OptaDOS: User Guide
Version 1.0

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Chapter 1

Introduction

1.1 Background

OptaDOS is a code for calculating optical, core-level excitation spectra along with full, partial and joint electronic density of states (DOS). The code was developed by merging the LinDOS code of Andrew Morris and Chris Pickard at University College London with the optical properties code of Rebecca Nicholls and Jonathan Yates at Oxford University. OptaDOS is written in Fortran 95 and may be run in parallel using MPI. At present OptaDOS interfaces with CASTEP output files, although it is extendible to perform calculations on any set of band eigenvalues and their derivatives generated by any electronic structure code.

The code is freely available through the GPL licence with the request that the following citation (quoted in full) is required in any publication resulting from the use of OptaDOS.

Andrew J. Morris, R. J. Nicholls, C. J. Pickard and Jonathan R. Yates, The OptaDOS code, Comp. Phys. Comm. (2011).

Further information and examples can be found at

www.optados.org

1.2 Features

OptaDOS generates optical, core-level excitation spectra along with full, partial and joint electronic DOS. The DOS, PDOS and JDOS take advantage of the linear and adaptive smearing schemes which are more accurate than standard Gaussian smearing since they exploit knowledge of the gradients of the bands at each k-point in the Brillouin zone. These DOS are the basis of the more advanced functionality of OptaDOS, the core and optical spectra.

Along with data text files OptaDOS also generates .agr files of results to be read by grace.

Chapter 2

Getting Started

2.1 Installation

`OptaDOS` is usually obtained in a gzipped tarball, `optados-X.X.tar.gz`. Extract this (`tar -xzf optados-X.X.tar.gz`) in the desired directory. Inside the `optados/` directory are a number of sub directories, `documents/`, `examples/`. The code may be compiled using the `Makefile` in the `optados/` directory. The `SYSTEM`, `BUILD`, `COMMS_ARCH` and `BIN_DIR` flags must be set, either in the `Makefile`, or from the command line (for example `make BUILD=fast`).

2.1.1 SYSTEM

Choose which compiler to use to make `OptaDOS`. The valid values are:

- `g95` (default)
- `gfortran`
- `ifort`
- `nag`
- `pathscale`
- `pgf90`
- `sun`

2.1.2 BUILD

Choose the level of optimisations required when making `OptaDOS`. The valid values are:

- `fast` (default) All optimisations
- `debug` No optimisations, full debug information

2.1.3 COMMS_ARCH

Whether to compile for serial or parallel execution. The valid values are:

- `serial` (default)
- `mpi`

2.1.4 BIN_DIR

Choose where to place the `OptaDOS` binary. The default is the `OptaDOS` directory.

2.2 Usage

```
optados.x86_64 [seedname]
```

- `seedname`: If a seedname string is given the code will read its input from a file `seedname.odi`. The default value is CASTEP.

Chapter 3

Parameters

3.1 `seedname.odi` File

The `OptaDOS` input file `seedname.odi` has a flexible free-form structure.

The ordering of the keywords is not significant. Case is ignored (so `smearing_width` is the same as `Smearing_Width`). Characters after !, or # are treated as comments. Most keywords have a default value that is used unless the keyword is given in `seedname.odi`. Keywords may be set in any of the following ways

```
smearing_width = 0.4
smearing_width :  0.4
smearing_width 0.4
```

A logical keyword can be set to `.true.` using any of the following strings: `T`, `true`, `.true.`.

3.2 Parameters

3.2.1 `character(len=20) :: task`

Tells the code what to compute.

The valid options for this parameter are:

- `dos` (default)
- `compare_dos`
- `compare_jdos`
- `jdos`
- `pdos`
- `optics`
- `core`
- `all`

Several taks can be specified *e.g.* to compute dos and jdos use `task : dos jdos`. However, the `compare_dos` and `compare_jdos` tasks can only be combined with each other, and no additional tasks. `compare_dos` and `compare_jdos` calculate the DOS and JDOS respectivly using all broadening schemes. It is good practice to check the quality of the underlying DOS before other tasks are requested.

3.2.2 `character(len=50) :: broadening`

Specified the scheme used to broaden a discrete sampling of the Brillouin Zone to a continuous spectral function.

The valid options for this parameter are:

- `adaptive` (default)
- `fixed`
- `linear`
- `quad` (not currently implimented)

3.2.3 `integer :: iprint`

This indicates the level of verbosity of the output from 1, the bare minimum: 2, with progress reports: to 3, which corresponds to full debugging output.

The default value is 1.

3.2.4 character(len=20) :: energy_unit

The energy unit to be used for writing quantities in the output files.

The valid options for this parameter are:

- eV (default)
- Ry
- Ha

3.2.5 logical :: legacy_file_format

- TRUE Read CASTEP input compatible with versions < 6.0.
- FALSE (Default) Read CASTEP input compatible for use with CASTEP versions 6.0+ and generated with the castep spectral task.

3.2.6 real(kind=dp) :: adaptive_smearing

Set the relative smearing in the adaptive scheme.

Default value is 1.4

3.2.7 real(kind=dp) :: fixed_smearing

Smearing width for fixed broadening.

If spectral_scheme = fixed default value is 0.3eV.

3.2.8 real(kind=dp) :: scissor_op

Value of the scissor operator.

Default value is 0 eV (*i.e.* not used)

3.2.9 logical :: compute_efermi

If compute_efermi=TRUE, then OptaDOS will use the value of the Fermi level computed from the integration of the DOS. If compute_efermi=FALSE, then the value set by fermi_energy will be used, if fermi_energy is not set the value from the bands file will be used.

The default value is FALSE.

3.2.10 `real(kind=dp) :: fermi_energy`

Value of the Fermi energy.

No default value

3.2.11 `character(len=20) :: output_format`

Format in which to output data.

The valid options for this parameter are:

- `gnuplot` (not implemented yet)
- `grace` (default)

3.2.12 `logical :: finite_bin_correction`

Force each Gaussian to be larger than a single energy bin. (Useful for adaptive smearing and semi-core states when `numerical\_intdos=TRUE`).

Default value `FALSE`.

3.2.13 `logical :: numerical_intdos`

Calculate the integrated dos by numerical integration instead of semi-analytically. (Useful for comparison with `LinDOS`.)

Default value `FALSE`.

3.2.14 `logical :: set_efermi_zero`

Shift energy scales so that the Fermi eergy is at 0.

Default value `TRUE`.

3.2.15 `logical :: compute_band_energy`

Compute the band energy by summing bands both using CASTEPś eignevalue and `OptaDOS`ś density of states.

Default value `TRUE`.

3.2.16 `logical :: dos_per_volume`

Present DOS per simulation cell volume

Default value FALSE.

3.2.17 real(kind=dp) :: dos_min_energy

Lower energy range for DOS and related properties.

Default value is 5eV below the lowest eigenvalue in the bands file.

3.2.18 real(kind=dp) :: dos_max_energy

Upper energy range for DOS and related properties.

Default value is 5eV above the highest eigenvalue in the bands file.

3.2.19 real(kind=dp) :: dos_nbins

Instead of setting a Default value dos_spacing the toal number of DOS bins may be given. (Useful for comparison with LinDOS.)

3.2.20 real(kind=dp) :: dos_spacing

Resolution at which to compute the DOS and related properties. Default value is 0.1eV

3.2.21 real(kind=dp) :: jdos_max_energy

Upper energy range for JDOS and related properties.

Default value is the difference between the valence band maximum (or Fermi level) and the highest eigenvalue in the bands file.

3.2.22 real(kind=dp) :: jdos_spacing

Resolution at which to compute the DOS and related properties. Default value is 0.01eV.

3.2.23 character(len=20) :: optics_geom

- polycrystalline (Isotropic average)
- polarized
- unpolarized
- tensor (Full dielectric tensor)

3.2.24 `real(kind=dp) :: optics_qdir(3)`

Direction of polarisation. Must be specified if `optics_geom :polarized` or `optics_geom : unpolarized` . No default

3.2.25 `character :: pdos`

Defines which components to include in the pdos analysis:

- `angular` (decompose as s,p,d *etc.*)
- `sites` (decompose onto atomic sites, C, H *etc.*)
- `species` (decompose onto atomic species C1, H1, H2 *etc.*)
- `species_ang` (decompose onto angular momentum channels and species C1s, C1p *etc.*)
- `C:H` (decompose onto Carbon and Hydrogen sites)
- `C1:C3:C4-C8` (decompose onto atoms C1, C2 and C4,C5,C6,C7,C8)
- `Si1[s;d]` (decompose onto 's' and 'd' channels for atom Si1)
- `sum:C1:C3:C4-C8` (decompose onto atoms C1, C2 and C4,C5,C6,C7,C8 and combine into the single projection)

3.2.26 `character(len=50) :: devel_flag`

Not a regular keyword. Its purpose is to allow a developer to pass a string into the code to be used inside a new routine as it is developed.

No default.

Chapter 4

Examples

Each example in the `examples/` directory contains example CASTEP input files and a sample `OptaDOS` input file.

4.1 DOS

See `examples/Si2_DOS/`. This is a simple example of using `OptaDOS` for calculating electronic density of states. We choose to recalculate the Fermi level using the calculated DOS, rather than use the Fermi level suggested by CASTEP. The DOS is outputted to `Si2.adaptive.dat`. A file suitable for plotting using `xmgrace` is written to `Si2.adaptive.agr`. If `TASK : compare_dos` is used instead, `OptaDOS` will calculate DOS using all the broadening methods, this is good practice to see whether the broadening widths are appropriate before more advanced tasks are carried out, such as JDOS, core and optical calculations.

4.2 PDOS

See `examples/Si2_PDOS/`. This is a simple example of using `OptaDOS` for calculating partial electronic density of states. We choose to decompse the DOS into angular momentum channels (`PDOS : angular`). We choose to recalculate the Fermi level using the calculated DOS, rather than use the Fermi level suggested by CASTEP. The output can be found in `Si2.pdos.dat`. Other things to try are:

- `PDOS : Si1;Si2(s)` – Output the PDOS on Si atom 1 and the PDOS on the s-channel of Si atom 2. (Resulting in two projectors)
- `PDOS : sum:Si1-2(s)` – Output the sum of the s-channels on the two Si atoms. (Resulting in one projector)
- `PDOS : Si1(p)` – Output the p-channel on Si atom 1. (Resulting in one projector)

4.3 JDOS

See `examples/Si2_JDOS/`. This is a simple example of using `OptaDOS` for calculating joint electronic density of states. This is a simple example of using `OptaDOS` for calculating joint electronic density of states. We choose to recalculate the Fermi level using the calculated DOS, rather than use the Fermi level suggested by CASTEP. If `TASK : compare_jdos` is used instead, `OptaDOS` will calculate the JDOS using all the broadening methods, this is good practice to see whether the broadening widths are appropriate before more advanced tasks are carried out. The JDOS is outputted to `Si2.jadaptive.dat`. A file suitable for plotting using `xmgrace` is written to `Si2.jadaptive.agr`.