FHI-aims File Format Description: geometry.in

1 Overview

FHI-aims requires two input files, which should contain all information needed to run a first-principles calculation.

All technical settings should be specified in a single file `control.in`.

A second input file, `geometry.in`, specifies the system geometry (placement and type of atoms, unit cell vectors, etc.) and any information that is linked directly to the system geometry, to the system's physical environment, or to specific atoms. No other technical information should be part of `geometry.in`. In particular, k-space related information is provided to the code in a generic format as a part of `control.in`, in fractional coordinates of the reciprocal space vectors, not of `geometry.in`.

In its simplest form, `geometry.in` is a generic format specification for files conveying the atomic structure of molecules or solids. This basic form is thus functionally equivalent to other, code-agnostic file specifications containing atomic structure information, such as .xyz, .cif, or .pdb . Like these other file formats, `geometry.in` can contain technical information beyond the actual atomic structure.

The present document focuses on aspects related to the basic atomic structure information (including information on specified initial spin moments, which may result in physically different outcomes for the structure in question). A full listing of all keywords related to `geometry.in` may be found in the FHI-aims code manual.

2 Examples

Any molecular geometry in FHI-aims requires only cartesian atomic coordinates of the position of a nucleus (in Å) and of the atomic species (usually, the chemical element) found at that position. No other information is required. Any `geometry.in` file that does not include a unit cell specification is automatically considered to correspond to the definition of an isolated molecule.

The `geometry.in` file for an isolated N_2 molecule might look like this:

```
atom 0. 0. 0.      N
atom 0. 0. 1.0976  N
```

Periodic systems are defined by specifying three lattice repeat vectors in cartesian units (Å). The `geometry.in` file for the primitive two-atom cell of a GaAs periodic crystal might look like this:

```
lattice_vector  2.826650         2.826650         0.000000
lattice_vector  0.000000         2.826650         2.826650
lattice_vector  2.826650         0.000000         2.826650

atom  0.000000         0.000000         0.000000  Ga
atom  1.413325         1.413325         1.413325  As
```

The previous version specifies the cartesian atomic coordinates in Å (`atom` keyword). Alternatively, a specification in fractional coordinates (units of the lattice vectors) is possible as well:

```
lattice_vector  2.826650         2.826650         0.000000
lattice_vector  0.000000         2.826650         2.826650
lattice_vector  2.826650         0.000000         2.826650

atom_frac  0.              0.              0.        Ga
atom_frac  0.25            0.25            0.25      As
```

The relation between lattice vectors $\{\boldsymbol{a}_i\}$, cartesian atomic coordinates $\{\boldsymbol{R}_I\}$ of atom I and fractional atomic coordinates $\{\boldsymbol{f}_I\}$ is

$$R_{I,j} = \sum_k f_{I,k} a_{k,j} \tag{1}$$

The index j denotes the cartesian coordinates of the kth lattice vector in the order provided in `geometry.in`.

3 Format and Keywords

In `geometry.in`, whitespace separates keywords and their values. Empty lines are ignored and comment lines can be inserted starting with the '#' character. The order of lines is generally arbitrary, with the exception of keywords that pertain to a specific atom. Keywords that pertain to a specific atom (such as an `initial_moment` spin moment specification or a constraint on the atomic position) must be specified after the `atom` or `atom_frac` line of that atom, and before the `atom` or `atom_frac` line indicating the next atom.

Keywords descriptions:
(restricted to the keywords that do not refer to code-specific technical features)

`atom`

Usage: `atom x y z species_name`

Purpose: Specifies the initial location and type of an atom.

`x`, `y`, `z` are real numbers (in Å) which specify the atomic position.

`species_name` is a string descriptor which names the element on this atomic position; it must match with one of the species descriptions given in `control.in`.

`atom_frac`

Usage: `atom_frac` n_1 n_2 n_3 `species_name`

Purpose: Specifies the initial location and type of an atom in fractional coordinates.

n_i is a real multiple of lattice vector i. `species_name` is a string descriptor which names the element on this atomic position; it must match with one of the species descriptions given in `control.in`.

Fractional coordinates are only meaningful in periodic calculations.

`lattice_vector`

Usage: `lattice_vector x y z`

Purpose: Specifies one lattice vector for periodic boundary conditions.

`x`, `y`, `z` are real numbers (in Å) which specify the direction and length of a unit cell vector.

If up to three lattice vectors are specified, FHI-aims automatically assumes periodic boundary conditions in those directions. *Note* that the order of lattice vectors matters, as the order of k space divisions (given in `control.in`) depends on it!

`initial_moment`

Usage: `initial_moment moment`

Purpose: Allows to place an initial spin moment on an `atom` in file `geometry.in`.

`moment` is a real number, referring to the electron difference $N^{\uparrow} - N^{\downarrow}$ on that site. Default: Zero, unless `default_initial_moment` is set explicitly.

The `initial_moment` keyword always applies to the immediately preceding `atom` specified in input file `geometry.in`. The moment is introduced by using a spin-polarized instead of an unpolarized spherical free-atom density on that site in the initial superposition-of-free-atoms density. Note that initial charge densities are generated by the functional specified with `xc` for DFT-LDA/GGA, but refer to `pw-lda` densities for all other functionals (hybrid functionals, Hartree-Fock, ...).