Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information (ESI) for

Rashba effect originates from the reduction of point-group symmetries

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Notation

The point-group symmetry is denoted by the Hermann–Mauguin notation. The representation is referred to the Bilbao Crystallographic Server [S1]. The representation is described for the single group as Γ and the double group as $\overline{\Gamma}$. The character table is summarized for BiTeI of $P3m1$ in Tables S I–S IV.

Representation of atomic orbital

The atomic orbital is represented in the full-rotation group by $\Gamma^{\mathrm{orb}}_{jl}$ and composed of an orbital function and spin function. The orbital function and spin function are transformed by the rotation, while only the orbital function is transformed by the inversion. The character χ^{orb}_{jl} of the point-group symmetry is thus described as [S2, S3]

$$\chi^{\mathrm{orb}}_{jl}\{\alpha\} = \frac{\sin(j+\frac{1}{2})\alpha}{\sin\frac{1}{2}\alpha} \;, \qquad \chi^{\mathrm{orb}}_{jl}\{\bar{\alpha}\} = (-1)^{l}\frac{\sin(j+\frac{1}{2})\alpha}{\sin\frac{1}{2}\alpha} \;, \tag{S1}$$

where j is the total angular quantum number, l is the orbital angular quantum number, $\{\alpha\}$ is the $\frac{2\pi}{\alpha}$-fold rotation, and $\{\bar{\alpha}\}$ is the $\frac{2\pi}{\alpha}$-fold rotoinversion. The atomic orbital is then subducted to the space group of a condensed-matter system and represented by Γ^{orb}. The Γ^{orb}'s at the Γ and A, M and L, and K and H points are summarized for BiTeI in Tables S V–S VII.

Representation of atomic arrangement

The atomic arrangement is represented in the space group by Γ^{arr} and described by the Bloch function as

$$f_{\mathbf{k}}(\mathbf{r}) = g_{\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}} \;, \qquad g_{\mathbf{k}}(\mathbf{r}) = \sum_i \delta(\mathbf{r}-\mathbf{r}_i) \;, \tag{S2}$$

where $g_{\mathbf{k}}(\mathbf{r})$ is the cell-periodic function and $\mathbf{r}_i$ is the atomic position. The character χ^{arr} of the space-group symmetry is thus described as [S4–S6]

$$\begin{aligned}
&\chi^{\mathrm{arr}}\{P|\boldsymbol{\tau}+\mathbf{R}\} \\
&= \langle f_{\mathbf{k}}|\{P|\boldsymbol{\tau}+\mathbf{R}\}f_{\mathbf{k}}\rangle \\
&= e^{-i\mathbf{k}\cdot\mathbf{R}}e^{-i(\mathbf{k}+\mathbf{G})\cdot\boldsymbol{\tau}}\langle g_{\mathbf{k}}|e^{i\mathbf{G}\cdot\mathbf{r}}\{P|\boldsymbol{\tau}+\mathbf{R}\}g_{\mathbf{k}}\rangle \\
&= e^{-i\mathbf{k}\cdot\mathbf{R}}e^{-i(\mathbf{k}+\mathbf{G})\cdot\boldsymbol{\tau}} \\
&\quad\times\sum_i\langle\delta(\mathbf{r}-\mathbf{r}_i)|e^{i\mathbf{G}\cdot\mathbf{r}}\delta(\{P|\boldsymbol{\tau}+\mathbf{R}\}^{-1}\mathbf{r}-\mathbf{r}_i)\rangle \\
&= e^{-i\mathbf{k}\cdot\mathbf{R}}e^{-i(\mathbf{k}+\mathbf{G})\cdot\boldsymbol{\tau}}\sum_i e^{i\mathbf{G}\cdot\mathbf{r}_i}\delta(\{P|\boldsymbol{\tau}+\mathbf{R}\}^{-1}\mathbf{r}_i-\mathbf{r}_i) \\
&= e^{-i\mathbf{k}\cdot\mathbf{R}}e^{-i(\mathbf{k}+\mathbf{G})\cdot\boldsymbol{\tau}}\sum_i e^{i\mathbf{G}\cdot\mathbf{r}_i}\delta[P^{-1}(\mathbf{r}_i-\boldsymbol{\tau})-\mathbf{r}_i] \;,
\end{aligned} \tag{S3}$$

where P is the point-group symmetry, $\boldsymbol{\tau}$ is the fractional lattice vector, $\mathbf{R}$ is the lattice vector, $\mathbf{G}$ is the reciprocal lattice vector, and $\mathbf{k}\cdot P^{-1}[\mathbf{r}-(\boldsymbol{\tau}+\mathbf{R})] = P\mathbf{k}\cdot[\mathbf{r}-(\boldsymbol{\tau}+\mathbf{R})]$ and $P\mathbf{k}=\mathbf{k}+\mathbf{G}$ are employed. The atomic arrangement can be reduced in the symmorphic group of $\boldsymbol{\tau}=\mathbf{0}$ as

$$\chi^{\mathrm{arr}}\{P|\mathbf{R}\} = e^{-i\mathbf{k}\cdot\mathbf{R}}\sum_i e^{i\mathbf{G}\cdot\mathbf{r}_i}\delta(P^{-1}\mathbf{r}_i-\mathbf{r}_i) \;. \tag{S4}$$

The Γ^{arr}'s at the Γ and A, M and L, and K and H points are summarized for BiTeI in Tables S VIII–S X.

Representation of atomic wavefunction

The atomic wavefunction is represented by the direct product of the atomic orbital and atomic arrangement as $\Gamma^{\mathrm{orb}}\otimes\Gamma^{\mathrm{arr}}$. The representations at the Γ and A, M and L, and K and H points are summarized for BiTeI in Tables S XI–S XIII.

[S1] M. I. Aroyo, A. Kirov, C. Capillas, J. M. Perez-Mato, and H. Wondratschek, Bilbao Crystallographic Server. II. Representations of crystallographic point groups and space groups, Acta Crystallogr., Sect. A: Found. Crystallogr. **62**, 115 (2006); L. Elcoro, B. Bradlyn, Z. Wang, M. G. Vergniory, J. Cano, C. Felser, B. A. Bernevig, D. Orobengoa, G. de la Flor, and M. I. Aroyo, Double crystallographic groups and their representations on the Bilbao Crystallographic Server, J. Appl. Crystallogr. **50**, 1457 (2017).

[S2] M. Lax, *Symmetry Principles in Solid State and Molecular Physics* (Dover Publications, Inc., Mineola, 2001).

[S3] M. Tinkham, *Group Theory and Quantum Mechanics* (Dover Publications, Inc., Mineola, 2003).

[S4] W. M. Lomer, The valence bands in two-dimensional graphite, Proc. R. Soc. London, Ser. A **227**, 330 (1955).

[S5] M. S. Dresselhaus, G. Dresselhaus, and A. Jorio, *Group Theory* (Springer-Verlag, Berlin, 2008).

[S6] K. Okamura, Focus on the overlap density of wavefunctions in *GW* approximations, Phys. Chem. Chem. Phys. **22**, 5366 (2020); Bloch state constrained by spatial and time-reversal symmetries, J. Phys. A: Math. Theor. **56**, 335003 (2023).

TABLE S I. Character table at the Γ [$\mathbf{k}_\Gamma = (0,0,0)$], A [$\mathbf{k}_A = \frac{2\pi}{c}(0,0,\frac{1}{2})$], and Δ [$\mathbf{k}_\Delta = \frac{2\pi}{c}(0,0,u)$, where $0 < u < \frac{1}{2}$] points of the space group $P3m1$, which transforms isomorphically to the point group $3m\,(C_{3v})$.

	$\{1\}^{\mathrm{a}}$	$\{3\}^{\mathrm{b}}$	$\{m_{010}\}^{\mathrm{c}}$	$\{m_{100}\}^{\mathrm{d}}$	$\{^{\mathrm{d}}1\}^{\mathrm{e}}$	$\{^{\mathrm{d}}3\}^{\mathrm{f}}$
Γ_1	$1 \cdot T^{\mathrm{g}}$	1	1	1	1	1
Γ_2	$1 \cdot T$	1	-1	-1	1	1
Γ_3	$2 \cdot T$	-1	0	0	2	-1
$\overline{\Gamma}_4$	$1 \cdot T$	-1	$-i$	i	-1	1
$\overline{\Gamma}_5$	$1 \cdot T$	-1	i	$-i$	-1	1
$\overline{\Gamma}_6$	$2 \cdot T$	1	0	0	-2	-1

[a] $\{1|\mathbf{R}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3\}$, where $\mathbf{a}_1 = a(1,0,0)$, $\mathbf{a}_2 = a(-\frac{1}{2}, \frac{\sqrt{3}}{2}, 0)$, and $\mathbf{a}_3 = c(0,0,1)$ and n_1, n_2, and n_3 are integer.
[b] $\{3^+_{001}|(0,0,0)\}, \{3^-_{001}|(0,0,0)\}$.
[c] $\{m_{010}|(0,0,0)\}, \{m_{110}|(0,0,0)\}, \{^{\mathrm{d}}m_{100}|(0,0,0)\}$.
[d] $\{m_{100}|(0,0,0)\}, \{^{\mathrm{d}}m_{010}|(0,0,0)\}, \{^{\mathrm{d}}m_{110}|(0,0,0)\}$.
[e] $\{^{\mathrm{d}}1|(0,0,0)\}$.
[f] $\{^{\mathrm{d}}3^+_{001}|(0,0,0)\}, \{^{\mathrm{d}}3^-_{001}|(0,0,0)\}$.
[g] T represents $T_\Gamma = e^{-i\mathbf{k}_\Gamma \cdot \mathbf{R}_n}$, $T_A = e^{-i\mathbf{k}_A \cdot \mathbf{R}_n}$, and $T_\Delta = e^{-i\mathbf{k}_\Delta \cdot \mathbf{R}_n}$.

TABLE S II. Character table at the M [$\mathbf{k}_M = \frac{2\pi}{a}(\frac{1}{2},0,0)$], L [$\mathbf{k}_L = (\frac{2\pi}{a}\frac{1}{2}, 0, \frac{2\pi}{c}\frac{1}{2})$], Σ [$\mathbf{k}_\Sigma = \frac{2\pi}{a}(u,0,0)$, where $0 < u < \frac{1}{2}$], and R [$\mathbf{k}_R = (\frac{2\pi}{a}u, 0, \frac{2\pi}{c}\frac{1}{2})$, where $0 < u < \frac{1}{2}$] points of the space group $P3m1$, which transforms isomorphically to the point group $m\,(C_s)$.

	$\{1\}^{\mathrm{a}}$	$\{m_{010}\}^{\mathrm{b}}$	$\{^{\mathrm{d}}1\}^{\mathrm{c}}$	$\{^{\mathrm{d}}m_{010}\}^{\mathrm{d}}$
M_1	$1 \cdot T^{\mathrm{e}}$	1	1	1
M_2	$1 \cdot T$	-1	1	-1
$\overline{M}_3$	$1 \cdot T$	$-i$	-1	i
$\overline{M}_4$	$1 \cdot T$	i	-1	$-i$

[a] $\{1|\mathbf{R}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3\}$, where $\mathbf{a}_1 = a(1,0,0)$, $\mathbf{a}_2 = a(-\frac{1}{2}, \frac{\sqrt{3}}{2}, 0)$, and $\mathbf{a}_3 = c(0,0,1)$ and n_1, n_2, and n_3 are integer.
[b] $\{m_{010}|(0,0,0)\}$.
[c] $\{^{\mathrm{d}}1|(0,0,0)\}$.
[d] $\{^{\mathrm{d}}m_{010}|(0,0,0)\}$.
[e] T represents $T_M = e^{-i\mathbf{k}_M \cdot \mathbf{R}_n}$, $T_L = e^{-i\mathbf{k}_L \cdot \mathbf{R}_n}$, $T_\Sigma = e^{-i\mathbf{k}_\Sigma \cdot \mathbf{R}_n}$, and $T_R = e^{-i\mathbf{k}_R \cdot \mathbf{R}_n}$.

TABLE S III. Character table at the K [$\mathbf{k}_K = \frac{2\pi}{a}(\frac{1}{3}, \frac{1}{3}, 0)$] and H [$\mathbf{k}_H = (\frac{2\pi}{a}\frac{1}{3}, \frac{2\pi}{a}\frac{1}{3}, \frac{2\pi}{c}\frac{1}{2})$] points of the space group $P3m1$, which transforms isomorphically to the point group $3\,(C_3)$.

	$\{1\}^{\mathrm{a}}$	$\{3^+\}^{\mathrm{b}}$	$\{3^-\}^{\mathrm{c}}$	$\{^{\mathrm{d}}1\}^{\mathrm{d}}$	$\{^{\mathrm{d}}3^+\}^{\mathrm{e}}$	$\{^{\mathrm{d}}3^-\}^{\mathrm{f}}$
K_1	$1 \cdot T^{\mathrm{g}}$	1	1	1	1	1
K_2	$1 \cdot T$	$\exp(i\frac{2\pi}{3})$	$\exp(-i\frac{2\pi}{3})$	1	$\exp(i\frac{2\pi}{3})$	$\exp(-i\frac{2\pi}{3})$
K_3	$1 \cdot T$	$\exp(-i\frac{2\pi}{3})$	$\exp(i\frac{2\pi}{3})$	1	$\exp(-i\frac{2\pi}{3})$	$\exp(i\frac{2\pi}{3})$
$\overline{K}_4$	$1 \cdot T$	-1	-1	-1	1	1
$\overline{K}_5$	$1 \cdot T$	$-\exp(i\frac{2\pi}{3})$	$-\exp(-i\frac{2\pi}{3})$	-1	$\exp(i\frac{2\pi}{3})$	$\exp(-i\frac{2\pi}{3})$
$\overline{K}_6$	$1 \cdot T$	$-\exp(-i\frac{2\pi}{3})$	$-\exp(i\frac{2\pi}{3})$	-1	$\exp(-i\frac{2\pi}{3})$	$\exp(i\frac{2\pi}{3})$

[a] $\{1|\mathbf{R}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3\}$, where $\mathbf{a}_1 = a(1,0,0)$, $\mathbf{a}_2 = a(-\frac{1}{2}, \frac{\sqrt{3}}{2}, 0)$, and $\mathbf{a}_3 = c(0,0,1)$ and n_1, n_2, and n_3 are integer.
[b] $\{3^+_{001}|(0,0,0)\}$.
[c] $\{3^-_{001}|(0,0,0)\}$.
[d] $\{^{\mathrm{d}}1|(0,0,0)\}$.
[e] $\{^{\mathrm{d}}3^+_{001}|(0,0,0)\}$.
[f] $\{^{\mathrm{d}}3^-_{001}|(0,0,0)\}$.
[g] T represents $T_K = e^{-i\mathbf{k}_K \cdot \mathbf{R}_n}$ and $T_H = e^{-i\mathbf{k}_H \cdot \mathbf{R}_n}$.

TABLE S IV. Character table at the Λ [$\mathbf{k}_\Lambda = \frac{2\pi}{a}(u,u,0),$ where $0<u<\frac{1}{3}$] and Q [$\mathbf{k}_Q = (\frac{2\pi}{a}u, \frac{2\pi}{a}u, \frac{2\pi}{c}\frac{1}{2}),$ where $0<u<\frac{1}{3}$] points of the space group $P3m1$, which transforms isomorphically to the point group $1\,(C_1)$.

	$\{1\}$[a]	$\{^{d}1\}$[b]
Λ_1	$1\cdot T$[c]	1
$\overline{\Lambda}_2$	$1\cdot T$	-1

[a] $\{1|\mathbf{R}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3\}$, where $\mathbf{a}_1 = a(1,0,0)$, $\mathbf{a}_2 = a(-\frac{1}{2}, \frac{\sqrt{3}}{2}, 0)$, and $\mathbf{a}_3 = c(0,0,1)$ and n_1, n_2, and n_3 are integer.
[b] $\{^{d}1|(0,0,0)\}$.
[c] T represents $T_\Lambda = e^{-i\mathbf{k}_\Lambda\cdot\mathbf{R}_n}$ and $T_Q = e^{-i\mathbf{k}_Q\cdot\mathbf{R}_n}$.

TABLE S V. Representation of the atomic orbital at the Γ and A points of the space group $P3m1$.

	$\{1\}$	$\{3\}$	$\{m_{010}\}$	$\{m_{100}\}$	Decomposition
$\Gamma_s^{\rm orb}$	1	1	1	1	Γ_1
$\Gamma_p^{\rm orb}$	3	0	1	1	$\Gamma_1 \oplus \Gamma_3$
$\Gamma_d^{\rm orb}$	5	-1	1	1	$\Gamma_1 \oplus 2\Gamma_3$
$\Gamma_{s\,1/2}^{\rm orb}$	2	1	0	0	$\overline{\Gamma}_6$
$\Gamma_{p\,1/2}^{\rm orb}$	2	1	0	0	$\overline{\Gamma}_6$
$\Gamma_{p\,3/2}^{\rm orb}$	4	-1	0	0	$\overline{\Gamma}_4 \oplus \overline{\Gamma}_5 \oplus \overline{\Gamma}_6$
$\Gamma_{d\,3/2}^{\rm orb}$	4	-1	0	0	$\overline{\Gamma}_4 \oplus \overline{\Gamma}_5 \oplus \overline{\Gamma}_6$
$\Gamma_{d\,5/2}^{\rm orb}$	6	0	0	0	$\overline{\Gamma}_4 \oplus \overline{\Gamma}_5 \oplus 2\overline{\Gamma}_6$

TABLE S VI. Representation of the atomic orbital at the M and L points of the space group $P3m1$.

	$\{1\}$	$\{m_{010}\}$	Decomposition
$M_s^{\rm orb}$	1	1	M_1
$M_p^{\rm orb}$	3	1	$2M_1 \oplus M_2$
$M_d^{\rm orb}$	5	1	$3M_1 \oplus 2M_2$
$M_{s\,1/2}^{\rm orb}$	2	0	$\overline{M}_3 \oplus \overline{M}_4$
$M_{p\,1/2}^{\rm orb}$	2	0	$\overline{M}_3 \oplus \overline{M}_4$
$M_{p\,3/2}^{\rm orb}$	4	0	$2\overline{M}_3 \oplus 2\overline{M}_4$
$M_{d\,3/2}^{\rm orb}$	4	0	$2\overline{M}_3 \oplus 2\overline{M}_4$
$M_{d\,5/2}^{\rm orb}$	6	0	$3\overline{M}_3 \oplus 3\overline{M}_4$

TABLE S VII. Representation of the atomic orbital at the K and H points of the space group $P3m1$.

	$\{1\}$	$\{3^+\}$	$\{3^-\}$	Decomposition
$K_s^{\rm orb}$	1	1	1	K_1
$K_p^{\rm orb}$	3	0	0	$K_1 \oplus K_2 \oplus K_3$
$K_d^{\rm orb}$	5	-1	-1	$K_1 \oplus 2K_2 \oplus 2K_3$
$K_{s\,1/2}^{\rm orb}$	2	1	1	$\overline{K}_5 \oplus \overline{K}_6$
$K_{p\,1/2}^{\rm orb}$	2	1	1	$\overline{K}_5 \oplus \overline{K}_6$
$K_{p\,3/2}^{\rm orb}$	4	-1	-1	$2\overline{K}_4 \oplus \overline{K}_5 \oplus \overline{K}_6$
$K_{d\,3/2}^{\rm orb}$	4	-1	-1	$2\overline{K}_4 \oplus \overline{K}_5 \oplus \overline{K}_6$
$K_{d\,5/2}^{\rm orb}$	6	0	0	$2\overline{K}_4 \oplus 2\overline{K}_5 \oplus 2\overline{K}_6$

TABLE S VIII. Representation of the atomic arrangement of Bi $(0,0,0)$, Te $(\frac{2}{3}, \frac{1}{3}, 0.75)$, and I $(\frac{1}{3}, \frac{2}{3}, 0.31)$ at the Γ and A points of the space group $P3m1$.

	$\{1\}$	$\{3\}$	$\{m_{010}\}$	$\{m_{100}\}$	Decomposition
$\frac{a}{2\pi}\mathbf{G}$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	$\mathbf{0}$	
$\Gamma_{\rm Bi}^{\rm arr}$	1	1	1	1	Γ_1
$\Gamma_{\rm Te}^{\rm arr}$	1	1	1	1	Γ_1
$\Gamma_{\rm I}^{\rm arr}$	1	1	1	1	Γ_1

TABLE S IX. Representation of the atomic arrangement of Bi $(0,0,0)$, Te $(\frac{2}{3},\frac{1}{3},0.75)$, and I $(\frac{1}{3},\frac{2}{3},0.31)$ at the M and L points of the space group $P3m1$.

	$\{1\}$	$\{m_{010}\}$	Decomposition
$\frac{a}{2\pi}\mathbf{G}$	$\mathbf{0}$	$\mathbf{0}$	
$M^{\mathrm{arr}}_{\mathrm{Bi}}$	1	1	M_1
$M^{\mathrm{arr}}_{\mathrm{Te}}$	1	1	M_1
$M^{\mathrm{arr}}_{\mathrm{I}}$	1	1	M_1

TABLE S X. Representation of the atomic arrangement of Bi $(0,0,0)$, Te $(\frac{2}{3},\frac{1}{3},0.75)$, and I $(\frac{1}{3},\frac{2}{3},0.31)$ at the K and H points of the space group $P3m1$.

	$\{1\}$	$\{3^+\}$	$\{3^-\}$	Decomposition
$\frac{a}{2\pi}\mathbf{G}$	$\mathbf{0}$	$(-1,0,0)$	$(0,-1,0)$	
$K^{\mathrm{arr}}_{\mathrm{Bi}}$	1	1	1	K_1
$K^{\mathrm{arr}}_{\mathrm{Te}}$	1	$\exp(i\frac{2\pi}{3})$	$\exp(-i\frac{2\pi}{3})$	K_2
$K^{\mathrm{arr}}_{\mathrm{I}}$	1	$\exp(-i\frac{2\pi}{3})$	$\exp(i\frac{2\pi}{3})$	K_3

TABLE S XI. Representation of the atomic wavefunction of Bi $(0,0,0)$, Te $(\frac{2}{3},\frac{1}{3},0.75)$, and I $(\frac{1}{3},\frac{2}{3},0.31)$ at the Γ and A points of the space group $P3m1$.

	$\{1\}$	$\{3\}$	$\{m_{010}\}$	$\{m_{100}\}$	Decomposition
Bi s	1	1	1	1	Γ_1
Bi p	3	0	1	1	$\Gamma_1 \oplus \Gamma_3$
Bi d	5	-1	1	1	$\Gamma_1 \oplus 2\Gamma_3$
Te s	1	1	1	1	Γ_1
Te p	3	0	1	1	$\Gamma_1 \oplus \Gamma_3$
Te d	5	-1	1	1	$\Gamma_1 \oplus 2\Gamma_3$
I s	1	1	1	1	Γ_1
I p	3	0	1	1	$\Gamma_1 \oplus \Gamma_3$
I d	5	-1	1	1	$\Gamma_1 \oplus 2\Gamma_3$
Bi $s_{1/2}$	2	1	0	0	$\overline{\Gamma}_6$
Bi $p_{1/2}$	2	1	0	0	$\overline{\Gamma}_6$
Bi $p_{3/2}$	4	-1	0	0	$\overline{\Gamma}_4 \oplus \overline{\Gamma}_5 \oplus \overline{\Gamma}_6$
Bi $d_{3/2}$	4	-1	0	0	$\overline{\Gamma}_4 \oplus \overline{\Gamma}_5 \oplus \overline{\Gamma}_6$
Bi $d_{5/2}$	6	0	0	0	$\overline{\Gamma}_4 \oplus \overline{\Gamma}_5 \oplus 2\overline{\Gamma}_6$
Te $s_{1/2}$	2	1	0	0	$\overline{\Gamma}_6$
Te $p_{1/2}$	2	1	0	0	$\overline{\Gamma}_6$
Te $p_{3/2}$	4	-1	0	0	$\overline{\Gamma}_4 \oplus \overline{\Gamma}_5 \oplus \overline{\Gamma}_6$
Te $d_{3/2}$	4	-1	0	0	$\overline{\Gamma}_4 \oplus \overline{\Gamma}_5 \oplus \overline{\Gamma}_6$
Te $d_{5/2}$	6	0	0	0	$\overline{\Gamma}_4 \oplus \overline{\Gamma}_5 \oplus 2\overline{\Gamma}_6$
I $s_{1/2}$	2	1	0	0	$\overline{\Gamma}_6$
I $p_{1/2}$	2	1	0	0	$\overline{\Gamma}_6$
I $p_{3/2}$	4	-1	0	0	$\overline{\Gamma}_4 \oplus \overline{\Gamma}_5 \oplus \overline{\Gamma}_6$
I $d_{3/2}$	4	-1	0	0	$\overline{\Gamma}_4 \oplus \overline{\Gamma}_5 \oplus \overline{\Gamma}_6$
I $d_{5/2}$	6	0	0	0	$\overline{\Gamma}_4 \oplus \overline{\Gamma}_5 \oplus 2\overline{\Gamma}_6$

TABLE S XII. Representation of the atomic wavefunction of Bi $(0, 0, 0)$, Te $(\frac{2}{3}, \frac{1}{3}, 0.75)$, and I $(\frac{1}{3}, \frac{2}{3}, 0.31)$ at the M and L points of the space group $P3m1$.

	{1}	$\{m_{010}\}$	Decomposition
Bi s	1	1	M_1
Bi p	3	1	$2M_1 \oplus M_2$
Bi d	5	1	$3M_1 \oplus 2M_2$
Te s	1	1	M_1
Te p	3	1	$2M_1 \oplus M_2$
Te d	5	1	$3M_1 \oplus 2M_2$
I s	1	1	M_1
I p	3	1	$2M_1 \oplus M_2$
I d	5	1	$3M_1 \oplus 2M_2$
Bi $s_{1/2}$	2	0	$\overline{M}_3 \oplus \overline{M}_4$
Bi $p_{1/2}$	2	0	$\overline{M}_3 \oplus \overline{M}_4$
Bi $p_{3/2}$	4	0	$2\overline{M}_3 \oplus 2\overline{M}_4$
Bi $d_{3/2}$	4	0	$2\overline{M}_3 \oplus 2\overline{M}_4$
Bi $d_{5/2}$	6	0	$3\overline{M}_3 \oplus 3\overline{M}_4$
Te $s_{1/2}$	2	0	$\overline{M}_3 \oplus \overline{M}_4$
Te $p_{1/2}$	2	0	$\overline{M}_3 \oplus \overline{M}_4$
Te $p_{3/2}$	4	0	$2\overline{M}_3 \oplus 2\overline{M}_4$
Te $d_{3/2}$	4	0	$2\overline{M}_3 \oplus 2\overline{M}_4$
Te $d_{5/2}$	6	0	$3\overline{M}_3 \oplus 3\overline{M}_4$
I $s_{1/2}$	2	0	$\overline{M}_3 \oplus \overline{M}_4$
I $p_{1/2}$	2	0	$\overline{M}_3 \oplus \overline{M}_4$
I $p_{3/2}$	4	0	$2\overline{M}_3 \oplus 2\overline{M}_4$
I $d_{3/2}$	4	0	$2\overline{M}_3 \oplus 2\overline{M}_4$
I $d_{5/2}$	6	0	$3\overline{M}_3 \oplus 3\overline{M}_4$

TABLE S XIII. Representation of the atomic wavefunction of Bi $(0, 0, 0)$, Te $(\frac{2}{3}, \frac{1}{3}, 0.75)$, and I $(\frac{1}{3}, \frac{2}{3}, 0.31)$ at the K and H points of the space group $P3m1$.

	{1}	$\{3^+\}$	$\{3^-\}$	Decomposition
Bi s	1	1	1	K_1
Bi p	3	0	0	$K_1 \oplus K_2 \oplus K_3$
Bi d	5	-1	-1	$K_1 \oplus 2K_2 \oplus 2K_3$
Te s	1	$\exp(i\frac{2\pi}{3})$	$\exp(-i\frac{2\pi}{3})$	K_2
Te p	3	0	0	$K_1 \oplus K_2 \oplus K_3$
Te d	5	$-\exp(i\frac{2\pi}{3})$	$-\exp(-i\frac{2\pi}{3})$	$2K_1 \oplus K_2 \oplus 2K_3$
I s	1	$\exp(-i\frac{2\pi}{3})$	$\exp(i\frac{2\pi}{3})$	K_3
I p	3	0	0	$K_1 \oplus K_2 \oplus K_3$
I d	5	$-\exp(-i\frac{2\pi}{3})$	$-\exp(i\frac{2\pi}{3})$	$2K_1 \oplus 2K_2 \oplus K_3$
Bi $s_{1/2}$	2	1	1	$\overline{K}_5 \oplus \overline{K}_6$
Bi $p_{1/2}$	2	1	1	$\overline{K}_5 \oplus \overline{K}_6$
Bi $p_{3/2}$	4	-1	-1	$2\overline{K}_4 \oplus \overline{K}_5 \oplus \overline{K}_6$
Bi $d_{3/2}$	4	-1	-1	$2\overline{K}_4 \oplus \overline{K}_5 \oplus \overline{K}_6$
Bi $d_{5/2}$	6	0	0	$2\overline{K}_4 \oplus 2\overline{K}_5 \oplus 2\overline{K}_6$
Te $s_{1/2}$	2	$\exp(i\frac{2\pi}{3})$	$\exp(-i\frac{2\pi}{3})$	$\overline{K}_4 \oplus \overline{K}_6$
Te $p_{1/2}$	2	$\exp(i\frac{2\pi}{3})$	$\exp(-i\frac{2\pi}{3})$	$\overline{K}_4 \oplus \overline{K}_6$
Te $p_{3/2}$	4	$-\exp(i\frac{2\pi}{3})$	$-\exp(-i\frac{2\pi}{3})$	$\overline{K}_4 \oplus 2\overline{K}_5 \oplus \overline{K}_6$
Te $d_{3/2}$	4	$-\exp(i\frac{2\pi}{3})$	$-\exp(-i\frac{2\pi}{3})$	$\overline{K}_4 \oplus 2\overline{K}_5 \oplus \overline{K}_6$
Te $d_{5/2}$	6	0	0	$2\overline{K}_4 \oplus 2\overline{K}_5 \oplus 2\overline{K}_6$
I $s_{1/2}$	2	$\exp(-i\frac{2\pi}{3})$	$\exp(i\frac{2\pi}{3})$	$\overline{K}_4 \oplus \overline{K}_5$
I $p_{1/2}$	2	$\exp(-i\frac{2\pi}{3})$	$\exp(i\frac{2\pi}{3})$	$\overline{K}_4 \oplus \overline{K}_5$
I $p_{3/2}$	4	$-\exp(-i\frac{2\pi}{3})$	$-\exp(i\frac{2\pi}{3})$	$\overline{K}_4 \oplus \overline{K}_5 \oplus 2\overline{K}_6$
I $d_{3/2}$	4	$-\exp(-i\frac{2\pi}{3})$	$-\exp(i\frac{2\pi}{3})$	$\overline{K}_4 \oplus \overline{K}_5 \oplus 2\overline{K}_6$
I $d_{5/2}$	6	0	0	$2\overline{K}_4 \oplus 2\overline{K}_5 \oplus 2\overline{K}_6$