Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic supplementary information (ESI): Focus on the overlap density of wavefunctions in *GW* approximations

Koshi Okamura*

Ronin Institute, Montclair, New Jersey 07043, USA

E-mail: koshi.okamura@ronininstitute.org

S1 PAW datasets

$\mathrm{PAW^{GS}}$ and $\mathrm{PAW^{QP}}$ are listed in Table S1. $\mathrm{PAW^{GS}}$ is a slight modification to the JTH atomic datasets library v1.0 provided with ABINIT code, and $\mathrm{PAW^{QP}}$ is an extension to $\mathrm{PAW^{GS}}$ with additional sets of partial waves and projector function.

S2 Character tables of space group #221

The character tables of the symmorphic space group #221 at high symmetry points and along symmetry axes are summarized in Tables S2-S9. Point group operations $\{R_\alpha\}$ are described in the Hermann-Mauguin notation. The irreducible representations in the first, second, and third column are given in the notations of the Bilbao Crystallographic Server (Bilbao),[S1,S2] Bouckaert-Smoluchowski-Wigner (BSW),[S3] and point group (PG),[S4] respectively.

S3 Representation of an atomic orbital

An atomic orbital has the representation of the full rotation group Γ^{atom}. The character χ^{atom} for an angular quantum number l and for either proper rotations $\{\alpha\}$ or improper rotations $\{\bar{\alpha}\}$ is described as

$$\begin{aligned} \chi_l^{\text{atom}}\{\alpha\} &= & \frac{\sin(l+\frac{1}{2})\alpha}{\sin\frac{1}{2}\alpha} \\ \chi_l^{\text{atom}}\{\bar{\alpha}\} &= (-1)^l & \frac{\sin(l+\frac{1}{2})\alpha}{\sin\frac{1}{2}\alpha} \end{aligned} \tag{S1}$$

The Γ^{atom}'s of s, p, and d orbitals for the groups of the wavevector at high symmetry points are summarized in Tables S10-S13 and decomposed into the irreducible representations. This procedure is based on ref. S5.

S4 Character of an equivalence representation

The character χ^{equiv} of an equivalence representation Γ^{equiv} for a space group operation $\{R_\alpha|\mathbf{R}_n\}$ is expressed by the trace of a matrix representation as

$$\chi^{\text{equiv}}\{R_\alpha|\mathbf{R}_n\} = \text{tr}\langle f_{\mathbf{k}}|\{R_\alpha|\mathbf{R}_n\}f_{\mathbf{k}}\rangle \tag{S2}$$

where $f_{\mathbf{k}}(\mathbf{r})$ is written in the form of a Bloch function with a cell-periodic function $g_{\mathbf{k}}(\mathbf{r})$ as

$$f_{\mathbf{k}}(\mathbf{r}) = \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}g_{\mathbf{k}}(\mathbf{r}) \tag{S3}$$

Here, $\mathbf{k}\cdot R_\alpha^{-1}\mathbf{r} = R_\alpha\mathbf{k}\cdot\mathbf{r}$ and $R_\alpha\mathbf{k} = \mathbf{k}+\mathbf{K}_\alpha$, where $\mathbf{K}_\alpha$ is a reciprocal lattice vector, and

$$\{R_\alpha|\mathbf{R}_n\}f_{\mathbf{k}}(\mathbf{r}) = \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}_n}\mathrm{e}^{\mathrm{i}(\mathbf{k}+\mathbf{K}_\alpha)\cdot\mathbf{r}}\{R_\alpha|\mathbf{R}_n\}g_{\mathbf{k}}(\mathbf{r}) \tag{S4}$$

Eqn (S2) then results in

$$\chi^{\mathrm{equiv}}\{R_\alpha|\mathbf{R}_n\} = \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}_n}\mathrm{tr}\langle g_{\mathbf{k}}|\mathrm{e}^{\mathrm{i}\mathbf{K}_\alpha\cdot\mathbf{r}}|\{R_\alpha|\mathbf{R}_n\}g_{\mathbf{k}}\rangle \tag{S5}$$

Note that the phase factor $\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}_n}$ comes from the translation operation $\{\mathbf{R}_n\}$.

S5 Equivalence representation of an atomic arrangement

An atomic arrangement is expressed by a Bloch function in the form of eqn (S3) with

$$g_{\mathbf{k}}(\mathbf{r}) = \sum_j \delta(\mathbf{r} - \mathbf{r}_j) \tag{S6}$$

where $\mathbf{r}_j$ is the position of atoms. Eqn (S5) then leads to

$$\chi^{\mathrm{equiv}}\{R_\alpha|\mathbf{R}_n\} = \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}_n}\sum_j \mathrm{e}^{\mathrm{i}\mathbf{K}_\alpha\cdot\mathbf{r}_j}\delta(\{R_\alpha^{-1}|\mathbf{R}_n\}\mathbf{r}_j - \mathbf{r}_j) \tag{S7}$$

The Γ^{equiv}'s of Ti, Sr, and O_3 atoms for the groups of the wavevector at high symmetry points are summarized in Tables S14-S17 and decomposed into the irreducible representations.

S6 Equivalence representation of a set of plane waves

Plane waves are sorted by $|\mathbf{k}+\mathbf{G}|$ and a set of plane waves is expressed by a Bloch function in the form of eqn (S3) with

$$g_{\mathbf{k}}(\mathbf{r}) = \sum_j \mathrm{e}^{\mathrm{i}\mathbf{G}_j\cdot\mathbf{r}} \tag{S8}$$

where $\mathbf{G}_j$ is the reciprocal lattice vector. Here, $\mathbf{G}_j \cdot R_\alpha^{-1}\mathbf{r} = R_\alpha\mathbf{G}_j \cdot \mathbf{r}$ and $R_\alpha\mathbf{G}_j = \mathbf{G}_j + \mathbf{K}_{\alpha,j}$, where $\mathbf{K}_{\alpha,j}$ is a reciprocal lattice vector. Eqn (S5) then leads to

$$\chi^{\mathrm{equiv}}\{R_\alpha|\mathbf{R}_n\} = \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}_n}\sum_j \delta(\mathbf{K}_\alpha + \mathbf{K}_{\alpha,j}) \tag{S9}$$

The Γ^{equiv}'s of sets of plane waves for the groups of the wavevector at high symmetry points are summarized in Tables S18-S21 and decomposed into the irreducible representations. These procedures in Sections S4-S6 are based partially on ref. S5.

Table S1: Description of PAW$^{\text{GS}}$ and PAW$^{\text{QP}}$ specifying the state, matching radius r_c, and reference energy E_{ref}

Atom	State	PAW$^{\text{GS}}$		PAW$^{\text{QP}}$	
		r_c (a_0)	E_{ref} (E_{h})	r_c (a_0)	E_{ref} (E_{h})
Sr	4s	1.81	−1.47	1.81	−1.47
	5s	1.81	−0.13	1.81	−0.13
	5s			1.81	1.50
	4p	2.01	−0.81	2.01	−0.81
	5p	2.01	1.00	2.01	0.25
	5p			2.01	1.00
	5p			2.01	1.75
	4d	2.21	−0.04	2.21	−0.04
	4d			2.21	1.00
	5d	2.21	1.50	2.21	1.50
Ti	3s	2.30	−2.17	2.30	−2.17
	4s	2.30	−0.14	2.30	−0.14
	4s			2.30	1.50
	3p	2.11	−1.31	2.11	−1.31
	4p	2.11	0.75	2.11	0.00
	4p			2.11	1.00
	4p			2.11	1.50
	3d	2.11	−0.08	2.11	−0.08
	4d	2.11	0.75	2.11	0.75
	4d			2.11	1.50
	4d			2.11	2.25
O	2s	1.41	−0.87	1.41	−0.87
	3s	1.41	1.00	1.41	0.50
	3s			1.41	1.50
	2p	1.41	−0.34	1.41	−0.34
	3p	1.41	1.00	1.41	0.75
	3p			1.41	1.50

Table S2: Character table for the group of the wavevector at the Γ point [$\mathbf{k}_\Gamma = \frac{2\pi}{a}(0,0,0)$] of the space group #221, which transforms isomorphically to the point group $m\bar{3}m$ (O_h)

Bilbao	BSW	PG	1^a	2^b	$2'^c$	3^d	4^e	$\bar{1}^f$	m^g	m'^h	$\bar{3}^i$	$\bar{4}^j$
Γ_1^+	Γ_1^+	A_{1g}	1	1	1	1	1	1	1	1	1	1
Γ_1^-	Γ_1^-	A_{1u}	1	1	1	1	1	−1	−1	−1	−1	−1
Γ_2^+	Γ_2^+	A_{2g}	1	1	−1	1	−1	1	1	−1	1	−1
Γ_2^-	Γ_2^-	A_{2u}	1	1	−1	1	−1	−1	−1	1	−1	1
Γ_3^+	Γ_{12}^+	E_g	2	2	0	−1	0	2	2	0	−1	0
Γ_3^-	Γ_{12}^-	E_u	2	2	0	−1	0	−2	−2	0	1	0
Γ_4^+	Γ_{15}^+	T_{1g}	3	−1	−1	0	1	3	−1	−1	0	1
Γ_4^-	Γ_{15}^-	T_{1u}	3	−1	−1	0	1	−3	1	1	0	−1
Γ_5^+	Γ_{25}^+	T_{2g}	3	−1	1	0	−1	3	−1	1	0	−1
Γ_5^-	Γ_{25}^-	T_{2u}	3	−1	1	0	−1	−3	1	−1	0	1

[a] $1 : \{1|\mathbf{R}_n\}$, where $\mathbf{R}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$, $\mathbf{a}_1 = a(1,0,0)$, $\mathbf{a}_2 = a(0,1,0)$, and $\mathbf{a}_3 = a(0,0,1)$, and n_1, n_2, and n_3 are integer.

[b] $2 : \{2_{001}|0\}, \{2_{010}|0\}, \{2_{100}|0\}$.

[c] $2' : \{2_{110}|0\}, \{2_{1\bar{1}0}|0\}, \{2_{101}|0\}, \{2_{\bar{1}01}|0\}, \{2_{011}|0\}, \{2_{01\bar{1}}|0\}$.

[d] $3 : \{3^+_{111}|0\}, \{3^+_{\bar{1}\bar{1}1}|0\}, \{3^+_{\bar{1}1\bar{1}}|0\}, \{3^+_{1\bar{1}\bar{1}}|0\}, \{3^-_{111}|0\}, \{3^-_{\bar{1}\bar{1}1}|0\}, \{3^-_{\bar{1}1\bar{1}}|0\}, \{3^-_{1\bar{1}\bar{1}}|0\}$.

[e] $4 : \{4^+_{001}|0\}, \{4^+_{010}|0\}, \{4^+_{100}|0\}, \{4^-_{001}|0\}, \{4^-_{010}|0\}, \{4^-_{100}|0\}$.

[f] $\bar{1} : \{\bar{1}|0\}$.

[g] $m : \{m_{001}|0\}, \{m_{010}|0\}, \{m_{100}|0\}$.

[h] $m' : \{m_{110}|0\}, \{m_{1\bar{1}0}|0\}, \{m_{101}|0\}, \{m_{\bar{1}01}|0\}, \{m_{011}|0\}, \{m_{01\bar{1}}|0\}$.

[i] $\bar{3} : \{\bar{3}^+_{111}|0\}, \{\bar{3}^+_{\bar{1}\bar{1}1}|0\}, \{\bar{3}^+_{\bar{1}1\bar{1}}|0\}, \{\bar{3}^+_{1\bar{1}\bar{1}}|0\}, \{\bar{3}^-_{111}|0\}, \{\bar{3}^-_{\bar{1}\bar{1}1}|0\}, \{\bar{3}^-_{\bar{1}1\bar{1}}|0\}, \{\bar{3}^-_{1\bar{1}\bar{1}}|0\}$.

[j] $\bar{4} : \{\bar{4}^+_{001}|0\}, \{\bar{4}^+_{010}|0\}, \{\bar{4}^+_{100}|0\}, \{\bar{4}^-_{001}|0\}, \{\bar{4}^-_{010}|0\}, \{\bar{4}^-_{100}|0\}$.

Table S3: Character table for the group of the wavevector at an X point $[\mathbf{k}_{\mathrm{X}} = \frac{2\pi}{a}(0, \frac{1}{2}, 0)]$ of the space group #221, which transforms isomorphically to $4/mmm$ (D_{4h})

Bilbao	BSW	PG	1^a	$2_y{}^b$	$2_h{}^c$	$2_{h'}{}^d$	$4_y{}^e$	$\bar{1}^f$	$m_y{}^g$	$m_v{}^h$	$m_d{}^i$	$\bar{4}_y{}^j$
X_1^+	X_1^+	$\mathrm{A_{1g}}$	$1 \cdot T_{\mathbf{R}_n}{}^k$	1	1	1	1	1	1	1	1	1
X_1^-	X_1^-	$\mathrm{A_{1u}}$	$1 \cdot T_{\mathbf{R}_n}$	1	1	1	1	−1	−1	−1	−1	−1
X_2^+	X_2^+	$\mathrm{B_{1g}}$	$1 \cdot T_{\mathbf{R}_n}$	1	1	−1	−1	1	1	1	−1	−1
X_2^-	X_2^-	$\mathrm{B_{1u}}$	$1 \cdot T_{\mathbf{R}_n}$	1	1	−1	−1	−1	−1	−1	1	1
X_3^+	X_4^+	$\mathrm{A_{2g}}$	$1 \cdot T_{\mathbf{R}_n}$	1	−1	−1	1	1	1	−1	−1	1
X_3^-	X_4^-	$\mathrm{A_{2u}}$	$1 \cdot T_{\mathbf{R}_n}$	1	−1	−1	1	−1	−1	1	1	−1
X_4^+	X_3^+	$\mathrm{B_{2g}}$	$1 \cdot T_{\mathbf{R}_n}$	1	−1	1	−1	1	1	−1	1	−1
X_4^-	X_3^-	$\mathrm{B_{2u}}$	$1 \cdot T_{\mathbf{R}_n}$	1	−1	1	−1	−1	−1	1	−1	1
X_5^+	X_5^+	$\mathrm{E_g}$	$2 \cdot T_{\mathbf{R}_n}$	−2	0	0	0	2	−2	0	0	0
X_5^-	X_5^-	$\mathrm{E_u}$	$2 \cdot T_{\mathbf{R}_n}$	−2	0	0	0	−2	2	0	0	0

[a] $1 : \{1|\mathbf{R}_n\}$, where $\mathbf{R}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$, $\mathbf{a}_1 = a(1,0,0)$, $\mathbf{a}_2 = a(0,1,0)$, and $\mathbf{a}_3 = a(0,0,1)$, and n_1, n_2, and n_3 are integer.

[b] $2_y : \{2_{010}|0\}$.

[c] $2_h : \{2_{001}|0\}, \{2_{100}|0\}$.

[d] $2_{h'} : \{2_{101}|0\}, \{2_{\bar{1}01}|0\}$.

[e] $4_y : \{4^+_{010}|0\}, \{4^-_{010}|0\}$.

[f] $\bar{1} : \{\bar{1}|0\}$.

[g] $m_y : \{m_{010}|0\}$.

[h] $m_v : \{m_{001}|0\}, \{m_{100}|0\}$.

[i] $m_d : \{m_{101}|0\}, \{m_{\bar{1}01}|0\}$.

[j] $\bar{4}_y : \{\bar{4}^+_{010}|0\}, \{\bar{4}^-_{010}|0\}$.

[k] $T_{\mathbf{R}_n} = \mathrm{e}^{\mathrm{i}\pi n_2}$

Table S4: Character table for the group of the wavevector at an M point [$\mathbf{k}_\mathrm{M} = \frac{2\pi}{a}(\frac{1}{2}, \frac{1}{2}, 0)$] of the space group #221, which transforms isomorphically to $4/mmm$ (D_{4h})

Bilbao	BSW	PG	1^a	$2_z{}^b$	$2_h{}^c$	$2_{h'}{}^d$	$4_z{}^e$	$\bar{1}^f$	$m_z{}^g$	$m_v{}^h$	$m_d{}^i$	$\bar{4}_z{}^j$
M_1^+	M_1^+	$\mathrm{A_{1g}}$	$1 \cdot T_{\mathbf{R}_n}{}^k$	1	1	1	1	1	1	1	1	1
M_1^-	M_1^-	$\mathrm{A_{1u}}$	$1 \cdot T_{\mathbf{R}_n}$	1	1	1	1	−1	−1	−1	−1	−1
M_2^+	M_2^+	$\mathrm{B_{1g}}$	$1 \cdot T_{\mathbf{R}_n}$	1	1	−1	−1	1	1	1	−1	−1
M_2^-	M_2^-	$\mathrm{B_{1u}}$	$1 \cdot T_{\mathbf{R}_n}$	1	1	−1	−1	−1	−1	−1	1	1
M_3^+	M_4^+	$\mathrm{A_{2g}}$	$1 \cdot T_{\mathbf{R}_n}$	1	−1	−1	1	1	1	−1	−1	1
M_3^-	M_4^-	$\mathrm{A_{2u}}$	$1 \cdot T_{\mathbf{R}_n}$	1	−1	−1	1	−1	−1	1	1	−1
M_4^+	M_3^+	$\mathrm{B_{2g}}$	$1 \cdot T_{\mathbf{R}_n}$	1	−1	1	−1	1	1	−1	1	−1
M_4^-	M_3^-	$\mathrm{B_{2u}}$	$1 \cdot T_{\mathbf{R}_n}$	1	−1	1	−1	−1	−1	1	−1	1
M_5^+	M_5^+	$\mathrm{E_g}$	$2 \cdot T_{\mathbf{R}_n}$	−2	0	0	0	2	−2	0	0	0
M_5^-	M_5^-	$\mathrm{E_u}$	$2 \cdot T_{\mathbf{R}_n}$	−2	0	0	0	−2	2	0	0	0

[a] $1 : \{1|\mathbf{R}_n\}$, where $\mathbf{R}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$, $\mathbf{a}_1 = a(1,0,0)$, $\mathbf{a}_2 = a(0,1,0)$, and $\mathbf{a}_3 = a(0,0,1)$, and n_1, n_2, and n_3 are integer.

[b] $2_z : \{2_{001}|0\}$.

[c] $2_h : \{2_{010}|0\}, \{2_{100}|0\}$.

[d] $2_{h'} : \{2_{110}|0\}, \{2_{1\bar{1}0}|0\}$.

[e] $4_z : \{4^+_{001}|0\}, \{4^-_{001}|0\}$.

[f] $\bar{1} : \{\bar{1}|0\}$.

[g] $m_z : \{m_{001}|0\}$.

[h] $m_v : \{m_{010}|0\}, \{m_{100}|0\}$.

[i] $m_d : \{m_{110}|0\}, \{m_{1\bar{1}0}|0\}$.

[j] $\bar{4}_z : \{\bar{4}^+_{001}|0\}, \{\bar{4}^-_{001}|0\}$.

[k] $T_{\mathbf{R}_n} = \mathrm{e}^{\mathrm{i}\pi(n_1+n_2)}$

Table S5: Character table for the group of the wavevector at an R point [$\mathbf{k}_{\mathrm{R}} = \frac{2\pi}{a}(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$] of the space group #221, which transforms isomorphically to the point group $m\bar{3}m$ (O_h)

Bilbao	BSW	PG	1[a]	2[b]	2′[c]	3[d]	4[e]	$\bar{1}$[f]	m[g]	m'[h]	$\bar{3}$[i]	$\bar{4}$[j]
R_1^+	R_1^+	$\mathrm{A_{1g}}$	$1 \cdot T_{\mathbf{R}_n}$[k]	1	1	1	1	1	1	1	1	1
R_1^-	R_1^-	$\mathrm{A_{1u}}$	$1 \cdot T_{\mathbf{R}_n}$	1	1	1	1	−1	−1	−1	−1	−1
R_2^+	R_2^+	$\mathrm{A_{2g}}$	$1 \cdot T_{\mathbf{R}_n}$	1	−1	1	−1	1	1	−1	1	−1
R_2^-	R_2^-	$\mathrm{A_{2u}}$	$1 \cdot T_{\mathbf{R}_n}$	1	−1	1	−1	−1	−1	1	−1	1
R_3^+	R_{12}^+	$\mathrm{E_g}$	$2 \cdot T_{\mathbf{R}_n}$	2	0	−1	0	2	2	0	−1	0
R_3^-	R_{12}^-	$\mathrm{E_u}$	$2 \cdot T_{\mathbf{R}_n}$	2	0	−1	0	−2	−2	0	1	0
R_4^+	R_{15}^+	$\mathrm{T_{1g}}$	$3 \cdot T_{\mathbf{R}_n}$	−1	−1	0	1	3	−1	−1	0	1
R_4^-	R_{15}^-	$\mathrm{T_{1u}}$	$3 \cdot T_{\mathbf{R}_n}$	−1	−1	0	1	−3	1	1	0	−1
R_5^+	R_{25}^+	$\mathrm{T_{2g}}$	$3 \cdot T_{\mathbf{R}_n}$	−1	1	0	−1	3	−1	1	0	−1
R_5^-	R_{25}^-	$\mathrm{T_{2u}}$	$3 \cdot T_{\mathbf{R}_n}$	−1	1	0	−1	−3	1	−1	0	1

[a] $1 : \{1|\mathbf{R}_n\}$, where $\mathbf{R}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$, $\mathbf{a}_1 = a(1,0,0)$, $\mathbf{a}_2 = a(0,1,0)$, and $\mathbf{a}_3 = a(0,0,1)$, and n_1, n_2, and n_3 are integer.

[b] $2 : \{2_{001}|0\}, \{2_{010}|0\}, \{2_{100}|0\}$.

[c] $2' : \{2_{110}|0\}, \{2_{1\bar{1}0}|0\}, \{2_{101}|0\}, \{2_{\bar{1}01}|0\}, \{2_{011}|0\}, \{2_{01\bar{1}}|0\}$.

[d] $3 : \{3^+_{111}|0\}, \{3^+_{\bar{1}\bar{1}1}|0\}, \{3^+_{\bar{1}1\bar{1}}|0\}, \{3^+_{1\bar{1}\bar{1}}|0\}, \{3^-_{111}|0\}, \{3^-_{\bar{1}\bar{1}1}|0\}, \{3^-_{\bar{1}1\bar{1}}|0\}, \{3^-_{1\bar{1}\bar{1}}|0\}$.

[e] $4 : \{4^+_{001}|0\}, \{4^+_{010}|0\}, \{4^+_{100}|0\}, \{4^-_{001}|0\}, \{4^-_{010}|0\}, \{4^-_{100}|0\}$.

[f] $\bar{1} : \{\bar{1}|0\}$.

[g] $m : \{m_{001}|0\}, \{m_{010}|0\}, \{m_{100}|0\}$.

[h] $m' : \{m_{110}|0\}, \{m_{1\bar{1}0}|0\}, \{m_{101}|0\}, \{m_{\bar{1}01}|0\}, \{m_{011}|0\}, \{m_{01\bar{1}}|0\}$.

[i] $\bar{3} : \{\bar{3}^+_{111}|0\}, \{\bar{3}^+_{\bar{1}\bar{1}1}|0\}, \{\bar{3}^+_{\bar{1}1\bar{1}}|0\}, \{\bar{3}^+_{1\bar{1}\bar{1}}|0\}, \{\bar{3}^-_{111}|0\}, \{\bar{3}^-_{\bar{1}\bar{1}1}|0\}, \{\bar{3}^-_{\bar{1}1\bar{1}}|0\}, \{\bar{3}^-_{1\bar{1}\bar{1}}|0\}$.

[j] $\bar{4} : \{\bar{4}^+_{001}|0\}, \{\bar{4}^+_{010}|0\}, \{\bar{4}^+_{100}|0\}, \{\bar{4}^-_{001}|0\}, \{\bar{4}^-_{010}|0\}, \{\bar{4}^-_{100}|0\}$.

[k] $T_{\mathbf{R}_n} = \mathrm{e}^{\mathrm{i}\pi(n_1+n_2+n_3)}$

Table S6: Character table for the group of the wavevector along a Δ axis [$\mathbf{k}_{\Delta} = \frac{2\pi}{a}(0, \frac{1}{2}u, 0)$, where $0 < u < 1$] of the space group #221, which transforms isomorphically to $4mm$ (C_{4v})

Bilbao	BSW	PG	1[a]	2[b]	4[c]	m_v[d]	m_d[e]
Δ_1	Δ_1	$\mathrm{A_1}$	$1 \cdot T_{\mathbf{R}_n}$[f]	1	1	1	1
Δ_2	Δ_2	$\mathrm{B_1}$	$1 \cdot T_{\mathbf{R}_n}$	1	−1	1	−1
Δ_3	$\Delta_{2'}$	$\mathrm{B_2}$	$1 \cdot T_{\mathbf{R}_n}$	1	−1	−1	1
Δ_4	$\Delta_{1'}$	$\mathrm{A_2}$	$1 \cdot T_{\mathbf{R}_n}$	1	1	−1	−1
Δ_5	Δ_5	E	$2 \cdot T_{\mathbf{R}_n}$	−2	0	0	0

[a] $1 : \{1|\mathbf{R}_n\}$, where $\mathbf{R}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$, $\mathbf{a}_1 = a(1,0,0)$, $\mathbf{a}_2 = a(0,1,0)$, and $\mathbf{a}_3 = a(0,0,1)$, and n_1, n_2, and n_3 are integer.

[b] $2 : \{2_{010}|0\}$.

[c] $4 : \{4^+_{010}|0\}, \{4^-_{010}|0\}$.

[d] $m_v : \{m_{001}|0\}, \{m_{100}|0\}$.

[e] $m_d : \{m_{101}|0\}, \{m_{\bar{1}01}|0\}$.

[f] $T_{\mathbf{R}_n} = \mathrm{e}^{\mathrm{i}\pi n_2 u}$

Table S7: Character table for the group of the wavevector along a Σ axis [$\mathbf{k}_\Sigma = \frac{2\pi}{a}(\frac{1}{2}u, \frac{1}{2}u, 0)$, where $0 < u < 1$] of the space group #221, which transforms isomorphically to $mm2$ (C_{2v})

Bilbao	BSW	PG	1^a	$2'^b$	${m_z}^c$	m'^d
Σ_1	Σ_1	A_1	$1 \cdot {T_{\mathbf{R}_n}}^e$	1	1	1
Σ_2	Σ_4	B_2	$1 \cdot T_{\mathbf{R}_n}$	-1	1	-1
Σ_3	Σ_3	B_1	$1 \cdot T_{\mathbf{R}_n}$	-1	-1	1
Σ_4	Σ_2	A_2	$1 \cdot T_{\mathbf{R}_n}$	1	-1	-1

[a] $1 : \{1|\mathbf{R}_n\}$, where $\mathbf{R}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$, $\mathbf{a}_1 = a(1,0,0)$, $\mathbf{a}_2 = a(0,1,0)$, and $\mathbf{a}_3 = a(0,0,1)$, and n_1, n_2, and n_3 are integer.
[b] $2' : \{2_{110}|0\}$.
[c] $m_z : \{m_{001}|0\}$.
[d] $m' : \{m_{1\bar{1}0}|0\}$.
[e] $T_{\mathbf{R}_n} = \mathrm{e}^{\mathrm{i}\pi(n_1 u + n_2 u)}$

Table S8: Character table for the group of the wavevector along a Λ axis [$\mathbf{k}_\Lambda = \frac{2\pi}{a}(\frac{1}{2}u, \frac{1}{2}u, \frac{1}{2}u)$, where $0 < u < 1$] of the space group #221, which transforms isomorphically to $3m$ (C_{3v})

Bilbao	BSW	PG	1^a	3^b	${m_d}^c$
Λ_1	Λ_1	A_1	$1 \cdot {T_{\mathbf{R}_n}}^d$	1	1
Λ_2	Λ_2	A_2	$1 \cdot T_{\mathbf{R}_n}$	1	-1
Λ_3	Λ_3	E	$2 \cdot T_{\mathbf{R}_n}$	-1	0

[a] $1 : \{1|\mathbf{R}_n\}$, where $\mathbf{R}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$, $\mathbf{a}_1 = a(1,0,0)$, $\mathbf{a}_2 = a(0,1,0)$, and $\mathbf{a}_3 = a(0,0,1)$, and n_1, n_2, and n_3 are integer.
[b] $3 : \{3^+_{111}|0\}, \{3^-_{111}|0\}$.
[c] $m_d : \{m_{1\bar{1}0}|0\}, \{m_{\bar{1}01}|0\}, \{m_{01\bar{1}}|0\}$.
[d] $T_{\mathbf{R}_n} = \mathrm{e}^{\mathrm{i}\pi(n_1 u + n_2 u + n_3 u)}$

Table S9: Character table for the group of the wavevector along a Z axis [$\mathbf{k}_\mathrm{Z} = \frac{2\pi}{a}(\frac{1}{2}u, \frac{1}{2}, 0)$, where $0 < u < 1$] of the space group #221, which transforms isomorphically to $mm2$ (C_{2v})

Bilbao	BSW	PG	1^a	${2_x}^b$	${m_z}^c$	${m_y}^d$
Z_1	Z_1	A_1	$1 \cdot {T_{\mathbf{R}_n}}^e$	1	1	1
Z_2	Z_2	A_2	$1 \cdot T_{\mathbf{R}_n}$	1	-1	-1
Z_3	Z_4	B_2	$1 \cdot T_{\mathbf{R}_n}$	-1	-1	1
Z_4	Z_3	B_1	$1 \cdot T_{\mathbf{R}_n}$	-1	1	-1

[a] $1 : \{1|\mathbf{R}_n\}$, where $\mathbf{R}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$, $\mathbf{a}_1 = a(1,0,0)$, $\mathbf{a}_2 = a(0,1,0)$, and $\mathbf{a}_3 = a(0,0,1)$, and n_1, n_2, and n_3 are integer.
[b] $2_x : \{2_{100}|0\}$.
[c] $m_z : \{m_{001}|0\}$.
[d] $m_y : \{m_{010}|0\}$.
[e] $T_{\mathbf{R}_n} = \mathrm{e}^{\mathrm{i}\pi(n_1 u + n_2)}$

Table S10: Representations of s, p, and d orbitals for the group of the wavevector at the Γ point of the space group #221

$m\bar{3}m$	1	2	$2'$	3	4	$\bar{1}$	m	m'	$\bar{3}$	$\bar{4}$	Irreducible representations
$\Gamma_{\mathrm{s}}^{\mathrm{atom}}$	1	1	1	1	1	1	1	1	1	1	Γ_1^+
$\Gamma_{\mathrm{p}}^{\mathrm{atom}}$	3	−1	−1	0	1	−3	1	1	0	−1	Γ_4^-
$\Gamma_{\mathrm{d}}^{\mathrm{atom}}$	5	1	1	−1	−1	5	1	1	−1	−1	$\Gamma_3^+ \oplus \Gamma_5^+$

Table S11: Representations of s, p, and d orbitals for the group of the wavevector at an X point of the space group #221

$4/mmm$	1	2_y	2_h	$2_{h'}$	4_y	$\bar{1}$	m_y	m_v	m_d	$\bar{4}_y$	Irreducible representations
$\mathrm{X}_{\mathrm{s}}^{\mathrm{atom}}$	1	1	1	1	1	1	1	1	1	1	X_1^+
$\mathrm{X}_{\mathrm{p}}^{\mathrm{atom}}$	3	−1	−1	−1	1	−3	1	1	1	−1	$\mathrm{X}_3^- \oplus \mathrm{X}_5^-$
$\mathrm{X}_{\mathrm{d}}^{\mathrm{atom}}$	5	1	1	1	−1	5	1	1	1	−1	$\mathrm{X}_1^+ \oplus \mathrm{X}_2^+ \oplus \mathrm{X}_4^+ \oplus \mathrm{X}_5^+$

Table S12: Representations of s, p, and d orbitals for the group of the wavevector at an M point of the space group #221

$4/mmm$	1	2_z	2_h	$2_{h'}$	4_z	$\bar{1}$	m_z	m_v	m_d	$\bar{4}_z$	Irreducible representations
$\mathrm{M}_{\mathrm{s}}^{\mathrm{atom}}$	1	1	1	1	1	1	1	1	1	1	M_1^+
$\mathrm{M}_{\mathrm{p}}^{\mathrm{atom}}$	3	−1	−1	−1	1	−3	1	1	1	−1	$\mathrm{M}_3^- \oplus \mathrm{M}_5^-$
$\mathrm{M}_{\mathrm{d}}^{\mathrm{atom}}$	5	1	1	1	−1	5	1	1	1	−1	$\mathrm{M}_1^+ \oplus \mathrm{M}_2^+ \oplus \mathrm{M}_4^+ \oplus \mathrm{M}_5^+$

Table S13: Representations of s, p, and d orbitals for the group of the wavevector at an R point of the space group #221

$m\bar{3}m$	1	2	$2'$	3	4	$\bar{1}$	m	m'	$\bar{3}$	$\bar{4}$	Irreducible representations
$\mathrm{R}_{\mathrm{s}}^{\mathrm{atom}}$	1	1	1	1	1	1	1	1	1	1	R_1^+
$\mathrm{R}_{\mathrm{p}}^{\mathrm{atom}}$	3	−1	−1	0	1	−3	1	1	0	−1	R_4^-
$\mathrm{R}_{\mathrm{d}}^{\mathrm{atom}}$	5	1	1	−1	−1	5	1	1	−1	−1	$\mathrm{R}_3^+ \oplus \mathrm{R}_5^+$

Table S14: Equivalence representations of Ti, Sr, and O_3 atoms in $SrTiO_3$ for the group of the wavevector at the Γ point of the space group #221

$m\bar{3}m$	1	2	$2'$	3	4	$\bar{1}$	m	m'	$\bar{3}$	$\bar{4}$	Irreducible representations
$\Gamma_{\mathrm{Ti}}^{\mathrm{equiv}}$	1	1	1	1	1	1	1	1	1	1	Γ_1^+
$\Gamma_{\mathrm{Sr}}^{\mathrm{equiv}}$	1	1	1	1	1	1	1	1	1	1	Γ_1^+
$\Gamma_{\mathrm{O_3}}^{\mathrm{equiv}}$	3	3	1	0	1	3	3	1	0	1	$\Gamma_1^+ \oplus \Gamma_3^+$

Table S15: Equivalence representations of Ti, Sr, and O_3 atoms in $SrTiO_3$ for the group of the wavevector at an X point of the space group #221

$4/mmm$	1	2_y	2_h	$2_{h'}$	4_y	$\bar{1}$	m_y	m_v	m_d	$\bar{4}_y$	Irreducible representations
$\mathrm{X}_{\mathrm{Ti}}^{\mathrm{equiv}}$	1	1	1	1	1	1	1	1	1	1	X_1^+
$\mathrm{X}_{\mathrm{Sr}}^{\mathrm{equiv}}$	1	1	−1	−1	1	−1	−1	1	1	−1	X_3^-
$\mathrm{X}_{\mathrm{O_3}}^{\mathrm{equiv}}$	3	3	1	−1	1	1	1	3	1	−1	$\mathrm{X}_1^+ \oplus \mathrm{X}_2^+ \oplus \mathrm{X}_3^-$

Table S16: Equivalence representations of Ti, Sr, and O_3 atoms in $SrTiO_3$ for the group of the wavevector at an M point of the space group #221

$4/mmm$	1	2_z	2_h	$2_{h'}$	4_z	$\bar{1}$	m_z	m_v	m_d	$\bar{4}_z$	Irreducible representations
M^{equiv}_{Ti}	1	1	1	1	1	1	1	1	1	1	M_1^+
M^{equiv}_{Sr}	1	1	−1	1	−1	1	1	−1	1	−1	M_4^+
$M^{equiv}_{O_3}$	3	−1	1	1	1	−1	3	1	1	1	$M_1^+ \oplus M_5^-$

Table S17: Equivalence representations of Ti, Sr, and O_3 atoms in $SrTiO_3$ for the group of the wavevector at an R point of the space group #221

$m\bar{3}m$	1	2	$2'$	3	4	$\bar{1}$	m	m'	$\bar{3}$	$\bar{4}$	Irreducible representations
R^{equiv}_{Ti}	1	1	1	1	1	1	1	1	1	1	R_1^+
R^{equiv}_{Sr}	1	1	−1	1	−1	−1	−1	1	−1	1	R_2^-
$R^{equiv}_{O_3}$	3	−1	−1	0	1	−3	1	1	0	−1	R_4^-

Table S18: Equivalence representations of sets of plane waves $e^{i(\mathbf{k}_\Gamma+\mathbf{G})\cdot\mathbf{r}}$ for the group of the wavevector at the Γ point $[\mathbf{k}_\Gamma = \frac{2\pi}{a}(0,0,0)]$ of the space group #221, which transforms isomorphically to $m\bar{3}m$ (O_h). Plane waves are sorted by $|\mathbf{k}_\Gamma+\mathbf{G}|$ and labeled by $\frac{a}{2\pi}\{\mathbf{k}_\Gamma+\mathbf{G}\}$

$\frac{a}{2\pi}\{\mathbf{k}_\Gamma+\mathbf{G}\}$	1	2	$2'$	3	4	$\bar{1}$	m	m'	$\bar{3}$	$\bar{4}$	Irreducible representations
$\{0,0,0\}$	1	1	1	1	1	1	1	1	1	1	Γ_1^+
$\{1,0,0\}$	6	2	0	0	2	0	4	2	0	0	$\Gamma_1^+ \oplus \Gamma_3^+ \oplus \Gamma_4^-$
$\{1,1,0\}$	12	0	2	0	0	0	4	2	0	0	$\Gamma_1^+ \oplus \Gamma_3^+ \oplus \Gamma_4^- \oplus \Gamma_5^+ \oplus \Gamma_5^-$
$\{1,1,1\}$	8	0	0	2	0	0	0	4	0	0	$\Gamma_1^+ \oplus \Gamma_2^- \oplus \Gamma_4^- \oplus \Gamma_5^+$
$\{2,0,0\}$	6	2	0	0	2	0	4	2	0	0	$\Gamma_1^+ \oplus \Gamma_3^+ \oplus \Gamma_4^-$
$\{2,1,0\}$	24	0	0	0	0	0	8	0	0	0	$\Gamma_1^+ \oplus \Gamma_2^+ \oplus 2\Gamma_3^+ \oplus \Gamma_4^+ \oplus 2\Gamma_4^- \oplus \Gamma_5^+ \oplus 2\Gamma_5^-$
$\{2,1,1\}$	24	0	0	0	0	0	0	4	0	0	$\Gamma_1^+ \oplus \Gamma_2^- \oplus \Gamma_3^+ \oplus \Gamma_3^- \oplus \Gamma_4^+ \oplus 2\Gamma_4^- \oplus 2\Gamma_5^+ \oplus \Gamma_5^-$
$\{2,2,0\}$	12	0	2	0	0	0	4	2	0	0	$\Gamma_1^+ \oplus \Gamma_3^+ \oplus \Gamma_4^- \oplus \Gamma_5^+ \oplus \Gamma_5^-$
$\{2,2,1\}$	24	0	0	0	0	0	0	4	0	0	$\Gamma_1^+ \oplus \Gamma_2^- \oplus \Gamma_3^+ \oplus \Gamma_3^- \oplus \Gamma_4^+ \oplus 2\Gamma_4^- \oplus 2\Gamma_5^+ \oplus \Gamma_5^-$
$\{3,0,0\}$	6	2	0	0	2	0	4	2	0	0	$\Gamma_1^+ \oplus \Gamma_3^+ \oplus \Gamma_4^-$
$\{3,1,0\}$	24	0	0	0	0	0	8	0	0	0	$\Gamma_1^+ \oplus \Gamma_2^+ \oplus 2\Gamma_3^+ \oplus \Gamma_4^+ \oplus 2\Gamma_4^- \oplus \Gamma_5^+ \oplus 2\Gamma_5^-$
$\{3,1,1\}$	24	0	0	0	0	0	0	4	0	0	$\Gamma_1^+ \oplus \Gamma_2^- \oplus \Gamma_3^+ \oplus \Gamma_3^- \oplus \Gamma_4^+ \oplus 2\Gamma_4^- \oplus 2\Gamma_5^+ \oplus \Gamma_5^-$
$\{2,2,2\}$	8	0	0	2	0	0	0	4	0	0	$\Gamma_1^+ \oplus \Gamma_2^- \oplus \Gamma_4^- \oplus \Gamma_5^+$
$\{3,2,1\}$	48	0	0	0	0	0	0	0	0	0	$\Gamma_1^+ \oplus \Gamma_1^- \oplus \Gamma_2^+ \oplus \Gamma_2^- \oplus 2\Gamma_3^+ \oplus 2\Gamma_3^- \oplus 3\Gamma_4^+ \oplus 3\Gamma_4^-$ $\oplus 3\Gamma_5^+ \oplus 3\Gamma_5^-$

Table S19: Equivalence representations of sets of plane waves $e^{i(\mathbf{k}_X+\mathbf{G})\cdot\mathbf{r}}$ for the group of the wavevector at an X point $[\mathbf{k}_X=\frac{2\pi}{a}(0,\frac{1}{2},0)]$ of the space group #221, which transforms isomorphically to $4/mmm$ (D_{4h}). Plane waves are sorted by $|\mathbf{k}_X+\mathbf{G}|$ and labeled by $\frac{a}{2\pi}\{\mathbf{k}_X+\mathbf{G}\}$

$\frac{a}{2\pi}\{\mathbf{k}_X+\mathbf{G}\}$	1	2_y	2_h	$2_{h'}$	4_y	$\bar{1}$	m_y	m_v	m_d	$\bar{4}_y$	Irreducible representations
$\{0,\frac{1}{2},0\}^a$	2	2	0	0	2	0	0	2	2	0	$X_1^+ \oplus X_3^-$
$\{1,\frac{1}{2},0\}^b$	8	0	0	0	0	0	0	4	0	0	$X_1^+ \oplus X_2^+ \oplus X_3^- \oplus X_4^- \oplus X_5^+ \oplus X_5^-$
$\{0,\frac{3}{2},0\}^c$	2	2	0	0	2	0	0	2	2	0	$X_1^+ \oplus X_3^-$
$\{1,\frac{1}{2},1\}^d$	8	0	0	0	0	0	0	0	4	0	$X_1^+ \oplus X_2^- \oplus X_3^- \oplus X_4^+ \oplus X_5^+ \oplus X_5^-$
$\{1,\frac{3}{2},0\}^e$	8	0	0	0	0	0	0	4	0	0	$X_1^+ \oplus X_2^+ \oplus X_3^- \oplus X_4^- \oplus X_5^+ \oplus X_5^-$
$\{1,\frac{3}{2},1\}^f$	8	0	0	0	0	0	0	0	4	0	$X_1^+ \oplus X_2^- \oplus X_3^- \oplus X_4^+ \oplus X_5^+ \oplus X_5^-$
$\{2,\frac{1}{2},0\}^g$	8	0	0	0	0	0	0	4	0	0	$X_1^+ \oplus X_2^+ \oplus X_3^- \oplus X_4^- \oplus X_5^+ \oplus X_5^-$
$\{2,\frac{1}{2},1\}^h$	16	0	0	0	0	0	0	0	0	0	$X_1^+ \oplus X_1^- \oplus X_2^+ \oplus X_2^- \oplus X_3^+ \oplus X_3^-$ $\oplus X_4^+ \oplus X_4^- \oplus 2X_5^+ \oplus 2X_5^-$

[a] $\frac{a}{2\pi}\mathbf{G}$'s are $(0,0,0),(0,\bar{1},0)$.
[b] $\frac{a}{2\pi}\mathbf{G}$'s are $(1,0,0),(1,\bar{1},0),(\bar{1},0,0),(\bar{1},\bar{1},0),(0,0,1),(0,\bar{1},1),(0,0,\bar{1}),(0,\bar{1},\bar{1})$.
[c] $\frac{a}{2\pi}\mathbf{G}$'s are $(0,1,0),(0,\bar{2},0)$.
[d] $\frac{a}{2\pi}\mathbf{G}$'s are $(1,0,1),(1,\bar{1},1),(1,0,\bar{1}),(1,\bar{1},\bar{1}),(\bar{1},0,1),(\bar{1},\bar{1},1),(\bar{1},0,\bar{1}),(\bar{1},\bar{1},\bar{1})$.
[e] $\frac{a}{2\pi}\mathbf{G}$'s are $(1,1,0),(1,\bar{2},0),(\bar{1},1,0),(\bar{1},\bar{2},0),(0,1,1),(0,\bar{2},1),(0,1,\bar{1}),(0,\bar{2},\bar{1})$.
[f] $\frac{a}{2\pi}\mathbf{G}$'s are $(1,1,1),(1,\bar{2},1),(1,1,\bar{1}),(1,\bar{2},\bar{1}),(\bar{1},1,1),(\bar{1},\bar{2},1),(\bar{1},1,\bar{1}),(\bar{1},\bar{2},\bar{1})$.
[g] $\frac{a}{2\pi}\mathbf{G}$'s are $(2,0,0),(2,\bar{1},0),(\bar{2},0,0),(\bar{2},\bar{1},0),(0,0,2),(0,\bar{1},2),(0,0,\bar{2}),(0,\bar{1},\bar{2})$.
[h] $\frac{a}{2\pi}\mathbf{G}$'s are $(2,0,1),(2,\bar{1},1),(2,0,\bar{1}),(2,\bar{1},\bar{1}),(\bar{2},0,1),(\bar{2},\bar{1},1),$
$(\bar{2},0,\bar{1}),(\bar{2},\bar{1},\bar{1}),(1,0,2),(1,\bar{1},2),(\bar{1},0,2),(\bar{1},\bar{1},2),(1,0,\bar{2}),(1,\bar{1},\bar{2}),(\bar{1},0,\bar{2}),(\bar{1},\bar{1},\bar{2})$.

Table S20: Equivalence representations of sets of plane waves $e^{i(\mathbf{k}_M+\mathbf{G})\cdot\mathbf{r}}$ for the group of the wavevector at an M point $[\mathbf{k}_M=\frac{2\pi}{a}(\frac{1}{2},\frac{1}{2},0)]$ of the space group #221, which transforms isomorphically to $4/mmm$ (D_{4h}). Plane waves are sorted by $|\mathbf{k}_M+\mathbf{G}|$ and labeled by $\frac{a}{2\pi}\{\mathbf{k}_M+\mathbf{G}\}$

$\frac{a}{2\pi}\{\mathbf{k}_M+\mathbf{G}\}$	1	2_z	2_h	$2_{h'}$	4_z	$\bar{1}$	m_z	m_v	m_d	$\bar{4}_z$	Irreducible representations
$\{\frac{1}{2},\frac{1}{2},0\}^a$	4	0	0	2	0	0	4	0	2	0	$M_1^+ \oplus M_4^+ \oplus M_5^-$
$\{\frac{1}{2},\frac{1}{2},1\}^b$	8	0	0	0	0	0	0	0	4	0	$M_1^+ \oplus M_2^- \oplus M_3^- \oplus M_4^+ \oplus M_5^+ \oplus M_5^-$
$\{\frac{3}{2},\frac{1}{2},0\}^c$	8	0	0	0	0	0	8	0	0	0	$M_1^+ \oplus M_2^+ \oplus M_3^+ \oplus M_4^+ \oplus 2M_5^-$
$\{\frac{3}{2},\frac{1}{2},1\}^d$	16	0	0	0	0	0	0	0	0	0	$M_1^+ \oplus M_1^- \oplus M_2^+ \oplus M_2^- \oplus M_3^+ \oplus M_3^-$ $\oplus M_4^+ \oplus M_4^- \oplus 2M_5^+ \oplus 2M_5^-$

[a] $\frac{a}{2\pi}\mathbf{G}$'s are $(0,0,0),(\bar{1},0,0),(0,\bar{1},0),(\bar{1},\bar{1},0)$.
[b] $\frac{a}{2\pi}\mathbf{G}$'s are $(0,0,1),(\bar{1},0,1),(0,\bar{1},1),(\bar{1},\bar{1},1),(0,0,\bar{1}),(\bar{1},0,\bar{1}),(0,\bar{1},\bar{1}),(\bar{1},\bar{1},\bar{1})$.
[c] $\frac{a}{2\pi}\mathbf{G}$'s are $(1,0,0),(\bar{2},0,0),(1,\bar{1},0),(\bar{2},\bar{1},0),(0,1,0),(0,\bar{2},0),(\bar{1},1,0),(\bar{1},\bar{2},0)$.
[d] $\frac{a}{2\pi}\mathbf{G}$'s are $(1,0,1),(\bar{2},0,1),(1,\bar{1},1),(\bar{2},\bar{1},1),(0,1,1),(0,\bar{2},1),$
$(\bar{1},1,1),(\bar{1},\bar{2},1),(1,0,\bar{1}),(\bar{2},0,\bar{1}),(1,\bar{1},\bar{1}),(\bar{2},\bar{1},\bar{1}),(0,1,\bar{1}),(0,\bar{2},\bar{1}),(\bar{1},1,\bar{1}),(\bar{1},\bar{2},\bar{1})$.

Table S21: Equivalence representations of sets of plane waves $e^{i(\mathbf{k}_R+\mathbf{G})\cdot\mathbf{r}}$ for the group of the wavevector at an R point $[\mathbf{k}_R=\frac{2\pi}{a}(\frac{1}{2},\frac{1}{2},\frac{1}{2})]$ of the space group #221, which transforms isomorphically to $m\bar{3}m$ (O_h). Plane waves are sorted by $|\mathbf{k}_R+\mathbf{G}|$ and labeled by $\frac{a}{2\pi}\{\mathbf{k}_R+\mathbf{G}\}$

$\frac{a}{2\pi}\{\mathbf{k}_R+\mathbf{G}\}$	1	2	$2'$	3	4	$\bar{1}$	m	m'	$\bar{3}$	$\bar{4}$	Irreducible representations
$\{\frac{1}{2},\frac{1}{2},\frac{1}{2}\}^a$	8	0	0	2	0	0	0	4	0	0	$R_1^+ \oplus R_2^- \oplus R_4^- \oplus R_5^+$
$\{\frac{3}{2},\frac{1}{2},\frac{1}{2}\}^b$	24	0	0	0	0	0	0	4	0	0	$R_1^+ \oplus R_2^- \oplus R_3^+ \oplus R_3^- \oplus R_4^+ \oplus 2R_4^- \oplus 2R_5^+ \oplus R_5^-$
$\{\frac{3}{2},\frac{3}{2},\frac{1}{2}\}^c$	24	0	0	0	0	0	0	4	0	0	$R_1^+ \oplus R_2^- \oplus R_3^+ \oplus R_3^- \oplus R_4^+ \oplus 2R_4^- \oplus 2R_5^+ \oplus R_5^-$
$\{\frac{3}{2},\frac{3}{2},\frac{3}{2}\}^d$	8	0	0	2	0	0	0	4	0	0	$R_1^+ \oplus R_2^- \oplus R_4^- \oplus R_5^+$
$\{\frac{5}{2},\frac{1}{2},\frac{1}{2}\}^e$	24	0	0	0	0	0	0	4	0	0	$R_1^+ \oplus R_2^- \oplus R_3^+ \oplus R_3^- \oplus R_4^+ \oplus 2R_4^- \oplus 2R_5^+ \oplus R_5^-$
$\{\frac{5}{2},\frac{3}{2},\frac{1}{2}\}^f$	48	0	0	0	0	0	0	0	0	0	$R_1^+ \oplus R_1^- \oplus R_2^+ \oplus R_2^- \oplus 2R_3^+ \oplus 2R_3^- \oplus 3R_4^+$ $\oplus 3R_4^- \oplus 3R_5^+ \oplus 3R_5^-$

[a] $\frac{a}{2\pi}\mathbf{G}$'s are $(0,0,0),(0,\bar{1},0),(0,0,\bar{1}),(0,\bar{1},\bar{1}),(\bar{1},0,0),(\bar{1},\bar{1},0),(\bar{1},0,\bar{1}),(\bar{1},\bar{1},\bar{1})$.

[b] $\frac{a}{2\pi}\mathbf{G}$'s are
$(1,0,0),(1,\bar{1},0),(1,0,\bar{1}),(1,\bar{1},\bar{1}),(\bar{2},0,0),(\bar{2},\bar{1},0),(\bar{2},0,\bar{1}),(\bar{2},\bar{1},\bar{1}),(0,1,0),(\bar{1},1,0),(0,1,\bar{1}),(\bar{1},1,\bar{1}),$
$(0,\bar{2},0),(\bar{1},\bar{2},0),(0,\bar{2},\bar{1}),(\bar{1},\bar{2},\bar{1}),(0,0,1),(0,\bar{1},1),(\bar{1},0,1),(\bar{1},\bar{1},1),(0,0,\bar{2}),(0,\bar{1},\bar{2}),(\bar{1},0,\bar{2}),(\bar{1},\bar{1},\bar{2})$.

[c] $\frac{a}{2\pi}\mathbf{G}$'s are
$(1,1,0),(1,\bar{2},0),(1,1,\bar{1}),(1,\bar{2},\bar{1}),(\bar{2},1,0),(\bar{2},\bar{2},0),(\bar{2},1,\bar{1}),(\bar{2},\bar{2},\bar{1}),(1,0,1),(1,0,\bar{2}),(1,\bar{1},1),(1,\bar{1},\bar{2}),$
$(\bar{2},0,1),(\bar{2},0,\bar{2}),(\bar{2},\bar{1},1),(\bar{2},\bar{1},\bar{2}),(0,1,1),(0,\bar{2},1),(\bar{1},1,1),(\bar{1},\bar{2},1),(0,1,\bar{2}),(0,\bar{2},\bar{2}),(\bar{1},1,\bar{2}),(\bar{1},\bar{2},\bar{2})$.

[d] $\frac{a}{2\pi}\mathbf{G}$'s are $(1,1,1),(1,\bar{2},1),(1,1,\bar{2}),(1,\bar{2},\bar{2}),(\bar{2},1,1),(\bar{2},\bar{2},1),(\bar{2},1,\bar{2}),(\bar{2},\bar{2},\bar{2})$.

[e] $\frac{a}{2\pi}\mathbf{G}$'s are
$(2,0,0),(2,\bar{1},0),(2,0,\bar{1}),(2,\bar{1},\bar{1}),(\bar{3},0,0),(\bar{3},\bar{1},0),(\bar{3},0,\bar{1}),(\bar{3},\bar{1},\bar{1}),(0,2,0),(\bar{1},2,0),(0,2,\bar{1}),(\bar{1},2,\bar{1}),$
$(0,\bar{3},0),(\bar{1},\bar{3},0),(0,\bar{3},\bar{1}),(\bar{1},\bar{3},\bar{1}),(0,0,2),(0,\bar{1},2),(\bar{1},0,2),(\bar{1},\bar{1},2),(0,0,\bar{3}),(0,\bar{1},\bar{3}),(\bar{1},0,\bar{3}),(\bar{1},\bar{1},\bar{3})$.

[f] $\frac{a}{2\pi}\mathbf{G}$'s are
$(2,1,0),(2,\bar{2},0),(2,1,\bar{1}),(2,\bar{2},\bar{1}),(\bar{3},1,0),(\bar{3},\bar{2},0),(\bar{3},1,\bar{1}),(\bar{3},\bar{2},\bar{1}),(2,0,1),(2,0,\bar{2}),(2,\bar{1},1),(2,\bar{1},\bar{2}),$
$(\bar{3},0,1),(\bar{3},0,\bar{2}),(\bar{3},\bar{1},1),(\bar{3},\bar{1},\bar{2}),(1,2,0),(\bar{2},2,0),(1,2,\bar{1}),(\bar{2},2,\bar{1}),(1,\bar{3},0),(\bar{2},\bar{3},0),(1,\bar{3},\bar{1}),(\bar{2},\bar{3},\bar{1}),$
$(0,2,1),(0,2,\bar{2}),(\bar{1},2,1),(\bar{1},2,\bar{2}),(0,\bar{3},1),(0,\bar{3},\bar{2}),(\bar{1},\bar{3},1),(\bar{1},\bar{3},\bar{2}),(0,1,2),(0,\bar{2},2),(\bar{1},1,2),(\bar{1},\bar{2},2),$
$(0,1,\bar{3}),(0,\bar{2},\bar{3}),(\bar{1},1,\bar{3}),(\bar{1},\bar{2},\bar{3}),(1,0,2),(\bar{2},0,2),(1,\bar{1},2),(\bar{2},\bar{1},2),(1,0,\bar{3}),(\bar{2},0,\bar{3}),(1,\bar{1},\bar{3}),(\bar{2},\bar{1},\bar{3})$.

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