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# **Onsager Documentation**

***Release 1.0***

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Contents:



## ONSAGER

Documentation now available at the [Onsager github page](<http://dallastrinkle.github.io/Onsager/>). Please cite as [[DOI](<https://zenodo.org/badge/14172/DallasTrinkle/Onsager.svg>)](<https://zenodo.org/badge/latestdoi/14172/DallasTrinkle/Onsager>) or see [Onsager github](#) for current version doi information.

The Onsager package provides routines for the general calculation of transport coefficients in vacancy-mediated diffusion and interstitial diffusion. It does this using a Green function approach, combined with point group symmetry reduction for maximum efficiency.

Typical usage looks like:

```
#!/usr/bin/env python

from onsager import crystal
from onsager import OnsagerCalc

...
```

Many of the subpackages within Onsager are support for the main attraction, which is in `OnsagerCalc`. Interstitial calculation examples are available in `bin`, including three YAML input files, as well as a interstitial diffuser. An example of vacancy-mediated diffusion is shown in `bin/fivefreq.py`, which computes the well-known five-frequency model for substitutional solute transport in an FCC lattice.

The tests for the package are include in `test`; `tests.py` will run all of the tests in the directory with verbosity level 2. This can be time-consuming (on the order of several of minutes) to run all tests; coverage is currently >90%.

The code uses YAML files for input/output of diffusion data for the interstitial calculator. The vacancy-mediated calculator requires much more data, and uses HDF5 format to save/reload as needed. The vacancy-mediated calculator uses tags (unique human-readable-ish strings) to identify all (symmetry-unique) vacancy, solute, and complex states, and transitions between them.

Releases:

- 0.9. Full release of Interstitial calculator, along with theory paper (see References below).
- 0.9.1. Added spin degrees of freedom to `crystal` for symmetry purposes; added `supercell` class to aid in automated setup of calculation.
- 1.0 Now including automator for supercell calculations.





## REFERENCES

- Dallas R. Trinkle, “Diffusivity and derivatives for interstitial solutes: Activation energy, volume, and elastodiffusion tensors.” [arXiv:1605.03623](<http://arxiv.org/abs/1605.03623>)



## CONTRIBUTORS

- Dallas R. Trinkle, initial design, derivation, and implementation.
- Ravi Agarwal, testing of HCP interstitial calculations; testing of HCP vacancy-mediated diffusion calculations
- Abhinav Jain, testing of HCP vacancy-mediated diffusion calculations.

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## CRYSTAL

Crystal:

The crystal module defines the `crystal` class, and `GroupOp` for group operations. `Crystal` class

Class to store definition of a crystal, along with some analysis 1. geometric analysis (nearest neighbor displacements) 2. space group operations 3. point group operations for each basis position 4. Wyckoff position generation (for interstitials)

`crystal.CombineTensorBasis` (*b1*, *b2*, *symmetric=True*)

Combines (intersects) two tensor spaces into one; uses SVD to compute null space.

**Parameters**

- **b1** – list of tensors
- **b2** – list of tensors

**Return** **tensorbasis** list of 2nd-rank symmetric tensors making up the basis

`crystal.CombineVectorBasis` (*b1*, *b2*)

Combines (intersects) two vector spaces into one.

**Parameters**

- **b1** – (dim, vect) – dimensionality (0..3), vector defining line direction (1) or plane normal (2)
- **b2** – (dim, vect)

**Return** **dim** dimensionality, 0..3

**Return** **vect** vector defining line direction (1) or plane normal (2)

**class** `crystal.Crystal` (*lattice*, *basis*, *chemistry=None*, *spins=None*, *NOSYM=False*, *noreduce=False*)

A class that defines a crystal, as well as the symmetry analysis that goes along with it. Now includes optional spins. These can be vectors or “scalar” spins, for which we need to consider a phase factor. In general, they can be complex. Ideally, they should have magnitude either 0 or 1.

Specified by a lattice (3 vectors), a basis (list of lists of positions in direct coordinates). Can also name the elements (chemistry), and specify spin degrees of freedom.

**classmethod** `BCC` (*a0*, *chemistry=None*)

Create a body-centered cubic crystal with lattice constant *a0*

**Parameters** **a0** – lattice constant

**Return** **BCC crystal**

**classmethod** `FCC` (*a0*, *chemistry=None*)

Create a face-centered cubic crystal with lattice constant *a0*

**Parameters** **a0** – lattice constant

**Return** FCC crystal

**FullVectorBasis** (*chem=None*)

Generate our full vector basis, using the information from our crystal

**Parameters** **chem** – (optional) chemical index to consider; otherwise return a list of such

**Return** **VBfunctions** (list) of our unique vector basis lattice functions, normalized; each is an array (NVbasis x Nsites x 3)

**Return** **VVouter** (list) of our VV “outer” expansion (NVbasis x NVbasis for each chemistry)

**classmethod HCP** (*a0, c\_a=1.6329931618554521, chemistry=None*)

Create a hexagonal closed packed crystal with lattice constant a0, c/a ratio c\_a

**Parameters**

- **a0** – lattice constant
- **c\_a** – (optional) c/a ratio, default=ideal  $\sqrt{8/3}$

**Return** HCP crystal

**SymmTensorBasis** (*ind*)

Generates the symmetric tensor basis corresponding to an atomic site

**Parameters** **ind** – tuple index for atom

**Return** **tensorbasis** list of 2nd-rank symmetric tensors making up the basis

**VectorBasis** (*ind*)

Generates the vector basis corresponding to an atomic site

**Parameters** **ind** – tuple index for atom

**Return** **dim** dimensionality, 0..3

**Return** **vect** vector defining line direction (1) or plane normal (2)

**Wyckoffpos** (*uvec*)

Generates all the equivalent Wyckoff positions for a unit cell vector.

**Parameters** **uvec** – 3-vector (float) vector in direct coordinates

**Return** **Wyckofflist** list of equivalent Wyckoff positions

**\_\_init\_\_** (*lattice, basis, chemistry=None, spins=None, NOSYM=False, noreduce=False*)

Initialization; starts off with the lattice vector definition and the basis vectors. While it does not explicitly store the specific chemical elements involved, it does store that there are different elements.

**Parameters**

- **lattice** – array[3,3] or list of array[3] lattice vectors; if [3,3] array, then the vectors need to be in *column* format so that the first lattice vector is `lattice[:,0]`
- **basis** – list of array[3] or list of list of array[3] crystalline basis vectors, in unit cell coordinates. If a list of lists, then there are multiple chemical elements, with each list corresponding to a unique element
- **chemistry** – (optional) list of names of chemical elements
- **spins** – (optional) list of numbers (complex) / vectors or list of list of same spins for individual atoms; if not None, needs to match the basis. Can either be scalars or vectors, corresponding to collinear or non-collinear magnetism



- **NOSYM** – turn off all symmetry finding (except identity)
- **noreduce** – do not attempt to reduce the atomic basis

**\_\_repr\_\_()**

String representation of crystal (lattice + basis)

**\_\_str\_\_()**

Human-readable version of crystal (lattice + basis)

**\_\_weakref\_\_**

list of weak references to the object (if defined)

**addbasis** (*basis*, *chemistry=None*, *spins=None*)

Returns a new Crystal object that contains additional sites (assumed to be new chemistry). This is intended to “add in” interstitial sites. Note: if the symmetry is to be maintained, should be the output from Wyckoffpos().

#### Parameters

- **basis** – list (or list of lists) of new sites
- **chemistry** – (optional) list of chemistry names
- **spins** – (optional) list of spins

**Return Crystal** new crystal object, with additional sites

**calcmetric()**

Computes the volume of the cell and the metric tensor

**Return volume** cell volume

**Return metric tensor** 3x3

**cart2pos** (*v*)

Return the lattvec and index corresponding to an atomic position in cartesian coord.

**Parameters** **v** – 3-vector (float) position in Cartesian coordinates

**Return lattvec** 3-vector (integer) lattice vector in direct coordinates,

**Return (c,i)** tuple of matching basis atom; None if no match

**cart2unit** (*v*)

Return the lattvec and unit cell coord. corresponding to a position in cartesian coord.

**Parameters** **v** – 3-vector (float) position in Cartesian coordinates

**Return lattvec** 3-vector (integer) lattice vector in direct coordinates,

**Return uvec** 3-vector (float) inside unit cell, in direct coordinates

**center()**

Center the atoms in the cell if there is an inversion operation present.

**chemindex** (*chemistry*)

Return index corresponding to chemistry; None if not present.

**Parameters** **chemistry** – value to check

**Return index** corresponding to chemistry

**classmethod fromdict** (*yamldict*)

Creates a Crystal object from a *very simple* YAML-created dictionary

**Parameters** **yamldict** – dictionary; must contain ‘lattice’ (using *row* vectors!) and ‘basis’; can contain optional ‘lattice\_constant’

**Return** **Crystal(lattice.T, basis)** new crystal object

**fullkptmesh** (*Nmesh*)

Creates a k-point mesh of density given by *Nmesh*; does not symmetrize but does put the k-points inside the BZ. Does not return any *weights* as every point is equally weighted.

**Parameters** **Nmesh** – mesh divisions *Nmesh*[0] x *Nmesh*[1] x *Nmesh*[2]

**Return** **kpt** array[*Nkpt*][3] of kpoints

**g\_cart** (*g*, *x*)

Apply a space group operation to a (Cartesian) vector position

**Parameters**

- **g** – group operation (GroupOp)
- **x** – 3-vector position in space

**Return** **gx** 3-vector position in space (Cartesian coordinates)

**static g\_direct** (*g*, *direc*)

Apply a space group operation to a direction

**Parameters**

- **g** – group operation (GroupOp)
- **direc** – 3-vector direction

**Return** **gdirec** 3-vector direction

**g\_direct\_equivalent** (*d1*, *d2*, *threshold=1e-08*)

Tells us if two directions are equivalent by according to the space group

**Parameters**

- **d1** – direction one (array[3])
- **d2** – direction two (array[3])
- **threshold** – threshold for equality

**Return** **equivalent** True if equivalent by a point group operation

**g\_pos** (*g*, *lattvec*, *ind*)

Apply a space group operation to an atom position specified by its lattice and index

**Parameters**

- **g** – group operation (GroupOp)
- **lattvec** – 3-vector (integer) lattice vector in direct coordinates
- **ind** – two-tuple index specifying the atom: (atomtype, atomindex)

**Return** **glatt** 3-vector (integer) lattice vector in direct coordinates

**Return** **gindex** tuple of new basis atom

**static g\_tensor** (*g*, *tensor*)

Apply a space group operation to a 2nd-rank tensor

**Parameters**

- **g** – group operation (GroupOp)

- **tensor** – 2nd-rank tensor

**Return gtensor** 2nd-rank tensor

**static g\_vect** (*g, lattvec, uvec*)

Apply a space group operation to a vector position specified by its lattice and a location in the unit cell in direct coordinates

**Parameters**

- **g** – group operation (GroupOp)
- **lattvec** – 3-vector (integer) lattice vector in direct coordinates
- **uvec** – 3-vector (float) vector in direct coordinates
- **guvec** – 3-vector (float) vector in direct coordinates

**Return glatt** 3-vector (integer) lattice vector in direct coordinates

**genBZG** ()

Generates the reciprocal lattice G points that define the Brillouin zone.

**Return Garray** array of G vectors that define the BZ, in Cartesian coordinates

**genWyckoffsets** ()

Generate our Wyckoff sets.

**Return Wyckoffsets** set of sets of tuples of positions that correspond to identical Wyckoff positions

**gengroup** ()

Generate all of the space group operations. Now handles spins! Doesn't store spin phase factors for each group operation, though.

**Return Gset** frozenset of group operations

**genpoint** ()

Generate our point group indices. Done with crazy list comprehension due to the structure of our basis.

**Return Gpointlists** list of lists of frozensets of point group operations that leave a site unchanged

**inBZ** (*vec, BZG=None, threshold=1e-05*)

Tells us if vec is inside our set of defining points.

**Parameters**

- **vec** – array [3], vector to be tested
- **BZG** – array [:,3], optional (default = self.BZG), array of vectors that define the BZ
- **threshold** – double, optional, threshold to use for “equality”

**Return inBZ** False if outside the BZ, True otherwise

**jumpnetwork** (*chem, cutoff, closestdistance=0*)

Generate the full jump network for a specific chemical index, out to a cutoff. Organized by symmetry-unique transitions. Note that i->j and j->i are always related to one-another, but by equivalence of transition state, not symmetry. Now updated with closest-distance parameter.

**Parameters**

- **chem** – index corresponding to the chemistry to consider
- **cutoff** – distance cutoff

- **closestdistance** – closest distance allowed in transition (can be a list)

**Return jumpnetwork** list of symmetry-unique transitions; each is a list of tuples:  $((i, j), dx)$  corresponding to jump from  $i \rightarrow j$  with vector  $\delta x$

**jumpnetwork2lattice** (*chem, jumpnetwork*)

Convert a “standard” jumpnetwork (that specifies displacement vectors  $dx$ ) into a lattice representation, where we replace  $dx$  with the lattice vector from  $i$  to  $j$ .

#### Parameters

- **chem** – index corresponding to the chemistry to consider
- **jumpnetwork** – list of symmetry-unique transitions; each is a list of tuples:  $((i, j), dx)$  corresponding to jump from  $i \rightarrow j$  with vector  $\delta x$

**Return jumplattice** list of symmetry-unique transitions; each is a list of tuples:  $((i, j), R)$  corresponding to jump from  $i$  in unit cell 0  $\rightarrow j$  in unit cell  $R$

**minlattice** ()

Try to find the optimal lattice vector definition for a crystal. Our definition of optimal is (a) length of each lattice vector is minimal; (b) the vectors are ordered from shortest to longest; (c) the vectors have minimal dot product; (d) the basis is right-handed.

Works recursively, and in-place.

**nnlist** (*ind, cutoff*)

Generate the nearest neighbor list for a given cutoff. Only consider neighbor vectors for atoms of the same type. Returns a list of cartesian vectors.

#### Parameters

- **ind** – tuple index for atom
- **cutoff** – distance cutoff

**Return nnlist** list of nearest neighbor vectors

**pos2cart** (*lattvec, ind*)

Return the cartesian coordinates of an atom specified by its lattice and index

#### Parameters

- **lattvec** – 3-vector (integer) lattice vector in direct coordinates
- **ind** – two-tuple index specifying the atom: (atomtype, atomindex)

**Return v** 3-vector (float) in Cartesian coordinates

**reduce** (*threshold=1e-08*)

Reduces the lattice and basis, if needed. Works (tail) recursively.

**reducekptmesh** (*kptfull, threshold=1e-08*)

Takes a fully expanded mesh, and reduces it by symmetry. Assumes every point is equally weighted. We would need a different (more complicated) algorithm if not true...

#### Parameters

- **kptfull** – array[Nkpt][3] of kpoints
- **threshold** – threshold for symmetry equality

**Return kptsymm** array[Nsymm][3] of kpoints

**Return weight** array[Nsymm] of weights (integrates to 1)

**remapbasis** (*supercell*)

Takes the basis definition, and using a supercell definition, returns a new basis

**Parameters** **supercell** – integer array[3,3]

**Return atomic basis** list of list of positions

**simpleYAML** (*a0=1.0*)

Creates a simplified YAML dump, in case we don't want to output the full symmetry analysis

**Return YAML** string dump

**sitelist** (*chem*)

Return a list of lists of Wyckoff-related sites for a given chemistry. Done with a single list comprehension–useful as input for diffusion calculation

**Parameters** **chem** – index corresponding to chemistry to consider

**Return symmequivsites** list of lists of indices that are equivalent by symmetry

**strain** (*eps*)

Returns a new Crystal object that is a strained version of the current.

**Parameters** **eps** – strain tensor

**Return Crystal** new crystal object, strained

**unit2cart** (*lattvec, uvec*)

Return the cartesian coordinates of a position specified by its lattice and unit cell coordinates

**Parameters**

- **lattvec** – 3-vector (integer) lattice vector in direct coordinates
- **uvec** – 3-vector (float) unit cell vector in direct coordinates

**Return v** 3-vector (float) in Cartesian coordinates

**static vectlist** (*vb*)

Returns a list of orthonormal vectors corresponding to our vector basis.

**Parameters** **vb** – (dim, v)

**Return vlist** list of vectors

**class** `crystal.GroupOp`

A class corresponding to a group operation. Based on namedtuple, so it is immutable.

Intended to be used in combination with Crystal, we have a few operations that can be defined out-of-the-box.

**Parameters**

- **rot** – np.array(3,3) integer idempotent matrix
- **trans** – np.array(3) real vector
- **cartrot** – np.array(3,3) real unitary matrix
- **indexmap** – tuples of tuples, containing the atom mapping

**static GroupOp\_constructor** (*loader, node*)

Construct a GroupOp from YAML

**static GroupOp\_representer** (*dumper, data*)

Output a GroupOp

**\_\_add\_\_** (*other*)

Add a translation to our group operation

`__eq__ (other)`

Test for equality—we use `numpy.isclose` for comparison, since that’s what we usually care about

`__hash__ ()`

Hash, so that we can make sets of group operations

`__mul__ (other)`

Multiply two group operations to produce a new group operation

`__ne__ (other)`

Inequality == not `__eq__`

`__sane__ ()`

Return true if the cartrot and rot are consistent and ‘sane’

`__str__ ()`

Human-readable version of `groupop`

`__sub__ (other)`

Add a (negative) translation to our group operation

**eigen ()**

Returns the type of group operation (single integer) and eigenvectors. 1 = identity 2, 3, 4, 6 = n- fold rotation around an axis negative = rotation + mirror operation, perpendicular to axis “special cases”: -1 = mirror, -2 = inversion

`eigenvect[0]` = axis of rotation / mirror `eigenvect[1]`, `eigenvect[2]` = orthonormal vectors to define the plane giving a right-handed coordinate system and where rotation around [0] is positive, and the positive imaginary eigenvector for the complex eigenvalue is `[1] + i [2]`.

**Return type** integer

**Return eigenvectors** list of `[ev0, ev1, ev2]`

**classmethod ident** (*basis*)

Return a group operation corresponding to identity for a given basis

**incell ()**

Return a version of `groupop` where the translation is in the unit cell

**inhalf ()**

Return a version of `groupop` where the translation is in the centered unit cell

**inv ()**

Construct and return the inverse of the group operation

**static optype** (*rot*)

Returns the type of group operation (single integer) and eigenvectors. 1 = identity 2, 3, 4, 6 = n- fold rotation around an axis negative = rotation + mirror operation, perpendicular to axis “special cases”: -1 = mirror, -2 = inversion

**Parameters** **rot** – rotation matrix (can be the integer `rot`)

**Return type** integer

`crystal.ProjectTensorBasis` (*tensor, basis*)

Given a tensor, project it onto the basis.

**Parameters**

- **tensor** – tensor
- **basis** – list consisting of an orthonormal basis

**Return tensor** tensor, projected

`crystal.SymmTensorBasis (rottype, eigenvect)`

Returns a symmetric second-rank tensor basis corresponding to the optype and eigenvectors for a GroupOp

**Parameters**

- **rottype** – output from `eigen()`
- **eigenvect** – eigenvectors

**Return tensorbasis** list of 2nd-rank symmetric tensors making up the basis

`crystal.VectorBasis (rottype, eigenvect)`

Returns a vector basis corresponding to the optype and eigenvectors for a GroupOp

**Parameters**

- **rottype** – output from `eigen()`
- **eigenvect** – eigenvectors

**Return dim** dimensionality, 0..3

**Return vect** vector defining line direction (1) or plane normal (2)

`crystal.Voigtstrain (e1, e2, e3, e4, e5, e6)`

Returns a symmetric strain tensor from the Voigt reduced strain values.

**Parameters**

- **e1** – xx
- **e2** – yy
- **e3** – zz
- **e4** – yz + zx
- **e5** – zx + xz
- **e6** – xy + yx

**Return strain** symmetric strain tensor

`crystal.incell (vec)`

Returns the vector inside the unit cell (in [0,1]\*\*3)

**Parameters** **vec** – 3-vector (unit coord)

**Returns** 3-vector

`crystal.inhalf (vec)`

Returns the vector inside the centered cell (in [-0.5,0.5]\*\*3)

**Parameters** **vec** – 3-vector (unit coord)

**Returns** 3-vector

`crystal.maptranslation (oldpos, newpos, oldspins=None, newspins=None, threshold=1e-08)`

Given a list of transformed positions, identify if there's a translation vector that maps from the current positions to the new position.

The mapping specifies the index that the *translated* atom corresponds to in the original position set. If unable to construct a mapping, the mapping return is None; the translation vector will be meaningless.

If old/newspins are given then ONLY mappings that maintain spin are considered. This means that a loop is needed to consider possible spin phase factors.

**Parameters**

- **oldpos** – list of list of array[3]
- **newpos** – list of list of array[3], same layout as oldpos
- **oldspins** – (optional) list of list of numbers/arrays
- **newspins** – (optional) list of list of numbers/arrays

**Return translation** array[3]

**Return mapping** list of list of indices

`crystal.ndarray_representer(dumper, data)`

Output a numpy array



## CRYSTALSTARS

CrystalStars:

The crystalStars module defines the classes corresponding to stars (in this case, for solute-vacancy complexes that are equivalent by space group symmetry), and vector stars (the inclusion of a vector basis on the stars). These modules are primarily responsible for all the symmetry analysis, and converting that into matrix forms for rapid numerical evaluation as needed. Stars module, modified to work with crystal class

Classes to generate star sets, double star sets, and vector star sets; a lot of indexing functionality.

NOTE: The naming follows that of stars; the functionality is extremely similar, and this code was modified as little as possible to translate that functionality to *crystals* which possess a basis. In the case of a single atom basis, this should reduce to the stars object functionality.

The big changes are:

- Replacing NNvect star (which represents the jumps) with the jumpnetwork type found in crystal
- Using the jumpnetwork\_latt representation from crystal
- Representing a “point” as a solute + vacancy. In this case, it is a tuple (s,v) of unit cell indices and a vector dx or dR (dx = Cartesian vector pointing from solute to vacancy; dR = lattice vector pointing from unit cell of solute to unit cell of vacancy). This is equivalent to our old representation if the tuple (s,v) = (0,0) for all sites. Due to translational invariance, the solute always stays inside the unit cell
- Using indices into the point list rather than just making lists of the vectors themselves. This is because the “points” now have a more complex representation (see above).

`crystalStars.PSlist2array (PSlist)`

Take in a list of pair states; return arrays that can be stored in HDF5 format

**Parameters** **PSlist** – list of pair states

**Return** **ij** int\_array[N][2] = (i,j)

**Return** **R** int[N][3]

**Return** **dx** float[N][3]

**class** `crystalStars.PairState`

A class corresponding to a “pair” state; in this case, a solute-vacancy pair, but can also be a transition state pair. The solute (or initial state) is in unit cell 0, in position indexed i; the vacancy (or final state) is in unit cell R, in position indexed j. The cartesian vector dx connects them. We can add and subtract, negate, and “endpoint” subtract (useful for determining what Green function entry to use)

**Parameters**

- **i** – index of the first member of the pair (solute)
- **j** – index of the second member of the pair (vacancy)

- **R** – lattice vector pointing from unit cell of *i* to unit cell of *j*
- **dx** – Cartesian vector pointing from first to second member of pair

**static PairState\_constructor** (*loader, node*)

Construct a GroupOp from YAML

**static PairState\_representer** (*dumper, data*)

Output a PairState

**\_\_add\_\_** (*other*)

Add two states: works if and only if  $\text{self.j} == \text{other.i}$   $(i,j) R + (j,k) R' = (i,k) R+R'$  : works for thinking about transitions... Note:  $a + b \neq b + a$ , and may be that only one of those is even defined

**\_\_eq\_\_** (*other*)

Test for equality—we don't bother checking *dx*

**\_\_hash\_\_** ()

Hash, so that we can make sets of states

**\_\_ne\_\_** (*other*)

Inequality == not **\_\_eq\_\_**

**\_\_neg\_\_** ()

Negation of state (swap members of pair)  $-(i,j) R = (j,i) -R$  Note:  $a + (-a) == (-a) + a == 0$  because we define what “zero” is.

**\_\_sane\_\_** (*crys, chem*)

Determine if the *dx* value makes sense given everything else...

**\_\_str\_\_** ()

Human readable version

**\_\_sub\_\_** (*other*)

Add a negative:  $a-b$  points from initial of *a* to initial of *b* if same final state  $(i,j) R - (k,j) R' = (i,k) R-R'$  Note: this means that  $(a-b) + b = a$ , but  $b + (a-b)$  is an error.  $(b-a) + a = b$

**\_\_xor\_\_** (*other*)

Subtraction on the endpoints (sort of the “opposite” of  $a-b$ ):  $a^b$  points from final of *b* to final of *a* if same initial state  $(i,j) R \wedge (i,k) R' = (k,j) R-R'$  Note:  $b + (a^b) = a$  but  $(a^b) + b$  is an error.  $a + (b^a) = b$

**classmethod fromcrys** (*crys, chem, ij, dx*)

Convert (*i,j*), *dx* into PairState

**classmethod fromcrys\_latt** (*crys, chem, ij, R*)

Convert (*i,j*), *R* into PairState

**g** (*crys, chem, g*)

Apply group operation.

#### Parameters

- **crys** – crystal
- **chem** – chemical index
- **g** – group operation (from *crys*)

**Return** **g\*PairState** corresponding to group operation applied to self

**iszero** ()

Quicker than  $\text{self} == \text{PairState.zero}()$

**classmethod zero** (*n=0*)

Return a “zero” state

**class** `crystalStars.StarSet` (*jumpnetwork, crys, chem, Nshells=0, lattice=False*)

A class to construct crystal stars, and be able to efficiently index.

Takes in a `jumpnetwork`, which is used to construct the corresponding stars, a crystal object with which to operate, a specification of the chemical index for the atom moving (needs to be consistent with `jumpnetwork` and `crys`), and then the number of shells.

In this case, `shells` = number of successive “jumps” from a state. As an example, in FCC, 1 shell = 1st neighbor, 2 shell = 1-4th neighbors.

`__add__` (*other*)

Add two StarSets together; done by making a copy of one, and iadding

`__contains__` (*PS*)

Return true if PS is in the star

`__iadd__` (*other*)

Add another StarSet to this one; very similar to `generate()`

`__init__` (*jumpnetwork, crys, chem, Nshells=0, lattice=False*)

Initiates a star set generator for a given `jumpnetwork`, crystal, and specified chemical index.

#### Parameters

- **jumpnetwork** – list of symmetry unique jumps, as a list of list of tuples; either  $((i, j), dx)$  for jump from  $i$  to  $j$  with displacement  $dx$ , or  $((i, j), R)$  for jump from  $i$  in unit cell 0  $\rightarrow$   $j$  in unit cell  $R$
- **crys** – crystal where jumps take place
- **chem** – chemical index of atom to consider jumps
- **Nshells** – number of shells to generate
- **lattice** – which form does the `jumpnetwork` take?

`__str__` ()

Human readable version

`__weakref__`

list of weak references to the object (if defined)

**addhdf5** (*HDF5group*)

Adds an HDF5 representation of object into an HDF5group (needs to already exist).

Example: if  $f$  is an open HDF5, then `StarSet.addhdf5(f.create_group('StarSet'))` will (1) create the group named ‘StarSet’, and then (2) put the StarSet representation in that group.

**Parameters** **HDF5group** – HDF5 group

**copy** (*empty=False*)

Return a copy of the StarSet; done as efficiently as possible; empty means skip the shells, etc.

**diffgenerate** (*S1, S2, threshold=1e-08*)

Construct a starSet using endpoint subtraction from starset  $S1$  to starset  $S2$ . Can (will) include zero. Points from vacancy states of  $S1$  to vacancy states of  $S2$ .

#### Parameters

- **S1** – starSet for start
- **S2** – starSet for final
- **threshold** – threshold for sorting magnitudes (can influence symmetry efficiency)

**generate** (*Nshells, threshold=1e-08, originstates=False*)

Construct the points and the stars in the set. Now includes “origin states” by default; these are PairStates that `iszero()` is True; they are only included if they have a nonzero VectorBasis.

**Parameters**

- **Nshells** – number of shells to generate; this is interpreted as subsequent “sums” of jumplist (as we need the solute to be connected to the vacancy by at least one jump)
- **threshold** – threshold for determining equality with symmetry
- **originstates** – include origin states in generate?

**jumpnetwork\_omega1** ()

Generate a jumpnetwork corresponding to vacancy jumping while the solute remains fixed.

**Return jumpnetwork** list of symmetry unique jumps; list of list of tuples (i,f), dx where i,f index into states for the initial and final states, and dx = displacement of vacancy in Cartesian coordinates. Note: if (i,f), dx is present, so if (f,i), -dx

**Return jumptype** list of indices corresponding to the (original) jump type for each symmetry unique jump; useful for constructing a LIMB approximation

**Return starpair** list of tuples of the star indices of the i and f states for each symmetry unique jump

**jumpnetwork\_omega2** ()

Generate a jumpnetwork corresponding to vacancy exchanging with a solute.

**Return jumpnetwork** list of symmetry unique jumps; list of list of tuples (i,f), dx where i,f index into states for the initial and final states, and dx = displacement of vacancy in Cartesian coordinates. Note: if (i,f), dx is present, so if (f,i), -dx

**Return jumptype** list of indices corresponding to the (original) jump type for each symmetry unique jump; useful for constructing a LIMB approximation

**Return starpair** list of tuples of the star indices of the i and f states for each symmetry unique jump

**classmethod loadhdf5** (*crys, HDF5group*)

Creates a new StarSet from an HDF5 group.

**Parameters**

- **crys** – crystal object–MUST BE PASSED IN as it is not stored with the StarSet
- **HDFgroup** – HDF5 group

**Return StarSet** new StarSet object

**starindex** (*PS*)

Return the index for the star to which pair state PS belongs; None if not found

**stateindex** (*PS*)

Return the index of pair state PS; None if not found

**symmatch** (*PS1, PS2*)

True if there exists a group operation that makes PS1 == PS2.

**symmequivjumplist** (*i, f, dx*)

Returns a list of tuples of symmetry equivalent jumps

**Parameters**

- **i** – index of initial state

- **f** – index of final state
- **dx** – displacement vector

**Return symmjumplist** list of tuples of ((gi, gf), gdx) for every group op

**class** crystalStars.**VectorStarSet** (*starset=None*)

A class to construct vector star sets, and be able to efficiently index.

All based on a StarSet

**GFexpansion** (*VectorBasis=()*)

Construct the GF matrix expansion in terms of the star vectors, and indexed to GFstarset. Now takes in a VectorBasis; if not an empty set, returns the expansion of the vector stars to the “origin states” as represented by the VB.

**Parameters VectorBasis** – (optional) list of [Nsites, 3] the vector basis in the unit cell for the solute states

**Return GFexpansion** array[Nsv, Nsv, NGFstars] the GF matrix[i, j] = sum(GFexpansion[i, j, k] \* GF(starGF[k]))

**Return GFstarset** starSet corresponding to the GF

**Return GFOSexpansion** array[NVB, Nsv, NGFstars] the GF matrix[os, i] = sum(GFOSexpansion[os, i, k] \* GF(starGF[k]))

**\_\_init\_\_** (*starset=None*)

Initiates a vector-star generator; work with a given star.

**Parameters starset** – StarSet, from which we pull nearly all of the info that we need

**\_\_weakref\_\_**

list of weak references to the object (if defined)

**addhdf5** (*HDF5group*)

Adds an HDF5 representation of object into an HDF5group (needs to already exist).

**Example: if f is an open HDF5, then StarSet.addhdf5(f.create\_group(‘VectorStarSet’)) will** (1) create the group named ‘VectorStarSet’, and then (2) put the VectorStarSet representation in that group.

**Parameters HDF5group** – HDF5 group

**bareexpansions** (*jumpnetwork, jumptype*)

Construct the bare diffusivity expansion in terms of the jumpnetwork. We return the reference (0) contribution so that the change can be determined; this is useful for the vacancy contributions. This saves us from having to deal with issues with our outer shell where we only have a fraction of the escapes, but as long as the kinetic shell is one more than the thermodynamics (so that the interaction energy is 0, hence no change in probability), this will work. The PS (pair stars) is useful for including the probability factor for the endpoint of the jump; we just call it the ‘probfactor’ below.

Note also: this *currently assumes* that the displacement vector *does not change* between omega0 and omega(1/2).

**Parameters**

- **jumpnetwork** – jumpnetwork of symmetry unique omega1-type jumps, corresponding to our starset. List of lists of (IS, FS), dx tuples, where IS and FS are indices corresponding to states in our starset.
- **jumptype** – specific omega0 jump type that the jump corresponds to

**Return D0expansion** array[3,3, Njump\_omega0] the  $D0[a,b,jt] = \text{sum}(D0\text{expansion}[a,b, jt] * \text{sqrt}(\text{probfactor0}[\text{PS}[jt][0]] * \text{probfactor0}[\text{PS}[jt][1]) * \text{omega0}[jt])$

**Return D1expansion** array[3,3, Njump\_omega1] the  $D1[a,b,k] = \text{sum}(D1\text{expansion}[a,b, k] * \text{sqrt}(\text{probfactor}[\text{PS}[k][0]] * \text{probfactor}[\text{PS}[k][1]) * \text{omega}[k])$

**biasexpansions** (*jumpnetwork, jumptype*)

Construct the bias1 and bias0 vector expansion in terms of the jumpnetwork. We return the bias0 contribution so that the  $db = \text{bias1} - \text{bias0}$  can be determined. This saves us from having to deal with issues with our outer shell where we only have a fraction of the escapes, but as long as the kinetic shell is one more than the thermodynamics (so that the interaction energy is 0, hence no change in probability), this will work. The PS (pair stars) is useful for including the probability factor for the endpoint of the jump; we just call it the ‘probfactor’ below. *Note:* this used to be separated into bias1expansion, and bias2expansion, and had terms that are now in rateexpansions. Note also that if jumpnetwork\_omega2 is passed, it also works for that. However, in that case we have a different approach for the calculation of bias1expansion: if there are origin states, they get the negative summed bias of the others.

**Parameters**

- **jumpnetwork** – jumpnetwork of symmetry unique omega1-type jumps, corresponding to our starset. List of lists of (IS, FS), dx tuples, where IS and FS are indices corresponding to states in our starset.
- **jumptype** – specific omega0 jump type that the jump corresponds to

**Return bias0expansion** array[Nsv, Njump\_omega0] the  $\text{gen0 vector}[i] = \text{sum}(\text{bias0expansion}[i, k] * \text{sqrt}(\text{probfactor0}[\text{PS}[k]]) * \text{omega0}[k])$

**Return bias1expansion** array[Nsv, Njump\_omega1] the  $\text{gen1 vector}[i] = \text{sum}(\text{bias1expansion}[i, k] * \text{sqrt}(\text{probfactor}[\text{PS}[k]] * \text{omega1}[k])$

**generate** (*starset, threshold=1e-08*)

Construct the actual vectors stars

**Parameters starset** – StarSet, from which we pull nearly all of the info that we need

**generateouter** ()

Generate our outer products for our star-vectors.

**Return outer** array [3, 3, Nvstars, Nvstars]  $\text{outer}[:, :, i, j]$  is the 3x3 tensor outer product for two vector-stars  $\text{vs}[i]$  and  $\text{vs}[j]$

**classmethod loadhdf5** (*SSet, HDF5group*)

Creates a new VectorStarSet from an HDF5 group.

**Parameters**

- **SSet** – StarSet–MUST BE PASSED IN as it is not stored with the VectorStarSet
- **HDFgroup** – HDF5 group

**Return VectorStarSet** new VectorStarSet object

**periodicvectorexpansion** (*elemtype='solute'*)

Construct the expansion from vectors on sites in the cell that are periodic to our vectorstar basis. This is used to map from the rate-bias correction vectors into the vectorstar basis, to correct for situations where the vacancy jumps themselves have bias.

**Parameters elemtype** – ‘solute’ or ‘vacancy’, depending on which site we need to check.

**Return periodicexpansion** [Nvstars, Nsites, 3], to map Nsites,3 into Nvstars

**rateexpansions** (*jumpnetwork, jumptype, VectorBasis=()*)

Construct the omega0 and omega1 matrix expansions in terms of the jumpnetwork; includes the escape

terms separately. The escape terms are tricky because they have probability factors that differ from the transitions; the PS (pair stars) is useful for finding this. We just call it the ‘probfactor’ below. *Note:* this used to be separated into rate0expansion, and rate1expansion, and partly in bias1expansion. Note also that if jumpnetwork\_omega2 is passed, it also works for that. However, in that case we have a different approach for the calculation of rate0expansion: if there are origin states, then we need to “jump” to those; if there is a non-empty VectorBasis we will want to account for them there.

#### Parameters

- **jumpnetwork** – jumpnetwork of symmetry unique omega1-type jumps, corresponding to our starset. List of lists of (IS, FS), dx tuples, where IS and FS are indices corresponding to states in our starset.
- **jumptype** – specific omega0 jump type that the jump corresponds to
- **VectorBasis** – (optional) list of [Nsites, 3] the vector basis in the unit cell for the solute states

**Return rate0expansion** array[Nsv, Nsv, Njump\_omega0] the omega0 matrix[i, j] = sum(rate0expansion[i, j, k] \* omega0[k]); *IF* NVB>0 we “hijack” this and use it for [NVB, Nsv, Njump\_omega0], as we’re doing an omega2 calc and rate0expansion won’t be used *anyway*.

**Return rate0escape** array[Nsv, Njump\_omega0] the escape contributions: omega0[i,i] += sum(rate0escape[i,k]\*omega0[k]\*probfactor(PS[k]))

**Return rate1expansion** array[Nsv, Nsv, Njump\_omega1] the omega1 matrix[i, j] = sum(rate1expansion[i, j, k] \* omega1[k])

**Return rate1escape** array[Nsv, Njump\_omega1] the escape contributions: omega1[i,i] += sum(rate1escape[i,k]\*omega0[k]\*probfactor(PS[k]))

**unitcellVectorBasisfolddown** (*VectorBasis, elemtype='solute'*)

Construct the expansion to “fold down” from starvector to a VectorBasis in the unit cell :param VectorBasis: list of (N,3) matrices, corresponding to (normalized) vectors :param elemtype: ‘solute’ of ‘vacancy’, depending on which site we need to reduce :return: folddown: [NV, Nvstars] to map vstars to VectorBasis

**crystalStars.array2PSlist** (*ij, R, dx*)

Take in arrays of ij, R, dx (from HDF5), return a list of PairStates

#### Parameters

- **ij** – int\_array[N][2] = (i,j)
- **R** – int[N][3]
- **dx** – float[N][3]

**Return PSlist** list of pair states

**crystalStars.doublelist2flatlistindex** (*listlist*)

Takes a list of lists, returns a flattened list and an index array

**Parameters listlist** – list of lists of objects

**Return flatlist** flat list of objects (preserving order)

**Return indexarray** array indexing which original list it came from

**crystalStars.flatlistindex2doublelist** (*flatlist, indexarray*)

Takes a flattened list and an index array, returns a list of lists

#### Parameters

- **flatlist** – flat list of objects (preserving order)

- **indexarray** – array indexing which original list it came from

**Return listlist** list of lists of objects



## SUPERCCELL

Supercell:

The supercell module defines the `supercell` class for building supercells from `crystal.Crystal` classes.  
Supercell class

Class to store supercells of crystals. A supercell is a lattice model of a crystal, with periodically repeating unit cells. In that framework we can

1. add/remove/substitute atoms
2. find the transformation map between two different representations of the same supercell
3. output POSCAR format (possibly other formats?)

**class** `supercell.Supercell` (*crys, super, interstitial=(), Nsolute=0, empty=False, NOSYM=False*)

A class that defines a Supercell of a crystal.

Takes in a crystal, a supercell (3x3 integer matrix). We can identify sites as interstitial sites, and specify if we'll have solutes.

**KrogerVink** ()

Attempt to make a “simple” string based on the defectindices, using Kroger-Vink notation. That is, we identify: vacancies, antisites, and interstitial sites, and return a string. NOTE: there is no relative charges, so this is a pseudo-KV notation.

**Return KV** string representation

**POSCAR** (*name=None, stoichiometry=True*)

Return a VASP-style POSCAR, returned as a string.

**Parameters**

- **name** – (optional) name to use for first list
- **stoichiometry** – (optional) if True, append stoichiometry to name

**Return POSCAR** string

**\_\_eq\_\_** (*other*)

Return True if two supercells are equal; this means they should have the same occupancy. *and* the same ordering

**Parameters other** – supercell for comparison

**Returns** True if same crystal, supercell, occupancy, and ordering; False otherwise

**\_\_getitem\_\_** (*key*)

Index into supercell

**Parameters key** – index (either an int, a slice, or a position)

**Returns** chemical occupation at that point

`__imul__ (other)`

Multiply by a GroupOp, in place.

**Parameters** *other* – must be a GroupOp (and *should* be a GroupOp of the supercell!)

**Returns** self

`__init__ (crys, super, interstitial=(), Nsolute=0, empty=False, NOSYM=False)`

Initialize our supercell to an empty supercell.

**Parameters**

- **crys** – crystal object
- **super** – 3x3 integer matrix
- **interstitial** – (optional) list/tuple of indices that correspond to interstitial sites
- **Nsolute** – (optional) number of substitutional solute elements to consider; default=0
- **empty** – (optional) designed to allow “copy” to work—skips all derived info
- **NOSYM** – (optional) does not do symmetry analysis (intended ONLY for testing purposes)

`__mul__ (other)`

Multiply by a GroupOp; returns a new supercell (constructed via copy).

**Parameters** *other* – must be a GroupOp (and *should* be a GroupOp of the supercell!)

**Returns** rotated supercell

`__ne__ (other)`

Inequality == not `__eq__`

`__rmul__ (other)`

Multiply by a GroupOp; returns a new supercell (constructed via copy).

**Parameters** *other* – must be a GroupOp (and *should* be a GroupOp of the supercell!)

**Returns** rotated supercell

`__sane__ ()`

Return True if supercell occupation and chemorder are consistent

`__setitem__ (key, value)`

Set specific composition for site; uses same indexing as `__getitem__`

**Parameters**

- **key** – index (either an int, a slice, or a position)
- **value** – chemical occupation at that point

`__str__ ()`

Human readable version of supercell

`__weakref__`

list of weak references to the object (if defined)

`copy ()`

Make a copy of the supercell; initializes, then copies over `__copyattr__` and `__eqattr__`.

**Returns** new supercell object, copy of the original

`defectindices ()`

Return a dictionary that corresponds to the “defect” content of the supercell.

**Return defects** dictionary, keyed by defect type, with a set of indices of corresponding defects

**definesolute** (*c, chemistry*)

Set the name of the chemistry of chemical index *c*. Only works for substitutional solutes.

**Parameters**

- **c** – index
- **chemistry** – string

**equivalencemap** (*other*)

Given the super *other* we want to find a group operation that transforms *self* into *other*. This is a GroupOp *along* with an index mapping of chemorder. The index mapping is to get the occposlist to match up: `(g*self).occposlist()[c][mapping[c][i]] == other.occposlist()[c][i]` (We can write a similar expression using chemorder, since chemorder indexes into pos). We're going to return both *g* and mapping.

*Remember:* *g* does not change the presentation ordering; mapping is necessary for full equivalence. If no such equivalence, return `None, None`.

**Parameters** **other** – Supercell

**Return g** GroupOp to transform sites from *self* to *other*

**Return mapping** list of maps, such that `(g*self).chemorder[c][mapping[c][i]] == other.chemorder[c][i]`

**fillperiodic** (*ci, Wyckoff=True*)

Occupies all of the (Wyckoff) sites corresponding to chemical index with the appropriate chemistry.

**Parameters**

- **ci** – tuple of (chem, index) in crystal
- **Wyckoff** – (optional) if False, *only* occupy the specific tuple, but still periodically

**Return self**

**gengroup** ()

Generate the group operations internal to the supercell

**Return G** set of GroupOps

**index** (*pos, threshold=1.0*)

Return the index that corresponds to the position *closest* to *pos* in the supercell. Done in direct coordinates of the supercell, using periodic boundary conditions.

**Parameters**

- **pos** – 3-vector
- **threshold** – (optional) minimum squared “distance” in supercell for a match; default=1.

**Return index** index of closest position

**makesites** ()

Generate the array corresponding to the sites; the indexing is based on the translations and the atomindices in *cryst*. These may not all be filled when the supercell is finished.

**Return pos** array [N\*size, 3] of supercell positions in direct coordinates

**static maketrans** (*super*)

Takes in a supercell matrix, and returns a list of all translations of the unit cell that remain inside the supercell

**Parameters** **super** – 3x3 integer matrix

**Return size** integer, corresponding to number of unit cells

**Return invsuper** integer matrix inverse of supercell (needs to be divided by size)

**Return translist** list of integer vectors (to be divided by `size`) corresponding to unit cell positions

**Return transdict** dictionary of tuples and their corresponding index (inverse of trans)

**occposlist** ()

Returns a list of lists of occupied positions, in (chem)order.

**Return occposlist** list of lists of supercell coord. positions

**reorder** (*mapping*)

Reorder (in place) the occupied sites. Does not change the occupancies, only the ordering for “presentation”.

**Parameters** **mapping** – list of maps; will make `newchemorder[c][i] = chemorder[c][mapping[c][i]]`

**Return self**

If mapping is not a proper permutation, raises `ValueError`.

**setocc** (*ind*, *c*)

Set the occupancy of position indexed by `ind`, to chemistry `c`. Used by all the other algorithms.

**Parameters**

- **ind** – integer index
- **c** – chemistry index

**stoichiometry** ()

Return a string representing the current stoichiometry

## POWEREXPANSION

PowerExpansion:

The PowerExpansion module defines the `Taylor3D` class, which is for 3-dimensional (xyz) Taylor expansions of functions. It's primary purpose is to be used in the calculation of the vacancy Green function, as it allows fairly straightforward block evaluation of the small  $k$  (large distance) transition matrix, and its inverse. This is key to removing the pole in the Green function evaluation. Power expansion class

Class to store and manipulate 3-dimensional Taylor (power) expansions of functions Particularly useful for inverting the FT of the evolution matrix, and subtracting off analytically calculated IFT for the Green function.

Really designed to get used by other code.

**class** `PowerExpansion.Taylor3D` (*coefflist=[]*, *Lmax=4*, *nodeeppcopy=False*)

Class that stores a Taylor expansion of a function in 3D, and defines some arithmetic

`__add__` (*other*)

Add a set of Taylor expansions

`__call__` (*u*, *fnu=None*)

Method for evaluating our 3D Taylor expansion. We have two approaches: if we are passed a dictionary in *fnu* that will map (n,l) tuple pairs to either (a) values or (b) functions of a single parameter *umagn*, then we will compute and return the function value. Otherwise, we return a dictionary mapping (n,l) tuple pairs into values, and leave it at that.

### Parameters

- **u** – three vector to evaluate; may (or may not) be normalized
- **fnu** – dictionary of (n,l): value or function pairs.

**Return value or dictionary** depending on *fnu*; default is dictionary

`__getitem__` (*key*)

Indexes (or even slices) into our Taylor expansion.

**Parameters** **key** – indices for our Taylor expansion

**Return** **Taylor3D** Taylor expansion after indexing

`__iadd__` (*other*)

Add a set of Taylor expansions

**classmethod** `__initTaylor3Dindexing__` (*Lmax*)

This calls *all* the class methods defined above, and stores them *for the class*. This is intended to be done *once*

**Parameters** **Lmax** – maximum power / orbital angular momentum

`__init__` (*coefflist*=[], *Lmax*=4, *nodeepcopy*=False)  
 Initializes a Taylor3D object, with *coefflist* (default = empty)

**Parameters**

- **coefflist** – list((n, lmax, powexpansion)). No type checking; default empty
- **Lmax** – maximum power / orbital angular momentum; can be set only once the first time a Taylor expansion is constructed, and is set for all objects
- **nodeepcopy** – true if we don’t want to copy the matrices on creation of object (i.e., deep copy, which is the default) **Note:** deep copy is strongly preferred. The *only* real reason to use *nodeepcopy* is when returning slices / indexing in arrays, but even then we have to be careful about doing things like reductions, etc., that modify matrices *in place*. We always copy the list, but that doesn’t make copies of the underlying matrices.

`__isub__` (*other*)  
 Subtract a set of Taylor expansions

`__mul__` (*other*)  
 Multiply our expansion

**Parameters** *other* –

**Return** Taylor3D expansion of product

`__neg__` ()  
 Return -T3D

`__pos__` ()  
 Return +T3D

`__radd__` (*other*)  
 Add a set of Taylor expansions

`__rmul__` (*other*)  
 Multiply our expansion

**Parameters** *other* –

**Return** Taylor3D expansion of product

`__rsub__` (*other*)  
 Subtract a set of Taylor expansions

`__setitem__` (*key*, *value*)  
 Indexes (or even slices) into our Taylor expansion and “sets”; really only intended to work with another Taylor expansion

**Parameters**

- **key** – indices for our Taylor expansion
- **value** – assignment value; really, should be

**Returns** Taylor expansion after indexing

`__str__` ()  
 Human readable string representation

`__sub__` (*other*)  
 Subtract a set of Taylor expansions

`__weakref__`  
 list of weak references to the object (if defined)

**addhdf5** (*HDF5group*)

Adds an HDF5 representation of object into an HDF5group (needs to already exist). Example: if f is an open HDF5, then T3D.addhdf5(f.create\_group('T3D')) will (1) create the group named 'T3D', and then (2) put the T3D representation in that group.

**Parameters** **HDF5group** – HDF5 group

**addterms** (*coefflist*)

Add additional coefficients into our object. No type checking. Only works if terms are completely non-overlapping (otherwise, need to use sum).

**Parameters** **coefflist** – list((n, lmax, powexpansion))

**classmethod checkinternalsHDF5** (*HDF5group*)

Reads the power expansion internals into an HDF5group, and performs sanity check

**Parameters** **HDF5group** – HDF5 group

**classmethod coeffproductcoeff** (*a, b*)

Takes a direction expansion a and b, and returns the product expansion.

**Parameters**

- **a** – list((n, lmax, powexpansion))
- **b** – list((n, lmax, powexpansion)) written as a series of coefficients; n defines the magnitude function, which is additive; lmax is the largest cumulative power of coefficients, and powexpansion is a numpy array that can be multiplied. We assume that a and b have consistent shapes throughout—we *do not test this*; runtime will likely fail if not true. The entries in the list are *tuples* of n, lmax, pow

**Return** **c** list((n, lmax, powexpansion)), product of a and b

**classmethod collectcoeff** (*a, inplace=False, atol=1e-10*)

Collects coefficients: sums up all the common n values. Best to be done *after* reduce is called.

**Parameters**

- **a** – list((n, lmax, powexpansion)), expansion of function in powers
- **inplace** – modify a in place?

**Return** **coefflist** a

**classmethod constructexpansion** (*basis, N=-1, pre=None*)

Takes a “basis” for constructing an expansion – list of vectors and matrices – and constructs the expansions up to power N (default = Lmax) Takes a direction expansion a and b, and returns the sum of the expansions.

**Parameters**

- **= list((coeffmatrix, vect))** (*basis*) – expansions to create; sum(coeffmatrix \* (vect\*q)^n), for powers n = 0..N
- **N** – maximum power to consider; for N=-1, use Lmax
- **pre** – list of prefactors, defining the Taylor expansion. Default = 1

**Return** list((n, lmax, powexpansion)),... our expansion, as input to create Taylor3D objects

**copy** ()

Returns a copy of the current expansion

**dumpinternalsHDF5** (*HDF5group*)

Adds the initialized power expansion internals into an HDF5group—should be stored for a sanity check

**Parameters** **HDF5group** – HDF5 group

**ildot** (*c*)

Computes  $c \cdot self$  in place

**inv** (*Nmax=0*)

Return the inverse of the expansion, up to order Nmax

**Parameters** **Nmax** – maximum order in the inverse expansion

**Return** **Taylor3D<sup>-1</sup>** Taylor series of inverse

**classmethod** **inversecoeff** (*a*, *Nmax=0*)

Takes a direction expansion, and returns the inversion expansion (approximated based on the Taylor expansion of  $1/(1-x) = \sum_{i=0}^{\infty} x^i$ , or  $(A+B)^{-1} = ((1+BA^{-1})A)^{-1} = A^{-1}(1-(-BA^{-1}))^{-1} = A^{-1} \sum_{i=0}^{\infty} (-BA^{-1})^i$

NOTE: assumes SMALLEST n coefficient is the leading order; only works if that coefficient is also isotropic (l=0). Otherwise, raises an error. NOTE: there is no sanity check on whether Nmax is reasonable given the expansion and Lmax values; *caveat emptor*.

**Parameters**

- **a** – = list((n, lmax, powexpansion) written as a series of coefficients; n defines the magnitude function, which is additive; lmax is the largest cumulative power of coefficients, and powexpansion is a numpy array that can be multiplied. We assume that a and b have consistent shapes throughout—we *do not test this*; runtime will likely fail if not true. The entries in the list are *tuples* of n, lmax, pow
- **Nmax** – maximum remaining n value in expansion. Default value of 0 means up to a discontinuity correction in an inversion, but higher (or lower) values are possible.

**Return** **c** list((n, lmax, powexpansion)), inverse of a

**irdot** (*c*)

Computes  $self \cdot c$  in place

**irotrate** (*powtrans*)

Rotate in place.

**Parameters** **powtrans** – Npow x Npow matrix, of [oldpow,newpow] corresponding to the rotation

**Returns** **self**

**ldot** (*c*)

Returns  $c \cdot self$

**classmethod** **loadhdf5** (*HDF5group*)

Creates a new T3D from an HDF5 group.

**Parameters** **HDFgroup** – HDF5 group

**Return** **T3D** new T3D object

**classmethod** **makeLprojections** ()

Constructs a series of projection matrices for each l component in our power series

**Returns** projL[l][p][p'] projection of powers containing *only* l component. -1 component = sum(l=0..Lmax, projL[l]) = simplification projection

**classmethod** **makeYlmpow** ()

Construct the expansion of the Ylm's in powers of x,y,z. Done via brute force.

**Return** Ylmpow[lm, p] expansion of each Ylm in powers

**classmethod** **makedirectmult** ()



**Return `direcmult[p][p']`** index that corresponds to the multiplication of power indices  $p$  and  $p'$

**static `makeindexPowerYlm(Lmax)`**  
 Analyzes the spherical harmonics and powers for a given  $L_{\max}$ ; returns a series of index functions.

**Parameters `Lmax`** – maximum  $l$  value to consider; equal to the sum of powers

**Return `NYlm`** number of Ylm coefficients

**Return `Npower`** number of power coefficients

**Return `pow2ind[n1][n2][n3]`** powers to index

**Return `ind2pow[n]`** powers for a given index

**Return `Ylm2ind[l][m]`**  $(l,m)$  to index

**Return `ind2Ylm[lm]`**  $(l,m)$  for a given index

**Return `powlrange[l]`** upper limit of power indices for a given  $l$  value; note:  $[-1] = 0$

**classmethod `makepowYlm()`**  
 Construct the expansion of the powers in Ylm's. Done using recursion relations instead of direct calculation. Note: an alternative approach would be Gaussian quadrature.

**Return `powYlm[p][lm]`** expansion of powers in Ylm; uses indexing scheme above

**classmethod `makepowercoeff()`**  
 Make our power coefficients for our construct expansion method

**Return `powercoeff[n][p]`** vector we multiply by our power expansion to get the  $n$ 'th coefficients

**classmethod `negcoeff(a)`**  
 Negates a coefficient expansion  $a$

**Parameters = `list((n, lmax, powexpansion))`** ( $a$ ) – expansion of function in powers

**Return `coefflist`**  $-a$

**`nl()`**  
 Returns a list of  $(n,l)$  pairs in the `coefflist`

**Return `nl_list`** all of the  $(n,l)$  pairs that are present in our `coefflist`

**classmethod `powexp(u, normalize=True)`**  
 Given a vector  $u$ , normalize it and return the power expansion of  $u_{\text{vec}}$

**Parameters**

- **`u[3]`** – vector to apply
- **`normalize`** – do we normalize  $u$  first?

**Return `upow[Npower]`**  $u_x u_y u_z$  products of powers

**Return `umagn`** magnitude of  $u$  (if normalized)

**`rdot(c)`**  
 Returns  $\text{self} \cdot c$

**`reduce()`**  
 Reduce the coefficients: eliminate any  $n$  that has zero coefficients, collect all of the same values of  $n$  together. Done in place.

**classmethod `reducecoeff(a, inplace=False, atol=1e-10)`**  
 Projects coefficients through Ylm space, then eliminates any zero contributions (including possible reduction in  $l$  values, too).

### Parameters

- **a** – list((n, lmax, powexpansion), expansion of function in powers
- **inplace** – modify a in place?

### Return coefflist a

**rotate** (*powtrans*)

Return a rotated version of the expansion.

**Parameters** **powtrans** – Npow x Npow matrix, of [oldpow,newpow] corresponding to the rotation

**Return** **rTaylor3D** Taylor expansion, rotated

**classmethod rotatecoeff** (*a, npowtrans, inplace=False*)

Return a rotated version of the expansion. Needs to use pad to work with reduced representations.

### Parameters

- **a** – coefficient list
- **npowtrans** – Lmax+1 x Npow x Npow matrix, of [n,oldpow,newpow] corresponding to the rotation

**Return** **coeff** coefficient list, rotated

**classmethod rotatedirections** (*qptrans*)

Takes a transformation matrix qptrans, where  $q[i] = \sum_j qptrans[i][j] p[j]$ , and returns the Npow x Npow transformation matrix for the new components in terms of the old. NOTE: This is more complex than one might first realize. If we only work with cases where all of the entries for a given power n have those same n (that is, not reduced), then this is straightforward. However, we run into problems with *reductions*: e.g., for n=2, the power  $x^0 y^0 z^0$  is, in reality,  $x^2 + y^2 + z^2$ , and hence *it must be transformed* because we allow non-orthogonal transformation matrices.

**Parameters** **qptrans** – 3x3 matrix

**Return** **npowtrans** [Lmax +1][Npow][Npow] transformation matrix [n][original pow][new pow] for each n from 0 up to Lmax

**classmethod scalarproductcoeff** (*c, a, inplace=False*)

Multiplies an coefficient expansion a by a scalar c

### Parameters

- **c** – scalar or dictionary mapping (n,l) to scalars
- **= list((n, lmax, powexpansion) (a)** – expansion of function in powers
- **inplace** – modify a in place?

**Return** **coefflist** c\*a

**separate** ()

Separate out the coefficients into (n,l) terms where *only* l contributions appear in each.

**classmethod separaterecoeff** (*a, inplace=False, atol=1e-10*)

Projects coefficients through Ylm space, one by one. Assumes they've already been reduced and collected first; if not, could lead to duplicated (n,l) entries in list, which is inefficient (should still *evaluate* the same, just with extra steps). After this, each (n,l) term *only* contains terms equal to l, rather than terms  $\leq l$ .

### Parameters

- **a** – list((n, lmax, powexpansion), expansion of function in powers

- **inplace** – modify a in place?

**Return coefflist** a

**classmethod `sumcoeff`** (a, b, alpha=1, beta=1, inplace=False)

Takes Taylor3D expansion a and b, and returns the sum of the expansions.

**Param** a, b = list((n, lmax, powexpansion) written as a series of coefficients; n defines the magnitude function, which is additive; lmax is the largest cumulative power of coefficients, and powexpansion is a numpy array that can be multiplied. We assume that a and b have consistent shapes throughout—we *do not test this*; runtime will likely fail if not true. The entries in the list are *tuples* of n, lmax, pow

**Parameters**

- **beta** (*alpha*,) – optional scalars:  $c = \alpha a + \beta b$ ; allows for more efficient expansions
- **inplace** – True if the summation should modify a in place

**Return c** coeff of sum of a and b (! NOTE ! does not return the class!) sum of a and b

**classmethod `tensorproductcoeff`** (c, a, leftmultiply=True)

Multiplies an coefficient expansion a by a scalar c

**Parameters**

- **c** – array or dictionary mapping (n,l) to arrays
- **= list((n, lmax, powexpansion) (a)** – expansion of function in powers
- **leftmultiply** – `tensorproduct(c,a)` vs. `tensorproduct(a,c)`

**Return coefflist** c.a (or a.c)

**`truncate`** (Nmax, inplace=False)

Remove the coefficients above a given Nmax; normally returns a new object

**Parameters**

- **Nmax** – maximum coefficient to include
- **inplace** – do it in place?

**classmethod `truncatecoeff`** (a, Nmax, inplace=False)

Remove the coefficients above a given Nmax; normally returns a new object

**Parameters**

- **Nmax** – maximum coefficient to include
- **a** – list((n, lmax, powexpansion), expansion of function in powers
- **inplace** – do it in place?

**classmethod `zeros`** (nmin, nmax, shape, dtype=<class 'complex'>)

Constructs (and returns) a “zero” Taylor expansion with the prescribed shape. This will be useful for doing slicing assignments. Because of the manner in which slicing works for assignment, we create what looks like a *lot* of zeros, by explicitly making the full range of l values.

**Parameters**

- **nmin** – minimum value of n
- **nmax** – maximum value of n (inclusive)
- **shape** – shape of matrix, as zeros would expect.

**Return Taylor3D** Taylor3D, with a zero coefficient list

## GFCALC

GFcalc:

The GFcalc module defines the `GFCrystalcalc` class for the evaluation of the vacancy Green function. GFcalc module

Code to compute the lattice Green function for diffusion; this entails inverting the “diffusion” matrix, which is infinite, singular, and has translational invariance. The solution involves fourier transforming to reciprocal space, inverting, and inverse fourier transforming back to real (lattice) space. The complication is that the inversion produces a second order pole which must be treated analytically. Subtracting off the pole then produces a discontinuity at the gamma-point ( $q=0$ ), which also should be treated analytically. Then, the remaining function can be numerically inverse fourier transformed.

**class** `GFcalc.GFCrystalcalc` (*crys, chem, sitelist, jumpnetwork, Nmax=4*)

Class calculator for the Green function, designed to work with the Crystal class.

This computes the bare vacancy GF. It requires a crystal, chemical identity for the vacancy, list of symmetry unique sites (to define energies / entropies uniquely), and a corresponding jumpnetwork for that vacancy.

**BlockInvertOmegaTaylor** (*dd, dr, rd, rr, D*)

Returns block inverted omega as a Taylor expansion, up to  $N_{max} = 0$  (discontinuity correction). Needs to be rotated such that leading order of  $D$  is isotropic.

#### Parameters

- **dd** – diffusive/diffusive block (upper left)
- **dr** – diffusive/relaxive block (lower left)
- **rd** – relaxive/diffusive block (upper right)
- **rr** – relaxive/relaxive block (lower right)
- **D** –  $dd - dr(rr)^{-1}rd$  (diffusion)

**Return gT** Taylor expansion of  $g$  in block form, and reduced (collected terms)

**BlockRotateOmegaTaylor** (*omega\_Taylor\_rotate*)

Returns block partitioned Taylor expansion of a rotated omega Taylor expansion.

#### Parameters

- **omega\_Taylor\_rotate** – rotated into diffusive [0] / relaxive [1:] basis
- **dd** – diffusive/diffusive block (upper left)
- **dr** – diffusive/relaxive block (lower left)
- **rd** – relaxive/diffusive block (upper right)
- **rr** – relaxive/relaxive block (lower right)

- $D = dd - dr(rr)^{-1}rd$  (diffusion)

**BreakdownGroups** ( )

Takes in a crystal, and a chemistry, and constructs the indexing breakdown for each (i,j) pair. :return grouparray: array[NG][3][3] of the NG group operations :return indexpair: array[N][N][NG][2] of the index pair for each group operation

**DiagGamma** (*omega=None*)

Diagonalize the gamma point (q=0) term

**Parameters** **omega** – optional; the Taylor expansion to use. If None, use self.omega\_Taylor

**Return r** array of eigenvalues, sorted from 0 to decreasing values.

**Return vr** array of eigenvectors where vr[:,i] is the vector for eigenvalue r[i]

**Diffusivity** (*omega\_Taylor\_D=None*)

Return the diffusivity, or compute it if it's not already known. Uses omega\_Taylor\_D to compute with maximum efficiency.

**Parameters** **omega\_Taylor\_D** – Taylor expansion of the diffusivity component

**Return D** diffusivity [3,3] array

**FourierTransformJumps** (*jumpnetwork, N, kpts*)

Generate the Fourier transform coefficients for each jump

**Parameters**

- **jumpnetwork** – list of unique transitions, as lists of ((i,j), dx)
- **N** – number of sites
- **kpts** – array[Nkpt][3], in Cartesian (same coord. as dx)

**Return FTjumps** array[Njump][Nkpt][Nsite][Nsite] of FT of the jump network

**Return SEjumps** array[Nsite][Njump] multiplicity of jump on each site

**SetRates** (*pre, betaene, preT, betaeneT*)

(Re)sets the rates, given the prefactors and Arrhenius factors for the sites and transitions, using the ordering according to sitelist and jumpnetwork. Initiates all of the calculations so that GF calculation is (fairly) efficient for each input.

**Parameters**

- **pre** – list of prefactors for site probabilities
- **betaene** – list of beta\*E (energy/kB T) for each site
- **preT** – list of prefactors for transition states
- **betaeneT** – list of beta\*ET (energy/kB T) for each transition state

**SymmRates** (*pre, betaene, preT, betaeneT*)

Returns a list of lists of symmetrized rates, matched to jumpnetwork

**TaylorExpandJumps** (*jumpnetwork, N*)

Generate the Taylor expansion coefficients for each jump

**Parameters**

- **jumpnetwork** – list of unique transitions, as lists of ((i,j), dx)
- **N** – number of sites

**Return T3Djumps** list of Taylor3D expansions of the jump network

**\_\_call\_\_** (*i, j, dx*)

Evaluate the Green function from site *i* to site *j*, separated by vector *dx*

**Parameters**

- **i** – site index
- **j** – site index
- **dx** – vector pointing from *i* to *j* (can include lattice contributions)

**Return G** Green function value

**\_\_init\_\_** (*crys, chem, sitelist, jumpnetwork, Nmax=4*)

Initializes our calculator with the appropriate topology / connectivity. Doesn't require, at this point, the site probabilities or transition rates to be known.

**Parameters**

- **crys** – Crystal object
- **chem** – index identifying the diffusing species
- **sitelist** – list, grouped into Wyckoff common positions, of unique sites
- **jumpnetwork** – list of unique transitions as lists of ((*i,j*), *dx*)
- **Nmax** – maximum range as estimator for kpt mesh generation

**\_\_weakref\_\_**

list of weak references to the object (if defined)

**addhdf5** (*HDF5group*)

Adds an HDF5 representation of object into an HDF5group (needs to already exist).

Example: if *f* is an open HDF5, then `GFcalc.addhdf5(f.create_group('GFcalc'))` will (1) create the group named 'GFcalc', and then (2) put the GFcalc representation in that group.

**Parameters HDF5group** – HDF5 group

**biascorrection** (*etav=None*)

Return the bias correction, or compute it if it's not already known. Uses *etav* to compute.

**Parameters etav** – Taylor expansion of the bias correction

**Return eta** [N,3] array

**exp\_dxq** (*dx*)

Return the array of  $\exp(-i \cdot q \cdot dx)$  evaluated over the *q*-points, and accounting for symmetry

**Parameters dx** – vector

**Return exp(-i q · dx)** array of  $\exp(-i \cdot dx)$

**classmethod loadhdf5** (*crys, HDF5group*)

Creates a new GFcalc from an HDF5 group.

**Parameters**

- **crys** – crystal object–MUST BE PASSED IN as it is not stored with the GFcalc
- **HDFgroup** – HDF5 group

**Return GFcalc** new GFcalc object





## ONSAGERCALC

OnsagerCalc:

The OnsagerCalc module defines the `Interstitial` class (for computation of interstitial-mediated diffusion), and `VacancyMediated` class (for computation of vacancy-mediated diffusion). Onsager calculator module: Interstitialcy mechanism and Vacancy-mediated mechanism

Class to create an Onsager “calculator”, which brings two functionalities: 1. determines *what* input is needed to compute the Onsager (mobility, or L) tensors 2. constructs the function that calculates those tensors, given the input values.

This class is designed to be combined with code that can, e.g., automatically run some sort of atomistic-scale (DFT, classical potential) calculation of site energies, and energy barriers, and then in concert with scripts to convert such data into rates and probabilities, this will allow for efficient evaluation of transport coefficients.

This implementation will be for vacancy-mediated solute diffusion assumes the dilute limit. The mathematics is based on a Green function solution for the vacancy diffusion. The computation of the GF is included in the `GFcalc` module.

Now with HDF5 write / read capability for `VacancyMediated` module

**class** `OnsagerCalc.Interstitial` (*crys, chem, sitelist, jumpnetwork*)

A class to compute interstitial diffusivity; uses structure of crystal to do most of the heavy lifting in terms of symmetry.

Takes in a crystal that contains the interstitial as one of the chemical elements, to be specified by *chem*, the *sitelist* (list of symmetry equivalent sites), and *jumpnetwork*. Both of the latter can be computed automatically from *crys* methods, but as they are lists, can also be edited or constructed by hand.

**\_\_init\_\_** (*crys, chem, sitelist, jumpnetwork*)

Initialization; takes an underlying crystal, a choice of atomic chemistry, a corresponding Wyckoff site list and jump network.

### Parameters

- **crys** – Crystal object
- **chem** – integer, index into the basis of *crys*, corresponding to the chemical element that hops
- **sitelist** – list of lists of indices, site indices where the atom may hop; grouped by symmetry equivalency
- **jumpnetwork** – list of lists of tuples: ( (i, j), dx ) symmetry unique transitions; each list is all of the possible transitions from site i to site j with jump vector dx; includes i->j and j->i

**\_\_weakref\_\_**

list of weak references to the object (if defined)

**diffusivity** (*pre, betaene, preT, betaeneT, CalcDeriv=False*)

Computes the diffusivity for our element given prefactors and energies/kB T. Also returns the negative derivative of diffusivity with respect to beta (used to compute the activation barrier tensor) if CalcDeriv = True The input list order corresponds to the sitelist and jumpnetwork

**Parameters**

- **pre** – list of prefactors for unique sites
- **betaene** – list of site energies divided by kB T
- **preT** – list of prefactors for transition states
- **betaeneT** – list of transition state energies divided by kB T

**Return D[3,3]** diffusivity as a 3x3 tensor

**Return DE[3,3]** diffusivity times activation barrier (if CalcDeriv == True)

**elastodiffusion** (*pre, betaene, dipole, preT, betaeneT, dipoleT*)

Computes the elastodiffusion tensor for our element given prefactors, energies/kB T, and elastic dipoles/kB T The input list order corresponds to the sitelist and jumpnetwork

**Parameters**

- **pre** – list of prefactors for unique sites
- **betaene** – list of site energies divided by kB T
- **dipole** – list of elastic dipoles divided by kB T
- **preT** – list of prefactors for transition states
- **betaeneT** – list of transition state energies divided by kB T
- **dipoleT** – list of elastic dipoles divided by kB T

**Return D[3,3]** diffusivity as 3x3 tensor

**Return dD[3,3,3,3]** elastodiffusion tensor as 3x3x3x3 tensor

**generateJumpGroupOps** ()

Generates a list of group operations that transform the first jump in the jump network into all of the other members; one group operation for each.

**Return siteGroupOps** list of list of group ops that mirrors the structure of jumpnetwork.

**generateJumpSymmTensorBasis** ()

Generates a list of symmetric tensor bases for the first representative transition in our jump network

**Return TensorSet** list of list of symmetric tensors

**generateSiteGroupOps** ()

Generates a list of group operations that transform the first site in each site list into all of the other members; one group operation for each.

**Return siteGroupOps** list of list of group ops that mirrors the structure of site list

**generateSiteSymmTensorBasis** ()

Generates a list of symmetric tensor bases for the first representative site in our site list.

**Return TensorSet** list of symmetric tensors

**generatetags** ()

Create tags for unique interstitial states, and transition states.

**Return tags** dictionary of tags; each is a list-of-lists

**Return tagdict** dictionary that maps tag into the index of the corresponding list.

**Return tagdicttype** dictionary that maps tag into the key for the corresponding list.

**jumpDipoles** (*dipoles*)

Returns a list of the elastic dipole for each transition, given the dipoles for the representatives. (“populating” the full set of dipoles)

**Parameters** *dipoles* – list of dipoles for the first representative transition

**Return dipolelist** list of lists of dipole for each jump[site][3][3]

**static jumpnetworkYAML** (*jumpnetwork*)

Dumps a “sample” YAML formatted version of the jumpnetwork with data to be entered

**makesupercells** (*super\_n*)

Take in a supercell matrix, then generate all of the supercells needed to compute site energies and transitions (corresponding to the representatives).

**Parameters** *super\_n* – 3x3 integer matrix to define our supercell

**Return superdict** dictionary of states, transitions, transmapping, and indices that correspond to dictionaries with tags.

- superdict[‘states’][i] = supercell of site;
- superdict[‘transitions’][n] = (supercell initial, supercell final);
- superdict[‘transmapping’][n] = ((site tag, groupop, mapping), (site tag, groupop, mapping))
- superdict[‘indices’][tag] = index of tag, where tag is either a state or transition tag.

**ratelist** (*pre, betaene, preT, betaeneT*)

Returns a list of lists of rates, matched to jumpnetwork

**siteDipoles** (*dipoles*)

Returns a list of the elastic dipole on each site, given the dipoles for the representatives. (“populating” the full set of dipoles)

**Parameters** *dipoles* – list of dipoles for the first representative site

**Return dipolelist** array of dipole for each site [site][3][3]

**static sitelistYAML** (*sitelist*)

Dumps a “sample” YAML formatted version of the sitelist with data to be entered

**siteprob** (*pre, betaene*)

Returns our site probabilities, normalized, as a vector

**symmratelist** (*pre, betaene, preT, betaeneT*)

Returns a list of lists of symmetrized rates, matched to jumpnetwork

**class** OnsagerCalc.**VacancyMediated** (*crys, chem, sitelist, jumpnetwork, Nthermo=0*)

A class to compute vacancy-mediated solute transport coefficients, specifically  $L_{vv}$  (vacancy diffusion),  $L_{ss}$  (solute), and  $L_{sv}$  (off-diagonal). As part of that, it determines *what* quantities are needed as inputs in order to perform this calculation.

Based on crystal class. Also now includes its own GF calculator and cacheing, and storage in HDF5 format.

Requires a crystal, chemical identity of vacancy, list of symmetry-equivalent sites for that chemistry, and a jumpnetwork for the vacancy. The thermodynamic range (number of “shells” – see `crystalStars.StarSet` for precise definition).

**Lij** (*bFV, bFS, bFSV, bFT0, bFT1, bFT2*)

Calculates the transport coefficients:  $L_{vv}$ ,  $L_{0ss}$ ,  $L_{2ss}$ ,  $L_{1sv}$ ,  $L_{1vv}$  from the scaled free energies. The Green function entries are calculated from the  $\omega_0$  info. As this is the most time-consuming part of the calculation, we cache these values with a dictionary and hash function. Used by `Lij`.

**Parameters**

- **bFV[NWyckoff]** –  $\beta \cdot \text{eneV} - \ln(\text{preV})$  (relative to minimum value)
- **bFS[NWyckoff]** –  $\beta \cdot \text{eneS} - \ln(\text{preS})$  (relative to minimum value)
- **bFSV[Nthermo]** –  $\beta \cdot \text{eneSV} - \ln(\text{preSV})$  (excess)
- **bFT0[Nomega0]** –  $\beta \cdot \text{eneT0} - \ln(\text{preT0})$  (relative to minimum value of bFV)
- **bFT1[Nomega1]** –  $\beta \cdot \text{eneT1} - \ln(\text{preT1})$  (relative to minimum value of bFV + bFS)
- **bFT2[Nomega2]** –  $\beta \cdot \text{eneT2} - \ln(\text{preT2})$  (relative to minimum value of bFV + bFS)

**Return**  $L_{vv}[3, 3]$  vacancy-vacancy; needs to be multiplied by  $cv/kBT$

**Return**  $L_{ss}[3, 3]$  solute-solute; needs to be multiplied by  $cv \cdot cs/kBT$

**Return**  $L_{sv}[3, 3]$  solute-vacancy; needs to be multiplied by  $cv \cdot cs/kBT$

**Return**  $L_{vv1}[3, 3]$  vacancy-vacancy correction due to solute; needs to be multiplied by  $cv \cdot cs/kBT$

**\_\_init\_\_** (*crys, chem, sitelist, jumpnetwork, Nthermo=0*)

Create our diffusion calculator for a given crystal structure, chemical identity, jumpnetwork (for the vacancy) and thermodynamic shell.

**Parameters**

- **crys** – Crystal object
- **chem** – index identifying the diffusing species
- **sitelist** – list, grouped into Wyckoff common positions, of unique sites
- **jumpnetwork** – list of unique transitions as lists of  $((i,j), dx)$

**\_\_weakref\_\_**

list of weak references to the object (if defined)

**addhdf5** (*HDF5group*)

Adds an HDF5 representation of object into an HDF5group (needs to already exist).

Example: if `f` is an open HDF5, then `VacancyMediated.addhdf5(f.create_group('Diffuser'))` will (1) create the group named 'Diffuser', and then (2) put the `VacancyMediated` representation in that group.

**Parameters** **HDF5group** – HDF5 group

**generate** (*Nthermo*)

Generate the necessary stars, vector-stars, and jump networks based on the thermodynamic range.

**Parameters** **Nthermo** – range of thermodynamic interactions, in terms of “shells”, which is multiple summations of `jumpvect`

**generatematrices** ()

Generates all the matrices and “helper” pieces, based on our jump networks. This has been separated out in case the user wants to, e.g., prune / modify the networks after they’ve been created with `generate()`, then `generatematrices()` can be rerun.

### **generatetags ()**

Create tags for vacancy states, solute states, solute-vacancy complexes; omega0, omega1, and omega2 transition states.

**Return tags** dictionary of tags; each is a list-of-lists

**Return tagdict** dictionary that maps tag into the index of the corresponding list.

**Return tagdicttype** dictionary that maps tag into the key for the corresponding list.

### **interactlist ()**

Return a list of solute-vacancy configurations for interactions. The points correspond to a vector between a solute atom and a vacancy. Defined by Stars.

**Return statelist** list of PairStates for the solute-vacancy interactions

### **classmethod loadhdf5 (HDF5group)**

Creates a new VacancyMediated diffuser from an HDF5 group.

**Parameters HDFgroup** – HDF5 group

**Return VacancyMediated** new VacancyMediated diffuser object from HDF5

### **makeLIMBpreene (preS, eneS, preSV, eneSV, preT0, eneT0, \*\*ignoreextraarguments)**

Generates corresponding energies / prefactors for corresponding to LIMB (Linearized interpolation of migration barrier approximation). Returns a dictionary. (we ignore extra arguments so that a dictionary including additional entries can be passed)

#### **Parameters**

- **preS[NWyckoff]** – prefactor for solute formation
- **eneS[NWyckoff]** – solute formation energy
- **preSV[Nthermo]** – prefactor for solute-vacancy interaction
- **eneSV[Nthermo]** – solute-vacancy binding energy
- **preT0[Nomeg0]** – prefactor for vacancy jump transitions (follows jumpnetwork)
- **eneT0[Nomeg0]** – transition energy for vacancy jumps

**Return preT1[Nomega1]** prefactor for omega1-style transitions (follows om1\_jn)

**Return eneT1[Nomega1]** transition energy/kBT for omega1-style jumps

**Return preT2[Nomega2]** prefactor for omega2-style transitions (follows om2\_jn)

**Return eneT2[Nomega2]** transition energy/kBT for omega2-style jumps

### **makesupercells (super\_n)**

Take in a supercell matrix, then generate all of the supercells needed to compute site energies and transitions (corresponding to the representatives).

Note: the states are lone vacancy, lone solute, solute-vacancy complexes in our thermodynamic range. Note that there will be escape states are endpoints of some omega1 jumps. They are not relaxed, and have no pre-existing tag. They will only be output as a single endpoint of an NEB run; there may be symmetry equivalent duplicates, as we construct these supercells on an as needed basis.

We've got a few classes of warnings (from most egregious to least) that can issued if the supercell is too small; the analysis will continue despite any warnings:

1. Thermodynamic shell states map to different states in supercell
2. Thermodynamic shell states are not unique in supercell (multiplicity)
3. Kinetic shell states map to different states in supercell

4. Kinetic shell states are not unique in supercell (multiplicity)

The lowest level can still be run reliably but runs the risk of errors in escape transition barriers. Extreme caution should be used if any of the other warnings are raised.

**Parameters** **super\_n** – 3x3 integer matrix to define our supercell

**Return superdict** dictionary of states, transitions, transmapping, indices that correspond to dictionaries with tags; the final tag reference is the basesupercell for calculations without defects.

- **superdict['states']**[i] = supercell of state;
- **superdict['transitions']**[n] = (supercell initial, supercell final);
- **superdict['transmapping']**[n] = ((site tag, groupop, mapping), (site tag, groupop, mapping))
- **superdict['indices']**[tag] = (type, index) of tag, where tag is either a state or transition tag.
- **superdict['reference']** = supercell reference, no defects

**maketracerpreene** (*preT0, eneT0, \*\*ignoredextraarguments*)

Generates corresponding energies / prefactors for an isotopic tracer. Returns a dictionary. (we ignore extra arguments so that a dictionary including additional entries can be passed)

**Parameters**

- **preT0[Nomeg0]** – prefactor for vacancy jump transitions (follows jumpnetwork)
- **eneT0[Nomeg0]** – transition energy state for vacancy jumps

**Return preS[NWyckoff]** prefactor for solute formation

**Return eneS[NWyckoff]** solute formation energy

**Return preSV[Nthermo]** prefactor for solute-vacancy interaction

**Return eneSV[Nthermo]** solute-vacancy binding energy

**Return preT1[Nomega1]** prefactor for omega1-style transitions (follows om1\_jn)

**Return eneT1[Nomega1]** transition energy for omega1-style jumps

**Return preT2[Nomega2]** prefactor for omega2-style transitions (follows om2\_jn)

**Return eneT2[Nomega2]** transition energy for omega2-style jumps

**omegalist** (*fivefreqindex=1*)

Return a list of pairs of endpoints for a vacancy jump, corresponding to omega1 or omega2 Solute at the origin, vacancy hopping between two sites. Defined by om1\_jumpnetwork

**Parameters** **fivefreqindex** – 1 or 2, corresponding to omega1 or omega2

**Return omegalist** list of tuples of PairStates

**Return omegajumptype** index of corresponding omega0 jumptype

**static preene2betafree** (*kT, preV, eneV, preS, eneS, preSV, eneSV, preT0, eneT0, preT1, eneT1, preT2, eneT2, \*\*ignoredextraarguments*)

Read in a series of prefactors ( $\exp(S/k_B)$ ) and energies, and return  $\beta F$  for energies and transition state energies. Used to provide scaled values to Lij() and \_lij(). Can specify all of the entries using a dictionary; e.g., `preene2betafree(kT, **data_dict)` and then send that output as input to Lij: `Lij(*preene2betafree(kT, **data_dict))` (we ignore extra arguments so that a dictionary including additional entries can be passed)

**Parameters**

- **kT** – temperature times Boltzmann’s constant kB
- **preV** – prefactor for vacancy formation (prod of inverse vibrational frequencies)
- **eneV** – vacancy formation energy
- **preS** – prefactor for solute formation (prod of inverse vibrational frequencies)
- **eneS** – solute formation energy
- **preSV** – excess prefactor for solute-vacancy binding
- **eneSV** – solute-vacancy binding energy
- **preT0** – prefactor for vacancy transition state
- **eneT0** – energy for vacancy transition state (relative to eneV)
- **preT1** – prefactor for vacancy swing transition state
- **eneT1** – energy for vacancy swing transition state (relative to eneV + eneS + eneSV)
- **preT2** – prefactor for vacancy exchange transition state
- **eneT2** – energy for vacancy exchange transition state (relative to eneV + eneS + eneSV)

**Return bFV**  $\beta \text{eneV} - \ln(\text{preV})$  (relative to minimum value)

**Return bFS**  $\beta \text{eneS} - \ln(\text{preS})$  (relative to minimum value)

**Return bFSV**  $\beta \text{eneSV} - \ln(\text{preSV})$  (excess)

**Return bFT0**  $\beta \text{eneT0} - \ln(\text{preT0})$  (relative to minimum value of bFV)

**Return bFT1**  $\beta \text{eneT1} - \ln(\text{preT1})$  (relative to minimum value of bFV + bFS)

**Return bFT2**  $\beta \text{eneT2} - \ln(\text{preT2})$  (relative to minimum value of bFV + bFS)

**tags2preene** (*usertagdict*, *VERBOSE=False*)

Generates energies and prefactors based on a dictionary of tags.

#### Parameters

- **usertagdict** – dictionary where the keys are tags, and the values are tuples: (pre, ene)
- **VERBOSE** – (optional) if True, also return a dictionary of missing tags, duplicate tags, and bad tags

**Return thermodict** dictionary of ene’s and pre’s corresponding to usertagdict

**Return missingdict** dictionary with keys corresponding to tag types, and the values are lists of lists of symmetry equivalent tags that are missing

**Return duplicatelist** list of lists of tags in usertagdict that are (symmetry) duplicates

**Return badtaglist** list of all tags in usertagdict that aren’t found in our dictionary

**OnsagerCalc.arrays2vTKdict** (*vTKarray*, *valarray*, *vTKsplits*)

Takes two arrays of vTK keys and values, and the splits to separate vTKarray back into vTK and returns a dictionary indexed by the vTK.

#### Parameters

- **vTKarray** – array of vTK entries
- **valarray** – array of values
- **vTKsplits** – split placement for vTK entries

**Return vTKdict** dictionary, indexed by vTK objects, whose entries are arrays

`OnsagerCalc.vTKdict2arrays` (*vTKdict*)

Takes a dictionary indexed by vTK objects, returns two arrays of vTK keys and values, and the splits to separate vTKarray back into vTK

**Parameters** `vTKdict` – dictionary, indexed by vTK objects, whose entries are arrays

**Return** `vTKarray` array of vTK entries

**Return** `valarray` array of values

**Return** `vTKsplits` split placement for vTK entries

**class** `OnsagerCalc.vacancyThermoKinetics`

Class to store (in a hashable manner) the thermodynamics and kinetics for the vacancy

**Parameters**

- `pre` – prefactors for sites
- `betaene` – energy for sites / kBT
- `preT` – prefactors for transition states
- `betaeneT` – transition state energy for sites / kBT

**static** `vacancyThermoKinetics_constructor` (*loader, node*)

Construct a GroupOp from YAML

**static** `vacancyThermoKinetics_representer` (*dumper, data*)

Output a PairState



## AUTOMATOR

Automator:

The automator module defines functions that create a tarball from a supercell dictionary. Automator code

Functions to convert from a supercell dictionary (output from a Diffuser) into a tarball that contains all of the input files in an organized directory structure to run the atomic-scale transition state calculations. This includes:

1. All positions in POSCAR format (POSCAR files for states to relax, POS as reference for transition endpoints that need to be relaxed)
2. Transformation information from relaxed states to initial states.
3. INCAR files for relaxation and NEB runs; KPOINTS for each.
4. perl script to transform CONTCAR output from a state relaxation to NEB endpoints.
5. perl script to linearly interpolate between NEB endpoints.
6. Makefile to run everything (representing the “directed graph” of calculations)

`automator.map2string` (*tag, groupop, mapping*)

Takes in a map: tag, groupop, mapping and constructs a string representation to be dumped to a file. If we want to call using the tuple, `map2string(* (map))` will suffice.

### Parameters

- **tag** – string of initial state to rotate
- **groupop** – see `crystal.GroupOp`; we use the rot and trans. This is in the supercell coord.
- **mapping** – in “chemorder” format; list by chemistry of lists of indices of position in initial cell to use.

**Return string\_rep** string representation (to be used by an external script)

```

automator.supercelltar(tar, superdict, filemode=436, directmode=509, timestamp=None, IN-
CARrelax='SYSTEM = {system}\nPREC = High\nISIF = 2\nEDIFF
= 1E-8\nEDIFFG = -10E-3\nIBRION = 2\nNSW = 50\nISMEAR
= 1\nSIGMA = 0.1\n# ENCUT =\n# NGX =\n# NGY =\n# NGZ
=\n# NGXF =\n# NGYF =\n# NGZF =\n# NPAR =\nLWAVE =
.FALSE.\nLCHARG = .FALSE.\nLREAL = .FALSE.\nVOSKOWN = 1\n',
INCARNEB='SYSTEM = {system}\nPREC = High\nISIF = 2\nED-
IFF = 1E-8\nEDIFFG = -10E-3\nIBRION = 2\nNSW = 50\nISMEAR
= 1\nSIGMA = 0.1\n# ENCUT =\n# NGX =\n# NGY =\n# NGZ
=\n# NGXF =\n# NGYF =\n# NGZF =\n# NPAR =\nLWAVE =
.FALSE.\nLCHARG = .FALSE.\nLREAL = .FALSE.\nVOSKOWN = 1\nIM-
AGES = 1\nSPRING = -5\nLCLIMB = .TRUE.\nNELMIN = 4\nN-
FREE = 10\n', KPOINTS='Gamma\n1\nReciproca\n0. 0. 0. 1.\n',
basedir='', statename='relax.', transitionname='neb.', IDformat='{02d}',
JSONdict='tags.json', YAMLdef='supercell.yaml')

```

Takes in a tarfile (needs to be open for reading) and a supercelldict (from a diffuser) and creates the full directory structure inside the tarfile. Best used in a form like

```

with tarfile.open('supercells.tar.gz', mode='w:gz') as tar:
    automator.supercelltar(tar, supercelldict)

```

## Parameters

- **tar** – tarfile open for writing; may contain other files in advance.
- **superdict** – dictionary of states, transitions, transmapping, indices that correspond to dictionaries with tags; the final tag reference is the basesupercell for calculations without defects.
  - superdict['states'][i] = supercell of state;
  - superdict['transitions'][n] = (supercell initial, supercell final);
  - superdict['transmapping'][n] = ((site tag, groupop, mapping), (site tag, groupop, mapping))
  - superdict['indices'][tag] = (type, index) of tag, where tag is either a state or transition tag; or...
  - superdict['indices'][tag] = index of tag, where tag is either a state or transition tag.
  - superdict['reference'] = (optional) supercell reference, no defects
- **filemode** – mode to use for files (default: 664)
- **directmode** – mode to use for directories (default: 775)
- **timestamp** – UNIX time for files; if None, use current time (default)
- **INCARrelax** – contents of INCAR file to use for relaxation; must contain {system} to be replaced by tag value (default: automator.INCARrelax)
- **INCARNEB** – contents of INCAR file to use for NEB; must contain {system} to be replaced by tag value (default: automator.INCARNEB)
- **KPOINTS** – contents of KPOINTS file (default: gamma-point only calculation); if None or empty, no KPOINTS file at all
- **basedir** – prepended to all files/directories (default: '')
- **statename** – prepended to all state names, before 2 digit number (default: relax.)

- **transitionname** – prepended to all transition names, before 2 digit number (default: neb.)
- **IDformat** – format for integer tags (default: {:02d})
- **JSONdict** – name of JSON file storing the tags corresponding to each directory (default: tags.json)
- **YAMLdef** – YAML file containing full definition of supercells, relationship, etc. (default: supercell.yaml); set to None to not output. **may want to change this to None for the future**



## INDICES AND TABLES

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