

# The *system.am* file format description

The *system.am* file has a tag-based format. This leads to a flexibility of adding new tags/data fields to a file.

```
...
& tagname
  data field
...
```

Ampersand (&) starts a section name followed by a tagname. Next line(s) contain(s) a data field in a formatted form, which depends on the data. The section has to be finished with an empty line. The order of sections is completely arbitrary and some of them can be optional. Comments can be placed between sections and should be separated by empty lines.

Below, a list of all tags with its description is presented.

| Tagname                          | Attribute                   | Description  |
|----------------------------------|-----------------------------|--|
| <i>hash</i>                      | optional                    | internal identifier, that can be used to check the consistency of different files. The UNIX timestamp is usually used.   |
| <i>codestamp</i>                 | optional                    | name of the band structure package in which <i>system.am</i> file was generated.   |
| <i>cell</i>                      | mandatory                   | scaling parameter ( <i>alat</i> ) and crystal lattice vectors in Cartesian coordinates (the first line defines the first vector and so on). The data are in atomic units.  |
| <i>crystcoord</i>                | optional<br>(default=false) | use crystal (or fractional) coordinates (true) or Cartesian coordinates (false) for atomic positions (in units of <i>alat</i> ).   |
| <i>atoms</i>                     | mandatory                   | contains information about atoms. The first line provides a number of atoms. The rest of the lines set atomic labels and atomic positions in units that depend on <i>crystcoord</i> .  |
| <i>nelec</i>                     | optional                    | number of electrons to adjust Fermi level.   |
| <i>efermi</i> or<br><i>fermi</i> | optional                    | self-consistent value of the Fermi level obtained in DFT calculation (in eV).  |
| <i>basis</i>                     | mandatory                   | defines a localized (Wannier-like) basis functions of the Hamiltonian. The first line sets the total basis dimension and number of the basis functions. Then, for each basis (Wannier) function, there is a line, which defines next parameters: atomic label, reference to atom, orbital symmetry of a wave function, position in the Hamiltonian and order of the cubic harmonics. |

The example of *system.am* file for bcc-Fe with explanations is shown below.

```

# This file was written on: 03.12.2018 08:20:35

& hash
  1544430035

&Codestamp
  exciting-plus

&cell
  1.000000000
  2.76987 2.76987 2.76987
  2.76987 2.76987 -2.76987
  2.76987 -2.76987 2.76987

&fermi
  8.86799076094252

&crystcoord
  true

# The tag below is absent in the real exciting-plus output but
# we added it for educative purpose

& NELEC
  8

&atoms
  1
  Fe 0.00000 0.00000 0.00000

# Basis description:
# dim, nblocks
# atom_sym, atom_num, l_sym, block_dim, block_start, orbitals(1:block_dim)
&basis
  9 3
  Fe 1 s 1 1 1
  Fe 1 p 3 2 2 3 4
  Fe 1 d 5 5 5 6 7 8 9

```

Most of tags are well explained, and hence, we will concentrate how the data from *system.am* file can be transferred to the *amulet.ini* and *impurity\_X.ini* files. In case of iron, the total valence charge is 16 (*grep* 'Total valence charge' INFO.OUT), while the *nelec* provides 8 electrons only. The difference is due to a projection to energy bands close to the Fermi level, or in the other words, due to the elimination of the occupied semicore 3s and 3p bands (8 electrons). The value of *nelec* can be used as *ntotal* token in the *amulet.ini* file. The *fermi* tag provides a self-consistent value for the Fermi energy out of the DFT calculation and it can be used as an initial value for

the token *mu* in the *amulet.ini* file.

The *basis* tag contains the information that can be directly utilized in the *impurity-X.ini* file. The first line sets a total number of the basis functions (dimension of the Hamiltonian) and a number of groups of Wannier functions with different symmetry. Then each group is described. In the above example, all orbital groups belong to Fe atom number one (unfortunately, in this example there is one atom only). Then the orbital symmetry is specified (*s*, *p* and *d* in our case) followed by degeneracy (1, 3, 5). Then the starting positions in the Hamiltonian (1, 2 and 5) are provided. The rest of the data sets the order of cubic harmonics (for numbering of cubic harmonics see table 1).

Thus, if one wants to use Fe *d* states as correlated in the DFT+DMFT calculations, we should setup next tokens in the *impurity\_1.ini* file.

```

name = Fe                                ! label
nlm = 5                                  ! degeneracy
himppos = 5                              ! starting position in the Hamiltonian
cubic_harmonic_order = 5 6 7 8 9        ! order of cubic harmonic
...

```

Table 1: Numbering of the cubic harmonics.

|          |                      |                      |                      |                       |                       |                                  |                       |  |  |                        |                                   |                                  |                                   |   |  |
|----------|----------------------|----------------------|----------------------|-----------------------|-----------------------|----------------------------------|-----------------------|--|--|------------------------|-----------------------------------|----------------------------------|-----------------------------------|---|--|
| 1        | 2                    | 3                    | 4                    | 5                     | 6                     | 7                                | 8                     | 9  | 10   | 11                     | 12                                | 13                               | 14                                | 15  | 16   |
| <i>s</i> | <i>p<sub>y</sub></i> | <i>p<sub>z</sub></i> | <i>p<sub>x</sub></i> | <i>d<sub>xy</sub></i> | <i>d<sub>yz</sub></i> | <i>d<sub>z<sup>2</sup></sub></i> | <i>d<sub>xz</sub></i> | <i>d<sub>x<sup>2</sup>-y<sup>2</sup></sub></i> | <i>f<sub>y(3x<sup>2</sup>-y<sup>2</sup>)</sub></i> | <i>f<sub>xyz</sub></i> | <i>f<sub>yz<sup>2</sup></sub></i> | <i>f<sub>z<sup>3</sup></sub></i> | <i>f<sub>xz<sup>2</sup></sub></i> | <i>f<sub>z(x<sup>2</sup>-y<sup>2</sup>)</sub></i> | <i>f<sub>x(x<sup>2</sup>-3y<sup>2</sup>)</sub></i> |