Model for "GaAs"

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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, E, T_1, T_2]
  - 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, E, T_1, T_2]
  - 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, E, T_1, T_2]
- 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, E, T_1, T_2]
- Max. neighbor: `10`
- Search cell range: `(-2, 3), (-2, 3), (-2, 3)`
- Toroidal priority: `false`

Group and Unit Cell

- Group: SG No. 216 T_{d}^2 $F\bar{4}3m$ [cubic]
- Associated point group: PG No. 216 T_{d} $\bar{4}3m$ [cubic]
- Unit cell:
  $a =$ `1.00000`, $b =$ `1.00000`, $c =$ `1.00000`, $\alpha =$ `90.0`, $\beta =$ `90.0`, $\gamma =$ `90.0`
- Lattice vectors (conventional cell):
  $\boldsymbol{a}_1 =$ `[ 1.00000, 0.00000, 0.00000]`
  $\boldsymbol{a}_2 =$ `[ 0.00000, 1.00000, 0.00000]`
  $\boldsymbol{a}_3 =$ `[ 0.00000, 0.00000, 1.00000]`

- Plus sets:
  $+[0,\,0,\,0],\ \ +[0,\,\frac{1}{2},\,\frac{1}{2}],\ \ +[\frac{1}{2},\,0,\,\frac{1}{2}],\ \ +[\frac{1}{2},\,\frac{1}{2},\,0]$

Symmetry Operation

Table 1: Symmetry operation

#	SO	#	SO	#	SO	#	SO	#	SO
1	$\{1\|0\}$	2	$\{2_{001}\|0\}$	3	$\{2_{010}\|0\}$	4	$\{2_{100}\|0\}$	5	$\{3^{+}_{111}\|0\}$
6	$\{3^{+}_{-11-1}\|0\}$	7	$\{3^{+}_{1-1-1}\|0\}$	8	$\{3^{+}_{-1-11}\|0\}$	9	$\{3^{-}_{111}\|0\}$	10	$\{3^{-}_{1-1-1}\|0\}$
11	$\{3^{-}_{-1-11}\|0\}$	12	$\{3^{-}_{-11-1}\|0\}$	13	$\{\mathrm{m}_{1-10}\|0\}$	14	$\{\mathrm{m}_{110}\|0\}$	15	$\{-4^{+}_{001}\|0\}$
16	$\{-4^{-}_{001}\|0\}$	17	$\{\mathrm{m}_{01-1}\|0\}$	18	$\{-4^{+}_{100}\|0\}$	19	$\{-4^{-}_{100}\|0\}$	20	$\{\mathrm{m}_{011}\|0\}$
21	$\{\mathrm{m}_{-101}\|0\}$	22	$\{-4^{-}_{010}\|0\}$	23	$\{\mathrm{m}_{101}\|0\}$	24	$\{-4^{+}_{010}\|0\}$		

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	-	-	$\sqrt{15}xyz$
3	$\mathbb{G}_0(A_2)$	A_2	0	G, M	-	-	1
4	$\mathbb{G}_{2,1}(E)$	E	2	G, M	-	1	$-\frac{\sqrt{3}(x-y)(x+y)}{2}$

continued ...

Table 2

#	symbol	irrep.	rank	X	multiplicity	component	symmetry
5	$\mathbb{G}_{2,2}(E)$					2	$-\frac{x^2}{2}-\frac{y^2}{2}+z^2$
6	$\mathbb{Q}_{2,1}(E)$	E	2	Q, T	-	1	$-\frac{x^2}{2}-\frac{y^2}{2}+z^2$
7	$\mathbb{Q}_{2,2}(E)$					2	$\frac{\sqrt{3}(x-y)(x+y)}{2}$
8	$\mathbb{G}_{1,1}(T_1)$	T_1	1	G, M	-	1	x
9	$\mathbb{G}_{1,2}(T_1)$					2	y
10	$\mathbb{G}_{1,3}(T_1)$					3	z
11	$\mathbb{G}_{2,1}(T_1)$	T_1	2	G, M	-	1	$\sqrt{3}yz$
12	$\mathbb{G}_{2,2}(T_1)$					2	$\sqrt{3}xz$
13	$\mathbb{G}_{2,3}(T_1)$					3	$\sqrt{3}xy$
14	$\mathbb{Q}_{3,1}(T_1)$	T_1	3	Q, T	-	1	$\frac{\sqrt{15}x(y-z)(y+z)}{2}$
15	$\mathbb{Q}_{3,2}(T_1)$					2	$-\frac{\sqrt{15}y(x-z)(x+z)}{2}$
16	$\mathbb{Q}_{3,3}(T_1)$					3	$\frac{\sqrt{15}z(x-y)(x+y)}{2}$
17	$\mathbb{Q}_{1,1}(T_2)$	T_2	1	Q, T	-	1	x
18	$\mathbb{Q}_{1,2}(T_2)$					2	y
19	$\mathbb{Q}_{1,3}(T_2)$					3	z
20	$\mathbb{Q}_{2,1}(T_2)$	T_2	2	Q, T	-	1	$\sqrt{3}yz$
21	$\mathbb{Q}_{2,2}(T_2)$					2	$\sqrt{3}xz$
22	$\mathbb{Q}_{2,3}(T_2)$					3	$\sqrt{3}xy$
23	$\mathbb{Q}_{3,1}(T_2)$	T_2	3	Q, T	-	1	$\frac{x\left(2x^2-3y^2-3z^2\right)}{2}$
24	$\mathbb{Q}_{3,2}(T_2)$					2	$-\frac{y\left(3x^2-2y^2+3z^2\right)}{2}$
25	$\mathbb{Q}_{3,3}(T_2)$					3	$-\frac{z\left(3x^2+3y^2-2z^2\right)}{2}$

Basis in full matrix

Table 3: dimension = 6

	#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)	#	orbital@atom(SL)
	0	$\|p_x\rangle$ @As(1)	1	$\|p_y\rangle$ @As(1)	2	$\|p_z\rangle$ @As(1)	3	$\|p_x\rangle$ @Ga(1)	4	$\|p_y\rangle$ @Ga(1)
	5	$\|p_z\rangle$ @Ga(1)								

Table 4: Atomic basis (orbital part only)

orbital	definition
$\|p_x\rangle$	x
$\|p_y\rangle$	y
$\|p_z\rangle$	z

SAMB: 48 (all 48)

- `As` : '`As`' site-cluster
  * bra: $\langle p_x|$, $\langle p_y|$, $\langle p_z|$
  * ket: $|p_x\rangle$, $|p_y\rangle$, $|p_z\rangle$
  * wyckoff: `4c`

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

  z6 $\quad \mathbb{Q}_{2,1}^{(c)}(E) = \dfrac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E)\mathbb{Q}_0^{(s)}(A_1)}{2}$

z7 $\mathbb{Q}^{(c)}_{2,2}(E) = \dfrac{\sqrt{2}\mathbb{Q}^{(a)}_{2,2}(E)\mathbb{Q}^{(s)}_{0}(A_1)}{2}$

z28 $\mathbb{Q}^{(c)}_{2,1}(T_2) = \dfrac{\sqrt{3}\mathbb{Q}^{(a)}_{2,1}(T_2)\mathbb{Q}^{(s)}_{0}(A_1)}{3}$

z29 $\mathbb{Q}^{(c)}_{2,2}(T_2) = \dfrac{\sqrt{3}\mathbb{Q}^{(a)}_{2,2}(T_2)\mathbb{Q}^{(s)}_{0}(A_1)}{3}$

z30 $\mathbb{Q}^{(c)}_{2,3}(T_2) = \dfrac{\sqrt{3}\mathbb{Q}^{(a)}_{2,3}(T_2)\mathbb{Q}^{(s)}_{0}(A_1)}{3}$

- `Ga` : '`Ga`' site-cluster
  * bra: $\langle p_x|$, $\langle p_y|$, $\langle p_z|$
  * ket: $|p_x\rangle$, $|p_y\rangle$, $|p_z\rangle$
  * wyckoff: `4a`

  z2 $\mathbb{Q}^{(c)}_{0}(A_1) = \mathbb{Q}^{(a)}_{0}(A_1)\mathbb{Q}^{(s)}_{0}(A_1)$

  z8 $\mathbb{Q}^{(c)}_{2,1}(E) = \dfrac{\sqrt{2}\mathbb{Q}^{(a)}_{2,1}(E)\mathbb{Q}^{(s)}_{0}(A_1)}{2}$

  z9 $\mathbb{Q}^{(c)}_{2,2}(E) = \dfrac{\sqrt{2}\mathbb{Q}^{(a)}_{2,2}(E)\mathbb{Q}^{(s)}_{0}(A_1)}{2}$

  z31 $\mathbb{Q}^{(c)}_{2,1}(T_2) = \dfrac{\sqrt{3}\mathbb{Q}^{(a)}_{2,1}(T_2)\mathbb{Q}^{(s)}_{0}(A_1)}{3}$

  z32 $\mathbb{Q}^{(c)}_{2,2}(T_2) = \dfrac{\sqrt{3}\mathbb{Q}^{(a)}_{2,2}(T_2)\mathbb{Q}^{(s)}_{0}(A_1)}{3}$

  z33 $\mathbb{Q}^{(c)}_{2,3}(T_2) = \dfrac{\sqrt{3}\mathbb{Q}^{(a)}_{2,3}(T_2)\mathbb{Q}^{(s)}_{0}(A_1)}{3}$

- `Ga;As_001_1` : '`As`'-'`Ga`' bond-cluster
  * bra: $\langle p_x|$, $\langle p_y|$, $\langle p_z|$
  * ket: $|p_x\rangle$, $|p_y\rangle$, $|p_z\rangle$
  * wyckoff: `16a@16e`

z3 $\mathbb{Q}_{0}^{(c)}(A_1) = \mathbb{Q}_{0}^{(a)}(A_1)\mathbb{Q}_{0}^{(b)}(A_1)$

z4 $\mathbb{Q}_{3}^{(c)}(A_1) = \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(T_2)\mathbb{Q}_{1,1}^{(b)}(T_2)}{3} + \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(T_2)\mathbb{Q}_{1,2}^{(b)}(T_2)}{3} + \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(a)}(T_2)\mathbb{Q}_{1,3}^{(b)}(T_2)}{3}$

z5 $\mathbb{G}_{0}^{(c)}(A_2) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(T_1)\mathbb{T}_{1,1}^{(b)}(T_2)}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(T_1)\mathbb{T}_{1,2}^{(b)}(T_2)}{3} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(a)}(T_1)\mathbb{T}_{1,3}^{(b)}(T_2)}{3}$

z10 $\mathbb{Q}_{2,1}^{(c)}(E) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E)\mathbb{Q}_{0}^{(b)}(A_1)}{2}$

z11 $\mathbb{Q}_{2,2}^{(c)}(E) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E)\mathbb{Q}_{0}^{(b)}(A_1)}{2}$

z12 $\mathbb{G}_{2,1}^{(c)}(E, a) = \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(T_2)\mathbb{Q}_{1,1}^{(b)}(T_2)}{6} + \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(T_2)\mathbb{Q}_{1,2}^{(b)}(T_2)}{6} - \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(a)}(T_2)\mathbb{Q}_{1,3}^{(b)}(T_2)}{3}$

z13 $\mathbb{G}_{2,2}^{(c)}(E, a) = -\frac{\mathbb{Q}_{2,1}^{(a)}(T_2)\mathbb{Q}_{1,1}^{(b)}(T_2)}{2} + \frac{\mathbb{Q}_{2,2}^{(a)}(T_2)\mathbb{Q}_{1,2}^{(b)}(T_2)}{2}$

z14 $\mathbb{G}_{2,1}^{(c)}(E, b) = -\frac{\mathbb{M}_{1,1}^{(a)}(T_1)\mathbb{T}_{1,1}^{(b)}(T_2)}{2} + \frac{\mathbb{M}_{1,2}^{(a)}(T_1)\mathbb{T}_{1,2}^{(b)}(T_2)}{2}$

z15 $\mathbb{G}_{2,2}^{(c)}(E, b) = -\frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(T_1)\mathbb{T}_{1,1}^{(b)}(T_2)}{6} - \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(T_1)\mathbb{T}_{1,2}^{(b)}(T_2)}{6} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(a)}(T_1)\mathbb{T}_{1,3}^{(b)}(T_2)}{3}$

z16 $\mathbb{Q}_{3,1}^{(c)}(T_1) = -\frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(E)\mathbb{Q}_{1,1}^{(b)}(T_2)}{6} - \frac{\mathbb{Q}_{2,2}^{(a)}(E)\mathbb{Q}_{1,1}^{(b)}(T_2)}{6} - \frac{\mathbb{Q}_{2,2}^{(a)}(T_2)\mathbb{Q}_{1,3}^{(b)}(T_2)}{3} + \frac{\mathbb{Q}_{2,3}^{(a)}(T_2)\mathbb{Q}_{1,2}^{(b)}(T_2)}{3}$

z17 $\mathbb{Q}_{3,2}^{(c)}(T_1) = \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(E)\mathbb{Q}_{1,2}^{(b)}(T_2)}{6} + \frac{\mathbb{Q}_{2,1}^{(a)}(T_2)\mathbb{Q}_{1,3}^{(b)}(T_2)}{3} - \frac{\mathbb{Q}_{2,2}^{(a)}(E)\mathbb{Q}_{1,2}^{(b)}(T_2)}{6} - \frac{\mathbb{Q}_{2,3}^{(a)}(T_2)\mathbb{Q}_{1,1}^{(b)}(T_2)}{3}$

z18 $\mathbb{Q}_{3,3}^{(c)}(T_1) = -\frac{\mathbb{Q}_{2,1}^{(a)}(T_2)\mathbb{Q}_{1,2}^{(b)}(T_2)}{3} + \frac{\mathbb{Q}_{2,2}^{(a)}(E)\mathbb{Q}_{1,3}^{(b)}(T_2)}{3} + \frac{\mathbb{Q}_{2,2}^{(a)}(T_2)\mathbb{Q}_{1,1}^{(b)}(T_2)}{3}$

z19 $\mathbb{G}_{1,1}^{(c)}(T_1) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(T_1)\mathbb{T}_{0}^{(b)}(A_1)}{3}$

z20 $\mathbb{G}_{1,2}^{(c)}(T_1) = \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(T_1)\mathbb{T}_{0}^{(b)}(A_1)}{3}$

z21 $$\mathbb{G}^{(c)}_{1,3}(T_1) = \frac{\sqrt{3}\mathbb{M}^{(a)}_{1,3}(T_1)\mathbb{T}^{(b)}_{0}(A_1)}{3}$$

z22 $$\mathbb{G}^{(c)}_{2,1}(T_1,a) = \frac{\sqrt{6}\mathbb{Q}^{(a)}_{2,1}(E)\mathbb{Q}^{(b)}_{1,1}(T_2)}{6} + \frac{\sqrt{2}\mathbb{Q}^{(a)}_{2,2}(E)\mathbb{Q}^{(b)}_{1,1}(T_2)}{6} - \frac{\sqrt{2}\mathbb{Q}^{(a)}_{2,2}(T_2)\mathbb{Q}^{(b)}_{1,3}(T_2)}{6} + \frac{\sqrt{2}\mathbb{Q}^{(a)}_{2,3}(T_2)\mathbb{Q}^{(b)}_{1,2}(T_2)}{6}$$

z23 $$\mathbb{G}^{(c)}_{2,2}(T_1,a) = -\frac{\sqrt{6}\mathbb{Q}^{(a)}_{2,1}(E)\mathbb{Q}^{(b)}_{1,2}(T_2)}{6} + \frac{\sqrt{2}\mathbb{Q}^{(a)}_{2,1}(T_2)\mathbb{Q}^{(b)}_{1,3}(T_2)}{6} + \frac{\sqrt{2}\mathbb{Q}^{(a)}_{2,2}(E)\mathbb{Q}^{(b)}_{1,2}(T_2)}{6} - \frac{\sqrt{2}\mathbb{Q}^{(a)}_{2,3}(T_2)\mathbb{Q}^{(b)}_{1,1}(T_2)}{6}$$

z24 $$\mathbb{G}^{(c)}_{2,3}(T_1,a) = -\frac{\sqrt{2}\mathbb{Q}^{(a)}_{2,1}(T_2)\mathbb{Q}^{(b)}_{1,2}(T_2)}{6} - \frac{\sqrt{2}\mathbb{Q}^{(a)}_{2,2}(E)\mathbb{Q}^{(b)}_{1,3}(T_2)}{3} + \frac{\sqrt{2}\mathbb{Q}^{(a)}_{2,2}(T_2)\mathbb{Q}^{(b)}_{1,1}(T_2)}{6}$$

z25 $$\mathbb{G}^{(c)}_{2,1}(T_1,b) = \frac{\sqrt{6}\mathbb{M}^{(a)}_{1,2}(T_1)\mathbb{T}^{(b)}_{1,3}(T_2)}{6} + \frac{\sqrt{6}\mathbb{M}^{(a)}_{1,3}(T_1)\mathbb{T}^{(b)}_{1,2}(T_2)}{6}$$

z26 $$\mathbb{G}^{(c)}_{2,2}(T_1,b) = \frac{\sqrt{6}\mathbb{M}^{(a)}_{1,1}(T_1)\mathbb{T}^{(b)}_{1,3}(T_2)}{6} + \frac{\sqrt{6}\mathbb{M}^{(a)}_{1,3}(T_1)\mathbb{T}^{(b)}_{1,1}(T_2)}{6}$$

z27 $$\mathbb{G}^{(c)}_{2,3}(T_1,b) = \frac{\sqrt{6}\mathbb{M}^{(a)}_{1,1}(T_1)\mathbb{T}^{(b)}_{1,2}(T_2)}{6} + \frac{\sqrt{6}\mathbb{M}^{(a)}_{1,2}(T_1)\mathbb{T}^{(b)}_{1,1}(T_2)}{6}$$

z34 $$\mathbb{Q}^{(c)}_{1,1}(T_2,a) = \frac{\sqrt{3}\mathbb{Q}^{(a)}_{0}(A_1)\mathbb{Q}^{(b)}_{1,1}(T_2)}{3}$$

z35 $$\mathbb{Q}^{(c)}_{1,2}(T_2,a) = \frac{\sqrt{3}\mathbb{Q}^{(a)}_{0}(A_1)\mathbb{Q}^{(b)}_{1,2}(T_2)}{3}$$

z36 $$\mathbb{Q}^{(c)}_{1,3}(T_2,a) = \frac{\sqrt{3}\mathbb{Q}^{(a)}_{0}(A_1)\mathbb{Q}^{(b)}_{1,3}(T_2)}{3}$$

z37 $$\mathbb{Q}^{(c)}_{1,1}(T_2,b) = -\frac{\sqrt{30}\mathbb{Q}^{(a)}_{2,1}(E)\mathbb{Q}^{(b)}_{1,1}(T_2)}{30} + \frac{\sqrt{10}\mathbb{Q}^{(a)}_{2,2}(E)\mathbb{Q}^{(b)}_{1,1}(T_2)}{10} + \frac{\sqrt{10}\mathbb{Q}^{(a)}_{2,2}(T_2)\mathbb{Q}^{(b)}_{1,3}(T_2)}{10} + \frac{\sqrt{10}\mathbb{Q}^{(a)}_{2,3}(T_2)\mathbb{Q}^{(b)}_{1,2}(T_2)}{10}$$

z38 $$\mathbb{Q}^{(c)}_{1,2}(T_2,b) = -\frac{\sqrt{30}\mathbb{Q}^{(a)}_{2,1}(E)\mathbb{Q}^{(b)}_{1,2}(T_2)}{30} + \frac{\sqrt{10}\mathbb{Q}^{(a)}_{2,1}(T_2)\mathbb{Q}^{(b)}_{1,3}(T_2)}{10} - \frac{\sqrt{10}\mathbb{Q}^{(a)}_{2,2}(E)\mathbb{Q}^{(b)}_{1,2}(T_2)}{10} + \frac{\sqrt{10}\mathbb{Q}^{(a)}_{2,3}(T_2)\mathbb{Q}^{(b)}_{1,1}(T_2)}{10}$$

z39 $$\mathbb{Q}^{(c)}_{1,3}(T_2,b) = \frac{\sqrt{30}\mathbb{Q}^{(a)}_{2,1}(E)\mathbb{Q}^{(b)}_{1,3}(T_2)}{15} + \frac{\sqrt{10}\mathbb{Q}^{(a)}_{2,1}(T_2)\mathbb{Q}^{(b)}_{1,2}(T_2)}{10} + \frac{\sqrt{10}\mathbb{Q}^{(a)}_{2,2}(T_2)\mathbb{Q}^{(b)}_{1,1}(T_2)}{10}$$

z40 $$\mathbb{Q}^{(c)}_{1,1}(T_2,c) = \frac{\sqrt{6}\mathbb{M}^{(a)}_{1,2}(T_1)\mathbb{T}^{(b)}_{1,3}(T_2)}{6} - \frac{\sqrt{6}\mathbb{M}^{(a)}_{1,3}(T_1)\mathbb{T}^{(b)}_{1,2}(T_2)}{6}$$

z41 $$\mathbb{Q}^{(c)}_{1,2}(T_2,c) = -\frac{\sqrt{6}\mathbb{M}^{(a)}_{1,1}(T_1)\mathbb{T}^{(b)}_{1,3}(T_2)}{6} + \frac{\sqrt{6}\mathbb{M}^{(a)}_{1,3}(T_1)\mathbb{T}^{(b)}_{1,1}(T_2)}{6}$$

z42 $$\mathbb{Q}^{(c)}_{1,3}(T_2,c) = \frac{\sqrt{6}\mathbb{M}^{(a)}_{1,1}(T_1)\mathbb{T}^{(b)}_{1,2}(T_2)}{6} - \frac{\sqrt{6}\mathbb{M}^{(a)}_{1,2}(T_1)\mathbb{T}^{(b)}_{1,1}(T_2)}{6}$$

z43 $$\mathbb{Q}^{(c)}_{2,1}(T_2) = \frac{\sqrt{3}\mathbb{Q}^{(a)}_{2,1}(T_2)\mathbb{Q}^{(b)}_{0}(A_1)}{3}$$

z44 $$\mathbb{Q}^{(c)}_{2,2}(T_2) = \frac{\sqrt{3}\mathbb{Q}^{(a)}_{2,2}(T_2)\mathbb{Q}^{(b)}_{0}(A_1)}{3}$$

z45 $$\mathbb{Q}^{(c)}_{2,3}(T_2) = \frac{\sqrt{3}\mathbb{Q}^{(a)}_{2,3}(T_2)\mathbb{Q}^{(b)}_{0}(A_1)}{3}$$

z46 $$\mathbb{Q}^{(c)}_{3,1}(T_2) = -\frac{\sqrt{5}\mathbb{Q}^{(a)}_{2,1}(E)\mathbb{Q}^{(b)}_{1,1}(T_2)}{10} + \frac{\sqrt{15}\mathbb{Q}^{(a)}_{2,2}(E)\mathbb{Q}^{(b)}_{1,1}(T_2)}{10} - \frac{\sqrt{15}\mathbb{Q}^{(a)}_{2,2}(T_2)\mathbb{Q}^{(b)}_{1,3}(T_2)}{15} - \frac{\sqrt{15}\mathbb{Q}^{(a)}_{2,3}(T_2)\mathbb{Q}^{(b)}_{1,2}(T_2)}{15}$$

z47 $$\mathbb{Q}^{(c)}_{3,2}(T_2) = -\frac{\sqrt{5}\mathbb{Q}^{(a)}_{2,1}(E)\mathbb{Q}^{(b)}_{1,2}(T_2)}{10} - \frac{\sqrt{15}\mathbb{Q}^{(a)}_{2,1}(T_2)\mathbb{Q}^{(b)}_{1,3}(T_2)}{15} - \frac{\sqrt{15}\mathbb{Q}^{(a)}_{2,2}(E)\mathbb{Q}^{(b)}_{1,2}(T_2)}{10} - \frac{\sqrt{15}\mathbb{Q}^{(a)}_{2,3}(T_2)\mathbb{Q}^{(b)}_{1,1}(T_2)}{15}$$

z48 $$\mathbb{Q}^{(c)}_{3,3}(T_2) = \frac{\sqrt{5}\mathbb{Q}^{(a)}_{2,1}(E)\mathbb{Q}^{(b)}_{1,3}(T_2)}{5} - \frac{\sqrt{15}\mathbb{Q}^{(a)}_{2,1}(T_2)\mathbb{Q}^{(b)}_{1,2}(T_2)}{15} - \frac{\sqrt{15}\mathbb{Q}^{(a)}_{2,2}(T_2)\mathbb{Q}^{(b)}_{1,1}(T_2)}{15}$$

Atomic SAMB

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

x1 $$\mathbb{Q}^{(a)}_{0}(A_1) = \begin{bmatrix} \frac{\sqrt{3}}{3} & 0 & 0 \\ 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & \frac{\sqrt{3}}{3} \end{bmatrix}$$

x2 $$\mathbb{Q}^{(a)}_{2,1}(E) = \begin{bmatrix} -\frac{\sqrt{6}}{6} & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{6} & 0 \\ 0 & 0 & \frac{\sqrt{6}}{3} \end{bmatrix}$$

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

x4 $\mathbb{Q}^{(a)}_{2,1}(T_2) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2}}{2} \\ 0 & \frac{\sqrt{2}}{2} & 0 \end{bmatrix}$

x5 $\mathbb{Q}^{(a)}_{2,2}(T_2) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{2}}{2} \\ 0 & 0 & 0 \\ \frac{\sqrt{2}}{2} & 0 & 0 \end{bmatrix}$

x6 $\mathbb{Q}^{(a)}_{2,3}(T_2) = \begin{bmatrix} 0 & \frac{\sqrt{2}}{2} & 0 \\ \frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$

x7 $\mathbb{M}^{(a)}_{1,1}(T_1) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{2}i}{2} \\ 0 & \frac{\sqrt{2}i}{2} & 0 \end{bmatrix}$

x8 $\mathbb{M}^{(a)}_{1,2}(T_1) = \begin{bmatrix} 0 & 0 & \frac{\sqrt{2}i}{2} \\ 0 & 0 & 0 \\ -\frac{\sqrt{2}i}{2} & 0 & 0 \end{bmatrix}$

x9 $\mathbb{M}^{(a)}_{1,3}(T_1) = \begin{bmatrix} 0 & -\frac{\sqrt{2}i}{2} & 0 \\ \frac{\sqrt{2}i}{2} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$

Cluster SAMB

- Site cluster

** Wyckoff: `4c`

y1 $\mathbb{Q}_0^{(s)}(A_1) = [1]$

** Wyckoff: `4a`

y2 $\mathbb{Q}_0^{(s)}(A_1) = [1]$

- Bond cluster

** Wyckoff: `16a@16e`

y3 $\mathbb{Q}_0^{(s)}(A_1) = \left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$

y4 $\mathbb{T}_0^{(s)}(A_1) = \left[\frac{i}{2}, \frac{i}{2}, \frac{i}{2}, \frac{i}{2}\right]$

y5 $\mathbb{Q}_{1,1}^{(s)}(T_2) = \left[\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}\right]$

y6 $\mathbb{Q}_{1,2}^{(s)}(T_2) = \left[\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}\right]$

y7 $\mathbb{Q}_{1,3}^{(s)}(T_2) = \left[\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}\right]$

y8 $\mathbb{T}_{1,1}^{(s)}(T_2) = \left[\frac{i}{2}, -\frac{i}{2}, -\frac{i}{2}, \frac{i}{2}\right]$

y9 $\mathbb{T}_{1,2}^{(s)}(T_2) = \left[\frac{i}{2}, -\frac{i}{2}, \frac{i}{2}, -\frac{i}{2}\right]$

y10 $\mathbb{T}_{1,3}^{(s)}(T_2) = \left[\frac{i}{2}, \frac{i}{2}, -\frac{i}{2}, -\frac{i}{2}\right]$

Site and Bond

Table 5: Orbital of each site

#	site	orbital
1	`As`	$\|p_x\rangle$, $\|p_y\rangle$, $\|p_z\rangle$
2	`Ga`	$\|p_x\rangle$, $\|p_y\rangle$, $\|p_z\rangle$

Table 6: Neighbor and bra-ket of each bond

#	head	tail	neighbor	head (bra)	tail (ket)
1	`As`	`Ga`	`[1]`	`[p]`	`[p]`

Site in Unit Cell

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

Table 7: '`As`' (#1) site cluster (`4c`), `-43m`

SL	position ($\boldsymbol{s}$)	mapping
1	`[ 0.25000, 0.25000, 0.25000]`	`[1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24]`

Table 8: 'Ga' (#2) site cluster (4a), -43m

SL	position ($\boldsymbol{s}$)	mapping
1	[0.00000, 0.00000, 0.00000]	[1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24]

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 'As'-'Ga' [1] (#1) bond cluster (16a@16e), D, $|\boldsymbol{v}|$= 0.43301 (cartesian)

SL	vector ($\boldsymbol{v}$)	center ($\boldsymbol{c}$)	mapping	head	tail	$\boldsymbol{R}$ (primitive)
1	[0.25000, 0.25000, 0.25000]	[0.12500, 0.12500, 0.12500]	[1,5,9,13,17,21]	(1,1)	(1,1)	[0,0,0]
2	[-0.25000,-0.25000, 0.25000]	[0.87500, 0.87500, 0.12500]	[2,7,12,14,19,24]	(1,4)	(1,1)	[0,0,1]
3	[-0.25000, 0.25000,-0.25000]	[0.87500, 0.12500, 0.87500]	[3,8,10,16,18,23]	(1,3)	(1,1)	[0,1,0]
4	[0.25000,-0.25000,-0.25000]	[0.12500, 0.87500, 0.87500]	[4,6,11,15,20,22]	(1,2)	(1,1)	[1,0,0]