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`

- Unit cell:
  $a = 2.435,\ b = 2.435,\ c = 10.0,\ \alpha = 90.0,\ \beta = 90.0,\ \gamma = 120.0$
- Lattice vectors:
  $\boldsymbol{a}_1 = \begin{pmatrix} 2.435 & 0 & 0 \end{pmatrix}$
  $\boldsymbol{a}_2 = \begin{pmatrix} -1.2175 & 2.10877185821511 & 0 \end{pmatrix}$
  $\boldsymbol{a}_3 = \begin{pmatrix} 0 & 0 & 10.0 \end{pmatrix}$

Table 1: High-symmetry line: Γ-X.

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

- 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	#	$\boldsymbol{b}$@$\boldsymbol{c}$	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:

$\boxed{\text{No. 1}}$ $\hat{\mathbb{Q}}_{0}^{(A_1')}$ $[\mathrm{M}_1, \mathrm{S}_1]$

$$\hat{\mathbb{Z}}_1 = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_1')}] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s,A_1')}]$$

$\boxed{\text{No. 2}}$ $\hat{\mathbb{Q}}_{0}^{(A_1')}$ $[\mathrm{M}_2, \mathrm{S}_2]$

$$\hat{\mathbb{Z}}_2 = \mathbb{X}_2[\mathbb{Q}_0^{(a,A_1')}] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(s,A_1')}]$$

$\boxed{\text{No. 3}}$ $\hat{\mathbb{Q}}_{0}^{(A_1')}$ $[\mathrm{M}_3, \mathrm{B}_1]$

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

$\boxed{\text{No. 4}}$ $\hat{\mathbb{Q}}_{0}^{(A_1')}$ $[\mathrm{M}_1, \mathrm{B}_2]$

$$\hat{\mathbb{Z}}_4 = \mathbb{X}_1[\mathbb{Q}_0^{(a,A_1')}] \otimes \mathbb{Y}_5[\mathbb{Q}_0^{(b,A_1')}]$$

$\boxed{\text{No. 5}}$ $\hat{\mathbb{Q}}_{0}^{(A_1')}$ $[\mathrm{M}_2, \mathrm{B}_3]$

$$\hat{\mathbb{Z}}_5 = \mathbb{X}_2[\mathbb{Q}_0^{(a,A_1')}] \otimes \mathbb{Y}_6[\mathbb{Q}_0^{(b,A_1')}]$$

$\boxed{\text{No. 6}}$ $\hat{\mathbb{Q}}_{3}^{(A_1')}$ $[\mathrm{M}_2, \mathrm{B}_3]$

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

$\boxed{\text{No. 7}}$ $\hat{\mathbb{Q}}_{3}^{(A_1')}$ $[\mathrm{M}_2, \mathrm{B}_3]$

$$\hat{\mathbb{Z}}_7 = \mathbb{X}_5[\mathbb{M}_1^{(a,A_2')}] \otimes \mathbb{Y}_9[\mathbb{T}_3^{(b,A_2')}]$$

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
$\mathbb{X}_1$	$\mathbb{Q}_0^{(a,A_1')}$	M_1	$\begin{pmatrix} 1 \end{pmatrix}$
$\mathbb{X}_2$	$\mathbb{Q}_0^{(a,A_1')}$	M_2	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{X}_3$	$\mathbb{Q}_{2,0}^{(a,E')}$	M_2	$\begin{pmatrix} 0 & -\frac{\sqrt{2}}{2} \\ -\frac{\sqrt{2}}{2} & 0 \end{pmatrix}$
$\mathbb{X}_4$	$\mathbb{Q}_{2,1}^{(a,E')}$	M_2	$\begin{pmatrix} -\frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{pmatrix}$
$\mathbb{X}_5$	$\mathbb{M}_1^{(a,A_2')}$	M_2	$\begin{pmatrix} 0 & -\frac{\sqrt{2}i}{2} \\ \frac{\sqrt{2}i}{2} & 0 \end{pmatrix}$
$\mathbb{X}_6$	$\mathbb{Q}_{1,0}^{(a,E')}$	M_3	$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$
$\mathbb{X}_7$	$\mathbb{Q}_{1,1}^{(a,E')}$	M_3	$\begin{pmatrix} 0 \\ 1 \end{pmatrix}$

Table 7: Cluster SAMB.

symbol	type	cluster	form
$\mathbb{Y}_1$	$\mathbb{Q}_0^{(s,A_1')}$	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'	–	–	$\frac{\sqrt{10}x\left(x^2-3y^2\right)}{4}$

Table 9: Axial harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{G}_1^{(A_2')}$	1	A_2'	–	–	Z

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

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								
$\mathbb{Q}_{3,1}^{(E'')}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{6}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$
	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{6}$								
$\mathbb{Q}_{4}^{(A_1'')}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$
	$-\frac{\sqrt{3}}{6}$	$-\frac{\sqrt{3}}{6}$								