Supplementary information (SI) for

Graphene has a finite band gap originating from the exchange term of self-energy

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Character tables of $P6/mmm$

The character tables at the Γ, M, and K points of the space group $P6/mmm$ are summarized in Tables S I–S III.

Representation of atomic orbital

The atomic orbital is represented in the full-rotation group by $\Gamma^{\rm orb}_{jl}$ 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 $\chi^{\rm orb}_{jl}$ of the point-group symmetry is thus described as [S1, S2]

$$\chi^{\rm orb}_{jl}\{\alpha\} = \frac{\sin(j+\frac{1}{2})\alpha}{\sin\frac{1}{2}\alpha} \ , \tag{S1}$$

$$\chi^{\rm orb}_{jl}\{\bar{\alpha}\} = (-1)^l \frac{\sin(j+\frac{1}{2})\alpha}{\sin\frac{1}{2}\alpha} \ , \tag{S2}$$

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 subduced to the space group of a condensed-matter system and represented by $\Gamma^{\rm orb}$. $\Gamma^{\rm orb}$'s at the Γ, M, and K points of the space group $P6/mmm$ are summarized in Tables S IV–S VI.

Representation of atomic arrangement

The atomic arrangement is represented in the space group by $\Gamma^{\rm arr}$ and described by the Bloch function as

$$\begin{aligned} f_{\mathbf{k}}(\mathbf{r}) &= g_{\mathbf{k}}(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} \ , \\ g_{\mathbf{k}}(\mathbf{r}) &= \sum_i \delta(\mathbf{r}-\mathbf{r}_i) \ , \end{aligned} \tag{S3}$$

where $g_{\mathbf{k}}(\mathbf{r})$ is the cell-periodic function and $\mathbf{r}_i$ is the atomic position. The character $\chi^{\rm arr}$ of the space-group symmetry $\{P|\boldsymbol{\tau}+\mathbf{R}\}$ is thus described as [S3–S6]

$$\begin{aligned} &\chi^{\rm arr}\{P|\boldsymbol{\tau}+\mathbf{R}\} \\ &= \langle f_{\mathbf{k}}|\{P|\boldsymbol{\tau}+\mathbf{R}\} f_{\mathbf{k}}\rangle \\ &= e^{-i\mathbf{k}\cdot\mathbf{R}} e^{-i(\mathbf{k}+\mathbf{G})\cdot\boldsymbol{\tau}} \langle g_{\mathbf{k}}| e^{i\mathbf{G}\cdot\mathbf{r}} \{P|\boldsymbol{\tau}+\mathbf{R}\} g_{\mathbf{k}}\rangle \\ &= e^{-i\mathbf{k}\cdot\mathbf{R}} e^{-i(\mathbf{k}+\mathbf{G})\cdot\boldsymbol{\tau}} \\ &\quad \times \sum_i \langle \delta(\mathbf{r}-\mathbf{r}_i)| e^{i\mathbf{G}\cdot\mathbf{r}} \delta(\{P|\boldsymbol{\tau}+\mathbf{R}\}^{-1}\mathbf{r}-\mathbf{r}_i)\rangle \\ &= e^{-i\mathbf{k}\cdot\mathbf{R}} e^{-i(\mathbf{k}+\mathbf{G})\cdot\boldsymbol{\tau}} \sum_i e^{i\mathbf{G}\cdot\mathbf{r}_i} \delta(\{P|\boldsymbol{\tau}+\mathbf{R}\}^{-1}\mathbf{r}_i-\mathbf{r}_i) \\ &= e^{-i\mathbf{k}\cdot\mathbf{R}} e^{-i(\mathbf{k}+\mathbf{G})\cdot\boldsymbol{\tau}} \sum_i e^{i\mathbf{G}\cdot\mathbf{r}_i} \delta[P^{-1}(\mathbf{r}_i-\boldsymbol{\tau})-\mathbf{r}_i] \ , \end{aligned} \tag{S4}$$

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 described in the symmorphic group of $\boldsymbol{\tau} = \mathbf{0}$ as

$$\chi^{\rm arr}\{P|\mathbf{R}\} = e^{-i\mathbf{k}\cdot\mathbf{R}} \sum_i e^{i\mathbf{G}\cdot\mathbf{r}_i} \delta(P^{-1}\mathbf{r}_i-\mathbf{r}_i) \ . \tag{S5}$$

$\Gamma^{\rm equiv}$'s of graphene at the Γ, M, and K points of the space group $P6/mmm$ are summarized in Tables S VII–S IX.

Representation of atomic wavefunction

The atomic wavefunction is represented by the direct product of the atomic orbital and atomic arrangement as $\Gamma^{\rm orb}\otimes\Gamma^{\rm arr}$. The representations of graphene at the Γ, M, and K points of the space group $P6/mmm$ are summarized in Tables S X–S XII.

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[S4] M. S. Dresselhaus, G. Dresselhaus, and A. Jorio, *Group Theory* (Springer-Verlag, Berlin, 2008).

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TABLE S I. Character table at the Γ point $[\mathbf{k}_\Gamma = \frac{2\pi}{a}(0,0,0)]$ of the space group $P6/mmm$, which transforms isomorphically to the point group $6/mmm\,(D_{6h})$.

	$\{1\}$[a]	$\{2\}$[b]	$\{2_v\}$[c]	$\{2_{v'}\}$[d]	$\{3\}$[e]	$\{6\}$[f]	$\{\bar{1}\}$[g]	$\{m\}$[h]	$\{m_v\}$[i]	$\{m_{v'}\}$[j]	$\{\bar{3}\}$[k]	$\{\bar{6}\}$[l]	$\{^{d}1\}$[m]	$\{^{d}3\}$[n]	$\{^{d}6\}$[o]	$\{^{d}\bar{1}\}$[p]	$\{^{d}\bar{3}\}$[q]	$\{^{d}\bar{6}\}$[r]	Type[s]
Γ_1^+	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	(a)
Γ_1^-	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	1	1	1	−1	−1	−1	(a)
Γ_2^+	1	1	−1	−1	1	1	1	1	−1	−1	1	1	1	1	1	1	1	1	(a)
Γ_2^-	1	1	−1	−1	1	1	−1	−1	1	1	−1	−1	1	1	1	−1	−1	−1	(a)
Γ_3^+	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1	1	1	−1	1	1	−1	(a)
Γ_3^-	1	−1	1	−1	1	−1	−1	1	−1	1	−1	1	1	1	−1	−1	−1	1	(a)
Γ_4^+	1	−1	−1	1	1	−1	1	−1	−1	1	1	−1	1	1	−1	1	1	−1	(a)
Γ_4^-	1	−1	−1	1	1	−1	−1	1	1	−1	−1	1	1	1	−1	−1	−1	1	(a)
Γ_5^+	2	2	0	0	−1	−1	2	2	0	0	−1	−1	2	−1	−1	2	−1	−1	(a)
Γ_5^-	2	2	0	0	−1	−1	−2	−2	0	0	1	1	2	−1	−1	−2	1	1	(a)
Γ_6^+	2	−2	0	0	−1	1	2	−2	0	0	−1	1	2	−1	1	2	−1	1	(a)
Γ_6^-	2	−2	0	0	−1	1	−2	2	0	0	1	−1	2	−1	1	−2	1	−1	(a)
$\overline{\Gamma}_7$	2	0	0	0	−2	0	2	0	0	0	−2	0	−2	2	0	−2	2	0	(b)
$\overline{\Gamma}_8$	2	0	0	0	1	$-\sqrt{3}$	2	0	0	0	1	$-\sqrt{3}$	−2	−1	$\sqrt{3}$	−2	−1	$\sqrt{3}$	(b)
$\overline{\Gamma}_9$	2	0	0	0	1	$\sqrt{3}$	2	0	0	0	1	$\sqrt{3}$	−2	−1	$-\sqrt{3}$	−2	−1	$-\sqrt{3}$	(b)
$\overline{\Gamma}_{10}$	2	0	0	0	−2	0	−2	0	0	0	2	0	−2	2	0	2	−2	0	(b)
$\overline{\Gamma}_{11}$	2	0	0	0	1	$-\sqrt{3}$	−2	0	0	0	−1	$\sqrt{3}$	−2	−1	$\sqrt{3}$	2	1	$-\sqrt{3}$	(b)
$\overline{\Gamma}_{12}$	2	0	0	0	1	$\sqrt{3}$	−2	0	0	0	−1	$-\sqrt{3}$	−2	−1	$-\sqrt{3}$	2	1	$\sqrt{3}$	(b)

[a] $\{1|\mathbf{R}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3\}$, where $\mathbf{a}_1 = a(\frac{\sqrt{3}}{2}, -\frac{1}{2}, 0)$, $\mathbf{a}_2 = a(0,1,0)$, and $\mathbf{a}_3 = c(0,0,1)$ and n_1, n_2, and n_3 are integer.
[b] $\{2_{001}|0\}, \{^{d}2_{001}|0\}$.
[c] $\{2_{100}|0\}, \{2_{010}|0\}, \{2_{110}|0\}, \{^{d}2_{100}|0\}, \{^{d}2_{010}|0\}, \{^{d}2_{110}|0\}$.
[d] $\{2_{1\bar{1}0}|0\}, \{2_{120}|0\}, \{2_{210}|0\}, \{^{d}2_{1\bar{1}0}|0\}, \{^{d}2_{120}|0\}, \{^{d}2_{210}|0\}$.
[e] $\{3^+_{001}|0\}, \{3^-_{001}|0\}$.
[f] $\{6^+_{001}|0\}, \{6^-_{001}|0\}$.
[g] $\{\bar{1}|0\}$.
[h] $\{m_{001}|0\}, \{^{d}m_{001}|0\}$.
[i] $\{m_{100}|0\}, \{m_{010}|0\}, \{m_{110}|0\}, \{^{d}m_{100}|0\}, \{^{d}m_{010}|0\}, \{^{d}m_{110}|0\}$.
[j] $\{m_{1\bar{1}0}|0\}, \{m_{120}|0\}, \{m_{210}|0\}, \{^{d}m_{1\bar{1}0}|0\}, \{^{d}m_{120}|0\}, \{^{d}m_{210}|0\}$.
[k] $\{\bar{3}^+_{001}|0\}, \{\bar{3}^-_{001}|0\}$.
[l] $\{\bar{6}^+_{001}|0\}, \{\bar{6}^-_{001}|0\}$.
[m] $\{^{d}1|0\}$.
[n] $\{^{d}3^+_{001}|0\}, \{^{d}3^-_{001}|0\}$.
[o] $\{^{d}6^+_{001}|0\}, \{^{d}6^-_{001}|0\}$.
[p] $\{^{d}\bar{1}|0\}$.
[q] $\{^{d}\bar{3}^+_{001}|0\}, \{^{d}\bar{3}^-_{001}|0\}$.
[r] $\{^{d}\bar{6}^+_{001}|0\}, \{^{d}\bar{6}^-_{001}|0\}$.
[s] Type (a), (b), and (c) correspond to the Frobenius–Schur test of +1, −1, and 0, respectively.

TABLE S II. Character table at the M point $[\mathbf{k}_M = \frac{2\pi}{a}(\frac{1}{2},0,0)]$ of the space group $P6/mmm$, which transforms isomorphically to the point group $mmm\,(D_{2h})$.

	$\{1\}$[a]	$\{2\}$[b]	$\{2_v\}$[c]	$\{2_{v'}\}$[d]	$\{\bar{1}\}$[e]	$\{m\}$[f]	$\{m_v\}$[g]	$\{m_{v'}\}$[h]	$\{^{\mathrm{d}}1\}$[i]	$\{^{\mathrm{d}}\bar{1}\}$[j]	Type[k]
M_1^+	$1 \cdot T_M$[l]	1	1	1	1	1	1	1	1	1	(a)
M_1^-	$1 \cdot T_M$	1	1	1	−1	−1	−1	−1	1	−1	(a)
M_2^+	$1 \cdot T_M$	1	−1	−1	1	1	−1	−1	1	1	(a)
M_2^-	$1 \cdot T_M$	1	−1	−1	−1	−1	1	1	1	−1	(a)
M_3^+	$1 \cdot T_M$	−1	1	−1	1	−1	1	−1	1	1	(a)
M_3^-	$1 \cdot T_M$	−1	1	−1	−1	1	−1	1	1	−1	(a)
M_4^+	$1 \cdot T_M$	−1	−1	1	1	−1	−1	1	1	1	(a)
M_4^-	$1 \cdot T_M$	−1	−1	1	−1	1	1	−1	1	−1	(a)
$\overline{M}_5$	$2 \cdot T_M$	0	0	0	2	0	0	0	−2	−2	(b)
$\overline{M}_6$	$2 \cdot T_M$	0	0	0	−2	0	0	0	−2	2	(b)

[a] $\{1|\mathbf{R}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3\}$, where $\mathbf{a}_1 = a(\frac{\sqrt{3}}{2}, -\frac{1}{2}, 0)$, $\mathbf{a}_2 = a(0,1,0)$, and $\mathbf{a}_3 = c(0,0,1)$ and n_1, n_2, and n_3 are integer.
[b] $\{2_{001}|0\}, \{^{\mathrm{d}}2_{001}|0\}$.
[c] $\{2_{010}|0\}, \{^{\mathrm{d}}2_{010}|0\}$.
[d] $\{2_{210}|0\}, \{^{\mathrm{d}}2_{210}|0\}$.
[e] $\{\bar{1}|0\}$.
[f] $\{m_{001}|0\}, \{^{\mathrm{d}}m_{001}|0\}$.
[g] $\{m_{010}|0\}, \{^{\mathrm{d}}m_{010}|0\}$.
[h] $\{m_{210}|0\}, \{^{\mathrm{d}}m_{210}|0\}$.
[i] $\{^{\mathrm{d}}1|0\}$.
[j] $\{^{\mathrm{d}}\bar{1}|0\}$.
[k] Type (a), (b), and (c) correspond to the Frobenius–Schur test of +1, −1, and 0, respectively.
[l] $T_M = e^{-i\mathbf{k}_M \cdot \mathbf{R}_n}$

TABLE S III. Character table at the K point $[\mathbf{k}_K = \frac{2\pi}{a}(\frac{1}{3},\frac{1}{3},0)]$ of the space group $P6/mmm$, which transforms isomorphically to the point group $\bar{6}m2\,(D_{3h})$.

	$\{1\}$[a]	$\{2_v\}$[b]	$\{3\}$[c]	$\{m\}$[d]	$\{m_{v'}\}$[e]	$\{\bar{6}\}$[f]	$\{^{\mathrm{d}}1\}$[g]	$\{^{\mathrm{d}}3\}$[h]	$\{^{\mathrm{d}}\bar{6}\}$[i]	Type[j]
K_1	$1 \cdot T_K$[k]	1	1	1	1	1	1	1	1	(a)
K_2	$1 \cdot T_K$	1	1	−1	−1	−1	1	1	−1	(a)
K_3	$1 \cdot T_K$	−1	1	−1	1	−1	1	1	−1	(a)
K_4	$1 \cdot T_K$	−1	1	1	−1	1	1	1	1	(a)
K_5	$2 \cdot T_K$	0	−1	2	0	−1	2	−1	−1	(a)
K_6	$2 \cdot T_K$	0	−1	−2	0	1	2	−1	1	(a)
$\overline{K}_7$	$2 \cdot T_K$	0	−2	0	0	0	−2	2	0	(b)
$\overline{K}_8$	$2 \cdot T_K$	0	1	0	0	$-\sqrt{3}$	−2	−1	$\sqrt{3}$	(b)
$\overline{K}_9$	$2 \cdot T_K$	0	1	0	0	$\sqrt{3}$	−2	−1	$-\sqrt{3}$	(b)

[a] $\{1|\mathbf{R}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3\}$, where $\mathbf{a}_1 = a(\frac{\sqrt{3}}{2}, -\frac{1}{2}, 0)$, $\mathbf{a}_2 = a(0,1,0)$, and $\mathbf{a}_3 = c(0,0,1)$ and n_1, n_2, and n_3 are integer.
[b] $\{2_{100}|0\}, \{2_{010}|0\}, \{2_{110}|0\}, \{^{\mathrm{d}}2_{100}|0\}, \{^{\mathrm{d}}2_{010}|0\}, \{^{\mathrm{d}}2_{110}|0\}$.
[c] $\{3^+_{001}|0\}, \{3^-_{001}|0\}$.
[d] $\{m_{001}|0\}, \{^{\mathrm{d}}m_{001}|0\}$.
[e] $\{m_{1\bar{1}0}|0\}, \{m_{120}|0\}, \{m_{210}|0\}, \{^{\mathrm{d}}m_{1\bar{1}0}|0\}, \{^{\mathrm{d}}m_{120}|0\}, \{^{\mathrm{d}}m_{210}|0\}$.
[f] $\{\bar{6}^+_{001}|0\}, \{\bar{6}^-_{001}|0\}$.
[g] $\{^{\mathrm{d}}1|0\}$.
[h] $\{^{\mathrm{d}}3^+_{001}|0\}, \{^{\mathrm{d}}3^-_{001}|0\}$.
[i] $\{^{\mathrm{d}}\bar{6}^+_{001}|0\}, \{^{\mathrm{d}}\bar{6}^-_{001}|0\}$.
[j] Type (a), (b), and (c) correspond to the Frobenius–Schur test of +1, −1, and 0, respectively.
[k] $T_K = e^{-i\mathbf{k}_K \cdot \mathbf{R}_n}$

TABLE S IV. Representation of the atomic orbital at the Γ point of the space group $P6/mmm$.

	{1}	{2}	$\{2_v\}$	$\{2_{v'}\}$	{3}	{6}	$\{\bar{1}\}$	$\{m\}$	$\{m_v\}$	$\{m_{v'}\}$	$\{\bar{3}\}$	$\{\bar{6}\}$	Decomposition
Γ_s^{orb}	1	1	1	1	1	1	1	1	1	1	1	1	Γ_1^+
Γ_p^{orb}	3	−1	−1	−1	0	2	−3	1	1	1	0	−2	$\Gamma_2^- \oplus \Gamma_6^-$
Γ_d^{orb}	5	1	1	1	−1	1	5	1	1	1	−1	1	$\Gamma_1^+ \oplus \Gamma_5^+ \oplus \Gamma_6^+$
$\Gamma_{s\,1/2}^{\mathrm{orb}}$	2	0	0	0	1	$\sqrt{3}$	2	0	0	0	1	$\sqrt{3}$	$\overline{\Gamma}_9$
$\Gamma_{p\,1/2}^{\mathrm{orb}}$	2	0	0	0	1	$\sqrt{3}$	−2	0	0	0	−1	$-\sqrt{3}$	$\overline{\Gamma}_{12}$
$\Gamma_{p\,3/2}^{\mathrm{orb}}$	4	0	0	0	−1	$\sqrt{3}$	−4	0	0	0	1	$-\sqrt{3}$	$\overline{\Gamma}_{10} \oplus \overline{\Gamma}_{12}$
$\Gamma_{d\,3/2}^{\mathrm{orb}}$	4	0	0	0	−1	$\sqrt{3}$	4	0	0	0	−1	$\sqrt{3}$	$\overline{\Gamma}_7 \oplus \overline{\Gamma}_9$
$\Gamma_{d\,5/2}^{\mathrm{orb}}$	6	0	0	0	0	0	6	0	0	0	0	0	$\overline{\Gamma}_7 \oplus \overline{\Gamma}_8 \oplus \overline{\Gamma}_9$

TABLE S V. Representation of the atomic orbital at the M point of the space group $P6/mmm$.

	{1}	{2}	$\{2_v\}$	$\{2_{v'}\}$	$\{\bar{1}\}$	$\{m\}$	$\{m_v\}$	$\{m_{v'}\}$	Decomposition
M_s^{orb}	1	1	1	1	1	1	1	1	M_1^+
M_p^{orb}	3	−1	−1	−1	−3	1	1	1	$M_2^- \oplus M_3^- \oplus M_4^-$
M_d^{orb}	5	1	1	1	5	1	1	1	$2M_1^+ \oplus M_2^+ \oplus M_3^+ \oplus M_4^+$
$M_{s\,1/2}^{\mathrm{orb}}$	2	0	0	0	2	0	0	0	$\overline{M}_5$
$M_{p\,1/2}^{\mathrm{orb}}$	2	0	0	0	−2	0	0	0	$\overline{M}_6$
$M_{p\,3/2}^{\mathrm{orb}}$	4	0	0	0	−4	0	0	0	$2\overline{M}_6$
$M_{d\,3/2}^{\mathrm{orb}}$	4	0	0	0	4	0	0	0	$2\overline{M}_5$
$M_{d\,5/2}^{\mathrm{orb}}$	6	0	0	0	6	0	0	0	$3\overline{M}_5$

TABLE S VI. Representation of the atomic orbital at the K point of the space group $P6/mmm$.

	{1}	$\{2_v\}$	{3}	$\{m\}$	$\{m_{v'}\}$	$\{\bar{6}\}$	Decomposition
K_s^{orb}	1	1	1	1	1	1	K_1
K_p^{orb}	3	−1	0	1	1	−2	$K_3 \oplus K_5$
K_d^{orb}	5	1	−1	1	1	1	$K_1 \oplus K_5 \oplus K_6$
$K_{s\,1/2}^{\mathrm{orb}}$	2	0	1	0	0	$\sqrt{3}$	$\overline{K}_9$
$K_{p\,1/2}^{\mathrm{orb}}$	2	0	1	0	0	$-\sqrt{3}$	$\overline{K}_8$
$K_{p\,3/2}^{\mathrm{orb}}$	4	0	−1	0	0	$-\sqrt{3}$	$\overline{K}_7 \oplus \overline{K}_8$
$K_{d\,3/2}^{\mathrm{orb}}$	4	0	−1	0	0	$\sqrt{3}$	$\overline{K}_7 \oplus \overline{K}_9$
$K_{d\,5/2}^{\mathrm{orb}}$	6	0	0	0	0	0	$\overline{K}_7 \oplus \overline{K}_8 \oplus \overline{K}_9$

TABLE S VII. Representation of the atomic arrangement of C_2 $(\frac{2}{3}, \frac{1}{3}, 0)$ and $(\frac{1}{3}, \frac{2}{3}, 0)$ at the Γ point of the space group $P6/mmm$.

	{1}	{2}	$\{2_v\}$	$\{2_{v'}\}$	{3}	{6}	$\{\bar{1}\}$	$\{m\}$	$\{m_v\}$	$\{m_{v'}\}$	$\{\bar{3}\}$	$\{\bar{6}\}$	Decomposition
G	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	
$\Gamma_{C_2}^{\mathrm{arr}}$	2	0	0	2	2	0	0	2	2	0	0	2	$\Gamma_1^+ \oplus \Gamma_4^-$

TABLE S VIII. Representation of the atomic arrangement of C_2 $(\frac{2}{3}, \frac{1}{3}, 0)$ and $(\frac{1}{3}, \frac{2}{3}, 0)$ at the M point of the space group $P6/mmm$.

	{1}	{2}	$\{2_v\}$	$\{2_{v'}\}$	$\{\bar{1}\}$	$\{m\}$	$\{m_v\}$	$\{m_{v'}\}$	Decomposition
G	**0**	(−1, 0, 0)	(−1, 0, 0)	**0**	(−1, 0, 0)	**0**	**0**	(−1, 0, 0)	
$M_{C_2}^{\mathrm{arr}}$	2	0	0	2	0	2	2	0	$M_1^+ \oplus M_4^-$

TABLE S IX. Representation of the atomic arrangement of C_2 $(\frac{2}{3}, \frac{1}{3}, 0)$ and $(\frac{1}{3}, \frac{2}{3}, 0)$ at the K point of the space group $P6/mmm$.

	{1}	$\{2_v\}$	{3}	$\{m\}$	$\{m_{v'}\}$	$\{\bar{6}\}$	Decomposition
G	**0**	(0, −1, 0)	(−1, 0, 0)	**0**	**0**	(0, −1, 0)	
$K_{C_2}^{\mathrm{arr}}$	2	0	−1	2	0	−1	K_5

TABLE S X. Representation of the atomic wavefunction of C_2 $(\frac{2}{3},\frac{1}{3},0)$ and $(\frac{1}{3},\frac{2}{3},0)$ at the Γ point of the space group $P6/mmm$.

	$\{1\}$	$\{2\}$	$\{2_v\}$	$\{2_{v'}\}$	$\{3\}$	$\{6\}$	$\{\bar{1}\}$	$\{m\}$	$\{m_v\}$	$\{m_{v'}\}$	$\{\bar{3}\}$	$\{\bar{6}\}$	Decomposition
$C_2\, s$	2	0	0	2	2	0	0	2	2	0	0	2	$\Gamma_1^+ \oplus \Gamma_4^-$
$C_2\, p$	6	0	0	-2	0	0	0	2	2	0	0	-4	$\Gamma_2^- \oplus \Gamma_3^+ \oplus \Gamma_5^+ \oplus \Gamma_6^-$
$C_2\, d$	10	0	0	2	-2	0	0	2	2	0	0	2	$\Gamma_1^+ \oplus \Gamma_4^- \oplus \Gamma_5^+ \oplus \Gamma_5^- \oplus \Gamma_6^+ \oplus \Gamma_6^-$
$C_2\, s_{1/2}$	4	0	0	0	2	0	0	0	0	0	0	$2\sqrt{3}$	$\overline{\Gamma}_9 \oplus \overline{\Gamma}_{11}$
$C_2\, p_{1/2}$	4	0	0	0	2	0	0	0	0	0	0	$-2\sqrt{3}$	$\overline{\Gamma}_8 \oplus \overline{\Gamma}_{12}$
$C_2\, p_{3/2}$	8	0	0	0	-2	0	0	0	0	0	0	$-2\sqrt{3}$	$\overline{\Gamma}_7 \oplus \overline{\Gamma}_8 \oplus \overline{\Gamma}_{10} \oplus \overline{\Gamma}_{12}$
$C_2\, d_{3/2}$	8	0	0	0	-2	0	0	0	0	0	0	$2\sqrt{3}$	$\overline{\Gamma}_7 \oplus \overline{\Gamma}_9 \oplus \overline{\Gamma}_{10} \oplus \overline{\Gamma}_{11}$
$C_2\, d_{5/2}$	12	0	0	0	0	0	0	0	0	0	0	0	$\overline{\Gamma}_7 \oplus \overline{\Gamma}_8 \oplus \overline{\Gamma}_9 \oplus \overline{\Gamma}_{10} \oplus \overline{\Gamma}_{11} \oplus \overline{\Gamma}_{12}$

TABLE S XI. Representation of the atomic wavefunction of C_2 $(\frac{2}{3},\frac{1}{3},0)$ and $(\frac{1}{3},\frac{2}{3},0)$ at the M point of the space group $P6/mmm$.

	$\{1\}$	$\{2\}$	$\{2_v\}$	$\{2_{v'}\}$	$\{\bar{1}\}$	$\{m\}$	$\{m_v\}$	$\{m_{v'}\}$	Decomposition
$C_2\, s$	2	0	0	2	0	2	2	0	$M_1^+ \oplus M_4^-$
$C_2\, p$	6	0	0	-2	0	2	2	0	$M_1^+ \oplus M_2^+ \oplus M_2^- \oplus M_3^+ \oplus M_3^- \oplus M_4^-$
$C_2\, d$	10	0	0	2	0	2	2	0	$2M_1^+ \oplus M_1^- \oplus M_2^+ \oplus M_2^- \oplus M_3^+ \oplus M_3^- \oplus M_4^- \oplus 2M_4^-$
$C_2\, s_{1/2}$	4	0	0	0	0	0	0	0	$\overline{M}_5 \oplus \overline{M}_6$
$C_2\, p_{1/2}$	4	0	0	0	0	0	0	0	$\overline{M}_5 \oplus \overline{M}_6$
$C_2\, p_{3/2}$	8	0	0	0	0	0	0	0	$2\overline{M}_5 \oplus 2\overline{M}_6$
$C_2\, d_{3/2}$	8	0	0	0	0	0	0	0	$2\overline{M}_5 \oplus 2\overline{M}_6$
$C_2\, d_{5/2}$	12	0	0	0	0	0	0	0	$3\overline{M}_5 \oplus 3\overline{M}_6$

TABLE S XII. Representation of the atomic wavefunction of C_2 $(\frac{2}{3},\frac{1}{3},0)$ and $(\frac{1}{3},\frac{2}{3},0)$ at the K point of the space group $P6/mmm$.

	$\{1\}$	$\{2_v\}$	$\{3\}$	$\{m\}$	$\{m_{v'}\}$	$\{\bar{6}\}$	Decomposition
$C_2\, s$	2	0	-1	2	0	-1	K_5
$C_2\, p$	6	0	0	2	0	2	$K_1 \oplus K_4 \oplus K_5 \oplus K_6$
$C_2\, d$	10	0	1	2	0	-1	$K_1 \oplus K_2 \oplus K_3 \oplus K_4 \oplus 2K_5 \oplus K_6$
$C_2\, s_{1/2}$	4	0	-1	0	0	$-\sqrt{3}$	$\overline{K}_7 \oplus \overline{K}_8$
$C_2\, p_{1/2}$	4	0	-1	0	0	$\sqrt{3}$	$\overline{K}_7 \oplus \overline{K}_9$
$C_2\, p_{3/2}$	8	0	1	0	0	$\sqrt{3}$	$\overline{K}_7 \oplus \overline{K}_8 \oplus 2\overline{K}_9$
$C_2\, d_{3/2}$	8	0	1	0	0	$-\sqrt{3}$	$\overline{K}_7 \oplus 2\overline{K}_8 \oplus \overline{K}_9$
$C_2\, d_{5/2}$	12	0	0	0	0	0	$2\overline{K}_7 \oplus 2\overline{K}_8 \oplus 2\overline{K}_9$