

# Model for “GaAs”

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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<sub>1</sub>, A<sub>2</sub>, E, T<sub>1</sub>, T<sub>2</sub>]
  - 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<sub>1</sub>, A<sub>2</sub>, E, T<sub>1</sub>, T<sub>2</sub>]
  - Spin (s): [0, 1]
- Site-cluster selection:
  - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
  - Irrep.: [A<sub>1</sub>, A<sub>2</sub>, E, T<sub>1</sub>, T<sub>2</sub>]
- Bond-cluster selection:
  - Type: [Q, G, M, T]
  - Rank: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
  - Irrep.: [A<sub>1</sub>, A<sub>2</sub>, E, T<sub>1</sub>, T<sub>2</sub>]
- 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. 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):  
 $a_1 = [1.00000, 0.00000, 0.00000]$   
 $a_2 = [0.00000, 1.00000, 0.00000]$   
 $a_3 = [0.00000, 0.00000, 1.00000]$

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

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### Symmetry Operation

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Table 1: Symmetry operation

#	SO	#	SO	#	SO	#	SO	#	SO
1	{1 0}	2	{2 <sub>001</sub>  0}	3	{2 <sub>010</sub>  0}	4	{2 <sub>100</sub>  0}	5	{3 <sub>111</sub> <sup>+</sup>  0}
6	{3 <sub>-11-1</sub> <sup>+</sup>  0}	7	{3 <sub>1-1-1</sub> <sup>+</sup>  0}	8	{3 <sub>-1-11</sub> <sup>+</sup>  0}	9	{3 <sub>111</sub> <sup>-</sup>  0}	10	{3 <sub>1-1-1</sub> <sup>-</sup>  0}
11	{3 <sub>-1-11</sub> <sup>-</sup>  0}	12	{3 <sub>-11-1</sub> <sup>-</sup>  0}	13	{m <sub>1-10</sub>  0}	14	{m <sub>110</sub>  0}	15	{-4 <sub>001</sub> <sup>+</sup>  0}
16	{-4 <sub>001</sub> <sup>-</sup>  0}	17	{m <sub>01-1</sub>  0}	18	{-4 <sub>100</sub> <sup>+</sup>  0}	19	{-4 <sub>100</sub> <sup>-</sup>  0}	20	{m <sub>011</sub>  0}
21	{m <sub>-101</sub>  0}	22	{-4 <sub>010</sub> <sup>-</sup>  0}	23	{m <sub>101</sub>  0}	24	{-4 <sub>010</sub> <sup>+</sup>  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	$Q, T$	-	-	$\sqrt{15}xyz$
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	$\frac{x(2x^2-3y^2-3z^2)}{2}$
24	$\mathbb{Q}_{3,2}(T_2)$					2	$-\frac{y(3x^2-2y^2+3z^2)}{2}$
25	$\mathbb{Q}_{3,3}(T_2)$					3	$-\frac{z(3x^2+3y^2-2z^2)}{2}$

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— Basis in full matrix —

Table 3: dimension = 6

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

Table 4: Atomic basis (orbital part only)

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

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— 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

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

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

$$\boxed{z7} \quad \mathbb{Q}_{2,2}^{(c)}(E) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E)\mathbb{Q}_0^{(s)}(A_1)}{2}$$

$$\boxed{z28} \quad \mathbb{Q}_{2,1}^{(c)}(T_2) = \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(T_2)\mathbb{Q}_0^{(s)}(A_1)}{3}$$

$$\boxed{z29} \quad \mathbb{Q}_{2,2}^{(c)}(T_2) = \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(T_2)\mathbb{Q}_0^{(s)}(A_1)}{3}$$

$$\boxed{z30} \quad \mathbb{Q}_{2,3}^{(c)}(T_2) = \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(a)}(T_2)\mathbb{Q}_0^{(s)}(A_1)}{3}$$

- **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**

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

$$\boxed{z8} \quad \mathbb{Q}_{2,1}^{(c)}(E) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E)\mathbb{Q}_0^{(s)}(A_1)}{2}$$

$$\boxed{z9} \quad \mathbb{Q}_{2,2}^{(c)}(E) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E)\mathbb{Q}_0^{(s)}(A_1)}{2}$$

$$\boxed{z31} \quad \mathbb{Q}_{2,1}^{(c)}(T_2) = \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(T_2)\mathbb{Q}_0^{(s)}(A_1)}{3}$$

$$\boxed{z32} \quad \mathbb{Q}_{2,2}^{(c)}(T_2) = \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(T_2)\mathbb{Q}_0^{(s)}(A_1)}{3}$$

$$\boxed{z33} \quad \mathbb{Q}_{2,3}^{(c)}(T_2) = \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(a)}(T_2)\mathbb{Q}_0^{(s)}(A_1)}{3}$$

- **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**

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

$$\boxed{\text{z4}} \quad \mathbb{Q}_3^{(c)}(A_1) = \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(T_2)\mathbb{Q}_{1,1}^{(b)}(T_2)}{3} + \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(T_2)\mathbb{Q}_{1,2}^{(b)}(T_2)}{3} + \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(a)}(T_2)\mathbb{Q}_{1,3}^{(b)}(T_2)}{3}$$

$$\boxed{\text{z5}} \quad \mathbb{G}_0^{(c)}(A_2) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(T_1)\mathbb{T}_{1,1}^{(b)}(T_2)}{3} + \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(T_1)\mathbb{T}_{1,2}^{(b)}(T_2)}{3} + \frac{\sqrt{3}\mathbb{M}_{1,3}^{(a)}(T_1)\mathbb{T}_{1,3}^{(b)}(T_2)}{3}$$

$$\boxed{\text{z10}} \quad \mathbb{Q}_{2,1}^{(c)}(E) = \frac{\sqrt{2}\mathbb{Q}_{2,1}^{(a)}(E)\mathbb{Q}_0^{(b)}(A_1)}{2}$$

$$\boxed{\text{z11}} \quad \mathbb{Q}_{2,2}^{(c)}(E) = \frac{\sqrt{2}\mathbb{Q}_{2,2}^{(a)}(E)\mathbb{Q}_0^{(b)}(A_1)}{2}$$

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

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

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

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

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

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

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

$$\boxed{\text{z19}} \quad \mathbb{G}_{1,1}^{(c)}(T_1) = \frac{\sqrt{3}\mathbb{M}_{1,1}^{(a)}(T_1)\mathbb{T}_0^{(b)}(A_1)}{3}$$

$$\boxed{\text{z20}} \quad \mathbb{G}_{1,2}^{(c)}(T_1) = \frac{\sqrt{3}\mathbb{M}_{1,2}^{(a)}(T_1)\mathbb{T}_0^{(b)}(A_1)}{3}$$

$$\boxed{z21} \quad \mathbb{G}_{1,3}^{(c)}(T_1) = \frac{\sqrt{3}\mathbb{M}_{1,3}^{(a)}(T_1)\mathbb{T}_0^{(b)}(A_1)}{3}$$

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

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

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

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

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

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

$$\boxed{z34} \quad \mathbb{Q}_{1,1}^{(c)}(T_2, a) = \frac{\sqrt{3}\mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_{1,1}^{(b)}(T_2)}{3}$$

$$\boxed{z35} \quad \mathbb{Q}_{1,2}^{(c)}(T_2, a) = \frac{\sqrt{3}\mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_{1,2}^{(b)}(T_2)}{3}$$

$$\boxed{z36} \quad \mathbb{Q}_{1,3}^{(c)}(T_2, a) = \frac{\sqrt{3}\mathbb{Q}_0^{(a)}(A_1)\mathbb{Q}_{1,3}^{(b)}(T_2)}{3}$$

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

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

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

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

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

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

$$\boxed{\text{z43}} \quad \mathbb{Q}_{2,1}^{(c)}(T_2) = \frac{\sqrt{3}\mathbb{Q}_{2,1}^{(a)}(T_2)\mathbb{Q}_0^{(b)}(A_1)}{3}$$

$$\boxed{\text{z44}} \quad \mathbb{Q}_{2,2}^{(c)}(T_2) = \frac{\sqrt{3}\mathbb{Q}_{2,2}^{(a)}(T_2)\mathbb{Q}_0^{(b)}(A_1)}{3}$$

$$\boxed{\text{z45}} \quad \mathbb{Q}_{2,3}^{(c)}(T_2) = \frac{\sqrt{3}\mathbb{Q}_{2,3}^{(a)}(T_2)\mathbb{Q}_0^{(b)}(A_1)}{3}$$

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

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

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

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### Atomic SAMB

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

$$\boxed{\text{x1}} \quad \mathbb{Q}_0^{(a)}(A_1) = \begin{bmatrix} \frac{\sqrt{3}}{3} & 0 & 0 \\ 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & \frac{\sqrt{3}}{3} \end{bmatrix}$$

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

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

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

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

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

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

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

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

— Cluster SAMB —————

- Site cluster

\*\* Wyckoff: 4c

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

\*\* Wyckoff: 4a

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

- Bond cluster

\*\* Wyckoff: 16a@16e

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

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

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

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

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

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

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

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

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]

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— Site in Unit Cell —————

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

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

SL	position ( <i>s</i> )	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 ( $s$ )	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]

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

SL	vector ( $v$ )	center ( $c$ )	mapping	head	tail	$R$ (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]