Model for "grapheneAB"

Generated on 2026-02-01 11:16:32 by MultiPie 2.0.7

General Condition

- Basis type: lg
- 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

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):
  $\boldsymbol{a}_1 =$ [2.43500, 0.00000, 0.00000]
  $\boldsymbol{a}_2 =$ [-1.21750, 2.10877, 0.00000]
  $\boldsymbol{a}_3 =$ [0.00000, 0.00000,10.00000]

Symmetry Operation

Table 1: Symmetry operation

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

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

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

SAMB

25 (all 25) SAMBs

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

z1 $\mathbb{Q}_0^{(c)}(A_1') = \mathbb{Q}_0^{(a)}(A_1')\mathbb{Q}_0^{(s)}(A_1')$

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

z2 $\mathbb{Q}_0^{(c)}(A_1') = \mathbb{Q}_0^{(a)}(A_1')\mathbb{Q}_0^{(s)}(A_1')$

z10 $\mathbb{Q}_{2,1}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_0^{(s)}(A_1')}{2}$

z11 $\mathbb{Q}_{2,2}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_0^{(s)}(A_1')}{2}$

- 'A'-'A' bond-cluster : A;A_001_1
  * bra: $\langle s|$
  * ket: $|s\rangle$
  * wyckoff: 3b@3j

z3 $\mathbb{Q}_0^{(c)}(A_1') = \mathbb{Q}_0^{(a)}(A_1')\mathbb{Q}_0^{(b)}(A_1')$

z12 $\mathbb{Q}_{1,1}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_1')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

z13 $\mathbb{Q}_{1,2}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_1')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

- 'A'-'B' bond-cluster : B;A_001_1

  * bra: $\langle s|$
  * ket: $|p_x\rangle$, $|p_y\rangle$
  * wyckoff: `3a@3j`

z4 $\mathbb{Q}_0^{(c)}(A_1') = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2} + \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

z8 $\mathbb{G}_1^{(c)}(A_2') = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} - \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

z14 $\mathbb{Q}_{1,1}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{1,1}^{(a)}(E')\mathbb{Q}_0^{(b)}(A_1')}{2}$

z15 $\mathbb{Q}_{1,2}^{(c)}(E') = \frac{\sqrt{2}\mathbb{Q}_{1,2}^{(a)}(E')\mathbb{Q}_0^{(b)}(A_1')}{2}$

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

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

- '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`

z5 $\mathbb{Q}_0^{(c)}(A_1', a) = \mathbb{Q}_0^{(a)}(A_1')\mathbb{Q}_0^{(b)}(A_1')$

z6 $\mathbb{Q}_0^{(c)}(A_1', b) = \mathbb{M}_1^{(a)}(A_2')\mathbb{M}_1^{(b)}(A_2')$

z7 $\mathbb{Q}_3^{(c)}(A_1') = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

z9 $\mathbb{Q}_3^{(c)}(A_2') = -\frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{1,2}^{(b)}(E')}{2} + \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

z18 $\mathbb{Q}_{1,1}^{(c)}(E', a) = \frac{\sqrt{2}\mathbb{Q}_0^{(a)}(A_1')\mathbb{Q}_{1,1}^{(b)}(E')}{2}$

z19 $\mathbb{Q}_{1,2}^{(c)}(E',a) = \dfrac{\sqrt{2}\mathbb{Q}_{0}^{(a)}(A_1')\mathbb{Q}_{1,2}^{(b)}(E')}{2}$

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

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

z22 $\mathbb{Q}_{1,1}^{(c)}(E',c) = -\dfrac{\sqrt{2}\mathbb{M}_{1}^{(a)}(A_2')\mathbb{T}_{1,2}^{(b)}(E')}{2}$

z23 $\mathbb{Q}_{1,2}^{(c)}(E',c) = \dfrac{\sqrt{2}\mathbb{M}_{1}^{(a)}(A_2')\mathbb{T}_{1,1}^{(b)}(E')}{2}$

z24 $\mathbb{Q}_{2,1}^{(c)}(E') = \dfrac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E')\mathbb{Q}_{0}^{(b)}(A_1')}{2}$

z25 $\mathbb{Q}_{2,2}^{(c)}(E') = \dfrac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E')\mathbb{Q}_{0}^{(b)}(A_1')}{2}$

Atomic SAMB

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

x1 $\mathbb{Q}_{0}^{(a)}(A_1') = \begin{bmatrix} 1 \end{bmatrix}$

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

x2 $\mathbb{Q}_{0}^{(a)}(A_1') = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{bmatrix}$

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

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

x5 $\mathbb{M}^{(a)}_{1}(A'_2) = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{2} \\ \frac{\sqrt{2}i}{2} & 0 \end{bmatrix}$

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

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

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

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

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

Cluster SAMB

- Site cluster

** Wyckoff: `1e`

y1 $\mathbb{Q}^{(s)}_{0}(A'_1) = [1]$

** Wyckoff: `1c`

y2 $\mathbb{Q}^{(s)}_{0}(A'_1) = [1]$

- Bond cluster

** Wyckoff: `3a@3j`

y3 $\mathbb{Q}^{(s)}_{0}(A'_1) = \left[\frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3} \right]$

y4 $\mathbb{T}^{(s)}_{0}(A'_1) = \left[\frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{3}, \frac{\sqrt{3}i}{3} \right]$

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

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

y7 $\mathbb{T}^{(s)}_{1,1}(E') = \left[\frac{\sqrt{2}i}{2},\, 0,\, -\frac{\sqrt{2}i}{2}\right]$

y8 $\mathbb{T}^{(s)}_{1,2}(E') = \left[-\frac{\sqrt{6}i}{6},\, \frac{\sqrt{6}i}{3},\, -\frac{\sqrt{6}i}{6}\right]$

** Wyckoff: `3b@3j`

y9 $\mathbb{Q}^{(s)}_{0}(A'_1) = \left[\frac{\sqrt{3}}{3},\, \frac{\sqrt{3}}{3},\, \frac{\sqrt{3}}{3}\right]$

y10 $\mathbb{M}^{(s)}_{1}(A'_2) = \left[\frac{\sqrt{3}i}{3},\, \frac{\sqrt{3}i}{3},\, \frac{\sqrt{3}i}{3}\right]$

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

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

y13 $\mathbb{T}^{(s)}_{1,1}(E') = \left[\frac{\sqrt{6}i}{6},\, -\frac{\sqrt{6}i}{3},\, \frac{\sqrt{6}i}{6}\right]$

y14 $\mathbb{T}^{(s)}_{1,2}(E') = \left[\frac{\sqrt{2}i}{2},\, 0,\, -\frac{\sqrt{2}i}{2}\right]$

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

Bond in Unit Cell

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, $|\boldsymbol{v}|$= 2.435 (cartesian)

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (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, $|\boldsymbol{v}|$= 1.40585 (cartesian)

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (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, $|\boldsymbol{v}|$= 2.435 (cartesian)

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (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]