma^0, \Gamma^2, \Gamma^7, \Gamma^1$ | 6'/m | $\Gamma^0, \Gamma^1, \Gamma^6, \Gamma^3$ | 4'3'm | $\Gamma^0, \Gamma^3, \Gamma^9, \Gamma^8$ |
| m'm'm | $\Gamma^0, \Gamma^3, \Gamma^4, \Gamma^3$ | 4/m'mmm | $\Gamma^0, \Gamma^4, \Gamma^2, \Gamma^7$ | 622 | $\Gamma^0, \Gamma^2, \Gamma^3, \Gamma^6$ | 6'm'3 | $\Gamma^0, \Gamma^1, \Gamma^7, \Gamma^9$ |
| m'm'm' | $\Gamma^0, \Gamma^3, \Gamma^4, \Gamma^1$ | 4'/m'm'm | $\Gamma^0, \Gamma^2, \Gamma^8, \Gamma^1$ | 6'2'2 | $\Gamma^0, \Gamma^3, \Gamma^6, \Gamma^2$ | 6'm3 | $\Gamma^0, \Gamma^8, \Gamma^9, \Gamma^1$ |
| m'mm | $\Gamma^0, \Gamma^3, \Gamma^4, \Gamma^1$ | 4'/m'm'm' | $\Gamma^0, \Gamma^2, \Gamma^8, \Gamma^1$ | 6'2'2' | $\Gamma^0, \Gamma^2, \Gamma^6, \Gamma^3$ | 6'm'3 | $\Gamma^0, \Gamma^8, \Gamma^9, \Gamma^1$ |
| 4   | $\Gamma^0, \Gamma^7$ | 4/m'm'm' | $\Gamma^0, \Gamma^3, \Gamma^2, \Gamma^7$ | 6mm | $\Gamma^0, \Gamma^3, \Gamma^4, \Gamma^6$ | 6'm'3 | $\Gamma^0, \Gamma^1, \Gamma^3, \Gamma^9, \Gamma^7$ |
| 4'  | $\Gamma^0, \Gamma^3, \Gamma^7$ | 3 | $\Gamma^0, \Gamma^6$ | 6m'm' | $\Gamma^0, \Gamma^3, \Gamma^6, \Gamma^4$ |
| 4'' | $\Gamma^0, \Gamma^8$ | 3 | $\Gamma^0, \Gamma^1, \Gamma^6$ | 6'm'm' | $\Gamma^0, \Gamma^4, \Gamma^6, \Gamma^3$ |
SIII. SYMMETRY ANALYSIS

Since there are published papers working on some groups and symmetry analysis, here we give a comparison between their derivation and this work.

| Research Object | Symmetry Analysis | References |
|-----------------|-------------------|------------|
| $D_{cd}$        | List the allowed point group: $C_1, C_{1v}, O, T, D_{2d}, S_4, C_n, C_{nv}, D_n (n = 2, 3, 4, 6)$. | Ref. [1] |
| $\chi_{\text{BCD}}^{abc}$ | Give the 2d matrix representations for 16 point group: $C_1, C_{1v}, D_{2d}, S_4, C_n, C_{nv}, D_n (n = 2, 3, 4, 6)$. | Ref. [8] |
| $\chi_{\text{BCD/BCP}}^{xyy}$ and $\chi_{\text{BCD/BCP}}^{yyx}$ | List and compare the contraints of common point group operations. | Ref. [4] |
| $\chi_{\text{BCD/BCP/D}}^{abc}$ | Classify the MPGs by the existence or absence $\chi_{abc}^{\text{BCD/BCP/D}}$. | Ref. [3] |
| $\chi_{\text{BCD(s)}}^{abc}$ | List the conditions of the Néel vector in 15 allowed PT-MPGs (except for $\Gamma$). | Ref. [9] |
| $\chi_{\text{BCD/BCP/D}}^{abc}$ and $\chi_{\text{BCD/BCP/D(s)}}^{abc}$ | Present the allowed MPGs and all matrix representations. | In this work |

A. The second-order charge response tensor

Firstly, we give a list of all the MPGs that allow $\chi_{\text{BCD}}^{abc}$ in Table S4. The first column is the class of the MPGs, where the parentheses indicate the number of MPGs allowed and the total number of MPGs. For instance, the second row, the first column tells us that there are 16 of 32 Class I MPGs in which the $\chi_{\text{BCD}}^{abc}$ exists. The last column point out the sequence number of the table represented by the corresponding matrix representations. The corresponding results of the BCP and Drude terms are shown in Table S5 and S6.

It is worth to mentioning that the second-order charge response tensor also can be represented as a rank-two pseudo-tensor Berry curvature dipole $D_{ab} = \int_k f_0 (\partial_a \Omega_b)$. According to the Eq. S8, we have

$$\chi_{\text{BCD}}^{abc} = \frac{e^2 \tau}{\hbar} \epsilon_{abc} D_{cd}$$  \hspace{1cm} (S22)

For the MPG 23 (T) and 432(O), we have

$$D = \begin{pmatrix} D_{xx} & 0 & 0 \\ 0 & D_{xx} & 0 \\ 0 & 0 & D_{xx} \end{pmatrix}$$ \hspace{1cm} (S23)

Hence, the second-order charge response tensor can be written,

$$\chi_{x}^{\text{BCD}} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & xyz \\ 0 & -xyz & 0 \end{pmatrix}, \quad \chi_{y}^{\text{BCD}} = \begin{pmatrix} 0 & 0 & -xyz \\ 0 & 0 & 0 \\ xyz & 0 & 0 \end{pmatrix}, \quad \chi_{z}^{\text{BCD}} = \begin{pmatrix} 0 & xyz & 0 \\ -xyz & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$ \hspace{1cm} (S24)

Hence we can get the charge current

$$j_x = \sum_{bc} \chi_{x}^{\text{BCD}} E_b E_c = (\chi_{xyy}^{\text{BCD}} + \chi_{xzz}^{\text{BCD}}) E_y E_z = (\chi_{x}^{\text{BCD}} - \chi_{yy}^{\text{BCD}}) E_y E_z = 0,$$ \hspace{1cm} (S25)

$$j_y = \sum_{bc} \chi_{y}^{\text{BCD}} E_b E_c = 0,$$ \hspace{1cm} (S26)

$$j_z = \sum_{bc} \chi_{z}^{\text{BCD}} E_b E_c = 0.$$ \hspace{1cm} (S27)

Hence, there is no second-order response current for the MPGs T(23) and O(432).
### TABLE S4. 53 MPGs classified by the existence of $\upsilon_{BCD}$.

| Class    | MPGs                                                                 | Matrix representations |
|----------|----------------------------------------------------------------------|------------------------|
| I (16/32)| 1, 2, 3, 4, 6, m, 2mm, 3m, 4mm, 6mm, 222, 32, 422, 622, 42m, 4        | Table S10              |
| II (16/32)| 11', 21', 31', 41', 61', m1', 2mm1', 3m1', 4mm1', 6mm1', 2221', 321', 4221', 6221', 42m1', 41' | Table S11              |
| III (21/58)| 2', m', 22'2', 2m'm', 2'm'm', 4', 6', 4'22, 42'2', 32', 6'22', 62'2', 42'm', 4'2'm, 4'm', 4'm'          | Table S11              |
|          | 6'm'm', 4m'm', 3m', 6m'm'                                             |                        |

### TABLE S5. 53 MPGs classified by the existence of $\upsilon_{BCP}$.

| Class    | MPGs                                                                 | Matrix representations |
|----------|----------------------------------------------------------------------|------------------------|
| I (16/32)| 1, 2, 3, 4, 6, m, 2mm, 3m, 4mm, 6mm, 222, 32, 422, 622, 42m, 4        | Table S12              |
| II (0/32)| none                                                                  |                        |
| III (37/58)| 1', 2', m', 2'/m', 2'/m, 22'2', 2m'm', 2'm'm', m'm'm', m'm'm, 4', 4'/m', 4'/m', 4'22, 42'2'          | Table S13              |
|          | 4'm'm', 4m'm', 4'2'm, 42'm', 4/m'm, 4'/m'm'm', 4'2'm', 4/m'm'm', 3m', 3', 32', 3'm', 3'm, 6'm', 6'/m, 6/m'm, 6/m'm' |                        |

### TABLE S6. 58 MPGs classified by the existence of $\upsilon_D$.

| Class    | MPGs                                                                 | Matrix representations |
|----------|----------------------------------------------------------------------|------------------------|
| I (18/32)| 1, 2, m, 222, 2mm, 4, 4, 4mm, 42m, 3, 32, 3m, 6, 6, 6mm, 6m2, 23, 43m | Table S14              |
| II (0/32)| none                                                                  |                        |
| III (40/58)| 1', 2', m', 2'/m', 2'/m, 22'2', 2m'm', 2'm'm', m'm'm', m'm'm, 4', 4'/m', 4'/m', 4'22, 42'2'          | Table S15              |
|          | 4'm'm', 4'2'm, 42'm', 4/m'm, 4'/m'm'm', 3', 3m', 32', 3'm', 3'm, 6', 6'/m, 6'/m, 6'/m, 6'/m, 6'/m, 6'/m, 6'/m, 6'/m |                        |
B. The second-order spin response tensor

In order to distinction, we call these spin-dependent BCD, BCP and Drude terms. The lists of allowed MPGs are shown for spin-dependent BCD (Table S7), BCP (Table S8) and Drude terms (Table S9).

| Class   | MPGs                                                                 | Matrix representations |
|---------|----------------------------------------------------------------------|------------------------|
| II (0/32) | none                                                                 |                        |
| III (37/58) | $\bar{1}', 2', m', 2'/m, 2'/m, 22'2', 2m'm', 2'm'm', m'm'm', m'm'm', 4', $4'/m', $4'/m'$, 42'2', 42'2', $4'$22, 4m'm', 4'm'm', 42'24'm', 4/m'm'm', 4/m'm'm', 4/m'm'm', 3', 32', 3'm', 3'3', 3'm', 3'm$, 6', 6/m'm', 62'2', 6m'm', 6'/m'm', 6/m'm |

Table S16

| Class   | MPGs                                                                 | Matrix representations |
|---------|----------------------------------------------------------------------|------------------------|
| II (16/32) | 11', 21', 31', 41', 61', 1m', 2mm1', 3m1', 4mm1', 6mm1', 2221', 321', 4221', 6221', 42m1', 41' |                        |
| III (21/58) | 2', 2'm', 2'm2', 2'm'm', 2'm'm', 4', 42', 42'22', 4'm', 4'm'm', 42'm', 42'm', 42'm', 42'm', 42'm', 42'm', 42'm', 32', 3'm', 6', 62'2', 6m2', 6'm', 6'mm' |

Table S17

| Class   | MPGs                                                                 | Matrix representations |
|---------|----------------------------------------------------------------------|------------------------|
| II (18/32) | 11', 21', 1m', 2221', 2mm1', 41', 441', 4mm1', 42m1', 31', 321', 3m1', 61', 6m1', 6m21', 231', 43m1' |                        |
| III (21/58) | 2', 2'm', 22'2', 2'm', 2'm', 2'm', 4', 44', 4m'm', 4m'm', 42'm', 42'm', 42'm', 32', 3'm', 6', 6'm', 6'mm', 6'mm', 6'mm', 6'mm', 6'mm' |

Table S19

According to the Table S4–S9, we can find the Class II omitted in Table S5, S6 and S7 but presented in S4, S8 and S9. This issue is due to the time reversal operator. Class II contains $\mathcal{T}$ as an element to satisfy the time reversal symmetry (TRS). If the tensor does not satisfy the TRS, the Class II MPGs must forbid the corresponding current. Under the time reversal operator, we have

$$
\chi^{\text{BCD/BCP/D(}\sigma\text{)}}_{abc}(\mathbf{k}) \xrightarrow{\mathcal{T}} \chi^{\text{BCD/BCP/D(}\sigma\text{)}}_{abc}(-\mathbf{k}).
$$

(S28)

According to Eq. (S8),

$$
\chi^{\text{BCP/D(}\sigma\text{)}}_{abc}(-\mathbf{k}) = -\chi^{\text{BCP/D(}\sigma\text{)}}_{abc}(\mathbf{k})
$$

(S29)

and

$$
\chi^{\text{BCD(}\sigma\text{)}}_{abc}(-\mathbf{k}) = \chi^{\text{BCD(}\sigma\text{)}}_{abc}(\mathbf{k}).
$$

(S30)

For the second charge current contributed by the BCD,

$$
\chi^{\text{BCD}}_{abc}(\mathbf{k}) = \chi^{\text{BCD(}\uparrow\text{)}}_{abc}(\mathbf{k}) + \chi^{\text{BCD(}\downarrow\text{)}}_{abc}(\mathbf{k})
\xrightarrow{\mathcal{T}} \chi^{\text{BCD(}\downarrow\text{)}}_{abc}(-\mathbf{k}) + \chi^{\text{BCD(}\uparrow\text{)}}_{abc}(-\mathbf{k}) = \chi^{\text{BCD(}\downarrow\text{)}}_{abc}(\mathbf{k}) + \chi^{\text{BCD(}\uparrow\text{)}}_{abc}(\mathbf{k}) = \chi^{\text{BCD}}_{abc}(\mathbf{k}).
$$

(S30)
Thus, the BCD term satisfies the time reversal symmetry.

For the BCP and Drude terms,
\[
\chi_{abc}^{BCP/D}(k) = \chi_{abc}^{BCP/D(\uparrow)}(k) + \chi_{abc}^{BCP/D(\downarrow)}(k)
\]
\[
\mathcal{T} \chi_{abc}^{BCP/D(\downarrow)}(-k) + \chi_{abc}^{BCP/D(\uparrow)}(-k) = -\chi_{abc}^{BCP/D(\downarrow)}(k) - \chi_{abc}^{BCP/D(\uparrow)}(k) = -\chi_{abc}^{BCP/D}(k),
\] (S31)
they are both zero for the time reversal symmetry. Therefore, the existence of time reversal symmetry enables the BCP and Drude vanishing but BCD existing, which leads to the Class II ($\mathcal{T}$ is an element for Class II MPG) omitted in Table S5 (BCP) and S6 (Drude) while presented in S4 (BCD).

For the spin current, the spin BCD, BCP and Drude terms are defined as
\[
\chi_{abc}^{BCD/B/CP/D(s)}(k) = \chi_{abc}^{BCD/B/CP/D(\uparrow)}(k) - \chi_{abc}^{BCD/B/CP/D(\downarrow)}(k)
\] (S32)
By analogy with Eq. (S30) and Eq. (S31), we have
\[
\chi_{abc}^{BCD(s)}(k) = \chi_{abc}^{BCD(\uparrow)}(k) - \chi_{abc}^{BCD(\downarrow)}(k)
\]
\[
\mathcal{T} \chi_{abc}^{BCD(\downarrow)}(-k) - \chi_{abc}^{BCD(\uparrow)}(-k) = \chi_{abc}^{BCD(\downarrow)}(k) - \chi_{abc}^{BCD(\uparrow)}(k) = -\chi_{abc}^{BCD(s)}(k).
\] (S33)
And,
\[
\chi_{abc}^{BCD(s)}(k) = \chi_{abc}^{BCD(\uparrow)}(k) - \chi_{abc}^{BCD(\downarrow)}(k)
\]
\[
\mathcal{T} \chi_{abc}^{BCD(\downarrow)}(-k) - \chi_{abc}^{BCD(\uparrow)}(-k) = -\chi_{abc}^{BCD(\downarrow)}(k) + \chi_{abc}^{BCD(\uparrow)}(k) = \chi_{abc}^{BCD(s)}(k).
\] (S34)

For time reversal symmetry, the spin-dependent BCD is zero, while the spin-dependent BCP and Drude are allowed. So the Class II omitted in Table S7 (spin-dependent BCD) but presented in Table S8 (spin-dependent BCP) and S9 (spin-dependent Drude).

Another important message is that the third line in Table S4 (BCD for Class III) is identical to the third line in Table S8 (spin-BCP for class III), while the third line in Table S5 (BCP for Class III) is identical to the second line in Table S7 (spin-BCD for class III).

For the second charge conductivity,
\[
\lambda_{abc}^{BCP/D} = \lambda_{abc}^{BCP/D(\uparrow)} + \lambda_{abc}^{BCP/D(\downarrow)} \mathcal{T} \sum_{i,j,k} \Gamma_{ai}^{\uparrow} \Gamma_{bj}^{\downarrow} \Gamma_{ck}^{\downarrow} \chi_{ijk}^{BCP/D(\downarrow)} + \sum_{i,j,k} \Gamma_{ai}^{\uparrow} \Gamma_{bj}^{\downarrow} \Gamma_{ck}^{\downarrow} \chi_{ijk}^{BCP/D(\uparrow)}
\]
\[
\lambda_{abc}^{BCP/D} = \lambda_{abc}^{BCP/D(\uparrow)} + \lambda_{abc}^{BCP/D(\downarrow)} \mathcal{T} \sum_{i,j,k} \Gamma_{ai}^{\uparrow} \Gamma_{bj}^{\downarrow} \chi_{ijk}^{BCP/D(\downarrow)} - \sum_{i,j,k} \Gamma_{ai}^{\uparrow} \Gamma_{bj}^{\downarrow} \chi_{ijk}^{BCP/D(\uparrow)} - \sum_{i,j,k} \Gamma_{ai}^{\uparrow} \Gamma_{bj}^{\downarrow} \Gamma_{ck}^{\downarrow} \chi_{ijk}^{BCP/D(\downarrow)}.
\]
(S35)

As the component of charge and spin response tensors is unchanged before and after the symmetry operation, we can find every nonzero component of the tensors. Based on Eq. (S35), the condition of non-zero charge current is
\[
\chi_{abc}^{BCD(\uparrow)} = \sum_{i,j,k} \Gamma_{ai}^{\uparrow} \Gamma_{bj}^{\downarrow} \Gamma_{ck}^{\downarrow} \chi_{ijk}^{BCD(\downarrow)}, \chi_{abc}^{BCD(\downarrow)} = \sum_{i,j,k} \Gamma_{ai}^{\uparrow} \Gamma_{bj}^{\downarrow} \Gamma_{ck}^{\downarrow} \chi_{ijk}^{BCD(\uparrow)}
\]
\[
\chi_{abc}^{BCP/D(\uparrow)} = \sum_{i,j,k} \Gamma_{ai}^{\uparrow} \Gamma_{bj}^{\downarrow} \Gamma_{ck}^{\downarrow} \chi_{ijk}^{BCP/D(\downarrow)}, \chi_{abc}^{BCP/D(\downarrow)} = -\sum_{i,j,k} \Gamma_{ai}^{\uparrow} \Gamma_{bj}^{\downarrow} \Gamma_{ck}^{\downarrow} \chi_{ijk}^{BCP/D(\uparrow)}.
\] (S36)

For the second spin conductivity,
\[
\chi_{abc}^{BCD(s)} = \chi_{abc}^{BCD(\uparrow)} - \chi_{abc}^{BCD(\downarrow)} \mathcal{T} \sum_{i,j,k} \Gamma_{ai}^{\uparrow} \Gamma_{bj}^{\downarrow} \Gamma_{ck}^{\downarrow} \chi_{ijk}^{BCD(\downarrow)} - \sum_{i,j,k} \Gamma_{ai}^{\uparrow} \Gamma_{bj}^{\downarrow} \Gamma_{ck}^{\downarrow} \chi_{ijk}^{BCD(\uparrow)}
\]
\[
\chi_{abc}^{BCP/D(s)} = \chi_{abc}^{BCP/D(\uparrow)} - \chi_{abc}^{BCP/D(\downarrow)} \mathcal{T} \sum_{i,j,k} \Gamma_{ai}^{\uparrow} \Gamma_{bj}^{\downarrow} \chi_{ijk}^{BCP/D(\downarrow)} - \sum_{i,j,k} \Gamma_{ai}^{\uparrow} \Gamma_{bj}^{\downarrow} \Gamma_{ck}^{\downarrow} \chi_{ijk}^{BCP/D(\uparrow)} + \sum_{i,j,k} \Gamma_{ai}^{\uparrow} \Gamma_{bj}^{\downarrow} \Gamma_{ck}^{\downarrow} \chi_{ijk}^{BCP/D(\downarrow)}.
\] (S37)
And,
\[
\chi_{abc}^{BCD(\uparrow)} = -\sum_{i,j,k} \Gamma_{ai}^{\uparrow} \Gamma_{bj}^{\downarrow} \Gamma_{ck}^{\downarrow} \chi_{ijk}^{BCD(\downarrow)}, \chi_{abc}^{BCD(\downarrow)} = -\sum_{i,j,k} \Gamma_{ai}^{\uparrow} \Gamma_{bj}^{\downarrow} \Gamma_{ck}^{\downarrow} \chi_{ijk}^{BCD(\uparrow)}
\]
\[
\chi_{abc}^{BCP/D(\uparrow)} = \sum_{i,j,k} \Gamma_{ai}^{\uparrow} \Gamma_{bj}^{\downarrow} \Gamma_{ck}^{\downarrow} \chi_{ijk}^{BCP/D(\downarrow)}, \chi_{abc}^{BCP/D(\downarrow)} = \sum_{i,j,k} \Gamma_{ai}^{\uparrow} \Gamma_{bj}^{\downarrow} \Gamma_{ck}^{\downarrow} \chi_{ijk}^{BCP/D(\uparrow)}.
\] (S38)
Because the BCD and spin-dependent BCP have the same independent components, the first line in Eq. (S36) for BCD is the same as the second line in Eq. (S38) for the spin-dependent BCP term. Thus, the third line in Table S4 (BCD for Class III) is identical to the third line in Table S8 (spin-BCP for class III).

Since the second line in Eq. (S36) for BCP is the same as the first in Eq. (S37) for spin-dependent BCD term, the third line in Table S5 (BCP for Class III) is identical to the second line in Table S7 (spin-BCD for class III).

However, the Drude term IS interchangeably symmetric for any two indices, and has 10 independent components, which causes the Drude term is special and have more allowed Class III MPGs (Table S6 and S9).

Next we give all corresponding matrix representations and candidate materials in Table S10 – S20.
Table S10: Matrix representations and candidate materials of second-order charge response tensor $\chi_{\text{BCD}}$ for Class I MPGs.

| Class I MPGs | $\sigma_{\text{BCD}}^x$ | $\sigma_{\text{BCD}}^y$ | $\sigma_{\text{BCD}}^z$ | Shortened form | Candidate materials |
|--------------|----------------|----------------|----------------|--------------|-------------------|
| 1            | $\begin{pmatrix} 0 & 0 & 0 \\ xy & xy & xy \\ xz & xz & xz \end{pmatrix}$ | $\begin{pmatrix} -xy & -xy & -xy \\ 0 & 0 & 0 \\ yz & yz & yz \end{pmatrix}$ | $\begin{pmatrix} -zx & -zy & -zx \\ -yz & -zy & -yz \\ 0 & 0 & 0 \end{pmatrix}$ | $A_{\text{BCD}}$ | twisted bilayer graphene [10]* |
| 2            | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & xy \\ xz & xz & xz \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & -xy \\ 0 & 0 & 0 \\ yz & yz & yz \end{pmatrix}$ | $\begin{pmatrix} -zx & -zy & 0 \\ -yz & -yz & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $B_{\text{BCD}}$ | LiFeP$_2$O$_7$ [11] |
| m            | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & xz \\ xy & xy & xy \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ yz & yz & yz \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & -xz \\ 0 & 0 & 0 \\ xz & xz & xz \end{pmatrix}$ | $C_{\text{BCD}}$ | Bilayer WTe$_2$ [12]*, Graphene [13]* |
| 222          | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & xy \\ 0 & xy & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & -xy \\ 0 & 0 & 0 \\ yz & yz & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & -xy & 0 \\ -yz & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $D_{\text{BCD}}$ | FePO$_4$ [14] |
| 2mm          | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ xz & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ yz & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ -zx & 0 & 0 \end{pmatrix}$ | $E_{\text{BCD}}$ | FeSb$_2$O$_4$ [15] |
| 4            | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & xy \\ xz & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ yz & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ -zx & -zy & 0 \end{pmatrix}$ | $F_{\text{BCD}}$ | Ce$_2$TeO$_6$ [16] |
| 3            | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & xy \\ xz & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ yz & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ xz & xz & 0 \end{pmatrix}$ | $F_{\text{BCD}}$ | Cu$_2$OSeO$_3$ [17] |
| 6            | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & xz \\ xy & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ yz & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ xz & xz & 0 \end{pmatrix}$ | $H_{\text{BCD}}$ | ScMnO$_3$ [18] |
| 4            | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & xz \\ xy & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ yz & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ xz & xz & 0 \end{pmatrix}$ | $H_{\text{BCD}}$ | – |
| 422          | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ xz & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ yz & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ xz & xz & 0 \end{pmatrix}$ | $J_{\text{BCD}}$ | Ho$_2$Ge$_2$O$_7$ [19] |
| 32           | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ xz & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ yz & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ xz & xz & 0 \end{pmatrix}$ | $J_{\text{BCD}}$ | La1/3Sr2/3FeO$_3$ [20] |
| 622          | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & xz \\ xy & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ yz & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ xz & xz & 0 \end{pmatrix}$ | $J_{\text{BCD}}$ | – |
| 4mm          | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ xz & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ yz & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ xz & xz & 0 \end{pmatrix}$ | $J_{\text{BCD}}$ | PbNiO$_3$ [21] |
| 3m           | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ xz & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ yz & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ xz & xz & 0 \end{pmatrix}$ | $J_{\text{BCD}}$ | (Y,Ho)MnO$_3$ [18, 22] |
| 6mm          | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ xz & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ yz & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ xz & xz & 0 \end{pmatrix}$ | $K_{\text{BCD}}$ | HgTe [23]* |

*Nonlinear charge current contributed by the BCD has been reported.
### TABLE S11: Matrix representations of second-order charge response tensor $\chi^{BCD}$ for Class II and III MPGs.

| Class MPGs | Shortened form | Candidate materials |
|------------|----------------|---------------------|
| 11'        | $A^{BCD}$      | NiPS$_3$ [24]       |
| 21' 2'     | $B^{BCD}$      | HoNiO$_3$ [11]      |
|            |                | U$_3$Al$_2$Si$_3$ [25] |
| m1' m'     | $C^{BCD}$      | Na$_2$MnF$_3$ [26]  |
|            |                | MnTiO$_3$ [27]       |
| 2221' 22'  | $D^{BCD}$      | AgNiO$_2$ [28]      |
|            |                | (Cs,Rb)NiCl$_3$ [29, 30] |
| 2mm1' 2'm' | $E^{BCD}$      | MnS$_2$ [31]        |
|            |                | MnSO$_4$ [32], TbCrO$_3$ [33] |
|            |                | MnSe$_2$ [34]       |
| 41' 31' 6' | $F^{BCD}$      | CeAuAl$_3$ [35]     |
|            |                | Ni$_3$TeO$_6$ [36]  |
|            |                | –                   |
| 4' 6'      |                | YMnO$_3$ [37]       |
| 4'         | $H^{BCD}$      | –                   |
|            |                | CsCoF$_4$ [38]      |
| 4221' 321' | $I^{BCD}$      | MnO$_2$ [39]        |
|            |                | SrFeO$_3$ [40]      |
| 6221' 4'2' |                | ScMn$_6$Ge$_6$ [41] |
| 42' 2'     |                | Er$_2$Ge$_2$O$_7$ [42] |
| 32' 6'2'   |                | Nd$_5$Si$_4$ [25]   |
|            |                | NaMnFeF$_6$ [43]    |
|            |                | –                   |
|            |                | EuIn$_2$As$_2$ [44], DyMn$_6$Ge$_6$ [45] |
| 4mm1' 3m'  | $J^{BCD}$      | CeAlGe [46]         |
|            |                | CuMnSb [47]         |
| 6mm1' 4'   |                | –                   |
| 4'm'       |                | Ce(Co,Ir)Ge$_3$ [48, 49] |
| 3m' 6'6'   |                | GaV$_4$S$_8$ [50], GaV$_4$S$_8$ [50] |
|            |                | (Yb,Ho,Mn)O$_3$ [37, 51] |
|            |                | (Yb,Ho,Sc,Mn)O$_3$ [18, 37, 51] |
| 42m1' 4'2'm| $K^{BCD}$      | GeCu$_3$O$_4$ [52] |
| 4'2'm      |                | Pb$_2$MnO$_4$ [53], Ce$_4$Sb$_3$ [54] |
| 4'2'm      |                | –                   |
| 4'2'm      |                | EuCr$_2$As$_2$ [55], MgCr$_2$O$_4$ [56] |
TABLE S12: Matrix representations and candidate materials of second-order charge response tensor $\chi^{BCP}$ for Class I MPGs.

| Class I MPGs | $\chi_{x}^{BCP}$ | $\chi_{y}^{BCP}$ | $\chi_{z}^{BCP}$ | Shortened form | Candidate materials |
|--------------|-------------------|-------------------|-------------------|---------------|-------------------|
| 1            | $\begin{bmatrix} 0 & 0 & 0 \\ yzy & yzy & yzy \\ xzx & xzy & xzz \end{bmatrix}$ | $\begin{bmatrix} -xyz & -xyz & -xyz \\ yzy & yzy & yzy \\ xzx & xzy & xzz \end{bmatrix}$ | $\begin{bmatrix} -xyz & -xyz & -xyz \\ -xyz & -xyz & -xyz \\ 0 & 0 & 0 \end{bmatrix}$ | $A^{BCP}$ |
| 2            | $\begin{bmatrix} 0 & 0 & 0 \\ yzy & yzy & yzy \\ xzx & xzy & xzz \end{bmatrix}$ | $\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ yzy & yzy & yzy \end{bmatrix}$ | $\begin{bmatrix} -xyz & -xyz & -xyz \\ 0 & 0 & 0 \\ yzy & yzy & yzy \end{bmatrix}$ | $B^{BCP}$ |
| m            | $\begin{bmatrix} xyx & xyx & xyx \\ yzy & yzy & yzy \\ xzx & xzy & xzz \end{bmatrix}$ | $\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ yzy & yzy & yzy \end{bmatrix}$ | $\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ yzy & yzy & yzy \end{bmatrix}$ | $C^{BCP}$ |
| 222          | $\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ xzy & xzy & xzza \end{bmatrix}$ | $\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ yzy & yzy & yzy \end{bmatrix}$ | $\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ yzy & yzy & yzy \end{bmatrix}$ | $D^{BCP}$ |
| 2mm          | $\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ xzy & xzy & xzza \end{bmatrix}$ | $\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ yzy & yzy & yzy \end{bmatrix}$ | $\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ yzy & yzy & yzy \end{bmatrix}$ | $E^{BCP}$ |
| 4, 3, 6      | $\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ xzy & xzy & xzza \end{bmatrix}$ | $\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ yzy & yzy & yzy \end{bmatrix}$ | $\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ yzy & yzy & yzy \end{bmatrix}$ | $F^{BCP}$ |
| $\bar{4}$    | $\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ xzy & xzy & xzza \end{bmatrix}$ | $\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ yzy & yzy & yzy \end{bmatrix}$ | $\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ yzy & yzy & yzy \end{bmatrix}$ | $G^{BCP}$ |
| 422, 32, 622 | $\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ xzy & xzy & xzza \end{bmatrix}$ | $\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ yzy & yzy & yzy \end{bmatrix}$ | $\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ yzy & yzy & yzy \end{bmatrix}$ | $H^{BCP}$ |
| 4mm, 3m, 6mm | $\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ xzy & xzy & xzza \end{bmatrix}$ | $\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ yzy & yzy & yzy \end{bmatrix}$ | $\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ yzy & yzy & yzy \end{bmatrix}$ | $I^{BCP}$ |
| $\bar{4}2m$  | $\begin{bmatrix} 0 & 0 & 0 \\ xzy & xzy & xzza \end{bmatrix}$ | $\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ yzy & yzy & yzy \end{bmatrix}$ | $\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ yzy & yzy & yzy \end{bmatrix}$ | $J^{BCP}$ |

$^1$The first column MPGs are same as in TABLE S11, so the candidates materials are not repeated here.
TABLE S13: Matrix representations and candidate materials of second-order charge response tensor $\chi^{BCP}$ for Class III MPGs.

| Class III MPGs | Shortened form | Candidate materials |
|----------------|----------------|---------------------|
| $\bar{1}'$    | $A^{BCP}$      | $\text{Cr}_2\text{S}_3$ [57] |
| $m'$          | $B^{BCP}$      | $\text{MnTiO}_3$ [27] $\text{ErGe}_3$ [58] |
| $2/m'$        | $C^{BCP}$      | $\text{U}_3\text{Al}_2\text{Si}_3$ [25] $\text{CuMnAs}$ [3]$\ast$, $\text{Cr}_2\text{O}_3$ [59] |
| $2'$          | $D^{BCP}$      | $\text{MnSO}_4$ [32], $\text{TbCrO}_3$ [33] $\text{RbFeO}_2$ [60] |
| $2'/m$        | $E^{BCP}$      | $(\text{Cs, Rb})\text{NiCl}_3$ [29, 30], $\text{MnSe}_2$ [34] $\text{Mn}_2\text{Au}$ [4]$\ast$ |
| $m'm'm'$      | $F^{BCP}$      | $\text{NdB}_4$ [61] $\text{Mn}(\text{Ti, Ge, Mg})_3$O$_3$ [62] $\text{Cu}_{0.82}\text{Mn}_{1.18}\text{As}$ [63] $\text{Cu}_{14}\text{Au}_{51}$ [64] |
| $4'$          | $G^{BCP}$      | $\text{Nd}_2\text{Ge}_2\text{O}_7$ [42] $\text{EuCr}_2\text{As}_2$ [55] $\text{MgCr}_2\text{O}_4$ [56] $\text{LiFeCr}_4\text{O}_8$ [72] $\text{CoAl}_2\text{O}_4$ [73] |

$\ast$Nonlinear charge current contributed by the BCP has been reported.
TABLE S14: Matrix representations and candidate materials of second-order charge response tensor $\chi^D$ for Class I MPGs.

| Class I MPGs | $\sigma_x^D$ | $\sigma_y^D$ | $\sigma_z^D$ | Shortened Candidate materials
|--------------|--------------|--------------|--------------|-----------------------------------|
| 1            | $\begin{pmatrix} xx & xy & xz \\ xy & xz & xz \\ xz & xz & xz \end{pmatrix}$ | $\begin{pmatrix} xy & xyy & xyy \\ xyy & xzy & xzy \\ xzy & xzy & xzy \end{pmatrix}$ | $\begin{pmatrix} xz & xzy & xzy \\ xzy & xyy & xyy \\ xzy & xzy & xzy \end{pmatrix}$ | $A^D$ |
| 2            | $\begin{pmatrix} 0 & 0 & xz \\ 0 & 0 & xz \\ xz & xz & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & xy \\ 0 & 0 & xy \\ xy & xy & 0 \end{pmatrix}$ | $\begin{pmatrix} xz & xzy & xzy \\ xzy & xyy & xyy \\ xzy & xzy & xzy \end{pmatrix}$ | $B^D$ |
| m            | $\begin{pmatrix} xx & yyy & 0 \\ xz & xzy & 0 \\ 0 & 0 & xz \end{pmatrix}$ | $\begin{pmatrix} xx & yyy & 0 \\ xz & xzy & 0 \\ 0 & 0 & xz \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & yz \\ 0 & 0 & yz \\ xz & yz & 0 \end{pmatrix}$ | $C^D$ |
| 222, 32m     | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} xx & 0 & 0 \\ xy & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $D^D$ |
| 23           | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} xz & 0 & 0 \\ xy & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $E^D$ |
| 33m          | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} xx & 0 & 0 \\ xx & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $F^D$ |
| 4            | $\begin{pmatrix} xx & xz & yz \\ 0 & 0 & 0 \\ xz & xz & 0 \end{pmatrix}$ | $\begin{pmatrix} xx & xz & yz \\ 0 & 0 & 0 \\ xz & xz & 0 \end{pmatrix}$ | $\begin{pmatrix} xx & xz & 0 \\ xx & xz & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $H^D$ |
| 32           | $\begin{pmatrix} xx & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} xx & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $I^D$ |
| 6m2          | $\begin{pmatrix} xx & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} xx & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $J^D$ |
| 3            | $\begin{pmatrix} xx & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} xx & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $K^D$ |
| 3m           | $\begin{pmatrix} xx & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} xx & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $L^D$ |

*Nonlinear charge current contributed by the Drude has been reported.
| Class III MPGs | shortened form | Candidate materials |
|----------------|---------------|----------------------|
| ċ'             | A^D           | Cr_2S_3 [57]         |
| m', 2/m'       | B^D           | MnTiO_3 [27], ErGe_3 [58] |
| 2', 2'/m       | C^D           | U_3Al_2Si_3 [25], Cr_2O_3 [59] |

|                | D^D           |                      |
|----------------|---------------|----------------------|
| 4'^32, m'^3m   |               | BaCuTe_2O_6 [80]     |
| m'^3           |               | --                   |
| 4'^mm          |               |  --                  |
| 2m'/m', m'/m'm', 4'/22 | | MnSO_4 [32], TbCrO_3 [33], RbFeO_2 [60] |
| 4'/m'/m'm'     |               | Er_2Ge_2O_7 [42], EuCr_2As_2 [55], CoAl_2O_4 [73] |

|                | E^D           |                      |
|----------------|---------------|----------------------|
| 22'2', 2'm'm', m'mmm |             | (Cs,Rb)NiCl_3 [29, 30], MnSe_2 [34], Mn_2Au [81] |

|                | F^D           |                      |
|----------------|---------------|----------------------|
| 3', 4'/m'm', 4'2'2' |             | NdBr_3 [61], Nd_2Si_4 [25] |
| 4'2'm, 4'/m'm'm, 6' |               | Co_3Al_2Si_2O_12 [69], Cu_0.82Mn_1.18As [63] |
| 6'/m', 6'2'2', 6'm2' |               | Cu_14Au_5 [64], EuIn_2As_2 [44], DyMn_6Ge_6 [45], CaFeCl_3 [71] |
| 6'/m'mm         |               | --                   |

|                | H^D           |                      |
|----------------|---------------|----------------------|
| 3'             | I^D           | Mn(Ti,Ge,Mg)O_3 [62] |

|                | J^D           |                      |
|----------------|---------------|----------------------|
| 6m'2'          |               | CsMnBr_3 [82]        |
| 6'/mmm'        |               | --                   |
| 3m', 3'm', 6'2'2', 6'm'm' | | GaV_4S_8 [50], GaV_4S_8 [50], Cr_2O_3 [67], (Yb, Ho)MnO_3 [37, 51] |

|                | K^D           |                      |
|----------------|---------------|----------------------|
| 32', 3'm       |               | NaMnFeF_6 [43], Ca_2(Y,La)Zr_2Fe_3O_12 [70] |

|                | L^D           |                      |
|----------------|---------------|----------------------|
| 6'             |               | YMnO_3 [37]          |
| 6'/m           |               | U_14Au_5 [83]        |
In this table, the candidate materials are not repeated, which are the same as the TABLE S11.

| Class III MPGs | $\chi^{BCD(s)}_{x}$ | $\chi^{BCD(s)}_{y}$ | $\chi^{BCD(s)}_{z}$ | Shortened Form |
|----------------|---------------------|---------------------|---------------------|----------------|
| $\bar{1}''$    | $\begin{pmatrix} 0 & 0 & 0 \\ xyz & xyy & xyz \\ xzx & xzy & xzz \end{pmatrix}$ | $\begin{pmatrix} -xzx & -xyz & -xzy \\ yzx & yzy & yzz \end{pmatrix}$ | $\begin{pmatrix} -yxx & -xzy & -yzz \\ 0 & 0 & 0 \end{pmatrix}$ | $A^{BCD(s)}$ |
| $m'', 2/m'$    | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -xyz \\ xzx & xzy & xzz \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ yxx & yxy & yzy \end{pmatrix}$ | $\begin{pmatrix} -yxx & -xyz & -yzy \\ 0 & 0 & 0 \end{pmatrix}$ | $B^{BCD(s)}$ |
| $2', 2'/m$     | $\begin{pmatrix} 0 & 0 & 0 \\ xyx & xyy & 0 \\ 0 & 0 & yzz \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & -xyz \\ 0 & 0 & 0 \end{pmatrix}$ | $C^{BCD(s)}$ |
| $2m''', \bar{3}''2m', m''m'm'$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -xyz \\ xyx & xyy & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} -yxx & 0 & 0 \\ -yzz & 0 & 0 \end{pmatrix}$ | $D^{BCD(s)}$ |
| $222', m'\overline{2}$ | $\begin{pmatrix} 0 & 0 & 0 \\ xzx & xzy & xzz \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $E^{BCD(s)}$ |
| $4/m', 3'/6/m', 3'/6'$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -xyz \\ xzx & xzy & xzz \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ xyy & xzy & xzz \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $F^{BCD(s)}$ |
| $4', 4'/m'$    | $\begin{pmatrix} 0 & 0 & 0 \\ xzx & xzy & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} -xzx & 0 & 0 \\ -xyz & 0 & 0 \end{pmatrix}$ | $H^{BCD(s)}$ |
| $4m'', 4/m''m'', 3m'$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -xyz \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ xzy & xzy & xzz \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $I^{BCD(s)}$ |
| $2m'$         | $\begin{pmatrix} 0 & 0 & 0 \\ xyx & xyy & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $L^{BCD(s)}$ |
| $422', 4/m''m', 32', 3'm, 622'2', 6'm2', 6/m'\overline{2}, 4'2'm$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ xzx & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $M^{BCD(s)}$ |
| $4'22m, 42'2', 4'/m'm'm$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $N^{BCD(s)}$ |
| $4'm'$        | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ xxz & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ | $O^{BCD(s)}$ |

TABLE S16: Matrix representations of second-order spin response tensor $\chi^{BCD(s)}$ for Class III MPGs.
### TABLE S17: Matrix representations of second-order spin response tensor $\chi_{\text{BCP(s)}}$ for Class II MPGs.

| Class II MPGs | $\chi_{\text{BCP(s)}}^{x}$ | $\chi_{\text{BCP(s)}}^{y}$ | $\chi_{\text{BCP(s)}}^{z}$ | Shortened form |
|---------------|-----------------------------|-----------------------------|-----------------------------|----------------|
| 11'           | (0 0 0)                     | (0 0 0)                     | (0 0 0)                     | $A_{\text{BCP(s)}}$ |
|               | (xy xz yz)                  | (xz yz yz)                  | (xz yz yz)                  | $B_{\text{BCP(s)}}$ |
| 21'           | (0 0 0)                     | (0 0 0)                     | (0 0 0)                     | $C_{\text{BCP(s)}}$ |
| m1'           | (0 0 0)                     | (0 0 0)                     | (0 0 0)                     | $D_{\text{BCP(s)}}$ |
| 2mm1'         | (0 0 0)                     | (0 0 0)                     | (0 0 0)                     | $E_{\text{BCP(s)}}$ |
| 41', 31', 61' | (0 0 0)                     | (0 0 0)                     | (0 0 0)                     | $F_{\text{BCP(s)}}$ |
| 41'           | (0 0 0)                     | (0 0 0)                     | (0 0 0)                     | $G_{\text{BCP(s)}}$ |
| 4221', 321', 6221' | (0 0 0)                     | (0 0 0)                     | (0 0 0)                     | $H_{\text{BCP(s)}}$ |
| 4mm1', 3m1', 6mm1' | (0 0 0)                     | (0 0 0)                     | (0 0 0)                     | $I_{\text{BCP(s)}}$ |
| 32m1'         | (0 0 0)                     | (0 0 0)                     | (0 0 0)                     | $J_{\text{BCP(s)}}$ |

In this table, the candidate materials are not repeated, which are the same as the TABLE S13.

### TABLE S18: Matrices expressions of second-order charge response tensor $\chi_{\text{BCP(s)}}$ for Class III MPGs.

| Class III MPGs | shortened form | Candidate materials |
|----------------|----------------|---------------------|
| 2'             | $B_{\text{BCP(s)}}$ | U$_3$Al$_2$Si$_3$ [84] |
| m'             | $C_{\text{BCP(s)}}$ | U$_3$Al$_2$Si$_3$ [25] |
| 222'2'         | $D_{\text{BCP(s)}}$ | (Cs,Rb)NiCl$_3$ [29, 30] |
| 2m',2'm'       | $E_{\text{BCP(s)}}$ | MnSO$_4$ [32], TbCrO$_3$ [33], MnSe$_2$ [34] |
| 4', 6'         | $F_{\text{BCP(s)}}$ | YMnO$_3$ [37] |
| 4'             | $H_{\text{BCP(s)}}$ | CsCoF$_4$ [38] |
| 4'22, 42'2', 32', 6'22', 62'2' | $I_{\text{BCP(s)}}$ | Er$_2$Ga$_2$O$_7$ [42], Nd$_5$Si$_4$ [25], NaMnFeF$_6$ [43], EuIn$_2$As$_2$ [44], DyMn$_6$Ge$_6$ [45] |
| 4'm', 4m', 3m', 6'm', 6m'm' | $J_{\text{BCP(s)}}$ | Ce(Co,Ir)Ge$_3$ [48, 49], GaV$_4$S$_8$ [50], CrSe [85], (Yb,Ho,Sc)MnO$_3$ [18, 37, 51] |
| 4'2m', 4'2'm, 42'm' | $K_{\text{BCP(s)}}$ | Pb$_2$MnO$_4$ [53], Ce$_4$Sb$_3$ [54], EuCr$_2$As$_2$ [55], MgCr$_2$O$_4$ [56], liFeCr$_4$O$_8$ [72] |
| Class II MPGs | $\chi^D_x$ | $\chi^D_y$ | $\chi^D_z$ | Shortened form | Candidate materials |
|--------------|----------|----------|----------|----------------|-------------------|
| 11′          | $xxy$    | $xxy$    | $xxy$    | $A^D(s)$       | NiPS$_3$ [24]    |
|              | $xxz$    | $yyz$    | $yyz$    |                |                   |
| 21′          | 0        | 0        | $xxz$    | $B^D(s)$       | HoNiO$_3$ [11]   |
|              | 0        | 0        | $xyz$    |                |                   |
| m1′          | $xxz$    | $yyz$    | 0        | $C^D(s)$       | Na$_2$MnF$_5$ [26]|
|              | 0        | 0        | 0        |                |                   |
| 231′         | 0        | 0        | 0        | $D^D(s)$       | Gd$_2$Ti$_2$O$_6$ [86] |
| 43m1′        | 0        | 0        | 0        |                |                   |
| 222′, 42m1′  | 0        | 0        | 0        | $E^D(s)$       | MnS$_2$ [31]     |
|              | 0        | 0        | 0        |                |                   |
| 41′, 4mm1′, 61′, 6mm1′ | 0        | 0        | 0        | $F^D(s)$       | CeAuAl$_3$ [35], CeAlGe [46] |
|              | 0        | 0        | 0        |                |                   |
| 41′          | 0        | 0        | 0        | $H^D(s)$       |                   |
|              | 0        | 0        | 0        |                |                   |
| 321′         | $xxx$    | 0        | 0        | $I^D(s)$       | SrFeO$_3$ [40]   |
| 62m1′        | 0        | $xxx$    | 0        |                | Ba$_6$Co$_6$ClO$_{15.5}$ [87] |
|              | 0        | 0        | 0        |                |                   |
| 31′          | $xxx$    | $-yyy$   | $xxx$   | $J^D(s)$       | Ni$_3$TeO$_6$ [36] |
|              | $-yyy$   | $xxx$   | 0        |                |                   |
| 3m1′         | 0        | $-yyy$   | $xxx$   | $K^D(s)$       | CuMnSb [47]      |
|              | $-yyy$   | 0        | $xxx$   |                |                   |
| 61′          | $xxx$    | $-yyy$   | 0        | $L^D(s)$       | TmPdIn [88]      |
|              | $-yyy$   | $xxx$   | 0        |                |                   |

**TABLE S19:** Matrix representations of second-order spin response tensor $\chi^D(s)$ for Class II MPGs.
### TABLE S20: Matrix representations of second-order spin response tensor $\chi^{D(s)}$ for Class III MPs.

| MPGs | $\chi^D(s)$ | $\chi^D(s)$ | $\chi^D(s)$ | Shortened form | Candidate materials |
|------|--------------|--------------|--------------|---------------|--------------------|
| 2'   | $\begin{pmatrix} 0 & 0 & xxz \\ xxz & xyz & 0 \\ 0 & 0 & zzz \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & xyz \\ xyz & yzy & 0 \\ 0 & 0 & zzz \end{pmatrix}$ | $\begin{pmatrix} xxz & xyz & 0 \\ xyz & yzy & 0 \\ 0 & 0 & zzz \end{pmatrix}$ | $B^D(s)$ | $U_3\text{Al}_2\text{Si}_3$ [84] |
| m'   | $\begin{pmatrix} xxy & xyy & 0 \\ 0 & 0 & xxz \\ xyy & yzy & 0 \end{pmatrix}$ | $\begin{pmatrix} xxy & xyy & 0 \\ 0 & 0 & zzz \\ yzy & yzy & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & yyz \\ xyy & yzy & 0 \\ 0 & 0 & zzz \end{pmatrix}$ | $C^D(s)$ | $U_3\text{Al}_2\text{Si}_3$ [25] |
| 22'2' 4'3m' | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & yzy \\ 0 & 0 & zzz \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & zzz \\ yzy & yzy & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & zzz \\ zzz & yzy & 0 \end{pmatrix}$ | $D^D(s)$ | (Cs,Rb)NiCl$_3$ [29, 30] |
| 2m'm', 2'm'm' | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & zzz \\ 0 & 0 & zzz \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & zzz \\ 0 & 0 & zzz \\ zzz & yzy & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & yzy \\ 0 & 0 & zzz \\ zzz & yzy & 0 \end{pmatrix}$ | $E^D(s)$ | MnSO$_4$ [32], TbCrO$_3$ [33] |
| 4', 4'm', 4'm', 6m', 6'm', 6'm', 6'm' | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & xzz \\ 0 & 0 & xzz \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & xzz \\ 0 & 0 & xzz \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & xzz \\ 0 & 0 & xzz \end{pmatrix}$ | $F^D(s)$ | YMnO$_3$ [37], Cs(Co,Ir)Ge$_3$ [48, 49] |
| 6'm', 6'm' | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & xzz \\ 0 & 0 & xzz \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & xzz \\ 0 & 0 & xzz \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & xzz \\ 0 & 0 & xzz \end{pmatrix}$ | $G^D(s)$ | (Yb, Ho, Sc)MnO$_3$ [18, 37, 51] |
| 4' | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & xzz \\ xzz & xzy & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & xzz \\ 0 & 0 & xzz \\ xzz & xzy & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & xzz \\ 0 & 0 & xzz \\ xzz & xzy & 0 \end{pmatrix}$ | $H^D(s)$ | CsCoF$_4$ [38] |
| 6'm, 2'm | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & xzz \\ xzz & xzy & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & xzz \\ 0 & 0 & xzz \\ xzz & xzy & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & xzz \\ 0 & 0 & xzz \\ xzz & xzy & 0 \end{pmatrix}$ | $I^D(s)$ | RbFeCl$_3$ [68] |
| 6' | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & xzz \\ xzz & xzy & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & xzz \\ 0 & 0 & xzz \\ xzz & xzy & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & xzz \\ 0 & 0 & xzz \\ xzz & xzy & 0 \end{pmatrix}$ | $L^D(s)$ | Cu$_{0.82}$Mn$_{1.18}$As [63] |
| 42'm', 4'2'm | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & xzz \\ xzz & xzy & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & xzz \\ xzz & xzy & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & xzz \\ xzz & xzy & 0 \end{pmatrix}$ | $M^D(s)$ | EuCr$_2$As$_2$ [55], MgCr$_2$O$_4$ [56] |
| 32', 6m2' | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & xzz \\ xzz & xzy & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & xzz \\ xzz & xzy & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & xzz \\ xzz & xzy & 0 \end{pmatrix}$ | $N^D(s)$ | NaMnFeF$_6$ [43], CsMnBr$_3$ [82] |
| 6'm2 | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & xzz \\ xzz & xzy & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & xzz \\ xzz & xzy & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & xzz \\ xzz & xzy & 0 \end{pmatrix}$ | $O^D(s)$ | GaV$_4$S$_8$ [50], GaV$_4$S$_8$ [50] |
C. Two-dimensional matrix representations for all response tensors

The second-order charge and spin response tensors can be expressed as \( j_a^{(\sigma)} = \sum_{b,c} \chi_{abc}^{(\sigma)} E_b E_c \), where the \( \chi_{abc} \) is a rank-three tensor and can be used a three-dimensional matrix to represent. Straightforwardly, we can also use a two-dimensional matrix to describe due to the commutative symmetry of the electric field components \( E_b \) and \( E_c \).

Hence, we blackefine a matrix to represent it \[89\],

\[
\mathcal{E} = \begin{pmatrix} E_1 & E_2 & E_3 & E_4 & E_5 & E_6 \\ E_7 & E_8 & E_9 & E_{10} & E_{11} & E_{12} \end{pmatrix} = \begin{pmatrix} \chi_{11} & \chi_{12} & \chi_{13} & \chi_{14} & \chi_{15} & \chi_{16} \\ \chi_{21} & \chi_{22} & \chi_{23} & \chi_{24} & \chi_{25} & \chi_{26} \\ \chi_{31} & \chi_{32} & \chi_{33} & \chi_{34} & \chi_{35} & \chi_{36} \end{pmatrix}
\]

(S39)

The current density is

\[
\begin{pmatrix} j_1^{(\sigma)} \\ j_2^{(\sigma)} \\ j_3^{(\sigma)} \end{pmatrix} = \begin{pmatrix} \chi_{11} & \chi_{12} & \chi_{13} & \chi_{14} & \chi_{15} & \chi_{16} \\ \chi_{21} & \chi_{22} & \chi_{23} & \chi_{24} & \chi_{25} & \chi_{26} \\ \chi_{31} & \chi_{32} & \chi_{33} & \chi_{34} & \chi_{35} & \chi_{36} \end{pmatrix} \begin{pmatrix} \mathcal{E}_1 \\ \mathcal{E}_2 \\ \mathcal{E}_3 \\ \mathcal{E}_4 \\ \mathcal{E}_5 \\ \mathcal{E}_6 \end{pmatrix}
\]

(S40)

where \( j_1^{(\sigma)}, j_2^{(\sigma)}, j_3^{(\sigma)} = j_x^{(\sigma)}, j_y^{(\sigma)}, j_z^{(\sigma)} \), the \( \chi_1^{(\sigma)} = \chi_{xx}, \chi_2^{(\sigma)} = \chi_{xy}, \chi_3^{(\sigma)} = \chi_{xz}, \chi_4^{(\sigma)} = \chi_{yy}, \chi_5^{(\sigma)} = \chi_{yz}, \chi_6^{(\sigma)} = \chi_{zz} \). Thus, the three term of the second conductivity can be written as

\[
\chi_{BCD/BCP}^{(\sigma)} = \begin{pmatrix} 0 & xy & xz & xz + xy & xz & xy \\ -xy & 0 & yz & -xy + yz & -xy & yz \\ -xz & -yz & 0 & -xz & -xz & -yz - yz \end{pmatrix}
\]

(S41)

\[
\chi_{D}^{(\sigma)} = \begin{pmatrix} xx & xy & xz & 2xy & 2xz & 2xy \\ xz & yy & yz & 2xz & 2xy & 2yy \\ xz & yy & zz & 2yz & 2xz & 2yy \end{pmatrix}
\]

(S42)

So, we give the two-dimensional matrix representations for the second-order charge and spin response tensor in the Table S21 and S23. This result is also completely consistent with the discussion about BCD term \( \chi_{BCD} \), which is \( \chi_{in} \) in the Ref. [8].
TABLE S21: Two-dimensional matrix representations for $\chi_{BCD}$ and $\chi_{BCD(s)}$.

| Shortened form | 2-d matrix representations |
|---------------|-----------------------------|
| $A_{BCD/BCD(s)}$ | $\begin{pmatrix} 0 & xyy & xzz & xyz + xzy & xzx & yx \n -xyx & 0 & yzz & yzy & -xyz + yzx & -xyx \n -xxx & -yzy & 0 & -yzz & -xzz & -xzy - yzx \end{pmatrix}$ |
| $B_{BCD/BCD(s)}$ | $\begin{pmatrix} 0 & 0 & 0 & xzy + xzy & xzx & 0 \n 0 & 0 & 0 & yzy & -xyz + yzx & 0 \n -xxx & -yzy & 0 & 0 & 0 & -xzy - yzx \end{pmatrix}$ |
| $C_{BCD/BCD(s)}$ | $\begin{pmatrix} 0 & xyy & xzz & 0 & 0 & yx \n -xyx & 0 & yzz & 0 & 0 & -xyz \end{pmatrix}$ |
| $D_{BCD/BCD(s)}$ | $\begin{pmatrix} 0 & 0 & 0 & xyz + xzy & 0 & 0 \n 0 & 0 & 0 & -xyz + yzx & 0 & 0 \n 0 & 0 & 0 & 0 & 0 & -xzy - yzx \end{pmatrix}$ |
| $E_{BCD/BCD(s)}$ | $\begin{pmatrix} 0 & 0 & 0 & 0 & xzy & 0 \n 0 & 0 & 0 & yzy & 0 & 0 \n -xxx & -yzy & 0 & 0 & 0 \end{pmatrix}$ |
| $F_{BCD/BCD(s)}$ | $\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & xzy \n 0 & 0 & 0 & 0 & 0 & xzy \n 0 & 0 & 0 & 0 & 0 & 0 \n -xxx & -xzy & 0 & 0 & 0 \end{pmatrix}$ |
| $H_{BCD/BCD(s)}$ | $\begin{pmatrix} 0 & 0 & 0 & 0 & xzy & xzx \n 0 & 0 & 0 & -xxx & xzy \n -xxx & xzx & 0 & 0 & 0 \n 0 & 0 & 0 & 0 & -2xyx \end{pmatrix}$ |
| $I_{BCD/BCD(s)}$ | $\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \n 0 & 0 & 0 & 0 & 0 & 0 \n 0 & 0 & 0 & 0 & 0 & 0 \n 0 & 0 & 0 & 0 & 0 & 0 \n 0 & 0 & 0 & 0 & 0 & 0 \n 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$ |
| $J_{BCD}$ | $\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & xxx \n 0 & 0 & 0 & 0 & 0 & xxx \n 0 & 0 & 0 & 0 & 0 & xxx \n -xxx & -xxx & 0 & 0 & 0 \end{pmatrix}$ |
| $K_{BCD}$ | $\begin{pmatrix} 0 & 0 & 0 & 0 & xzy & 0 \n 0 & 0 & 0 & 0 & xzy & 0 \n 0 & 0 & 0 & 0 & 0 & 0 \n 0 & 0 & 0 & 0 & 0 & 0 \n 0 & 0 & 0 & 0 & 0 & 0 \n 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$ |
| $L_{BCD(s)}$ | $\begin{pmatrix} 0 & xyy & xxx & 0 & 0 \n 0 & 0 & 0 & 0 & 0 \n 0 & 0 & 0 & 0 & 0 \n 0 & 0 & 0 & 0 & 0 \n 0 & 0 & 0 & 0 & 0 \n 0 & 0 & 0 & 0 & 0 \end{pmatrix}$ |
| $M_{BCD(s)}$ | $\begin{pmatrix} 0 & 0 & 0 & 0 & xxx \n 0 & 0 & 0 & 0 & xxx \n 0 & 0 & 0 & 0 & xxx \n -xxx & -xxx & 0 & 0 & 0 \end{pmatrix}$ |
| $N_{BCD(s)}$ | $\begin{pmatrix} 0 & 0 & 0 & 0 & 0 \n 0 & 0 & 0 & 0 & 0 \n 0 & 0 & 0 & 0 & 0 \n 0 & 0 & 0 & 0 & 0 \n 0 & 0 & 0 & 0 & 0 \n 0 & 0 & 0 & 0 & 0 \end{pmatrix}$ |
| $O_{BCD(s)}$ | $\begin{pmatrix} 0 & 0 & 0 & 0 & xxx \n 0 & 0 & 0 & 0 & xxx \n 0 & 0 & 0 & 0 & xxx \n -xxx & -xxx & 0 & 0 & 0 \end{pmatrix}$ |
TABLE S22: Two-dimensional matrix representations for $\chi^\text{BCP}$ and $\chi^\text{BCP(s)}$.

| Shortened form | 2-d matrix representations |
|----------------|-----------------------------|
| $A^\text{BCP/BCP(s)}$ | $\begin{pmatrix} 0 & xyy & xzz & xyz + xzy & xly & xyx \\ -xyx & 0 & yzy & -xyz + yzx & -xyy \\ -xzz & -yzy & 0 & -yzz & -zzz & -xzy - yzx \end{pmatrix}$ |
| $B^\text{BCP/BCP(s)}$ | $\begin{pmatrix} 0 & 0 & 0 & xyz + xzy & xzz & 0 \\ 0 & 0 & 0 & yzy & -xyz + yzx & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$ |
| $C^\text{BCP/BCP(s)}$ | $\begin{pmatrix} 0 & xyy & xzz & 0 & 0 & xyx \\ -xyx & 0 & yzy & 0 & 0 & -xyy \\ 0 & 0 & 0 & -yzz & -zzz & 0 \end{pmatrix}$ |
| $D^\text{BCP/BCP(s)}$ | $\begin{pmatrix} 0 & 0 & 0 & xyz + xzy & 0 & 0 \\ 0 & 0 & 0 & -xyz + yzx & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$ |
| $E^\text{BCP/BCP(s)}$ | $\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & xzz \\ 0 & 0 & 0 & yzy & 0 & 0 \\ 0 & 0 & 0 & -yzz & -zzz & 0 \end{pmatrix}$ |
| $F^\text{BCP/BCP(s)}$ | $\begin{pmatrix} 0 & 0 & 0 & xyz + xzy & 0 \\ 0 & 0 & 0 & xzz & -xyz - xzy & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$ |
| $H^\text{BCP/BCP(s)}$ | $\begin{pmatrix} 0 & 0 & 0 & xyy & xzz & 0 \\ 0 & 0 & 0 & -xyx & -zzz & 0 \\ 0 & 0 & 0 & 0 & 0 & -2xyz \end{pmatrix}$ |
| $I^\text{BCP/BCP(s)}$ | $\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$ |
| $J^\text{BCP/BCP(s)}$ | $\begin{pmatrix} 0 & 0 & 0 & xyy & 0 \\ 0 & 0 & 0 & -xyx & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$ |
| $K^\text{BCP/BCP(s)}$ | $\begin{pmatrix} 0 & 0 & 0 & xyx & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$ |
TABLE S23: Two-dimensional matrix representations for $\chi^D$ and $\chi^{D(s)}$.

| Shortened form | 2-d matrix representations |
|----------------|----------------------------|
| $A^{D/D(s)}$   | $\begin{pmatrix} xxx & xxx & 2xyz & 2xxz & 2xxz & 2xxy \\ xxx & xxx & 2xyz & 2xxz & 2xxz & 2xxy \\ xxy & xxy & xxx & 2yyz & 2yyz & 2yyz \\ xxx & xxx & 2xyz & 2xxz & 2xxz & 2xxy \\ xxx & xxx & 2xyz & 2xxz & 2xxz & 2xxy \\ xxx & xxx & 2xyz & 2xxz & 2xxz & 2xxy \end{pmatrix}$ |
| $B^{D/D(s)}$   | $\begin{pmatrix} 0 & 0 & 0 & 2xyz & 0 & 0 \\ 0 & 0 & 0 & 2xyz & 0 & 0 \\ xxx & xxx & 0 & 0 & 2xxy & 0 \\ xxx & xxx & 0 & 0 & 2xxy & 0 \\ xxx & xxx & 0 & 0 & 2xxy & 0 \end{pmatrix}$ |
| $C^{D/D(s)}$   | $\begin{pmatrix} xxx & xxx & 0 & 0 & 2xxy & 0 \\ xxx & xxx & 0 & 0 & 2xxy & 0 \\ xxx & xxx & 0 & 0 & 2xxy & 0 \\ xxx & xxx & 0 & 0 & 2xxy & 0 \\ xxx & xxx & 0 & 0 & 2xxy & 0 \\ xxx & xxx & 0 & 0 & 2xxy & 0 \end{pmatrix}$ |
| $D^{D/D(s)}$   | $\begin{pmatrix} 0 & 0 & 0 & 2xyz & 0 & 0 \\ 0 & 0 & 0 & 2xyz & 0 & 0 \\ xxx & xxx & 0 & 0 & 2xxy & 0 \\ xxx & xxx & 0 & 0 & 2xxy & 0 \\ xxx & xxx & 0 & 0 & 2xxy & 0 \end{pmatrix}$ |
| $E^{D/D(s)}$   | $\begin{pmatrix} 0 & 0 & 0 & 2xyz & 0 & 0 \\ 0 & 0 & 0 & 2xyz & 0 & 0 \\ xxx & xxx & 0 & 0 & 2xxy & 0 \\ xxx & xxx & 0 & 0 & 2xxy & 0 \\ xxx & xxx & 0 & 0 & 2xxy & 0 \end{pmatrix}$ |
| $F^{D/D(s)}$   | $\begin{pmatrix} 0 & 0 & 0 & 2xyz & 0 & 0 \\ 0 & 0 & 0 & 2xyz & 0 & 0 \\ xxx & xxx & 0 & 0 & 2xxy & 0 \\ xxx & xxx & 0 & 0 & 2xxy & 0 \\ xxx & xxx & 0 & 0 & 2xxy & 0 \end{pmatrix}$ |
| $H^{D/D(s)}$   | $\begin{pmatrix} 0 & 0 & 0 & 2xyz & 0 & 0 \\ 0 & 0 & 0 & 2xyz & 0 & 0 \\ xxx & xxx & 0 & 0 & 2xxy & 0 \\ xxx & xxx & 0 & 0 & 2xxy & 0 \end{pmatrix}$ |
| $J^{D/D(s)}$   | $\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ xxx & xxx & 0 & 0 & 0 & 0 \\ xxx & xxx & 0 & 0 & 0 & 0 \end{pmatrix}$ |
| $J^{D/D(s)}$   | $\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ xxx & xxx & 0 & 0 & 0 & 0 \\ xxx & xxx & 0 & 0 & 0 & 0 \end{pmatrix}$ |
| $K^{D/D(s)}$   | $\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ xxx & xxx & 0 & 0 & 0 & 0 \\ xxx & xxx & 0 & 0 & 0 & 0 \end{pmatrix}$ |
| $L^{D/D(s)}$   | $\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ xxx & xxx & 0 & 0 & 0 & 0 \\ xxx & xxx & 0 & 0 & 0 & 0 \end{pmatrix}$ |
| $M^{D(s)}$     | $\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ xxx & xxx & 0 & 0 & 0 & 0 \\ xxx & xxx & 0 & 0 & 0 & 0 \end{pmatrix}$ |
| $N^{D(s)}$     | $\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ xxx & xxx & 0 & 0 & 0 & 0 \\ xxx & xxx & 0 & 0 & 0 & 0 \end{pmatrix}$ |
| $O^{D(s)}$     | $\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ xxx & xxx & 0 & 0 & 0 & 0 \\ xxx & xxx & 0 & 0 & 0 & 0 \end{pmatrix}$ |
J. A. Gonzalo, D. E. Cox, and G. Shirane, “The magnetic structure of FeSb$_2$,” Phys. Rev. Lett. 112, 166601 (2014).

Chong Wang, Yang Gao, and Di Xiao, “Intrinsic nonlinear hall effect in antiferromagnetic tetragonal CuMnAs,” Phys. Rev. Lett. 127, 277201 (2021).

Huiying Liu, Jianzhou Zhao, Yue-Xin Huang, Weikang Wu, Xian-Lei Sheng, Cong Xiao, and Shengyuan A. Yang, “Intrinsic second-order anomalous hall effect and its application in compensated antiferromagnets,” Phys. Rev. Lett. 127, 277202 (2021).

Yang Gao, “Semiclassical dynamics and nonlinear charge current,” Front. Phys. 14 (2019), 10.1007/s11467-019-0887-2.

J. Železný, Z. Fang, K. Olejník, J. Patchett, F. Gerhard, C. Gould, L. W. Molenkamp, C. Gomez-Olivella, J. Zemen, T. Tichý, T. Jungwirth, and C. Ciccarelli, “Unidirectional magnetoresistance and spin-orbit torque in NiMnSb,” Phys. Rev. B 104, 054429 (2021).

C. L. Kane and E. J. Mele, “Quantum spin hall effect in graphene,” Phys. Rev. Lett. 95, 226801 (2005).

Z. Z. Du, C. M. Wang, Hai-Peng Sun, Hai-Zhou Lu, and X. C. Xie, “Quantum theory of the nonlinear hall effect,” Nat Commun 12, 5038 (2021).

Satoru Hayami, Megumi Yatsushiro, and Hiroaki Kusunose, “Nonlinear spin hall effect in PT-symmetric collinear magnets,” Phys. Rev. B 106, 024405 (2022).

Cheng-Ping Zhang, Jiewen Xiao, Benjamin T. Zhou, and Jin-Xin, “Giant nonlinear hall effect in strained twisted bilayer graphene,” arXiv:2010.08333 (2022).

M. T. Fernández-Díaz, J. A. Alonso, M. J. Martínez-Lope, M. T. Casais, and J. L. García-Muñoz, “Magnetic structure of the HoNiO$_3$ perovskite,” Phys. Rev. B 64, 144417 (2001).

Z. Z. Du, C. M. Wang, Hai-Zhou Lu, and X. C. Xie, “Band signatures for strong nonlinear hall effect in bilayer WTe$_2$,” Phys. Rev. Lett. 121, 266601 (2018).

Raffaele Battilomo, Niccolò Scopigno, and Carmine Ortix, “Berry curvature dipole in strained graphene: A fermi surface warping effect,” Phys. Rev. Lett. 123, 196403 (2019).

G. Rousse, J. Rodríguez-Carvajal, S. Patoux, and C. Masquelier, “Magnetic structures of the triphylite LiFePO$_4$ and of its delithiated form FePO$_4$,,” Chem. Mater. 15, 4082–4090 (2003).

J. A. Gonzalo, D. E. Cox, and G. Shirane, “The magnetic structure of FeSb$_2$O$_4$,” Phys. Rev. 147, 415–418 (1966).

Stanislav Podchezevsek, Nicolas Barrier, Alain Pautrat, Emmanuelle Saud, Marí a Returto, Jose Antonio Alonso, María Teresa Fernández-Díaz, and Juan Rodríguez-Carvajal, “Influence of polymorphism on the magnetic properties of c0$_5$Te$_{08}$ spinel,” Inorg. Chem. 60, 13990–14001 (2021).

Jan-Willem G. Bos, Claire V. Colin, and Thomas T. M. Palstra, “Magneetoelectric coupling in the cubic ferrimagnet Cu$_2$OSeO$_3$,,” Phys. Rev. B 78, 094416 (2008).

A. Muñoz, J. A. Alonso, M. J. Martínez-Lope, M. T. Casais, J. L. Martínez, and M. T. Fernández-Díaz, “Magnetic structure of hexagonal RMnO$_4$(R=Y,Sc): Thermal evolution from neutron powder diffraction data,” Phys. Rev. B 62, 9498–9510 (2000).

E. Morosan, J. A. Fleitman, Q. Huang, J. W. Lynn, Y. Chen, X. Ke, M. L. Dahlberg, P. Schiffer, C. R. Crangle, and R. J. Cava, “Structure and magnetic properties of the Ho$_2$Ge$_2$O$_7$ pyrogermanate,” Phys. Rev. B 77, 224423 (2008).

F. Li, V. Pomjakushin, T. Mazet, R. Sibille, B. Malaman, R. Yadav, L. Keller, M. Medarde, K. Conder, and E. Pomjakushina, “Revisiting the magnetic structure and charge ordering in La$_{1/3}$Sr$_{2/3}$FeO$_3$ by neutron powder diffraction and nmsbauer spectroscopy,” Phys. Rev. B 97, 174418 (2018).

X. F. Hao, A. Stroppa, S. Picozzi, A. Filippetti, and C. Franchini, “Exceptionally large room-temperature ferroelectric polarizability in the PbNiO$_3$ multiferroic nickelate: First-principles study,” Phys. Rev. B 86, 014116 (2012).

A. Muñoz, J. A. Alonso, M. J. Martínez-Lope, M. T. Casais, J. L. Martínez, and M. T. Fernández-Díaz, “Evolution of the magnetic structure of hexagonal HoMnO$_3$ from neutron powder diffraction data,” Chem. Mater. 13, 1497–1505 (2001).

Cheng Chen, Huaqiang Wang, Dinghui Wang, and Haijun Zhang, “Strain-engineeblacks nonlinear hall effect in HgTe,” SPIN 09, 1940017 (2019).

A. R. Wildes, V. Simonet, E. Ressouche, G. J. McIntyre, M. Avdeev, E. Suard, S. A. J. Kimber, D. Lançon, G. Pepe, B. Moubaraki, and T. J. Hicks, “Magnetic structure of the quasi-two-dimensional antiferromagnet Ni$_2$MnF$_5$,,” Solid State Commun. 92, 601–605 (1994).

Angel M. Arévalo-López and J. Paul Attfield, “Weak ferromagnetism and domain effects in multiferroic LiNbO$_3$-type MnTiO$_3$,,” Phys. Rev. B 88, 104416 (2013).

E. Wawrzyńiak, R. Coldea, E. M. Wheeler, T. Srgel, M. Jansen, R. M. Ibberson, P. G. Radselli, and M. M. Koza, “Charge disproportionation and collinear magnetic order in the frustrated triangular antiferromagnet AgNiO$_2$,,” Phys. Rev. B 77,
M. Smidman, D. T. Adroja, A. D. Hillier, L. C. Chapon, J. W. Taylor, V. K. Anand, R. P. Singh, M. R. Lees, E. A. T. Chattopadhyay, J. Rossat-Mignod, and H. Fjellvåg, “Magnetic ordering in MnSe$_2$,” Solid State Commun. 8, 1001–1005 (1970).

L. M. Corliss, N. Elliott, and J. M. Hastings, “Antiferromagnetic structures of MnS$_2$, MnSe$_2$ and MnTe$_2$,” J. Appl. Phys. 29, 391–392 (1958).

G. Will, B. C. Frazer, G. Shirane, D. E. Cox, and P. J. Brown, “Magnetic structure of MnS$_4$,” Phys. Rev. 140, A2139–A2142 (1965).

E. F. Bertaut, J. Chappert, J. Mareschal, J. P. Rebonnault, and J. Sivardière, “Structures magnétiques de TbFeO$_3$,” Solid State Commun. 5, 293–298 (1967).

T. Chattopadhyay, J. Rossat-Mignod, and H. Fjellvåg, “Magnetic ordering in MnSe$_2$,” Solid State Commun. 63, 65–67 (1987).

D. T. Adroja, C. de la Fuente, A. Fraile, A. D. Hillier, A. Daoud-Aladine, W. Kockelmann, J. W. Taylor, M. M. Koza, E. Burzuri, F. Luis, J. I. Arnaudas, and A. del Moral, “Muon spin rotation and neutron scattering study of the noncentrosymmetric tetragonal compound CeAuAl$_3$,” Phys. Rev. B 91, 134425 (2015).

I. Živković, K. Prša, O. Zaharko, and H. Berger, “Ni$_3$TeO$_6$ — a collinear antiferromagnet with ferromagnetic honeycomb planes,” J. Phys.: Condens. Matter 20, 056002 (2010).

P. Lacorre, J. Pannetier, T. Fleischer, R. Hoppe, and G. Ferey, “Ordeblack magnetic frustration: XVI. magnetic structure of $\text{cscof}_{4}$ at 1.5 k,” J. Solid State Chem. 93, 37–45 (1991).

Hirohiko Sato, Koji Wakiya, Toshiaki Enoki, Takashi Kiyama, Yusuke Wakabayashi, Hironori Nakao, and Youichi Murakami, “Magnetic structure of $\beta$-MnO$_2$: X-ray magnetic scattering study,” J. Phys. Soc. Jpn. 70, 37–40 (2001).

M. Reehuis, C. Ulrich, A. Maljuk, Ch. Niedermayer, B. Ouladdiaf, A. Hoser, T. Hofmann, and B. Keimer, “Neutron diffraction study of spin and charge ordering in SrFeO$_{3-\delta}$,” Phys. Rev. B 85, 184109 (2012).

P. Schobinger-Papamantellos, J. Rodríguez-Carvajal, and K. H. J. Buschow, “Magnetic ordering of ScMnGe$_6$ by neutron diffraction,” J. Magn. Magn. Mater. 369, 243–248 (2014).

K. M. Taddei, L. Sanjeeva, J. W. Kolis, A. S. Sefat, C. de la Cruz, and D. M. Pajerowski, “Localized-type magnetic order and metamagnetism in the rare-earth pyrogermanate $\text{Er}_2\text{Ge}_2\text{O}_7$,” Phys. Rev. Materials 3, 014405 (2019).

G. Courbion and M. Leblanc, “The magnetic structure of NaMnFeF$_4$,” J. Magn. Magn. Mater. 74, 158–164 (1988).

S. X. M. Riberolles, T. V. Trevisan, B. Kuthanazhi, T. W. Heitmann, F. Ye, D. C. Johnston, S. L. Bud’ko, D. H. Ryan, G. Courbion, and M. Leblanc, “Structures magnetiques de TbFeO$_3$,” Phys. Rev. B 29, 2024–2027 (1973).

R. Hoppe, and G. Ferey, “Ordeblack magnetic frustration: XVI. magnetic structure of $\text{cscof}_{4}$ at 1.5 k,” J. Solid State Chem. 93, 37–45 (1991).

H. Shaked, J. M. Hastings, and L. M. Corliss, “Magnetic structure of magnesium chromite,” Phys. Rev. B 3, 3116–3124 (1970).

E. F. Bertaut, J. Cohen, B. Lambert-Andron, and P. Mollard, “Étude de Cr$_2$S$_3$ rhomboédrique par diffraction neutronique et mesures magnétiques,” J. Phys. 29, 813–824 (1968).
[58] P. Schobinger-Papamantellos, G. André, J. Rodríguez-Carvajal, C.H. de Groot, and K.H.J. Buschow, “The magnetic ordering of the novel compound ErGe₂,” J. Alloys 232, 165–168 (1996).

[59] M. Fiebig, D. Fröhlich, and H. J. Thiele, “Determination of spin direction in the spin-flop phase of Cr₂O₃,” Phys. Rev. B 54, R12681–R12684 (1996).

[60] D Sheptyakov, N Z Ali, and M Jansen, “A neutron diffraction study of structural and magnetic transformations in AFeO₃(a = K, Rb and Cs),” J. Phys.: Condens. Matter 22, 426001 (2010).

[61] Hiroki Yamauchi, Naoto Metoki, Ryuta Watanuki, Kazuya Suzuki, Hiroshi Fukazawa, Songxue Chi, and Jaime A. Fernandez-Baca, “Magnetic structure and quadrupolar order parameter driven by geometrical frustration effect in NdB₃,” J. Phys. Soc. Jpn. 86, 044705 (2017).

[62] Gen Shirane, S. J. Pickart, and Yoshikazu Ishikawa, “Neutron diffraction study of antiferromagnetic MnTiO₃ and NiTiO₃,” J. Phys. Soc. Jpn. 14, 1352–1360 (1959).

[63] P J Brown, J B Forsyth, E Leliévre-Berna, and F Tasset, “Determination of the magnetization distribution in CrO₂,” J. Phys.: Condens. Matter. 9, 4729–4742 (1997).

[64] Manohar H. Karigerasi, Kisung Kang, Arun Ramanathan, Danielle L. Gray, Matthias D. Frontzek, Huibo Cao, André Schleife, and Daniel P. Shoemaker, “In-plane hexagonal antiferromagnet in the Cu-Mn-As system Cu₉₀₈₂Mnₑ₈As,” Phys. Rev. Mat. 3, 111402 (2019).

[65] P J Brown, J Crangle, K-U Neumann, J G Smith, and K R A Ziebeck, “The structure and magnetic moment distribution in the antiferromagnetic phase of Cu₁₄Au₅₁,” J. Phys.: Condens. Matter 9, 381–384 (1991).

[66] A. Dommann, H.R. Ott, F. Hulliger, and P. Fischer, “The crystal structure and the magnetic order of U₃₃₄₅Au,” Journal of the Less Common Metals 160, 171–180 (1990).

[67] A G Gukasov, P Rogl, P J Brown, M Mihalik, and A Menovsky, “Site susceptibility tensors and magnetic structure of U₃Al₂Si₁₃: a polarized neutron diffraction study,” J. Phys.: Condens. Matter 14, 8841–8851 (2002).
[85] L. M. Corliss, N. Elliott, J. M. Hastings, and R. L. Sass, “Magnetic structure of chromium selenide,” Phys. Rev. 122, 1402–1406 (1961).

[86] J R Stewart, G Ehlers, A S Wills, S T Bramwell, and J S Gardner, “Phase transitions, partial disorder and multi-k structures in Gd$_2$Ti$_2$O$_6$,” J. Phys.: Condens. Matter 16, L321–L326 (2004).

[87] Olivier Mentré, Matthieu Kauffmann, Ghislaine EHota, Sylvie Daviero-Minaud, Francis Abraham, and Pascal Roussel, “Structure, dimensionality and magnetism of new cobalt oxyhalides,” Solid State Sci. 10, 471–475 (2008).

[88] S. Baran, A. Szytula, D. Kaczorowski, and F. Damay, “Magnetic structures in TmPdIn and TmAgSn,” J. Alloys 662, 11–15 (2016).

[89] R. E. Newnham, Properties of materials: anisotropy, symmetry, structure (Oxford University Press, 2005).