

# Model for “grapheneAB”

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## General Condition

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- 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

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- 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):  
 $a_1 = [ 2.43500, 0.00000, 0.00000 ]$   
 $a_2 = [-1.21750, 2.10877, 0.00000 ]$   
 $a_3 = [ 0.00000, 0.00000, 10.00000 ]$

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 — Symmetry Operation —

Table 1: Symmetry operation

#	SO	#	SO	#	SO	#	SO	#	SO
1	{1 0}	2	{3 <sup>+</sup> <sub>001</sub>  0}	3	{3 <sup>-</sup> <sub>001</sub>  0}	4	{m <sub>001</sub>  0}	5	{-6 <sup>-</sup> <sub>001</sub>  0}
6	{-6 <sup>+</sup> <sub>001</sub>  0}	7	{m <sub>110</sub>  0}	8	{m <sub>100</sub>  0}	9	{m <sub>010</sub>  0}	10	{2 <sub>1-10</sub>  0}
11	{2 <sub>120</sub>  0}	12	{2 <sub>210</sub>  0}						

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 — Harmonics —

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	$\frac{\sqrt{3}(x-y)(x+y)}{2}$

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Basis in full matrix

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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$	$z$

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**SAMB**

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25 (all 25) SAMBs

- 'A' site-cluster : A
  - \* bra:  $\langle s |$
  - \* ket:  $| s \rangle$
  - \* wyckoff: 1c

$$\boxed{z1} \quad Q_0^{(c)}(A'_1) = Q_0^{(a)}(A'_1)Q_0^{(s)}(A'_1)$$

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

$$\boxed{z2} \quad Q_0^{(c)}(A'_1) = Q_0^{(a)}(A'_1)Q_0^{(s)}(A'_1)$$

$$\boxed{z10} \quad Q_{2,1}^{(c)}(E') = \frac{\sqrt{2}Q_{2,1}^{(a)}(E')Q_0^{(s)}(A'_1)}{2}$$

$$\boxed{z11} \quad Q_{2,2}^{(c)}(E') = \frac{\sqrt{2}Q_{2,2}^{(a)}(E')Q_0^{(s)}(A'_1)}{2}$$

- 'A'-'A' bond-cluster : A;A\_001\_1
  - \* bra:  $\langle s |$
  - \* ket:  $| s \rangle$
  - \* wyckoff: 3b@3j

$$\boxed{z3} \quad Q_0^{(c)}(A'_1) = Q_0^{(a)}(A'_1)Q_0^{(b)}(A'_1)$$

$$\boxed{z12} \quad Q_{1,1}^{(c)}(E') = \frac{\sqrt{2}Q_0^{(a)}(A'_1)Q_{1,1}^{(b)}(E')}{2}$$

$$\boxed{z13} \quad Q_{1,2}^{(c)}(E') = \frac{\sqrt{2}Q_0^{(a)}(A'_1)Q_{1,2}^{(b)}(E')}{2}$$

- 'A'-'B' bond-cluster : B;A\_001\_1

\* bra:  $\langle s |$

\* ket:  $|p_x\rangle, |p_y\rangle$

\* wyckoff: 3a@3j

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

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

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

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

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

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

• 'B'-'B' bond-cluster : B;B\_001\_1

\* bra:  $\langle p_x |, \langle p_y |$

\* ket:  $|p_x\rangle, |p_y\rangle$

\* wyckoff: 3b@3j

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

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

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

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

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

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

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

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

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

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

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

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

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### — Atomic SAMB —

- 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:  $|p_x\rangle, |p_y\rangle$

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

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

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

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

- bra:  $\langle s |$

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

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

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

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

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

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### — Cluster SAMB —

- Site cluster

\*\* Wyckoff: **1c**

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

\*\* Wyckoff: **1e**

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

- Bond cluster

\*\* Wyckoff: **3b@3j**

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

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

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

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

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

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

\*\* Wyckoff: 3a@3j

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

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

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

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

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

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

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]

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— Site in Unit Cell —

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

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

SL	position ( $s$ )	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 ( $s$ )	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 (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]	[ 0.83333, 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]