

SAMB for “graphene”

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- Group: No. 191 D_{6h}^1 $P6/mmm$ [hexagonal]
- Associated point group: No. 27 D_{6h} $6/mmm$ [hexagonal]
- Generation condition
 - model type: **tight_binding**
 - time-reversal type: **electric**
 - irrep: [A1g]
 - spinful

- Unit cell:
 - $a = 1.0$, $b = 1.0$, $c = 1.0$, $\alpha = 90.0$, $\beta = 90.0$, $\gamma = 120.0$
- Lattice vectors:
 - $\mathbf{a}_1 = (1.0 \ 0 \ 0)$
 - $\mathbf{a}_2 = (-0.5 \ 0.86602540378444 \ 0)$
 - $\mathbf{a}_3 = (0 \ 0 \ 1.0)$

Table 1: High-symmetry line: Γ -M-K- Γ -K’.

symbol	position	symbol	position	symbol	position
Γ	$\begin{pmatrix} 0 & 0 & 0 \end{pmatrix}$	M	$\begin{pmatrix} \frac{1}{2} & 0 & 0 \end{pmatrix}$	K	$\begin{pmatrix} \frac{1}{3} & \frac{1}{3} & 0 \end{pmatrix}$
K’	$\begin{pmatrix} -\frac{1}{3} & -\frac{1}{3} & 0 \end{pmatrix}$				

- Kets: dimension = 4

Table 2: Hilbert space for full matrix.

No.	ket	No.	ket	No.	ket	No.	ket
1	$(p_z, \uparrow)@A_1$	2	$(p_z, \downarrow)@A_1$	3	$(p_z, \uparrow)@A_2$	4	$(p_z, \downarrow)@A_2$

- Sites in (primitive) unit cell:

Table 3: Site-clusters.

	site	position	mapping
S ₁ [2c: -6m2]	A ₁	$\begin{pmatrix} \frac{1}{3} & \frac{2}{3} & 0 \end{pmatrix}$	[1,6,7,8,9,10,14,15,16,17,23,24]
	A ₂	$\begin{pmatrix} \frac{2}{3} & \frac{1}{3} & 0 \end{pmatrix}$	[2,3,4,5,11,12,13,18,19,20,21,22]

- Bonds in (primitive) unit cell:

Table 4: Bond-clusters.

	bond	tail	head	n	#	$\mathbf{b@c}$	mapping
B ₁ [3f: mmm]	b ₁	A ₂	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,-3,6,-13,14,17,-18]
	b ₂	A ₂	A ₁	1	1	$\begin{pmatrix} \frac{1}{3} & -\frac{1}{3} & 0 \end{pmatrix} @ \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$	[-4,7,10,-11,15,-19,-22,23]
	b ₃	A ₂	A ₁	1	1	$\begin{pmatrix} -\frac{2}{3} & -\frac{1}{3} & 0 \end{pmatrix} @ \begin{pmatrix} 0 & \frac{1}{2} & 0 \end{pmatrix}$	[-5,8,9,-12,16,-20,-21,24]

- SAMB:

$$\boxed{\text{No. 1}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [M_1, S_1]$$

$$\hat{\mathbb{Z}}_1 = \mathbb{X}_1[\mathbb{Q}_0^{(a, A_{1g})}] \otimes \mathbb{Y}_1[\mathbb{Q}_0^{(s, A_{1g})}]$$

$$\boxed{\text{No. 2}} \quad \hat{\mathbb{Q}}_0^{(A_{1g})} [\mathbb{M}_1, \mathbb{B}_1]$$

$$\hat{\mathbb{Z}}_2 = \mathbb{X}_1[\mathbb{Q}_0^{(a, A_{1g})}] \otimes \mathbb{Y}_2[\mathbb{Q}_0^{(b, A_{1g})}]$$

Table 5: Atomic SAMB group.

group	bra	ket
\mathbb{M}_1	$(p_z, \uparrow), (p_z, \downarrow)$	$(p_z, \uparrow), (p_z, \downarrow)$

Table 6: Atomic SAMB.

symbol	type	group	form
\mathbb{X}_1	$\mathbb{Q}_0^{(a, A_{1g})}$	\mathbb{M}_1	$\begin{pmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{pmatrix}$

Table 7: Cluster SAMB.

symbol	type	cluster	form
\mathbb{Y}_1	$\mathbb{Q}_0^{(s, A_{1g})}$	\mathbb{S}_1	$\begin{pmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$
\mathbb{Y}_2	$\mathbb{Q}_0^{(b, A_{1g})}$	\mathbb{B}_1	$\begin{pmatrix} \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} & \frac{\sqrt{3}}{3} \end{pmatrix}$

Table 8: Polar harmonics.

No.	symbol	rank	irrep.	mul.	comp.	form
1	$\mathbb{Q}_0^{(A_{1g})}$	0	A_{1g}	—	—	1

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- Group info.: Generator = $\{3_{001}^+|0\}$, $\{2_{001}|0\}$, $\{2_{110}|0\}$, $\{-1|0\}$

Table 9: Conjugacy class (point-group part).

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

Table 10: Symmetry operations.

No.	SO	No.	SO	No.	SO	No.	SO	No.	SO
1	$\{1 0\}$	2	$\{2_{001} 0\}$	3	$\{2_{100} 0\}$	4	$\{2_{010} 0\}$	5	$\{2_{110} 0\}$

continued ...

Table 10

	No.	SO	No.	SO	No.	SO	No.	SO	No.	SO
	6	$\{2_{120} 0\}$	7	$\{2_{210} 0\}$	8	$\{2_{1-10} 0\}$	9	$\{3_{001}^+ 0\}$	10	$\{3_{001}^- 0\}$
	11	$\{6_{001}^+ 0\}$	12	$\{6_{001}^- 0\}$	13	$\{-1 0\}$	14	$\{m_{100} 0\}$	15	$\{m_{010} 0\}$
	16	$\{m_{110} 0\}$	17	$\{m_{001} 0\}$	18	$\{m_{120} 0\}$	19	$\{m_{210} 0\}$	20	$\{m_{1-10} 0\}$
	21	$\{-3_{001}^+ 0\}$	22	$\{-3_{001}^- 0\}$	23	$\{-6_{001}^+ 0\}$	24	$\{-6_{001}^- 0\}$		

Table 11: Character table (point-group part).

	1	2 ₀₀₁	2 ₁₀₀	2 ₁₂₀	3 ₀₀₁ ⁺	6 ₀₀₁ ⁺	-1	m ₁₀₀	m ₀₀₁	m ₁₂₀	-3 ₀₀₁ ⁺	-6 ₀₀₁ ⁺
<i>A</i> _{1g}	1	1	1	1	1	1	1	1	1	1	1	1
<i>A</i> _{2g}	1	1	-1	-1	1	1	1	-1	1	-1	1	1
<i>B</i> _{1g}	1	-1	-1	1	1	-1	1	-1	-1	1	1	-1
<i>B</i> _{2g}	1	-1	1	-1	1	-1	1	1	-1	-1	1	-1
<i>E</i> _{1g}	2	-2	0	0	-1	1	2	0	-2	0	-1	1
<i>E</i> _{2g}	2	2	0	0	-1	-1	2	0	2	0	-1	-1
<i>A</i> _{1u}	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1
<i>A</i> _{2u}	1	1	-1	-1	1	1	-1	1	-1	1	-1	-1
<i>B</i> _{1u}	1	-1	-1	1	1	-1	-1	1	1	-1	-1	1
<i>B</i> _{2u}	1	-1	1	-1	1	-1	-1	-1	1	1	-1	1
<i>E</i> _{1u}	2	-2	0	0	-1	1	-2	0	2	0	1	-1
<i>E</i> _{2u}	2	2	0	0	-1	-1	-2	0	-2	0	1	1

Table 12: Parity conversion.

\leftrightarrow	\leftrightarrow	\leftrightarrow	\leftrightarrow	\leftrightarrow
<i>A</i> _{1g} (<i>A</i> _{1u})	<i>A</i> _{2g} (<i>A</i> _{2u})	<i>B</i> _{1g} (<i>B</i> _{1u})	<i>B</i> _{2g} (<i>B</i> _{2u})	<i>E</i> _{1g} (<i>E</i> _{1u})
<i>E</i> _{2g} (<i>E</i> _{2u})	<i>A</i> _{1u} (<i>A</i> _{1g})	<i>A</i> _{2u} (<i>A</i> _{2g})	<i>B</i> _{1u} (<i>B</i> _{1g})	<i>B</i> _{2u} (<i>B</i> _{2g})
<i>E</i> _{1u} (<i>E</i> _{1g})	<i>E</i> _{2u} (<i>E</i> _{2g})			

Table 13: Symmetric product, $[\Gamma \otimes \Gamma']_+$.

	A_{1g}	A_{2g}	B_{1g}	B_{2g}	E_{1g}	E_{2g}	A_{1u}	A_{2u}	B_{1u}	B_{2u}	E_{1u}	E_{2u}
A_{1g}	A_{1g}	A_{2g}	B_{1g}	B_{2g}	E_{1g}	E_{2g}	A_{1u}	A_{2u}	B_{1u}	B_{2u}	E_{1u}	E_{2u}
A_{2g}		A_{1g}	B_{2g}	B_{1g}	E_{1g}	E_{2g}	A_{2u}	A_{1u}	B_{2u}	B_{1u}	E_{1u}	E_{2u}
B_{1g}			A_{1g}	A_{2g}	E_{2g}	E_{1g}	B_{1u}	B_{2u}	A_{1u}	A_{2u}	E_{2u}	E_{1u}
B_{2g}				A_{1g}	E_{2g}	E_{1g}	B_{2u}	B_{1u}	A_{2u}	A_{1u}	E_{2u}	E_{1u}
E_{1g}					$A_{1g} + E_{2g}$	$B_{1g} + B_{2g} + E_{1g}$	E_{1u}	E_{1u}	E_{2u}	E_{2u}	$A_{1u} + A_{2u} + E_{2u}$	$B_{1u} + B_{2u} + E_{1u}$
E_{2g}						$A_{1g} + E_{2g}$	E_{2u}	E_{2u}	E_{1u}	E_{1u}	$B_{1u} + B_{2u} + E_{1u}$	$A_{1u} + A_{2u} + E_{2u}$
A_{1u}							A_{1g}	A_{2g}	B_{1g}	B_{2g}	E_{1g}	E_{2g}
A_{2u}								A_{1g}	B_{2g}	B_{1g}	E_{1g}	E_{2g}
B_{1u}									A_{1g}	A_{2g}	E_{2g}	E_{1g}
B_{2u}										A_{1g}	E_{2g}	E_{1g}
E_{1u}											$A_{1g} + E_{2g}$	$B_{1g} + B_{2g} + E_{1g}$
E_{2u}												$A_{1g} + E_{2g}$

Table 14: Anti-symmetric product, $[\Gamma \otimes \Gamma]_-$.

A_{1g}	A_{2g}	B_{1g}	B_{2g}	E_{1g}	E_{2g}	A_{1u}	A_{2u}	B_{1u}	B_{2u}	E_{1u}	E_{2u}
—	—	—	—	A_{2g}	A_{2g}	—	—	—	—	A_{2g}	A_{2g}

Table 15: Virtual-cluster sites.

No.	position	No.	position	No.	position	No.	position
1	$\begin{pmatrix} 1 + \sqrt{3} & -1 + \sqrt{3} & 1 \end{pmatrix}$	2	$\begin{pmatrix} -\sqrt{3} - 1 & 1 - \sqrt{3} & 1 \end{pmatrix}$	3	$\begin{pmatrix} 2 & 1 - \sqrt{3} & -1 \end{pmatrix}$	4	$\begin{pmatrix} -\sqrt{3} - 1 & -2 & -1 \end{pmatrix}$
5	$\begin{pmatrix} -1 + \sqrt{3} & 1 + \sqrt{3} & -1 \end{pmatrix}$	6	$\begin{pmatrix} -2 & -1 + \sqrt{3} & -1 \end{pmatrix}$	7	$\begin{pmatrix} 1 + \sqrt{3} & 2 & -1 \end{pmatrix}$	8	$\begin{pmatrix} 1 - \sqrt{3} & -\sqrt{3} - 1 & -1 \end{pmatrix}$
9	$\begin{pmatrix} 1 - \sqrt{3} & 2 & 1 \end{pmatrix}$	10	$\begin{pmatrix} -2 & -\sqrt{3} - 1 & 1 \end{pmatrix}$	11	$\begin{pmatrix} 2 & 1 + \sqrt{3} & 1 \end{pmatrix}$	12	$\begin{pmatrix} -1 + \sqrt{3} & -2 & 1 \end{pmatrix}$
13	$\begin{pmatrix} -\sqrt{3} - 1 & 1 - \sqrt{3} & -1 \end{pmatrix}$	14	$\begin{pmatrix} -2 & -1 + \sqrt{3} & 1 \end{pmatrix}$	15	$\begin{pmatrix} 1 + \sqrt{3} & 2 & 1 \end{pmatrix}$	16	$\begin{pmatrix} 1 - \sqrt{3} & -\sqrt{3} - 1 & 1 \end{pmatrix}$
17	$\begin{pmatrix} 1 + \sqrt{3} & -1 + \sqrt{3} & -1 \end{pmatrix}$	18	$\begin{pmatrix} 2 & 1 - \sqrt{3} & 1 \end{pmatrix}$	19	$\begin{pmatrix} -\sqrt{3} - 1 & -2 & 1 \end{pmatrix}$	20	$\begin{pmatrix} -1 + \sqrt{3} & 1 + \sqrt{3} & 1 \end{pmatrix}$
21	$\begin{pmatrix} -1 + \sqrt{3} & -2 & -1 \end{pmatrix}$	22	$\begin{pmatrix} 2 & 1 + \sqrt{3} & -1 \end{pmatrix}$	23	$\begin{pmatrix} -2 & -\sqrt{3} - 1 & -1 \end{pmatrix}$	24	$\begin{pmatrix} 1 - \sqrt{3} & 2 & -1 \end{pmatrix}$

Table 16: Virtual-cluster basis.

[illegible]

continued ...

[illegible]

continued ...

Table 16

symbol	1	2	3	4	5	6	7	8	9	10
	$-\frac{1}{4}$	0	$-\frac{1}{4}$	$-\frac{1}{4}$	0	$\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	0	$\frac{1}{4}$
	0	$\frac{1}{4}$	$\frac{1}{4}$	0						
$\mathbb{Q}_6^{(A_{2g})}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$
	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$						
$\mathbb{Q}_{6,0}^{(E_{1g},1)}$	$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$
	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$	$-\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$	$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$
	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{6}}{12}$						
$\mathbb{Q}_{6,1}^{(E_{1g},1)}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$
	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$	$-\frac{\sqrt{2}}{8} - \frac{\sqrt{6}}{24}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$
	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{24} + \frac{\sqrt{2}}{8}$	$-\frac{\sqrt{2}}{8} + \frac{\sqrt{6}}{24}$	$-\frac{\sqrt{6}}{12}$						
$\mathbb{Q}_7^{(A_{1u})}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$
	$\frac{\sqrt{6}}{12}$	$\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$
	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$	$-\frac{\sqrt{6}}{12}$						