

EXC!TING input reference

exciting devteam

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1 Root element input

The input element is the root element of the exciting input file. XML may contain only one root element. The input element must contain one structure element and one groundstate element. Every input file must contain a structure element to specify the domain and the atoms. Unless explicitly stated otherwise, EXCITING uses atomic units. In this system $\hbar = 1$, the electron mass $m = 1$, the Bohr radius $a_0 = 1$ and the electron charge $e = 1$ (note that the electron charge is positive, so that the atomic numbers Z are negative). Thus, the atomic unit of length is 0.52917720859(36) Å, and the atomic unit of energy is the Hartree which equals 27.21138386(68) eV. The unit of the external magnetic fields is defined such that one unit of magnetic field in `exciting.in` equals 1717.2445320376 Tesla.

Attributes:

xsltpath type xs:anyURI

default-value ../../xml

scratchpath This is the path to scratch space where the eigenvector files EVECFV.OUT, EVECSV.OUT and OCCSV.OUT will be written. If the local directory is accessed via a network then scrpath can be set to a directory on a local disk

type xs:anyURI

use optional

id The id is a unique identifier in an input set. The inputset element is currently not used by the exciting code.

type xs:ID

depends The depends attribute can be used to specify a dependence from another simulation in the same input set. The inputset element is currently not used by the exciting code.

type xs:IDREFS

2 title element

Title of the input file.

3 structure element

The structure element contains all structural information such as atoms atom positions and symmetries.

Attributes:

speciespath gives the path to the directory containing the species files

type xs:anyURI

use required

molecule has to be set to true if one wants to calculate an isolated molecule. is **true** , then the atomic positions, **a**, are assumed to be in Cartesian coordinates. The lattice vectors are also set up automatically with the i-th lattice vector given by

$$\mathbf{A}^i = A_i \hat{\mathbf{e}}^i, \quad (1)$$

where

$$A_i = \max_{\alpha, \beta} \left| \mathbf{a}_i^\alpha - \mathbf{a}_i^\beta \right| + d_{\text{vac}} \quad (2)$$

with α and β labeling atoms, and d_{vac} determines the size of the vacuum around the molecule. The last variable is set by the attribute **vacuum** .

type xs:boolean

default-value false

vacuum determines the size of the vacuum around the molecule.

type fortrandouble

default-value 10

epsflat vectors with lengths less than this are considered zero.

type fortrandouble

default-value 1e-6

autormt If true automatic determination of the muffin tin radii is allowed.

type xs:boolean

default-value false

primcell allows the primitive unit cell to be determined automatically from the conventional cell. This is done by searching for lattice vectors among all those which connect atomic sites, and using the three shortest ones which produce a unit cell with non-zero volume.

type xs:boolean

default-value false

tshift Set to it to "true" if the crystal can be shifted such that the atom closest to the origin is exactly at the origin.

type xs:boolean

default-value true

3.1 symmetries element

This element is used by the spacegroup tool to generate structures and super-cells. The symmetries element is output from the spacegroup program; the values are currently not used in the exciting program.

Attributes:

HermannMauguinSymbol Herman Mauguin symbol giving the spacegroup

type xs:string

use required

HallSymbol **type** xs:string

SchoenfliesSymbol **type** xs:string

spaceGroupNumber **type** xs:string

3.1.1 lattice element

defines lattice from a,b,c, and angles

Attributes:

a **type** fortrandouble

use required

b **type** fortrandouble

use required

c **type** fortrandouble

use required

ab **type** fortrandouble

use required

ac **type** fortrandouble

use required

bc **type** fortrandouble

use required

ncell number of repeated cells in each direction

type integertriple

use optional

default-value 1 1 1

3.1.2 WyckoffPositions element

wspecies element

Attributes:

speciesfile type xs:string

wpos element

Attributes:

coord type vect3d

3.2 crystal element

defines the unit cell of the calculation. unit cell is spanned by 3 basevectors that define the lattice coordinates.

Attributes:

scale scales all the lattice vectors. This is useful for varying the volume.

type fortrandouble

default-value 1

stretch allows for a separate scaling of each lattice vector. 1 1 1 means no scaling.

type vect3d

default-value 1.0d0 1.0d0 1.0d0

3.2.1 basevect element

are the basis vectors or lattice vectors in Bohr.

3.3 species element

for each atom type (species) a species element is defined containing all the atom positions

Attributes:

speciesfile defines the file from which the species definition is read. It is looked up in the species directory specified by the species path.

type xs:anyURI
use required

chemicalSymbol can be given to simplify visualisation and converters. is ignored by exciting

type xs:string
use optional
default-value

atomicNumber can be given to simplify visualisation and converters. is ignored by exciting

type xs:integer
use optional

rmt muffin tin radius this optional parameter allows to override speciesfile or automatic tetemination

type fortrandouble
use optional
default-value -1

3.3.1 atom element

atomic position in lattice coordinates for atom

Attributes:

coord position in lattice coordinates

type vect3d
use required

bfcmt muffin-tin external magnetic field in Cartesian coordinates for atom

type vect3d
use optional
default-value 0 0 0

mommtfix **type** vect3d
use optional

3.3.2 LDAplusU element

If present defines ldaplusU parameters for species

Attributes:

L **type** fortrandouble
default-value 0

U **type** fortrandouble
default-value 0

J **type** fortrandouble
default-value 0

4 groundstate element

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

Attributes:

do Decides if the groundstate is read from file or recalculated or continued from file.

type select:

- fromscratch
- fromfile
- skip

default-value fromscratch

ngridk Number of k grid points along the basis vector directions.

type integertriple

use required

rgkmax This sets the maximum length for the $\mathbf{G} + \mathbf{k}$ vectors, defined as **rgkmax** divided by the smallest muffin-tin radius.

type fortrandouble

default-value 7

epspt If the RMS change in the effective potential and magnetic field is smaller than **epspt**, 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

use optional

default-value 1e-6

rmtapm parameters governing the automatic generation of the muffin-tin radii. When @autormt is set to true, the muffin-tin radii are found automatically from the formula

$$R_i \propto 1 + \zeta |Z_i|^{1/3}, \quad (3)$$

where Z_i is the atomic number of the i th species, ζ is stored in @rmtapm(1) and the value which governs the distance between the muffin-tins is stored in @rmtapm(2). When @rmtapm(2) = 1, the closest muffin-tins will touch.

type vect2d

default-value 0.25d0 0.95d0

swidth width of the smooth approximation to the Dirac delta function.

type fortrandouble

default-value 0.001d0

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

type select:

- Gaussian
- Methfessel-Paxton 1
- Methfessel-Paxton 2
- Fermi Dirac
- Square-wave impulse

default-value Gaussian

findlinetype select method to determine the linearization energies.

type select:

- simple
- advanced

default-value advanced

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

type xs:integer

default-value -1

gmaxvr maximum length of ---G--- for expanding the interstitial density and potential.

type fortrandouble

default-value 12

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-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 xs:integer

default-value 5

nosym when set to **.true.** no symmetries, apart from the identity, are used anywhere in the code.

type xs:boolean

default-value false

frozenscore when set to **true** the frozen core approximation is applied, i.e., the core states are fixed to the atomic states.

type xs:boolean

default-value false

autokpt if the-point set is to be determined automatically

type xs:boolean

default-value false

radkpt Used for the automatic determination of the-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

default-value 40

reducek **reducek** set to **true** if the k -point set is to be reduced with the crystal symmetries.

type xs:boolean

default-value true

tfibs See 10. 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.

tforce See 10. if the force should be calculated at the end of the self-consistent cycle.

lmaxapw angular momentum cut-off for the APW functions.

type `xs:integer`
default-value 10

maxscl upper limit for the selfconsistency loop.

type `xs:integer`
default-value 200

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`
default-value 0

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 wavefunction 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 wavefunction at the muffin-tin radius is zero. This energy, E_b , is at the bottom of the band. The band energy is taken as $(E_t + E_b)/2$. If either E_t or E_b cannot be found then the band energy is set to the default value.

type `fortrandouble`
default-value 0.0025d0

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

type `fortrandouble`
default-value 1.0d-3

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

type `fortrandouble`

default-value 1e-8

mixer select the mixing (relaxation) scheme for SCF

type select:

- lin
- msec
- pulay

default-value msec

beta0 initial value for mixing parameter. Used in linear mixing.

type fortrandouble

default-value 0.4

betainc mixing parameter increase. Used in linear mixing.

type fortrandouble

default-value 1.1

betadec mixing parameter decrease. Used in linear mixing.

type fortrandouble

default-value 0.6

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 xs:integer

default-value 4

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

type xs:integer

default-value 4

xctype type of exchange-correlation functional to be used

- No exchange-correlation functional ($E_{xc} \equiv 0$)
- LDA, Perdew-Zunger/Ceperley-Alder, *Phys. Rev. B*, 5048 (1981)
- LSDA, Perdew-Wang/Ceperley-Alder, *Phys. Rev. B*, 13244 (1992)
- LDA, X-alpha approximation, J. C. Slater, *Phys. Rev.*, 385 (1951)

- LSDA, von Barth-Hedin, *J. Phys. C* , 1629 (1972)
- GGA, Perdew-Burke-Ernzerhof, *Phys. Rev. Lett.* , 3865 (1996)
- GGA, Revised PBE, Zhang-Yang, *Phys. Rev. Lett.*, 890 (1998)
- GGA, PBEsol, arXiv:0707.2088v1 (2007)
- GGA, Wu-Cohen exchange (WC06) with PBE correlation, *Phys. Rev. B* , 235116 (2006)
- GGA, Armiento-Mattsson (AM05) spin-unpolarised functional, *Phys. Rev. B*, 085108 (2005)

type select:

- LDAPerdew-Zunger
- LSDAPerdew-Wang
- LDA-X-alpha
- LSDA-Barth-Hedin
- GGAPerdew-Burke-Ernzerhof
- GGArevPBE
- GGAPBEsol
- GGA-Wu-Cohen
- GGAArmiento-Mattsson
- EXX
- none

default-value LSDAPerdew-Wang

evalmin Any valence states with eigenvalues below evalmin are not occupied and a warning message is issued.

type fortrandouble

default-value -4.5d0

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

type xs:integer

default-value 6

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

type fortrandouble

default-value 0.25d0

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 xs:integer
default-value 2

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

type xs:integer
default-value 5

vkloff the k-point offset vector in lattice coordinates.

type vect3d
default-value 0 0 0

npsden **type** xs:integer
default-value 9

cf damp damping coefficient for characteristic function.

type fortrandouble
default-value 0

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

type xs:boolean
default-value false

tevecsv tevecsv is true if second-variational eigenvectors are calculated

type xs:boolean
default-value false

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 xs:integer
default-value 0

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

type xs:boolean
default-value true

4.1 spin element

If present calculation is done with spin polarization it may be switched off with the `spinpol` attribute set to `false`

Attributes:

momfix the desired total moment for a FSM calculation.

type vect3d
default-value 0 0 0

bfieldc allows to apply a constant B field This is a constant magnetic field applied throughout the entire unit cell and enters the second-variational Hamiltonian as

$$\frac{g_e \alpha}{4} \vec{\sigma} \cdot \mathbf{B}_{\text{ext}}, \quad (4)$$

where g_e is the electron g -factor (2.0023193043718). This 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 \mathbf{B} -field energy reported in `INFO.OUT` should be added to the total by hand. This field is applied throughout the entire unit cell. To apply magnetic fields in particular muffin-tins use the `bfcmt` vectors in the `atoms` block. Collinear calculations are more efficient if the field is applied in the z -direction.

type vect3d
default-value 0 0 0

spinorb if a spin-orbit coupling is required If `spinorb` is `.true.`, then a $\sigma \cdot \mathbf{L}$ term is added to the second-variational Hamiltonian. See `spinpol`.

type xs:boolean

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 xs:boolean

vqlss the \mathbf{q} -vector of the spin-spiral state in lattice coordinates Spin-spirals arise from spinor states assumed to be of the form

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

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

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

where m_x , m_y and m_z are lattice periodic. See also `spinprl`.

type vect3d
default-value 0 0 0

taufsm type fortrandouble
default-value 0.01d0

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 atoms.

type fortrandouble
default-value 1

fixspin type select:

- none
- total FSM
- localmt FSM
- both

default-value none

4.2 HartreeFock element

If preset HartreeFock calculation is triggered.

Attributes:

epsengy energy convergence tolerance

type fortrandouble
use optional
default-value 1e-7

4.3 solver element

Optional configuration options for eigenvector solver.

Attributes:

type select the eigenvalue solver for the first variational equation

type select:

- Lapack
- Arpack

- DIIS

default-value Lapack

packedmatrixstorage In the default calculation the matrix is stored in packed form. When using multithreaded BLAS setting this parameter to false increases efficiency.

type xs:boolean

use optional

default-value true

epsarpack Tolerance parameter for the ARPACK shift invert solver

type fortrandouble

default-value 1.0e-8

evaltol error tolerance for the first-variational eigenvalues using the LAPACK Solver

type fortrandouble

default-value 1e-8

4.4 OEP element

If present exact exchange calculation is triggered. (experimental)

Attributes:

maxitoe maximum number of iterations when solving the exact exchange integral equations

type xs:integer

default-value 120

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 maxitoe.

type vect3d

default-value 1.0 0.2 1.5

4.5 RDMFT element

If present Reduced Density Matrix Functional Theory calculation is triggered

Attributes:

rdmxctype xc functional.

type xs:integer
default-value 2

rdmmaxscl maximum number of self-consistent loops.

type xs:integer
default-value 1

maxitn maximum number of iteration for occupation number optimisation.

type xs:integer
default-value 250

maxitc maximum number of iteration for natural orbital optimisation.

type xs:integer
default-value 10

taurdmn step size for occupation numbers.

type fortrandouble
default-value 1.0

taurdmc step size for natural orbital coefficients.

type fortrandouble
default-value 0.5

rdmalpha exponent for the functional.

type fortrandouble
default-value 0.7

rdmtemp temperature.

type fortrandouble
default-value 0.0

5 structureoptimization element

The structure optimization element triggers if present a geometry relaxation. structural optimisation run starting from the atomic densities, with atomic positions written to `GEOMETRY.OUT` .

Attributes:

epsforce convergence tolerance for the forces during a structural optimisation run.

type fortrandouble

default-value 5e-5

tau0atm the step size to be used for structural optimisationThe position of atom α is updated on step m of a structural optimisation run using

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

where τ_α is set to **tau0atm** for $m = 0$, and incremented by the same amount if the atom is moving in the same direction between steps. If the direction changes then τ_α is reset to **tau0atm**.

type fortrandouble

default-value 0.2d0

resume Resumption of structural optimisation run using density in `STATE.OUT` but with positions from `exciting.in`.

type xs:boolean

default-value false

6 properties element

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

6.1 bandstructure element

If present a bandstructure is calculated. Create a bandstructure. Must contain `plot1d` element for bandstructure path.

Attributes:

scissor See 10. value to shift bandgap.

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

type xs:boolean

default-value false

6.1.1 plot1d element

See 9.3

6.2 STM element

6.2.1 plot2d element

See 9.4

6.3 wfplot element

wavefunction plot. Plot the wave function at a set of kpoints

6.3.1 kstlist element

See 9.7 List of kpoints of which the wave functions should be plotted.

6.3.2 plot1d element

See 9.3

6.3.3 plot2d element

See 9.4

6.3.4 plot3d element

See 9.5

6.4 dos element

If present a DOS calculation is started. DOS and optics plots require integrals of the kind

$$g(\omega_i) = \frac{\Omega}{(2\pi)^3} \int_{\text{BZ}} f(\mathbf{k}) \delta(\omega_i - e(\mathbf{k})) d\mathbf{k}. \quad (8)$$

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 .

Attributes:

sqados spin-quantisation axis in Cartesian coordinates used when plotting the spin-resolved DOS (z-axis by default)

type vect3d

default-value 0.0 0.0 1.0

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 xs:boolean

default-value false

nwdos number of frequency/energy points in the DOS

type xs:integer

default-value 500

ngrdos effective k-point mesh size to be used for Brillouin zone integration.

type xs:integer

default-value 100

scissor See 10.

nsmdos level of smoothing applied to DOS/optics output integer 0

type xs:integer

default-value 0

winddos frequency/energy window for the DOS or optics plot

type vect2d

default-value .5 .5

6.5 LSJ element

Output L, S and J expectation values.

6.5.1 kstlist element

See 9.7 *i*th k-point and state pair

6.6 `masstensor` element

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

Attributes:

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

type `fortrandouble`

default-value `0.025d0`

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

type `xs:integer`

default-value `1`

`vklem` the k-point in lattice coordinates at which to compute the effective mass tensors.

type `vect3d`

default-value `0 0 0`

6.7 `chargedensityplot` element

Plot the charge density

6.7.1 `plot1d` element

See 9.3

6.7.2 `plot2d` element

See 9.4

6.7.3 `plot3d` element

See 9.5

6.8 `exccplot` element

exchange-correlation and Coulomb potential plots.

6.8.1 `plot1d` element

See 9.3

6.8.2 plot2d element

See 9.4

6.8.3 plot3d element

See 9.5

6.9 elfplot element

electron localisation function (ELF)

6.9.1 plot1d element

See 9.3

6.9.2 plot2d element

See 9.4

6.9.3 plot3d element

See 9.5

6.10 mvecfield element

plot of magnetisation vector field

6.10.1 plot2d element

See 9.4

6.10.2 plot3d element

See 9.5

6.11 xcmvecfield element

plot of exchange-correlation magnetic vector field

6.11.1 plot2d element

See 9.4

6.11.2 plot3d element

See 9.5

6.12 electricfield element

writes the electric field to file.

6.12.1 plot2d element

See 9.4

6.12.2 plot3d element

See 9.5

6.13 gradmvecfield element

plot of the gradient of the magnetic vector field.

6.13.1 plot1d element

See 9.3

6.13.2 plot2d element

See 9.4

6.13.3 plot3d element

See 9.5

6.14 fermisurfaceplot element

writes fermisurface data to file.

Attributes:

nstfsp number of states to be included in the Fermi surface plot file

type xs:integer

default-value 6

separate type xs:boolean

6.15 EFG element

Calculation of electric field gradient (EFG), contact charge

6.16 momentummatrix element

6.17 linresponsetensor element

Linear optical response tensor.

Attributes:

scissor See 10.

6.17.1 optcomp element

the components of the first- or second-order optical tensor to be calculated

6.18 mossbauer element

6.19 dielectric element

6.20 expiqr element

6.21 elnes element

Attributes:

vecql q-vector in lattice coordinates for calculating ELNES

type vect3d

6.22 eliashberg element

Attributes:

mustar Coulomb pseudopotential, *, used in the McMillan-Allen-Dynes equation

type fortrandouble

default-value 0.15

7 phonons element

Phonon frequencies and eigen vectors for an arbitrary q-point. The phonon element must contain one or more q-point elements

Attributes:

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

type xs:boolean

default-value true

deltaph Phonon calculations are performed by constructing a supercell corresponding to a particular \mathbf{q} -vector and making a small periodic displacement of the atoms. The magnitude of this displacement is given by `deltaph`. This should not be made too large, as anharmonic terms could then become significant, neither should it be too small as this can introduce numerical error.

type fortrandouble

default-value 0.03

7.1 `qpointset` element

See 9.9

7.2 `phonondos` element

Phonon density of states.

7.3 `phonondisplot` element

Phonon dispersion plot.

7.3.1 `plot1d` element

See 9.3

8 `xs` element

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).

Attributes:

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

type xs:integer

default-value 1

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

type xs:boolean

default-value false

lmaxapwwf maximum angular momentum for APW functions for q -dependent matrix elements

type xs:integer
default-value -1

lmaxemat maximum angular momentum for Rayleigh expansion of q -dependent plane wave factor

type xs:integer
default-value 3

emaxdf energy cutoff for the unoccupied states in the Kohn-Sahm response function and screening

type fortrandouble
default-value 1d10

broad Lorentzian broadening for all spectra

type fortrandouble
default-value 0.01d0

tevout true if energy outputs are in eV

type xs:boolean
default-value false

xstype Should TDDFT be used or BSE

type select:

- TDDFT
- BSE

use required

symmorph True if only symmorphic space-group operations are to be considered, i.e. only symmetries without non-primitive translations are allowed.

type xs:boolean
default-value false

fastpmat if 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 xs:boolean
default-value true

fastemat if true, a fast method to calculate APW-lo, lo-APW and lo-lo parts of the \mathbf{q} -dependent matrix elements in the muffin-tin is used.

type xs:boolean
default-value true

gather **type** xs:boolean
default-value false

tappinfo **type** xs:boolean
default-value false

dbglev **type** xs:integer
default-value 0

usegdf **type** xs:boolean
default-value false

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

type fortrandouble
default-value 0

nosym nosym is true if no symmetry information should be used

type xs:boolean
default-value false

ngridk k-point grid sizes

type integertriple
default-value 1 1 1

vkloff k-point offset

type vect3d
default-value 0 0 0

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

type xs:boolean
default-value true

ngridq q-point grid sizes

type integertriple

default-value 1 1 1

reduceq reduceq is true if q-points are to be reduced (with crystal symmetries)

type xs:boolean

default-value true

rgkmax smallest muffin-tin radius times gkmax

type fortrandouble

default-value 7

swidth width of the smooth approximation to the Dirac delta function

type fortrandouble

default-value 0.001d0

lmaxpw angular momentum cut-off for the APW functions

type xs:integer

default-value 10

lmaxmat angular momentum cut-off for the outer-most loop in the hamiltonian and overlap matrix setup

type xs:integer

default-value 5

nempty number of empty states

type xs:integer

default-value 5

scissor See 10. scissors correction

8.1 tddft element

Attributes:

intraband intraband is true if the intraband term is to be added to the optical matrix (q=0)

type xs:boolean

default-value false

torddf **type** xs:boolean

default-value false

tordfxc **type** xs:boolean
default-value false

aresdf true if to consider the anti-resonant part for the dielectric function
type xs:boolean
default-value true

aresfxc true if to consider the anti-resonant part for the BSE-derived xc-kernels
type xs:boolean
default-value true

fxcbseplit split parameter for degeneracy in energy differences of BSE-derived kernel
type fortrandouble
default-value 1d-5

acon true if analytic continuation from the imaginary axis to the real axis is to be performed
type xs:boolean
default-value false

nwacont number of energy intervals (on imaginary axis) for analytic continuation
type xs:integer
default-value 0

lindhard true if Lindhard like function is calculated (trivial matrix elements)
type xs:boolean
default-value false

epsdfde smallest energy difference for which the square of its inverse will be considered in the Kohn-Sham response function
type fortrandouble
default-value 1.0d-8

kerndiag **type** xs:boolean
default-value false

lmaxalda angular momentum cutoff for Rayleigh expansion of exponential factor for ALDA-kernel

type xs:integer
default-value 3

alphaLRC alpha-parameter for the static long range contribution (LRC) model xc kernel

type fortrandouble
default-value 0

alphaLRCdyn alpha-parameter for the dynamical long range contribution (LRC) model xc kernel

type fortrandouble
default-value 0

betaLRCdyn beta-parameter for the dynamical long range contribution (LRC) model xc kernel

type fortrandouble

mdfqttype 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 $\mathbf{Q} = \mathbf{q} + \mathbf{G}_q$ and the $(\mathbf{Q}_q, \mathbf{Q}_q)$ component of the microscopic dielectric matrix is used.

type xs:integer
default-value 0

fxctype defines which xc kernel is to be used

type select:

- RPA
- LRCstatic_NLF
- LRCstatic
- LRCdyn_NLF
- LRCdyn
- ALDA
- MB1_NLF
- MB1

default-value RPA

resumeFromKernel true if the TDDFT calculation is to be resumed starting from a new xc kernel.

type xs:boolean
default-value false

8.1.1 dftrans element

trans element

8.2 screening element

Attributes:

run type select:

- fromscratch
- skip

default-value fromscratch

nosym nosym is true if no symmetry information should be used

type xs:boolean

default-value false

ngridk k-point grid sizes

type integertriple

default-value 0 0 0

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

type xs:boolean

default-value false

vkloff k-point offset

type vect3d

default-value -1 -1 -1

rgkmax smallest muffin-tin radius times gkmax

type fortrandouble

default-value 0

nempty number of empty states

type xs:integer

default-value 0

screeintype defines which screening is used

type select:

- full
- diag
- noinvdiag
- longrange

default-value full

8.3 BSE element

Attributes:

nosym type xs:boolean
default-value false

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

type xs:boolean
default-value false

vkloff k-point offset

type vect3d
default-value -1 -1 -1

rgkmax smallest muffin-tin radius times gkmax

type fortrandouble
default-value 0

scrherm type xs:integer
default-value 0

fbzq type xs:boolean
default-value false

sciavtype defines how the screened Coulomb interaction matrix is to be averaged (important for the singular terms)

type select:
• spherical
• screendiag
• invscreendiag
default-value spherical

sciavbd true if the body of the screened Coulomb interaction is to be averaged (q=0)

type xs:boolean
default-value false

sciavqhd true if the head of the screened Coulomb interaction is to be averaged (q!=0)

type xs:boolean

default-value false

sciavqwg true if the wings of the screened Coulomb interaction is to be averaged ($q \neq 0$)

type xs:boolean
default-value false

sciavqbd true if the body of the screened Coulomb interaction is to be averaged ($q \neq 0$)

type xs:boolean
default-value false

bsedirsing **type** xs:boolean
default-value false

lmaxdielt angular momentum cutoff of the spherical harmonics expansion of the dielectric matrix

type xs:integer
default-value 14

nleblaik number of points used for the Lebedev-Laikov grids (must be selected according to Ref.LebLaik)

type xs:integer
default-value 5810

nexcitmax **type** xs:integer
default-value 100

nstlbse number of states below and above the Fermi level

type integerpair
default-value 0 0

nstlce **type** integerpair
default-value 0 0

bsetype defines which parts of the BSE Hamiltonian are to be considered

type select:

- ip
- rpa
- singlet
- triplet

default-value singlet

8.4 qpointset element

See 9.9finite momentum transfer $\mathbf{G} + \mathbf{q}$ vector

8.5 tetra element

Attributes:

tetraocc type xs:boolean
default-value false

tetradf true if tetrahedron method is used for the k-space integration in the Kohn-Sham response function

type xs:boolean
default-value false

kordexc type xs:boolean
default-value false

cw1k type xs:boolean
default-value false

qweights type xs:integer
default-value 1

8.6 dosWindow element

Attributes:

points number of points to be sampled linearly inside the energy interval

type xs:integer
default-value 500

intv energy interval for the density of states

type vect2d
default-value -0.5 0.5

nsmdos type xs:integer
default-value 0

8.7 plan element

8.7.1 doonly element

Attributes:

task type select:

- xsgeneigvec
- tetcalccw
- writepmatxs
- writeemat
- df
- df2
- idf
- scrgeneigvec
- scrtetcalccw
- scrwritepmat
- screen
- scrcoulint
- exccoulint
- BSE
- kernxc_bse
- writebandgapgrid
- writepmat
- dielectric
- writepmatasc
- pmatxs2orig
- writeematasc
- writepwmatt
- emattest
- x0toasc
- x0tobin
- epsconv
- fxc_alda_check
- kernxc_bse3
- testxs
- xsestimate
- xstiming
- testmain
- portstate(1)
- portstate(2)
- portstate(-1)
- portstate(-2)

use required

9 reused Elements

These elements make sense in more than only one context. In this documentation there are references placed if one of these applies.

9.1 origin element

Attributes:

coord type vect3d

9.2 point element

Attributes:

coord type vect3d

label type xs:string
default-value

9.3 plot1d element

plot1d specifies sample points along a path. The coordinate space is chosen in the context of the parent

9.3.1 path element

Attributes:

steps type xs:integer
use required

outfileprefix See 10.

point element See 9.2

9.4 plot2d element

defines a 2d plot domain

9.4.1 parallelogram element

Attributes:

grid type integerpair
use required

outfileprefix See 10.

origin element See 9.1

point element See 9.2

9.5 plot3d element

defines a 3d plot domain

9.5.1 box element

Attributes:

grid type integertriple

use required

outfileprefix See 10.

origin element See 9.1

point element See 9.2

9.6 pointstatepair element

k-point and state index pair

9.7 kstlist element

kstlist 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.

9.7.1 pointstatepair element

See 9.6

9.8 inputset element

The inputset element can be used to store a set of input elements. It is not used by exciting now but will be usefull eventually.

9.8.1 input element

See 1

9.9 qpointset element

9.9.1 qpoint element

a q-point is given in reciprocal space coordinates

10 reused attributes

These attributes make sense in more than only one context. In this documentation there are references placed if one of these applies. input schema

Attributes:

outfileprefix a prefix to be prepended to the output files

type xs:string

tfibs if the IBS correction to the force should be calculated 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 xs:boolean

default-value true

tforce set to **.true**. if the force should be calculated at the end of the self-consistent cycle This variable is automatically set to **.true**. pre when performing structural optimization.

type xs:boolean

default-value false

scissor the scissors correction This is the scissors shift applied to states above the Fermi energy. Affects DOS, optics and band structure plots.

type fortrandouble

default-value 0