exciting input reference

exciting carbon

December 2015

About this Document

In order to perform an **exciting** calculation an **XML** input file called **input.xml** must be provided.

This web page lists all **elements** and **attributes** that can be used in the input file of an **exciting** calculation:

- **elements** are defined according to the **general XML conventions** (http://en.wikipedia.org/wiki/XML#Key_terminology). **Example:** The element groundstate is used to set up a self-consistent calculation of the ground-state energy.
- **attributes** are also defined from the **general XML conventions** (http://en.wikipedia.org/wiki/XML#Key_terminology). An attribute is always connected to an element. In **exciting** an attribute generally specifies a parameter or a set of parameters which are connected to the corresponding element. **Example:** The attribute xctype of the element groundstate defines which exchange-correlation potential is used in the self-consistent calculation.

The input file of an **exciting** calculation has the default name **input.xml**. Simple examples for input files can be found in the available **Tutorials** (http://exciting-code.org/tutorials-carbon). The input file **input.xml** must be a valid **XML** file and it must contain the root element input.

Unless explicitly stated otherwise, **exciting** uses atomic units, setting $\hbar = m_e = e = 1$. Relevant units are:

- Energies are given in Hartree:
$$1 \text{ Ha} = 2 \text{ Ry} = 27.21138386(68) \text{ eV} = 4.35926 \cdot 10^{-18} \text{ J}$$
- Lengths are given in Bohr:
$$1\ a_{\text{Bohr}} = 0.52917720859(36)\ \text{Å} = 0.52917720859(36) \cdot 10^{-10} \text{ m}$$
- Magnetic fields are given in units of
$$1 \text{ a.u.} = \frac{e}{a_{\text{Bohr}}^2} = 1717.2445320376 \text{ Tesla.}$$

Note: The electron charge is positive, so that the atomic numbers Z are negative.

Part I
Input Elements

1 Element: input

The **XML** element input is the root element of the **exciting** input file. It must contain at least the elements title, structure, and groundstate, each

of them must be present only one time.

Contains:	`title` (1 times)
	`structure` (1 times)
	`groundstate` (1 times)
	`relax` (optional)
	`properties` (optional)
	`phonons` (optional)
	`xs` (optional)
	`gw` (optional)
	`eph` (optional)
	`keywords` (optional)
XPath:	`/input`

This element allows for specification of the following attributes:

`sharedfs`

1.1 Attribute: sharedfs

This attributes tells if a parallel job has a shared file system. Set it to `false` if the processes of the job do not share a common file system. It gives **exciting** a chance to adapt the file IO accordingly

Type:	boolean
Default:	"`true`"
Use:	optional
XPath:	`/input/@sharedfs`

2 Element: title

The title of the input file, *e.g.*, "Ground-State Calculation for Aluminum".

Type:	string
XPath:	`/input/title`

3 Element: keywords

The keywords tag can contain a space separated list of keywords classifying the calculation for archiving purposes. It is not used by the **exciting** program.

Type:	string
XPath:	`/input/keywords`

4 Element: structure

This element contains all structural information, such as unit-cell parameters as well as type and position of each atom. The presence of the subelement species is necessary unless one wants to perform an empty-lattice calculation. The attribute speciespath must be specified.

Contains: crystal (1 times)
species (zero or more)
XPath: /input/structure

This element allows for specification of the following attributes:

speciespath (required), autormt, cartesian, epslat, primcell, rmtapm, tshift

4.1 Attribute: autormt

If "true", the muffin-tin radius of each species is automatically set according to the variables specified by the attribute rmtapm.

Type: boolean
Default: "false"
Use: optional
XPath: /input/structure/@autormt

4.2 Attribute: cartesian

If "true" the input atomic positions are given in cartesian coordinates.

Type: boolean
Default: "false"
Use: optional
XPath: /input/structure/@cartesian

4.3 Attribute: epslat

This attribute defines the accuracy up to which two vectors can be considered numerically identical. Vectors with lengths less than this are considered zero.

Type: fortrandouble (114.1)
Default: "1.0d-6"
Use: optional
Unit: Bohr
XPath: /input/structure/@epslat

4.4 Attribute: primcell

If "true", the primitive unit cell is determined automatically from the conventional cell defined by the basis vectors given by the basevect elements. The primitive unit cell is determined by searching for lattice vectors among all vectors connecting atomic sites and choosing the three shortest ones which produce a unit cell with non-zero volume.

Type: boolean
Default: "false"
Use: optional
XPath: /input/structure/@primcell

4.5 Attribute: rmtapm

This attribute assigns the two parameters governing the automatic generation of the muffin-tin radii. When the attribute autormt is set to "true", the muffin-tin radii are determined according to the following expression

$$R_i \propto 1 + \zeta |Z_i|^{1/3}, \tag{1}$$

where Z_i is the atomic number of the i th species, ζ is stored in rmtapm(1). The distance between the muffin-tin speheres is determined by the value of rmtapm(2): When rmtapm(2)=1, the closest muffin-tin spheres will touch each other.

Type: vect2d (114.7)
Default: "0.25d0 0.95d0"
Use: optional
XPath: /input/structure/@rmtapm

4.6 Attribute: speciespath

The path to the directory containing the species files. Alternatively, it can be defined as an HTTP URL, in this case the **wget** (http://exciting-code.org/wget) utility must be installed.

Type: anyURI
Use: required
XPath: /input/structure/@speciespath

4.7 Attribute: tshift

If "true", the crystal is shifted such that the atom closest to the origin is exactly at the origin.

Type: boolean

Default: "true"
Use: optional
XPath: /input/structure/@tshift

5 Element: crystal

Defines the unit cell of the crystal via the 3 basis vectors.

Contains: basevect (3 times)
XPath: /input/structure/crystal

This element allows for specification of the following attributes:

scale, stretch

5.1 Attribute: scale

Scales all the lattice vectors by the same factor. This is useful for varying the volume.

Type: fortrandouble (114.1)
Default: "1.0d0"
Use: optional
Unit: 1
XPath: /input/structure/crystal/@scale

5.2 Attribute: stretch

Allows for an individual scaling of each lattice vector separately. "1 1 1" means no scaling.

Type: vect3d (114.6)
Default: "1.0d0 1.0d0 1.0d0 "
Use: optional
XPath: /input/structure/crystal/@stretch

6 Element: basevect

Defines one basis vector in Cartesian coordinates.

Type: vect3d (114.6)
Unit: Bohr
XPath: /input/structure/crystal/basevect

7 Element: species

Defines the atomic species, *i.e.*, the chemical element. Aatomic coordinates and, optionally, quantities relevant for magnetic calculations are defined in the subelement(s) atom.

Contains:	atom (1 times or more)
	LDAplusU (optional)
	dfthalfparam (optional)
XPath:	/input/structure/species

This element allows for specification of the following attributes:

speciesfile (required), rmt

7.1 Attribute: rmt

Defines the muffin-tin radius. This optional parameter allows to override the value either specified in the species file or generated by automatic determination. The muffin-tin radius defines the region around the atomic nucleus where the wave function is expanded in terms of atomic-like functions. In contrast, the interstitial region, *i.e.*, the region not belonging to any muffin-tin sphere, is described by planewaves.

Type:	fortrandouble (114.1)
Default:	"-1.0d0"
Use:	optional
Unit:	Bohr
XPath:	/input/structure/species/@rmt

7.2 Attribute: speciesfile

Defines the file that contains the species definition. It is looked up in the species directory specified by speciespath. By default, the name of the file is *element*.xml, *e.g.*, Ag.xml.

Type:	anyURI
Use:	required
XPath:	/input/structure/species/@speciesfile

8 Element: atom

Defines the position and other attributes of one atom in the unit cell.

Type:	no content
XPath:	/input/structure/species/atom

This element allows for specification of the following attributes:

coord (required), bfcmt, lockxyz, mommtfix

8.1 Attribute: bfcmt

Muffin-tin external magnetic field in Cartesian coordinates.

Type: vect3d (114.6)
Default: "0.0d0 0.0d0 0.0d0"
Use: optional
XPath: /input/structure/species/atom/@bfcmt

8.2 Attribute: coord

Atom position in lattice coordinates.

Type: vect3d (114.6)
Use: required
Unit: lattice coordinates
XPath: /input/structure/species/atom/@coord

8.3 Attribute: lockxyz

Switches to constrain atomic movement along x/y/z directions.

Type: booleantriple (114.3)
Default: "false false false"
Use: optional
XPath: /input/structure/species/atom/@lockxyz

8.4 Attribute: mommtfix

The desired muffin-tin moment for a Fixed Spin Moment (FSM) calculation.

Type: vect3d (114.6)
Default: "0.0d0 0.0d0 0.0d0"
Use: optional
XPath: /input/structure/species/atom/@mommtfix

9 Element: LDAplusU

The LADplusU element is used to specify the J, U, and l parameters of an atomic species. To switch on the LDAplusU feature one needs to set the ldapu attribute of the groundstate element.

Type: no content
XPath: /input/structure/species/LDAplusU

This element allows for specification of the following attributes:

J, U, l

9.1 Attribute: J

Type: fortrandouble (114.1)
Default: "0.0d0"
Use: optional
XPath: /input/structure/species/LDAplusU/@J

9.2 Attribute: U

Type: fortrandouble (114.1)
Default: "0.0d0"
Use: optional
XPath: /input/structure/species/LDAplusU/@U

9.3 Attribute: l

Type: integer
Default: "-1"
Use: optional
XPath: /input/structure/species/LDAplusU/@l

10 Element: dfthalfparam

This element specifies some of the fundamentals parameters (for each species) regarding a **DFT-1/2** calculation. Do not forget to specify the subelement dfthalf inside the element groundstate, otherwise no **DFT-1/2** correction will be done (even though you specify the parameters).

Contains: shell (1 times or more)
XPath: /input/structure/species/dfthalfparam

This element allows for specification of the following attributes:

ampl, cut, exponent

10.1 Attribute: ampl

Specifies the amplitude of the self-energy potential.

Type: fortrandouble (114.1)
Default: "1.00"
Use: optional
XPath: /input/structure/species/dfthalfparam/@ampl

10.2 Attribute: cut

Specifies the value of r_{cut} (in Bohrs) for the self-energy potential, which determines the range of the correction. Note that this can/should be specified for each species.

Type: fortrandouble (114.1)
Default: "0.0d0"
Use: optional
Unit: Bohr
XPath: /input/structure/species/dfthalfparam/@cut

10.3 Attribute: exponent

Specifies the exponent n of the cutoff-function (for the self-energy potential)

$$\Theta(r) = A\left[1 - \left(\frac{r}{r_{\text{cut}}}\right)^n\right]^3$$

for $r \leq r_{\text{cut}}$.

Type: integer
Default: "8"
Use: optional
XPath: /input/structure/species/dfthalfparam/@exponent

11 Element: shell

This element specifies the shell to which the **DFT-1/2** correction should be applied to.

Type: no content
XPath: /input/structure/species/dfthalfparam/shell

This element allows for specification of the following attributes:

ionization, number

11.1 Attribute: ionization

Specifies the degree of ionization.

Type:	fortrandouble (114.1)
Default:	"0.5d0"
Use:	optional
Unit:	Bohr
XPath:	/input/structure/species/dfthalfparam/shell/@ionization

11.2 Attribute: number

Specifies the number of the shell to be ionized. For instance, a number equal to 1 will ionize the first shell, a number equal to 2, the second, and so on. The default value of 0 corresponds to the last shell specified in the species file.

Type:	integer
Default:	"0"
Use:	optional
XPath:	/input/structure/species/dfthalfparam/shell/@number

12 Element: groundstate

The groundstate element is required for any calculation. Its attributes are parameters and methods which are used to calculate the ground-state density.

Contains:	DFTD2parameters (optional) TSvdWparameters (optional) spin (optional) dfthalf (optional) Hybrid (optional) solver (optional) OEP (optional) output (optional) libxc (optional)
XPath:	/input/groundstate

This element allows for specification of the following attributes:

CoreRelativity, ExplicitKineticEnergy, PrelimLinSteps, SymmetricKineticEnergy, ValenceRelativity, autokpt, beta0, betadec, betainc, cfdamp, chgexs, deband, dipolecorrection, dipoleposition, dlinengyfermi, do, energyref, epsband, epschg, epsengy, epsforcescf, epsocc, epspot, fermilinengy, findlinentype, fracinr, frozencore, gmaxvr, isgkmax, ldapu, lmaxapw, lmaxinr, lmaxmat, lmaxvr, lorecommendation, lradstep, maxscl, mixer, mixerswitch, modifiedsv, msecStoredSteps,

nempty, ngridk, niterconvcheck, nktot, nosource, nosym, nprad, npsden, nwrite, outputlevel, ptnucl, radialgridtype, radkpt, reducek, rgkmax, scfconv, stype, swidth, symmorph, tevecsv, tfibs, tforce, tpartcharges, vdWcorrection, vkloff, xctype

12.1 Attribute: CoreRelativity

Chooses between relativistic/non-relativistic descriptions for core electrons. Pick either "dirac" or "none".

Type:	**choose from:**
	dirac
	none
Default:	"dirac"
Use:	optional
XPath:	/input/groundstate/@CoreRelativity

12.2 Attribute: ExplicitKineticEnergy

If true, the kinetic energy expectation values are calculated explicitly and, then, they are used for calculating the total energy.

Type:	boolean
Default:	"true"
Use:	optional
XPath:	/input/groundstate/@ExplicitKineticEnergy

12.3 Attribute: PrelimLinSteps

After which SCF iteration is msec mixing supposed to be turned on. Until then linear mixing is applied. Used in msec mixing as choosen with mixer.

Type:	integer
Default:	"2"
Use:	optional
XPath:	/input/groundstate/@PrelimLinSteps

12.4 Attribute: SymmetricKineticEnergy

If "true", the kinetic-energy matrix elements of muffin-tin functions are calculated by applying gradient to both bra and ket. Otherwise, the whole kinetic-energy operator is applied to ket only, and the surface-term correction is applied to make the hamiltonian hermitian.

Type:	boolean
Default:	"true"
Use:	optional

XPath: /input/groundstate/@SymmetricKineticEnergy

12.5 Attribute: ValenceRelativity

Relativistic Hamiltonian to use in groundstate calculations.

- none - solves non-relativistic Schoedinger equation (SE)
- zora - solves scalar-relativistic SE within zero-order regular approximation (ZORA)
- iora* - solves scalar-relativistic SE within infinite-order regular approximation (IORA), the small component is neglected
- iora - solves scalar-relativistic SE within infinite-order regular approximation (IORA), the small component is included
- kh* - solves scalar-relativistic SE for the large component, the small component is neglected
- kh - solves scalar-relativistic SE for the large component, the small component is included

iora, kh* and kh are implemented only for atoms.

Type: **choose from:**
`zora`
`iora*`
`iora`
`kh*`
`kh`
`none`
Default: "`zora`"
Use: optional
XPath: /input/groundstate/@ValenceRelativity

12.6 Attribute: autokpt

If `"true"`, the set of **k**-points is determined automatically according to `radkpt`.

Type: boolean
Default: "`false`"
Use: optional
XPath: /input/groundstate/@autokpt

12.7 Attribute: beta0

Initial value for mixing parameter. Used in linear mixing as choosen with `mixer`.

Type: fortrandouble (114.1)
Default: "0.4d0"
Use: optional
XPath: /input/groundstate/@beta0

12.8 Attribute: betadec

Mixing parameter decrease. Used in linear mixing.

Type: fortrandouble (114.1)
Default: "0.6d0"
Use: optional
XPath: /input/groundstate/@betadec

12.9 Attribute: betainc

Mixing parameter increase. Used in linear mixing.

Type: fortrandouble (114.1)
Default: "1.1d0"
Use: optional
XPath: /input/groundstate/@betainc

12.10 Attribute: cfdamp

Damping coefficient for characteristic function.

Type: fortrandouble (114.1)
Default: "0.0d0"
Use: optional
XPath: /input/groundstate/@cfdamp

12.11 Attribute: chgexs

This controls the amount of charge in the unit cell beyond that required to maintain neutrality. It can be set positive or negative depending on whether electron or hole doping is required.

Type: fortrandouble (114.1)
Default: "0.0d0"
Use: optional
XPath: /input/groundstate/@chgexs

12.12 Attribute: deband

Initial band energy step size The initial step length used when searching for the band energy, which is used as the APW linearisation energy. This is done by first searching upwards in energy until the radial wave-function at the muffin-tin radius is zero. This is the energy at the top of the band, denoted E_{t}. A downward search is now performed from E_{t} until the slope of the radial wave-function at the muffin-tin radius is zero. This energy, E_{b}, is at the bottom of the band. The band energy is taken as $(E_{\mathrm{t}} + E_{\mathrm{b}})/2$. If either E_{t} or E_{b} cannot be found then the band energy is set to the default value.

Type: fortrandouble (114.1)
Default: "0.0025d0"
Use: optional
Unit: Hartree
XPath: /input/groundstate/@deband

12.13 Attribute: dipolecorrection

If "true", the dipole correction is applied for slabs oriented along the z-direction.

Type: boolean
Default: "false"
Use: optional
XPath: /input/groundstate/@dipolecorrection

12.14 Attribute: dipoleposition

The value of this attribute indicates the position of the jump in electrostatic potential, after the compensating potential (*i.e.*, the dipole correction) is applied. The position is given as a fractional coordinate in the vertical direction. Please note that this jump position should be located within the vacuum region enough far away from the atomic layers, otherwise the compensating potential cannot be correctly applied. It is recommended to put the jump position at the middle of the vacuum layer.

Type: fortrandouble (114.1)
Default: "1.0d0"
Use: optional
XPath: /input/groundstate/@dipoleposition

12.15 Attribute: dlinengyfermi

Energy difference between linearisation and Fermi energy.

Type: fortrandouble (114.1)
Default: "-0.1d0"

Use: optional
Unit: Hartree
XPath: /input/groundstate/@dlinengyfermi

12.16 Attribute: do

Decides if the ground state is calculated starting from scratch, using the densities from file, or if its calculation is skipped and only the associated input parameters are read in.

Type: **choose from:**
`fromscratch`
`fromfile`
`skip`
Default: "`fromscratch`"
Use: optional
XPath: /input/groundstate/@do

12.17 Attribute: energyref

Energy reference ε_{ref} for the scalar-relativistic ZORA. It enters the kinetic energy expression $T = \mathbf{p}\frac{c^2}{2c^2+\varepsilon-v(\mathbf{r})}\mathbf{p}$.

Type: fortrandouble (114.1)
Default: "`0.0d0`"
Use: optional
XPath: /input/groundstate/@energyref

12.18 Attribute: epsband

Energy tolerance for search of linearisation energies.

Type: fortrandouble (114.1)
Default: "`1.0d-6`"
Use: optional
Unit: Hartree
XPath: /input/groundstate/@epsband

12.19 Attribute: epschg

Convergence criterion for the maximum allowed error in the calculated total charge beyond which a warning message will be issued.

Type: fortrandouble (114.1)
Default: "`1.0d-5`"
Use: optional

XPath: /input/groundstate/@epschg

12.20 Attribute: epsengy

Energy convergence tolerance.

Type: fortrandouble (114.1)
Default: "1.0d-6"
Use: optional
Unit: Hartree
XPath: /input/groundstate/@epsengy

12.21 Attribute: epsforcescf

Convergence tolerance for forces (not including IBS contribution) during the SCF run.

Type: fortrandouble (114.1)
Default: "5.0d-5"
Use: optional
XPath: /input/groundstate/@epsforcescf

12.22 Attribute: epsocc

smallest occupancy for which a state will contribute to the density.

Type: fortrandouble (114.1)
Default: "1.0d-8"
Use: optional
XPath: /input/groundstate/@epsocc

12.23 Attribute: epspot

If the RMS change in the effective potential and magnetic field is smaller than epspot, then the self-consistent loop is considered converged and exited. For structural optimization runs this results in the forces being calculated, the atomic positions updated and the loop restarted. See also maxscl.

Type: fortrandouble (114.1)
Default: "1.0d-6"
Use: optional
XPath: /input/groundstate/@epspot

12.24 Attribute: fermilinengy

If "true" the linearization energies marked as non-varying are set to the Fermi level plus dlinengyfermi.

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/groundstate/@fermilinengy

12.25 Attribute: findlinentype

Select method to determine the linearisation energies.

Type:	**choose from:**
	Wigner_Seitz
	lcharge
	logderiv
	no_search
Default:	"Wigner_Seitz"
Use:	optional
XPath:	/input/groundstate/@findlinentype

12.26 Attribute: fracinr

Fraction of the muffin-tin radius up to which lmaxinr is used as the angular momentum cut-off.

Type:	fortrandouble (114.1)
Default:	"0.02d0"
Use:	optional
XPath:	/input/groundstate/@fracinr

12.27 Attribute: frozencore

When set to "true" the frozen core approximation is applied, i.e., the core states are fixed to the atomic states.

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/groundstate/@frozencore

12.28 Attribute: gmaxvr

Maximum length of —G— for expanding the interstitial density and potential.

Type: fortrandouble (114.1)
Default: "12.0d0"
Use: optional
XPath: /input/groundstate/@gmaxvr

12.29 Attribute: isgkmax

Species for which the muffin-tin radius will be used for calculating gkmax.

Type: integer
Default: "-1"
Use: optional
XPath: /input/groundstate/@isgkmax

12.30 Attribute: ldapu

Type of LDA+U method to be used.

Type: **choose from:**
none
FullyLocalisedLimit
AroundMeanField
FFL-AMF-interpolation
Default: "none"
Use: optional
XPath: /input/groundstate/@ldapu

12.31 Attribute: lmaxapw

Angular momentum cut-off for the APW functions.

Type: integer
Default: "8"
Use: optional
XPath: /input/groundstate/@lmaxapw

12.32 Attribute: lmaxinr

Close to the nucleus, the density and potential is almost spherical and therefore the spherical harmonic expansion can be truncated a low angular momentum. See also fracinr.

Type: integer
Default: "2"
Use: optional
XPath: /input/groundstate/@lmaxinr

12.33 Attribute: lmaxmat

Angular momentum cut-off for the outer-most loop in the hamiltonian and overlap matrix setup.

Type: integer
Default: "8"
Use: optional
XPath: /input/groundstate/@lmaxmat

12.34 Attribute: lmaxvr

Angular momentum cut-off for the muffin-tin density and potential.

Type: integer
Default: "8"
Use: optional
XPath: /input/groundstate/@lmaxvr

12.35 Attribute: lorecommendation

Local orbitals may be used for improving unoccupied states. But what energy parameters to use? Set this parameter to true, and you will get a list of energies at which the radial wavefunction turns to zero on the muffin-tin sphere. These energies are calculated using atomic potential, and to make them transferable to a general system, use the average of two consecutive atomic energies.

Type: boolean
Default: "false"
Use: optional
XPath: /input/groundstate/@lorecommendation

12.36 Attribute: lradstep

Some muffin-tin functions (such as the density) are calculated on a coarse radial mesh and then interpolated onto a fine mesh. This is done for the sake of efficiency. lradstp defines the step size in going from the fine to the coarse radial mesh. If it is too large, loss of precision may occur.

Type: integer
Default: "1"
Use: optional
XPath: /input/groundstate/@lradstep

12.37 Attribute: maxscl

Upper limit for the self-consistency loop.

Type: integer
Default: "200"
Use: optional
XPath: /input/groundstate/@maxscl

12.38 Attribute: mixer

Select the mixing (relaxation) scheme for the SCF loop. One has the following options:

Linear mixer ("lin"):

Given the input μ^i and output ν^i vectors of the ith iteration, the next input vector to the $(i+1)$th iteration is generated using an adaptive mixing scheme. The jth component of the output vector is mixed with a fraction of the same component of the input vector:

$$\mu_j^{i+1} = \beta_j^i \nu_j^i + (1 - \beta_j^i)\mu_j^i, \tag{2}$$

where β_j^i is set to β_0 at initialisation and increased by scaling with β_{inc} (> 1) if $f_j^i \equiv \nu_j^i - \mu_j^i$ does not change sign between loops. If f_j^i does change sign, then β_j^i is scaled by β_{dec} (> 1).

Multisecant Broyden potential mixing ("msec")

Pulay mixing ("pulay"):

Pulay's mixing scheme which uses direct inversion in the iterative subspace (DIIS). See *Chem. Phys. Lett.* **73**, 393 (1980).

Type: **choose from:**
lin
msec
pulay
Default: "msec"
Use: optional
XPath: /input/groundstate/@mixer

12.39 Attribute: mixerswitch

Switch between potential (1) and density (2) mixing.

Type: integer
Default: "1"
Use: optional
XPath: /input/groundstate/@mixerswitch

12.40 Attribute: modifiedsv

If "true", the construction of the second-variational hamiltonian involves wavefunctions in the basis representation and wavefunctions are not evaluated ex-

plicitly. Otherwise, the usual second-variational procedure is used. The first of the two approaches is generally recommended, but it is not implemented for non-collinear and LDA+U calculations.

Type: boolean
Default: "false"
Use: optional
XPath: /input/groundstate/@modifiedsv

12.41 Attribute: msecStoredSteps

How many potentials from previous steps to store. Used in msec mixing as choosen with mixer.

Type: integer
Default: "8"
Use: optional
XPath: /input/groundstate/@msecStoredSteps

12.42 Attribute: nempty

Defines the number of eigenstates beyond that required for charge neutrality. When running metals it is not known *a priori* how many states will be below the Fermi energy for each **k**-point. Setting nempty greater than zero allows the additional states to act as a buffer in such cases. Furthermore, magnetic calculations use the first-variational eigenstates as a basis for setting up the second-variational Hamiltonian, and thus nempty will determine the size of this basis set. Convergence with respect to this quantity should be checked.

Type: integer
Default: "5"
Use: optional
XPath: /input/groundstate/@nempty

12.43 Attribute: ngridk

Number of k grid points along the basis vector directions. Alternatively give autokpt and radkpt, or nktot. In the latter cases any value given for ngridk is not used. Notes: Phonon calculations using supercells adjust the k-grid according to the supercell size; if the element xs is given, the present attribute is overwritten by the value in xs for xs-related groundstate calculations; the values of the present attribute are also relevant for calculations related to the element gw.

Type: integertriple (114.8)
Default: "1 1 1"

Use: optional
XPath: /input/groundstate/@ngridk

12.44 Attribute: niterconvcheck

Number of self-consistency iterations over which to test convergence. For example, if niterconvcheck=2, then both the second and third to last iterations are compared to the last one to check convergence. The convergence criteria used are those set up by scfconv.

Type: integer
Default: "2"
Use: optional
XPath: /input/groundstate/@niterconvcheck

12.45 Attribute: nktot

Used for the automatic determination of the **k**-point mesh from the total number of **k**-points. If nktot is set, then the mesh will be determined in such a way that the number of **k**-points is proportional to the length of the reciprocal lattice vector in each direction and that the total number of **k**-points is less than or equal to nktot.

Type: integer
Default: "0"
Use: optional
XPath: /input/groundstate/@nktot

12.46 Attribute: nosource

When set to "true", source fields are projected out of the exchange-correlation magnetic field. experimental feature.

Type: boolean
Default: "false"
Use: optional
XPath: /input/groundstate/@nosource

12.47 Attribute: nosym

When set to "true" no symmetries, apart from the identity, are used anywhere in the code.

Type: boolean
Default: "false"
Use: optional
XPath: /input/groundstate/@nosym

12.48 Attribute: nprad

(Obsolete) Order of predictor-corrector polynomial.

Type:	integer
Default:	"4"
Use:	optional
XPath:	/input/groundstate/@nprad

12.49 Attribute: npsden

Order of polynomial for pseudo-charge density.

Type:	integer
Default:	"9"
Use:	optional
XPath:	/input/groundstate/@npsden

12.50 Attribute: nwrite

Normally, the density and potentials are written to the file STATE.OUT only after completion of the self-consistent loop. By setting nwrite to a positive integer the file will be written during the loop every nwrite iterations.

Type:	integer
Default:	"0"
Use:	optional
XPath:	/input/groundstate/@nwrite

12.51 Attribute: outputlevel

Specify amount of information which is printed to files:

- none - no output is produced
- low - minimal output is produced
- normal - (default) standard information
- high - detailed output

Type:	**choose from:**
	none
	low
	normal
	high
Default:	"normal"
Use:	optional
XPath:	/input/groundstate/@outputlevel

12.52 Attribute: ptnucl

The attrubute ptnucl is "true" if the nuclei are to be treated as point charges, if "false" the nuclei have a finite spherical distribution.

Type:	boolean
Default:	"true"
Use:	optional
XPath:	/input/groundstate/@ptnucl

12.53 Attribute: radialgridtype

The parameter defines a functional form how radial-grid points are distributed. Choose from "cubic", "exponential" and "expocubic". "cubic" is the most suitable one for a majority of calculations, but switch to "expocubic" if you set the innermost grid point very close to a nucleus.

Type:	string
Default:	"cubic"
Use:	optional
XPath:	/input/groundstate/@radialgridtype

12.54 Attribute: radkpt

Used for the automatic determination of the **k**-point mesh. If autokpt is set to "true" then the mesh sizes will be determined by $n_i = \lambda / |\mathbf{A}_i| + 1$.

Type:	fortrandouble (114.1)
Default:	"40.0d0"
Use:	optional
XPath:	/input/groundstate/@radkpt

12.55 Attribute: reducek

If the attribute reducek is "true" the **k**-point set is reduced with the crystal symmetries.

Type:	boolean
Default:	"true"
Use:	optional
XPath:	/input/groundstate/@reducek

12.56 Attribute: rgkmax

The parameter rgkmax implicitly determines the number of basis functions and is one of the crucial parameters for the accuracy of the calculation. It represents the product of two quantities: $R_{MT,\,Min}$, the smallest of all muffin-tin radii, and

$|\mathbf{G}+\mathbf{k}|_{max}$, the maximum length for the $\mathbf{G}+\mathbf{k}$ vectors. Because each $\mathbf{G}+\mathbf{k}$ vector represents one basis function, `rgkmax` gives the number of basis functions used for solving the Kohn-Sham equations. Typical values of `rgkmax` are between 6 and 9. However, for systems with very short bond-lengths, significantly smaller values may be sufficient. This may especially be the case for materials containing carbon, where `rgkmax` may be 4.5-5, or hydrogen, where even values between 3 and 4 may be sufficient. In any case, a convergence check is indispensible for a proper choice of this parameter for your system!

Type: fortrandouble (114.1)
Default: "`7.0d0`"
Use: optional
XPath: `/input/groundstate/@rgkmax`

12.57 Attribute: scfconv

Specify the SCF convergence criteria

- "energy" - only the total energy of the system is used as a convergence criterion. If the calculation of the atomic forces is required (e.g., in the optimization of the atomic positions) the non-IBS contribution to the atomic forces is added as a further convergence criterion.
- "potential" - only the Kohn-Sham potential is used as a convergence criterion. If atomic forces are required the convergence criterion is extended to include non-IBS forces.
- "multiple" - total energy, Kohn-Sham potential, and total electronic charge of the system are used as convergence criteria. If atomic forces are required the convergence criterion is extended to include non-IBS forces.

Type: string
Default: "`multiple`"
Use: optional
XPath: `/input/groundstate/@scfconv`

12.58 Attribute: stype

A smooth approximation to the Dirac delta function is needed to compute the occupancies of the Kohn-Sham states. The attribute `swidth` determines the width of the approximate delta function.

Type: **choose from:**
`Gaussian`
`Methfessel-Paxton 1`
`Methfessel-Paxton 2`
`Fermi Dirac`

Square-wave impulse
libbzint
Default: "Gaussian"
Use: optional
XPath: /input/groundstate/@stype

12.59 Attribute: swidth

Width of the smooth approximation to the Dirac delta function (must be greater than zero).

Type: fortrandouble (114.1)
Default: "0.001d0"
Use: optional
Unit: Hartree
XPath: /input/groundstate/@swidth

12.60 Attribute: symmorph

When set to "true" only symmorphic space-group operations are to be considered, i.e. only symmetries without non-primitive translations are used anywhere in the code.

Type: boolean
Default: "false"
Use: optional
XPath: /input/groundstate/@symmorph

12.61 Attribute: tevecsv

The attribute tevecsv is "true" if second-variational eigenvectors are calculated.

Type: boolean
Default: "false"
Use: optional
XPath: /input/groundstate/@tevecsv

12.62 Attribute: tfibs

Because calculation of the incomplete basis set (IBS) correction to the force is fairly time- consuming, it can be switched off by setting tfibs to "false" This correction can then be included only when necessary, i.e. when the atoms are close to equilibrium in a structural relaxation run.

Type: boolean
Default: "true"

Use: optional
XPath: /input/groundstate/@tfibs

12.63 Attribute: tforce

Decides if the force should be calculated at the end of the self-consistent cycle.

Type: boolean
Default: "false"
Use: optional
XPath: /input/groundstate/@tforce

12.64 Attribute: tpartcharges

The attribute tpartcharges is "true" if partial charges for each state j, atom alpha and for each lm combination are calculated.

Type: boolean
Default: "false"
Use: optional
XPath: /input/groundstate/@tpartcharges

12.65 Attribute: vdWcorrection

Adds dispersion (van-der-Waals) correction to total energy after the last SCF iteration. If forces are calculated, an appropriate dispersion correction is applied. Available methods are

- "DFTD2": This is the **DFT-D2** method by Stefan Grimme which is introduced in *Semiempirical GGA-type density functional constructed with a long-range dispersion correction*, J. Comput. Chem. **27**, 1787-1799 (2006).
- "TSvdW": This is the **TS-vdW** method by Alexandre Tkatchenko and Matthias Scheffler introduced in *Accurate molecular van-der-Waals interactions from ground-state electron density and free-atom reference data*, Phys. Rev. Lett. **102**, 073005 (2009).

Parameters corresponding to each method can be specified using the subelements DFTD2parameters and TSvdWparameters inside the element groundstate. It is also possible to decouple these van-der-Waals corrections from a complete ground-state calculation. In this case, you can use the subelements DFTD2 and TSvdW inside the element properties.

Type: **choose from:**
none
DFTD2

	`TSvdW`
Default:	"`none`"
Use:	optional
XPath:	`/input/groundstate/@vdWcorrection`

12.66 Attribute: vkloff

The **k**-point offset vector in lattice coordinates.

Type:	vect3d (114.6)
Default:	"`0.0d0 0.0d0 0.0d0`"
Use:	optional
XPath:	`/input/groundstate/@vkloff`

12.67 Attribute: xctype

Type of exchange-correlation functional to be used

- No exchange-correlation funtional ($E_{\mathrm{xc}} \equiv 0$)
- LDA, Perdew-Zunger/Ceperley-Alder, *Phys. Rev. B* **23**, 5048 (1981)
- LSDA, Perdew-Wang/Ceperley-Alder, *Phys. Rev. B* **45**, 13244 (1992)
- LDA, X-alpha approximation, J. C. Slater, *Phys. Rev.* **81**, 385 (1951)
- LSDA, von Barth-Hedin, *J. Phys. C* **5**, 1629 (1972)
- GGA, Perdew-Burke-Ernzerhof (PBE), *Phys. Rev. Lett.* **77**, 3865 (1996)
- GGA, Revised PBE, Zhang-Yang, *Phys. Rev. Lett.* **80**, 890 (1998)
- GGA, PBEsol, arXiv:0707.2088v1 (2007)
- GGA, asymptotically corrected PBE (acPBE), arXiv:1409.4834 (2014)
- GGA, Wu-Cohen exchange (WC06) with PBE correlation, *Phys. Rev. B* **73**, 235116 (2006)
- GGA, Armiento-Mattsson (AM05) spin-unpolarised functional, *Phys. Rev. B* **72**, 085108 (2005)
- EXX, Exact Exchange, *Phys. Rev. Lett.* **95**, 136402 (2005)
- Hybrid, PBE0, *J. Chem. Phys.* **110**, 5029 (1999)

Type:	**choose from:**
	`LDA_PZ`
	`LDA_PW`
	`LDA_XALPHA`

LDA_vBH
GGA_PBE
GGA_PBE_R
GGA_PBE_SOL
GGA_WC
GGA_AM05
GGA_AC_PBE
HYB_PBE0
HYB_LDA0
EXX
none

Default: "GGA_PBE"
Use: optional
XPath: /input/groundstate/@xctype

13 Element: DFTD2parameters

This element allows to customize parameters when either the option "DFTD2" of the attribute vdWcorrection is chosen, or the subelement DFTD2 of the element properties is specified.

Type: no content
XPath: /input/groundstate/DFTD2parameters

This element allows for specification of the following attributes:

cutoff, d, s6, sr6

13.1 Attribute: cutoff

Cutoff distance of interatomic interactions for the method "DFTD2". In the sum over all pairwise interactions, only pairs of atoms are considered which are closer to each other than the value of the cutoff attribute.

Type: fortrandouble (114.1)
Default: "95.0d0"
Use: optional
XPath: /input/groundstate/DFTD2parameters/@cutoff

13.2 Attribute: d

This damping constant determines the steepnes of the damping function for the method "DFTD2".

Type: fortrandouble (114.1)
Default: "20.0d0"

Use: optional
XPath: /input/groundstate/DFTD2parameters/@d

13.3 Attribute: s6

Global scaling factor for all C_6-dispersion coefficients for the method "DFTD2". This factor depends on the exchange-correlation functional in use. The default value suits PBE calculations.

Type: fortrandouble (114.1)
Default: "0.75d0"
Use: optional
XPath: /input/groundstate/DFTD2parameters/@s6

13.4 Attribute: sr6

Scaling factor for van-der-Waals radii for the method "DFTD2". This factor depends on the exchange-correlation functional in use. The default value suits PBE calculations.

Type: fortrandouble (114.1)
Default: "1.1d0"
Use: optional
XPath: /input/groundstate/DFTD2parameters/@sr6

14 Element: TSvdWparameters

This element allows to customize parameters when either the option "TSvdW" of the attribute vdWcorrection is chosen, or the subelement TSvdW of the element properties is specified.

Type: no content
XPath: /input/groundstate/TSvdWparameters

This element allows for specification of the following attributes:

cutoff, d, nr, nsph, s6, sr6

14.1 Attribute: cutoff

Cutoff distance of interatomic interactions for the method "TSvdW". In the sum over all pairwise interactions, only pairs of atoms are considered which are closer to each other than the value of the cutoff attribute.

Type: fortrandouble (114.1)
Default: "95.0d0"

Use: optional
XPath: /input/groundstate/TSvdWparameters/@cutoff

14.2 Attribute: d

This damping constant determines the steepnes of the damping function for the method "TSvdW".

Type: fortrandouble (114.1)
Default: "20.0d0"
Use: optional
XPath: /input/groundstate/TSvdWparameters/@d

14.3 Attribute: nr

Number of radial grid points for the Gauss-Chebyshev quadrature.

Type: integer
Default: "120"
Use: optional
XPath: /input/groundstate/TSvdWparameters/@nr

14.4 Attribute: nsph

Number of Lebedev grid points. The **only** possible values are: "1", "6", "14", "26", "38", "50", "74", "86", "110", "146", "170", "194", "230", "266", "302", "350", "434", "590", "770", "974", "1202", "1454", "1730", "2030", "2354", "2702", "3074", "3740", "3890", "4334", "4802", "5294", "5810".

Type: integer
Default: "590"
Use: optional
XPath: /input/groundstate/TSvdWparameters/@nsph

14.5 Attribute: s6

Global scaling factor for all C_6-dispersion coefficients for the method "TSvdW".

Type: fortrandouble (114.1)
Default: "1.0d0"
Use: optional
XPath: /input/groundstate/TSvdWparameters/@s6

14.6 Attribute: sr6

Scaling factor for van-der-Waals radii for the method `"TSvdW"`. This factor depends on the exchange-correlation functional in use. The default value suits PBE calculations.

Type: fortrandouble (114.1)
Default: "`0.94d0`"
Use: optional
XPath: `/input/groundstate/TSvdWparameters/@sr6`

15 Element: spin

If the `spin` element is present, calculation is done with spin polarization.

Type: no content
XPath: `/input/groundstate/spin`

This element allows for specification of the following attributes:

`bfieldc`, `fixspin`, `momfix`, `reducebf`, `spinorb`, `spinsprl`, `taufsm`, `vqlss`

15.1 Attribute: bfieldc

Allows to apply a constant $\mathbf{B}_{\mathtt{ext}}$ field. This is an external constant magnetic field applied throughout the entire unit cell and enters the second-variational Hamiltonian as

$$\frac{g_e\,\alpha}{4}\,\vec{\sigma}\cdot\mathbf{B}_{\mathtt{ext}}\,, \tag{3}$$

where g_e is the electron g-factor (g_e=2.0023193043718). The external magnetic field is normally used to break spin symmetry for spin-polarised calculations and considered to be infinitesimal with no direct contribution to the total energy. In cases where the magnetic field is finite (for example when computing magnetic response) the external **B**-field energy reported in `INFO.OUT` (when the attribute `outputlevel` is set to`"high"`) should be added to the total energy by hand. This external magnetic field is applied hroughout the entire unit cell. To apply magnetic fields in particular muffin-tins use the `bfcmt` vectors in the `atom` elements. Collinear calculations are more efficient if the field is applied in the z-direction.

Type: vect3d (114.6)
Default: "`0.0d0 0.0d0 0.0d0 `"
Use: optional
XPath: `/input/groundstate/spin/@bfieldc`

15.2 Attribute: fixspin

Type:	**choose from:**
	`none`
	`total FSM`
	`localmt FSM`
	`both`

Default:	"`none`"
Use:	optional
XPath:	`/input/groundstate/spin/@fixspin`

15.3 Attribute: momfix

The desired total moment for a fixed spin moment (`FSM`) calculation.

Type:	vect3d (114.6)
Default:	"`0.0d0 0.0d0 0.0d0`"
Use:	optional
XPath:	`/input/groundstate/spin/@momfix`

15.4 Attribute: reducebf

After each iteration the external magnetic fields are multiplied with reducebf. This allows for a large external magnetic field at the start of the self-consistent loop to break spin symmetry, while at the end of the loop the field will be effectively zero, i.e. infinitesimal. See `bfieldc` and atom element.

Type:	fortrandouble (114.1)
Default:	"`1.0d0`"
Use:	optional
XPath:	`/input/groundstate/spin/@reducebf`

15.5 Attribute: spinorb

If `spinorb` is `"true"`, then a $\boldsymbol{\sigma} \cdot \mathbf{L}$ term is added to the second-variational Hamiltonian.

Type:	boolean
Default:	"`false`"
Use:	optional
XPath:	`/input/groundstate/spin/@spinorb`

15.6 Attribute: spinsprl

Set to `"true"` if a spin-spiral calculation is required. Experimental feature for the calculation of spin-spiral states. See `vqlss` for details.

Type: boolean
Default: "`false`"
Use: optional
XPath: `/input/groundstate/spin/@spinsprl`

15.7 Attribute: taufsm

The effective magnetic field required for fixing the spin moment to a given value, is updated according to

$$\mathbf{B}_{\mathtt{FSM}}^{i+1} = \mathbf{B}_{\mathtt{FSM}}^{i} + \tau_{\mathtt{FSM}} \left(\boldsymbol{\mu}^{i} - \boldsymbol{\mu}_{\mathtt{FSM}} \right) , \tag{4}$$

for iteration i. It must be positive.

Type: fortrandouble (114.1)
Default: "`0.01d0`"
Use: optional
XPath: `/input/groundstate/spin/@taufsm`

15.8 Attribute: vqlss

This attribute allows to specify the **q**-vector of the spin-spiral state in lattice coordinates. Spin-spirals arise from spinor states assumed to be of the form

$$\Psi_{\mathbf{k}}^{\mathbf{q}}(\mathbf{r}) = \begin{pmatrix} U_{\mathbf{k}}^{\mathbf{q}\uparrow}(\mathbf{r})\, e^{i(\mathbf{k}+\mathbf{q}/\mathbf{2})\cdot\mathbf{r}} \\ \\ U_{\mathbf{k}}^{\mathbf{q}\downarrow}(\mathbf{r})\, e^{i(\mathbf{k}-\mathbf{q}/\mathbf{2})\cdot\mathbf{r}} \end{pmatrix} . \tag{5}$$

These spin-spirals are determined using a second-variational approach, and give rise to a magnetization density of the form

$$\mathbf{m}^{\mathbf{q}}(\mathbf{r}) = [m_x(\mathbf{r})\, \cos(\mathbf{q}\cdot\mathbf{r}),\ m_y(\mathbf{r})\, \sin(\mathbf{q}\cdot\mathbf{r}),\ m_z(\mathbf{r})] , \tag{6}$$

where m_x, m_y, and m_z have the periodicity of the lattice. See also `spinsprl`.

Type: vect3d (114.6)
Default: "`0.0d0 0.0d0 0.0d0`"
Use: optional
XPath: `/input/groundstate/spin/@vqlss`

16 Element: dfthalf

The presence of this element triggers **DFT-1/2** calculations.

Type: no content
XPath: `/input/groundstate/dfthalf`

This element allows for specification of the following attributes:

printVSfile

16.1 Attribute: printVSfile

When set to "true", the self-energy correction potential $V_S(\mathbf{r})$ (as defined in the **DFT-1/2** method) is calculated for each constituent atomic species and written into the files VS_S*.OUT, where * ranges from **1** to the number of atomic species. The exciting run quits after the printing. In this case, a serial calculation is suggested. It is useful to visualize the self-energy potential, or for debugging purposes.

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/groundstate/dfthalf/@printVSfile

17 Element: Hybrid

Options for hybrid functionals.

Type:	no content
XPath:	/input/groundstate/Hybrid

This element allows for specification of the following attributes:

exchangetype, excoeff, maxscl

17.1 Attribute: exchangetype

Type of exchange (Hartree Fock or OEP) to be used for the exact exchange.

Type:	**choose from:**
	HF
	OEP
Default:	"HF"
Use:	optional
XPath:	/input/groundstate/Hybrid/@exchangetype

17.2 Attribute: excoeff

Define value of the mixing parameter for exact exchange. ATTENTION: If you are using libxc, the libxc settings will be employed and your choice of this parameter will be ignored.

Type:	fortrandouble (114.1)

Default: "0.25d0"
Use: optional
XPath: /input/groundstate/Hybrid/@excoeff

17.3 Attribute: maxscl

Upper limit for the Hybrids self-consistency loop.

Type: integer
Default: "50"
Use: optional
XPath: /input/groundstate/Hybrid/@maxscl

18 Element: solver

Optional configuration options for eigenvector solver.

Type: no content
XPath: /input/groundstate/solver

This element allows for specification of the following attributes:

ArpackImproveInverse, ArpackLinSolve, ArpackShift, ArpackUserDefinedShift, DecompPrec, epsarpack, evaltol, packedmatrixstorage, type

18.1 Attribute: ArpackImproveInverse

Tells whether iterative improvement should be applied during the shift-and-invert procedure. Setting to true may be useful, for instance, when DecompPrec is set to "sp".

Type: boolean
Default: "false"
Use: optional
XPath: /input/groundstate/solver/@ArpackImproveInverse

18.2 Attribute: ArpackLinSolve

Linear solve method during shift-and-invert process in ARPACK. Pick either LDL, LU, LL, Diag and InvertOnce.

Type: **choose from:**
LDL
LL
LU
Diag

	`InvertOnce`
Default:	"`LDL`"
Use:	optional
XPath:	`/input/groundstate/solver/@ArpackLinSolve`

18.3 Attribute: ArpackShift

Energy shift in the shift-and-invert procedure in the ARPACK solver.

Type:	fortrandouble (114.1)
Default:	"`-1.0d0`"
Use:	optional
Unit:	Hartree
XPath:	`/input/groundstate/solver/@ArpackShift`

18.4 Attribute: ArpackUserDefinedShift

ArpackShift will be used if this flag is set to true, otherwise the energy shift will be determined internally.

Type:	boolean
Default:	"`false`"
Use:	optional
XPath:	`/input/groundstate/solver/@ArpackUserDefinedShift`

18.5 Attribute: DecompPrec

Precision used during the factorization in ARPACK. Pick either sp or dp.

Type:	**choose from:**
	`sp`
	`dp`
Default:	"`dp`"
Use:	optional
XPath:	`/input/groundstate/solver/@DecompPrec`

18.6 Attribute: epsarpack

Tolerance parameter for the ARPACK shift invert solver

Type:	fortrandouble (114.1)
Default:	"`1.0d-14`"
Use:	optional
XPath:	`/input/groundstate/solver/@epsarpack`

18.7 Attribute: evaltol

Error tolerance for the first-variational eigenvalues using the LAPACK Solver

Type:	fortrandouble (114.1)
Default:	"1.0d-14"
Use:	optional
Unit:	Hartree
XPath:	/input/groundstate/solver/@evaltol

18.8 Attribute: packedmatrixstorage

In the default calculation the matrix is sored in packed form. When using multi-threaded BLAS setting this parameter to "false" increases efficiency.

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/groundstate/solver/@packedmatrixstorage

18.9 Attribute: type

Selects the eigenvalue solver for the first variational equation

Type:	**choose from:**
	Lapack
	Arpack
Default:	"Lapack"
Use:	optional
XPath:	/input/groundstate/solver/@type

19 Element: OEP

Necessary, if exact exchange calculation is to be performed.

Type:	no content
XPath:	/input/groundstate/OEP

This element allows for specification of the following attributes:

convoep, maxitoep, tauoep

19.1 Attribute: convoep

Convergence tolerance for OEP residue when solving the exact exchange integral equations.

Type: fortrandouble (114.1)
Default: "1e-11"
Use: optional
XPath: /input/groundstate/OEP/@convoep

19.2 Attribute: maxitoep

Maximum number of iterations when solving the exact exchange integral equations.

Type: integer
Default: "300"
Use: optional
XPath: /input/groundstate/OEP/@maxitoep

19.3 Attribute: tauoep

The optimised effective potential is determined using an iterative method. *Phys. Rev. Lett.* **98**, 196405 (2007). At the first iteration the step length is set to tauoep(1). During subsequent iterations, the step length is scaled by tauoep(2) or tauoep(3), when the residual is increasing or decreasing, respectively. See also maxitoep.

Type: vect3d (114.6)
Default: "1.0d0 0.2d0 1.5d0"
Use: optional
XPath: /input/groundstate/OEP/@tauoep

20 Element: output

Specifications on the file formats for output files.

Type: no content
XPath: /input/groundstate/output

This element allows for specification of the following attributes:

state

20.1 Attribute: state

Selects the file format of the STATE file.

Type: **choose from:**
binary
XML

Default: "binary"
Use: optional
XPath: /input/groundstate/output/@state

21 Element: libxc

Type: no content
XPath: /input/groundstate/libxc

This element allows for specification of the following attributes:

correlation, exchange, xc

21.1 Attribute: correlation

Type: **choose from:**
none
XC_LDA_C_WIGNER
XC_LDA_C_RPA
XC_LDA_C_HL
XC_LDA_C_GL
XC_LDA_C_XALPHA
XC_LDA_C_VWN
XC_LDA_C_VWN_RPA
XC_LDA_C_PZ
XC_LDA_C_PZ_MOD
XC_LDA_C_OB_PZ
XC_LDA_C_PW
XC_LDA_C_PW_MOD
XC_LDA_C_OB_PW
XC_LDA_C_2D_AMGB
XC_LDA_C_2D_PRM
XC_LDA_C_vBH
XC_LDA_C_1D_CSC
XC_LDA_C_ML1
XC_LDA_C_ML2
XC_LDA_C_GOMBAS
XC_LDA_C_PW_RPA
XC_LDA_C_1D_LOOS
XC_LDA_C_RC04
XC_LDA_C_VWN_1
XC_LDA_C_VWN_2
XC_LDA_C_VWN_3
XC_LDA_C_VWN_4

XC_GGA_C_OP_XALPHA
XC_GGA_C_OP_G96
XC_GGA_C_OP_PBE
XC_GGA_C_OP_B88
XC_GGA_C_FT97
XC_GGA_C_SPBE
XC_GGA_C_REVTCA
XC_GGA_C_TCA
XC_GGA_C_PBE
XC_GGA_C_LYP
XC_GGA_C_P86
XC_GGA_C_PBE_SOL
XC_GGA_C_PW91
XC_GGA_C_AM05
XC_GGA_C_XPBE
XC_GGA_C_LM
XC_GGA_C_PBE_JRGX
XC_GGA_C_RGE2
XC_GGA_C_WL
XC_GGA_C_WI
XC_GGA_C_SOGGA11
XC_GGA_C_WI0
XC_GGA_C_SOGGA11_X
XC_GGA_C_APBE
XC_GGA_C_OPTC

Default: "XC_GGA_C_PBE"
Use: optional
XPath: /input/groundstate/libxc/@correlation

21.2 Attribute: exchange

Type: **choose from:**
none
XC_LDA_X
XC_LDA_X_2D
XC_LDA_X_1D
XC_GGA_X_SSB_SW
XC_GGA_X_SSB
XC_GGA_X_SSB_D
XC_GGA_X_BPCCAC
XC_GGA_X_PBE
XC_GGA_X_PBE_R
XC_GGA_X_B86
XC_GGA_X_HERMAN
XC_GGA_X_B86_MGC

XC_GGA_X_B88
XC_GGA_X_G96
XC_GGA_X_PW86
XC_GGA_X_PW91
XC_GGA_X_OPTX
XC_GGA_X_DK87_R1
XC_GGA_X_DK87_R2
XC_GGA_X_LG93
XC_GGA_X_FT97_A
XC_GGA_X_FT97_B
XC_GGA_X_PBE_SOL
XC_GGA_X_RPBE
XC_GGA_X_WC
XC_GGA_X_MPW91
XC_GGA_X_AM05
XC_GGA_X_PBEA
XC_GGA_X_MPBE
XC_GGA_X_XPBE
XC_GGA_X_2D_B86_MGC
XC_GGA_X_BAYESIAN
XC_GGA_X_PBE_JSJR
XC_GGA_X_2D_B88
XC_GGA_X_2D_B86
XC_GGA_X_2D_PBE
XC_GGA_X_OPTB88_VDW
XC_GGA_X_PBEK1_VDW
XC_GGA_X_OPTPBE_VDW
XC_GGA_X_RGE2
XC_GGA_X_RPW86
XC_GGA_X_KT1
XC_GGA_X_MB88
XC_GGA_X_SOGGA
XC_GGA_X_SOGGA11
XC_GGA_X_C09X
XC_GGA_X_LB
XC_GGA_X_LBM
XC_GGA_X_OL2
XC_GGA_X_APBE
XC_GGA_X_HTBS
XC_GGA_X_AIRY
XC_GGA_X_LAG

Default: "XC_GGA_X_PBE"
Use: optional
XPath: /input/groundstate/libxc/@exchange

21.3 Attribute: xc

Combined functionals. If set it overrides the exchange and the correlation attributes.

Type: **choose from:**

`none`
`XC_LDA_XC_TETER93`
`XC_GGA_XC_HCTH_407P`
`XC_GGA_XC_HCTH_P76`
`XC_GGA_XC_HCTH_P14`
`XC_GGA_XC_B97_GGA1`
`XC_GGA_XC_HCTH_A`
`XC_GGA_XC_KT2`
`XC_GGA_XC_TH1`
`XC_GGA_XC_TH2`
`XC_GGA_XC_TH3`
`XC_GGA_XC_TH4`
`XC_GGA_XC_HCTH_93`
`XC_GGA_XC_HCTH_120`
`XC_GGA_XC_HCTH_147`
`XC_GGA_XC_HCTH_407`
`XC_GGA_XC_EDF1`
`XC_GGA_XC_XLYP`
`XC_GGA_XC_B97`
`XC_GGA_XC_B97_1`
`XC_GGA_XC_B97_2`
`XC_GGA_XC_B97_D`
`XC_GGA_XC_B97_K`
`XC_GGA_XC_B97_3`
`XC_GGA_XC_PBE1W`
`XC_GGA_XC_MPWLYP1W`
`XC_GGA_XC_PBELYP1W`
`XC_GGA_XC_SB98_1a`
`XC_GGA_XC_SB98_1b`
`XC_GGA_XC_SB98_1c`
`XC_GGA_XC_SB98_2a`
`XC_GGA_XC_SB98_2b`
`XC_GGA_XC_SB98_2c`
`XC_GGA_XC_MOHLYP`
`XC_GGA_XC_MOHLYP2`
`XC_GGA_XC_TH_FL`
`XC_GGA_XC_TH_FC`
`XC_GGA_XC_TH_FCFO`
`XC_GGA_XC_TH_FCO`
`XC_HYB_GGA_XC_B3PW91`
`XC_HYB_GGA_XC_B3LYP`

XC_HYB_GGA_XC_B3P86
XC_HYB_GGA_XC_O3LYP
XC_HYB_GGA_XC_mPW1K
XC_HYB_GGA_XC_PBEH
XC_HYB_GGA_XC_B97
XC_HYB_GGA_XC_B97_1
XC_HYB_GGA_XC_B97_2
XC_HYB_GGA_XC_X3LYP
XC_HYB_GGA_XC_B1WC
XC_HYB_GGA_XC_B97_K
XC_HYB_GGA_XC_B97_3
XC_HYB_GGA_XC_MPW3PW
XC_HYB_GGA_XC_B1LYP
XC_HYB_GGA_XC_B1PW91
XC_HYB_GGA_XC_mPW1PW
XC_HYB_GGA_XC_MPW3LYP
XC_HYB_GGA_XC_SB98_1a
XC_HYB_GGA_XC_SB98_1b
XC_HYB_GGA_XC_SB98_1c
XC_HYB_GGA_XC_SB98_2a
XC_HYB_GGA_XC_SB98_2b
XC_HYB_GGA_XC_SB98_2c
XC_HYB_GGA_XC_BHANDH
XC_HYB_GGA_XC_BHANDHLYP
XC_HYB_GGA_XC_MB3LYP_RC04

Default: "none"
Use: optional
XPath: /input/groundstate/libxc/@xc

22 Element: relax

The element relax activates the optimization of atomic positions at fixed lattice parameters.

Type: no content
XPath: /input/relax

This element allows for specification of the following attributes:

addtohistory, endbfgs, epsforce, history, historyformat, maxbfgs, maxsteps, method, outputlevel, printtorque, taubfgs, taunewton

22.1 Attribute: addtohistory

If history is "true", this switch allows newly computed optimization steps to be appended to a previously generated history file.

Type: boolean
Default: "false"
Use: optional
XPath: /input/relax/@addtohistory

22.2 Attribute: endbfgs

When using the "bfgs" method, specifies the method employed for the relaxation if the "bfgs" scheme fails to converge.

- "newton" - Simple (Newton-like) method, see also method.
- "harmonic" - Method based on the combination of the "newton" method and the harmonic approximation, see also method.
- "stop" - Stops the "bfgs" optimization procedure at the last accepted configuration.

Type: string
Default: "harmonic"
Use: optional
XPath: /input/relax/@endbfgs

22.3 Attribute: epsforce

The optimization stops when the maximum amplitude of the force acting on the atoms is lower then the value specified by epsforce. Notice that, in particular for the "bfgs" method, high accuracy in the calculated forces requires high accuracy in the calculated total energy (see the attribute epsengy of the groundstate element).

Type: fortrandouble (114.1)
Default: "2.0d-4"
Use: optional
XPath: /input/relax/@epsforce

22.4 Attribute: history

If "true" the atomic configuration at each relaxation step is written in a history file which is generated in one of the formats specified in historyformat.

Type: boolean

Default: "false"
Use: optional
XPath: /input/relax/@history

22.5 Attribute: historyformat

If history is "true", the history file, containig atomic configurations at each optimization step, is generated in one of the following formats:

- "xyz" molecular format. The first line of this file the total number of atoms. The second line is a comment line with total energy in eV. Finally, starting from line three, one finds atomic species, cartesian coordinates in Angstrom, and forces in eV/Angstrom. This format is repeated for each optimization step.
- "gulp" format, which is useful to visualize crystal structure changes using the GDIS program.

Type: string
Default: "xyz"
Use: optional
XPath: /input/relax/@historyformat

22.6 Attribute: maxbfgs

Maximum number of atomic configurations that can be investigated in a single "bfgs" optimization step.

Type: integer
Default: "5"
Use: optional
XPath: /input/relax/@maxbfgs

22.7 Attribute: maxsteps

Maximum number of optimization steps.

Type: integer
Default: "200"
Use: optional
XPath: /input/relax/@maxsteps

22.8 Attribute: method

Specify the method used for atomic relaxation:

- `"newton"` - Simple (Newton-like) method. At each step m of a structural optimization run, the atom α is displaced according to

$$\mathbf{r}_\alpha^{(m+1)} = \mathbf{r}_\alpha^{(m)} + \tau_\alpha^{(m)} \left(\mathbf{F}_\alpha^{(m)} + \mathbf{F}_\alpha^{(m-1)} \right), \tag{7}$$

  i.e., the magnitude of the displacement at the step m is proportional to $\tau_\alpha^{(m)}$. For the initial step, $\tau_\alpha^{(0)}$ is set to `taunewton`. If the forces of two subsequent optimization steps have the same sign, $\tau_\alpha^{(m)}$ is increased by $\tau_\alpha^{(0)}$. Otherwise, $\tau_\alpha^{(m)}$ is reset to $\tau_\alpha^{(0)}$.

- `"harmonic"` - Method based on the combination of the `"newton"` method and the harmonic approximation. Contrary to `"newton"`, all cartesian components of the position vector of each atom are treated independently. At the optimization step m, each cartesian component of the position vector of each atom is updated using the same algorithm as in `"newton"` ("newton step") unless the "harmonic condition", either

$$\beta \equiv \frac{\mathbf{F}_\alpha^{(m-1)}}{\mathbf{F}_\alpha^{(m)}} \in \left] -\infty, 0 \right] \tag{8}$$

  or

$$\beta \in [3, \infty[\,, \tag{9}$$

  is fulfilled. In this case ("harmonic step"), atomic positions are updated according to

$$\mathbf{r}_\alpha^{(m+1)} = \frac{\mathbf{r}_\alpha^{(m-1)} - \beta\, \mathbf{r}_\alpha^{(m)}}{1 - \beta}\,. \tag{10}$$

  The `"harmonic"` method is of general validity and it is particularly efficient when the atomic configuration is close to the optimized one and the internal degrees of freedom are weakly coupled.

- `"bfgs"` - Limited memory algorithm for bound constrained optimization, see `Byrd, et al., SIAM J. Scientific Computing 16, 1190 (1995)`. This method requires high accuracy for the determination of the total energy in dependence of the maximum allowed for the residual atomic force. For this reason, the default value of the attribute `epsengy` is decreased in order to be at least equal to the value of the attribute `epsforce` of the `relax` element multiplied by a factor `0.02`.

Type: string
Default: "`bfgs`"
Use: optional
XPath: `/input/relax/@method`

22.9 Attribute: outputlevel

Specify the amount of information which is printed to output files:

- `"low"` - Minimal output is produced. For each optimization steps, the main output file `"INFO.OUT"` contains information on the number of SCF cicles performed, the value of the maximum force acting on the atoms, and the calculated total energy.
- `"normal"` - (default) Standard information. In addition to the output level `"low"`, the atomic configuration (in lattice coordinates) and the total forces (in cartesian coordinates) acting on the atoms are also given. If a constrained optimization is performed, the constrained (unconstrained) cartesian components of each atom are labeled by `"T"` (`"F"`).
- `"high"` - Detailed output. In addition to the output level `"normal"`, partial charges and the different force contributions are also specified.

Type:	**choose from:**
	`low`
	`normal`
	`high`
Default:	"`normal`"
Use:	optional
XPath:	`/input/relax/@outputlevel`

22.10 Attribute: printtorque

If `"true"` the total torque with respect to cartesian axes with origin in the center of mass is written on the output file `INFO.OUT`. This option is useful when dealing with isolated molecules when checking if the molecule is rotating as a whole during the optimization. If `printtorque` is set to `"true"` the cartesian coordinates of the center of mass are also written. Notice that the definition of a `center of mass` is unique only for isolated molecules.

Type:	boolean
Default:	"`false`"
Use:	optional
XPath:	`/input/relax/@printtorque`

22.11 Attribute: taubfgs

Maximum atomic displacement for atomic relaxation when using the `"bfgs"` method. At each optimization step, the optimized value of each cartesian coordinate of each atom is searched in a range of size $2\tau_{\texttt{BFGS}}$ centered at the actual value of the coordinate.

Type: fortrandouble (114.1)
Default: "5.0d0"
Use: optional
XPath: /input/relax/@taubfgs

22.12 Attribute: taunewton

Parameter determining the initial amplitude of atomic displacement for the "newton" method of atomic relaxation.

Type: fortrandouble (114.1)
Default: "0.2d0"
Use: optional
XPath: /input/relax/@taunewton

23 Element: properties

Properties listed in this element can be calculated from the groundstate. It works also from a saved state from a previous run.

Contains:
bandstructure (optional)
stm (optional)
wfplot (optional)
dos (optional)
LSJ (optional)
masstensor (optional)
chargedensityplot (optional)
TSvdW (optional)
DFTD2 (optional)
exccplot (optional)
elfplot (optional)
mvecfield (optional)
xcmvecfield (optional)
electricfield (optional)
gradmvecfield (optional)
fermisurfaceplot (optional)
EFG (optional)
mossbauer (optional)
expiqr (optional)
elnes (optional)
eliashberg (optional)
momentummatrix (optional)
dielmat (optional)
boltzequ (optional)
raman (optional)

moke (optional)
shg (optional)
wannier (optional)
wannierplot (optional)
wanniergap (optional)

XPath: /input/properties

24 Element: bandstructure

If present a banstructure is calculated.

Contains: plot1d
XPath: /input/properties/bandstructure

This element allows for specification of the following attributes:

character, deriv, scissor, wannier

24.1 Attribute: character

Band structure plot which includes angular momentum characters for every atom.

Type: boolean
Default: "false"
Use: optional
XPath: /input/properties/bandstructure/@character

24.2 Attribute: deriv

In addition, the first and second band-derivative is computed using Wannier interpolation.

Type: boolean
Default: "false"
Use: optional
XPath: /input/properties/bandstructure/@deriv

24.3 Attribute: scissor

Value to shift bandgap.

Type: fortrandouble (114.1)
Default: "0.0d0"
Use: optional
Unit: Hartree

XPath: /input/properties/shg/@scissor

24.4 Attribute: wannier

Wannier interpolation is used for calculating the band-structure.

Type: boolean
Default: "false"
Use: optional
XPath: /input/properties/bandstructure/@wannier

25 Element: stm

Contains: plot2d (optional)
region (optional)
XPath: /input/properties/stm

This element allows for specification of the following attributes:

bias, stmmode, stmtype

25.1 Attribute: bias

Value of the STM bias voltage in Hartree. A positive value gives an empty states STM image while a negative bias gives a filled states images.

Type: fortrandouble (114.1)
Default: "0.0d0"
Use: optional
Unit: Hartree
XPath: /input/properties/stm/@bias

25.2 Attribute: stmmode

Specifies the STM mode of operation to be simulated.

- constantHeight (default): Calculates the property defined in the "stmtype" attribute on a two-dimensional mesh defined by the plot2d element.
- topographic: (to be implemented) Calculates the iso-surface of the property defined in the "stmtype" attribute.

Type: **choose from:**
constantHeight
topographic

Default: "constantHeight"
Use: optional
XPath: /input/properties/stm/@stmmode

25.3 Attribute: stmtype

Specifies the type of STM calculation.

- differentialConductance (default): calculation of the LDOS at an energy Ef+bias.
- integratedLDOS: integrates the LDOS in the range [Ef,Ef+bias] for positive bias and in the range [Ef+bias, Ef] for negative bias.

Type: **choose from:**
differentialConductance
integratedLDOS
Default: "differentialConductance"
Use: optional
XPath: /input/properties/stm/@stmtype

26 Element: region

Type: no content
XPath: /input/properties/stm/region

This element allows for specification of the following attributes:

grid2d, grid3d, height, zrange

26.1 Attribute: grid2d

Number of grid points along first and second unit cell vectors, respectively.

Type: integerpair (114.10)
Default: "10 10"
Use: optional
XPath: /input/properties/stm/region/@grid2d

26.2 Attribute: grid3d

Number of grid points along first and second unit cell vectors and along the segment between zmin and zmax along the third cell vector.

Type: integertriple (114.8)

Default: "10 10 10"
Use: optional
XPath: /input/properties/stm/region/@grid3d

26.3 Attribute: height

Height (z-coordinate) of the STM tip in Bohr radius, measured from the absolute origin of the unit cell as defined in the structure element. Assumes the surface is in xy plane.

Type: fortrandouble (114.1)
Default: "0.0d0"
Use: optional
Unit: Bohr
XPath: /input/properties/stm/region/@height

26.4 Attribute: zrange

Pair of floats giving the minimum and maximum z coordinate of the volumetric region for sampling the differential-conductance or integrated-LDOS in topographic mode.

Type: vect2d (114.7)
Default: "0.0 0.0"
Use: optional
Unit: Bohr
XPath: /input/properties/stm/region/@zrange

27 Element: wfplot

Wavefunction plot.

Contains: kstlist (1 times)
plot1d (optional)
plot2d (optional)
plot3d (optional)
XPath: /input/properties/wfplot

This element allows for specification of the following attributes:

version

27.1 Attribute: version

(Temporal solution) 'old' and 'new' version of the visualization subroutine. All tutorials are currently supporting only 'old' version.

Type: string
Default: "old"
Use: optional
XPath: /input/properties/wfplot/@version

28 Element: dos

If present a DOS calculation is started.

DOS and optics plots require integrals of the kind

$$g(\omega_i) = \frac{\Omega}{(2\pi)^3} \int_{\mathrm{BZ}} f(\mathbf{k})\delta(\omega_i - e(\mathbf{k}))d\mathbf{k}. \tag{11}$$

These are calculated by first interpolating the functions $e(\mathbf{k})$ and $f(\mathbf{k})$ with the trilinear method on a much finer mesh whose size is determined by ngrdos. Then the ω-dependent histogram of the integrand is accumulated over the fine mesh. If the output function is noisy then either ngrdos should be increased or nwdos decreased. Alternatively, the output function can be artificially smoothed up to a level given by nsmdos. This is the number of successive 3-point averages to be applied to the function g.

Type: no content
XPath: /input/properties/dos

This element allows for specification of the following attributes:

jdos, lmirep, lonly, newint, ngrdos, ngridkint, nsmdos, nwdos, scissor, sqados, wannier, winddos

28.1 Attribute: jdos

If true, in addition, the joint density of states is computed.

Type: boolean
Default: "false"
Use: optional
XPath: /input/properties/dos/@jdos

28.2 Attribute: lmirep

When lmirep is set to "true", the spherical harmonic basis is transformed into one in which the site symmetries are block diagonal. Band characters determined from the density matrix expressed in this basis correspond to irreducible representations, and allow the partial DOS to be resolved into physically relevant contributions, for example eg and t2g.

Type: boolean
Default: "`false`"
Use: optional
XPath: `/input/properties/dos/@lmirep`

28.3 Attribute: lonly

If true, the partial density of states is computed only l-resolved but not l- and m-resoveld.

Type: boolean
Default: "`false`"
Use: optional
XPath: `/input/properties/dos/@lonly`

28.4 Attribute: newint

If true, a new (partially analytical) routine for the BZ integration is used. It is more efficient for high values of `ngrdos` and give less noisy results.

Type: boolean
Default: "`false`"
Use: optional
XPath: `/input/properties/dos/@newint`

28.5 Attribute: ngrdos

Type: integer
Default: "`100`"
Use: optional
XPath: `/input/properties/dos/@ngrdos`

28.6 Attribute: ngridkint

The dense integration grid on which the energies are interpolated when `wannier` is set to `true`.

Type: integertriple (114.8)
Default: "`0 0 0`"
Use: optional
XPath: `/input/properties/dos/@ngridkint`

28.7 Attribute: nsmdos

This attribute indicates the type of smearing for the resulting DOS. In particular, the value 0 means no smearing at all, 1 that a three nearest point averaging is performed, 2 that two such consecutive averagings are done, etc.

Type: integer
Default: "0"
Use: optional
XPath: /input/properties/dos/@nsmdos

28.8 Attribute: nwdos

Type: integer
Default: "500"
Use: optional
XPath: /input/properties/dos/@nwdos

28.9 Attribute: scissor

The scissor operator is applied, i.e. all bands above the fermi-level are shifted by the given value.

Type: fortrandouble (114.1)
Default: "0.0d0"
Use: optional
Unit: Hartree
XPath: /input/properties/shg/@scissor

28.10 Attribute: sqados

Spin-quantization axis in Cartesian coordinates used when plotting the spin-resolved DOS (z-axis by default).

Type: vect3d (114.6)
Default: "0.0d0 0.0d0 1.0d0"
Use: optional
XPath: /input/properties/dos/@sqados

28.11 Attribute: wannier

If true, Wannier interpolation is used to perform the BZ integration.

Type: boolean
Default: "false"
Use: optional

XPath: /input/properties/dos/@wannier

28.12 Attribute: winddos

Frequency/energy window for the DOS or optics plot.

Type: vect2d (114.7)
Default: "-0.5d0 0.5d0"
Use: optional
Unit: Hartree
XPath: /input/properties/dos/@winddos

29 Element: LSJ

Output L, S and J expectation values.

Contains: kstlist (optional)
XPath: /input/properties/LSJ

30 Element: masstensor

Compute the effective mass tensor at the **k**-point given by vklem.

Type: no content
XPath: /input/properties/masstensor

This element allows for specification of the following attributes:

deltaem, ndspem, vklem

30.1 Attribute: deltaem

The size of the **k**-vector displacement used when calculating numerical derivatives for the effective mass tensor.

Type: fortrandouble (114.1)
Default: "0.025d0"
Use: optional
XPath: /input/properties/masstensor/@deltaem

30.2 Attribute: ndspem

The number of **k**-vector displacements in each direction around vklem when computing the numerical derivatives for the effective mass tensor.

Type: integer
Default: "1"
Use: optional
XPath: /input/properties/masstensor/@ndspem

30.3 Attribute: vklem

The **k**-point in lattice coordinates at which to compute the effective mass tensors.

Type: vect3d (114.6)
Default: "0.0d0 0.0d0 0.0d0"
Use: optional
XPath: /input/properties/masstensor/@vklem

31 Element: chargedensityplot

Plot the charge density

Contains: plot1d (optional)
plot2d (optional)
plot3d (optional)
XPath: /input/properties/chargedensityplot

This element allows for specification of the following attributes:

nocore

31.1 Attribute: nocore

Visualize only the density of valence electrons.

Type: boolean
Default: "false"
Use: optional
XPath: /input/properties/chargedensityplot/@nocore

32 Element: TSvdW

If the subelement TSvdW is specified inside the element properties, the **TS-vdW** method (find reference here: vdWcorrection) for van-der-Waals correction to the total energy is used. The energy correction is written to a file called TSvdW.OUT. Since this method makes use of the electron density of the specific system under investigation, the **TS-vdW** correction can only be obtained in combination with a standard DFT ground-state calculation. In case

you skip the ground-state calculation (do="skip"), you should make sure that a STATE.OUT-file from a previous calculation is contained in your working directory. The electron density will then be read in from this file. If you are interested in changing any of the **TS-vdW** parameters, you can use the element TSvdWparameters to do so.

Type: no content
XPath: /input/properties/TSvdW

33 Element: DFTD2

If the subelement DFTD2 is specified inside the element properties, the **DFT-D2** method (find reference here: vdWcorrection) for van-der-Waals correction to the total energy is used. The energy correction is written to a file called DFTD2.OUT. It is not necessary to perform a ground-state calculation, so you could choose do="skip" and only calculate the van-der-Waals correction. Only the input file input.xml with the declaration of the structure of interest must be provided. If you are interested in changing any of the **DFT-D2** parameters, you can use the element DFTD2parameters to do so.

Type: no content
XPath: /input/properties/DFTD2

34 Element: exccplot

Exchange-correlation and Coulomb potential plots.

Contains: plot1d (optional)
plot2d (optional)
plot3d (optional)
XPath: /input/properties/exccplot

35 Element: elfplot

Electron localization function (ELF).

Contains: plot1d (optional)
plot2d (optional)
plot3d (optional)
XPath: /input/properties/elfplot

36 Element: mvecfield

Plot of magnetization vector field.

Contains:	plot2d (optional) plot3d (optional)
XPath:	/input/properties/mvecfield

37 Element: xcmvecfield

Plot of exchange-correlation magnetic vector field.

Contains:	plot2d (optional) plot3d (optional)
XPath:	/input/properties/xcmvecfield

38 Element: electricfield

Writes the electric field to file.

Contains:	plot2d (optional) plot3d (optional)
XPath:	/input/properties/electricfield

39 Element: gradmvecfield

Plot of he gradient of the magnetic vector field.

Contains:	plot1d (optional) plot2d (optional) plot3d (optional)
XPath:	/input/properties/gradmvecfield

40 Element: fermisurfaceplot

Writes Fermi surface data to file.

Contains:	plot2d (optional) plot3d (optional)
XPath:	/input/properties/fermisurfaceplot

This element allows for specification of the following attributes:

nstfsp

40.1 Attribute: nstfsp

Number of states to be included in the Fermi surface plot file.

Type: integer
Default: "6"
Use: optional
XPath: /input/properties/fermisurfaceplot/@nstfsp

41 Element: EFG

Calculation of electric field gradient (EFG), contact charge.

Type: no content
XPath: /input/properties/EFG

42 Element: mossbauer

Type: no content
XPath: /input/properties/mossbauer

43 Element: expiqr

Contains: kstlist (optional)
XPath: /input/properties/expiqr

44 Element: elnes

Type: no content
XPath: /input/properties/elnes

This element allows for specification of the following attributes:

ngrid, vecql, wgrid, wmax, wmin

44.1 Attribute: ngrid

Type: integer
Default: "100"
Use: optional
XPath: /input/properties/elnes/@ngrid

44.2 Attribute: vecql

Gives the q-vector in lattice coordinates for calculating ELNES.

Type: vect3d (114.6)
Default: "0.0d0 0.0d0 0.0d0"
Use: optional
XPath: /input/properties/elnes/@vecql

44.3 Attribute: wgrid

Number of grid points inside [wmin,wmax] interval.

Type: integer
Default: "100"
Use: optional
XPath: /input/properties/elnes/@wgrid

44.4 Attribute: wmax

Upper energy limit.

Type: fortrandouble (114.1)
Default: "0.5"
Use: optional
XPath: /input/properties/elnes/@wmax

44.5 Attribute: wmin

Lower energy limit.

Type: fortrandouble (114.1)
Default: "0.0"
Use: optional
XPath: /input/properties/elnes/@wmin

45 Element: eliashberg

Type: no content
XPath: /input/properties/eliashberg

This element allows for specification of the following attributes:

mustar

45.1 Attribute: mustar

Coulomb pseudopotential, $\mu*$, used in the McMillan-Allen-Dynes equation.

Type: fortrandouble (114.1)
Default: "0.15d0"
Use: optional
XPath: /input/properties/eliashberg/@mustar

46 Element: momentummatrix

Generate matrix elements of the momentum operator and store them in PMAT.OUT.

Type: no content
XPath: /input/properties/momentummatrix

This element allows for specification of the following attributes:

fastpmat

46.1 Attribute: fastpmat

apply generalised DFT correction of L. Fritsche and Y. M. Gu, Phys. Rev. B 48, 4250 (1993)

Type: boolean
Default: "true"
Use: optional
XPath: /input/properties/momentummatrix/@fastpmat

47 Element: dielmat

Calculate the dielectric tensor in IP-RPA (without local-field effect) for q=0.

Contains: epscomp (optional)
XPath: /input/properties/dielmat

This element allows for specification of the following attributes:

drude, intraband, scissor, swidth, tevout, wgrid, wmax

47.1 Attribute: drude

Parameters for the Drude term used for calculating the intraband contribution: First value determines the plasma frequency, second - the lifetime broadening.

Type: vect2d (114.7)

Default: "0.0d0 0.0d0"
Use: optional
XPath: /input/properties/dielmat/@drude

47.2 Attribute: intraband

The intraband attribute is "true" if the intraband term is to be added to the optical matrix.

Type: boolean
Default: "false"
Use: optional
XPath: /input/xs/screening/@intraband

47.3 Attribute: scissor

Value of the "scissor" correction.

Type: fortrandouble (114.1)
Default: "0.0d0"
Use: optional
XPath: /input/properties/dielmat/@scissor

47.4 Attribute: swidth

Broadening factor to fit the experimental resolution.

Type: fortrandouble (114.1)
Default: "0.01d0"
Use: optional
XPath: /input/properties/dielmat/@swidth

47.5 Attribute: tevout

"true" if energy outputs are in eV.

Type: boolean
Default: "false"
Use: optional
XPath: /input/properties/dielmat/@tevout

47.6 Attribute: wgrid

Number of grid points inside [0,wmax] interval.

Type: integer

Default: "400"
Use: optional
XPath: /input/properties/dielmat/@wgrid

47.7 Attribute: wmax

Upper energy limit for the dielectric matrix calculations.

Type: fortrandouble (114.1)
Default: "0.30"
Use: optional
XPath: /input/properties/dielmat/@wmax

48 Element: epscomp

Components of the dielectric tensor to be calculated.

Type: integerpair (114.10)
XPath: /input/properties/dielmat/epscomp

49 Element: boltzequ

Calculate the electronic transport coefficients from the Boltzmann equation.

Contains: condcomp (optional)
XPath: /input/properties/boltzequ

This element allows for specification of the following attributes:

mugrid, nwtdf, swidth, tevout, tgrid, tsiout, windmu, windtdf, windtemp

49.1 Attribute: mugrid

Number of chemical potential points.

Type: integer
Default: "1"
Use: optional
XPath: /input/properties/boltzequ/@mugrid

49.2 Attribute: nwtdf

Number of frequency (or energy) points for the evaluation of the transport distribution function.

Type: integer
Default: "100"
Use: optional
XPath: /input/properties/boltzequ/@nwtdf

49.3 Attribute: swidth

Broadening factor used in the calculation of the transport distribution function.

Type: fortrandouble (114.1)
Default: "0.01d0"
Use: optional
XPath: /input/properties/boltzequ/@swidth

49.4 Attribute: tevout

If "true", output energies are in eV.

Type: boolean
Default: "false"
Use: optional
XPath: /input/properties/boltzequ/@tevout

49.5 Attribute: tgrid

Number of temperature points.

Type: integer
Default: "1"
Use: optional
XPath: /input/properties/boltzequ/@tgrid

49.6 Attribute: tsiout

If "true", output transport coefficients are given in SI units: Seebeck coefficient in V/K , electrical conductivity over relaxation time in S/(m s) , thermal conductivity over relaxation time in W/(mK s).

Type: boolean
Default: "false"
Use: optional
XPath: /input/properties/boltzequ/@tsiout

49.7 Attribute: windmu

Chemical potential window for the evaluation of the transport coefficients.

Type: vect2d (114.7)
Default: "0.0d0 0.0d0"
Use: optional
XPath: /input/properties/boltzequ/@windmu

49.8 Attribute: windtdf

Frequency (or energy) window for the evaluation of the transport distribution function.

Type: vect2d (114.7)
Default: "-0.5d0 0.5d0"
Use: optional
XPath: /input/properties/boltzequ/@windtdf

49.9 Attribute: windtemp

Temperature window for the evaluation of the transport coefficients in Kelvin.

Type: vect2d (114.7)
Default: "300.0d0 300.0d0"
Use: optional
XPath: /input/properties/boltzequ/@windtemp

50 Element: condcomp

Components of the tensors for the electronic transport coefficients to be calculated.

Type: integerpair (114.10)
XPath: /input/properties/boltzequ/condcomp

51 Element: raman

Compute first order Raman spectra.

Contains: eigvec (zero or more)
energywindow (1 times)
XPath: /input/properties/raman

This element allows for specification of the following attributes:

broad, degree, displ, doequilibrium, elaser, elaserunit, getphonon, mode, molecule, ninter, nstate, nstep, temp, useforces, usesym, writefunc, xmax, xmin

51.1 Attribute: broad

Lorentzian broadening in cm^{-1} for simulation of experimental spectra.

Type:	fortrandouble (114.1)
Default:	"10.0d0"
Use:	optional
XPath:	/input/properties/raman/@broad

51.2 Attribute: degree

Degree of fitting polynomial for the potential. The default of 2 results in a harmonic oscillator. For the dielectric function also a polynomial of degree degree is fitted, but only the first derivative used.

Type:	integer
Default:	"2"
Use:	optional
XPath:	/input/properties/raman/@degree

51.3 Attribute: displ

Step length for each displacement along normal coordinate, $|\mathbf{u}_i|$ in Bohr. For solids, a value of 0.01-0.02 times the number of atoms in the unit cell is often a good choice. In any case check the obtained potential and dielectric functions carefully.

Type:	fortrandouble (114.1)
Default:	"0.02d0"
Use:	optional
XPath:	/input/properties/raman/@displ

51.4 Attribute: doequilibrium

Specifiy whether the true equilibirum geometry should be included in the frozen phonon calculations. On one hand the symmetry of the equilibrium might be higher and the properties slightly changed; on the other hand the same equilibrium structure is used for all active modes and thus some computer time can be saved. The default is false, which means that a close-to-equilibrium structure with the same symmetry as the mode is used. For every mode this is a slightly different structure.

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/properties/raman/@doequilibrium

51.5 Attribute: elaser

Energy of the incident laser beam. Specify it in units of `elaserunit`

Type:	fortrandouble (114.1)
Default:	"0.0"
Use:	optional
XPath:	/input/properties/raman/@elaser

51.6 Attribute: elaserunit

Units of `elaser`: electron volts, photon wave length in nm, reciprocal centimeters or Hartree.

Type:	**choose from:**
	eV
	nm
	cm-1
	Ha
Default:	"nm"
Use:	optional
XPath:	/input/properties/raman/@elaserunit

51.7 Attribute: getphonon

Prior to the calculation of Raman intensities, the normal coordinates of the phonon modes have to be ready. Four choices are available: `fromscratch` triggers a supercell phonon calculation for the Γ-point (i.e. the supercell is just the unit cell), note that the relevant attributes given with the element phonons will be overwritten by suitable values; `fromfile` reads the dynamical matrix from `DYN_*.OUT` files produced in a previous phonon calculation; `readinput` enables you to input a phonon eigenvector manually; and `symvec` constructs symmetry vectors from the crystal symmetries and uses them instead of eigenvectors (this is not generally meaningful, as the symmetry vectors are obtained as linear combinations of eigenvectors in case several phonon modes which belong to the same irreducible representation occur, so check the output carefully). `symveccheck` solely produces the symmetry vectors and stops.

Type:	**choose from:**
	fromscratch
	fromfile
	symvec
	symveccheck
	readinput
Default:	"fromscratch"
Use:	optional
XPath:	/input/properties/raman/@getphonon

51.8 Attribute: mode

Optionally choose a phonon mode to compute ($4 \leq$`mode`$\leq 3N_{\text{atm}}$). The default of 0 means compute spectra of all Raman active modes present.

Type: integer
Default: "0"
Use: optional
XPath: /input/properties/raman/@mode

51.9 Attribute: molecule

If `true`, an isolated molecule is assumed and some additional output created. The default of `false` means the calculation is done for the solid state limit.

Type: boolean
Default: "false"
Use: optional
XPath: /input/properties/raman/@molecule

51.10 Attribute: ninter

Number of intervals in numerical (FE) solution of the oscillator problem.

Type: integer
Default: "500"
Use: optional
XPath: /input/properties/raman/@ninter

51.11 Attribute: nstate

Number of vibrational states to solve for.

Type: integer
Default: "5"
Use: optional
XPath: /input/properties/raman/@nstate

51.12 Attribute: nstep

Create `nstep` distorted geometries to sample the potential and dielectric function. The distortion is done by displacing atoms along normal coordinate by $n*$`displ` with $-1/2$`nstep`$\leq n \leq 1/2$`nstep`.

Type: integer
Default: "5"
Use: optional

XPath: /input/properties/raman/@nstep

51.13 Attribute: temp

Temperature in K for which the Raman spectrum is computed. This affects the occupation of vibrational states.

Type: fortrandouble (114.1)
Default: "298.15"
Use: optional
XPath: /input/properties/raman/@temp

51.14 Attribute: useforces

Request the use forces to fit the potential along normal coordinates (if set to true), otherwise the total energy will be used (if set to false).

Type: boolean
Default: "true"
Use: optional
XPath: /input/properties/raman/@useforces

51.15 Attribute: usesym

Flag wether to use symmetry to analyze the Raman activity of phonon modes prior to running through all computation steps.

Type: boolean
Default: "true"
Use: optional
XPath: /input/properties/raman/@usesym

51.16 Attribute: writefunc

If true output eigenfunctions of oscillator problem to files.

Type: boolean
Default: "false"
Use: optional
XPath: /input/properties/raman/@writefunc

51.17 Attribute: xmax

Upper boundary of the oscillator problem, give a distance along the normal coordinate, $|\mathbf{u}_i|$ in Bohr.

Type: fortrandouble (114.1)

Default: "3.0d0"
Use: optional
XPath: /input/properties/raman/@xmax

51.18 Attribute: xmin

Lower boundary of the oscillator problem, give a distance along the normal coordinate, $|\mathbf{u}_i|$ in Bohr.

Type: fortrandouble (114.1)
Default: "-3.0d0"
Use: optional
XPath: /input/properties/raman/@xmin

52 Element: eigvec

Input manually the eigenvector of a normal mode. Note: Not normalized eigenvectors are renormalized by exciting.

Type: no content
XPath: /input/properties/raman/eigvec

This element allows for specification of the following attributes:

comp (required)

52.1 Attribute: comp

A component of the phonon eigenvector. The order of the given components must correspond to the order of the atoms given in structure, and consist of three times the element eigvec for each atom (for x, y and z). Each time specify two floating point numbers, which are the real and imaginary part of the component.

Type: vect2d (114.7)
Use: required
XPath: /input/properties/raman/eigvec/@comp

53 Element: moke

Type: no content
XPath: /input/properties/moke

This element allows for specification of the following attributes:

drude, intraband, scissor, swidth, tevout, wgrid, wmax

53.1 Attribute: drude

Parameters for the Drude term used for calculating the intraband contribution: First value determines the plasma frequency, second - the lifetime broadening.

Type: vect2d (114.7)
Default: "0.0d0 0.0d0"
Use: optional
XPath: /input/properties/moke/@drude

53.2 Attribute: intraband

Use the intraband term in calculations if the dielectric matrix.

Type: boolean
Default: "false"
Use: optional
XPath: /input/xs/screening/@intraband

53.3 Attribute: scissor

Scissors operator.

Type: fortrandouble (114.1)
Default: "0.0d0"
Use: optional
XPath: /input/properties/moke/@scissor

53.4 Attribute: swidth

Broadening factor.

Type: fortrandouble (114.1)
Default: "0.01d0"
Use: optional
XPath: /input/properties/moke/@swidth

53.5 Attribute: tevout

"true" if energy outputs are in eV.

Type: boolean
Default: "false"
Use: optional
XPath: /input/properties/moke/@tevout

53.6 Attribute: wgrid

Number of grid points inside [0,wmax] interval.

Type:	integer
Default:	"400"
Use:	optional
XPath:	/input/properties/moke/@wgrid

53.7 Attribute: wmax

Upper energy limit for the Kerr angle calculation.

Type:	fortrandouble (114.1)
Default:	"0.30"
Use:	optional
XPath:	/input/properties/moke/@wmax

54 Element: shg

Contains:	chicomp
XPath:	/input/properties/shg

This element allows for specification of the following attributes:

etol, scissor, swidth, tevout, wgrid, wmax

54.1 Attribute: etol

Tolerence factor (to avoid singularities).

Type:	fortrandouble (114.1)
Default:	"0.004d0"
Use:	optional
XPath:	/input/properties/shg/@etol

54.2 Attribute: scissor

Scissors operator.

Type:	fortrandouble (114.1)
Default:	"0.0d0"
Use:	optional
XPath:	/input/properties/shg/@scissor

54.3 Attribute: swidth

Broadening factor.

Type:	fortrandouble (114.1)
Default:	"0.01d0"
Use:	optional
XPath:	/input/properties/shg/@swidth

54.4 Attribute: tevout

"true" if energy outputs are in eV.

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/properties/shg/@tevout

54.5 Attribute: wgrid

Number of grid points inside [0,emax] interval.

Type:	integer
Default:	"400"
Use:	optional
XPath:	/input/properties/shg/@wgrid

54.6 Attribute: wmax

Upper energy limit for SHG calculations.

Type:	fortrandouble (114.1)
Default:	"0.3"
Use:	optional
XPath:	/input/properties/shg/@wmax

55 Element: chicomp

The components of the second-order optical tensor Chi(-2w,w,w) to be calculated.

Type:	integertriple (114.8)
Default:	"1 2 3"
XPath:	/input/properties/shg/chicomp

56 Element: wannier

When the wannier element is present, in addition Wannier functions are calculated.

Contains:	projection (optional)
	group (zero or more)
XPath:	/input/properties/wannier

This element allows for specification of the following attributes:

do, fermizero, input, mindist, printproj

56.1 Attribute: do

Specifies, whether Wannier functions are calculated from scratch, skipped, read in from file or maximally localized starting from a previous result from file.

Type:	**choose from:**
	fromscratch
	fromfile
	maxfromfile
	skip
Default:	"fromscratch"
Use:	optional
XPath:	/input/properties/wannier/@do

56.2 Attribute: fermizero

Set Fermi energy to zero.

Type:	boolean
Default:	"true"
Use:	optional
XPath:	/input/properties/wannier/@fermizero

56.3 Attribute: input

Specifies, which method was used for the input calculation.

Type:	**choose from:**
	gs
	gw
	hybrid
	qsgw
Default:	"gs"
Use:	optional

XPath: /input/properties/wannier/@input

56.4 Attribute: mindist

Use minimal distances for interpolation. This is more accurate for coarse k-grids but also more costly.

Type: boolean
Default: "true"
Use: optional
XPath: /input/properties/wannier/@mindist

56.5 Attribute: printproj

If true the projection functions are written to WANNIER_INFO.OUT.

Type: boolean
Default: "false"
Use: optional
XPath: /input/properties/wannier/@printproj

57 Element: projection

Various parameters on the local-orbital set for the projection.

Type: no content
XPath: /input/properties/wannier/projection

This element allows for specification of the following attributes:

dordmax, epsld, nprojtot, nunocc

57.1 Attribute: dordmax

Energy derivative up to which local-orbitals are added.

Type: integer
Default: "2"
Use: optional
XPath: /input/properties/wannier/projection/@dordmax

57.2 Attribute: epsld

Tolerance for removing linear dependent local-orbitals.

Type: fortrandouble (114.1)

Default: "1.0d-3"
Use: optional
XPath: /input/properties/wannier/projection/@epsld

57.3 Attribute: nprojtot

Total number of local-orbitals used for the projection

Type: integer
Default: "0"
Use: optional
XPath: /input/properties/wannier/projection/@nprojtot

57.4 Attribute: nunocc

Number of unoccupied states per atom for which local-orbitals are added.

Type: integer
Default: "20"
Use: optional
XPath: /input/properties/wannier/projection/@nunocc

58 Element: group

Defines a group of bands from which Wannier functions are calculated.

Contains: projector (zero or more)
XPath: /input/properties/wannier/group

This element allows for specification of the following attributes:

cg, epsdis, epsmaxloc, epsopf, fst, innerwindow, lambdaopf, ls, lst, maxit, method, minit, nproj, nwf, nwrite, outerwindow, step, uncertainty, writeconv

58.1 Attribute: cg

Specifies which conjugate gradient update parameter is used for the minimization. The options are steepest descent (sd), Hestenes-Stiefel (hs), Fletcher-Reeves (fr), Polak-Ribiere (pr) and Hager-Zhang (hz).

Type: **choose from:**
sd
hs
fr
pr

hz
Default: "hs"
Use: optional
XPath: /input/properties/wannier/group/@cg

58.2 Attribute: epsdis

Convergency cut-off for subspace disentanglement.

Type: fortrandouble (114.1)
Default: "1.0d-4"
Use: optional
XPath: /input/properties/wannier/group/@epsdis

58.3 Attribute: epsmaxloc

Convergency cut-off (gradient) for MLWFs. The minimization is stopped when the norm of the gradient of the spread functional is smaller than the given value.

Type: fortrandouble (114.1)
Default: "1.0d-6"
Use: optional
XPath: /input/properties/wannier/group/@epsmaxloc

58.4 Attribute: epsopf

Convergency cut-off for OPFs. The minimization is stopped when the change in the spread functional between the last two sweeps is smaller than the given value.

Type: fortrandouble (114.1)
Default: "1.0d-2"
Use: optional
XPath: /input/properties/wannier/group/@epsopf

58.5 Attribute: fst

Lowest state from which Wannier functions are constructed.

Type: integer
Default: "1"
Use: optional
XPath: /input/properties/wannier/group/@fst

58.6 Attribute: innerwindow

Inner energy-window for band-disentanglement.

Type: vect2d (114.7)
Default: "0.0d0 0.0d0"
Use: optional
XPath: /input/properties/wannier/group/@innerwindow

58.7 Attribute: lambdaopf

Lambda in the Lagrangian of the optimized projection functions (OPF).

Type: fortrandouble (114.1)
Default: "1.0d0"
Use: optional
XPath: /input/properties/wannier/group/@lambdaopf

58.8 Attribute: ls

If true, a line-search is made in the minimization.

Type: boolean
Default: "true"
Use: optional
XPath: /input/properties/wannier/group/@ls

58.9 Attribute: lst

Highest state from which Wannier functions are constructed.

Type: integer
Default: "1"
Use: optional
XPath: /input/properties/wannier/group/@lst

58.10 Attribute: maxit

Maximum number of interations for minimization.

Type: integer
Default: "2000"
Use: optional
XPath: /input/properties/wannier/group/@maxit

58.11 Attribute: method

Defines the method that is used for computing Wannier functions. The options are simple projection (`pro`), optimized projection functions (OPFs) (`opf`), maximal localization starting from simple projection (`promax`), maximal localization starting from OPFs (`opfmax`) and band-disentanglement (`disentangle`).

Type:	**choose from:**
	`pro`
	`prowan`
	`opf`
	`promax`
	`prowanmax`
	`opfmax`
	`scdm`
	`scdmmax`
	`disentangle`
Default:	"`opfmax`"
Use:	optional
XPath:	`/input/properties/wannier/group/@method`

58.12 Attribute: minit

Minimum number of interations for minimization.

Type:	integer
Default:	"`0`"
Use:	optional
XPath:	`/input/properties/wannier/group/@minit`

58.13 Attribute: nproj

Number of local-orbitals used for the projection in this group

Type:	integer
Default:	"`0`"
Use:	optional
XPath:	`/input/properties/wannier/group/@nproj`

58.14 Attribute: nwf

Number of Wannier functions to be created from the given energy windows.

Type:	integer
Default:	"`0`"
Use:	optional
XPath:	`/input/properties/wannier/group/@nwf`

58.15 Attribute: nwrite

Number of iterations after which the transformation matrices are written to file.

Type: integer
Default: "0"
Use: optional
XPath: /input/properties/wannier/group/@nwrite

58.16 Attribute: outerwindow

Outer energy-window for band-disentanglement.

Type: vect2d (114.7)
Default: "0.0d0 0.0d0"
Use: optional
XPath: /input/properties/wannier/group/@outerwindow

58.17 Attribute: step

Step-length used for minimization if no line-search is done.

Type: fortrandouble (114.1)
Default: "0.5d0"
Use: optional
XPath: /input/properties/wannier/group/@step

58.18 Attribute: uncertainty

Convergency cut-off (uncertainty) for MLWFs. The minimization is stopped when the uncertainty of the spread functional is smaller than the given value.

Type: fortrandouble (114.1)
Default: "0.0d0"
Use: optional
XPath: /input/properties/wannier/group/@uncertainty

58.19 Attribute: writeconv

Write convergence behaviour to file.

Type: boolean
Default: "false"
Use: optional
XPath: /input/properties/wannier/group/@writeconv

59 Element: projector

Defines a local-orbital to be used as projection function.

Type: no content
XPath: /input/properties/wannier/group/projector

This element allows for specification of the following attributes:

nr (required)

59.1 Attribute: nr

Number of the local-orbital.

Type: integer
Use: required
XPath: /input/properties/wannier/group/projector/@nr

60 Element: wannierplot

Wannier function plot.

Contains: plot1d (optional)
plot2d (optional)
plot3d (optional)
XPath: /input/properties/wannierplot

This element allows for specification of the following attributes:

fst, lst

60.1 Attribute: fst

First Wannier function.

Type: integer
Default: "0"
Use: optional
XPath: /input/properties/wannierplot/@fst

60.2 Attribute: lst

Last Wannier function.

Type: integer
Default: "0"

Use: optional
XPath: /input/properties/wannierplot/@lst

61 Element: wanniergap

Finds VBM and CBM and determines gap using Wannier interpolation.

Type: no content
XPath: /input/properties/wanniergap

This element allows for specification of the following attributes:

ngridkint

61.1 Attribute: ngridkint

Interpolation grid used for extrema search.

Type: integertriple (114.8)
Default: "0 0 0"
Use: optional
XPath: /input/properties/wanniergap/@ngridkint

62 Element: phonons

Compute the dynamical matrix.

This is done by constructing a supercell (attributes ngridq and reduceq), displacing atoms in it and obtaining the dynamical matrix from the forces. As all atoms are displaced four times in each direction, and this is done for every **q**-point, phonon calculations can become quite tedious. If the calculation was done already at an earlier point, and an existing dynamical matrix should be reused, the attribute do allows to skip a fresh calculation. Note also that the calculation of the dynamical matrix can be run in parallel.

To obtain phonon eigenvalues and eigenvectors for one or more **q**-points, add one of the elements qpointset, interpolate, phonondispplot or phonondos.

Contains: qpointset (optional)
phonondos (optional)
phonondispplot (optional)
reformatdynmat (optional)
interpolate (optional)
parts (optional)
XPath: /input/phonons

This element allows for specification of the following attributes:

deltaph, do, gamma, ngridq, reduceq

62.1 Attribute: deltaph

Phonon calculations are performed by constructing a supercell corresponding to a particular **q**-vector and making small periodic sin- and cos-like displacements of the atoms. The amplitude of this displacement, in cartesian coordinates for each component, is given by `deltaph` (in units of Bohr). Additionally a displacement of `2*deltaph` is done, so in general each atom is displaced four times.

`deltaph` should not be made too large, as anharmonic terms could then become significant, neither should it be too small as this can introduce a numerical error.

Type:	fortrandouble (114.1)
Default:	"`0.03d0`"
Use:	optional
XPath:	`/input/phonons/@deltaph`

62.2 Attribute: do

Specify if the phonon calculation is performed (value `fromscratch`) or skipped (value `skip`.) In the latter case the dynamical matrix is read from files produced in a previous run with the same parameters. The value `fromscratch` can also be used to continue an incomplete calculation.

Type:	**choose from:**
	`fromscratch`
	`skip`
Default:	"`fromscratch`"
Use:	optional
XPath:	`/input/phonons/@do`

62.3 Attribute: gamma

Determines how force constants at the Γ-point are computed. The numerical differentiation is done from (a) a displacement by `deltaphi` and the equilibirum (`onestep`), (b) displacements by ±`deltaphi` (`twostep`), or (c) displacements by `deltaphi` and 2`deltaphi` (`standard`) for each atom in each cartesian direction. Note that options (a) requires $3N+1$ computations, whereas option (b) and (c) require $6N$ for N atoms. In particular if only the Γ-point is to be computed, option (b) is more accurate and yields better eigenvectors than (a).

Type:	**choose from:**
	`onestep`
	`twostep`

	`standard`
Default:	"`twostep`"
Use:	optional
XPath:	`/input/phonons/@gamma`

62.4 Attribute: ngridq

Number of **q** grid points along the basis vector directions. This determines the size of the supercell.

Type:	integertriple (114.8)
Default:	"`1 1 1`"
Use:	optional
XPath:	`/input/phonons/@ngridq`

62.5 Attribute: reduceq

The attribute `reduceq` is set to `"true"` if the **q**-point set is to be reduced with the crystal symmetries.

Type:	boolean
Default:	"`true`"
Use:	optional
XPath:	`/input/phonons/@reduceq`

63 Element: phonondos

Compute the phonon density of states (DOS) $g(\omega)$ and thermodynamical properties. This is done by calculating the phonon eigenvalues on a dense grid, specified by `ngrdos`. The DOS is output to file `PHDOS.OUT`. Note that $\int_{\omega_{\min}}^{\omega_{\max}} d\omega\ g(\omega) = 3N_{\text{at}}$

From the DOS $g(\omega)$ the following thermodynamical properties are obtained:

- the zero-point energy $E_{\text{ZP}} = \frac{1}{2}\int_{\omega_{\min}}^{\omega_{\max}} d\omega\ \omega\, g(\omega)$
- the vibrational internal energy $E_{\text{vib}} = \frac{1}{2}\int_{\omega_{\min}}^{\omega_{\max}} d\omega\ \omega\, g(\omega) \coth \frac{\omega}{2k_BT}$
- the vibrational free energy $F_{\text{vib}} = k_BT \int_{\omega_{\min}}^{\omega_{\max}} d\omega\ g(\omega) \log\left(2\sinh\frac{\omega}{2k_BT}\right)$
- the vibrational entropy $S_{\text{vib}} = \frac{E_{\text{vib}}-F_{\text{vib}}}{T}$
- the heat capacity $c = k_B \int_{\omega_{\min}}^{\omega_{\max}} d\omega\ g(\omega) \left(\frac{\omega}{k_BT}\right)^2 \exp\left(\frac{\omega}{k_BT}\right)\left[\exp(\frac{\omega}{k_BT})-1\right]^{-2}$

where N_{at} is the number of atoms in the unit cell. These quantities are computed for the temperatures, specified by ntemp and written to files THERMO.OUT and thermo.xml.

Type: no content
XPath: /input/phonons/phonondos

This element allows for specification of the following attributes:

ngrdos, nsmdos, ntemp, nwdos

63.1 Attribute: ngrdos

Number of grid points in each lattice direction on which the eigenvalues are interpolated.

Type: integer
Default: "100"
Use: optional
XPath: /input/phonons/phonondos/@ngrdos

63.2 Attribute: nsmdos

Number of 3-point averaging runs to smoothen the DOS. One run corresponds to setting the DOS value for one frequency $g(\omega_i)$ to the average $1/3\,[g(\omega_{i-1}) + g(\omega_i) + g(\omega_{i+1})]$.

Type: integer
Default: "0"
Use: optional
XPath: /input/phonons/phonondos/@nsmdos

63.3 Attribute: ntemp

Number of temperatures in the range up to the maximal temperature T_{max} for the calculation of the thermodynamical properties from the phonon DOS This corresponds to the maximal phonon frequency ω_{max} by $T_{\mathrm{max}} = \omega_{\mathrm{max}}/k_B$.

Type: integer
Default: "200"
Use: optional
XPath: /input/phonons/phonondos/@ntemp

63.4 Attribute: nwdos

Number of steps between the lowest and highest phonon frequency for the DOS.

Type: integer

Default: "500"
Use: optional
XPath: /input/phonons/phonondos/@nwdos

64 Element: phonondispplot

Produce a phonon dispersion plot by interpolating phonon frequencies for points on a path through the Brillouin zone. The frequencies for all phonon modes along the path are written to file PHDISP.OUT, vertex lines are written to file PHDLINES.OUT. Use the element plot1d to specify the path in reciprocal lattice vectors.

Contains: plot1d
XPath: /input/phonons/phonondispplot

65 Element: reformatdynmat

Reads in the dynamical matrix rows from the corresponding files and outputs them as 3×3 blocks for each atom combination to the file DYNMAT.OUT. A corrected dynamical matrix which fulfills the accoustic sumrule is output to the file DYNMAT_SUMRULE.OUT. It is obtained by subtracting the three lowest eigenvectors from the original matrix: $D_{ij}^{\mathbf{q}} \rightarrow D_{ij}^{\mathbf{q}} - \sum_{k=1}^{3} (\omega_k^0)^2 v_{k;i}^0 v_{k;j}^0$ for all $\mathbf{q}$, where ω_k^0 is the kth eigenvalue of the $\mathbf{q} = 0$ dynamical matrix and $v_{k;i}^0$ the ith component of its eigenvector.

Symmetrized forms are written to the files DYNMAT_SYM.OUT and DYNMAT_SYM_SUMRULE.OUT.

Type: no content
XPath: /input/phonons/reformatdynmat

66 Element: interpolate

Interpolates the phonon frequencies, and optionally eigenvectors, on a given **q**-point grid and outputs them to file PHONON_INTERPOLATE.OUT.

Type: no content
XPath: /input/phonons/interpolate

This element allows for specification of the following attributes:

ngridq (required), vqloff, writeeigenvectors

66.1 Attribute: ngridq

q-point grid for interpolation.

Type: integertriple (114.8)
Use: required
XPath: /input/phonons/interpolate/@ngridq

66.2 Attribute: vqloff

The **q**-point offset vector in lattice coordinates.

Type: vect3d (114.6)
Default: "0.0d0 0.0d0 0.0d0"
Use: optional
XPath: /input/phonons/interpolate/@vqloff

66.3 Attribute: writeeigenvectors

Set to `true` if the phonon eigenvectors are to be interpolated and output in addition to the phonon frequencies.

Type: boolean
Default: "false"
Use: optional
XPath: /input/phonons/interpolate/@writeeigenvectors

67 Element: parts

Contains: dopart (zero or more)
XPath: /input/phonons/parts

68 Element: dopart

Type: no content
XPath: /input/phonons/parts/dopart

This element allows for specification of the following attributes:

id (required)

68.1 Attribute: id

This attribute is used to trigger lower-level tasks and is mainly used for testing, debugging, and the testing of new features. Do not use it unless you know what you are doing.

Type: string

Use: required
XPath: /input/phonons/parts/dopart/@id

69 Element: xs

If this element is present with valid configuration, the macroscopic dielectric function and related spectroscopic quantities in the linear regime are calculated through either time-dependent DFT (TDDFT) or the Bethe-Salpeter equation (BSE).

Contains: storeexcitons (optional)
writeexcitons (optional)
writekpathweights (optional)
excitonPlot (optional)
tddft (optional)
screening (optional)
BSE (optional)
transitions (optional)
qpointset (1 times)
tetra (optional)
energywindow (1 times)
plan (optional)
XPath: /input/xs

This element allows for specification of the following attributes:

xstype (required), bfieldc, broad, dbglev, dfoffdiag, dogroundstate, emattype, emaxdf, epsdfde, fastpmat, gqmax, gqmaxtype, lmaxapw, lmaxapwwf, lmaxemat, lmaxmat, maxscl, nempty, ngridk, ngridq, nosym, pwmat, reducek, reduceq, rgkmax, scissor, skipgnd, swidth, tappinfo, tevout, vkloff, writexsgrids

69.1 Attribute: bfieldc

This attribute overrides the homonym attribute from the groundstate/spin element.

Type: vect3d (114.6)
Default: "0.0d0 0.0d0 0.0d0 "
Use: optional
XPath: /input/xs/@bfieldc

69.2 Attribute: broad

Lorentzian broadening for all spectra

Type: fortrandouble (114.1)
Default: "0.01d0"
Use: optional
Unit: Hartree
XPath: /input/xs/@broad

69.3 Attribute: dbglev

Debugging level. Any value > 0 will produce additional debug output. The large the value, the more information is output.

Type: integer
Default: "0"
Use: optional
XPath: /input/xs/@dbglev

69.4 Attribute: dfoffdiag

"true" if also off-diagonal tensor elements for the interacting response function are to be calculated.

Type: boolean
Default: "false"
Use: optional
XPath: /input/xs/@dfoffdiag

69.5 Attribute: dogroundstate

Decides if the ground state is calculated starting from scratch or using the densities from file.

Type: **choose from:**
fromscratch
fromfile
Default: "fromfile"
Use: optional
XPath: /input/xs/@dogroundstate

69.6 Attribute: emattype

Type of matrix element generation (band-combinations). Should only be referenced for experimental features.

Type: integer
Default: "1"
Use: optional

XPath: /input/xs/@emattype

69.7 Attribute: emaxdf

Energy cutoff for the unoccupied states in the Kohn-Sham response function and screening. This parameter ensures a cutoff at the specified energy and is defined in addition to the nempty parameter.

Type: fortrandouble (114.1)
Default: "1.0d10"
Use: optional
XPath: /input/xs/@emaxdf

69.8 Attribute: epsdfde

The smallest energy difference for which the square of its inverse will be considered in the Kohn-Sham response function.

Type: fortrandouble (114.1)
Default: "1.0d-8"
Use: optional
Unit: Hartree
XPath: /input/xs/@epsdfde

69.9 Attribute: fastpmat

If set to "true", a fast method to calculate APW-lo, lo-APW and lo-lo parts of the momentum matrix elements in the muffin-tin is used.

Type: boolean
Default: "true"
Use: optional
XPath: /input/xs/@fastpmat

69.10 Attribute: gqmax

$|\mathbf{G}+\mathbf{q}|$ cutoff for Kohn-Sham response function, screening and for expansion of Coulomb potential

Type: fortrandouble (114.1)
Default: "0.0d0"
Use: optional
XPath: /input/xs/@gqmax

69.11 Attribute: gqmaxtype

Defines the way the gqmax cutoff is applied for the selection of the G-vectors. For "$|G+q|$" G vectors are selected such that $\mathbf{G}+\mathbf{q}$ lies within the gqmax cutoff. For "$|G|$" G vectors are selected such that $\mathbf{G}$ lies within the gqmax cutoff.

Type:	**choose from:**
	`|G+q|`
	`|G|`
Default:	"`|G+q|`"
Use:	optional
XPath:	`/input/xs/@gqmaxtype`

69.12 Attribute: lmaxapw

Angular momentum cut-off for the APW functions.

Type:	integer
Default:	"`10`"
Use:	optional
XPath:	`/input/xs/@lmaxapw`

69.13 Attribute: lmaxapwwf

Maximum angular momentum for APW functions for q-dependent matrix elements.

Type:	integer
Default:	"`-1`"
Use:	optional
XPath:	`/input/xs/@lmaxapwwf`

69.14 Attribute: lmaxemat

Maximum angular momentum for Rayleigh expansion of **q**-dependent plane wave factor.

Type:	integer
Default:	"`3`"
Use:	optional
XPath:	`/input/xs/@lmaxemat`

69.15 Attribute: lmaxmat

Angular momentum cut-off for the outer-most loop in the hamiltonian and overlap matrix setup.

Type: integer
Default: "5"
Use: optional
XPath: /input/xs/@lmaxmat

69.16 Attribute: maxscl

Upper limit of the self-consistency loop for the calculation of eigenvectors and eigenvalues from an existing ground-state calculation.

Type: integer
Default: "1"
Use: optional
XPath: /input/xs/@maxscl

69.17 Attribute: nempty

Number of empty states. This parameter determines the energy cutoff for the excitation spectra. For determining the number of states related to an energy cutoff, perform one iteration of a SCF calculation, setting nempty to a higher value and check the EIGVAL.OUT.

Type: integer
Default: "5"
Use: optional
XPath: /input/xs/@nempty

69.18 Attribute: ngridk

k-point grid sizes.

Type: integertriple (114.8)
Default: "1 1 1"
Use: optional
XPath: /input/xs/@ngridk

69.19 Attribute: ngridq

q-point grid sizes.

Type: integertriple (114.8)
Default: "1 1 1"
Use: optional
XPath: /input/xs/@ngridq

69.20 Attribute: nosym

nosym is "true" if no symmetry information should be used

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/xs/@nosym

69.21 Attribute: pwmat

Algorithm for calculating matrix elements of plane waves. Matrix multiplications (mm) are better suited for small systems, while fast Fourier transforms (fft) are appropriate for large systems.

Type:	**choose from:**
	fft
	mm
Default:	"fft"
Use:	optional
XPath:	/input/xs/@pwmat

69.22 Attribute: reducek

reducek is "true" if **k**-points are to be reduced (with crystal symmetries).

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/xs/@reducek

69.23 Attribute: reduceq

reducek is "true" if q-points are to be reduced (with crystal symmetries).

Type:	boolean
Default:	"true"
Use:	optional
XPath:	/input/xs/@reduceq

69.24 Attribute: rgkmax

Smallest muffin-tin radius times gkmax. If set to zero (the default), this value defaults to the rgkmax set in the groundstate element.

Type:	fortrandouble (114.1)
Default:	"0.0d0"

Use: optional
XPath: /input/xs/@rgkmax

69.25 Attribute: scissor

Scissors correction to correct the conduction band energies.

Type: fortrandouble (114.1)
Default: "0.0d0"
Use: optional
Unit: Hartree
XPath: /input/xs/@scissor

69.26 Attribute: skipgnd

If set to "true", recalculation of KS eigenvalues and eigenvectors is skipped.

Type: boolean
Default: "false"
Use: optional
XPath: /input/xs/@skipgnd

69.27 Attribute: swidth

Width of the smooth approximation to the Dirac delta function (must be ¿ 0).

Type: fortrandouble (114.1)
Default: "0.001d0"
Use: optional
Unit: Hartree
XPath: /input/xs/@swidth

69.28 Attribute: tappinfo

"true" to append info to output file.

Type: boolean
Default: "false"
Use: optional
XPath: /input/xs/@tappinfo

69.29 Attribute: tevout

"true" if energy outputs are in eV.

Type: boolean

Default: "`false`"
Use: optional
XPath: `/input/xs/@tevout`

69.30 Attribute: vkloff

The **k**-point set offset. All **k**-points of a regular **k**-mesh (a mesh containing the Gamma point) are shifted by a constant vector given by $(\text{vkloff}_1/N_1, \text{vkloff}_2/N_2, \text{vkloff}_3/N_3)$, where (N_1, N_2, N_3) is the division of the **k**-point mesh. It should be selected such that all symmetries among the **k**-points from the regular (non-shifted) mesh are broken. An exception is the case of optical spectra without local field effects where symmetries among **k**-points are explicitly taken into account.

Type: vect3d (114.6)
Default: "`0.0d0 0.0d0 0.0d0 `"
Use: optional
XPath: `/input/xs/@vkloff`

69.31 Attribute: writexsgrids

"`true`" to write out k, k+q, g, g+k, g+q grids to file.

Type: boolean
Default: "`false`"
Use: optional
XPath: `/input/xs/@writexsgrids`

69.32 Attribute: xstype

Should TDDFT be used or BSE.

Type: **choose from:**
`TDDFT`
`BSE`
Use: required
XPath: `/input/xs/@xstype`

70 Element: storeexcitons

When present this element allows to store the exciton components (BSE eigenvectors). The number of stored excitons starting from the lowest energy one is given by the attribute `MaxNumberExcitons`.

Type: no content
XPath: `/input/xs/storeexcitons`

This element allows for specification of the following attributes:

MaxEnergyExcitons, MaxNumberExcitons, MinEnergyExcitons, MinNumberExcitons, selectenergy, useev

70.1 Attribute: MaxEnergyExcitons

Upper limit of the energy interval for the stored excitons.

Type: fortrandouble (114.1)
Default: "100.0"
Use: optional
XPath: /input/xs/storeexcitons/@MaxEnergyExcitons

70.2 Attribute: MaxNumberExcitons

It represents the upper limit of the number of stored excitons.

Type: integer
Default: "10"
Use: optional
XPath: /input/xs/storeexcitons/@MaxNumberExcitons

70.3 Attribute: MinEnergyExcitons

Lower limit of the energy interval for the stored excitons.

Type: fortrandouble (114.1)
Default: "0.0"
Use: optional
XPath: /input/xs/storeexcitons/@MinEnergyExcitons

70.4 Attribute: MinNumberExcitons

It represents the lower limit of the number of stored excitons.

Type: integer
Default: "1"
Use: optional
XPath: /input/xs/storeexcitons/@MinNumberExcitons

70.5 Attribute: selectenergy

Set to "true" if excitons within a specified energy interval shall be stored.

Type: boolean
Default: "false"

Use: optional
XPath: /input/xs/storeexcitons/@selectenergy

70.6 Attribute: useev

"true" if energy input is in eV.

Type: boolean
Default: "true"
Use: optional
XPath: /input/xs/storeexcitons/@useev

71 Element: writeexcitons

When present this element allows to write the stored exciton components (BSE eigenvectors) to ASCII files. The range of excitons must lie within the stored range given by the attributes in the element storeexcitons.

Type: no content
XPath: /input/xs/writeexcitons

This element allows for specification of the following attributes:

MaxEnergyExcitons, MaxNumberExcitons, MinEnergyExcitons, MinNumberExcitons, abscutares, abscutres, selectenergy, useev

71.1 Attribute: MaxEnergyExcitons

Upper limit of the energy interval of the written excitons.

Type: fortrandouble (114.1)
Default: "100.0"
Use: optional
XPath: /input/xs/writeexcitons/@MaxEnergyExcitons

71.2 Attribute: MaxNumberExcitons

It represents the upper limit of the number of written excitons.

Type: integer
Default: "10"
Use: optional
XPath: /input/xs/writeexcitons/@MaxNumberExcitons

71.3 Attribute: MinEnergyExcitons

Lower limit of the energy interval of the written excitons.

Type:	fortrandouble (114.1)
Default:	"0.0"
Use:	optional
XPath:	/input/xs/writeexcitons/@MinEnergyExcitons

71.4 Attribute: MinNumberExcitons

It represents the lower limit of the number of written excitons.

Type:	integer
Default:	"1"
Use:	optional
XPath:	/input/xs/writeexcitons/@MinNumberExcitons

71.5 Attribute: abscutares

Cutoff interval for exciton eigenvector writeout (anit-resonant).

Type:	vect2d (114.7)
Default:	"0.0d0 1.0d10"
Use:	optional
XPath:	/input/xs/writeexcitons/@abscutares

71.6 Attribute: abscutres

Cutoff interval for exciton eigenvector writeout (resonant).

Type:	vect2d (114.7)
Default:	"0.0d0 1.0d10"
Use:	optional
XPath:	/input/xs/writeexcitons/@abscutres

71.7 Attribute: selectenergy

Set to "true" if excitons within a specified energy interval shall written.

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/xs/writeexcitons/@selectenergy

71.8 Attribute: useev

"true" if energy input is in eV.

Type:	boolean
Default:	"true"
Use:	optional
XPath:	/input/xs/writeexcitons/@useev

72 Element: writekpathweights

This element configures the interpolation of the excitonic weights onto a banstructure path performend by the writekpathweights task.

Type:	no content
XPath:	/input/xs/writekpathweights

This element allows for specification of the following attributes:

MaxEnergyExcitons, MaxNumberExcitons, MinEnergyExcitons, MinNumberExcitons, intorder, printgridweights, selectenergy, useev

72.1 Attribute: MaxEnergyExcitons

Upper limit of the energy interval of the written excitons.

Type:	fortrandouble (114.1)
Default:	"100.0"
Use:	optional
XPath:	/input/xs/writekpathweights/@MaxEnergyExcitons

72.2 Attribute: MaxNumberExcitons

It represents the upper limit of the number of written excitons.

Type:	integer
Default:	"1"
Use:	optional
XPath:	/input/xs/writekpathweights/@MaxNumberExcitons

72.3 Attribute: MinEnergyExcitons

Lower limit of the energy interval of the written excitons.

Type:	fortrandouble (114.1)
Default:	"0.0"

Use: optional
XPath: /input/xs/writekpathweights/@MinEnergyExcitons

72.4 Attribute: MinNumberExcitons

It represents the lower limit of the number of written excitons.

Type: integer
Default: "1"
Use: optional
XPath: /input/xs/writekpathweights/@MinNumberExcitons

72.5 Attribute: intorder

Spline order for the interpolation of the excitonic weights (polynomial order + 1).

Type: integer
Default: "2"
Use: optional
XPath: /input/xs/writekpathweights/@intorder

72.6 Attribute: printgridweights

"true" if the excitonic weights on the k-grid shall be printed to file.

Type: boolean
Default: "true"
Use: optional
XPath: /input/xs/writekpathweights/@printgridweights

72.7 Attribute: selectenergy

Set to "true" if excitons within a specified energy interval shall be considered.

Type: boolean
Default: "false"
Use: optional
XPath: /input/xs/writekpathweights/@selectenergy

72.8 Attribute: useev

"true" if energy input is in eV.

Type: boolean
Default: "true"

Use: optional
XPath: /input/xs/writekpathweights/@useev

73 Element: excitonPlot

Parameters for the electron-hole visualization.

Contains: exciton (zero or more)
hole (1 times)
electron (1 times)
XPath: /input/xs/excitonPlot

This element allows for specification of the following attributes:

epstol

73.1 Attribute: epstol

Threshold value for selecting states which contribute to the exciton.

Type: fortrandouble (114.1)
Default: "1.0d-4"
Use: optional
XPath: /input/xs/excitonPlot/@epstol

74 Element: exciton

Electron-hole pair descriptor.

Type: no content
XPath: /input/xs/excitonPlot/exciton

This element allows for specification of the following attributes:

fix, lambda

74.1 Attribute: fix

Fix position (in lattice coordinates) either of the "hole" or "electron".

Type: string
Default: "hole"
Use: optional
XPath: /input/xs/excitonPlot/exciton/@fix

74.2 Attribute: lambda

The index of the stored exciton.

Type:	integer
Default:	"1"
Use:	optional
XPath:	/input/xs/excitonPlot/exciton/@lambda

75 Element: hole

For the exciton wavefunction visualization: Real space grid for the hole distribution.

Contains:	plot1d (optional) plot2d (optional) plot3d (optional)
XPath:	/input/xs/excitonPlot/hole

76 Element: electron

For the exciton wavefunction visualization: Real space grid for the electron distribution.

Contains:	plot1d (optional) plot2d (optional) plot3d (optional)
XPath:	/input/xs/excitonPlot/electron

77 Element: tddft

Type:	no content
XPath:	/input/xs/tddft

This element allows for specification of the following attributes:

acont, ahc, alphalrc, alphalrcdyn, aresdf, aresfxc, betalrcdyn, do, drude, fxcbsesplit, fxctype, intraband, kerndiag, lindhard, lmaxalda, mdfqtype, nwacont, torddf, tordfxc

77.1 Attribute: acont

Set to "true" if analytic continuation from the imaginary axis to the real axis is to be performed.

Type: boolean
Default: "`false`"
Use: optional
XPath: `/input/xs/tddft/@acont`

77.2 Attribute: ahc

By setting it to "`true`", the anomalous Hall conductivity (AHC) term is included in the calculation of the dielectric tensor [see PRB 86, 125139 (2012)]. In this case, the MOKE.OUT output file is generated, containing the MOKE spectrum. This attribute only has effect when local field effects are neglected (gqmax=0) and q=0.

Type: boolean
Default: "`false`"
Use: optional
XPath: `/input/xs/tddft/@ahc`

77.3 Attribute: alphalrc

α-parameter for the static long range contribution (LRC) model xc kernel.

Type: fortrandouble (114.1)
Default: "`0.0d0`"
Use: optional
XPath: `/input/xs/tddft/@alphalrc`

77.4 Attribute: alphalrcdyn

α-parameter for the dynamical long range contribution (LRC) model xc kernel.

Type: fortrandouble (114.1)
Default: "`0.0d0`"
Use: optional
XPath: `/input/xs/tddft/@alphalrcdyn`

77.5 Attribute: aresdf

Set to "`true`" if to consider the anti-resonant part for the dielectric function.

Type: boolean
Default: "`true`"
Use: optional
XPath: `/input/xs/tddft/@aresdf`

77.6 Attribute: aresfxc

Set to "true" if to consider the anti-resonant part for the MBPT derived xc-kernels.

Type: boolean
Default: "true"
Use: optional
XPath: /input/xs/tddft/@aresfxc

77.7 Attribute: betalrcdyn

β-parameter for the dynamical long range contribution (LRC) model xc kernel.

Type: fortrandouble (114.1)
Use: optional
XPath: /input/xs/tddft/@betalrcdyn

77.8 Attribute: do

Decides if the TDDFT calculation is to be resumed starting from a new xc kernel or is to be skipped.

Type: **choose from:**
fromscratch
fromkernel
Default: "fromscratch"
Use: optional
XPath: /input/xs/tddft/@do

77.9 Attribute: drude

Parameters defining semiclassical Drude approximation to intraband term. The first value determines the plasma frequency ω_p and the second the inverse relaxation time ω_τ:$\chi_0^D = \frac{1}{\omega}\frac{\omega_p^2}{\omega+i\omega_\tau}$

Type: vect2d (114.7)
Default: "0.0d0 0.0d0"
Use: optional
XPath: /input/xs/tddft/@drude

77.10 Attribute: fxcbsesplit

Split parameter for degeneracy in energy differences of MBPT derived xc kernels. See A. Marini, Phys. Rev. Lett., 91, (2003) 256402.

Type: fortrandouble (114.1)

Default: "1.0d-5"
Use: optional
Unit: Hartree
XPath: /input/xs/tddft/@fxcbsesplit

77.11 Attribute: fxctype

Defines which xc kernel is to be used. Examples on the use of the different kernels can be found online on the Tutorial "TDDFT Calculations with Different Kernels" on www.exciting-code.org. In the options indicated below, if the suffix "_NLF" is present, then local-field effects are neglected (scalar kernel). Otherwise the kernel is a matrix of the size of the number of **G**-vectors, whose diagonal elements are all equal. The available kernels f_{xc} are:

- "RPA" - Random-phase approximation kernel. $f_{xc} = 0$
- "LRCstatic[_NLF]" - Long-range correction kernel.

$$f_{xc} = -\frac{\alpha}{\mathbf{q}^2}. \tag{12}$$

  See S. Botti et al., Phys. Rev. B 69, 155112 (2004)

- "LRCdyn[_NLF]" - Dynamical long-range correction kernel.

$$f_{xc} = -\frac{\alpha + \beta\omega^2}{\mathbf{q}^2} \tag{13}$$

  with α given by the value of alphalrcdyn and β given by the value of betalrcdyn. See S. Botti et al., Phys. Rev. B 72, 125203 (2005)

- "ALDA" - Adiabatic LDA kernel.

$$f_{xc}(\mathbf{r}, \mathbf{r}', t - t') = \frac{\delta V_{xc}(\mathbf{r})}{\delta n(\mathbf{r}')}\delta(t - t'). \tag{14}$$

  In this implementation, $V_{xc}(\mathbf{r})$ is the spin-unpolarised exchange-correlation potential corresponding to the Perdew-Wang parameterisation of Ceperley-Alder's Monte-Carlo data (see Phys. Rev. B 45, 13244 (1992) and Phys. Rev. Lett. 45, 566 (1980)).

- "MB1[_NLF]" - BSE derived xc kernel. See L. Reining et al., Phys. Rev. Lett. 88, 066404 (2002) and A. Marini et al., Phys. Rev. Lett. 91, 256402 (2003).

- "BO" - Bootstrap kernel.

$$f_{xc} = \frac{\varepsilon^{-1}(\omega = 0)}{\chi_{00}(\omega = 0)}. \tag{15}$$

  See S. Sharma et al., Phys. Rev. Lett. 107, 186401 (2011).

- "BO_SCALAR" - Scalar version of the bootstrap kernel. $f_{xc} = [\varepsilon_M(\omega = 0)\chi_{00}(\omega = 0)]^{-1}$. See S. Sharma et al., Phys. Rev. Lett. 107, 186401 (2011).
- "RBO" - RPA bootstrap kernel. $f_{xc} = \left[\varepsilon_M^{RPA}(\omega = 0)\overline{\chi}_{00}^{RPA}(\omega = 0)\right]^{-1}$. See S. Rigamonti et al., Phys. Rev. Lett. 114, 146402 (2015).

Type:	**choose from:**
	RPA
	LRCstatic_NLF
	LRCstatic
	LRCdyn_NLF
	LRCdyn
	ALDA
	MB1_NLF
	MB1
	BO
	BO_SCALAR
	RBO
Default:	"RPA"
Use:	optional
XPath:	/input/xs/tddft/@fxctype

77.12 Attribute: intraband

By setting it to "true", the intraband contribution is included in the calculation for the finite q.

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/xs/screening/@intraband

77.13 Attribute: kerndiag

Set to "true" if only diagonal part of xc-kernel is to be used.

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/xs/tddft/@kerndiag

77.14 Attribute: lindhard

Set to "true" if Lindhard-like function is to be calculated.

Type:	boolean

Default: "false"
Use: optional
XPath: /input/xs/tddft/@lindhard

77.15 Attribute: lmaxalda

Angular momentum cutoff for Rayleigh expansion of exponential factor for ALDA-kernel.

Type: integer
Default: "3"
Use: optional
XPath: /input/xs/tddft/@lmaxalda

77.16 Attribute: mdfqtype

Treatment of macroscopic dielectric function for $\mathbf{Q}$-point outside of Brillouin zone. A value of 0 uses the full $\mathbf{Q}$ and the $(\mathbf{0},\mathbf{0})$ component of the microscopic dielectric matrix is used. A value of 1 invokes a decomposition $\mathbf{Q}=\mathbf{q}+\mathbf{G}_\mathbf{q}$ and the $(\mathbf{Q}_\mathbf{q},\mathbf{Q}_\mathbf{q})$ component of the microscopic dielectric matrix is used.

Type: integer
Default: "0"
Use: optional
XPath: /input/xs/tddft/@mdfqtype

77.17 Attribute: nwacont

Number of energy intervals (on imaginary axis) for analytic continuation.

Type: integer
Default: "0"
Use: optional
XPath: /input/xs/tddft/@nwacont

77.18 Attribute: torddf

Set to "true" if to consider the time-ordered version of the dielectric function.

Type: boolean
Default: "false"
Use: optional
XPath: /input/xs/tddft/@torddf

77.19 Attribute: tordfxc

Set to "true" if to consider the time-ordered version of xc kernel (MBPT derived kernels only).

Type: boolean
Default: "false"
Use: optional
XPath: /input/xs/tddft/@tordfxc

78 Element: screening

Type: no content
XPath: /input/xs/screening

This element allows for specification of the following attributes:

do, intraband, nempty, ngridk, nosym, reducek, rgkmax, screentype, tr, vkloff

78.1 Attribute: do

Decides if the calculation of the screening is done from scratch or is to be skipped.

Type: **choose from:**
fromscratch
skip
Default: "fromscratch"
Use: optional
XPath: /input/xs/screening/@do

78.2 Attribute: intraband

Set to "false" to not use transition between states at same n but different k. Note: If the unit cell used in the calculation is not primitive, the n index does not corresponds to then physical band index due to the umklapp process at the cell boundaries.

Type: boolean
Default: "false"
Use: optional
XPath: /input/xs/screening/@intraband

78.3 Attribute: nempty

Number of empty states.

Type:	integer
Default:	"0"
Use:	optional
XPath:	/input/xs/screening/@nempty

78.4 Attribute: ngridk

k-point grid sizes for screening.

Type:	integertriple (114.8)
Default:	"0 0 0"
Use:	optional
XPath:	/input/xs/screening/@ngridk

78.5 Attribute: nosym

nosym is "true" if no symmetry information should be used for screening.

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/xs/screening/@nosym

78.6 Attribute: reducek

reducek is "true" if **k**-points are to be reduced with crystal symmetries for screening.

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/xs/screening/@reducek

78.7 Attribute: rgkmax

The smallest muffin-tin radius times gkmax for screening.

Type:	fortrandouble (114.1)
Default:	"0.0d0"
Use:	optional
XPath:	/input/xs/screening/@rgkmax

78.8 Attribute: screentype

Defines which type of screening is to be used.

Type:	**choose from:**
	`full`
	`diag`
	`noinvdiag`
	`longrange`
Default:	"`full`"
Use:	optional
XPath:	`/input/xs/screening/@screentype`

78.9 Attribute: tr

`tr` is `"true"` if the time reversal symmetry is used to equate the anit-resonant with the resonant part of Chi0 in the case of static screening without broadening.

Type:	boolean
Default:	"`true`"
Use:	optional
XPath:	`/input/xs/screening/@tr`

78.10 Attribute: vkloff

k-point offset for screening.

Type:	vect3d (114.6)
Default:	"`-1.0d0 -1.0d0 -1.0d0`"
Use:	optional
XPath:	`/input/xs/screening/@vkloff`

79 Element: BSE

Type:	no content
XPath:	`/input/xs/BSE`

This element allows for specification of the following attributes:

`aresbse`, `blocks`, `bsedirsing`, `bsetype`, `checkposdef`, `chibarq`, `coupling`, `cuttype`, `distribute`, `econv`, `eecs`, `efind`, `fbzq`, `iqmtrange`, `lmaxdielt`, `measure`, `nexc`, `ngridksub`, `nleblaik`, `nosym`, `nstlbse`, `nstlxas`, `outputlevel`, `reducek`, `rgkmax`, `sciavbd`, `sciavqbd`, `sciavqhd`, `sciavqwg`, `sciavtype`, `scrherm`, `vkloff`, `xas`, `xasatom`, `xasedge`, `xasspecies`

79.1 Attribute: aresbse

Is set to "true" if to consider the anti-resonant part for the BSE spectrum.

Type:	boolean
Default:	"true"
Use:	optional
XPath:	/input/xs/BSE/@aresbse

79.2 Attribute: blocks

Defines which blocks of the BSE Hamiltonian are to be set up (resonant-resonat, resonant-anti-resonant or both).

Type:	**choose from:**
	rr
	ra
	both
Default:	"both"
Use:	optional
XPath:	/input/xs/BSE/@blocks

79.3 Attribute: bsedirsing

"true" if effective singular part of direct term of BSE Hamiltonian is to be used.

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/xs/BSE/@bsedirsing

79.4 Attribute: bsetype

Defines which parts of the BSE Hamiltonian are to be considered.

Type:	**choose from:**
	IP
	RPA
	singlet
	triplet
Default:	"singlet"
Use:	optional
XPath:	/input/xs/BSE/@bsetype

79.5 Attribute: checkposdef

Set to "true" to check positive definitness of the auxilliary matrix used in BSE+TI.

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/xs/BSE/@checkposdef

79.6 Attribute: chibarq

Set to "true" to use the modified $\bar{\chi}$ also for finite q.

Type:	boolean
Default:	"true"
Use:	optional
XPath:	/input/xs/BSE/@chibarq

79.7 Attribute: coupling

Set to "true" to perform BSE without Tamm-Dancoff approximation.

Type:	boolean
Default:	"false"
Use:	optional
XPath:	/input/xs/BSE/@coupling

79.8 Attribute: cuttype

Defines how the Coulomb potential is to be truncated. Used for lower dimentional systems.

Type:	**choose from:**
	none
	0d
	2d
Default:	"none"
Use:	optional
XPath:	/input/xs/BSE/@cuttype

79.9 Attribute: distribute

Use ScaLAPACK or not.

Type:	boolean
Default:	"false"

Use: optional
XPath: /input/xs/BSE/@distribute

79.10 Attribute: econv

Additional energy for KS transitions to be included in the construction of the BSE hamiltoninan. Spectrum for a desired energy window needs to be converged with respect to this parameter. First/second entry is convergence energy for the lower/upper end of the spectrum.

Type: vect2d (114.7)
Default: "0.0d0 0.0d0"
Use: optional
XPath: /input/xs/BSE/@econv

79.11 Attribute: eecs

Estimated BSE eigenvalue cluster size.

Type: integer
Default: "3"
Use: optional
XPath: /input/xs/BSE/@eecs

79.12 Attribute: efind

Set to "true" to solve the BSE Hamiltonian only for needed solutions with respect to desired energy window.

Type: boolean
Default: "false"
Use: optional
XPath: /input/xs/BSE/@efind

79.13 Attribute: fbzq

Set to "true" if q-point set is to be taken from the first Brillouin zone.

Type: boolean
Default: "false"
Use: optional
XPath: /input/xs/BSE/@fbzq

79.14 Attribute: iqmtrange

For which points in the q-point list should the BSE Matrix be constructed. A value of iqmtrange(1)=-1 uses all listed Q-points.

Type: integerpair (114.10)
Default: "1 1"
Use: optional
XPath: /input/xs/BSE/@iqmtrange

79.15 Attribute: lmaxdielt

Angular momentum cutoff of the spherical harmonics expansion of the dielectric matrix.

Type: integer
Default: "14"
Use: optional
XPath: /input/xs/BSE/@lmaxdielt

79.16 Attribute: measure

Set to "true" to write out measures for the resonant-anti-resonat coupling.

Type: boolean
Default: "false"
Use: optional
XPath: /input/xs/BSE/@measure

79.17 Attribute: nexc

Number of excitons (eigensolutions) to be considered in a BSE calculation. The default corresponds to all.

Type: integer
Default: "-1"
Use: optional
XPath: /input/xs/BSE/@nexc

79.18 Attribute: ngridksub

The sub-grid of a BSE double grid run. Any value larger than 1 triggers a computation following this scheme: the BSE is solved several times on coarse grids, as given by ngridk and ngridq, which are shifted to all symmetry non-equivalent points of the sub-grid. The latter are distributed uniformly between the k-points of the coarse grid. The final results are obtained by averaging all the spectra yielded in this way, what is expected to be almost as good as solving

the BSE on the fine grid, at much less computational cost.

Type: integertriple (114.8)
Default: "1 1 1"
Use: optional
XPath: /input/xs/BSE/@ngridksub

79.19 Attribute: nleblaik

Number of points used for the Lebedev-Laikov grids must be selected according to V.I. Lebedev, and D.N. Laikov, Doklady Mathematics, 59 (1999) 477.

Type: integer
Default: "5810"
Use: optional
XPath: /input/xs/BSE/@nleblaik

79.20 Attribute: nosym

Set to "true" if no symmetry information should be used for BSE.

Type: boolean
Default: "false"
Use: optional
XPath: /input/xs/BSE/@nosym

79.21 Attribute: nstlbse

Range of bands included for the BSE calculation. The first pair of numbers corresponds to the band index for local orbitals and valence states (counted from the lowest eigenenergy), the second pair corresponds to the band index of the conduction states (counted from the Fermi level).

Type: integerquadrupel (114.9)
Default: "0 0 0 0"
Use: optional
XPath: /input/xs/BSE/@nstlbse

79.22 Attribute: nstlxas

Range of bands included for the BSE calculation. The pair corresponds to the band index of the conduction states (counted from the Fermi level).

Type: integerpair (114.10)
Default: "0 0"
Use: optional
XPath: /input/xs/BSE/@nstlxas

79.23 Attribute: outputlevel

Specify amount of information which is printed to files:

- normal - (default) standard information
- exper - detailed output

Type:	**choose from:**
	`normal`
	`expert`
Default:	"`normal`"
Use:	optional
XPath:	`/input/xs/BSE/@outputlevel`

79.24 Attribute: reducek

`reducek` is "`true`" if **k**-points are to be reduced with crystal symmetries for BSE.

Type:	boolean
Default:	"`false`"
Use:	optional
XPath:	`/input/xs/BSE/@reducek`

79.25 Attribute: rgkmax

Smallest muffin-tin radius times `gkmax`.

Type:	fortrandouble (114.1)
Default:	"`0.0d0`"
Use:	optional
XPath:	`/input/xs/BSE/@rgkmax`

79.26 Attribute: sciavbd

"`true`" if the body of the screened Coulomb interaction is to be averaged (q=0).

Type:	boolean
Default:	"`true`"
Use:	optional
XPath:	`/input/xs/BSE/@sciavbd`

79.27 Attribute: sciavqbd

"`true`" if the body of the screened Coulomb interaction is to be averaged (q!=0).

Type: boolean
Default: "false"
Use: optional
XPath: /input/xs/BSE/@sciavqbd

79.28 Attribute: sciavqhd

"true" if the head of the screened Coulomb interaction is to be averaged (q!=0).

Type: boolean
Default: "false"
Use: optional
XPath: /input/xs/BSE/@sciavqhd

79.29 Attribute: sciavqwg

"true" if the wings of the screened Coulomb interaction are to be averaged (q!=0).

Type: boolean
Default: "false"
Use: optional
XPath: /input/xs/BSE/@sciavqwg

79.30 Attribute: sciavtype

Defines how the screened Coulomb interaction matrix is to be averaged (important for the singular terms).

Type: **choose from:**
spherical
screendiag
invscreendiag
Default: "spherical"
Use: optional
XPath: /input/xs/BSE/@sciavtype

79.31 Attribute: scrherm

Method of how an almost Hermitian matrix is inverted. A value of 0: invert full matrix (matrix is allowed to be not strictly Hermitian); a value of 1: take the Hermitian average for inversion; a value of 2: assume Hermitian and use the upper triangle; a value of 3: assume Hermitian and use the lower triangle.

Type: integer
Default: "0"

Use: optional
XPath: /input/xs/BSE/@scrherm

79.32 Attribute: vkloff

k-point offset for BSE.

Type: vect3d (114.6)
Default: "-1.0d0 -1.0d0 -1.0d0"
Use: optional
XPath: /input/xs/BSE/@vkloff

79.33 Attribute: xas

Set to "true" to perform BSE X-rasy absorption spectroscopy (XAS) calculation

Type: boolean
Default: "false"
Use: optional
XPath: /input/xs/BSE/@xas

79.34 Attribute: xasatom

Atom number for which the XAS is calculated.

Type: integer
Default: "0"
Use: optional
XPath: /input/xs/BSE/@xasatom

79.35 Attribute: xasedge

Defines the initial states of the XAS calculation.

Type: **choose from:**
K
L1
L2
L3
L23
M1
M2
M3
M23
M4

M5
M45
Default: "K"
Use: optional
XPath: /input/xs/BSE/@xasedge

79.36 Attribute: xasspecies

Species number for which the XAS is calculated.

Type: integer
Default: "0"
Use: optional
XPath: /input/xs/BSE/@xasspecies

80 Element: transitions

Describe transitions between Kohn-Sham states for the calculation of the Kohn-Sham response function (and screening) here. Individual transitions as well as a range (or a list) of initial and final states can be defined.

Contains: individual (optional)
ranges (optional)
lists (optional)
XPath: /input/xs/transitions

81 Element: individual

A list of individual transitions consisting of an initial state a final state and a **k**-point is given here. If the list is empty, no transitions are considered.

Contains: trans (zero or more)
XPath: /input/xs/transitions/individual

82 Element: trans

An individual transition consisting of an initial state a final state and a **k**-point is given here. Values of zero correspond to the inclusion of all initial and final states and all **k**-points and can be used as "wildcards" (default). Therefore, an empty element amounts to include all transitions.

Type: no content
XPath: /input/xs/transitions/individual/trans

This element allows for specification of the following attributes:

`action`, `final`, `initial`, `kpointnumber`

82.1 Attribute: action

Select to include or exclude states. If a state is included as well as excluded several times the last definition (in the sequence of individual transitions) counts.

Type:	**choose from:**
	`include`
	`exclude`
Default:	"`include`"
Use:	optional
XPath:	`/input/xs/transitions/individual/trans/@action`

82.2 Attribute: final

Final state of individual transition. A value of zero (default) means to include all states.

Type:	integer
Default:	"`0`"
Use:	optional
XPath:	`/input/xs/transitions/individual/trans/@final`

82.3 Attribute: initial

Initial state of individual transition. A value of zero (default) means to include all states.

Type:	integer
Default:	"`0`"
Use:	optional
XPath:	`/input/xs/transitions/individual/trans/@initial`

82.4 Attribute: kpointnumber

Number of **k**-points to be considered. A value of zero (default) means to include all **k**-points.

Type:	integer
Default:	"`0`"
Use:	optional
XPath:	`/input/xs/transitions/individual/trans/@kpointnumber`

83 Element: ranges

A list of ranges of transitions (initial state as well as final state ranges) and a **k**-point are given here. An empty list amounts to no transitions at all.

Contains: range (zero or more)
XPath: /input/xs/transitions/ranges

84 Element: range

A range of transitions (for initial as well as final states) is given here. A range consists of a "start" and a "stop" values as well as a **k**-point. Values of zero correspond to starting at the first state and stopping at the last state and considering all **k**-points. They can be used as "wildcards" (default). Therefore, an empty element corresponds to the full initial/final state range for all **k**-points.

Type: no content
XPath: /input/xs/transitions/ranges/range

This element allows for specification of the following attributes:

statestype (required), action, kpointnumber, start, stop

84.1 Attribute: action

Select to include or exclude states. If a state is included as well as excluded several times the last definition (in the sequence of individual transitions) counts.

Type: **choose from:**
include
exclude
Default: "include"
Use: optional
XPath: /input/xs/transitions/ranges/range/@action

84.2 Attribute: kpointnumber

Number of **k**-point to be considered. A value of zero (default) means to include all **k**-point.

Type: integer
Default: "0"
Use: optional
XPath: /input/xs/transitions/ranges/range/@kpointnumber

84.3 Attribute: start

Start value (first state) for range. A value of zero (default) means to start from the first state.

Type: integer
Default: "0"
Use: optional
XPath: /input/xs/transitions/ranges/range/@start

84.4 Attribute: statestype

Select for initial or final state range.

Type: **choose from:**
initialstates
finalstates
Use: required
XPath: /input/xs/transitions/ranges/range/@statestype

84.5 Attribute: stop

Stop value (last state) for range. A value of zero (default) means to stop at the last state (no upper limit).

Type: integer
Default: "0"
Use: optional
XPath: /input/xs/transitions/ranges/range/@stop

85 Element: lists

A list of initial and final state entries to be considered for transitions. An empty list amounts to no transitions at all.

Contains: istate (zero or more)
XPath: /input/xs/transitions/lists

86 Element: istate

An initial or final state and corresponding **k**-point is given here. Values of zero correspond to considering all initial/final states for all **k**-points. They can be used as "wildcards" (default). Therefore, an empty element corresponds to the full initial/final state set for all **k**-points.

Type: no content

XPath: /input/xs/transitions/lists/istate

This element allows for specification of the following attributes:

statestype (required), action, kpointnumber, state

86.1 Attribute: action

Select to include or exclude states. If a state is included as well as excluded several times the last definition (in the sequence of individual transitions) counts.

Type:	**choose from:**
	include
	exclude
Default:	"include"
Use:	optional
XPath:	/input/xs/transitions/lists/istate/@action

86.2 Attribute: kpointnumber

Number of **k**-point to be consider. A value of zero (default) means to include all **k**-point.

Type:	integer
Default:	"0"
Use:	optional
XPath:	/input/xs/transitions/lists/istate/@kpointnumber

86.3 Attribute: state

The state to be considered. A value of zero (default) means to include all states.

Type:	integer
Default:	"0"
Use:	optional
XPath:	/input/xs/transitions/lists/istate/@state

86.4 Attribute: statestype

Select for initial or final state list.

Type:	**choose from:**
	initialstates
	finalstates
Use:	required
XPath:	/input/xs/transitions/lists/istate/@statestype

87 Element: tetra

Type: no content
XPath: /input/xs/tetra

This element allows for specification of the following attributes:

cw1k, kordexc, qweights, tetradf, tetraocc

87.1 Attribute: cw1k

Type: boolean
Default: "false"
Use: optional
XPath: /input/xs/tetra/@cw1k

87.2 Attribute: kordexc

Type: boolean
Default: "false"
Use: optional
XPath: /input/xs/tetra/@kordexc

87.3 Attribute: qweights

Choice of weights and nodes for the tetrahedron method and non-zero Q-point.

Type: integer
Default: "1"
Use: optional
XPath: /input/xs/tetra/@qweights

87.4 Attribute: tetradf

"true" if tetrahedron method is used for the **k**-space integration in the Kohn-Sham response function.

Type: boolean
Default: "false"
Use: optional
XPath: /input/xs/tetra/@tetradf

87.5 Attribute: tetraocc

Type: boolean
Default: "false"
Use: optional
XPath: /input/xs/tetra/@tetraocc

88 Element: plan

Contains: doonly (zero or more)
XPath: /input/xs/plan

89 Element: doonly

Type: no content
XPath: /input/xs/plan/doonly

This element allows for specification of the following attributes:

task (required)

89.1 Attribute: task

Type: **choose from:**
xsgeneigvec
tetcalccw
writepmatxs
writeemat
df
df2
idf
scrgeneigvec
scrtetcalccw
scrwritepmat
screen
scrcoulint
exccoulint
bse
bsegenspec
writeexcitons
writekpathweights
bsesurvey
kernxc_bse
writebandgapgrid
writepmat

dielectric
writepmatasc
pmatxs2orig
writeematasc
writepwmat
emattest
x0toasc
x0tobin
fxc_alda_check
kernxc_bse3
testxs
xsestimate
xstiming
testmain
excitonWavefunction
portstate(1)
portstate(2)
portstate(-1)
portstate(-2)

Use: required
XPath: /input/xs/plan/doonly/@task

90 Element: gw

G0W0 calculation setup.

Contains: plot1d
freqgrid (optional)
selfenergy (optional)
mixbasis (optional)
barecoul (optional)
scrcoul (optional)
XPath: /input/gw

This element allows for specification of the following attributes:

at1, at2, coreflag, debug, ibgw, ibmax, ibmax2, ibmin, ibmin2, igmax, igmin, iik, jjk, nbgw, nempty, ngridq, reduceq, rmax, rpath, rpmat, skipgnd, taskname, vqloff

90.1 Attribute: at1

First atom number (for test only)

Type: integer
Default: "1"

Use: optional
XPath: /input/gw/@at1

90.2 Attribute: at2

Second atom number (for test only).

Type: integer
Default: "1"
Use: optional
XPath: /input/gw/@at2

90.3 Attribute: coreflag

Option for treating core. Valid options are:

- all - All electron calculation
- val - Valence electron only calculation
- vab - Core electrons are excluded from the mixed product basis
- xal - All electron treatment of the exchange self-energy only

Type: string
Default: "all"
Use: optional
XPath: /input/gw/@coreflag

90.4 Attribute: debug

Print debugging information.

Type: boolean
Default: "false"
Use: optional
XPath: /input/gw/@debug

90.5 Attribute: ibgw

Lower band index for GW output.

Type: integer
Default: "1"
Use: optional
XPath: /input/gw/@ibgw

90.6 Attribute: ibmax

Upper bound for the band number (for test only).

Type: integer
Default: "1"
Use: optional
XPath: /input/gw/@ibmax

90.7 Attribute: ibmax2

Upper bound for the band number (for test only).

Type: integer
Default: "1"
Use: optional
XPath: /input/gw/@ibmax2

90.8 Attribute: ibmin

Lower bound for the band number (for test only).

Type: integer
Default: "1"
Use: optional
XPath: /input/gw/@ibmin

90.9 Attribute: ibmin2

Lower bound for the band number (for test only).

Type: integer
Default: "1"
Use: optional
XPath: /input/gw/@ibmin2

90.10 Attribute: igmax

Upper bound for the G-vector number (for test only).

Type: integer
Default: "1"
Use: optional
XPath: /input/gw/@igmax

90.11 Attribute: igmin

Lower bound for the G-vector number (for test only).

Type: integer
Default: "1"
Use: optional
XPath: /input/gw/@igmin

90.12 Attribute: iik

Lower bound for the k-point number (for test only).

Type: integer
Default: "1"
Use: optional
XPath: /input/gw/@iik

90.13 Attribute: jjk

Upper bound for the k-point number (for test only).

Type: integer
Default: "1"
Use: optional
XPath: /input/gw/@jjk

90.14 Attribute: nbgw

Upper band index for GW output. If not specified, the maximum number of the available states is used.

Type: integer
Default: "0"
Use: optional
XPath: /input/gw/@nbgw

90.15 Attribute: nempty

Number of empty states (cutoff parameter) used in GW. If not specified, the same number as for the groundstate calculations is used.

Type: integer
Default: "0"
Use: optional
XPath: /input/gw/@nempty

90.16 Attribute: ngridq

k/q-point grid size to be used in GW calculations. If not specified, (2,2,2) k-grid is used.

Type: integertriple (114.8)
Default: "0 0 0"
Use: optional
XPath: /input/gw/@ngridq

90.17 Attribute: reduceq

Use the crystal symmetry to calculate the dielectric function and perform q-point BZ integration (currently is not implemented).

Type: boolean
Default: "false"
Use: optional
XPath: /input/gw/@reduceq

90.18 Attribute: rmax

Determine the basis size for the Fourier-series based interpolation subroutine used for the QP bandstructure plot.

Type: fortrandouble (114.1)
Default: "40.0"
Use: optional
XPath: /input/gw/@rmax

90.19 Attribute: rpath

Type of the 1d real space path: "atoms" - connecting atoms specified in at1 and at2; "rad" - radial grid path in MT of at1; "azi" - azimuthal path in MT of at1.

Type: string
Default: "atoms"
Use: optional
XPath: /input/gw/@rpath

90.20 Attribute: rpmat

Skip calculation of the momentum matrix elements but read them from files PMATVV.OUT and PMATCV.OUT.

Type: boolean

Default: "false"
Use: optional
XPath: /input/gw/@rpmat

90.21 Attribute: skipgnd

Skip recalculation KS eigenvalues and eigenvectors for the complete k-point grid.

Type: boolean
Default: "false"
Use: optional
XPath: /input/gw/@skipgnd

90.22 Attribute: taskname

Type of calculations. Available tasks:

- g0w0 - G0W0 calculations
- g0w0_x - Exchange only (Hartree-Fock) G0W0 calculations
- gw0 - Partially self-consistent GW0 calculations
- cohsex - Coulomb-hole and screened-exchange (COHSEX) approximation
- band - QP banstructure as obtained by Fourier interpolation
- dos - QP density of states
- emac - Calculate the macroscopic dielectric function
- vxc - Calculate diagonal matrix elements of the exchange-correlation potential
- pmat - Calculate matrix elements of the momentum operator
- acon - Perform analytic continuation of the correlation self-energy from imaginary to real frequency and calculate QP energies
- wannier-

Type: string
Default: "g0w0"
Use: optional
XPath: /input/gw/@taskname

90.23 Attribute: vqloff

The $\mathbf{k}/q$-point offset vector in lattice coordinates.

Type: vect3d (114.6)
Default: "0.0d0 0.0d0 0.0d0"
Use: optional
XPath: /input/gw/@vqloff

91 Element: freqgrid

Frequecy grid parameters.

Type: no content
XPath: /input/gw/freqgrid

This element allows for specification of the following attributes:

fconv, fgrid, freqmax, nomeg

91.1 Attribute: fconv

Frequency convolution type: 'nofreq' - no frequecy dependence of the weights; 'refreq' - weights calculated for real frequecies; 'imfreq' - weights calculated for imaginary frequecies.

Type: string
Default: "imfreq"
Use: optional
XPath: /input/gw/freqgrid/@fconv

91.2 Attribute: fgrid

Frequency integration grid type: 'eqdis' - equidistant frequencies from 0 to freqmax; 'gaulag' - Gauss-Laguerre quadrature from 0 to infinity; 'gauleg' - Gauss-Legendre quadrature from 0 to freqmax; 'gaule2' (default) - double Gauss-Legendre quadrature from 0 to freqmax and from freqmax to infinity.

Type: string
Default: "gaule2"
Use: optional
XPath: /input/gw/freqgrid/@fgrid

91.3 Attribute: freqmax

Parameter of the double frequency grid technique.

Type: fortrandouble (114.1)
Default: "1.0d0"
Use: optional

XPath: /input/gw/freqgrid/@freqmax

91.4 Attribute: nomeg

Number of frequency (grid) points.

Type: integer
Default: "16"
Use: optional
XPath: /input/gw/freqgrid/@nomeg

92 Element: selfenergy

Options related to the calculations of the correlation self-energy.

Contains: SpectralFunctionPlot (optional)
XPath: /input/gw/selfenergy

This element allows for specification of the following attributes:

actype, iopes, nempty, npol, secordw, singularity

92.1 Attribute: actype

Analytical continuation scheme: 'pade': Pade's approximant (by H. J. Vidberg and J. W. Serence, J. Low Temp. Phys. 29, 179 (1977)) 'mpf': Multi-Pole Fitting (by H. N Rojas, R. W. Godby and R. J. Needs, Phys. Rev. Lett. 74, 1827 (1995))

Type: string
Default: "pade"
Use: optional
XPath: /input/gw/selfenergy/@actype

92.2 Attribute: iopes

Solution of the quasiparticle equation: 0 : perturbative G0W0 without energy shift; 1 : perturbative G0W0 with energy shift 2 - iterative G0W0 with energy shift; 3 - iterative G0W0 without energy shift.

Type: integer
Default: "0"
Use: optional
XPath: /input/gw/selfenergy/@iopes

92.3 Attribute: nempty

Number of empty states to be used to calculate the correlation self energy.

Type: integer
Default: "0"
Use: optional
XPath: /input/gw/selfenergy/@nempty

92.4 Attribute: npol

Number of poles used in the analytical continuation.

Type: integer
Default: "0"
Use: optional
XPath: /input/gw/selfenergy/@npol

92.5 Attribute: secordw

Calculate second order screened exchange contribution.

Type: boolean
Default: "false"
Use: optional
XPath: /input/gw/selfenergy/@secordw

92.6 Attribute: singularity

Treatment of the integrable singular terms: 'none': No special treatment (test purpose only); 'mpb' : Auxiliary function method by S. Massidda, M. Posternak, and A. Baldereschi, PRB 48, 5058 (1993); 'crg' : Auxiliary function method by P. Carrier, S. Rohra, and A. Goerling, PRB 75, 205126 (2007).

Type: string
Default: "mpb"
Use: optional
XPath: /input/gw/selfenergy/@singularity

93 Element: SpectralFunctionPlot

Parameters for the self-energy and spectral function visualization.

Type: no content
XPath: /input/gw/selfenergy/SpectralFunctionPlot

This element allows for specification of the following attributes:

axis, eta, nwgrid, wmax, wmin

93.1 Attribute: axis

Real ("real") or imaginary ("imag") frequency axis for visialization.

Type: string
Default: "real"
Use: optional
XPath: /input/gw/selfenergy/SpectralFunctionPlot/@axis

93.2 Attribute: eta

Smearing parameter (small number).

Type: fortrandouble (114.1)
Default: "1.0d-4"
Use: optional
Unit: Hartree
XPath: /input/gw/selfenergy/SpectralFunctionPlot/@eta

93.3 Attribute: nwgrid

Number of grid points within the visualization interval.

Type: integer
Default: "1001"
Use: optional
XPath: /input/gw/selfenergy/SpectralFunctionPlot/@nwgrid

93.4 Attribute: wmax

Upper bound for the visualization frequency interval.

Type: fortrandouble (114.1)
Default: "10"
Use: optional
Unit: Hartree
XPath: /input/gw/selfenergy/SpectralFunctionPlot/@wmax

93.5 Attribute: wmin

Lower bound for the visualization frequency interval.

Type: fortrandouble (114.1)

Default: "-10"
Use: optional
Unit: Hartree
XPath: /input/gw/selfenergy/SpectralFunctionPlot/@wmin

94 Element: mixbasis

Mixed basis parameters.

Type: no content
XPath: /input/gw/mixbasis

This element allows for specification of the following attributes:

epsmb, gmb, lmaxmb

94.1 Attribute: epsmb

Type: fortrandouble (114.1)
Default: "1.0d-4"
Use: optional
XPath: /input/gw/mixbasis/@epsmb

94.2 Attribute: gmb

Type: fortrandouble (114.1)
Default: "1.0"
Use: optional
XPath: /input/gw/mixbasis/@gmb

94.3 Attribute: lmaxmb

Type: integer
Default: "3"
Use: optional
XPath: /input/gw/mixbasis/@lmaxmb

95 Element: barecoul

Parameters for the bare coulomb potential: pwm - Maximum G for the pw basis (in gmaxvr*gmb units) stctol - Convergence tolerance of the struct. const. barcevtol - Tolerance to choose basis functions from bare Coulomb matrix eigenvectors.

Type: no content
XPath: /input/gw/barecoul

This element allows for specification of the following attributes:

barcevtol, basis, cutofftype, pwm, stctol

95.1 Attribute: barcevtol

Type: fortrandouble (114.1)
Default: "0.1d0"
Use: optional
XPath: /input/gw/barecoul/@barcevtol

95.2 Attribute: basis

Type: string
Default: "mb"
Use: optional
XPath: /input/gw/barecoul/@basis

95.3 Attribute: cutofftype

Type: string
Default: "none"
Use: optional
XPath: /input/gw/barecoul/@cutofftype

95.4 Attribute: pwm

Type: fortrandouble (114.1)
Default: "2.0d0"
Use: optional
XPath: /input/gw/barecoul/@pwm

95.5 Attribute: stctol

Type: fortrandouble (114.1)
Default: "1.0d-15"
Use: optional
XPath: /input/gw/barecoul/@stctol

96 Element: scrcoul

Parameters for the dynamically screened Coulomb potential:

Type: no content
XPath: /input/gw/scrcoul

This element allows for specification of the following attributes:

lmaxdielt, nleblaik, omegap, q0eps, sciavbd, sciavtype, scrtype

96.1 Attribute: lmaxdielt

Angular momentum cutoff in anisotropy treatment.

Type: integer
Default: "2"
Use: optional
XPath: /input/gw/scrcoul/@lmaxdielt

96.2 Attribute: nleblaik

Number of Lebedev-Laikov grid points in anisotropy treatment.

Type: integer
Default: "5810"
Use: optional
XPath: /input/gw/scrcoul/@nleblaik

96.3 Attribute: omegap

Plasmon-pole model fitting parameter (plasmon frequency).

Type: fortrandouble (114.1)
Default: "1.0d0"
Use: optional
XPath: /input/gw/scrcoul/@omegap

96.4 Attribute: q0eps

q0eps - averaging direction q $\rightarrow$ 0. Default: (1,1,1)

Type: vect3d (114.6)
Default: "1.0d0 1.0d0 1.0d0"
Use: optional
XPath: /input/gw/scrcoul/@q0eps

96.5 Attribute: sciavbd

Flag for anisotropic averaging of the dielectric tensor 'body' part.

Type: boolean
Default: "false"
Use: optional
XPath: /input/gw/scrcoul/@sciavbd

96.6 Attribute: sciavtype

Type of volume averaging: isotropic - Simple averaging along a specified direction using only diagonal components of the dielectric tensor; anisotropic - Anisotropic screening by C. Freysoldt et al., CPC 176, 1-13 (2007).

Type: string
Default: "isotropic"
Use: optional
XPath: /input/gw/scrcoul/@sciavtype

96.7 Attribute: scrtype

Model type: rpa - Full-frequency random-phase approximation; ppm - Godby-Needs plasmon-pole model.

Type: string
Default: "rpa"
Use: optional
XPath: /input/gw/scrcoul/@scrtype

97 Element: eph

Electron-phonon calculation setup.

Contains: freqgrideph (optional)
selfenergyeph (optional)
XPath: /input/eph

This element allows for specification of the following attributes:

debugeph, ibeph, ibsumeph, nbeph, nbsumeph, nemptyeph, ngridqeph, tasknameeph, vqloffeph

97.1 Attribute: debugeph

Print debugging information.

Type: boolean
Default: "false"
Use: optional
XPath: /input/eph/@debugeph

97.2 Attribute: ibeph

Lower band index for e-ph output.

Type: integer
Default: "1"
Use: optional
XPath: /input/eph/@ibeph

97.3 Attribute: ibsumeph

Lower band index for the summation in e-ph calculations.

Type: integer
Default: "1"
Use: optional
XPath: /input/eph/@ibsumeph

97.4 Attribute: nbeph

Upper band index for electron-phonon coupling output. If not specified, the maximum number of the available states is used.

Type: integer
Default: "0"
Use: optional
XPath: /input/eph/@nbeph

97.5 Attribute: nbsumeph

Upper band index for the summation electron-phonon coupling output.

Type: integer
Default: "0"
Use: optional
XPath: /input/eph/@nbsumeph

97.6 Attribute: nemptyeph

Number of empty states (cutoff parameter) used in e-ph. If not specified, the same number as for the groundstate calculations is used.

Type: integer
Default: "0"
Use: optional
XPath: /input/eph/@nemptyeph

97.7 Attribute: ngridqeph

k/q-point grid size to be used in e-ph calculations. If not specified, (2,2,2) k-grid is used.

Type: integertriple (114.8)
Default: "0 0 0"
Use: optional
XPath: /input/eph/@ngridqeph

97.8 Attribute: tasknameeph

Type of calculations. Available tasks:

- eph - eph calculations

Type: string
Default: "eph"
Use: optional
XPath: /input/eph/@tasknameeph

97.9 Attribute: vqloffeph

The $\mathbf{k}/q$-point offset vector in lattice coordinates.

Type: vect3d (114.6)
Default: "0.0d0 0.0d0 0.0d0"
Use: optional
XPath: /input/eph/@vqloffeph

98 Element: freqgrideph

Frequecy grid parameters.

Type: no content
XPath: /input/eph/freqgrideph

This element allows for specification of the following attributes:

freqmaxeph, nomegeph

98.1 Attribute: freqmaxeph

Parameter of the double frequency grid technique.

Type: fortrandouble (114.1)
Default: "1.0d0"
Use: optional
XPath: /input/eph/freqgrideph/@freqmaxeph

98.2 Attribute: nomegeph

Number of frequency (grid) points.

Type: integer
Default: "16"
Use: optional
XPath: /input/eph/freqgrideph/@nomegeph

99 Element: selfenergyeph

Options related to the calculations of the correlation self-energy.

Contains: SpectralFunctionPloteph (optional)
XPath: /input/eph/selfenergyeph

100 Element: SpectralFunctionPloteph

Parameters for the self-energy and spectral function visualization.

Type: no content
XPath: /input/eph/selfenergyeph/SpectralFunctionPloteph

This element allows for specification of the following attributes:

axis, eta, nwgrid, wmax, wmin

100.1 Attribute: axis

Real ("real") or imaginary ("imag") frequency axis for visialization.

Type: string
Default: "real"
Use: optional
XPath: /input/eph/selfenergyeph/SpectralFunctionPloteph/@axis

100.2 Attribute: eta

Smearing parameter (small number).

Type:	fortrandouble (114.1)
Default:	"1.0d-4"
Use:	optional
Unit:	Hartree
XPath:	/input/eph/selfenergyeph/SpectralFunctionPloteph/@eta

100.3 Attribute: nwgrid

Number of grid points within the visualization interval.

Type:	integer
Default:	"1001"
Use:	optional
XPath:	/input/eph/selfenergyeph/SpectralFunctionPloteph/@nwgrid

100.4 Attribute: wmax

Upper bound for the visualization frequency interval.

Type:	fortrandouble (114.1)
Default:	"10"
Use:	optional
Unit:	Hartree
XPath:	/input/eph/selfenergyeph/SpectralFunctionPloteph/@wmax

100.5 Attribute: wmin

Lower bound for the visualization frequency interval.

Type:	fortrandouble (114.1)
Default:	"-10"
Use:	optional
Unit:	Hartree
XPath:	/input/eph/selfenergyeph/SpectralFunctionPloteph/@wmin

Part II
Reused Elements

The following elements can occur more than once in the input file. Therefore they are listed separately.

101 Element: origin

Type: no content
XPath: /origin
Parent: /plot2d/parallelogram
/plot3d/box

This element allows for specification of the following attributes:

coord

101.1 Attribute: coord

Type: vect3d (114.6)
Use: optional
XPath: /origin/@coord

102 Element: point

Type: no content
XPath: /point
Parent: /plot1d/path
/plot2d/parallelogram
/plot3d/box

This element allows for specification of the following attributes:

coord (required), label

102.1 Attribute: coord

Type: vect3d (114.6)
Use: required
XPath: /point/@coord

102.2 Attribute: label

Type: string
Default: ""
Use: optional
XPath: /point/@label

103 Element: plot1d

The element plot1d specifies sample points along a path. The coordinate space (lattice or cartesian)is chosen in the context of the parent.

Contains: path (1 times)
XPath: /plot1d
Parent: /input/phonons/phonondispplot
/input/properties/bandstructure
/input/properties/wfplot
/input/properties/chargedensityplot
/input/properties/exccplot
/input/properties/elfplot
/input/properties/gradmvecfield
/input/properties/wannierplot
/input/xs/excitonPlot/hole
/input/xs/excitonPlot/electron
/input/gw

104 Element: path

Contains: point (1 times or more)
XPath: /plot1d/path

This element allows for specification of the following attributes:

steps (required), outfileprefix

104.1 Attribute: outfileprefix

Type: string
Use: optional
XPath: /plot1d/path/@outfileprefix

104.2 Attribute: steps

Type: integer
Use: required
XPath: /plot1d/path/@steps

105 Element: plot2d

Defines a 2d plot domain.

Contains: parallelogram (1 times)
XPath: /plot2d
Parent: /input/properties/stm
/input/properties/wfplot
/input/properties/chargedensityplot
/input/properties/exccplot
/input/properties/elfplot
/input/properties/mvecfield
/input/properties/xcmvecfield
/input/properties/electricfield
/input/properties/gradmvecfield
/input/properties/fermisurfaceplot
/input/properties/wannierplot
/input/xs/excitonPlot/hole
/input/xs/excitonPlot/electron

106 Element: parallelogram

Contains: origin (1 times)
point (2 times)
XPath: /plot2d/parallelogram

This element allows for specification of the following attributes:

grid (required), outfileprefix

106.1 Attribute: grid

Type: integerpair (114.10)
Use: required
XPath: /plot2d/parallelogram/@grid

106.2 Attribute: outfileprefix

Type: string
Use: optional
XPath: /plot2d/parallelogram/@outfileprefix

107 Element: plot3d

Defines a 3d plot domain.

Contains: box (1 times)

XPath: /plot3d
Parent: /input/properties/wfplot
/input/properties/chargedensityplot
/input/properties/exccplot
/input/properties/elfplot
/input/properties/mvecfield
/input/properties/xcmvecfield
/input/properties/electricfield
/input/properties/gradmvecfield
/input/properties/fermisurfaceplot
/input/properties/wannierplot
/input/xs/excitonPlot/hole
/input/xs/excitonPlot/electron

This element allows for specification of the following attributes:

usesym

107.1 Attribute: usesym

When set to "true", crystal symmetries are used in the determination of the 3D spatial grid. Also, in that case the whole unit cell is sampled.

Type: boolean
Default: "false"
Use: optional
XPath: /plot3d/@usesym

108 Element: box

Contains: origin (1 times)
point (3 times)
XPath: /plot3d/box

This element allows for specification of the following attributes:

grid (required), outfileprefix

108.1 Attribute: grid

Type: integertriple (114.8)
Use: required
XPath: /plot3d/box/@grid

108.2 Attribute: outfileprefix

Type: string
Use: optional
XPath: /plot3d/box/@outfileprefix

109 Element: kstlist

The kstlist element is used in the LSJ and wavefunction plot element This is a user-defined list of **k**-point and state index pairs which are those used for plotting wavefunctions and writing **L**, **S** and **J** expectation values.

Contains: pointstatepair (1 times or more)
XPath: /kstlist
Parent: /input/properties/wfplot
/input/properties/LSJ
/input/properties/expiqr

110 Element: pointstatepair

The element `pointstatepair` defines a **k**-point and state index pair.

Type: integerpair (114.10)
XPath: /kstlist/pointstatepair

111 Element: energywindow

Type: no content
XPath: /energywindow
Parent: /input/properties/raman
/input/xs

This element allows for specification of the following attributes:

intv, points

111.1 Attribute: intv

energy interval lower and upper limits.

Type: vect2d (114.7)
Default: "-0.5d0 0.5d0"
Use: optional
XPath: /energywindow/@intv

111.2 Attribute: points

number of points to be sampled linearly inside the energy interval including the lower limit.

Type:	integer
Default:	"500"
Use:	optional
XPath:	/energywindow/@points

112 Element: qpointset

Contains:	qpoint (1 times or more)
XPath:	/qpointset
Parent:	/input/phonons /input/xs

113 Element: qpoint

a q-point is given in reciprocal space coordinates

Type:	vect3d (114.6)
XPath:	/qpointset/qpoint

114 Data Types

The Input definition uses derived data types. These are described here.

114.1 Type fortrandouble

The type `fortrandouble` allows to use the letters `"eEdDqQ"` for exponent operators. This alters in what precision the number is parsed.

114.2 Type booleanlist

List of space separated booleans.

114.3 Type booleantriple

Space separated list of three booleans.
Example: `"true false true"`

114.4 Type vector

A vector is a space separated list of floating point numbers.
Example: `"1.3 2.3e4 3 90"`

114.5 Type integerlist

List of space separated integers.

114.6 Type vect3d

Three dimensional vector as three space separated floating point numbers.

114.7 Type vect2d

Two dimensional vector as two space separated floating point numbers.

114.8 Type integertriple

Space separated list of three integers.
Example: `"1 2 3"`

114.9 Type integerquadrupel

Space separated list of three integers.
Example: `"1 2 3 4"`

114.10 Type integerpair

Space separated list of two integers
Example: `"1 2"`