

geostats

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2. Introduction

geostats is a graphical frontend to the comatsci computational materials science toolkit developed by Jan M. Knaup.

Geostats allows calculating some basic statistical information on geometries, editing atomic data tables and preparing QM/MM coupling geometries based on the BCTC embedding scheme.

2.1. invoking geostats

The geostats command line optionally supports passing the name of one geometry file to be opened upon startup:

```
geostats <input file>
```

geostats supports reading input in the following formats:

.gen

DFTB generic file format, Cf. DFTB documentation or comatsci manual.

.xyz

Xmol xyz coordinate format, an optional 5th column is interpreted as atomic valence populations following DFTB+ convention. Cf. DFTB documentation or comatsci manual.

.fmg

Flexible molecular geometry xml format. Native comatsci format, cf. comatsci manual.

.cdh

Chemical data hierarchy format. Portable data interchange format based on HDF5.

3. Menu structure

3.1. Main window

geostats main window

The geostats main window

(cf. figure)

is composed of the main menu at the top and the text display area. This area will display all statistical reports and graphs generated. Its contents can be copy-pasted, saved as plain text and html or printed. On most systems, the print dialog also allows saving in PDF format.

3.2. File menu

.gen

DFTB generic file format, Cf. DFTB documentation or comatsci manual.

.xyz

Xmol xyz coordinate format, an optional 5th column is interpreted as atomic valence populations following DFTB+ convention. Cf. DFTB documentation or comatsci manual.

.fmg

Flexible molecular geometry xml format. Native comatsci format, cf. comatsci manual.

.cdh

Chemical data hierarchy format. Portable data interchange format based on HDF5.

.pdb

Protein database format. Periodic boundary conditions are only preserved in case of af an x-y-z aligned orthorhombic unit cell.

.fdf

Flexible data format. Standard input file format for SIESTA (<http://icmab.cat/leem/siesta/>).

.xyzq

x,y,z coordinates in Bohr and atomic charge in elementary charges per atom. Default format for external point charges in DFTB+

turbomole

Geometry file format for turbomole (<http://www.turbomole.com/>). The file name is fixed to “coord”, regardless if the user selection in the file name dialog!

aims

Geometry file format for FHI-aims (<https://aimsclub.fhi-berlin.mpg.de/>). The file name is fixed to “geometry.in”, regardless of the user selection in the file name dialog!

3.3. Edit menu

The edit menu entries are only available if a geometry is loaded.

Figure 2.

edit atoms dialog

Element

The chemical element.

Subtype

An arbitrary string describing the atom type. Defaults to the element symbol but may be changed to anything the user wishes. Autogenerated link-atoms will be labeled “H_1”

X,Y,Z

The atomic cartesian coordinates in Å.

Layer

Logical subdivision of the geometry. Similar in concept to fragments in the protein database but more flexible. For QM/MM embedding, layers are used to separate QM-zone and MM-zone parts of the geometry. If no layer information is stored in the input file format, atoms are placed in the “default layer”. Layer information is stored in the fragment columns in .pdf and .cdh formats, it is stored as the “<layer>” tag in .fmg. If a new layer name is entered that does not yet exist, the respective layer is created.

Charge

The atomic net charge in elementary charge units. (I.e. negative charge denotes excess electrons, positive charge denotes electron deficiency.)

Figure 3.

periodic expand dialog

3.4. Statistics menu

3.5. Help menu

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