Electronic tab

The *Electronic* tab allows you to set the parameters associated with the electronic Hamiltonian. These include the basis set, pseudopotentials, SCF convergence criteria, and k-point set.

Energy cutoff: Select the precision used for the plane wave basis set.

- Coarse
- Medium
- Fine
- Ultra-fine

The actual value of the energy cutoff corresponding to the selected quality for the current structure is also displayed.

Note: Calculation of the NMR parameters may require the *Energy cutoff* to be set to a higher value than for total energy or geometry optimization calculations. It is advisable to study the convergence of the results as the *Energy cutoff* parameter is increased. Generally, setting the cutoff to between 270 and 400 eV should produce convergence of the shielding constant to about 1 ppm, but in some cases, the cutoff has to be increased up to 550 eV.

SCF tolerance: Select the threshold used to determine whether an SCF has converged. Available options and associated convergence thresholds are:

- Coarse - 10^{-5} eV/atom
- Medium - 2×10^{-6} eV/atom
- Fine - 10^{-6} eV/atom
- Ultra-fine - 5×10^{-7} eV/atom

Note: When the main quality is set to Express the SCF tolerance is also set to Express which corresponds to 10^{-4} eV/cell.

Energy tolerances per: Specifies whether energy tolerances are calculated as the energy change per atom (Atom is the default setting) or per unit cell (the Cell value is enforced when the main quality, and hence the SCF tolerance quality, is set to Express).

k-point set: Define the number of integration points that will be used to integrate the wavefunction in reciprocal space. Available options are:

- Gamma - a single point at (0, 0, 0)
- Coarse
- Medium
- Fine

Pseudopotentials: Select the type of pseudopotential to be used. Two different types of pseudopotentials are available, ultrasoft and norm-conserving; both of them are available as either generated on the fly (OTFG) potentials or as tabulated potentials. OTFG potentials are generally preferred for reasons of accuracy and consistency. They are required for NMR calculations.

- OTFG ultrasoft (default) - the preferred option, ultrasoft pseudopotentials allow calculations to be performed with lower energy cutoffs. On-the-fly generation produces potentials that are consistent between solid state and pseudo-atom calculations since they use the same exchange-correlation functional throughout. The set of OTFG ultrasoft pseudopotentials introduced in Materials Studio 8.0 provides results in close agreement with all electron calculations and is very accurate for describing ground state structures.
- OTFG norm conserving - typically harder and therefore more computationally expensive than ultrasoft pseudopotentials. Norm-conserving potentials are currently required for linear response-based calculations of phonon properties and of polarizabilities and for calculations with nonlocal exchange-correlation functionals (for example, screened exchange).
- Ultrasoft - tabulated ultrasoft pseudopotentials, provided for compatibility with earlier versions of Materials Studio.
- Norm conserving - tabulated norm-conserving pseudopotentials, provided for compatibility with earlier versions of Materials Studio.

Note: It is not recommended to use PW91 exchange-correlation functional when requesting on the fly generation of pseudopotentials; PBE, RPBE, WC, BLYP, or PBESOL are better options when a GGA functional is required.

Note: When you specify the type of pseudopotential to be used in this way, the default pseudopotential of that type for each element will be used in the calculation.

Tip: Use the Electronic Options dialog to exercise more control over which pseudopotentials are used for each element.

Relativistic treatment: The way relativistic effects are incorporated into OTFG pseudopotentials. Options are:

- Schroedinger
- Koelling-Harmon (default)
- ZORA

Use core hole: Specify whether to include core holes in the calculation; core holes can be used in core level spectroscopy calculations and should be defined using the Core Hole tab of the Electronic Configuration dialog.

Note: For calculations exploiting core holes, on-the-fly pseudopotentials must be used.
If the *Use core hole* checkbox is not checked, any core holes in the input system will not be preserved during the calculation.

Note: CASTEP calculations with core holes assume by default that an electron is removed from the system, so it is treated as having a charge of 1 (or one more than specified in the *Charge* field on the Setup tab of the CASTEP Calculation dialog). In some circumstances, for example when studying impurities, it might be more appropriate to consider the system as charge neutral. In order to achieve this you should specify the *Charge* of -1 on the Setup tab, in this way the CASTEP input file will have a zero charge. It is also possible to edit the `seedname.param` file to specify a fractional charge. The strength of the core hole can be adjusted by editing the `seedname.cell` file and modifying the pseudopotential definition string (for example, change `{1s1}` to `{1s0.5}` to use a core hole with the charge of 0.5).

More...: Provides access to the CASTEP Electronic Options dialog, which allows you to set up and display further details of the electronic Hamiltonian.

Access methods

Menu	*Modules	CASTEP	Calculation	Electronic*
Toolbar	 *	Calculation	Electronic*

See Also:

Plane wave basis set
Pseudopotentials
Requesting core level spectroscopy
Setting up a core hole calculation
CASTEP Calculation dialog
CASTEP Electronic Options dialog