

Tight-Binding Coherent Potential Approximation

1.0

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Chapter 1

Data Type Index

1.1 Data Types List

Here are the data types with brief descriptions:

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Chapter 2

Data Type Documentation

2.1 concentration Module Reference

Public Attributes

- `real(kind=8) con`

Module for the concentration related variables of the CPA program.

2.1.1 Member Data Documentation

2.1.1.1 `real(kind=8) concentration::con`

Module for the concentration related variables of the CPA program.

Parameters

<code>con</code>	- The concentration of the first atom type (e.g. $FeSe_{con}Te_{1-con}$)
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The documentation for this module was generated from the following file:

- `global.f90`

2.2 converge Module Reference

Public Attributes

- `real(kind=8) cr`

Module for the convergence criterion related variables.

- `real(kind=8) ci`

2.2.1 Member Data Documentation

2.2.1.1 `real(kind=8) converge::cr`

Module for the convergence criterion related variables.

Parameters

<i>cr</i>	- Convergence criterion for the real part of the Newton-Raphson procedure
<i>ci</i>	- Convergence criterion for the imaginary part of the Newton-Raphson procedure

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- global.f90

2.3 global Module Reference

Public Attributes

- integer(kind=4) **vlvl**
Currently this global file is setup for calculations of P4/nmm Fe2Se/Te2.
- integer(kind=4) **mode**
- integer(kind=4), parameter **jsz** = 196
- integer(kind=4), parameter **ntype** = 2
- integer(kind=4), dimension(ntype),
parameter **natom** = (/ 2, 2 /)
- integer(kind=4), parameter **nse** = 4*natom(2)
- integer(kind=4), parameter **sec** = 9*2*2
- logical **verbose**
- real(kind=8), parameter **pi** = 4.0d0*datan(1.0d0)
- real(kind=8), parameter **pp** = 1.0d0/pi
- real(kind=8), parameter **small** = 1.0d-20
- character(len=75) **title**

2.3.1 Member Data Documentation

2.3.1.1 integer(kind=4) global::vlvl

Currently this global file is setup for calculations of P4/nmm Fe2Se/Te2.

Parameters

<i>jsz</i>	- Number of kpoints
<i>mode</i>	- Used to decide how the program is run 1 - Perform full CPA prgoram, including GG calculations 2 - Perform only GG calculations. Must have run mode 1 or 3 previously 3 - Perform VCA with DOS and GG calculations. Essentially skips setting and calculating self-energies.
<i>ntype</i>	- Number of different atom types
<i>natom(ntype)</i>	- Number of different atoms (# of atoms in should be given alphabetical order; i.e. UPd2Al3 should be (3,2,1))
<i>nse</i>	- Number of self energies
<i>pi</i>	Mathematical value of pi
<i>sec</i>	- Number of secular equations
<i>small</i>	Real value considered to be "small"
<i>title</i>	- Title from cpaper.in to be used in all output files
<i>verbose</i>	- Logical for debugging flags (.true. = debug info on)
<i>vlvl</i>	- Level of debugging verboseness

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- global.f90

2.4 green Module Reference

Public Attributes

- `complex(kind=8), dimension(sec, sec) grn`

The documentation for this module was generated from the following file:

- `global.f90`

2.5 hamiltonians Module Reference

Public Attributes

- `real(kind=8), dimension(jsz, sec, sec) hma`
- `real(kind=8), dimension(jsz, sec, sec) hmb`
- `real(kind=8), dimension(jsz, sec, sec) vsa`
- `real(kind=8), dimension(jsz, sec, sec) vsb`
- `complex(kind=8), dimension(jsz, sec, sec) ham`

The documentation for this module was generated from the following file:

- `global.f90`

2.6 onsite Module Reference

Public Attributes

- `real(kind=8), dimension(natom(2), sec) ons`
- `real(kind=8), dimension(sec) ons_bar`
- `complex(kind=8), dimension(nse, nse) onsa`
- `complex(kind=8), dimension(nse, nse) onsb`
- `complex(kind=8), dimension(nse, nse) onsavg`

The documentation for this module was generated from the following file:

- `global.f90`

2.7 sigma Module Reference

Public Attributes

- `complex(kind=8), dimension(nse) sig`

The documentation for this module was generated from the following file:

- `global.f90`

2.8 unitconvert Module Reference

Public Attributes

- `real(kind=8), parameter ang2m = 1.0d-10`
- `real(kind=8), parameter bohr2ang = 0.52917721092d0`
- `real(kind=8), parameter bohr2m = 0.52917721092d-11`
- `real(kind=8), parameter ev_aa2kg_ss = 16.0217656d0`
- `real(kind=8), parameter ev2hz = 2.417989348d14`
- `real(kind=8), parameter ev2j = 1.602176565d-18`
- `real(kind=8), parameter k2ev = 8.621738d-5`
- `real(kind=8), parameter k2mev = 8.621738d-2`
- `real(kind=8), parameter kg_ss2ev_aa = 6.2415094d-2`
- `real(kind=8), parameter mev2hz = 2.417989348d11`
- `real(kind=8), parameter ry2ev = 13.60569253d0`
- `real(kind=8), parameter u2kg = 1.660538921d-27`
- `real(kind=8), parameter u2ev_c2 = 931.494061d6`
- `real(kind=8), parameter ukk2ev_aa = 1.776386273d-6`
- `real(kind=8), parameter ukk2ev_aa2 = 4.504401531323d-8`

The documentation for this module was generated from the following file:

- `global.f90`

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