

SAMB for “grapheneAB”

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- Group: No. 187 D_{3h}^1 $P-6m2$ [hexagonal]
 - Associated point group: No. 26 D_{3h} $-6m2$ (-6m2 setting) [hexagonal]
 - Generation condition
 - model type: **tight_binding**
 - time-reversal type: **electric**
 - irrep: [A1']
 - spinless
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- Unit cell:
 - $a = 2.435$, $b = 2.435$, $c = 10.0$, $\alpha = 90.0$, $\beta = 90.0$, $\gamma = 120.0$
- Lattice vectors:
 - $\mathbf{a}_1 = (2.435 \ 0 \ 0)$
 - $\mathbf{a}_2 = (-1.2175 \ 2.10877185821511 \ 0)$
 - $\mathbf{a}_3 = (0 \ 0 \ 10.0)$

Table 1: High-symmetry line: Γ -X.

	symbol	position		symbol	position
	Γ	$\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$		X	$\begin{pmatrix} \frac{1}{2} & 0 & 0 \end{pmatrix}$

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- Kets: dimension = 3

Table 2: Hilbert space for full matrix.

No.	ket	No.	ket	No.	ket
1	$s@A_1$	2	$p_x@B_1$	3	$p_y@B_1$

- Sites in (primitive) unit cell:

Table 3: Site-clusters.

	site	position	mapping
S_1 [1c: -6m2]	A_1	$\begin{pmatrix} \frac{1}{3} & \frac{2}{3} & 0 \end{pmatrix}$	[1,2,3,4,5,6,7,8,9,10,11,12]
S_2 [1e: -6m2]	B_1	$\begin{pmatrix} \frac{2}{3} & \frac{1}{3} & 0 \end{pmatrix}$	[1,2,3,4,5,6,7,8,9,10,11,12]

- Bonds in (primitive) unit cell:

Table 4: Bond-clusters.

	bond	tail	head	n	#	$b@c$	mapping
B_1 [3j: mm2]	b_1	B_1	A_1	1	1	$\begin{pmatrix} \frac{1}{3} & \frac{2}{3} & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & 0 & 0 \end{pmatrix}$	[1,2,7,10]
	b_2	B_1	A_1	1	1	$\begin{pmatrix} \frac{1}{3} & -\frac{1}{3} & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$	[3,6,8,11]
	b_3	B_1	A_1	1	1	$\begin{pmatrix} -\frac{2}{3} & -\frac{1}{3} & 0 \end{pmatrix} @ \begin{pmatrix} 0 & \frac{1}{2} & 0 \end{pmatrix}$	[4,5,9,12]
B_2 [3j: mm2]	b_4	A_1	A_1	1	1	$\begin{pmatrix} 0 & 1 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{3} & \frac{1}{6} & 0 \end{pmatrix}$	[1,-3,-8,10]
	b_5	A_1	A_1	1	1	$\begin{pmatrix} 1 & 1 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{5}{6} & \frac{1}{6} & 0 \end{pmatrix}$	[2,-5,7,-12]
	b_6	A_1	A_1	1	1	$\begin{pmatrix} 1 & 0 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{5}{6} & \frac{2}{3} & 0 \end{pmatrix}$	[-4,6,-9,11]
B_3 [3j: mm2]	b_7	B_1	B_1	1	1	$\begin{pmatrix} 1 & 0 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{6} & \frac{1}{3} & 0 \end{pmatrix}$	[1,-2,-7,10]
	b_8	B_1	B_1	1	1	$\begin{pmatrix} 1 & 1 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{6} & \frac{5}{6} & 0 \end{pmatrix}$	[3,-6,8,-11]
	b_9	B_1	B_1	1	1	$\begin{pmatrix} 0 & 1 & 0 \end{pmatrix} @ \begin{pmatrix} \frac{2}{3} & \frac{5}{6} & 0 \end{pmatrix}$	[-4,5,-9,12]

- SAMB:

$$\boxed{\text{No. 1}} \quad \hat{\mathbb{Q}}_0^{(A'_1)} [\text{M}_1, \text{S}_1]$$

$$\hat{\mathbb{Z}}_1 = \mathbb{X}_1[\mathbb{Q}_0^{(a, A'_1)}] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s, A'_1)}]$$

$$\boxed{\text{No. 2}} \quad \hat{\mathbb{Q}}_0^{(A'_1)} [\text{M}_2, \text{S}_2]$$

$$\hat{\mathbb{Z}}_2 = \mathbb{X}_2[\mathbb{Q}_0^{(a, A'_1)}] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(s, A'_1)}]$$

$$\boxed{\text{No. 3}} \quad \hat{\mathbb{Q}}_0^{(A'_1)} [\text{M}_3, \text{B}_1]$$

$$\hat{\mathbb{Z}}_3 = \frac{\sqrt{2}\mathbb{X}_6[\mathbb{Q}_{1,0}^{(a, E')}] \otimes \mathbb{Y}_3[\mathbb{Q}_{1,0}^{(b, E')}] }{2} + \frac{\sqrt{2}\mathbb{X}_7[\mathbb{Q}_{1,1}^{(a, E')}] \otimes \mathbb{Y}_4[\mathbb{Q}_{1,1}^{(b, E')}] }{2}$$

$$\boxed{\text{No. 4}} \quad \hat{\mathbb{Q}}_0^{(A'_1)} [\text{M}_1, \text{B}_2]$$

$$\hat{\mathbb{Z}}_4 = \mathbb{X}_1[\mathbb{Q}_0^{(a, A'_1)}] \otimes \mathbb{Y}_5[\mathbb{Q}_0^{(b, A'_1)}]$$

$$\boxed{\text{No. 5}} \quad \hat{\mathbb{Q}}_0^{(A'_1)} [\text{M}_2, \text{B}_3]$$

$$\hat{\mathbb{Z}}_5 = \mathbb{X}_2[\mathbb{Q}_0^{(a, A'_1)}] \otimes \mathbb{Y}_6[\mathbb{Q}_0^{(b, A'_1)}]$$

$$\boxed{\text{No. 6}} \quad \hat{\mathbb{Q}}_3^{(A'_1)} [\text{M}_2, \text{B}_3]$$

$$\hat{\mathbb{Z}}_6 = -\frac{\sqrt{2}\mathbb{X}_3[\mathbb{Q}_{2,0}^{(a, E')}] \otimes \mathbb{Y}_7[\mathbb{Q}_{1,0}^{(b, E')}] }{2} - \frac{\sqrt{2}\mathbb{X}_4[\mathbb{Q}_{2,1}^{(a, E')}] \otimes \mathbb{Y}_8[\mathbb{Q}_{1,1}^{(b, E')}] }{2}$$

$$\boxed{\text{No. 7}} \quad \hat{\mathbb{Q}}_3^{(A'_1)} [\text{M}_2, \text{B}_3]$$

$$\hat{\mathbb{Z}}_7 = \mathbb{X}_5[\mathbb{M}_1^{(a, A'_2)}] \otimes \mathbb{Y}_9[\mathbb{T}_3^{(b, A'_2)}]$$

Table 5: Atomic SAMB group.

group	bra	ket
M ₁	s	s
M ₂	p_x, p_y	p_x, p_y
M ₃	p_x, p_y	s

Table 6: Atomic SAMB.

symbol	type	group	form
X ₁	$\mathbb{Q}_0^{(a, A'_1)}$	M ₁	$\begin{pmatrix} 1 \end{pmatrix}$
X ₂	$\mathbb{Q}_0^{(a, A'_1)}$	M ₂	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{pmatrix}$
X ₃	$\mathbb{Q}_{2,0}^{(a, E')}$	M ₂	$\begin{pmatrix} 0 & -\frac{\sqrt{2}}{2} \\ -\frac{\sqrt{2}}{2} & 0 \end{pmatrix}$
X ₄	$\mathbb{Q}_{2,1}^{(a, E')}$	M ₂	$\begin{pmatrix} -\frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{pmatrix}$
X ₅	$\mathbb{M}_1^{(a, A'_2)}$	M ₂	$\begin{pmatrix} 0 & -\frac{\sqrt{2}i}{2} \\ \frac{\sqrt{2}i}{2} & 0 \end{pmatrix}$
X ₆	$\mathbb{Q}_{1,0}^{(a, E')}$	M ₃	$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$
X ₇	$\mathbb{Q}_{1,1}^{(a, E')}$	M ₃	$\begin{pmatrix} 0 \\ 1 \end{pmatrix}$

Table 7: Cluster SAMB.

symbol	type	cluster	form
Y ₁	$\mathbb{Q}_0^{(s, A'_1)}$	S ₁	$\begin{pmatrix} 1 \end{pmatrix}$

continued ...

Table 7

symbol	type	cluster	form
\mathbb{Y}_2	$\mathbb{Q}_0^{(s, A'_1)}$	S_2	$\begin{pmatrix} 1 \end{pmatrix}$
\mathbb{Y}_3	$\mathbb{Q}_{1,0}^{(b, E')}$	B_1	$\begin{pmatrix} 0 & -\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$
\mathbb{Y}_4	$\mathbb{Q}_{1,1}^{(b, E')}$	B_1	$\begin{pmatrix} -\frac{\sqrt{6}}{3} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} \end{pmatrix}$
\mathbb{Y}_5	$\mathbb{Q}_0^{(b, A'_1)}$	B_2	$\begin{pmatrix} \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} \end{pmatrix}$
\mathbb{Y}_6	$\mathbb{Q}_0^{(b, A'_1)}$	B_3	$\begin{pmatrix} \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} \end{pmatrix}$
\mathbb{Y}_7	$\mathbb{Q}_{1,0}^{(b, E')}$	B_3	$\begin{pmatrix} 0 & -\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$
\mathbb{Y}_8	$\mathbb{Q}_{1,1}^{(b, E')}$	B_3	$\begin{pmatrix} -\frac{\sqrt{6}}{3} & \frac{\sqrt{6}}{6} & \frac{\sqrt{6}}{6} \end{pmatrix}$
\mathbb{Y}_9	$\mathbb{T}_3^{(b, A'_2)}$	B_3	$\begin{pmatrix} \frac{\sqrt{3}i}{3} & -\frac{\sqrt{3}i}{3} & \frac{\sqrt{3}i}{3} \end{pmatrix}$

Table 8: Polar harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{Q}_0^{(A'_1)}$	0	A'_1	—	—	1
2	$\mathbb{Q}_{1,0}^{(E')}$	1	E'	—	0	x
3	$\mathbb{Q}_{1,1}^{(E')}$	1	E'	—	1	y
4	$\mathbb{Q}_{2,0}^{(E')}$	2	E'	—	0	$-\sqrt{3}xy$
5	$\mathbb{Q}_{2,1}^{(E')}$	2	E'	—	1	$-\frac{\sqrt{3}(x-y)(x+y)}{2}$
6	$\mathbb{Q}_3^{(A'_2)}$	3	A'_2	—	—	$\frac{\sqrt{10}x(x^2-3y^2)}{4}$

Table 9: Axial harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{G}_1^{(A'_2)}$	1	A'_2	—	—	Z

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- Group info.: Generator = $\{3_{001}^+|0\}$, $\{m_{001}|0\}$, $\{m_{110}|0\}$

Table 10: Conjugacy class (point-group part).

rep. SO	symmetry operations
$\{1 0\}$	$\{1 0\}$
$\{2_{120} 0\}$	$\{2_{120} 0\}$, $\{2_{210} 0\}$, $\{2_{1-10} 0\}$
$\{3_{001}^+ 0\}$	$\{3_{001}^+ 0\}$, $\{3_{001}^- 0\}$
$\{m_{100} 0\}$	$\{m_{100} 0\}$, $\{m_{010} 0\}$, $\{m_{110} 0\}$
$\{m_{001} 0\}$	$\{m_{001} 0\}$
$\{-6_{001}^+ 0\}$	$\{-6_{001}^+ 0\}$, $\{-6_{001}^- 0\}$

Table 11: Symmetry operations.

No.	SO	No.	SO	No.	SO	No.	SO	No.	SO
1	$\{1 0\}$	2	$\{2_{120} 0\}$	3	$\{2_{210} 0\}$	4	$\{2_{1-10} 0\}$	5	$\{3_{001}^+ 0\}$
6	$\{3_{001}^- 0\}$	7	$\{m_{100} 0\}$	8	$\{m_{010} 0\}$	9	$\{m_{110} 0\}$	10	$\{m_{001} 0\}$
11	$\{-6_{001}^+ 0\}$	12	$\{-6_{001}^- 0\}$						

Table 12: Character table (point-group part).

	1	2 ₁₂₀	3 ⁺ ₀₀₁	m ₁₀₀	m ₀₀₁	-6 ⁺ ₀₀₁
A'_1	1	1	1	1	1	1
A'_2	1	-1	1	-1	1	1
A''_1	1	1	1	-1	-1	-1
A''_2	1	-1	1	1	-1	-1
E'	2	0	-1	0	2	-1
E''	2	0	-1	0	-2	1

Table 13: Parity conversion.

\leftrightarrow	\leftrightarrow	\leftrightarrow	\leftrightarrow	\leftrightarrow
$A'_1 (A''_1)$	$A'_2 (A''_2)$	$A''_1 (A'_1)$	$A''_2 (A'_2)$	$E'' (E')$
$E' (E'')$				

 Table 14: Symmetric product, $[\Gamma \otimes \Gamma']_+$.

	A'_1	A'_2	A''_1	A''_2	E'	E''
A'_1	A'_1	A'_2	A''_1	A''_2	E'	E''
A'_2		A'_1	A''_2	A''_1	E'	E''
A''_1			A'_1	A'_2	E''	E'
A''_2				A'_1	E''	E'
E'					$A'_1 + E'$	$A'_1 + A'_2 + E''$
E''						$A'_1 + E'$

 Table 15: Anti-symmetric product, $[\Gamma \otimes \Gamma']_-$.

A'_1	A'_2	A''_1	A''_2	E'	E''
-	-	-	-	A'_2	A'_2

Table 16: Virtual-cluster sites.

No.	position	No.	position	No.	position	No.	position
1	$\begin{pmatrix} -1 & -1 & 1 \end{pmatrix}$	2	$\begin{pmatrix} 0 & -1 & -1 \end{pmatrix}$	3	$\begin{pmatrix} -1 & 0 & -1 \end{pmatrix}$	4	$\begin{pmatrix} 1 & 1 & -1 \end{pmatrix}$
5	$\begin{pmatrix} 1 & 0 & 1 \end{pmatrix}$	6	$\begin{pmatrix} 0 & 1 & 1 \end{pmatrix}$	7	$\begin{pmatrix} 0 & -1 & 1 \end{pmatrix}$	8	$\begin{pmatrix} -1 & 0 & 1 \end{pmatrix}$
9	$\begin{pmatrix} 1 & 1 & 1 \end{pmatrix}$	10	$\begin{pmatrix} -1 & -1 & -1 \end{pmatrix}$	11	$\begin{pmatrix} 0 & 1 & -1 \end{pmatrix}$	12	$\begin{pmatrix} 1 & 0 & -1 \end{pmatrix}$

Table 17: Virtual-cluster basis.

symbol	1	2	3	4	5	6	7	8	9	10
$\mathbb{Q}_0^{(A_1')}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$
$\mathbb{Q}_1^{(A_2'')}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$
$\mathbb{Q}_{1,0}^{(E')}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$
$\mathbb{Q}_{1,1}^{(E')}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	0	$\frac{\sqrt{2}}{4}$	0	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	0	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$
$\mathbb{Q}_{2,0}^{(E')}$	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	0	$-\frac{\sqrt{2}}{4}$	0	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	0	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$
$\mathbb{Q}_{2,1}^{(E')}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
$\mathbb{Q}_{2,0}^{(E'')}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
$\mathbb{Q}_{2,1}^{(E'')}$	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	0	$-\frac{\sqrt{2}}{4}$	0	$\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	0	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$
$\mathbb{Q}_3^{(A_2')}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$

continued ...

Table 17

symbol	1	2	3	4	5	6	7	8	9	10
	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$								
$\mathbb{Q}_{3,0}^{(E'')}$	$-\frac{\sqrt{2}}{4}$	$-\frac{\sqrt{2}}{4}$	0	$\frac{\sqrt{2}}{4}$	0	$\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$	0	$-\frac{\sqrt{2}}{4}$	$\frac{\sqrt{2}}{4}$
	$-\frac{\sqrt{2}}{4}$	0								
$\mathbb{Q}_{3,1}^{(E'')}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$
	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{6}$								
$\mathbb{Q}_4^{(A_1'')}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$
	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$								