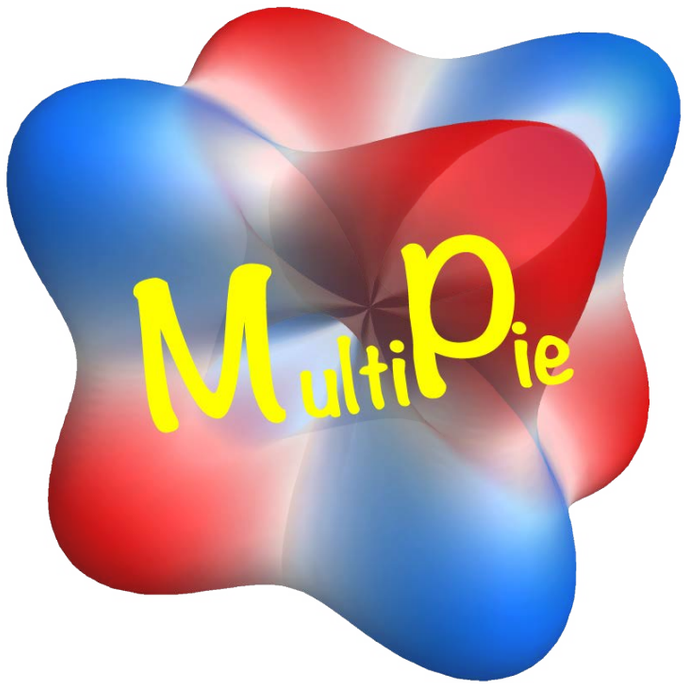
MultiPie and QtDraw Manual

MultiPie : ver. 1.2.0
QtDraw : ver. 1.1.20

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

MultiPie

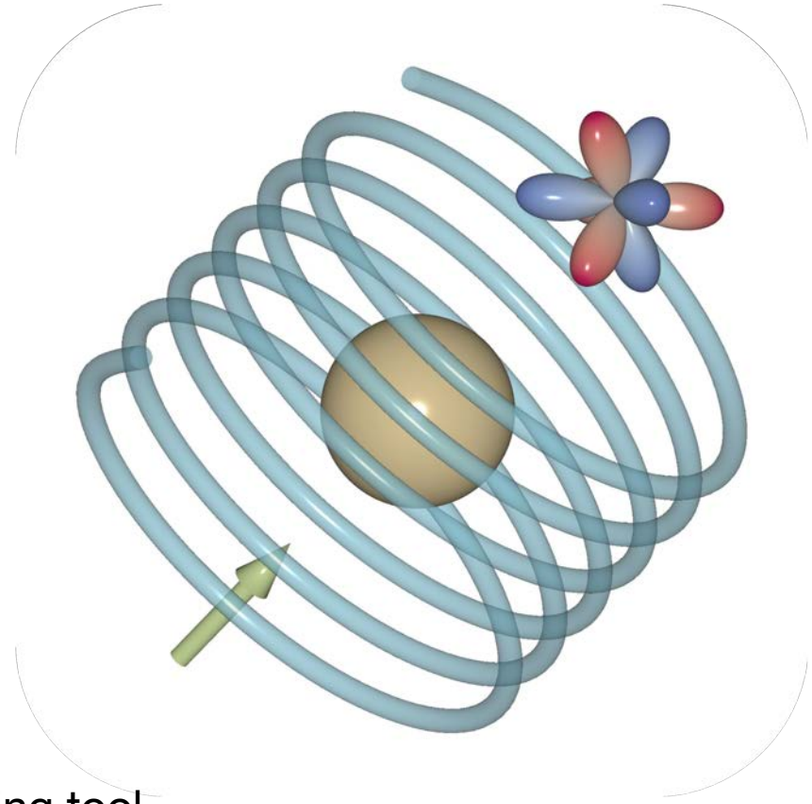


- Symmetry operations for point/space groups
- Symmetry-adapted basis construction

  ("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)

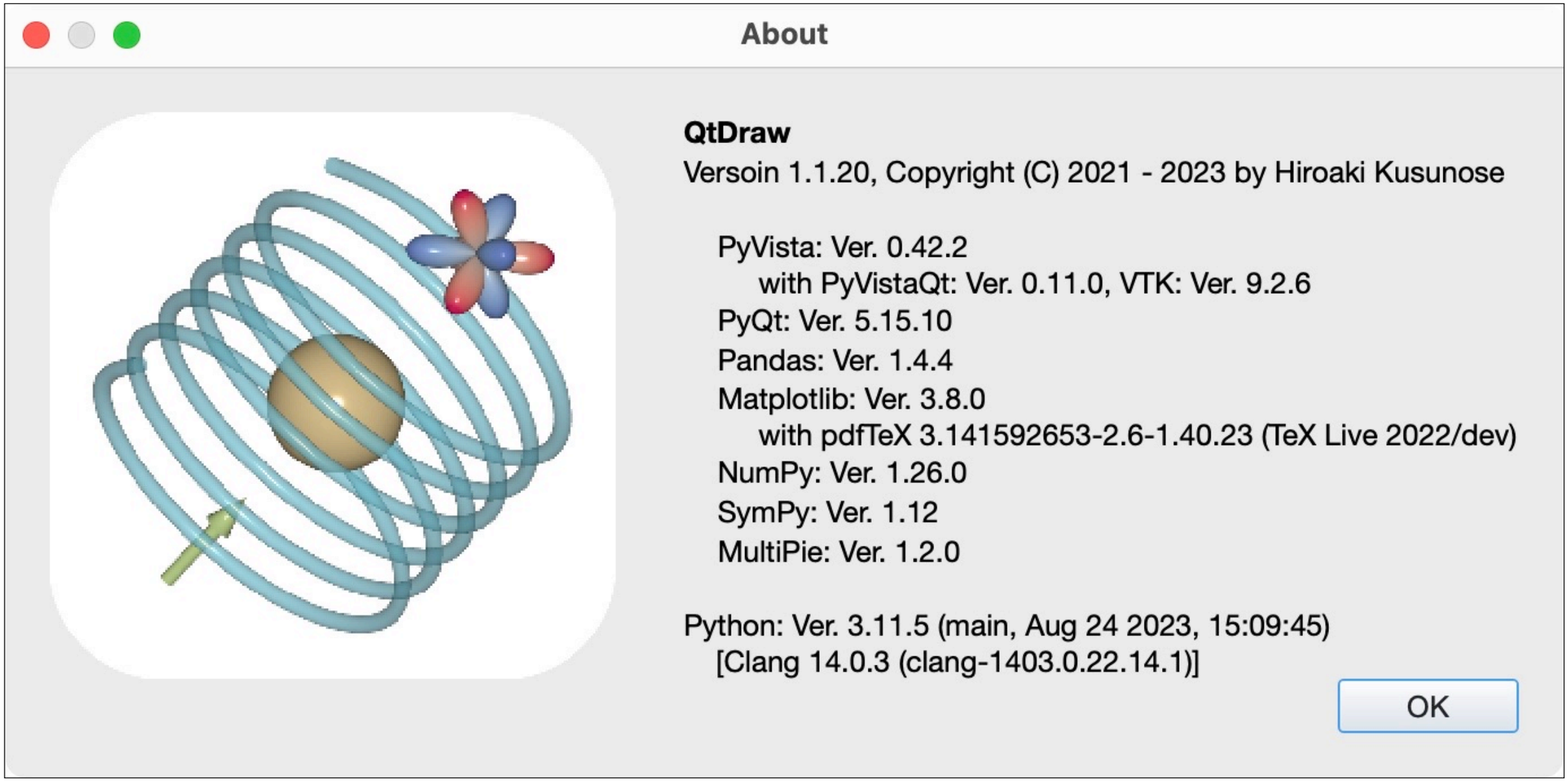
https://cmt-mu.github.io/QtDraw/

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 (**k** = 0 : Γ point in BZ)

Classification for Materials

For TP spherical systems

→ **Molecule and Crystal**

T : time-reversal (electric + or magnetic –)
P : spatial-inversion (polar or axial)
g : anisotropy (l, m)

Subgroup of spherical systems

Linear combination of spherical base

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

Type ($\mathbb{Z}_{lm}$)	Symbol	T	P		Charge	g
Electric (E)	$\mathbb{Q}_{lm}$	+	polar	$(-1)^l$	1	Y_{lm}
Magnetic (M)	$\mathbb{M}_{lm}$	–	axial	$-(-1)^l$	$i(\boldsymbol{e}_1 \times \boldsymbol{e}_2) \cdot \boldsymbol{e}_3$	Y_{lm}
Magnetic-Toroidal (MT)	$\mathbb{T}_{lm}$	–	polar	$(-1)^l$	i	Y_{lm}
Electric-Toroidal (ET)	$\mathbb{G}_{lm}$	+	axial	$-(-1)^l$	$(\boldsymbol{e}_1 \times \boldsymbol{e}_2) \cdot \boldsymbol{e}_3$	Y_{lm}

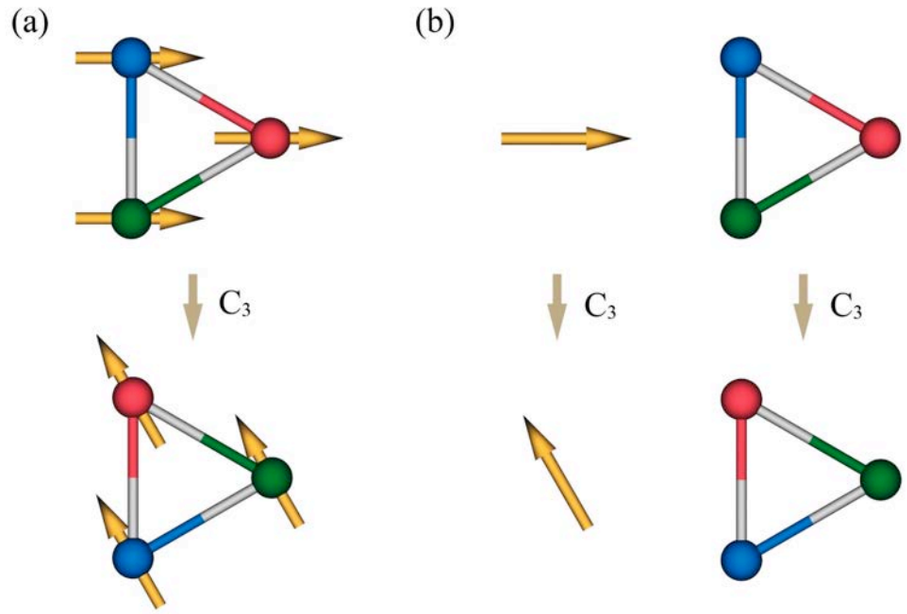
Construction of Basis

Basis for Materials

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

$$\mathbb{Z}_\alpha = \sum_{\beta\gamma} C_\alpha^{\beta,\gamma} \mathbb{X}_\beta \otimes \mathbb{Y}_\gamma$$

"Clebsch-Gordan" coefficient



Symmetry operation — atomic — site/bond

Atomic d.o.f

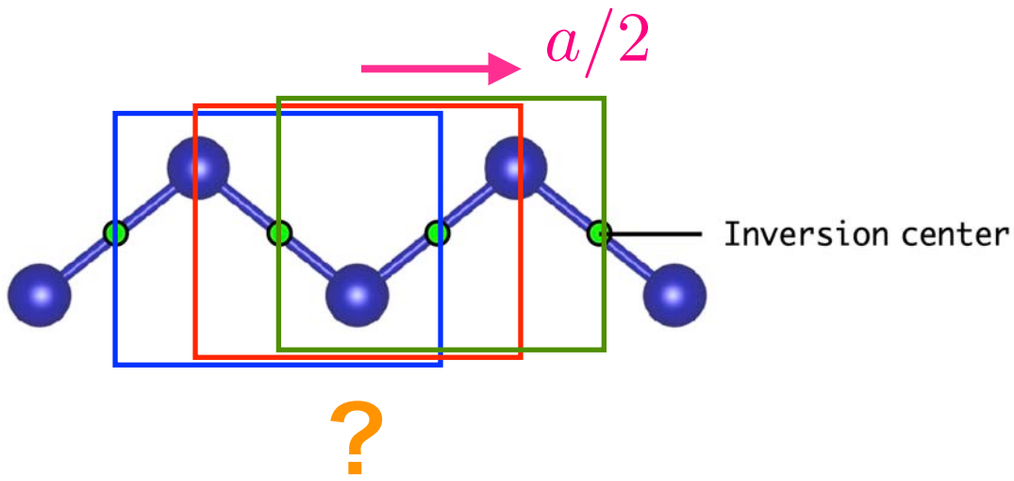
Given by quantum-mechanical expressions of complete set,
compute matrix elements by using general formula

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) ?



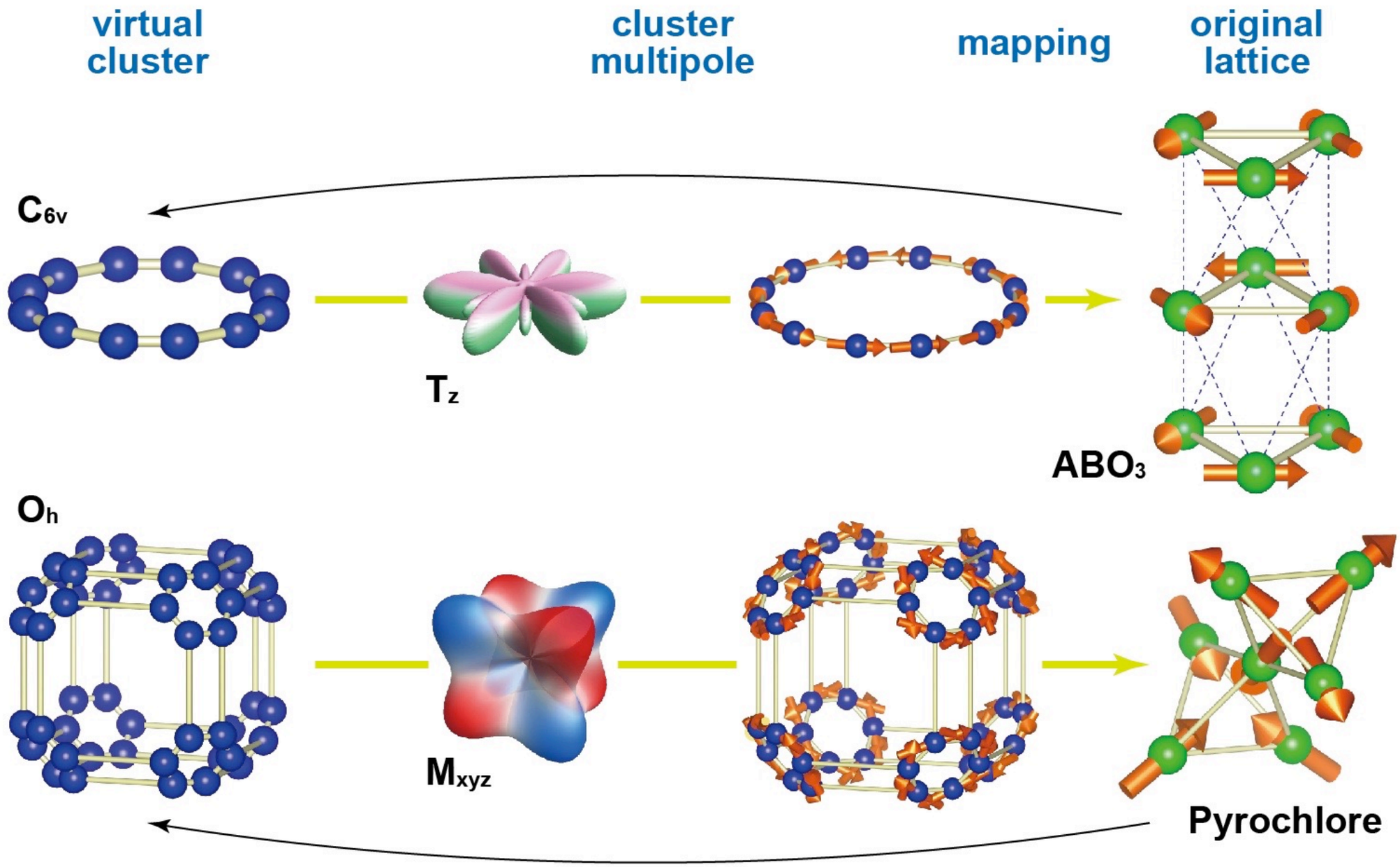
→ Use "Virtual Cluster"

Concept of Virtual Cluster

Virtual Cluster

Site-Cluster M.-T. Suzuki, et al., PRB **99**, 174407 (2019)

Site/Bond-Cluster HK, R. Oiwa, and S. Hayami, PRB **107**, 195118 (2023)



MultiPie - Example

Example for graphene

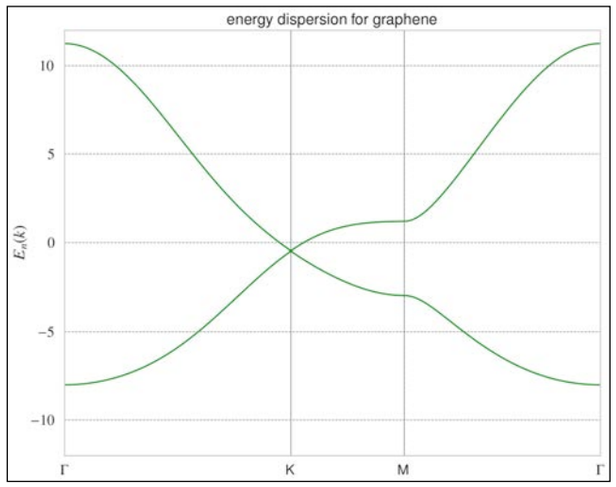
Download

`https://github.com/CMT-MU/MultiPie/tree/main/docs/example`

and try "**`python create_plot.py`**"

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.
}
```



Create Symmetry-Adapted Multipole Basis (SAMB)

```
create_samb graphene
```

In "graphene" folder

See, document for detailed dict structure

- graphene_model.py (Model info.)
- graphene_matrix.py (Full matrix form)
- graphene_samb.py (SAMB info.)
- 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 ⟶ $H = \sum_j z_j \mathbb{Z}_j$

graphene_matrix.py

```
graphene = {
    "model": "graphene",
    "molecule": False,
    "group": ("D6h^1", "space group No. 191 : D6h^1 / P6/mmm : PG D6h"),
    "dimension": 2,  # matrix size.
    "ket": ["pz@C_1", "pz@C_2"],  # Hilbert space : orbital @ site.
    "cell_site": {  # site : position, symmetry operations.
        "C_1": ("[1/3, 2/3, 0]", "[1,6,7,8,9,10,14,15,16,17,23,24]"),
        "C_2": ("[2/3, 1/3, 0]", "[2,3,4,5,11,12,13,18,19,20,21,22]"),
    },
    "version": "1.1.15",
    "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]]",  # unit vectors : [a1,a2,a3].
    "matrix": {  # SAMB.
        # z_# : { (n1, n2, n3, a, b), matrix element }, where lattice vector, R = [n1, n2, n3], a, b : row and col. in full matrix.
        "z_001": {(0, 0, 0, 0, 0): "sqrt(2)/2", (0, 0, 0, 1, 1): "sqrt(2)/2"},
            ...
        "z_007": {(2, 2, 0, 0, 0): "sqrt(3)/6", (-2, -2, 0, 0, 0): "sqrt(3)/6",
                  (2, 2, 0, 1, 1): "sqrt(3)/6", (-2, -2, 0, 1, 1): "sqrt(3)/6",
                  (0, 2, 0, 1, 1): "sqrt(3)/6", (0, -2, 0, 1, 1): "sqrt(3)/6",
                  (2, 0, 0, 1, 1): "sqrt(3)/6", (-2, 0, 0, 1, 1): "sqrt(3)/6",
                  (0, 2, 0, 0, 0): "sqrt(3)/6", (0, -2, 0, 0, 0): "sqrt(3)/6",
                  (2, 0, 0, 0, 0): "sqrt(3)/6", (-2, 0, 0, 0, 0): "sqrt(3)/6"},
}
```

Fourier transform of full matrix

$$[\mathbb{Z}_j(\boldsymbol{k})]_{a,b} = \sum_{n_1,n_2,n_3} z_j[(n_1,n_2,n_3,a,b)] e^{2\pi i \boldsymbol{\kappa}\cdot(\boldsymbol{R}+\boldsymbol{r}_a-\boldsymbol{r}_b)}$$

e.g. : ra = cell_site[ket[a].split("@")[1]] [0]
rb = cell_site[ket[b].split("@")[1]] [0]

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)

$\mathbb{Q}_{3,B_{1u}}$ "C" site-cluster

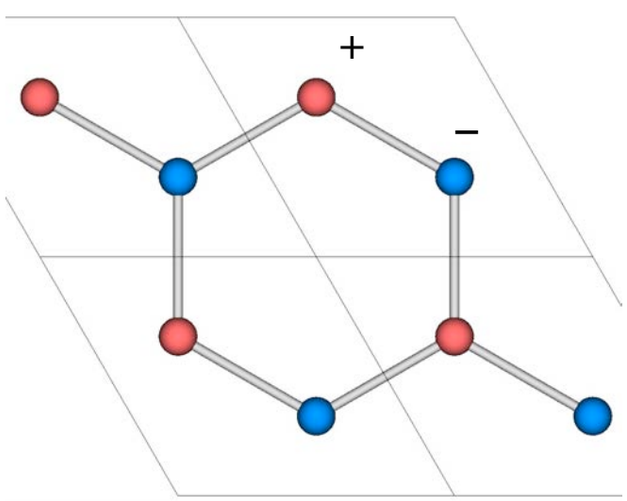
2. Haldane's magnetic flux term from kinetic SOC (spinless)

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

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

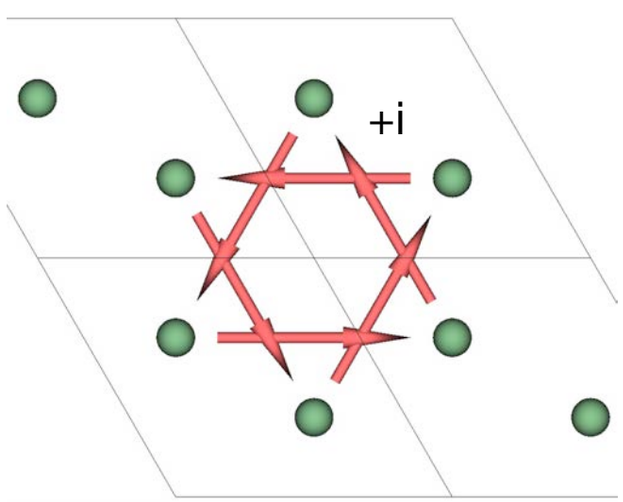
$\mathbb{Q}_{1,A_{2u}}$ "C-C" 1st neighbor bond-cluster

1. Mass term



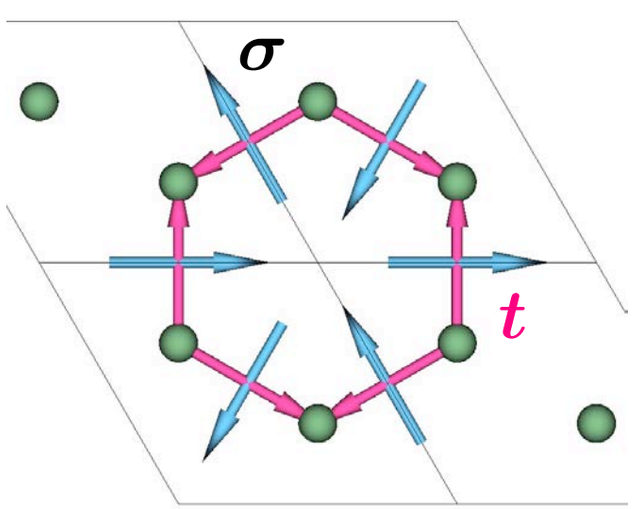
$-y(3x^2 - y^2)$

2. Haldane's M-flux



$Z \qquad (\boldsymbol{R} \times \boldsymbol{t})_z$

3. Rashba



$z \qquad (\boldsymbol{\sigma} \times \boldsymbol{t})_z$

QtDraw - Features

based on Qt Python and PyVista

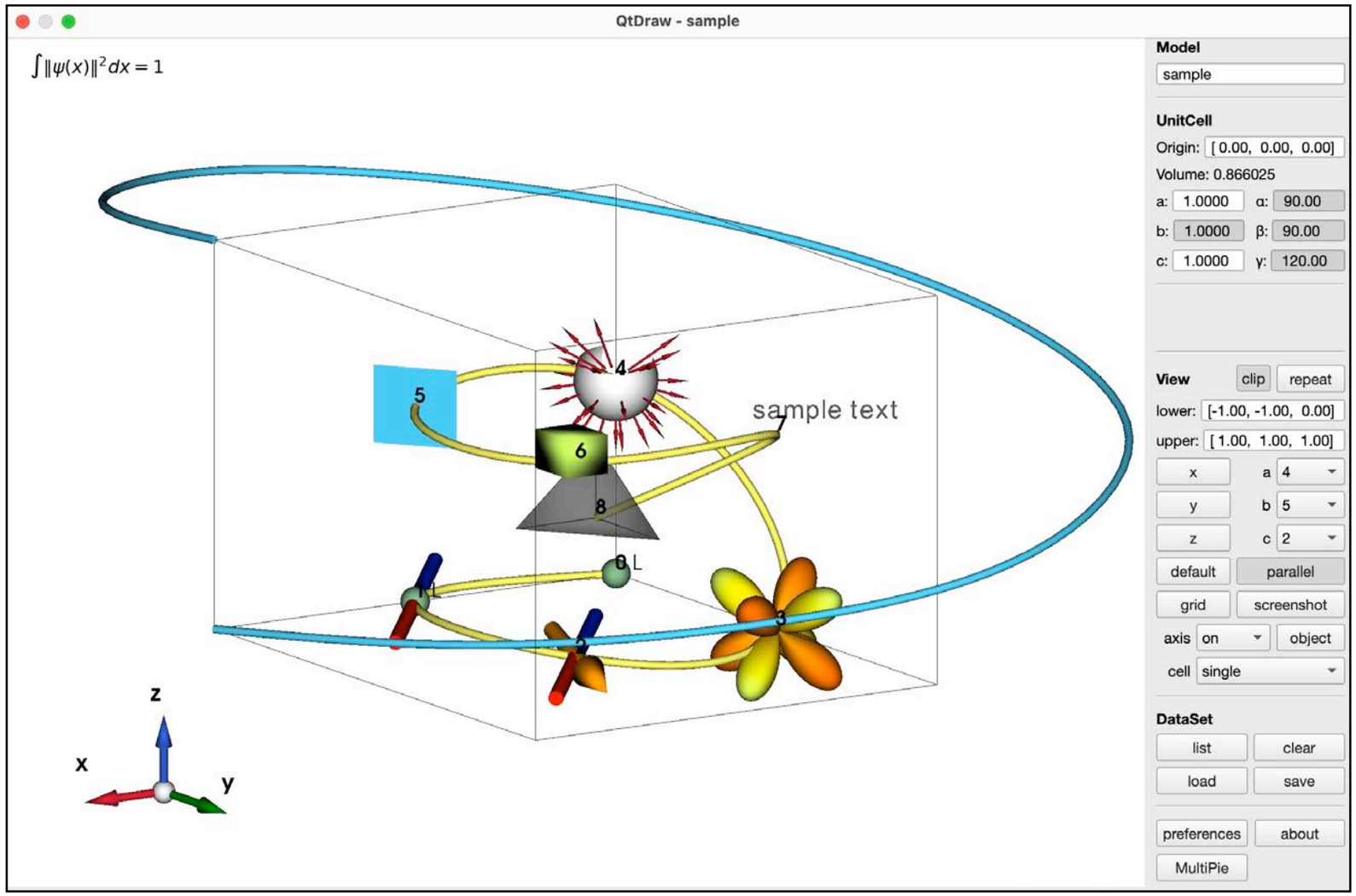
https://www.qt.io/qt-for-python

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



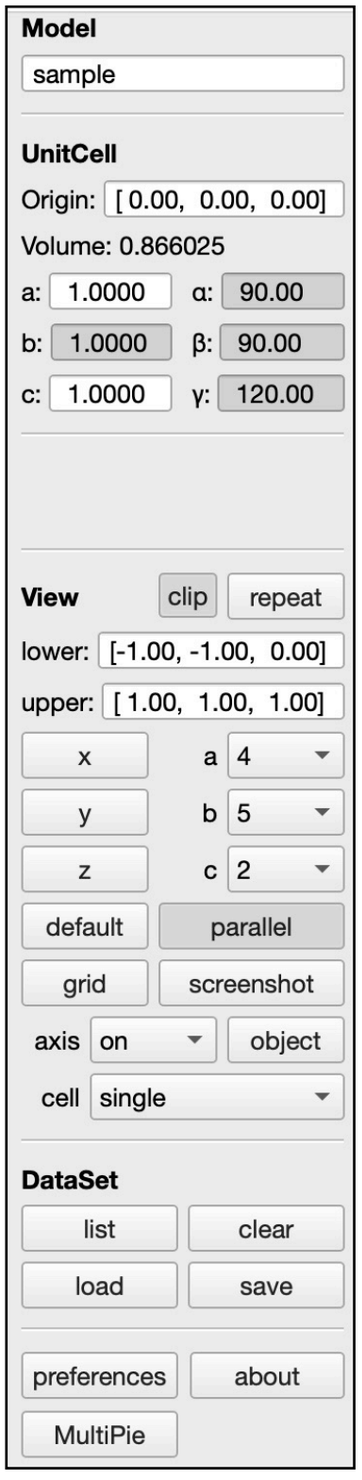
All objects can be drawn by calling Python API : easy to extend functionality of drawing

e.g. spin/orbital modulation patterns

QtDraw - Main Menu

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

Menu



model 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

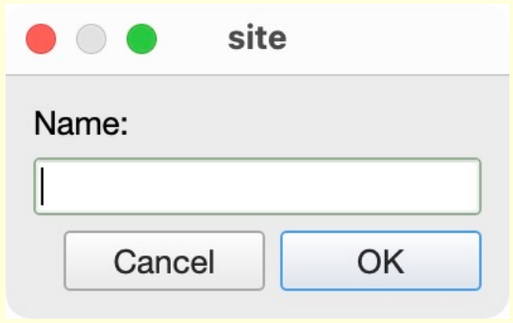
load/save data (**`.qtdw`** file)

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

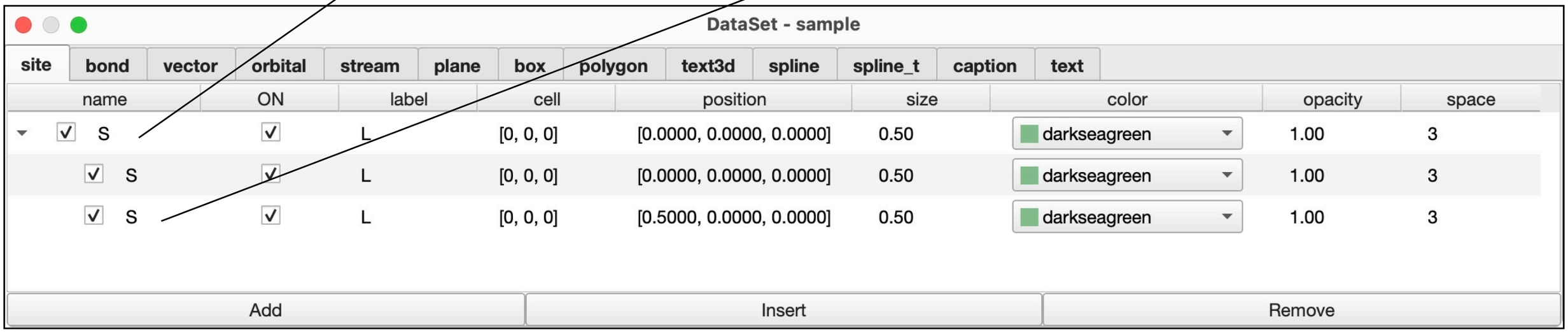
Draw objects in a Cell, and then repeat

QtDraw - List Panel

List Panel

Edit all objects in group

Edit individual object



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	darkseagreen

Bond

vector	width	color	color2
[-0.5000, -0.5000, 0.0000]	1.00	red	blue

Vector

vector	length	width	offset	color
[0.0000, 0.5000, 0.0000]	0.40	1.00	-0.43	orange

cartesian

Orbital

shape	surface	size	scale	theta0	theta1	phi0	phi1	color
xyz	xyz	0.20	☑	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	$\begin{pmatrix} x \\ y \\ z \end{pmatrix}$	0.10	0.15	1.00	☐	4	8	0	120	0	270	coolwarm	abs

stream on shape

vector at ***r***

arrow in (θ, ϕ)

θ range

ϕ range

color based on

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]	☐	☐	1.00	honeydew
reduced	reduced	reduced				

Polygon

point	connection	edge	wireframe	width	color
[0.0000, 0.0000, 0.0000] [0.2000, 0.0000, 0.0000] [0.0000, 0.2000, 0.0000] [0.0000, 0.0000, 0.2000]	[0, 1, 2] [0, 1, 3] [1, 2, 3] [2, 0, 3]	☑	☐	2.00	aluminum
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] [0.5000, 0.0000, 0.5000] [0.5000, 0.5000, 0.5000] [0.0000, 0.5000, 0.5000] [0.2500, 0.2500, 0.2500]	1.00	100	☐	☑	banana

natural spline

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	☐	☑	sky

natural spline

interpolation

reduced

Caption

caption	space	size	bold	color
0 1 2 3 4 5 6 7 8	0	18	☑	licorice

caption

text

Text (2d)

position	relative	caption	size	color	font
[0.02, 0.95]	☑	$\int \|\psi(x)\|^2 dx=1$	8	licorice	arial

position 2d (origin at left-top)

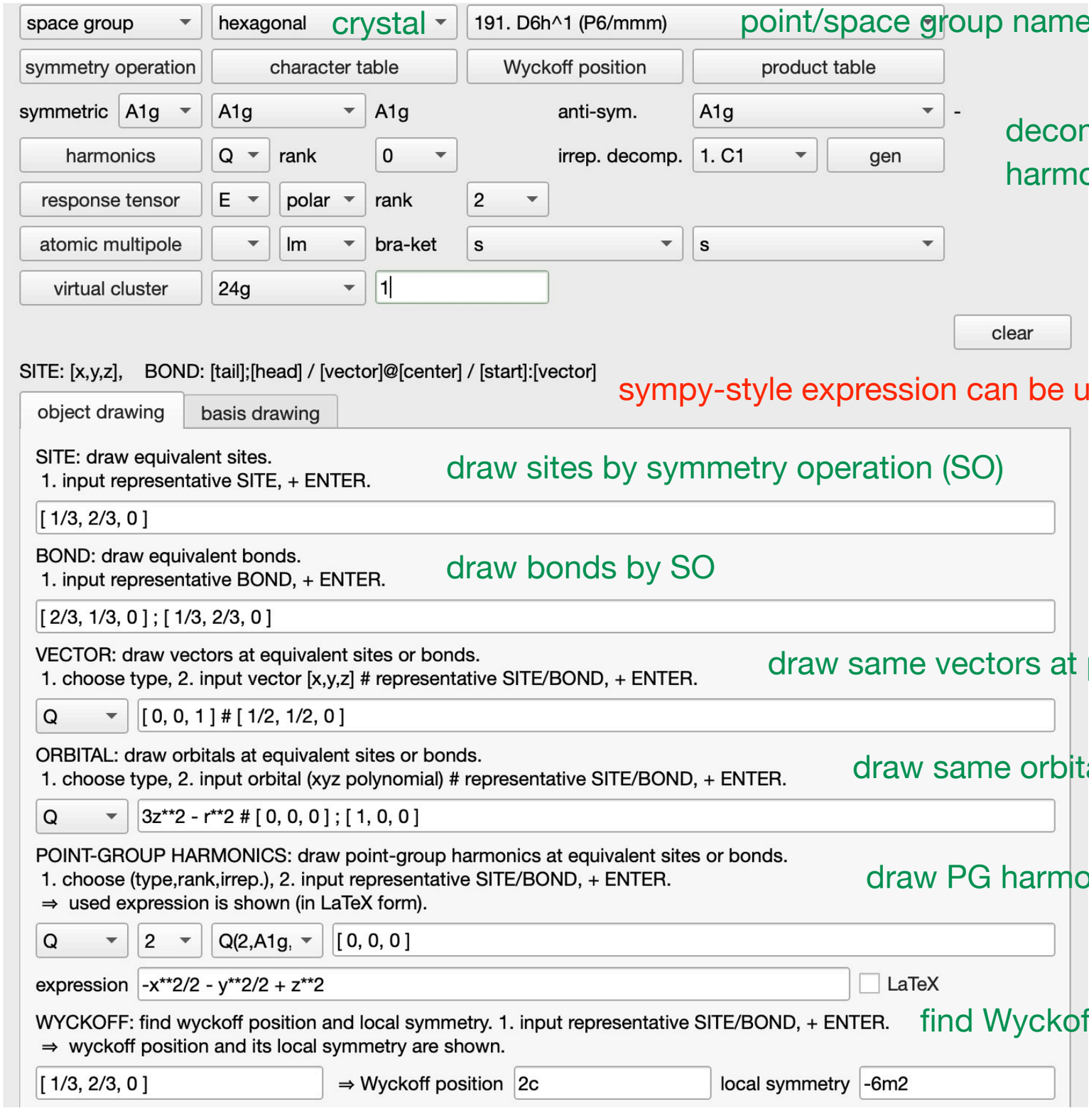
text (with simple LaTeX)

QtDraw with MultiPie Enhanced (QtDraw+)

Additional Panel by pushing "MultiPie" in Menu Group operations become available !

space/point group

product of irrep.
draw harmonics
active tensor
matrix element
draw VC at Wycoff



type of MP

type of MP

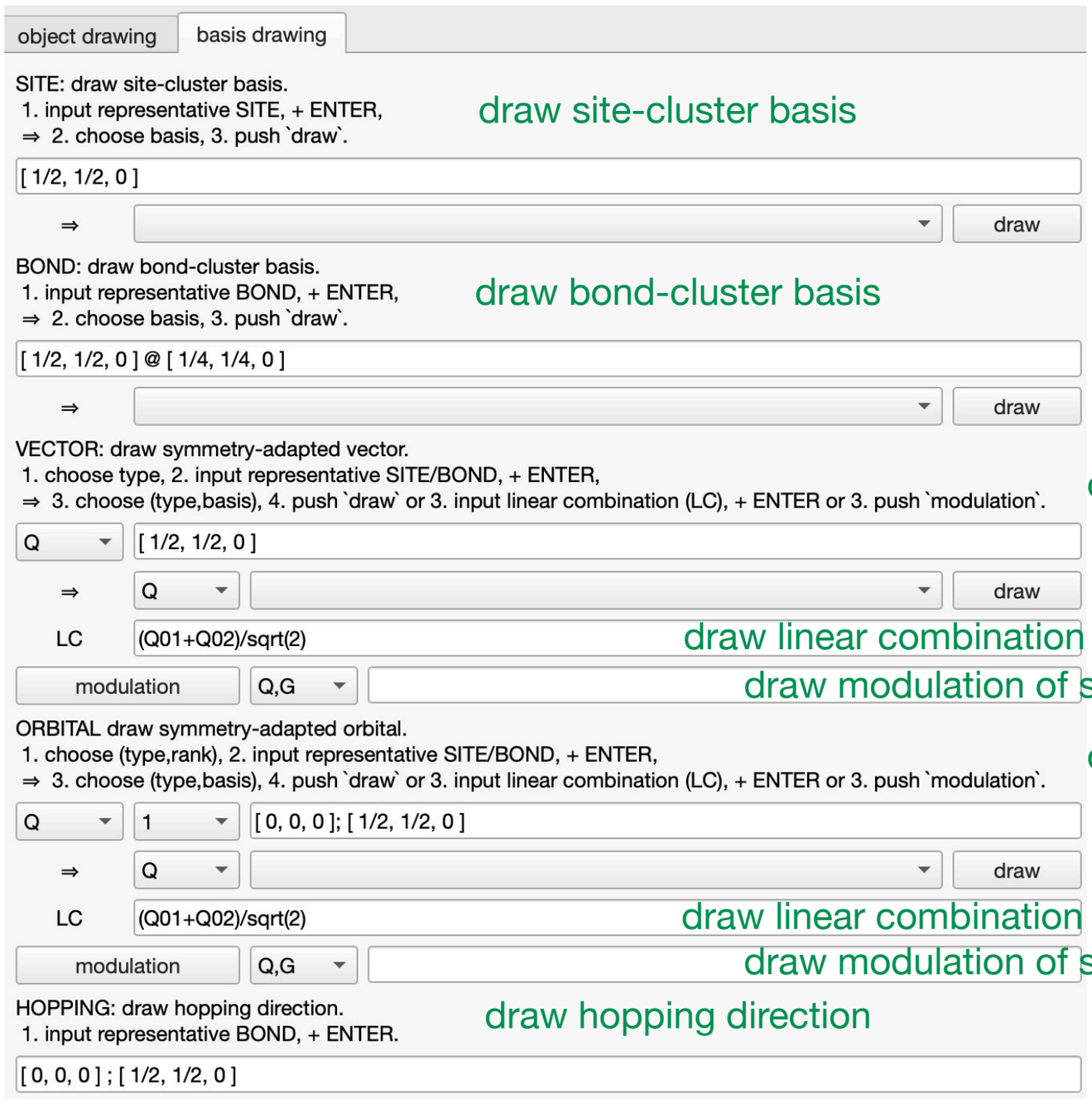
type, rank, PG-MP
definition of PG-MP

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

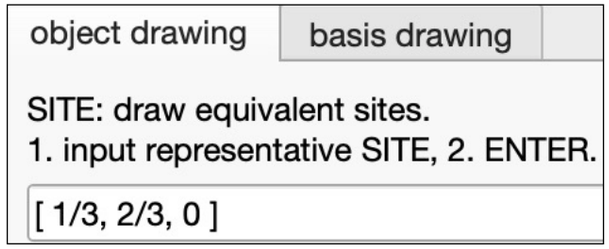


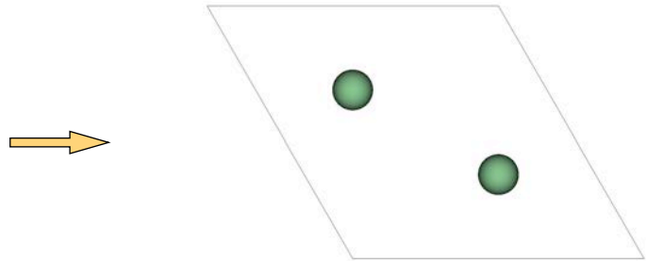
QtDraw+ - Crystal Structure Drawing

Example Draw "graphene"

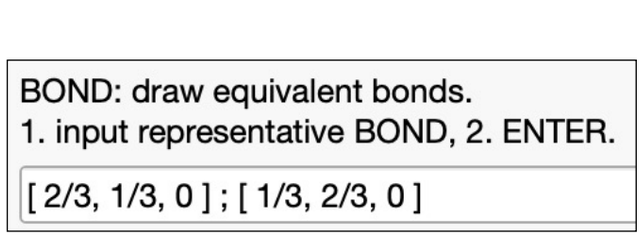
1. Choose space group

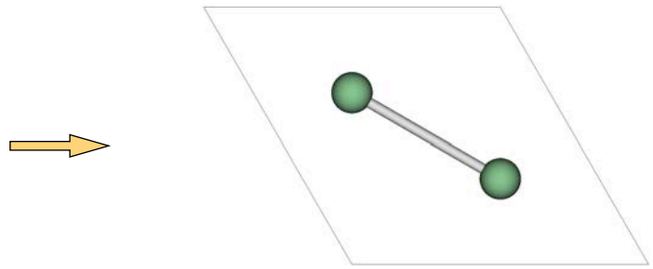
2. Input site



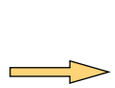


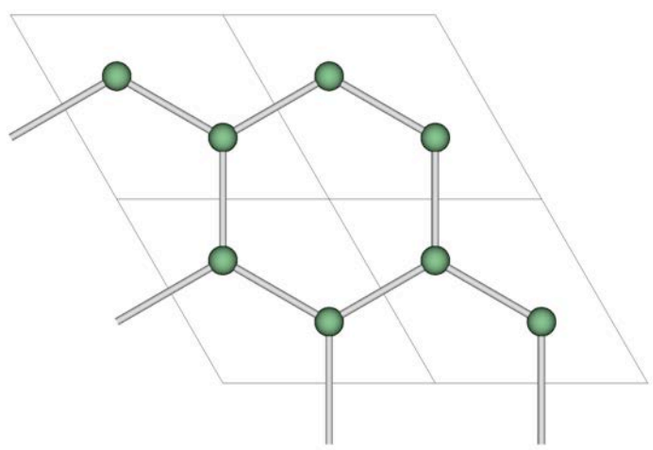
3. Input bond



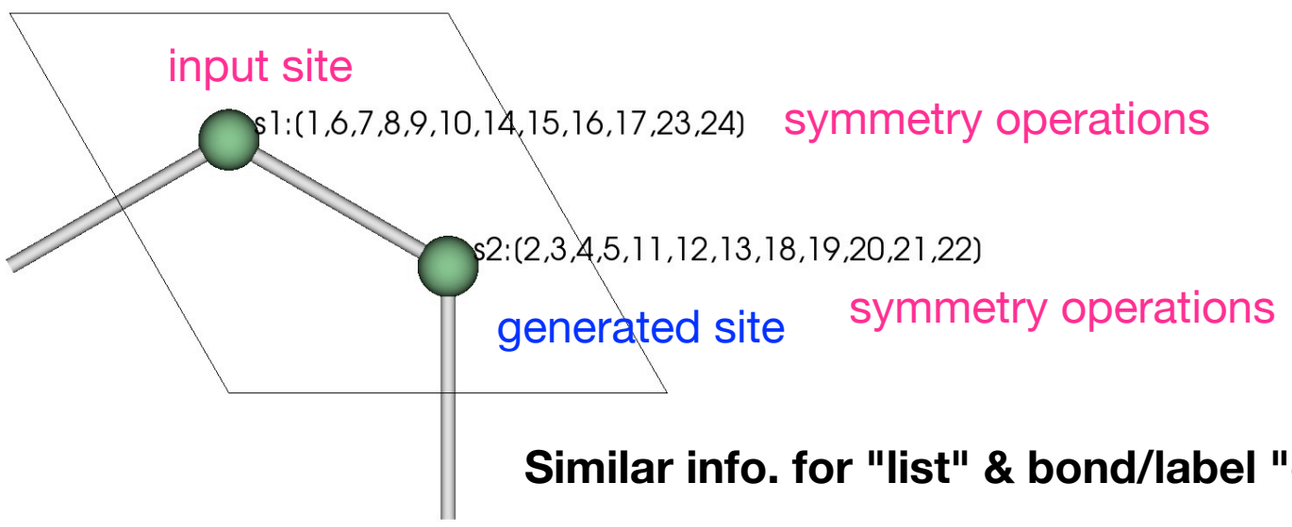


4. Push "clip" and "repeat"





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



Similar info. for "list" & bond/label "on"

QtDraw+ - SAMB Drawing

Draw SAMB for "graphene"

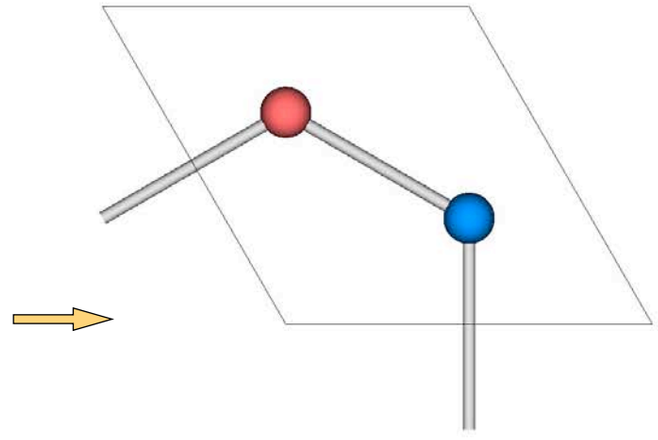
1. Draw "mass term"

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,) x Qs(3,B1u,) draw



Z MP basis atomic x site-cluster

2. Draw "Rashba SOC"

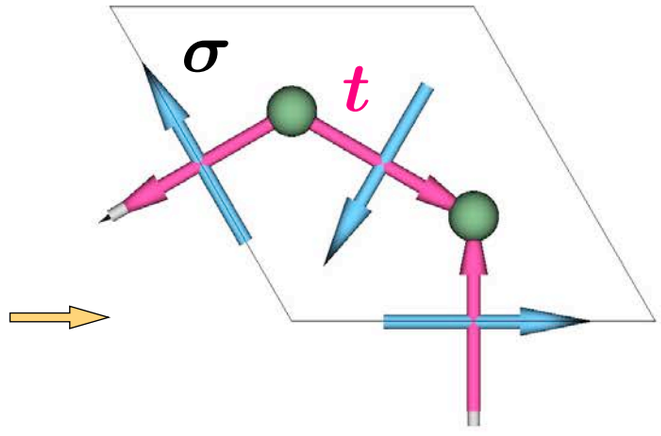
HOPPING: draw hopping direction.
1. input representative BOND, + ENTER. — draw hopping direction

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

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

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

⇒ Q Q01: Q(1,A2u,,) = Ma(1,E1g,) x Tb(1,E1u,) draw



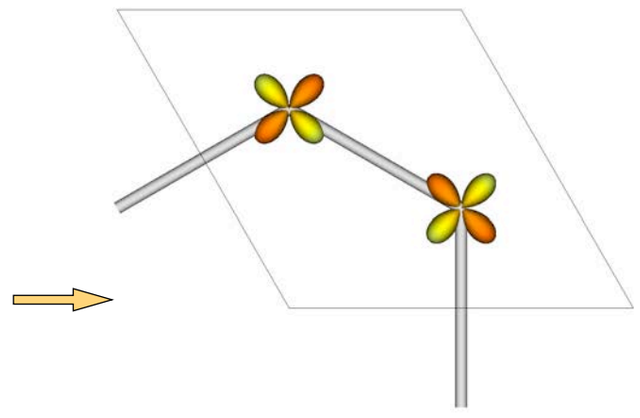
Z MP basis atomic x bond-cluster

3. Draw "cluster quadrupole order"

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

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

⇒ Q Q01: Q(1,E1u,,0) = Qa(2,E2g,) x Qs(3,B1u,) draw



Electric E_{1u} order

QtDraw+ - Modulation Drawing

SAMB modulation

$$\{\, \boldsymbol{X}_\eta(\boldsymbol{p}_s;\boldsymbol{R}) \,\} = \sum_i^{\text{coeff}} c_i \mathbb{X}_i \cos[\boldsymbol{k}_i \cdot (\boldsymbol{R}+\boldsymbol{p}_s) - \frac{\pi}{2} n_i]$$

basis · k · cell · plus set · phase

n = 0 : cos
n = 1 : sin

for given [[X, c, k, n]]

Draw SAMB modulation for "graphene"

1. Simple AFM (single-k)

2. Vortex-like AFM (triple-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
⇒ 3. choose (type,basis), 4. push `draw` o

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

(c) Open modulation panel, and edit

modulation | T,M

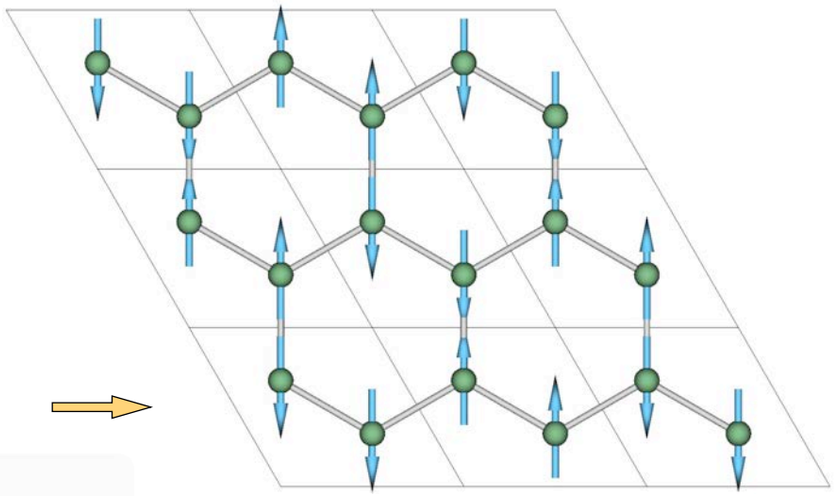
Modulation - vector

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



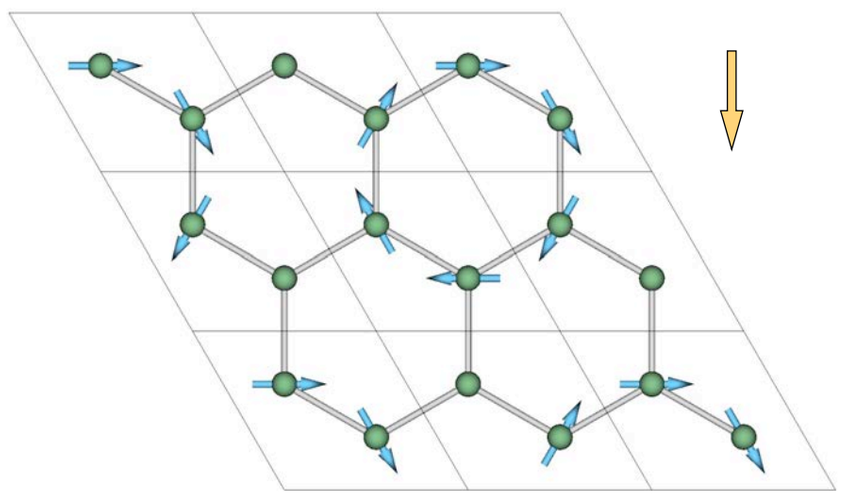
Modulation - vector

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. D3^4

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

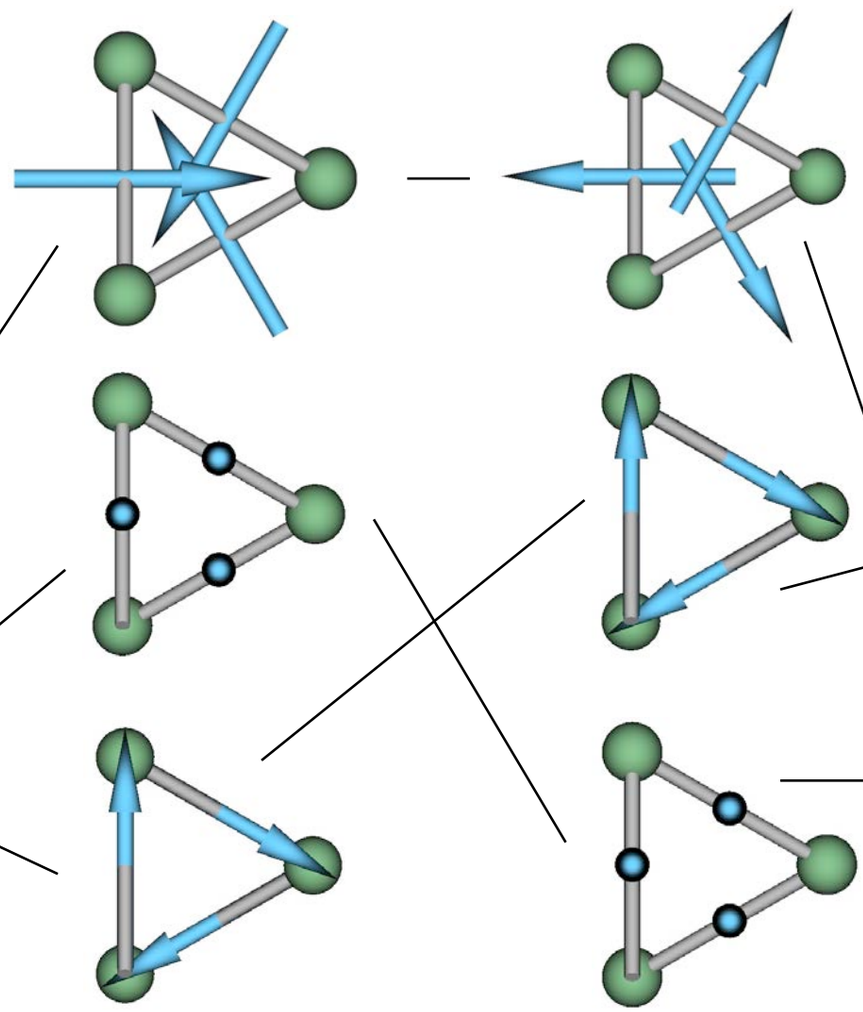
Q(1,A2,,) = Ma(1,E,) x Tb(1,E,)
Q(1,E,,0) = Ma(1,A2,) x Tb(1,E,)
Q(1,E,,1) = Ma(1,A2,) x Tb(1,E,)

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)

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(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

space group | trigonal | 152. D3^4

cf. Te

$$\chi_i^{\alpha\beta} = a_0 \mathbb{Q}_0 + \sum_\alpha b_\alpha \mathbb{Q}_{2,\alpha}$$

electric symmetric tensor = site-cluster mono/quadrupole

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`.

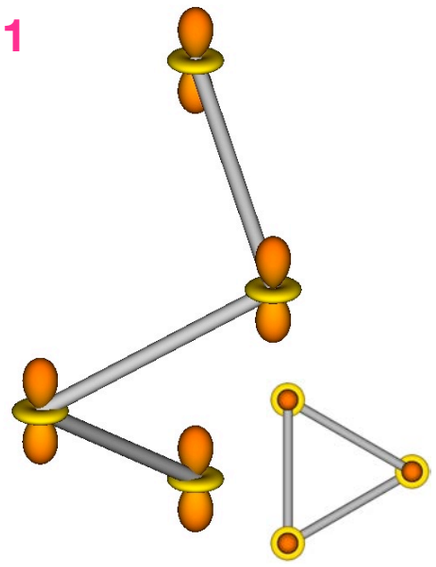
Q | 2 | [0.3, 0, 1/3]

	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,)
1	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,)
2	Q(3,A1,,) = Qa(2,E,2) x Qs(1,E,)
	Q(3,A2,2,) = Qa(2,E,2) x Qs(1,E,)

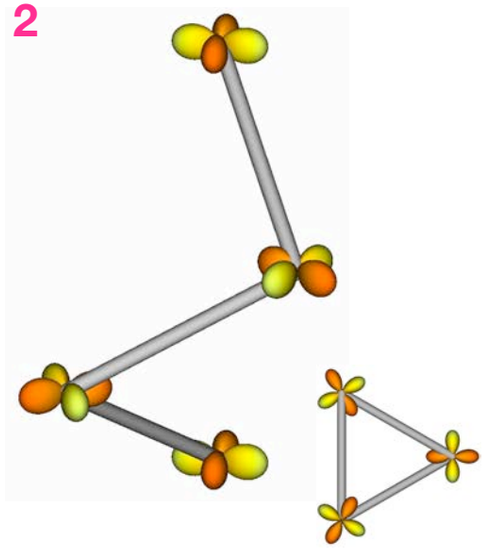
3	G(2,A1,,) = Qa(2,E,1) x Qs(1,E,)
	G(2,E,1,0) = Qa(2,A1,) x Qs(1,E,)
	G(2,E,1,1) = Qa(2,A1,) x Qs(1,E,)
	G(2,E,2,0) = Qa(2,E,1) x Qs(1,E,)
	G(2,E,2,1) = Qa(2,E,1) x Qs(1,E,)

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

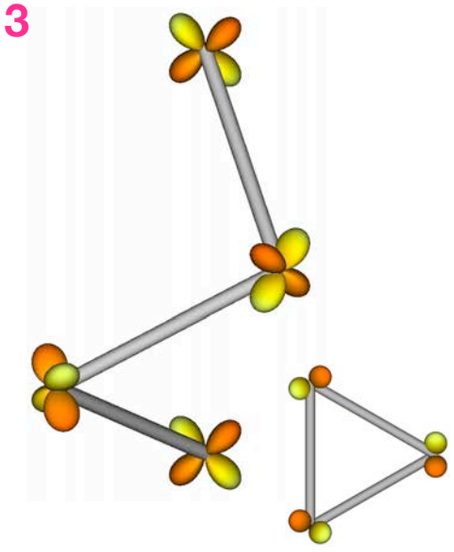
1



2



3



Application - SAMB Decomposition

Stiffness of Phonon

Te

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

$$g_{ij}^{\alpha\beta} = a_0 \mathbb{Q}_0 + \sum_\alpha b_\alpha \mathbb{Q}_{2,\alpha}$$

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`.

Q | 2 | [0.3, 0, 1/3] ; [0, 0.3, 2/3]

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

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

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

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

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

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

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

Q(2,E,2,0) = Qa(2,E,1) x Qb(2,E,1)

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

Q(2,E,2,1) = Qa(2,E,1) x Qb(2,E,1)

G(1,A2,,) = Qa(2,E,1) x Qb(2,E,1)

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

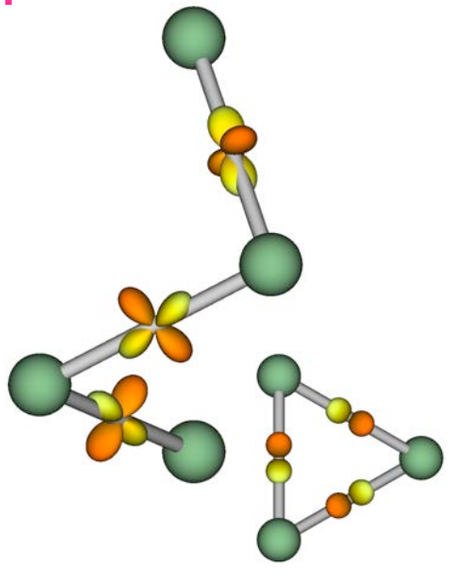
G(1,E,,1) = Qa(2,A1,) x Qb(2,E,1)

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

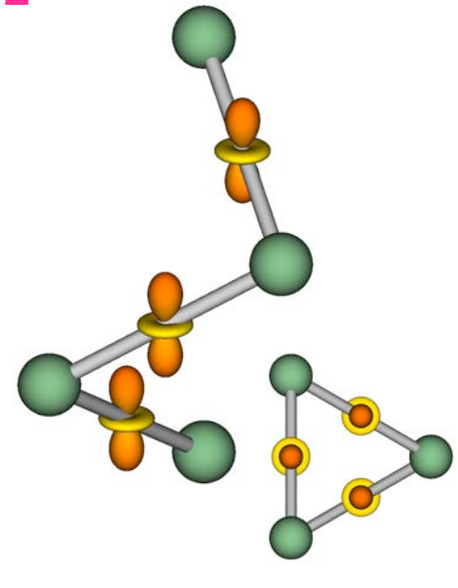
G(3,A2,2,) = Qa(2,E,2) x Qb(2,E,1)

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

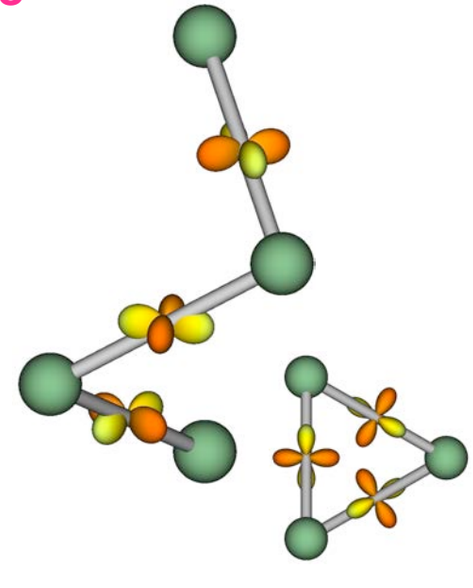
1



2



3



Application - SAMB Decomposition

Other Physical Quantities

Type	Expression	Correspondence	SAMB
Electric potential	ϕq	$q \to \mathbb{Q}^{(\mathrm{a})}_{0,0}$	(E) Atomic (s) & Site-cluster
Crystal field	$\phi_{lm} Q_{lm}$	$Q_{lm} \to \mathbb{Q}^{(\mathrm{a})}_{lm}$	(E) Atomic & Site-cluster
Zeeman term	$-h^a m^a$	$m^a \to \mathbb{M}^{(\mathrm{a})}_{1m}$	(M) Atomic (spinful) & Site-cluster
Spin-orbit int.	$\zeta l^a \sigma^a$	$l^a, \sigma^a \to \mathbb{M}^{(\mathrm{a})}_{1m}$	(E) Atomic (p-spinful) & Site-cluster
Density-density int.	$V_{ij} n_i n_j$	$n_i n_j \to \mathbb{Q}^{(\mathrm{a})}_{0,0}$	(E) Atomic (s) & Bond-cluster
Elastic energy	$\epsilon^{ab}_{ij} u^a_i u^b_j$	$u^a_i u^b_j \to \mathbb{Q}^{(\mathrm{a})}_{0,0}, \mathbb{Q}^{(\mathrm{a})}_{2m}$	(E) Atomic (p) & Bond-cluster
Exchange int.	$J^{ab}_{ij} S^a_i S^b_j$	$S^a_i S^b_j \to \mathbb{Q}^{(\mathrm{a})}_{0,0}, \mathbb{Q}^{(\mathrm{a})}_{2m}$	(E) Atomic (p) & Bond-cluster
DM int.	$D^c_{ij} \epsilon_{abc} S^a_i S^b_j$	$\epsilon_{abc} S^a_i S^b_j \to \mathbb{G}^{(\mathrm{a})}_{lm}$	(ET) Atomic (p) & Bond-cluster
Real hopping	$t_{ij} c^\dagger_i c_j + \mathrm{H.c.}$	$c^\dagger_i c_j + \mathrm{H.c.} \to \mathbb{Q}^{(\mathrm{b})}_{lm}$	(all) Atomic & Bond-cluster
Imaginary hopping	$\mathrm{i}\, t_{ij} c^\dagger_i c_j + \mathrm{H.c.}$	$\mathrm{i}\, c^\dagger_i c_j + \mathrm{H.c.} \to \mathbb{T}^{(\mathrm{b})}_{lm}$	(all) Atomic & Bond-cluster

Various quantities can be expressed by using SAMB