

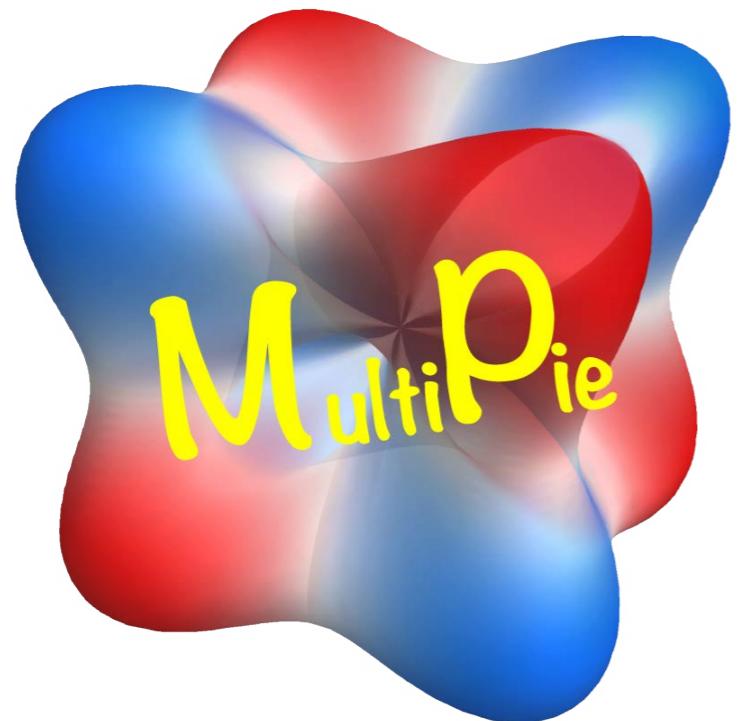
MultiPie and QtDraw Manual

MultiPie : ver. 1.1.13

QtDraw : ver. 1.1.15

Install Guide (in Japanese) https://cmt-mu.github.io/QtDraw/install_guide.pdf

MultiPie

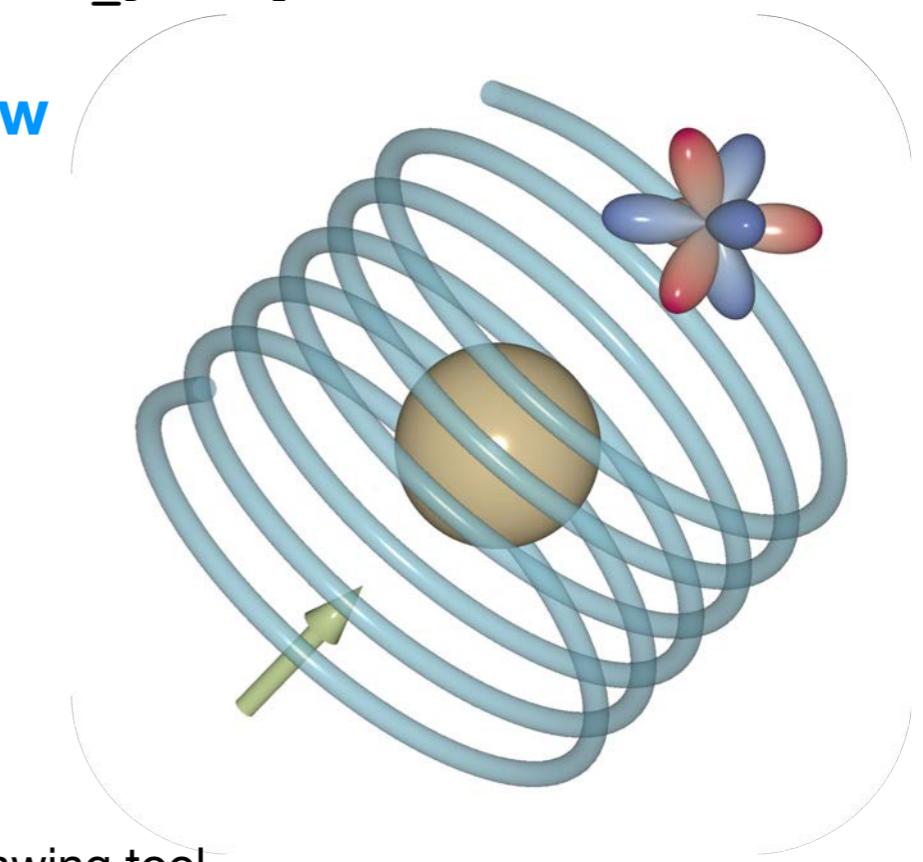


- Symmetry operations for point/space groups
- Symmetry-adapted basis construction

("MultiPy" was already registered in PyPI, umm...)

<https://cmt-mu.github.io/MultiPie/>

QtDraw



- 3D drawing tool
(including orbital, vector stream spline curve...)
- With MultiPie, draw symmetry-related objects, projection to each Irreps. (Symmetry-Adapted)

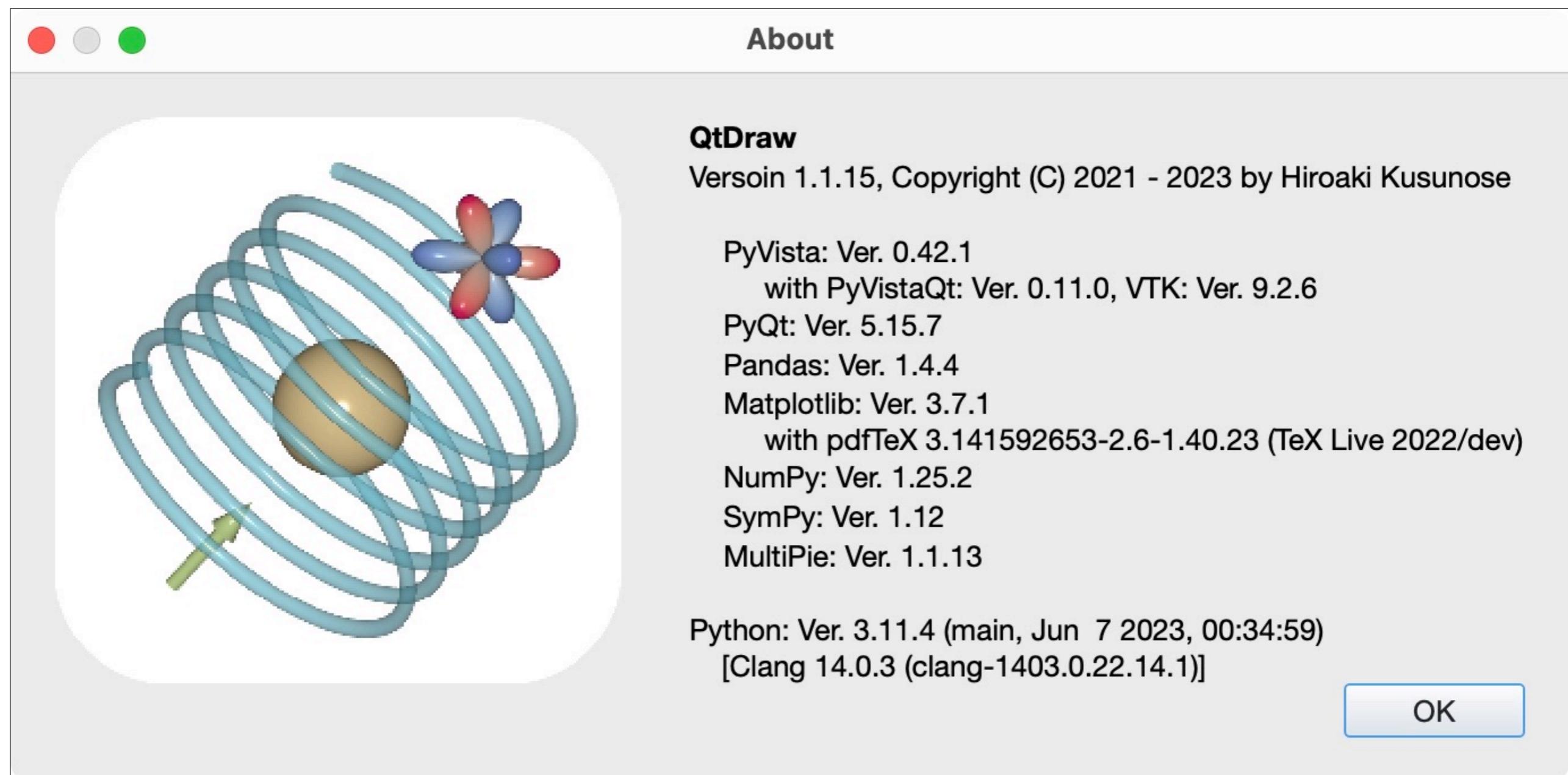
<https://cmt-mu.github.io/QtDraw/>

If you are using MultiPie and/or QtDraw in your scientific research, please help our scientific visibility by citing our work:

Hiroaki Kusunose, Rikuto Oiwa, and Satoru Hayami, Symmetry-adapted modeling for molecules and crystals, *Phys. Rev. B* **107**, 195118 (2023).

DOI: <https://doi.org/10.1103/PhysRevB.107.195118>

Checked Library Version for QtDraw



MacBook Air

15インチ、M2、2023

チップ Apple M2

メモリ 8 GB

シリアル番号

macOS Ventura 13.5

QtDraw can read

- **.qtdw** : QtDraw file
- **.cif** : CIF file
- **.vesta** : VESTA file

Concept of Symmetry-Adapted Basis

HK, R. Oiwa, and S. Hayami, PRB **107**, 195118 (2023)

Neumann Principle

Every physical phenomenon manifested by a crystal must possess an equivalent or higher symmetry as the crystal itself.



(Static) macroscopic response can be classified by POINT GROUP symmetry ($\mathbf{k} = 0 : \Gamma$ point in BZ)

Classification for Materials

For TP spherical systems



Molecule and Crystal

T : time-reversal (electric + or magnetic -)

Subgroup of spherical systems

P : spatial-inversion (polar or axial)

Linear combination of spherical base

g : anisotropy (l, m)

$$Z_{l\gamma}^{(\Gamma,n)} = \sum_m c_{\gamma m}^{(\Gamma,n)} Z_{lm}$$

Type (Z_{lm})	Symbol	T	P		Charge	g
Electric (E)	Q_{lm}	+	polar	$(-1)^l$	1	Y_{lm}
Magnetic (M)	M_{lm}	-	axial	$-(-1)^l$	$i(\mathbf{e}_1 \times \mathbf{e}_2) \cdot \mathbf{e}_3$	Y_{lm}
Magnetic-Toroidal (MT)	T_{lm}	-	polar	$(-1)^l$	i	Y_{lm}
Electric-Toroidal (ET)	G_{lm}	+	axial	$-(-1)^l$	$(\mathbf{e}_1 \times \mathbf{e}_2) \cdot \mathbf{e}_3$	Y_{lm}

Construction of Basis

Basis for Materials

Electronic degrees of freedom = (atomic d.o.f.) \otimes (site/bond d.o.f.)

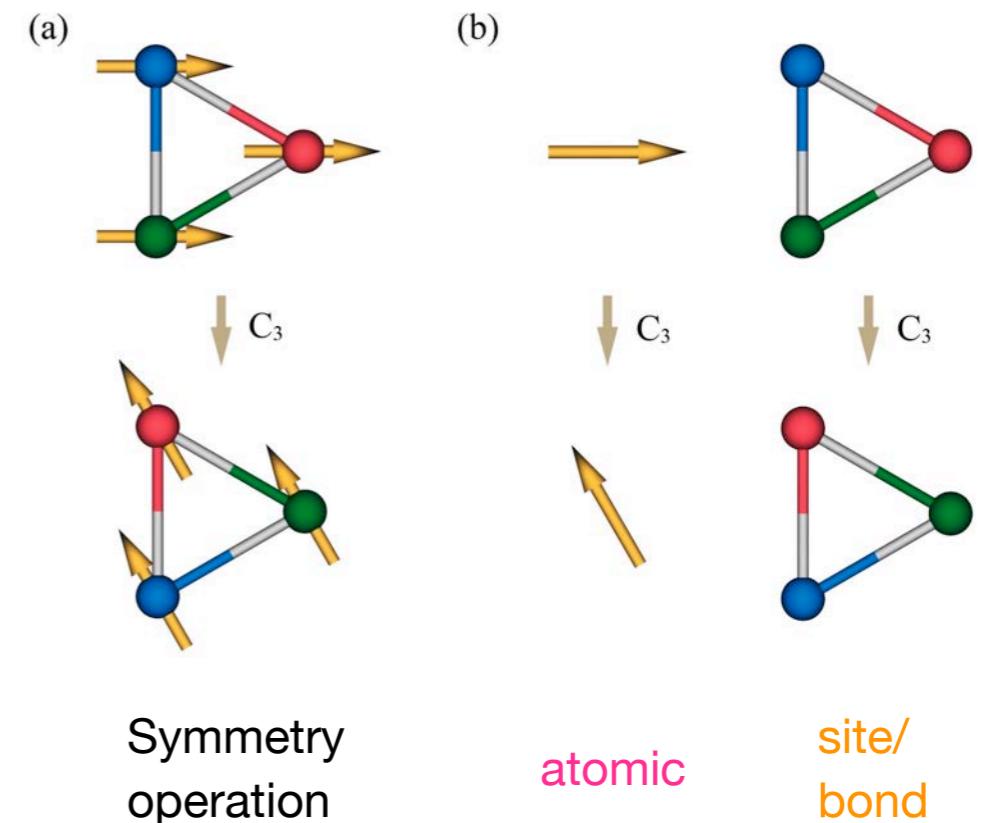
$$Z_\alpha = \sum_{\beta\gamma} C_{\alpha}^{\beta,\gamma} X_\beta \otimes Y_\gamma$$

"Clebsch-Gordan" coefficient

Atomic d.o.f

Given by quantum-mechanical expressions of complete set,
compute matrix elements by using general formula

HK, R. Oiwa, and S. Hayami, JPSJ **89**, 104704 (2020)



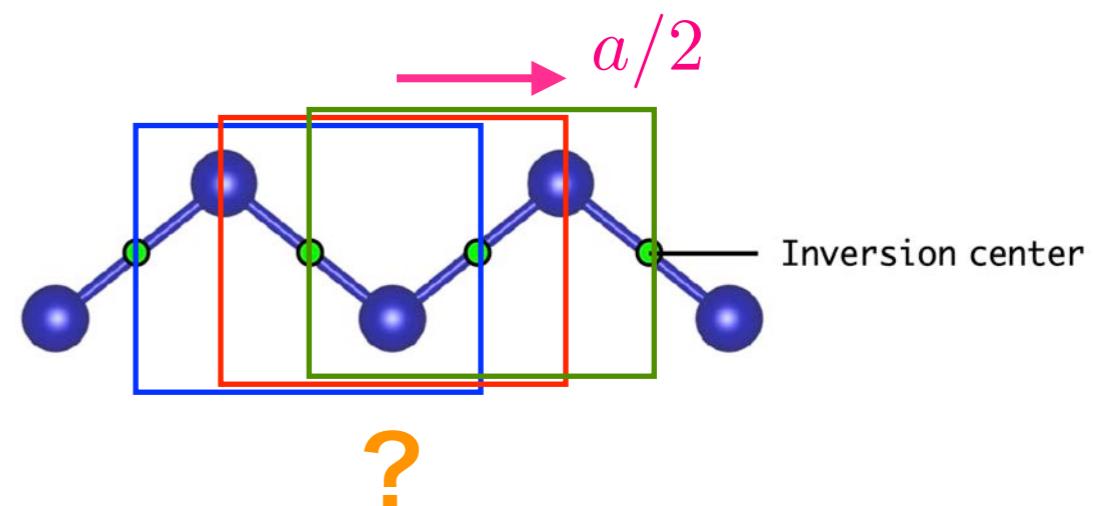
Site/Bond d.o.f

Ambiguity

- How to choose cluster and center (translation) ?
- Non isoradius (nonsymmorphic = screw or glide) ?



Use "Virtual Cluster"

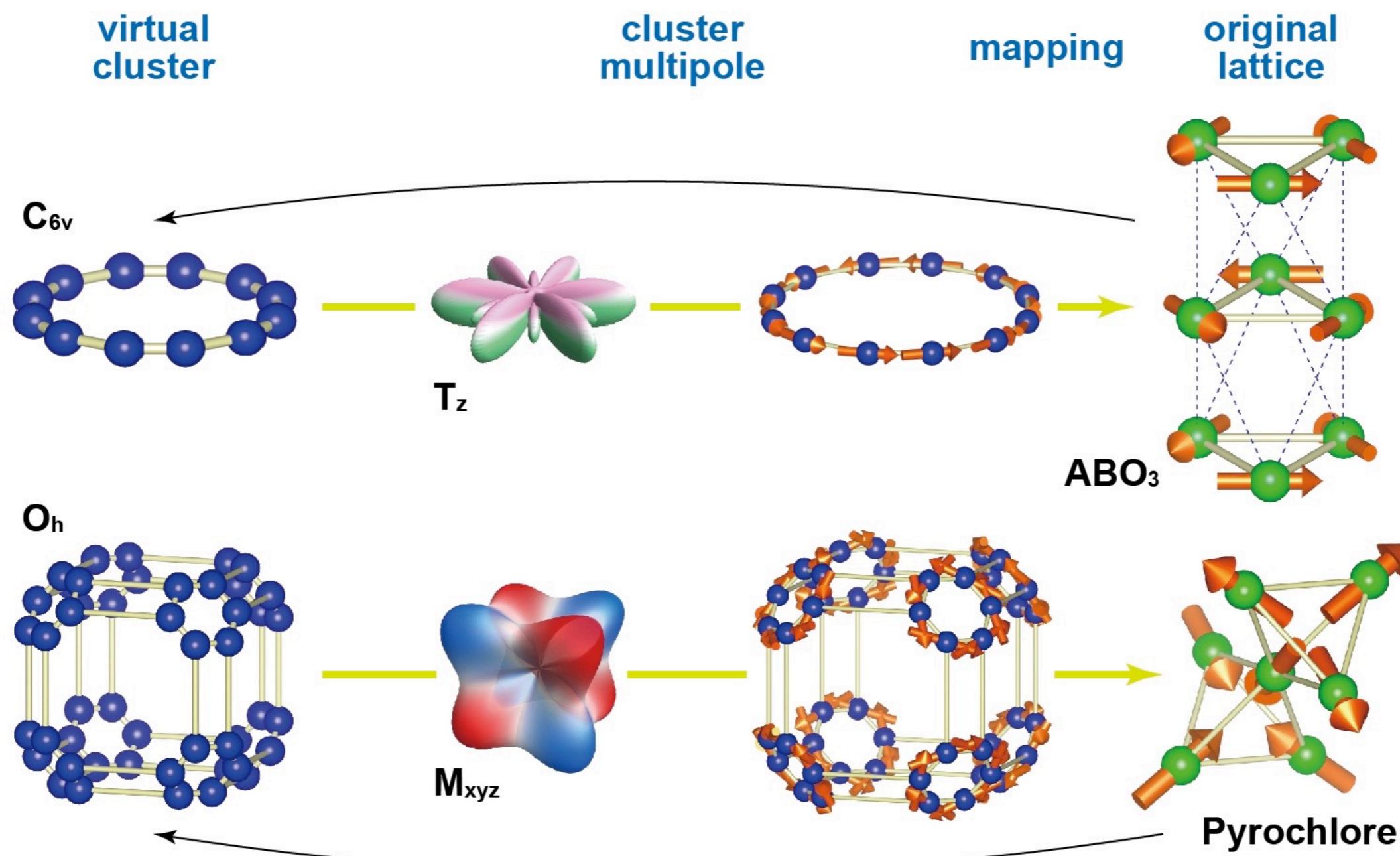


Concept of Virtual Cluster

Virtual Cluster

Site-Cluster
Site/Bond-Cluster

M.-T. Suzuki, et al., PRB **99**, 174407 (2019)
HK, R. Oiwa, and S. Hayami, PRB **107**, 195118 (2023)



MultiPie - Example

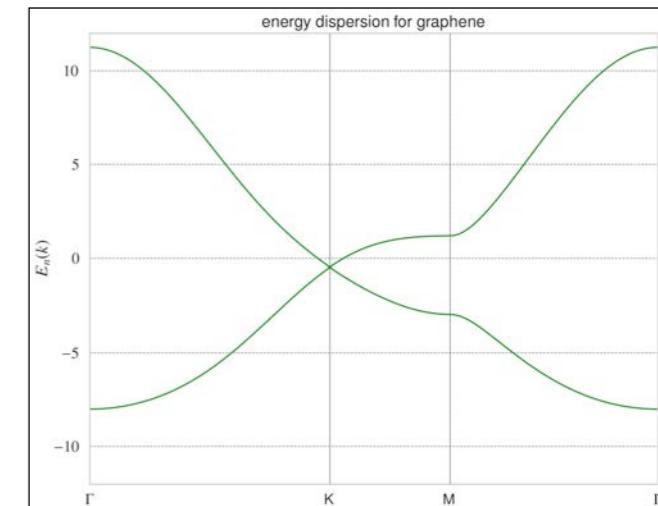
Example for graphene

Input file (`graphene.py` : Python dict format)

```
graphene = {
    "model": "graphene", # name of model.
    "group": 191, # No. of space group.
    "cell": {"c": 4}, # set large enough interlayer distance.
    #
    "site": {"C": ("[1/3,2/3,0]", "pz")}, # positions of C site and its orbital.
    "bond": [("C", "C", [1, 2, 3, 4, 5, 6])], # C-C bonds up to 6th neighbors.
    #
    "spinful": False, # spinless.
    #
    "k_point": {"Γ": "[0, 0, 0]", "M": "[1/2, 0, 0]", "K": "[1/3, 1/3, 0]"}, # def. of k points.
    "k_path": "Γ-K-M-Γ", # high-symmetry line.
}
```

Download

<https://github.com/CMT-MU/MultiPie/tree/main/docs/example>
and try "python `create_plot.py`"



Create Symmetry-Adapted Multipole Basis (SAMB)

```
create_samb graphene
```

→ In "graphene" folder

- `graphene_model.py` (Model info.)
- `graphene_matrix.py` (Full matrix form)
- `graphene_samb.py` (SAMB info.)

See, document for detailed dict structure

- `graphene_samb.tex`
- `graphene_samb.pdf` (SAMB info. for human)
- `graphene_view.qtdw` (structure QtDraw file)

MultiPie - Output of Full Matrix

Full matrix form file



$$H = \sum_j z_j \mathbb{Z}_j$$

Matrix elements
for each SAMB

```
graphene = {
    "model": "graphene",
    "molecule": False,
    "group": ("D6h^1", "space group No. 191 : D6h^1 / P6/mmm : PG D6h"),
    "dimension": 2,
    "ket": ["pz@C_1", "pz@C_2"],
    "version": "1.1.11",
    "k_point": {"Γ": "[0, 0, 0]", "M": "[1/2, 0, 0]", "K": "[1/3, 1/3, 0]"},
    "k_path": "Γ-K-M-Γ",
    "A": "[[1.0, -0.5, 0.0], [0.0, 0.86602540378444, 0.0], [0.0, 0.0, 4.0]]",
    "bond": {
        "bond_001": "[1/3, 2/3, 0]",
        "bond_002": "[1/3, -1/3, 0]",
        "bond_003": "[-2/3, -1/3, 0]",
        "bond_004": "[0, 1, 0]",
        "bond_005": "[0, 1, 0]",
        "bond_006": "[1, 1, 0]",
        "bond_007": "[1, 0, 0]",
        "bond_008": "[1, 1, 0]",
        ....
    }
}
```

Bond info.

$$\text{bond}_{\#\#\#} = \mathbf{b}_i$$

$$c_{\#\#\#} = \cos(\mathbf{k} \cdot \mathbf{b}_i)$$

$$s_{\#\#\#} = \sin(\mathbf{k} \cdot \mathbf{b}_i)$$

```
"matrix": {
    "z_001": "[[sqrt(2)/2, 0], [0, sqrt(2)/2]],
    "z_002": "[[0, sqrt(6)*c001/6 + sqrt(6)*c002/6 + sqrt(6)*c003/6 + sqrt(6)*I*s001/6 + sqrt(6)*I*s002/6 + sqrt(6)*I*s003/6], [sqrt(6)*c001/6 + sqrt(6)*c002/6 + sqrt(6)*c003/6 - sqrt(6)*I*s001/6 - sqrt(6)*I*s002/6 - sqrt(6)*I*s003/6, 0]],
    "z_003": "[[sqrt(3)*c004/3 + sqrt(3)*c006/3 + sqrt(3)*c007/3, 0], [0, sqrt(3)*c004/3 + sqrt(3)*c006/3 + sqrt(3)*c007/3]],
    "z_004": "[[0, sqrt(6)*c010/6 + sqrt(6)*c011/6 + sqrt(6)*c012/6 + sqrt(6)*I*s010/6 + sqrt(6)*I*s011/6 + sqrt(6)*I*s012/6], [sqrt(6)*c010/6 + sqrt(6)*c011/6 + sqrt(6)*c012/6 - sqrt(6)*I*s010/6 - sqrt(6)*I*s011/6 - sqrt(6)*I*s012/6, 0]],
    "z_005": "[[0, sqrt(3)*c013/6 + sqrt(3)*c014/6 + sqrt(3)*c015/6 + sqrt(3)*c016/6 + sqrt(3)*c017/6 + sqrt(3)*c018/6 + sqrt(3)*I*s013/6 + sqrt(3)*I*s014/6 + sqrt(3)*I*s015/6 + sqrt(3)*I*s016/6 + sqrt(3)*I*s017/6 + sqrt(3)*I*s018/6], [sqrt(3)*c013/6 + sqrt(3)*c014/6 + sqrt(3)*c015/6 + sqrt(3)*c016/6 + sqrt(3)*c017/6 + sqrt(3)*c018/6 - sqrt(3)*I*s013/6 - sqrt(3)*I*s014/6 - sqrt(3)*I*s015/6 - sqrt(3)*I*s016/6 - sqrt(3)*I*s017/6 - sqrt(3)*I*s018/6, 0]],
    "z_006": "[[sqrt(3)*c019/3 + sqrt(3)*c021/3 + sqrt(3)*c022/3, 0], [0, sqrt(3)*c019/3 + sqrt(3)*c021/3 + sqrt(3)*c022/3]],
    "z_007": "[[sqrt(3)*c025/3 + sqrt(3)*c027/3 + sqrt(3)*c028/3, 0], [0, sqrt(3)*c025/3 + sqrt(3)*c027/3 + sqrt(3)*c028/3]],
},
```

MultiPie - Output of Non-Identity Irrep.

Input file

```
graphene = {
    ...
    "generate": {
        "time_reversal_type" : "both",
        "irrep": ["A1g", "B1u", "A2g", "A2u"],
    },
    "spinful": True,
}
```

Consider "symmetry-breaking" terms

1. Mass term (spinless)

$$Q_{3,B_{1u}} \quad \text{"C" site-cluster}$$

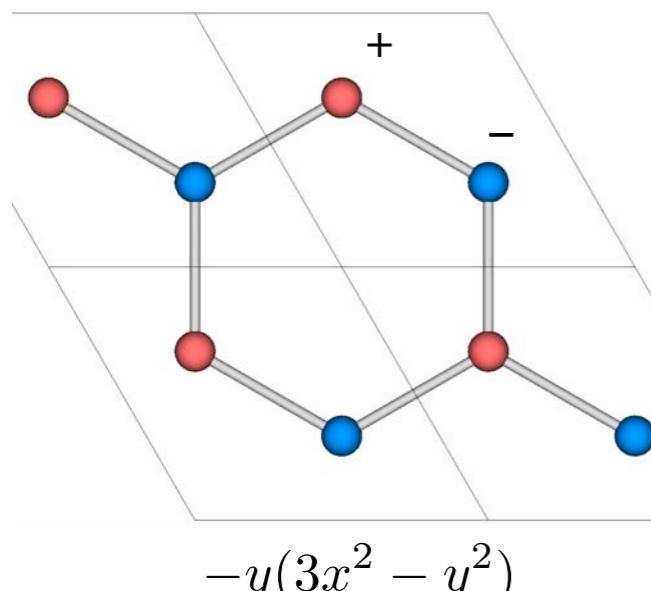
2. Haldane's magnetic flux term from kinetic SOC (spinless)

$$\mathbb{M}_{1,A_{2g}} \quad \text{"C-C" 2nd neighbor bond-cluster} \quad M_z \in A_{2g}$$

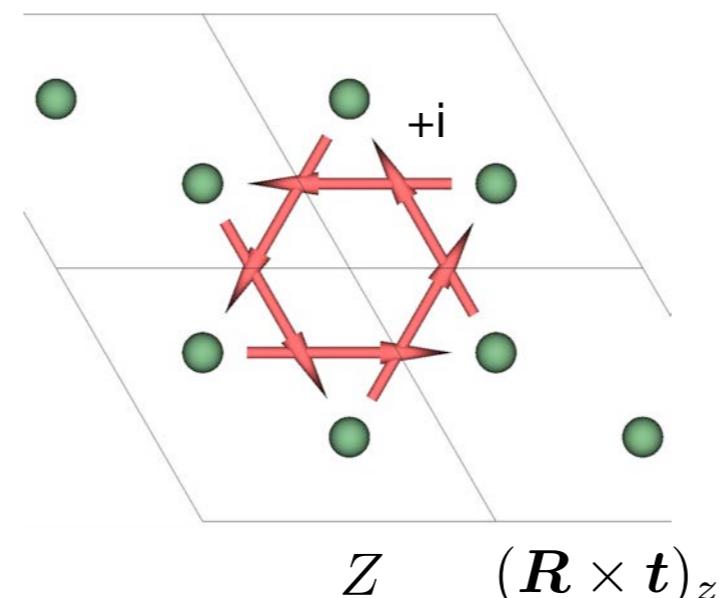
3. Surface Rashba term from z-polar field (spinful) $E_z \in A_{2u}$

$$Q_{1,A_{2u}} \quad \text{"C-C" 1st neighbor bond-cluster}$$

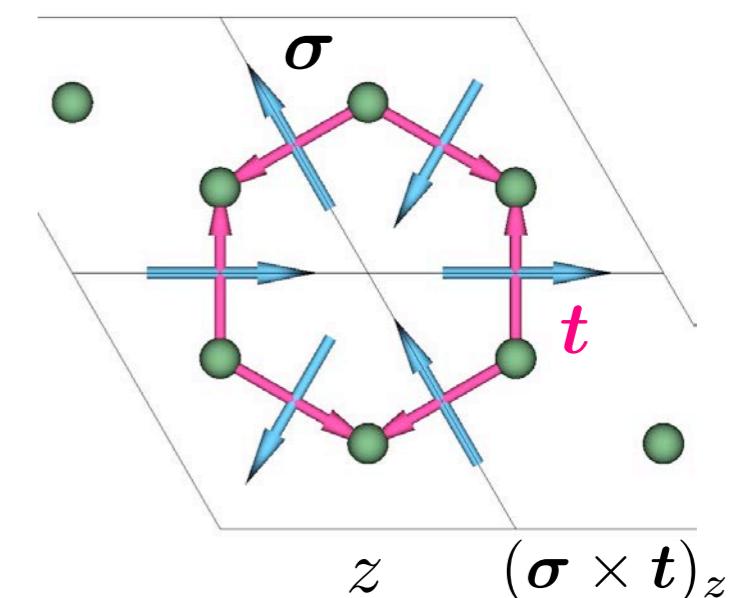
1. Mass term



2. Haldane's M-flux



3. Rashba



QtDraw - Features

based on Qt Python and PyVista

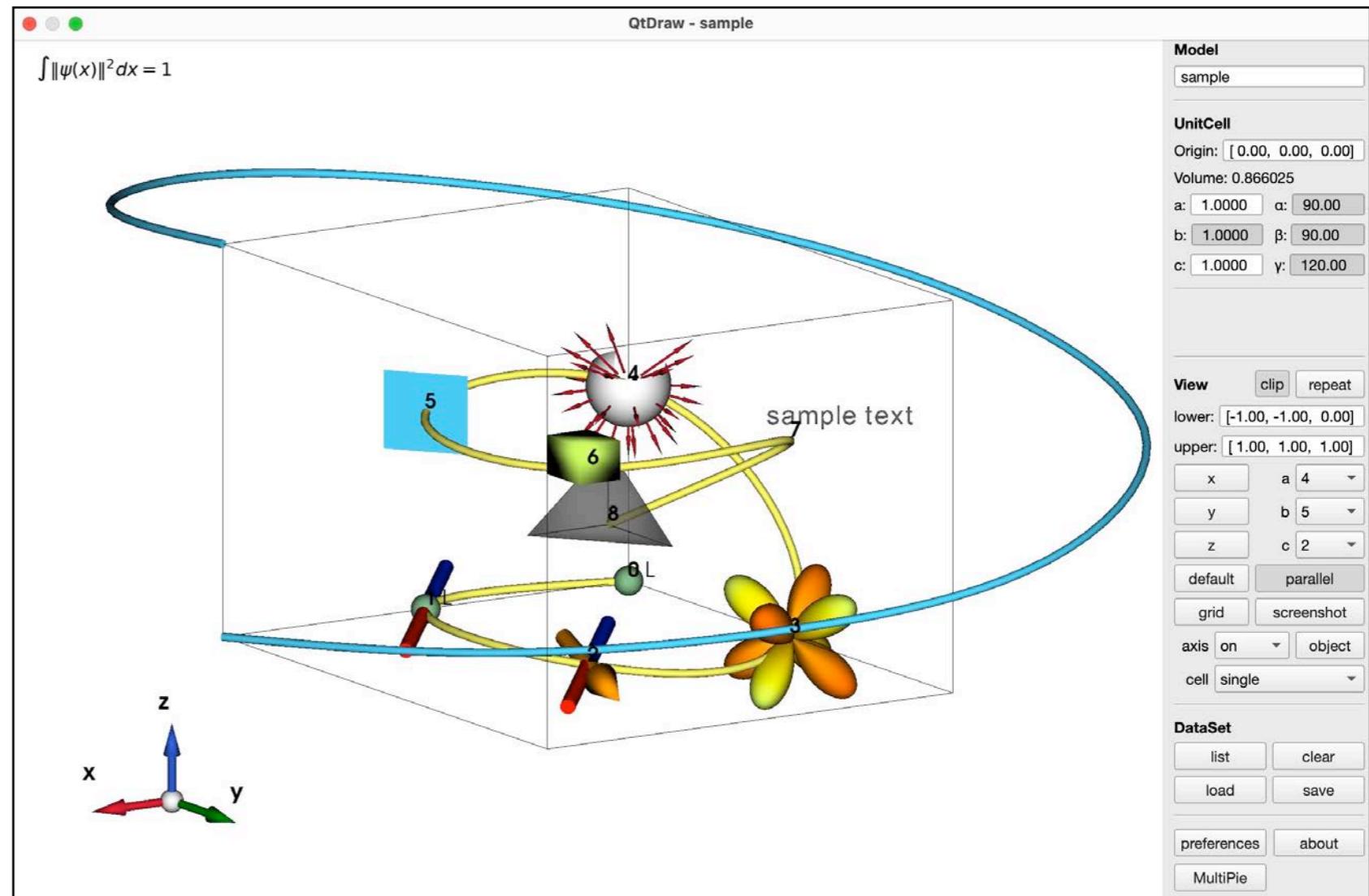
<https://www.qt.io/qt-for-python>

<https://docs.pyvista.org/version/stable/>

tested mainly on Mac (managed to work out on Windows, no check on Linux)

Drawable objects

- Sphere (site)
- Bond (monotone/two-tone color)
- Vector
- Stream vector
- Plane
- Box
- Polygon
- Text (3d, 2d)
- Spline curve (data or function)
- Caption



All objects can be drawn by calling **Python API** : easy to extend functionality of drawing

e.g. spin/orbital modulation patterns

QtDraw - Main Menu

*** NO UNDO functionality at this version ***

Menu

Model
sample

UnitCell
Origin: [0.00, 0.00, 0.00]
Volume: 0.866025
a: 1.0000 α: 90.00
b: 1.0000 β: 90.00
c: 1.0000 γ: 120.00

View clip repeat
lower: [-1.00, -1.00, 0.00]
upper: [1.00, 1.00, 1.00]
x a 4
y b 5
z c 2
default parallel
grid screenshot
axis on object
cell single

DataSet
list clear
load save
preferences about
MultiPie

model name

origin (reduced)

lattice const. & angle

clip/repeat on/off

clip/repeat range

viewpoint x/y/z/default

index (a,b,c)

parallel or perspective view

grid on/off, screenshot : **[png/bmp/tif/tiff/svg/eps/ps/pdf]**

axis, cell on/off

list/clear data

load/save data (.qtdw file)

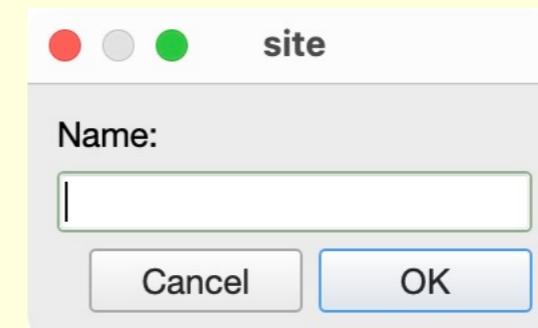
setting options

use MultiPie

- Create / add / remove objects

- Edit properties of objects

Add : create object in new group



specify group name

Edit properties of objects in group or individual object

Insert : insert object in selected group

Remove : remove selected object

Coordinate: reduced one with unit vectors

[**x, y, z**] in Cell + Cell position

Draw objects in a Cell, and then repeat

QtDraw - List Panel

List Panel

Edit all objects in group Edit individual object

DataSet - sample														
site	bond	vector	orbital	stream	plane	box	polygon	text3d	spline	spline_t	caption	text		
name	ON		label		cell		position		size		color		opacity	space
✓ S	ON		✓ L		[0, 0, 0]		[0.0000, 0.0000, 0.0000]		0.50		darkseagreen		1.00	3
✓ S	ON		✓ L		[0, 0, 0]		[0.0000, 0.0000, 0.0000]		0.50		darkseagreen		1.00	3
✓ S	ON		✓ L		[0, 0, 0]		[0.5000, 0.0000, 0.0000]		0.50		darkseagreen		1.00	3

Add Insert Remove

group name label on/off label name cell position position in Cell pre-space for label

object on/off

In equation-style property

orbital [shape/surface], stream [shape/vector], spline_t [expression]

sympy-style expression can be used (variables: **x**, **y**, **z**, **r**) + (**t** for spline_t)

e.g. "3sqrt(3)/2 cos(pi/3) (3z**2-r**2)", "0.3sin(2pi t)", etc.

QtDraw - Object Property

Site

size	color
0.50	<input type="color" value="darkseagreen"/> darkseagreen ▾

Bond

vector	width	color	color2
[-0.5000, -0.5000, 0.0000]	1.00	<input type="color" value="red"/> red ▾	<input type="color" value="blue"/> blue ▾

Vector

vector	length	width	offset	color
[0.0000, 0.5000, 0.0000]	0.40	1.00	-0.43	<input type="color" value="orange"/> orange ▾
cartesian				

Orbital

shape	surface	size	scale	theta0	theta1	phi0	phi1	color
xyz	xyz	0.20	<input checked="" type="checkbox"/>	0	180	0	360	 Wistia ▾
				θ range	φ range			

Stream

shape	vector	size	v_size	width	scale	theta	phi	theta0	theta1	phi0	phi1	color	component	
1 stream on shape	$\begin{pmatrix} x \\ y \\ z \end{pmatrix}$ vector at r	0.10	0.15	1.00	<input type="checkbox"/>	4	8	0	120	0	270	 coolwarm ▾	<input type="button" value="abs"/> ▾	
						# arrow in (θ, ϕ)	θ range	φ range					color based on	12

QtDraw - Object Property

Plane

normal	x	y	color
[1.00, 1.00, 0.00]	0.20	0.20	■ sky ▼
reduced		reduced	

Box

a1	a2	a3	edge	wireframe	width	color
[0.1000, 0.0000, 0.0000]	[0.0000, 0.1000, 0.0000]	[0.0000, 0.0000, 0.1000]	<input type="checkbox"/>	<input type="checkbox"/>	1.00	■ honeydew ▼
reduced	reduced	reduced				

Polygon

point	connection	edge	wireframe	width	color
[0.0000, 0.0000, 0.0000]	[0, 1, 2]				
[0.2000, 0.0000, 0.0000]	[0, 1, 3]	<input checked="" type="checkbox"/>	<input type="checkbox"/>		
[0.0000, 0.2000, 0.0000]	[1, 2, 3]				
[0.0000, 0.0000, 0.2000]	[2, 0, 3]				
reduced	connecting point #s				

Text3d

text	size	depth	normal	offset	color
sample text	1.00	3.00	[4.00, 5.00, 2.00]	[0.1000, 0.1000, 0.1000]	■ iron ▼
			reduced	reduced	

QtDraw - Object Property

Spline

point	width	n_interp	closed	natural	color
[0.0000, 0.0000, 0.0000] [0.5000, 0.0000, 0.0000] [0.5000, 0.5000, 0.0000] [0.0000, 0.5000, 0.0000] [0.0000, 0.0000, 0.5000]	1.00	100	<input type="checkbox"/>	<input checked="" type="checkbox"/>	banana
[0.5000, 0.0000, 0.5000] [0.5000, 0.5000, 0.5000] [0.0000, 0.5000, 0.5000]	natural spline				
[0.2500, 0.2500, 0.2500]	# interpolation				
reduced					

Spline_t

expression	t_range	width	n_interp	closed	natural	color
$\begin{pmatrix} \cos(2\pi t) \\ \sin(2\pi t) \\ t \end{pmatrix}$	[0.0000, 1.1000, 0.1000]	1.00	100	<input type="checkbox"/>	<input checked="" type="checkbox"/>	sky
natural spline						
# interpolation						
reduced						

Caption

caption	space	size	bold	color		
0						
1	caption					
2	text					
3						
4	0	18	<input checked="" type="checkbox"/>	licorice		
5						
6	Text (2d)					
7	position	relative	caption	size	color	font
8	[0.02, 0.95]	<input checked="" type="checkbox"/>	\$\int \psi(x) ^2 dx = 1\$	8	licorice	arial
position 2d (origin at left-top)			text (with simple LaTeX)			

QtDraw with MultiPie Enhanced (QtDraw⁺)

Additional Panel

space/point group

product of irrep.

draw harmonics

active tensor

matrix element

draw VC at Wyckoff

by pushing "MultiPie" in Menu

Group operations become available !

space group dropdown: hexagonal crystal dropdown: 191. D6h¹ (P6/mmm) point/space group name dropdown: A1g dropdown: A1g dropdown: A1g dropdown: A1g dropdown: anti-sym. dropdown: A1g dropdown: product table

symmetry operation dropdown: character table Wyckoff position dropdown: Wyckoff position dropdown: product table

symmetric dropdown: A1g dropdown: A1g dropdown: A1g dropdown: anti-sym. dropdown: A1g dropdown: product table

harmonics dropdown: Q dropdown: rank dropdown: 0 dropdown: irrep. decom. dropdown: 1. C1 dropdown: gen

response tensor dropdown: E dropdown: polar dropdown: rank dropdown: 2 dropdown: irrep. decom. dropdown: 1. C1 dropdown: gen

atomic multipole dropdown: Im dropdown: bra-ket dropdown: s dropdown: s

virtual cluster dropdown: 24g dropdown: 1| dropdown: clear

SITE: [x,y,z], BOND: [tail];[head] / [vector]@[center] / [start]:[vector]

object drawing basis drawing

sympy-style expression can be used

SITE: draw equivalent sites.

1. input representative SITE, + ENTER.

draw sites by symmetry operation (SO)

BOND: draw equivalent bonds.

1. input representative BOND, + ENTER.

draw bonds by SO

[1/3, 2/3, 0]

VECTOR: draw vectors at equivalent sites or bonds.

1. choose type, 2. input vector [x,y,z] # representative SITE/BOND, + ENTER.

draw same vectors at positions by SO

Q dropdown: [0, 0, 1] # [1/2, 1/2, 0]

ORBITAL: draw orbitals at equivalent sites or bonds.

1. choose type, 2. input orbital (xyz polynomial) # representative SITE/BOND, + ENTER.

draw same orbitals at positions by SO

Q dropdown: 3z² - r² # [0, 0, 0] ; [1, 0, 0]

POINT-GROUP HARMONICS: draw point-group harmonics at equivalent sites or bonds.

1. choose (type,rank,irrep.), 2. input representative SITE/BOND, + ENTER.

draw PG harmonics

⇒ used expression is shown (in LaTeX form).

Q dropdown: 2 dropdown: Q(2,A1g) dropdown: [0, 0, 0]

expression -x²/2 - y²/2 + z²

LaTeX

WYCKOFF: find wyckoff position and local symmetry. 1. input representative SITE/BOND, + ENTER.
⇒ wyckoff position and its local symmetry are shown.

find Wyckoff and local symmetry

[1/3, 2/3, 0]

⇒ Wyckoff position 2c

local symmetry -6m2

type of MP

type of MP

type, rank, PG-MP

definition of PG-MP

QtDraw+ - Drawing with Symmetry Operation

Bond expression

Tail-Head : [1/2,1/2,0] ; [0,0,0]
Vector-Center : [1/2,1/2,0] @ [0,0,0] ➔ object is drawn at bond center
Start-Vector : [1/2,1/2,0] : [0,0,0]

Basis drawing

<p>object drawing basis drawing</p> <p>SITE: draw site-cluster basis. 1. input representative SITE, + ENTER, ⇒ 2. choose basis, 3. push `draw`.</p> <p>[1/2, 1/2, 0] ⇒ <input type="button" value="draw"/></p> <p>BOND: draw bond-cluster basis. 1. input representative BOND, + ENTER, ⇒ 2. choose basis, 3. push `draw`.</p> <p>[1/2, 1/2, 0] @ [1/4, 1/4, 0] ⇒ <input type="button" value="draw"/></p> <p>VECTOR: draw symmetry-adapted vector. 1. choose type, 2. input representative SITE/BOND, + ENTER, ⇒ 3. choose (type,basis), 4. push `draw` or 3. input linear combination (LC), + ENTER or 3. push `modulation`.</p> <p>Q [1/2, 1/2, 0] ⇒ Q <input type="button" value="draw"/> LC (Q01+Q02)/sqrt(2) modulation Q,G <input type="button" value="draw"/></p> <p>ORBITAL draw symmetry-adapted orbital. 1. choose (type,rank), 2. input representative SITE/BOND, + ENTER, ⇒ 3. choose (type,basis), 4. push `draw` or 3. input linear combination (LC), + ENTER or 3. push `modulation`.</p> <p>Q 1 [0, 0, 0]; [1/2, 1/2, 0] ⇒ Q <input type="button" value="draw"/> LC (Q01+Q02)/sqrt(2) modulation Q,G <input type="button" value="draw"/></p> <p>HOPPING: draw hopping direction. 1. input representative BOND, + ENTER.</p> <p>[0, 0, 0] ; [1/2, 1/2, 0]</p>	<p>draw site-cluster basis</p> <p>draw bond-cluster basis</p> <p>draw symmetry-adapted vector</p> <p>draw linear combination of symmetry-adapted vectors</p> <p>draw modulation of symmetry-adapted vectors</p> <p>draw symmetry-adapted orbital</p> <p>draw linear combination of symmetry-adapted orbitals</p> <p>draw modulation of symmetry-adapted orbitals</p> <p>draw hopping direction</p>
--	---

QtDraw+ - Crystal Structure Drawing

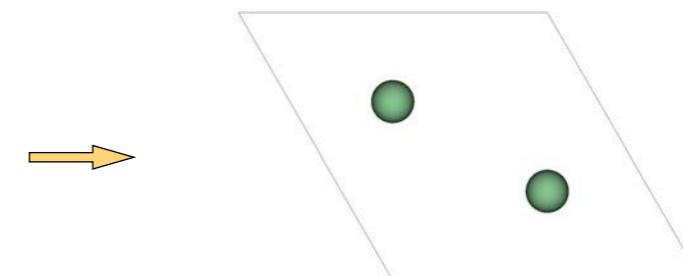
Example Draw "graphene"

1. Choose space group

space group ▾ hexagonal ▾ 191. D6h¹ (P6/mmm) ▾

2. Input site

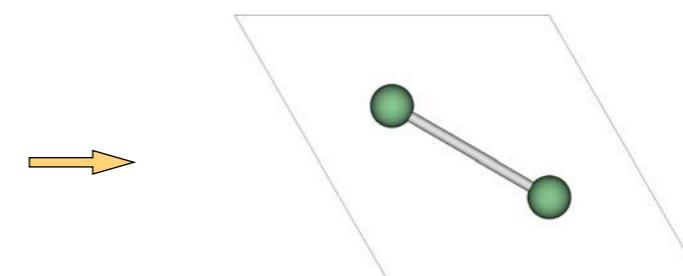
object drawing	basis drawing
SITE: draw equivalent sites. 1. input representative SITE, 2. ENTER.	
[1/3, 2/3, 0]	



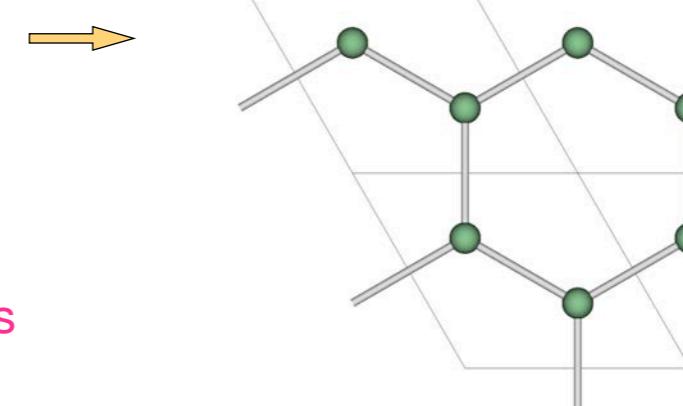
3. Input bond

BOND: draw equivalent bonds.
1. input representative BOND, 2. ENTER.

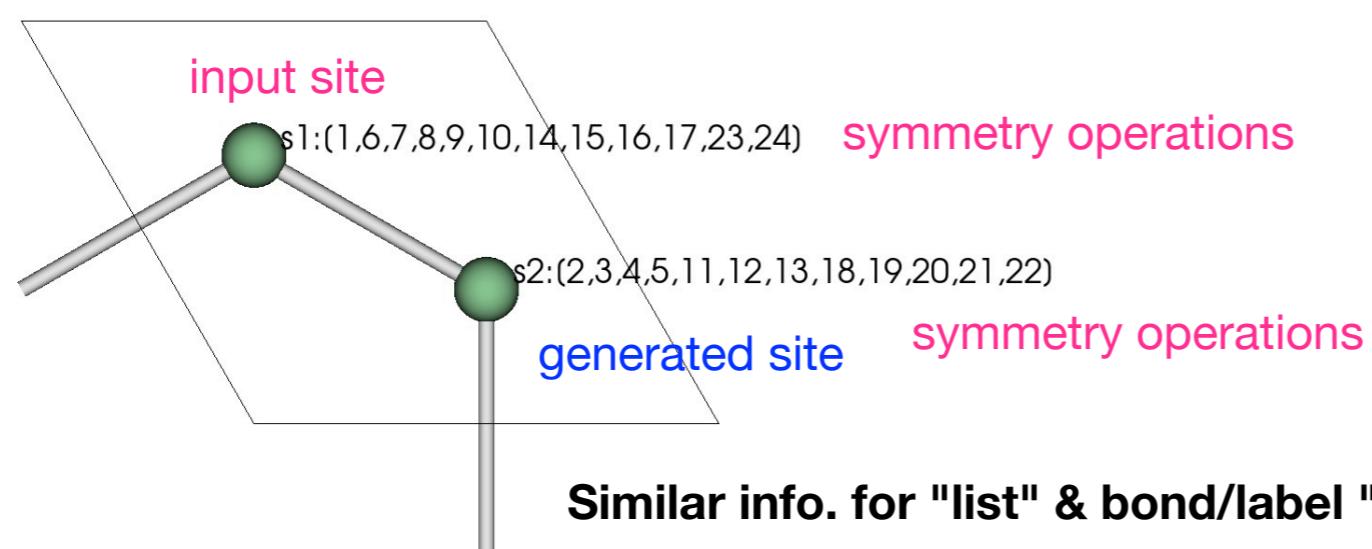
[2/3, 1/3, 0] ; [1/3, 2/3, 0]



4. Push "clip" and "repeat"



5. Push "repeat" and "list" & site/label "on"



QtDraw+ - SAMB Drawing

Draw SAMB for "graphene"

1. Draw "mass term"

object drawing basis drawing **draw weight of sites**

SITE: draw site-cluster basis.
1. input representative SITE, + ENTER,
⇒ 2. choose basis, 3. push `draw`.

[1/3, 2/3, 0]

⇒ Q02: $Q(3,B1u,,) = Qa(0,A1g,) \times Qs(3,B1u,,)$

draw

Z MP basis atomic x site-cluster

2. Draw "Rashba SOC"

HOPPING: draw hopping direction.
1. input representative BOND, + ENTER.

draw hopping direction

[1/3, 2/3, 0] ; [2/3, 1/3, 0]

VECTOR: draw symmetry-adapted vector.
1. choose type, 2. input representative SITE/BOND, + ENTER,
⇒ 3. choose (type,basis), 4. push `draw` or 3. input linear combination (LC), + ENTER or 3. push `modulation`.

M **draw spin direction**

[1/3, 2/3, 0] ; [2/3, 1/3, 0]

⇒ Q **draw**

Q01: $Q(1,A2u,,) = Ma(1,E1g,) \times Tb(1,E1u,,)$

Z MP basis atomic x bond-cluster

3. Draw "cluster quadrupole order"

ORBITAL draw symmetry-adapted orbital.
1. choose (type,rank), 2. input representative SITE/BOND, + ENTER,
⇒ 3. choose (type,basis), 4. push `draw` or 3. input linear combination (LC), + ENTER or 3. push `modulation`.

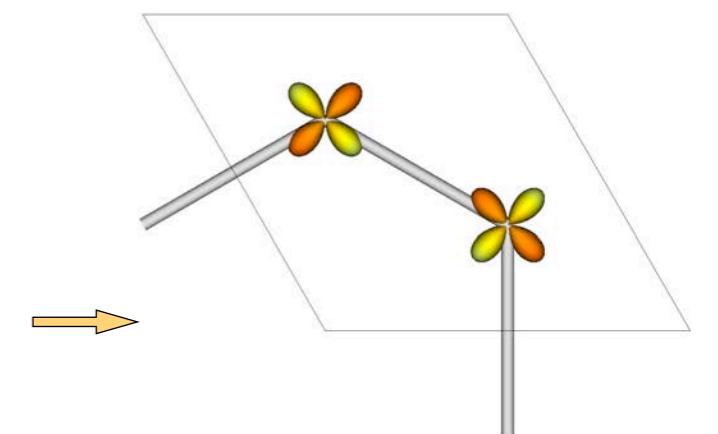
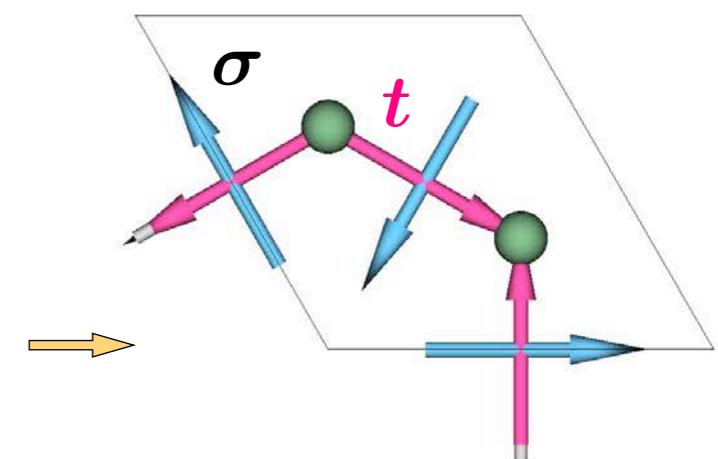
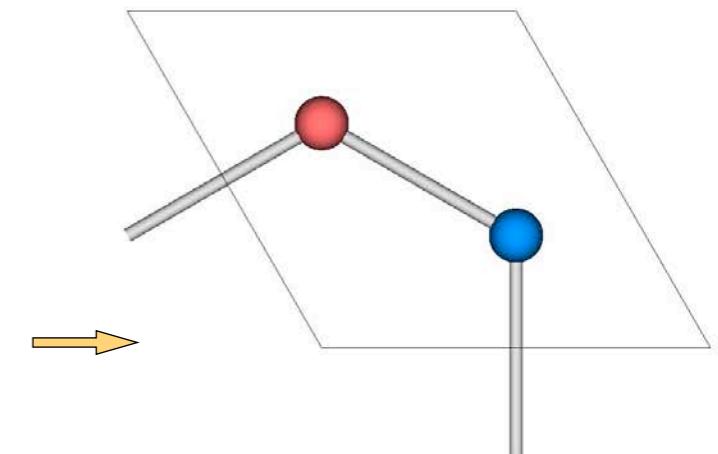
draw orbitals

Q 2 [1/3, 2/3, 0]

⇒ Q **draw**

Q01: $Q(1,E1u,,0) = Qa(2,E2g,) \times Qs(3,B1u,,)$

Electric E_{1u} order



QtDraw+ - Modulation Drawing

SAMB modulation

$$\{ X_\eta(\mathbf{p}_s; \mathbf{R}) \} = \sum_i c_i \mathbb{X}_i \cos[\mathbf{k}_i \cdot (\mathbf{R} + \mathbf{p}_s) - \frac{\pi}{2} n_i]$$

coeff basis k cell plus set phase

$n = 0 : \cos$
 $n = 1 : \sin$

for given $[[\mathbf{X}, \mathbf{c}, \mathbf{k}, \mathbf{n}]]$

Draw SAMB modulation for "graphene"

1. Simple AFM (single-k)

(a) First, draw sites & bonds, and repeat in range $[0,0,0]-[3,3,1]$

(b) Construct vector SAMB

VECTOR: draw symmetry-adapted vector.
 1. choose type, 2. input representative SIT
 \Rightarrow 3. choose (type,basis), 4. push `draw` o

M [1/3, 2/3, 0]

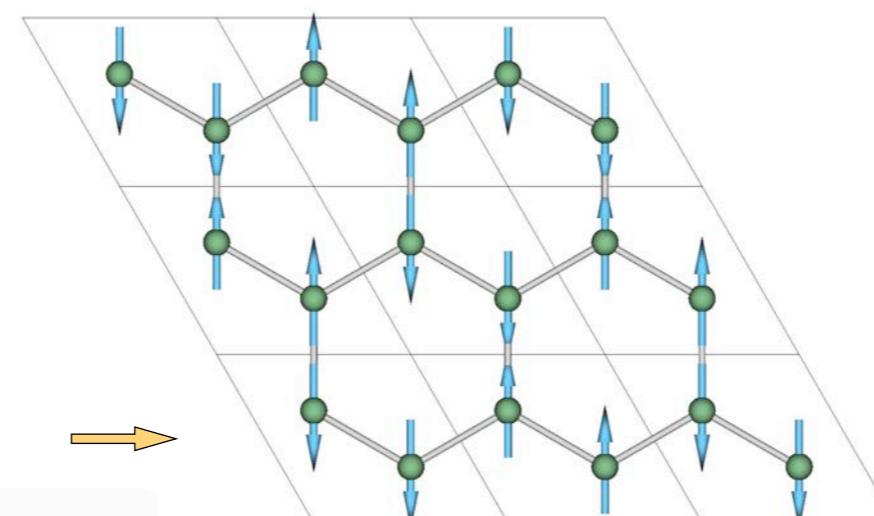
(c) Open modulation panel, and edit

modulation T,M []

Modulation - vector

basis	coeff	k	phase
M02	$\frac{7}{10}$	$(\frac{1}{2}, \frac{1}{2}, 0)$	cos

add remove
lower [0,0,0] repeat [3,3,1]
Apply Cancel OK

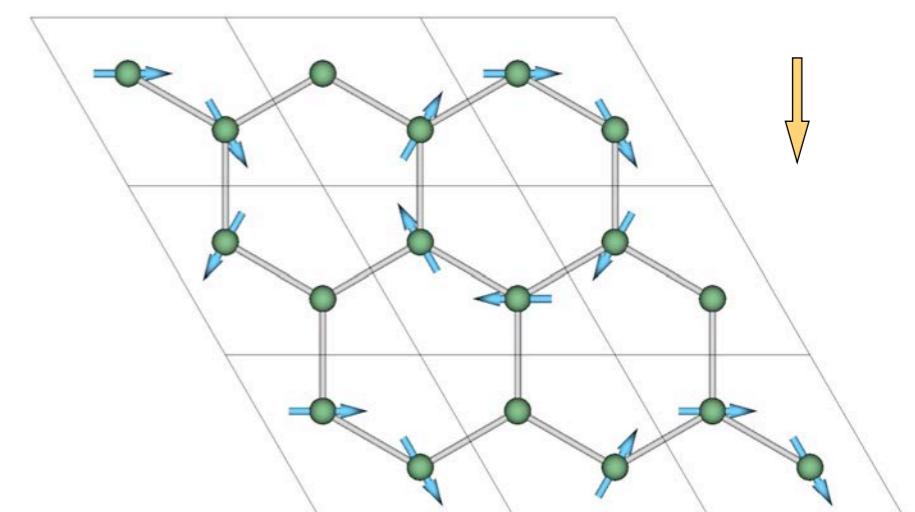


2. Vortex-like AFM (triple-k)

Modulation - vector

basis	coeff	k	phase
M03	$\frac{\sqrt{3}}{6}$	$(0, \frac{1}{2}, 0)$	cos
M02	$\frac{1}{4}$	$(\frac{1}{2}, 0, 0)$	cos
M03	$\frac{\sqrt{3}}{12}$	$(\frac{1}{2}, 0, 0)$	cos
M04	$\frac{\sqrt{3}}{12}$	$(\frac{1}{2}, \frac{1}{2}, 0)$	cos
M05	$\frac{1}{4}$	$(\frac{1}{2}, \frac{1}{2}, 0)$	cos

add remove
lower [0, 0, 0] repeat [3, 3, 1]
Apply Cancel OK



QtDraw+ - SAMB Name Ambiguity

Caveat

Sometime, MP base belonging to the same irreps. but with different rank cannot be distinguished !

Then, the displayed rank and type of MP differs for essentially the same basis.

Example

space group ▾ trigonal ▾ 152. D3⁴ ▾

M-vector on [0.3, 0, 1/3]; [0, 0.3, 2/3]

or

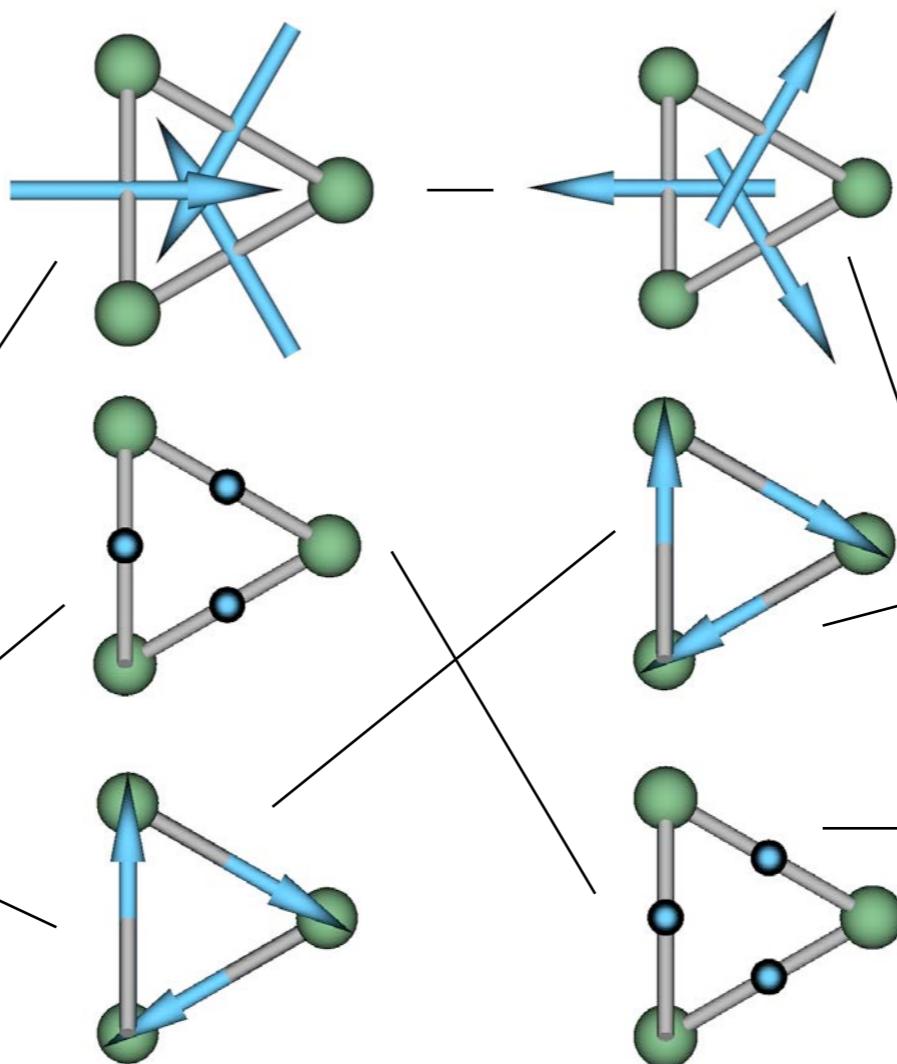
[-0.3, -0.3, 0]; [0.3, 0, 1/3]

Q(1,A2,,) = Ma(1,E,) x Tb(1,E,
Q(1,E,,0) = Ma(1,A2,) x Tb(1,E,
Q(1,E,,1) = Ma(1,A2,) x Tb(1,E,

G(0,A1,,) = Ma(1,A2,) x Tb(1,A2,)
G(2,A1,,) = Ma(1,A2,) x Tb(1,A2,)
G(2,E,1,0) = Ma(1,A2,) x Tb(1,E,)
G(2,E,1,1) = Ma(1,A2,) x Tb(1,E,)
G(2,E,2,0) = Ma(1,E,) x Tb(1,E,)
G(2,E,2,1) = Ma(1,E,) x Tb(1,E,)

T(2,A1,,) = Ma(1,E,) x Qb(2,E,1)
T(2,E,2,0) = Ma(1,E,) x Qb(2,E,1)
T(2,E,2,1) = Ma(1,E,) x Qb(2,E,1)

M(1,A2,,) = Ma(1,A2,) x Qb(0,A1,)
M(1,A2,,) = Ma(1,E,) x Qb(2,E,1)
M(1,E,,0) = Ma(1,E,) x Qb(0,A1,)
M(1,E,,0) = Ma(1,A2,) x Qb(2,E,1)
M(1,E,,1) = Ma(1,E,) x Qb(0,A1,)
M(1,E,,1) = Ma(1,A2,) x Qb(2,E,1)



Q(1,A2,,) = Ma(1,E,) x Tb(1,E,
Q(1,E,,0) = Ma(1,A2,) x Tb(1,E,
Q(1,E,,1) = Ma(1,A2,) x Tb(1,E,

G(0,A1,,) = Ma(1,A2,) x Tb(1,A2,)
G(2,A1,,) = Ma(1,A2,) x Tb(1,A2,)
G(2,E,1,0) = Ma(1,A2,) x Tb(1,E,)
G(2,E,1,1) = Ma(1,A2,) x Tb(1,E,)
G(2,E,2,0) = Ma(1,E,) x Tb(1,E,)
G(2,E,2,1) = Ma(1,E,) x Tb(1,E,)

T(1,A2,,) = Ma(1,E,) x Qb(1,E,
T(1,E,,0) = Ma(1,A2,) x Qb(1,E,
T(1,E,,1) = Ma(1,A2,) x Qb(1,E,

M(0,A1,,) = Ma(1,E,) x Qb(1,E,
M(1,A2,,) = Ma(1,A2,) x Qb(0,A1,)
M(1,E,,0) = Ma(1,E,) x Qb(0,A1,)
M(1,E,,1) = Ma(1,E,) x Qb(0,A1,)
M(2,E,2,0) = Ma(1,E,) x Qb(1,E,)
M(2,E,2,1) = Ma(1,E,) x Qb(1,E,)

Application - SAMB Decomposition

Local Susceptibility

$$\chi_i^{\alpha\beta} = a_0 Q_0 + \sum_{\alpha} b_{\alpha} Q_{2,\alpha}$$

electric symmetric tensor = site-cluster mono/quadrupole

space group ▾ trigonal ▾ 152. D3⁴ ▾ cf. Te

View clip repeat
lower: [-0.50, -0.50, 0.00]
upper: [0.50, 0.50, 1.01]

Site : [0.3, 0, 1/3]
Bond : [0.3, 0, 1/3]; [0, 0.3, 2/3]

ORBITAL draw symmetry-adapted orbital.

1. choose (type,rank), 2. input representative SITE/BOND, + ENTER,
 ⇒ 3. choose (type,basis), 4. push `draw` or 3. input linear combination (LC), + ENTER or 3. push `modulation`.

Q ▾ 2 ▾ [0.3, 0, 1/3]

1 Q(1,A2,,) = Qa(2,E,1) x Qs(1,E,)

Q(1,E,,0) = Qa(2,A1,) x Qs(1,E,)

Q(1,E,,1) = Qa(2,A1,) x Qs(1,E,)

2 Q(2,A1,,) = Qa(2,A1,) x Qs(0,A1,)

Q(2,E,1,0) = Qa(2,E,1) x Qs(0,A1,)

Q(2,E,1,1) = Qa(2,E,1) x Qs(0,A1,)

Q(2,E,2,0) = Qa(2,E,2) x Qs(0,A1,)

Q(2,E,2,1) = Qa(2,E,2) x Qs(0,A1,)

3 Q(3,A1,,) = Qa(2,E,2) x Qs(1,E,)

Q(3,A2,2,) = Qa(2,E,2) x Qs(1,E,)

3 G(2,A1,,) = Qa(2,E,1) x Qs(1,E,)

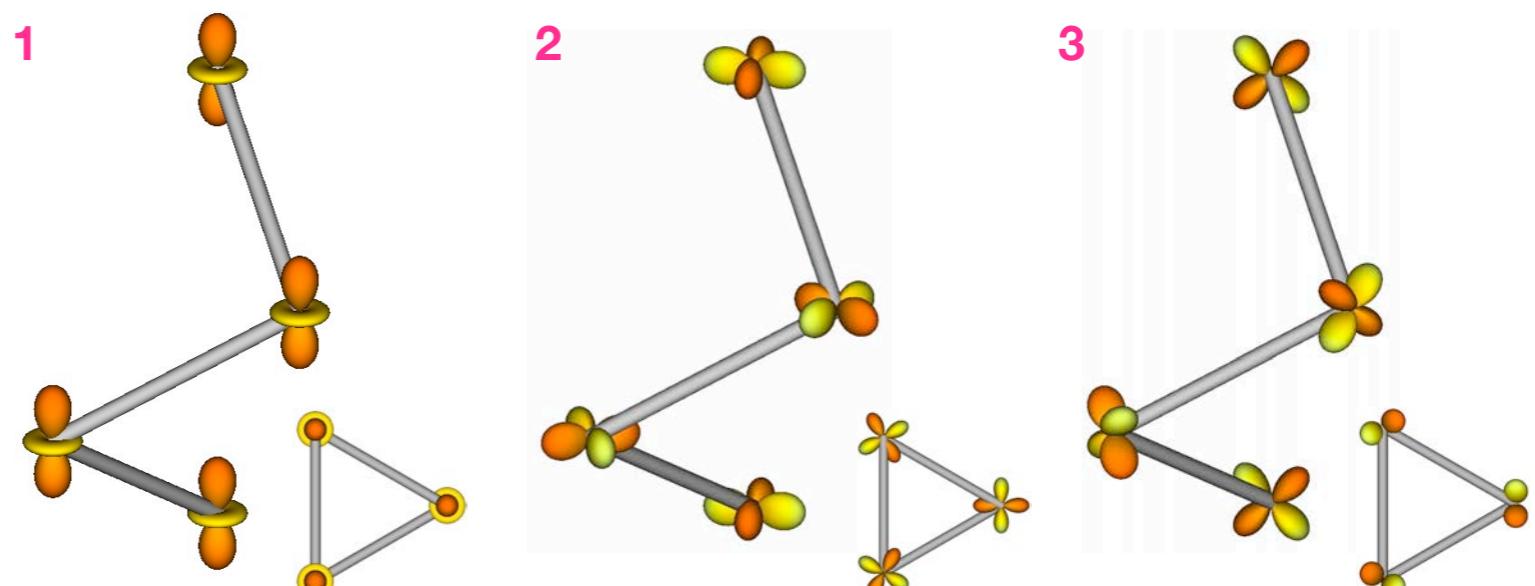
G(2,E,1,0) = Qa(2,A1,) x Qs(1,E,)

G(2,E,1,1) = Qa(2,A1,) x Qs(1,E,)

G(2,E,2,0) = Qa(2,E,1) x Qs(1,E,)

G(2,E,2,1) = Qa(2,E,1) x Qs(1,E,)

1 (monopole) + 3 identity irrep. (A₁)



Application - SAMB Decomposition

Stiffness of Phonon

Te

$$V = \frac{1}{2} g_{ij}^{\alpha\beta} (x_i^\alpha - x_{0i}^\alpha)(x_j^\beta - x_{0j}^\beta)$$

$$g_{ij}^{\alpha\beta} = a_0 Q_0 + \sum_{\alpha} b_{\alpha} Q_{2,\alpha}$$

electric symmetric tensor = bond-cluster mono/quadrupole

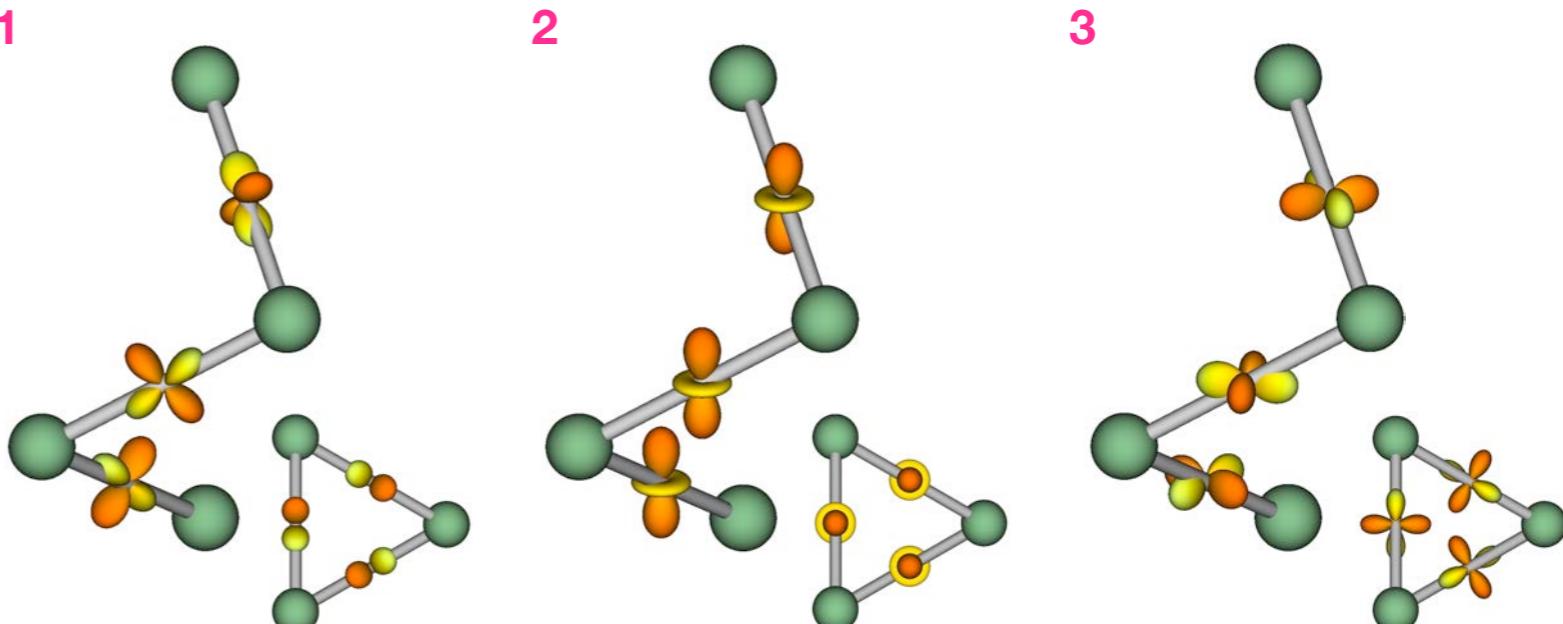
ORBITAL draw symmetry-adapted orbital.

1. choose (type,rank), 2. input representative SITE/BOND, + ENTER,
 ⇒ 3. choose (type,basis), 4. push `draw` or 3. input linear combination (LC), + ENTER or 3. push `modulation`.

1 $Q(0,A1,,) = Qa(2,E,1) \times Qb(2,E,1)$
2 $Q(2,A1,,) = Qa(2,A1,) \times Qb(0,A1,)$
 $Q(2,E,1,0) = Qa(2,E,1) \times Qb(0,A1,)$
 $Q(2,E,1,0) = Qa(2,A1,) \times Qb(2,E,1)$
 $Q(2,E,1,1) = Qa(2,E,1) \times Qb(0,A1,)$
 $Q(2,E,1,1) = Qa(2,A1,) \times Qb(2,E,1)$
 $Q(2,E,2,0) = Qa(2,E,2) \times Qb(0,A1,)$
 $Q(2,E,2,0) = Qa(2,E,1) \times Qb(2,E,1)$
 $Q(2,E,2,1) = Qa(2,E,2) \times Qb(0,A1,)$
 $Q(2,E,2,1) = Qa(2,E,1) \times Qb(2,E,1)$

3 $G(1,A2,,) = Qa(2,E,1) \times Qb(2,E,1)$
 $G(1,E,,0) = Qa(2,A1,) \times Qb(2,E,1)$
 $G(1,E,,1) = Qa(2,A1,) \times Qb(2,E,1)$
3 $G(3,A1,,) = Qa(2,E,2) \times Qb(2,E,1)$
 $G(3,A2,2,) = Qa(2,E,2) \times Qb(2,E,1)$

1 (monopole) + 3 identity irrep. (A_1)



Application - SAMB Decomposition

Other Physical Quantities

Type	Expression	Correspondence	SAMB
Electric potential	ϕq	$q \rightarrow Q_{0,0}^{(a)}$	(E) Atomic (s) & Site-cluster
Crystal field	$\phi_{lm} Q_{lm}$	$Q_{lm} \rightarrow Q_{lm}^{(a)}$	(E) Atomic & Site-cluster
Zeeman term	$-h^a m^a$	$m^a \rightarrow M_{1m}^{(a)}$	(M) Atomic (spinful) & Site-cluster
Spin-orbit int.	$\zeta l^a \sigma^a$	$l^a, \sigma^a \rightarrow M_{1m}^{(a)}$	(E) Atomic (p-spinful) & Site-cluster
Density-density int.	$V_{ij} n_i n_j$	$n_i n_j \rightarrow Q_{0,0}^{(a)}$	(E) Atomic (s) & Bond-cluster
Elastic energy	$\epsilon_{ij}^{ab} u_i^a u_j^b$	$u_i^a u_j^b \rightarrow Q_{0,0}^{(a)}, Q_{2m}^{(a)}$	(E) Atomic (p) & Bond-cluster
Exchange int.	$J_{ij}^{ab} S_i^a S_j^b$	$S_i^a S_j^b \rightarrow Q_{0,0}^{(a)}, Q_{2m}^{(a)}$	(E) Atomic (p) & Bond-cluster
DM int.	$D_{ij}^c \epsilon_{abc} S_i^a S_j^b$	$\epsilon_{abc} S_i^a S_j^b \rightarrow G_{lm}^{(a)}$	(ET) Atomic (p) & Bond-cluster
Real hopping	$t_{ij} c_i^\dagger c_j + \text{H.c.}$	$c_i^\dagger c_j + \text{H.c.} \rightarrow Q_{lm}^{(b)}$	(all) Atomic & Bond-cluster
Imaginary hopping	$i t_{ij} c_i^\dagger c_j + \text{H.c.}$	$i c_i^\dagger c_j + \text{H.c.} \rightarrow T_{lm}^{(b)}$	(all) Atomic & Bond-cluster

Various quantities can be expressed by using SAMB