

# Model for “grapheneAB”

Generated on 2026-01-25 20:45:20 by MultiPie 2.0.4

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## General Condition

- Basis type: **1g**
- SAMB selection:
  - Type: **[Q, G]**
  - Rank: **[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]**
  - Irrep.: **[ $A'_1$ ,  $A'_2$ ,  $A''_1$ ,  $A''_2$ ,  $E'$ ,  $E''$ ]**
  - Spin (s): **[0, 1]**
- Atomic selection:
  - Type: **[Q, G, M, T]**
  - Rank: **[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]**
  - Irrep.: **[ $A'_1$ ,  $A'_2$ ,  $A''_1$ ,  $A''_2$ ,  $E'$ ,  $E''$ ]**
  - Spin (s): **[0, 1]**
- Site-cluster selection:
  - Rank: **[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]**
  - Irrep.: **[ $A'_1$ ,  $A'_2$ ,  $A''_1$ ,  $A''_2$ ,  $E'$ ,  $E''$ ]**
- Bond-cluster selection:
  - Type: **[Q, G, M, T]**
  - Rank: **[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]**
  - Irrep.: **[ $A'_1$ ,  $A'_2$ ,  $A''_1$ ,  $A''_2$ ,  $E'$ ,  $E''$ ]**
- Max. neighbor: **10**
- Search cell range: **(-2, 3), (-2, 3), (-2, 3)**
- Toroidal priority: **false**

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## Group and Unit Cell

- Group: SG No. 187  $D_{3h}^1$   $P\bar{6}m2$  [ hexagonal ]
- Associated point group: PG No. 187  $D_{3h}$   $\bar{6}m2$  (-6m2 setting) [ hexagonal ]
- Unit cell:
  - $a = 2.43500$ ,  $b = 2.43500$ ,  $c = 10.00000$ ,  $\alpha = 90.0$ ,  $\beta = 90.0$ ,  $\gamma = 120.0$
- Lattice vectors (conventional cell):
  - $\mathbf{a}_1 = [ 2.43500, 0.00000, 0.00000 ]$
  - $\mathbf{a}_2 = [ -1.21750, 2.10877, 0.00000 ]$
  - $\mathbf{a}_3 = [ 0.00000, 0.00000, 10.00000 ]$

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## Symmetry Operation

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Table 1: Symmetry operation

#	SO	#	SO	#	SO	#	SO	#	SO
1	$\{1 0\}$	2	$\{3_{001}^+ 0\}$	3	$\{3_{001}^- 0\}$	4	$\{m_{001} 0\}$	5	$\{-6_{001}^- 0\}$
6	$\{-6_{001}^+ 0\}$	7	$\{m_{110} 0\}$	8	$\{m_{100} 0\}$	9	$\{m_{010} 0\}$	10	$\{2_{1-10} 0\}$
11	$\{2_{120} 0\}$	12	$\{2_{210} 0\}$						

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## Harmonics

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Table 2: Harmonics

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
1	$\mathbb{Q}_0(A'_1)$	$A'_1$	0	$Q, T$	-	-	1
2	$\mathbb{Q}_3(A'_1)$	$A'_1$	3	$Q, T$	-	-	$\frac{\sqrt{10}y(3x^2-y^2)}{4}$
3	$\mathbb{G}_1(A'_2)$	$A'_2$	1	$G, M$	-	-	$z$
4	$\mathbb{Q}_3(A'_2)$	$A'_2$	3	$Q, T$	-	-	$\frac{\sqrt{10}x(x^2-3y^2)}{4}$
5	$\mathbb{Q}_{1,1}(E')$	$E'$	1	$Q, T$	-	1	$x$
6	$\mathbb{Q}_{1,2}(E')$					2	$y$
7	$\mathbb{Q}_{2,1}(E')$	$E'$	2	$Q, T$	-	1	$\sqrt{3}xy$

*continued ...*

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
8	$\mathbb{Q}_{2,2}(E')$					2	$\frac{\sqrt{3}(x-y)(x+y)}{2}$

— Basis in full matrix —

Table 3: dimension = 3

#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)
0	$ s\rangle @A(1)$	1	$ p_x\rangle @B(1)$	2	$ p_y\rangle @B(1)$

Table 4: Atomic basis (orbital part only)

orbital	definition
$ s\rangle$	1
$ p_x\rangle$	$x$
$ p_y\rangle$	$y$
$ p_z\rangle$	$z$

25 (all 25) SAMBs

• 'A' site-cluster : A

- \* bra:  $\langle s|$
- \* ket:  $|s\rangle$
- \* wyckoff: 1c

$$\boxed{\text{z1}} \quad \mathbb{Q}_0^{(c)}(A'_1) = \mathbb{Q}_0^{(a)}(A'_1)\mathbb{Q}_0^{(s)}(A'_1)$$

• 'B' site-cluster : B

- \* bra:  $\langle p_x|, \langle p_y|$
- \* ket:  $|p_x\rangle, |p_y\rangle$
- \* wyckoff: 1e

$$\boxed{\text{z2}} \quad \mathbb{Q}_0^{(c)}(A'_1) = \mathbb{Q}_0^{(a)}(A'_1)\mathbb{Q}_0^{(s)}(A'_1)$$

$$\boxed{\text{z10}} \quad \mathbb{Q}_{2,1}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_0^{(s)}(A'_1)}{2}$$

$$\boxed{\text{z11}} \quad \mathbb{Q}_{2,2}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_0^{(s)}(A'_1)}{2}$$

• 'A'-'A' bond-cluster : A;A\_001\_1

- \* bra:  $\langle s|$
- \* ket:  $|s\rangle$
- \* wyckoff: 3b@3j

$$\boxed{\text{z3}} \quad \mathbb{Q}_0^{(c)}(A'_1) = \mathbb{Q}_0^{(a)}(A'_1)\mathbb{Q}_0^{(b)}(A'_1)$$

$$\boxed{\text{z12}} \quad \mathbb{Q}_{1,1}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A'_1)\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z13}} \quad \mathbb{Q}_{1,2}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A'_1)\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

• 'A'-'B' bond-cluster : B;A\_001\_1

\* bra:  $\langle s|$   
 \* ket:  $|p_x\rangle, |p_y\rangle$   
 \* wyckoff: **3a03j**

$$\boxed{\text{z4}} \quad \mathbb{Q}_0^{(c)}(A'_1) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z8}} \quad \mathbb{G}_1^{(c)}(A'_2) = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z14}} \quad \mathbb{Q}_{1,1}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_0^{(b)}(A'_1)}{2}$$

$$\boxed{\text{z15}} \quad \mathbb{Q}_{1,2}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_0^{(b)}(A'_1)}{2}$$

$$\boxed{\text{z16}} \quad \mathbb{Q}_{2,1}^{(c)}(E') = \frac{\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} + \frac{\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z17}} \quad \mathbb{Q}_{2,2}^{(c)}(E') = \frac{\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2} - \frac{\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

• 'B'-'B' bond-cluster : B;B\_001\_1

\* bra:  $\langle p_x|, \langle p_y|$   
 \* ket:  $|p_x\rangle, |p_y\rangle$   
 \* wyckoff: **3b03j**

$$\boxed{\text{z5}} \quad \mathbb{Q}_0^{(c)}(A'_1, a) = \mathbb{Q}_0^{(a)}(A'_1)\mathbb{Q}_0^{(b)}(A'_1)$$

$$\boxed{\text{z6}} \quad \mathbb{Q}_0^{(c)}(A'_1, b) = \mathbb{M}_1^{(a)}(A'_2)\mathbb{M}_1^{(b)}(A'_2)$$

$$\boxed{\text{z7}} \quad \mathbb{Q}_3^{(c)}(A'_1) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z9}} \quad \mathbb{Q}_3^{(c)}(A'_2) = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z18}} \quad \mathbb{Q}_{1,1}^{(c)}(E', a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A'_1)\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z19}} \quad \mathbb{Q}_{1,2}^{(c)}(E', a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A'_1)\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z20}} \quad \mathbb{Q}_{1,1}^{(c)}(E', b) = \frac{\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z21}} \quad \mathbb{Q}_{1,2}^{(c)}(E', b) = \frac{\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2} - \frac{\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z22}} \quad \mathbb{Q}_{1,1}^{(c)}(E', c) = -\frac{\sqrt{2}\mathbb{M}_1^{(a)}(A'_2)\mathbb{T}_{1,2}^{(b)}(E')}{2}$$

$$\boxed{\text{z23}} \quad \mathbb{Q}_{1,2}^{(c)}(E', c) = \frac{\sqrt{2}\mathbb{M}_1^{(a)}(A'_2)\mathbb{T}_{1,1}^{(b)}(E')}{2}$$

$$\boxed{\text{z24}} \quad \mathbb{Q}_{2,1}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_0^{(b)}(A'_1)}{2}$$

$$\boxed{\text{z25}} \quad \mathbb{Q}_{2,2}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_0^{(b)}(A'_1)}{2}$$

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## Atomic SAMB

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- bra:  $\langle s|$
- ket:  $|s\rangle$

$$\boxed{\text{x1}} \quad \mathbb{Q}_0^{(a)}(A'_1) = [1]$$

- bra:  $\langle p_x|, \langle p_y|$
- ket:  $|p_x\rangle, |p_y\rangle$

$$\boxed{\text{x2}} \quad \mathbb{Q}_0^{(a)}(A'_1) = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{bmatrix}$$

$$\boxed{\text{x3}} \quad \mathbb{Q}_{2,1}^{(a)}(E') = \begin{bmatrix} 0 & \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} & 0 \end{bmatrix}$$

$$\boxed{\text{x4}} \quad \mathbb{Q}_{2,2}^{(a)}(E') = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & -\frac{\sqrt{2}}{2} \end{bmatrix}$$

$$\boxed{\text{x5}} \quad \mathbb{M}_1^{(a)}(A'_2) = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{2} \\ \frac{\sqrt{2}i}{2} & 0 \end{bmatrix}$$

- bra:  $\langle s|$
- ket:  $|p_x\rangle, |p_y\rangle$

$$\boxed{\text{x6}} \quad \mathbb{Q}_{1,1}^{(a)}(E') = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 \end{bmatrix}$$

$$\boxed{\text{x7}} \quad \mathbb{Q}_{1,2}^{(a)}(E') = \begin{bmatrix} 0 & \frac{\sqrt{2}}{2} \end{bmatrix}$$

$$\boxed{\text{x8}} \quad \mathbb{T}_{1,1}^{(a)}(E') = \begin{bmatrix} \frac{\sqrt{2}i}{2} & 0 \end{bmatrix}$$

$$\boxed{\text{x9}} \quad \mathbb{T}_{1,2}^{(a)}(E') = \begin{bmatrix} 0 & \frac{\sqrt{2}i}{2} \end{bmatrix}$$

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#### Cluster SAMB

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- Site cluster

\*\* Wyckoff: 1c

$$\boxed{\text{y1}} \quad \mathbb{Q}_0^{(s)}(A'_1) = [1]$$

\*\* Wyckoff: 1e

$$\boxed{\text{y2}} \quad \mathbb{Q}_0^{(s)}(A'_1) = [1]$$

- Bond cluster

\*\* Wyckoff: 3b@3j

$$\boxed{\text{y3}} \quad \mathbb{Q}_0^{(s)}(A'_1) = \left[ \frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3} \right]$$

$$\boxed{\text{y4}} \quad \mathbb{M}_1^{(s)}(A'_2) = \left[ \frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{3} \right]$$

$$\boxed{\text{y5}} \quad \mathbb{Q}_{1,1}^{(s)}(E') = \left[ \frac{\sqrt{2}}{2}, 0, -\frac{\sqrt{2}}{2} \right]$$

$$\boxed{\text{y6}} \quad \mathbb{Q}_{1,2}^{(s)}(E') = \left[ -\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{3}, -\frac{\sqrt{6}}{6} \right]$$

$$\boxed{\text{y7}} \quad \mathbb{T}_{1,1}^{(s)}(E') = \left[ \frac{\sqrt{6}i}{6}, -\frac{\sqrt{6}i}{3}, \frac{\sqrt{6}i}{6} \right]$$

$$\boxed{\text{y8}} \quad \mathbb{T}_{1,2}^{(s)}(E') = \left[ \frac{\sqrt{2}i}{2}, 0, -\frac{\sqrt{2}i}{2} \right]$$

\*\* Wyckoff: 3a@3j

$$\boxed{\text{y9}} \quad \mathbb{Q}_0^{(s)}(A'_1) = \left[ \frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3} \right]$$

$$\boxed{\text{y10}} \quad \mathbb{T}_0^{(s)}(A'_1) = \left[ \frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{3} \right]$$

$$\boxed{\text{y11}} \quad \mathbb{Q}_{1,1}^{(s)}(E') = \left[ \frac{\sqrt{2}}{2}, 0, -\frac{\sqrt{2}}{2} \right]$$

$$\boxed{\text{y12}} \quad \mathbb{Q}_{1,2}^{(s)}(E') = \left[ -\frac{\sqrt{6}}{6}, \frac{\sqrt{6}}{3}, -\frac{\sqrt{6}}{6} \right]$$

$$\boxed{\text{y13}} \quad \mathbb{T}_{1,1}^{(s)}(E') = \left[ \frac{\sqrt{2}i}{2}, 0, -\frac{\sqrt{2}i}{2} \right]$$

$$\boxed{\text{y14}} \quad \mathbb{T}_{1,2}^{(s)}(E') = \left[ -\frac{\sqrt{6}i}{6}, \frac{\sqrt{6}i}{3}, -\frac{\sqrt{6}i}{6} \right]$$

— Site and Bond —



Table 5: Orbital of each site

#	site	orbital
1	A	$ s\rangle$
2	B	$ p_x\rangle,  p_y\rangle$

Table 6: Neighbor and bra-ket of each bond

#	head	tail	neighbor	head (bra)	tail (ket)
1	A	A	[1]	[s]	[s]
2	A	B	[1]	[s]	[p]
3	B	B	[1]	[p]	[p]

## — Site in Unit Cell —

Sites in (conventional) cell (no plus set), SL = sublattice

Table 7: 'A' (#1) site cluster (1c),  $-6m2$ 

SL	position ( $\mathbf{s}$ )	mapping
1	[ 0.33333, 0.66667, 0.00000]	[1,2,3,4,5,6,7,8,9,10,11,12]

Table 8: 'B' (#2) site cluster (1e),  $-6m2$ 

SL	position ( $\mathbf{s}$ )	mapping
1	[ 0.66667, 0.33333, 0.00000]	[1,2,3,4,5,6,7,8,9,10,11,12]

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**Bond in Unit Cell**


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Bonds in (conventional) cell (no plus set): tail, head = (SL, plus set), (N)D = (non)directional (listed up to 5th neighbor at most)

Table 9: 1-th 'A'-'A' [1] (#1) bond cluster (3b03j), ND,  $|\mathbf{v}|=2.435$  (cartesian)

SL	vector ( $\mathbf{v}$ )	center ( $\mathbf{c}$ )	mapping	head	tail	$\mathbf{R}$ (primitive)
1	[-1.00000, -1.00000, 0.00000]	[ 0.83333, 0.16667, 0.00000]	[1,4,-7,-10]	(1,1)	(1,1)	[1,1,0]
2	[ 1.00000, 0.00000, 0.00000]	[ 0.83333, 0.66667, 0.00000]	[2,5,-9,-12]	(1,1)	(1,1)	[-1,0,0]
3	[ 0.00000, 1.00000, 0.00000]	[ 0.33333, 0.16667, 0.00000]	[3,6,-8,-11]	(1,1)	(1,1)	[0,-1,0]

Table 10: 1-th 'A'-'B' [1] (#2) bond cluster (3a@3j), D,  $|\mathbf{v}|=1.40585$  (cartesian)

SL	vector ( $\mathbf{v}$ )	center ( $\mathbf{c}$ )	mapping	head	tail	$\mathbf{R}$ (primitive)
1	[-0.33333, 0.33333, 0.00000]	[ 0.50000, 0.50000, 0.00000]	[1,4,7,10]	(1,1)	(1,1)	[0,0,0]
2	[-0.33333,-0.66667, 0.00000]	[ 0.50000, 0.00000, 0.00000]	[2,5,9,12]	(1,1)	(1,1)	[0,1,0]
3	[ 0.66667, 0.33333, 0.00000]	[ 0.00000, 0.50000, 0.00000]	[3,6,8,11]	(1,1)	(1,1)	[-1,0,0]

Table 11: 1-th 'B'-'B' [1] (#3) bond cluster (3b@3j), ND,  $|\mathbf{v}|=2.435$  (cartesian)

SL	vector ( $\mathbf{v}$ )	center ( $\mathbf{c}$ )	mapping	head	tail	$\mathbf{R}$ (primitive)
1	[-1.00000,-1.00000, 0.00000]	[ 0.16667, 0.83333, 0.00000]	[1,4,-7,-10]	(1,1)	(1,1)	[1,1,0]
2	[ 1.00000, 0.00000, 0.00000]	[ 0.16667, 0.33333, 0.00000]	[2,5,-9,-12]	(1,1)	(1,1)	[-1,0,0]
3	[ 0.00000, 1.00000, 0.00000]	[ 0.66667, 0.83333, 0.00000]	[3,6,-8,-11]	(1,1)	(1,1)	[0,-1,0]