supercell

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A Scientific Tool

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Version 0.1

Abstract

supercell is a tool to convert a crystallographic structure with partial occupancy and/or vacancies to ordinary supercell structure suitable for calculations.

1 Synopsis

supercell **-h, --help**
supercell [**OPTIONS**] **-i** *input-file*
supercell [**OPTIONS**] **--input**=*input-file*

2 Description

supercell ... Some description here ...

3 Options

-h, --help Print help message and exit the program.

-v *level*, --verbose=*level* Change verbosity level from default 1. Level 0 - quiet mode, only error output. Level 1 suggested for regular users. Higher levels suggested to developers, bug tracking and long program execution times.

-i *input-file*, --input=*input-file* Required options. Input file with in CIF format. Only one file can be specified.

-d, --dry-run The option is highly recommended for the first run of the program with new input specified. With the option the program will do everything, but not write file. Be careful, if you switched **-m**, **--merge-by-distance** option. With the option dry-run should go through all crystal structures. So, it can take time.

-s *cell-size*, --cell-size=*cell-size* The option specifies the size of supercell. The format is AxBxC, where A, B, C are positive integer multipliers of a, b and c vectors of input sell. Default is "1x1x1".

-c *balance-type*, --charge-balance=*balance-type* The option helps you to charge balance the system. Be careful, charge balancing with wrong input charges will make output system composition far from desired or it can freeze the program. The possible arguments are

no No charge balancing. The option will set all charges to zero.

try Default. Try to charge balance system, if initial system is not charged.

yes Charge balance the system.

-p *labels-properties*, --property=*labels-properties* The option will allow you to specify some properties of atoms with specific label manually. The option allows you to use simple of extended syntax.

- Simple: <label>:<property_name>[=<property_value>].
- Extended: "<OPT>(<labels>):<properties>". DONT forget to put extended syntax in quotes.

Where <label> is a label of atom, which property you want to change, <labels> set of space separate labels. <OPT> is type of string processing you want to set for labels. The possible values of <OPT> are

p Treat the labels in parenthesis like a plain string.

w, "" Default for simple syntax. Treat the labels in parenthesis like a wild card. For example, N* means all labels, starting with N: N1, N12, but also Na3. You can use * - any numbers of any symbol and ? - any symbol (exactly one).

r Treat the labels in parenthesis like a Perl Regex. Syntax description you can find at `http://en.wikipedia.org/wiki/Regular_expression`.

The <property_name> is a name of the property you want to set for all specified atoms. Some properties can have values, which you should set using equal symbol. The properties can be

c[charge] Set charge of atoms with specified label(s). Floaing-point value in elementary charge units.

p[opulation] Number of atoms with specific label(s) in output supercell structure.

[not]fixed Exclude atoms from combinations. The output file will contain partial occupancy sites.

Some fancy examples you can find below.

-t *tolerance*, --tolerance=*tolerance* An argument of the option specify the maximum distance between sites, which will be treated like equivalent. Check carefully output of *supercell* before changing the parameter. Default *tolerance*=0.75.

-m, --merge-by-distance The options enables symmetry check algorithm for output structures. Structures, which can be transform to each other using crystallographic symmetry operation will be merged and stored as one structure. For cases with more than 10^4 of total combination it is recommended to treat execution of *supercell* using verbosity level 2 or higher to trace program execution.

-q, --coloumb-energy The option enable Coloumb energy calculations. The result energies for each structures are stored in file <output-prefix>_coloumb_energy.txt. The energies can help to consider the relevant regular structures for following calculations. Ewald summation algorithm is used for the calculations. Be careful, in case of charged cell the energy values can be meanless.

-o *output-prefix*, --output=*output-prefix* The options specify output file name prefix. The prefix can contain folder name but the folder should be created before run the program. For example, --output=myfolder/myfiles. The output files will be created according to templates. Fon non merging run the template will be ¡output-prefix¿_ind¡index¿.cif. For merging run the template will be <output-prefix>_ind<index>_w<weight>.cif, where <weight> - number of the structures merged to the structure. Be careful, all existing files with mask "<output-prefix>*.cif" will be deleted during not dry-run.

4 Files

`somthing` The LaTeX file containing this Man-page.

`1.pdf` The PDF version of this document.

5 Examples

6 Requirements

openbabel Need.

7 Bugs

In case of huge (more than 10^9) number of total combaintions *supercell* can work quite slow or even freeze. The situation most of the time appears with large supresses. Always try small cells first.

If you are merging significant number of combinations (more than 10^5) the program can make get all available physical memory and freeze your system. Control *supercell* with *top* etc.

8 See Also

openbabel(1).

9 Version

Version: 0.1 of January 23, 2014.

10 License and Copyright

Misc The actual version of *supercell* may be found on my homepage `https://github.com/orex/supercell`.

11 Author

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