User Manual

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Introduction

DensityTool is a FORTRAN program, designed to compute the local density of states (LDOS) $L(E, \mathbf{r})$ and local spin density of states (LSDOS) $S(E, \mathbf{r})$ from the output of the VASP package [1, 2]. The program includes various routines to further modify the density data for visualization. The main input are the PARCHG, CHGCAR and EIGENVAL files from a preceding VASP calculation.

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Methodology

DensityTool computes the energy-resolved LDOS and LSDOS from the band- and $\mathbf{k}$-decomposed partial charge densities and the band structure as calculated by VASP. The density of states (DOS) is defined as

$$D(E) = \frac{N_e}{(2\pi)^3} \sum_n \int_{\mathrm{BZ}} \delta(E - \epsilon_{n,\mathbf{k}})\ d^3k \tag{1}$$

with N_e the band occupancy (2 for non-magnetic and 1 for magnetic or non-collinear calculations). The partial charge density describes the probability to find an electron described by a wavefunction $\varphi_{n,\mathbf{k}}(\mathbf{r})$ with a given wavevector $\mathbf{k}$ and band index n in a given space region,

$$P_{n,\mathbf{k}}(\mathbf{r}) = |\varphi_{n,\mathbf{k}}(\mathbf{r})|^2 . \tag{2}$$

When spin is conserved (i.e., in absence of spin-orbit coupling and non-collinear magnetism), the wavefunction $\varphi_{n,\mathbf{k},\chi}(\mathbf{r})$ can be additionally labeled by its spin eigenvalue $\chi = \uparrow\downarrow$. We will now distinguish two different cases.

Spin not included

If the system is spin-degenerate ($N_e = 2$) or spin is not conserved ($N_e = 1$), then the total charge density is defined as

$$\rho(\mathbf{r}) = \frac{N_e \Omega_{\text{cell}}}{(2\pi)^3} \sum_n \int_{\text{BZ}} f_{n,\mathbf{k}} P_{n,\mathbf{k}}(\mathbf{r})\ d^3k, \tag{3}$$

where $f_{n,\mathbf{k}}$ is the Fermi-Dirac distribution, Ω_{cell} is the unit cell volume, $\Omega_{\text{cell}} = L_1 L_2 L_3 |\hat{L}_3 \cdot (\hat{L}_1 \times \hat{L}_2)|$, where L_i and $\hat{L}_i$ are the magnitude and unit vector of the lattice vectors spanning the unit cell, respectively.
The LDOS can be understood as a combination of the DOS and the partial charge density, and it is defined as

$$L(E, \mathbf{r}) = \frac{N_e}{(2\pi)^3} \sum_n \int_{\text{BZ}} \delta(E - \epsilon_{n,\mathbf{k}}) P_{n,\mathbf{k}}(\mathbf{r})\ d^3k. \tag{4}$$

Being a 5-dimensional quantity, in order to visualize it, restrictions to chosen subspaces of the unit cell or averaging of the data is necessary. A useful approach is to calculate planar-averaged LDOS. For this we choose one lattice vector direction, e.g., $\hat{L}_3$ with a coordinate r_3 measuring the position along this direction. The remaining two lattice vectors define a plane, over which the LDOS is averaged as

$$\bar{L}(E, r_3) = \frac{1}{A_{12}} \iint L(E, \mathbf{r}) |\hat{L}_1 \times \hat{L}_2| dr_1 dr_2, \tag{5}$$

where $A_{12} = L_1 L_2 |\hat{L}_1 \times \hat{L}_2|$ is the area of the cut of the plane spanned by $\hat{L}_1$ and $\hat{L}_2$ through the unit cell. Equation (5) can be further rewritten as

$$\bar{L}(E, r_3) = \frac{N_e}{(2\pi)^3} \sum_n \int_{\text{BZ}} \delta(E - \epsilon_{n,\mathbf{k}}) \bar{P}_{n,\mathbf{k}}(r_3)\ d^3k, \tag{6}$$

where $\bar{P}_{n,\mathbf{k}}(r_3)$ is the partial charge average (PCA) over the area A_{12},

$$\bar{P}_{n,\mathbf{k}}(r_3) = \frac{1}{A_{12}} \iint P_{n,\mathbf{k}}(\mathbf{r}) |\hat{L}_1 \times \hat{L}_2| dr_1 dr_2 = \frac{1}{L_1 L_2} \iint P_{n,\mathbf{k}}(\mathbf{r}) dr_1 dr_2. \tag{7}$$

Spin included

In magnetic systems with conserved spin, a special treatment is necessary. We define spin-resolved partial charge densities

$$P^{\uparrow\downarrow}_{n,\mathbf{k}}(\mathbf{r}) = \left| \varphi^{\uparrow\downarrow}_{n,\mathbf{k}}(\mathbf{r}) \right|^2 \tag{8}$$

and spin-resolved charge densities

$$\rho^{\uparrow\downarrow}(\mathbf{r}) = \frac{1}{(2\pi)^3} \sum_n \int_{\text{BZ}} f^{\uparrow\downarrow}_{n,\mathbf{k}} P^{\uparrow\downarrow}_{n,\mathbf{k}}(\mathbf{r})\ d^3k. \tag{9}$$

The total charge density is then defined as

$$\rho(\mathbf{r}) = \rho^{\uparrow}(\mathbf{r}) + \rho^{\downarrow}(\mathbf{r}) \tag{10}$$

and the spin density as

$$s(\mathbf{r}) = \rho^{\uparrow}(\mathbf{r}) - \rho^{\downarrow}(\mathbf{r}). \tag{11}$$

Using the above definition, the LDOS is expressed as

$$L(E,\mathbf{r}) = \frac{1}{(2\pi)^3}\sum_n \int_{\mathrm{BZ}} \left[\delta(E-\epsilon^{\uparrow}_{n,\mathbf{k}})P^{\uparrow}_{n,\mathbf{k}}(\mathbf{r}) + \delta(E-\epsilon^{\downarrow}_{n,\mathbf{k}})P^{\downarrow}_{n,\mathbf{k}}(\mathbf{r})\right] d^3k \tag{12}$$

and the LSDOS as

$$S(E,\mathbf{r}) = \frac{1}{(2\pi)^3}\sum_n \int_{\mathrm{BZ}} \left[\delta(E-\epsilon^{\uparrow}_{n,\mathbf{k}})P^{\uparrow}_{n,\mathbf{k}}(\mathbf{r}) - \delta(E-\epsilon^{\downarrow}_{n,\mathbf{k}})P^{\downarrow}_{n,\mathbf{k}}(\mathbf{r})\right] d^3k. \tag{13}$$

The plane-averaged charge and spin densities of states can be calculated in analogy to eqs. (5) to (7).

Computational details

Numerical calculations of electronic properties using a plane wave basis and periodic boundary conditions are performed using a discretized real and reciprocal space. Therefore, the above integrals in the reciprocal and real space are computed on a coarse mesh as

$$\frac{1}{(2\pi)^3}\int_{BZ} \dots\ d^3k \qquad \longrightarrow \qquad \frac{1}{\Omega_{\mathrm{cell}}}\sum_{\mathbf{k}\,\in\,BZ} \dots W_{\mathbf{k}} \tag{14}$$

and

$$\frac{1}{A_{12}}\iint \dots |\hat{L}_1 \times \hat{L}_2| dr_1 dr_2 \qquad \longrightarrow \qquad \frac{1}{N_1N_2}\sum_{r_1,r_2} \dots, \tag{15}$$

respectively. $W_{\mathbf{k}}$ are the weight coefficients of the wave vectors $\mathbf{k}$, depending on the discretization of the Brillouin zone. $N_{1,2}$ are the numbers of discrete points on the real space mesh along the lattice vectors $\hat{L}_{1,2}$ and they are given by the choice of the plane wave cutoff in the *ab-initio* calculation.

Most importantly, to visualize e.g. the plane-averaged LDOS (eq. (5)), it is convenient to compute it on an equidistant discrete energy mesh, in addition to the discretized r_3 coordinate. For this purpose, we approximate $\delta(E-\epsilon_{n,\mathbf{k}})$ by a normalized Gaussian as

$$\delta(E-\epsilon_{n,\mathbf{k}}) \qquad \longrightarrow \qquad g_{n,\mathbf{k}}(E,\sigma) = \frac{1}{\sigma\sqrt{2\pi}}\, e^{\frac{-(E-\epsilon_{n,\mathbf{k}})^2}{2\sigma^2}} \tag{16}$$

with a proper smearing value σ. We further introduce a threshold parameter η, redefining eq. (16) as

$$\tilde{g}_{n,\mathbf{k}}(E,\sigma) = \begin{cases} g_{n,\mathbf{k}}(E,\sigma) & \text{for } g_{n,\mathbf{k}}(E,\sigma) > \frac{\eta}{\sigma\sqrt{2\pi}} \\ 0 & \text{for } g_{n,\mathbf{k}}(E,\sigma) \leqslant \frac{\eta}{\sigma\sqrt{2\pi}}. \end{cases} \tag{17}$$

Using this treatment allows for each energy E to include only partial density contributions of states with $g_{n,\mathbf{k}}(E,\sigma) > \frac{\eta}{\sigma\sqrt{2\pi}}$ during the local density function calculations, substantially speeding it up. This definition ensures a systematic and stable treatment for different inputs. For each E, only states with energy in the range $\pm\sigma\sqrt{-2\ln(\eta)}$ around E are considered. $\eta = 0.001$ is a very good compromise between numerical precision and program speed up, recovering 99.98% of the distribution function area).

Program details

Code source and examples

DensityTool source is free. The FORTRAN code, input parameters file, manual and application examples can be found at:

`https://github.com/llodeiro/DensityTool`

Licensing provisions

Compilation and execution

The program can be compiled using a FORTRAN compiler, e.g.:

```
ifort -O2 -o DENSITYTOOL.X DENSITYTOOL.F90
```

or

```
gfortran -O3 -o DENSITYTOOL.X DENSITYTOOL.F90
```

We recommend `-O2` and `-O3` as optimizers for the respective compiler.

The executable `DENSITYTOOL.X` has to be executed in a folder with the VASP output and the input file, `DENSITYTOOL.IN`, if used, as

```
/PROGRAMFOLDER/DENSITYTOOL.X < DENSITYTOOL.IN > DENSITYTOOL.OUT
```

In `DENSITYTOOL.IN` the parameters of the calculation can be specified. If `DENSITYTOOL.IN` is not used, the parameters for the calculation are asked by the program and can be entered manually.

Input files

DensityTool requires three VASP output files as input: EIGENVAL, CHGCAR and the PARCHG files set. The program reads these files and extracts information necessary to compute LDOS and LSDOS. The name and format of these files is fixed.

- From EIGENVAL, the program extracts the number of atoms, bands, **k**-points, the Kohn-Sham eigenvalues $\epsilon_{n,\mathbf{k}}$, and the **k**-point weights, $W_{\mathbf{k}}$. **Note that EIGENVAL file from the original SCF calculation has to be used**, since the one from the non-SCF calculation of partial charge density is written in a different format.

- From CHGCAR, the program extracts the size of the real space mesh, i.e., the N_i values, and the unit cell dimensions.
- From the PARCHG files set the program extracts the partial charge density $P_{n,\mathbf{k}}(\mathbf{r})$. Only PARCHG files contributing to the energy window of interest (including those that contribute via the Gaussian smearing in eq. (17)) are necessary. The PARCHG name format is `PARCHG.nnnn.kkkk`, where *nnnn* is a four index of band number, and *kkkk* is a four index of **k**-point number, as VASP writes the PARCHG files names for individual bands and **k**-points.

Input parameters

The program is controlled by a set of input parameters which can be entered either manually after the execution or via `DENSITYTOOL.IN`. The parameters are:

- SIGMA (real), smearing σ in eV in the Gaussian eq. (16)
- EMIN (real), minimum of the energy window in eV
- EMAX (real), maximum of the energy window in eV
- NEN (integer), number of discrete energy values between EMIN and EMAX
- ETHR (real), threshold value from which the partial charge densities contribute to L(S)DOS
- SPINCASE (integer), type of system, 1: spin conserved, spin-degenerate, 2: spin conserved, spin-nondegenerate, 3: spin not conserved
- DIRECTION (integer), 1,2, or 3, choosing the lattice vector along which the data is NOT averaged in eq. (6)
- DOPCA (logical), switches on/off (T/F) the PCA routine (plane-averaged partial charge density)
- DOPSA (logical), switches on/off (T/F) the PSA routine (plane-averaged partial spin density)
- DOLDOS (logical), switches on/off (T/F) the LDOS routine (plane-averaged LDOS, using energy averages if SPINCASE = 2)
- DOLDOSFULL (logical), switches on/off (T/F) the LDOSFULL routine (LDOS, not averaged, using energy averages if SPINCASE = 2)
- DOLSDOS (logical), switches on/off (T/F) the LSDOS routine (plane-averaged LSDOS, using energy averages if SPINCASE = 2)
- DOLSDOSFULL (logical), switches on/off (T/F) the LSDOSFULL routine (LSDOS, not averaged, using energy averages if SPINCASE = 2)

- DOPARCHGSPIN (logical), switches on/off (T/F) the PARCHGSPIN routine (plane-averaged partial spin-resolved charge densities, only for SPINCASE = 2)
- DOCHGCARSPIN (logical), switches on/off (T/F) the CHGCARSPIN routine (plane-averaged spin-resolved total charge density, only for SPINCASE = 2)
- DOCHGCARAVG (logical), switches on/off (T/F) the CHGCARAVG routine (plane-averaged total charge and spin densities)
- DOLDOSMAG (logical), switches on/off (T/F) the LDOSMAG routine (plane-averaged LDOS, using correct spin-resolved energies)
- DOLSDOSMAG (logical), switches on/off (T/F) the LSDOSMAG routine (plane-averaged LSDOS, using correct spin-resolved energies)
- DOLDOSFULLMAG (logical), switches on/off (T/F) the LDOSFULLMAG routine (LDOS, not averaged, using correct spin-resolved energies)
- DOLSDOSFULLMAG (logical), switches on/off (T/F) the LSDOSFULLMAG routine (LSDOS, not averaged, using correct spin-resolved energies)

DensityTool working and output data

After initial read of the input variables, the program prints their values to the specified output file (e.g., `DENSITYTOOL.OUT`). Then, depending on the choice of the task, the program runs different routines with their own output. In case of file reading and writing problems, the program stops and informs in which file is the problem. To avoid problems with overwriting some output files, the program stops if the output file is already created. Note that the unit of all local functions is density unit ($\frac{e}{\mathrm{bohr}^3}$) as opposed to VASP output, which is in electronic charge unit.

Routines

PCA

In this routine, PCA is calculated according to eq. (7) for each partial charge density stored in `PARCHG.nnnn.kkkk`. The lattice direction along which the data remains spatially resolved is given by the parameter DIRECTION = $j \in [1, 2, 3]$.
For each band and **k**-point the routine writes the plane-averaged partial charge density into the file `PARCHG.nnnn.kkkk.Rj` where j = DIRECTION.
The output of this routine is necessary for the calculation of plane-averaged LDOS. Once PCA was calculated, LDOS can be easily recalculated for different energy windows and resolutions saving computational resources.

PSA

In this routine, plane-averaged partial spin density (PSA) is calculated for each partial spin density stored in `PARCHG.nnnn.kkkk`. The lattice direction along which the data remains spatially resolved is given by the parameter DIRECTION = $j \in [1, 2, 3]$.
For each band and **k**-point the routine writes the plane-averaged partial spin density into the file `PARCHG.nnnn.kkkk.SRj` where j = DIRECTION.
The output of this routine is necessary for the calculation of plane-averaged LSDOS. Once PSA was calculated, LSDOS can be easily recalculated for different energy windows and resolutions saving computational resources.
The PSA routine can be used only for SPINCASE = 2. While for SPINCASE = 1 the partial spin density is zero by definition, the case of SPINCASE = 3 cannot be evaluated, because currently VASP does not write the partial spin (magnetization) densities for non-collinear systems.

LDOS

In this routine, the plane-averaged LDOS is calculated. If spin is not included (SPINCASE = 1 or 3), eq. (6) is calculated. If spin is included (SPINCASE = 2), the spin-dependent energies are approximated by their average as $\epsilon^{\uparrow\downarrow}_{n,\mathbf{k}} \approx {}^{(\epsilon^{\uparrow}_{n,\mathbf{k}}+\epsilon^{\downarrow}_{n,\mathbf{k}})}/_2 =: \bar{\epsilon}_{n,\mathbf{k}}$, which allows for the use of eq. (6) also in this case. For a proper inclusion of the spin-resolved densities, please use the LDOSMAG routine.
As input, LDOS routine reads the PCAs stored in `PARCHG.nnnn.kkkk.Rj`. Therefore, a PCA calculation using the PCA routine must be performed before LDOS.
The LDOS is calculated for each of the NEN energy values between EMIN and EMAX. For each of them, the program performs a loop over all bands and **k**-points. For each $(n, \mathbf{k})$, if `PARCHG.nnnn.kkkk.Rj` file present, its name is written to the output, followed by the triple $g_{n,\mathbf{k}}$ $\epsilon_{n,\mathbf{k}}$ E. If the state contributes to the given energy E (i.e., $g_{n,\mathbf{k}}(E, \sigma) > \frac{\eta}{\sigma\sqrt{2\pi}}$), “YES” is written to the output.
As a result, for each energy an individual file `LDOS.Rj.eeee.dat` is written, with *eeee* the index of the energy E. The data can be plotted for each energy individually, or all in one figure (e.g. by using the `cat` command).

LSDOS

In this routine, the plane-averaged LSDOS is calculated if SPINCASE = 2. The spin-dependent energies are approximated by their average as $\epsilon^{\uparrow\downarrow}_{n,\mathbf{k}} \approx {}^{(\epsilon^{\uparrow}_{n,\mathbf{k}}+\epsilon^{\downarrow}_{n,\mathbf{k}})}/_2 =: \bar{\epsilon}_{n,\mathbf{k}}$. This approximation allows a faster evaluation, but it may be to crude for some applications. For a proper inclusion of the spin-resolved densities, please use the LSDOSMAG routine.
The input and output is analogous to the LDOS routine, the name format of the output being `LSDOS.Rj.eeee.dat`.

LDOSFULL

In this routine, the full LDOS is calculated in analogy to the LDOS routine. As input the program reads directly the VASP output `PARCHG.nnnn.kkkk`. The result is an individual file

`LDOS.FULL.eeee.dat` for each energy E. The output files are written in the format of the CHGCAR file as written by VASP. This enables a direct visualization of the data, e.g. by Vesta. The corresponding value of E is added in the corresponding title line of the file.
For a proper inclusion of the spin-resolved densities, please use the LDOSFULLMAG routine.

LSDOSFULL

In this routine, the full LSDOS is calculated if SPINCASE = 2 in analogy to the LDOSFULL routine. The output is written into the files `LSDOS.FULL.eeee.dat` in the CHGCAR format.
For a proper inclusion of the spin-resolved densities, please use the LSDOSFULLMAG routine.

PARCHGSPIN

In this routine, PCA is calculated if SPINCASE = 2 for each of the spin-up and -down density separately, in analogy to PCA routine. The output of this routine is necessary for a subsequent LDOS and LSDOS calculation with a proper treatment of the non-degenerate spin-up and -down states.
First, the spin-resolved partial charge densities are written into `PARCHG.nnnn.kkkk.ALPHA` and `PARCHG.nnnn.kkkk.BETA` (these files are written in the CHGCAR format), and the calculated PCA is written into the files `PARCHG.nnnn.kkkk.ALPHA.Rj` and `PARCHG.nnnn.kkkk.BETA.Rj` for the spin-up and -down densities, respectively.

CHGCARSPIN

In this routine, the plane-averaged spin-resolved total charge density is calculated if SPINCASE = 2. The routine reads directly the CHGCAR file.
The spin-resolved total charge densities are written into `CHGCAR.ALPHA` and `CHGCAR.BETA` (these files are written in the CHGCAR format), and the PCA data are written into `CHGCAR.ALPHA.Rj` and `CHGCAR.BETA.Rj`.

CHGCARAVG

In this routine, plane-averaged total charge density, spin density, and total magnetization are calculated. The input is the CHGCAR file.
For SPINCASE = 1, only the plane-averaged total charge density is calculated and written to `CHGCAR.Rj`.
For SPINCASE = 2, also the total spin (magnetization) density is written into `CHGCAR.S` and the calculated plane-averaged total spin (magnetization) density is written into `CHGCAR.SRj`. The magnetization and absolute magnetization are calculated and written into the output.
For SPINCASE = 3, also the total spin (magnetization) density is written into `CHGCAR.Sm` for each of the three orientations of the quantization axis m. The calculated plane-averaged total spin (magnetization) density is written into `CHGCAR.SmRj`. The three components of the magnetization and absolute magnetization are calculated and written into the output.
The files `CHGCAR.S` and `CHGCAR.Sm` are written in the CHGCAR format.

LDOSMAG

In this routine, the plane-averaged LDOS is calculated as in LDOS routine if SPINCASE = 2, but the non-degenerate spin-dependent energies are treated properly. The input are the `PARCHG.nnnn.kkkk.ALPHA.Rj` and `PARCHG.nnnn.kkkk.BETA.Rj` files calculated by the PARCHGSPIN routine.
The results for each energy are written into `LDOSMAG.Rj.eeee.dat`.

LSDOSMAG

In this routine, the plane-averaged LSDOS is calculated as in LDOSMAG routine if SPINCASE = 2, including the proper treatment of the non-degenerate spin-dependent energies. The input are the `PARCHG.nnnn.kkkk.ALPHA.Rj` and `PARCHG.nnnn.kkkk.BETA.Rj` files calculated by the PARCHGSPIN routine.
The results for each energy are written into `LSDOSMAG.Rj.eeee.dat`.

LDOSFULLMAG

In this routine, the LDOS is calculated without averaging as in LDOSFULL routine if SPINCASE = 2, including the proper treatment of the non-degenerate spin-dependent energies. The input are the `PARCHG.nnnn.kkkk.ALPHA` and `PARCHG.nnnn.kkkk.BETA` files calculated by the PARCHGSPIN routine.
The results for each energy are written into `LDOSMAG.FULL.eeee.dat` in the CHGCAR format.

LSDOSFULLMAG

In this routine, the LSDOS is calculated without averaging as in DOLSDOSFULL if SPINCASE = 2, including the proper treatment of the non-degenerate spin-dependent energies. The input are the `PARCHG.nnnn.kkkk.ALPHA` and `PARCHG.nnnn.kkkk.BETA` files calculated by the DOPARCHGSPIN routine.
The results for each energy are written into `LSDOSMAG.FULL.eeee.dat` in the CHGCAR format.

Examples

The following examples demonstrate the usage of DensityTool. Mostly the underlying VASP calculations are done with a small number of **k**-points to keep the amount of data low. Unless stated otherwise, the results should not be interpreted as physically meaningful. We provide all input and output files for all examples at the code repository, `https://github.com/llodeiro/DensityTool`.

Cubic C

The calculated system is diamond in the conventional unit cell (see Fig. 1a). The VASP calculation was done at the Γ point. The highest occupied level is located at $E = 9.73\,\mathrm{eV}$

and the lowest unoccupied one at $E = 14.5\,\mathrm{eV}$. Therefore, the LDOS has finite contributions only around these energies in the chosen energy range $E \in (8{,}15)\,\mathrm{eV}$.

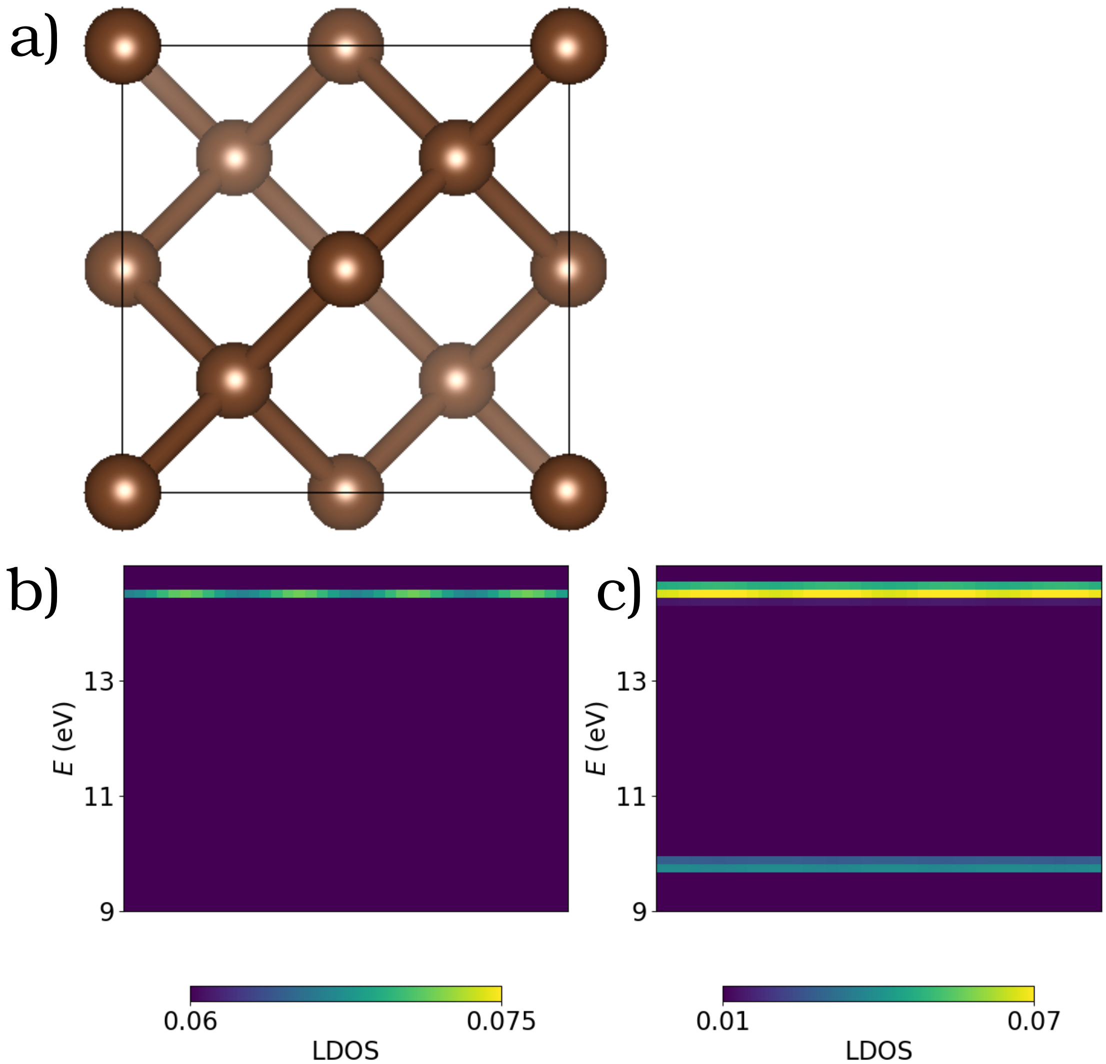

Figure 1: Diamond in the conventional cubic unit cell. a) atomic structure, b) and c) LDOS averaged in the x-y-plane of the unit cell. The data in both panels is identical, but in b) the range of visualized LDOS is (0.06, 0.075) whereas in c) it is (0.01,0.07).

For the material we calculated PCA by averaging the partial charge densities in the x-y-plane of the unit cell and in the next step we used it to calculate the plane-averaged LDOS. Following parameters were chosen as input of DensityTool to calculate PCA and LDOS in a single run:

```
0.10 !#Enter SIGMA value in eV
8.0 !#Enter EMIN value in eV
15.0 !#Enter EMAX value in eV
50 !#Enter NEN value (Integer)
0.001 !#Enter ETHR value in eV
```

```
3 !#Enter SPINCASE value (1,2 or 3)
3 !#Enter DIRECTION value (1,2,3)
T !#Enter DOPCA logical value (T or F)
F !#Enter DOPSA logical value (T or F)
T !#Enter DOLDOS logical value (T or F)
F !#Enter DOLDOSFULL logical value (T or F)
F !#Enter DOLSDOS logical value (T or F)
F !#Enter DOLSDOSFULL logical value (T or F)
F !#Enter DOPARCHGSPIN logical value (T or F)
F !#Enter DOCHGCARSPIN logical value (T or F)
F !#Enter DOCHGCARAVG logical value (T or F)
F !#Enter DOLDOSMAG logical value (T or F)
F !#Enter DOLDOSFULLMAG logical value (T or F)
F !#Enter DOLSDOSMAG logical value (T or F)
F !#Enter DOLSDOSFULLMAG logical value (T or F)
```

Owing to the single-point calculation, LDOS is finite only at the discrete energy levels corresponding to the band edges, as shown in Fig. 1c. The visualized in Fig. 1b was chosen to make the spatial variation of LDOS at the conduction band edge visible.

FCC Ni

In this example we demonstrate the difference between the exact treatment of the spin-polarized energies (PARCHG) of the magnetic system and the approximation (PCA/PSA). The input files from the VASP wiki `https://www.vasp.at/wiki/index.php/Fcc_Ni_(revisited)` were used to obtain the self-consistent charge density. It was then recalculated non-selfconsistently on a sparser $4\times4\times4$ **k**-point mesh to reduce the amount of data.
In both cases we averaged the partial charge or spin densities in the plane spanned by two of the lattice vectors of the FCC unit cell. For the exact treatment we used the routines PARCHG, followed by LDOSMAG and LSDOSMAG for the plane-averaged LDOS and LSDOS:

```
0.05 !#Enter SIGMA value in eV
3.5 !#Enter EMIN value in eV
5.5 !#Enter EMAX value in eV
100 !#Enter NEN value (Integer)
0.001 !#Enter ETHR value in eV
2 !#Enter SPINCASE value (1,2 or 3)
3 !#Enter DIRECTION value (1,2,3)
F !#Enter DOPCA logical value (T or F)
F !#Enter DOPSA logical value (T or F)
F !#Enter DOLDOS logical value (T or F)
F !#Enter DOLDOSFULL logical value (T or F)
F !#Enter DOLSDOS logical value (T or F)
F !#Enter DOLSDOSFULL logical value (T or F)
T !#Enter DOPARCHGSPIN logical value (T or F)
F !#Enter DOCHGCARSPIN logical value (T or F)
```

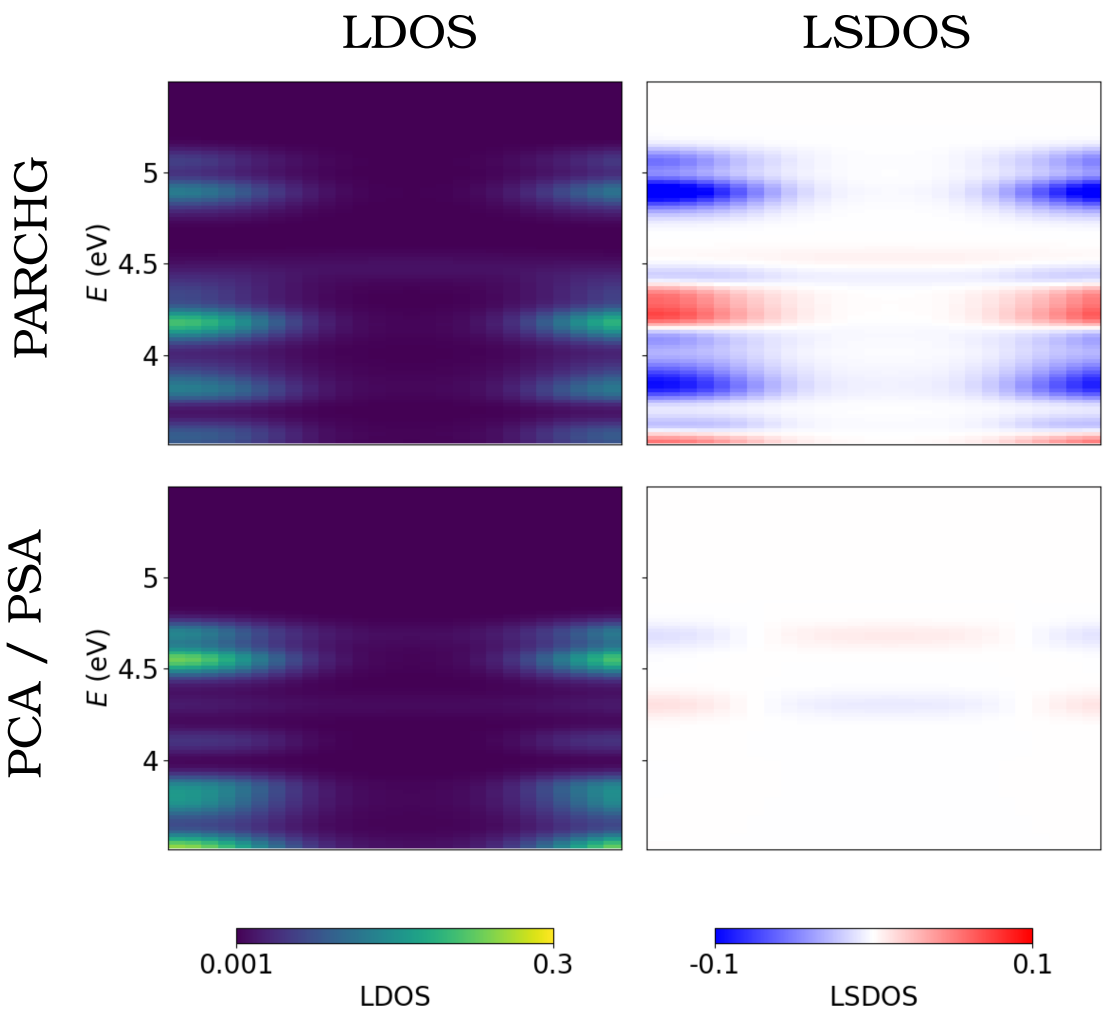

Figure 2: Ferromagnetic FCC Ni. Plane-averaged LDOS (left column) and LSDOS (right column) calculated using the exact spin-polarized energies (top row, PARCHG) and the approximation (bottom row, PCA/PSA).

```
F !#Enter DOCHGCARAVG logical value (T or F)
T !#Enter DOLDOSMAG logical value (T or F)
F !#Enter DOLDOSFULLMAG logical value (T or F)
T !#Enter DOLSDOSMAG logical value (T or F)
F !#Enter DOLSDOSFULLMAG logical value (T or F)
```

In the case of the approximation to the energies we used PCA and PSA, followed by LDOS and LSDOS:

```
0.05 !#Enter SIGMA value in eV
3.5 !#Enter EMIN value in eV
5.5 !#Enter EMAX value in eV
100 !#Enter NEN value (Integer)
0.001 !#Enter ETHR value in eV
```

```
2 !#Enter SPINCASE value (1,2 or 3)
3 !#Enter DIRECTION value (1,2,3)
T !#Enter DOPCA logical value (T or F)
T !#Enter DOPSA logical value (T or F)
T !#Enter DOLDOS logical value (T or F)
F !#Enter DOLDOSFULL logical value (T or F)
T !#Enter DOLSDOS logical value (T or F)
F !#Enter DOLSDOSFULL logical value (T or F)
F !#Enter DOPARCHGSPIN logical value (T or F)
F !#Enter DOCHGCARSPIN logical value (T or F)
F !#Enter DOCHGCARAVG logical value (T or F)
F !#Enter DOLDOSMAG logical value (T or F)
F !#Enter DOLDOSFULLMAG logical value (T or F)
F !#Enter DOLSDOSMAG logical value (T or F)
F !#Enter DOLSDOSFULLMAG logical value (T or F)
```

The results are shown in Fig. 2. It is obvious that in this case the spin splitting of the energy levels is so strong, that the approximation using the average of the spin-up and spin-down energies (PCA/PSA) leads to very different results compared to the exact treatment of the energies (PARCHG).

Hydrogenized Si(111) surface with adsorbed F6-TCNNQ molecule

The system studied in this example being a realistic model of a Si semiconductor surface with a F6-TCNNQ molecule attached to it, it can be seen as a prototypical example where DensityTool can help understanding the local electronic structure at different parts of the system. It was studied previously in Ref. [3] and the data used in this example was published in Ref. [4].

Since in the original calculation the partial charge densities are written by VASP for each **k**-point and band in the relevant energy window, the amount of stored data is very large. Therefore, for this example we provide only the plane-averaged spin-polarized partial charge densities calculated with the PARCHG routine. The LDOS is then obtained using the settings:

```
0.05 !#Enter SIGMA value in eV
3.5 !#Enter EMIN value in eV
5.5 !#Enter EMAX value in eV
100 !#Enter NEN value (Integer)
0.001 !#Enter ETHR value in eV
2 !#Enter SPINCASE value (1,2 or 3)
3 !#Enter DIRECTION value (1,2,3)
F !#Enter DOPCA logical value (T or F)
F !#Enter DOPSA logical value (T or F)
F !#Enter DOLDOS logical value (T or F)
F !#Enter DOLDOSFULL logical value (T or F)
F !#Enter DOLSDOS logical value (T or F)
```

```
F !#Enter DOLSDOSFULL logical value (T or F)
F !#Enter DOPARCHGSPIN logical value (T or F)
F !#Enter DOCHGCARSPIN logical value (T or F)
F !#Enter DOCHGCARAVG logical value (T or F)
T !#Enter DOLDOSMAG logical value (T or F)
F !#Enter DOLDOSFULLMAG logical value (T or F)
F !#Enter DOLSDOSMAG logical value (T or F)
F !#Enter DOLSDOSFULLMAG logical value (T or F)
```

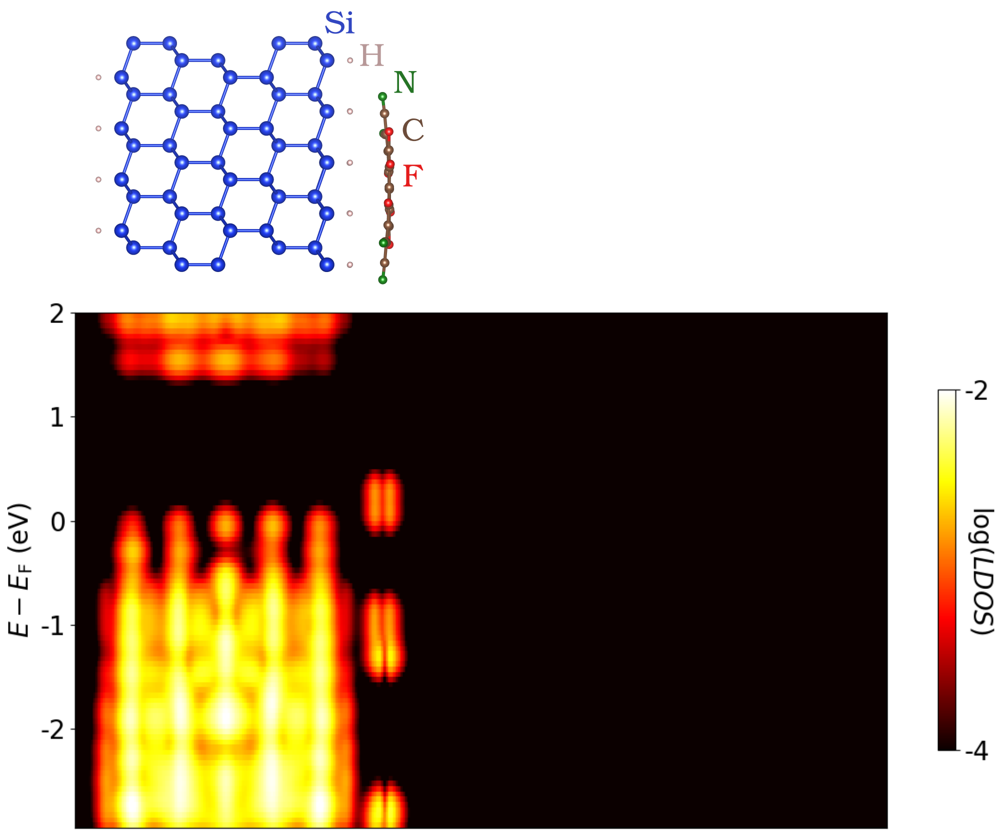

Figure 3: Hydrogenized Si(111) surface with adsorbed F6-TCNNQ molecule. Atomic structure (top) and plane-averaged LDOS (bottom).

The atomic structure of the system and the calculated plane-averaged LDOS for energies around the semiconductor band gap are shown in Fig. 3. The enhanced LDOS of the occupied stated below the Fermi energy E_F in the regions of the Si atomic planes are clearly recognizable, as well as the LDOS of the molecular orbitals adsorbed on the right surface of the Si slab.

Resume of variables used in different routines

Table 1: Resume of variables used in different routines of DensityTool. ✓means variable is used in routine.

Routine	SIGMA	EMAX	EMIN	NEN	ETHR	SPINCASE	DIRECTION
PCA							✓
PSA						✓	✓
LDOS	✓	✓	✓	✓	✓		✓
LSDOS	✓	✓	✓	✓	✓	✓	✓
LDOSFULL	✓	✓	✓	✓	✓		
LSDOSFULL	✓	✓	✓	✓	✓	✓	
PARCHGSPIN						✓	✓
CHGCARSPIN						✓	✓
CHGCARAVG						✓	✓
LDOSMAG	✓	✓	✓	✓	✓	✓	✓
LSDOSMAG	✓	✓	✓	✓	✓	✓	✓
LDOSFULLMAG	✓	✓	✓	✓	✓	✓	
LSDOSFULLMAG	✓	✓	✓	✓	✓	✓	

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