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I. INPUT FILE EXAMPLE

TEXT *** band structure calculation of Perovskite SrTiO3 ***

CONTROL iter_dft= 26 iter_hf= 0 iter_gw= 0 iter_qp= 20

admix= 0.150 adspin= 0.300 adm_gw= 0.200 acc_it_gw= 0.200

iexch= 005 scal_spin= 1.0000

nproc_tau= 24 nproc_k= 5

irel= 1 clight= 274.074e+00 rel_interst= F irel_core= 1

temperature= 1000.00

FILES

allfile= srtio3

SYM symgen= 'LR3D_R4Z_'

STRUCTURE par= 7.3793830 natom= 5 nsort= 3 istruc= 1

is= 1 2 3 3 3

b_a= 1.000000 c_a= 1.000000

a= 1.0000000000000000 0.0000000000000000 0.0000000000000000

b= 0.0000000000000000 1.0000000000000000 0.0000000000000000

c= 0.0000000000000000 0.0000000000000000 1.0000000000000000

tau= 0.0000000000000000 0.0000000000000000 0.0000000000000000

0.5000000000000000 0.5000000000000000 0.5000000000000000

0.0000000000000000 0.5000000000000000 0.5000000000000000

0.5000000000000000 0.0000000000000000 0.5000000000000000

0.5000000000000000 0.5000000000000000 0.0000000000000000

REAL SPACE MESHES mdiv= 18 18 18

nrdiv= 14 14 14

BASIS cut_lapw_ratio= 0.600 cut_pb_ratio= 0.950

eps_pb= 1.e-03

ZONES nbndf= 0

DOS emindos= -0.400 emaxdos= 0.400 ndos= 900

n_cont_frac= 28 e_small= 5.e-03

K_POINT ndiv= 4 4 4 metal= F n_k_div= 1 k_line= 001

MULTI_SCF vv0= 1.000

MAGNET b_extval= 0.000000 iter_h_ext= 00000

b_ext= 0.000 0.000 1.000

TAU MESH n_tau= 46 n_tau_int= 1000

OMEGA MESH n_omega_exa= 29 n_omega_asy= 18 omega_max= 200.00

interp_omega_d= 2

NU MESH n_nu_exa= 29 n_nu_asy= 18 nu_max= 200.00

interp_nu_d= 2

ATOMIC DATE -----

txtel= Sr z= 38.0 magn_shift= 0.000

smt= 3.37300 h= 0.0200 nrad= 616 z_dop= 0.0000

lmb= 6 lmpb= 6

lim_pb_mt= 10 8 6 6 6 6 6

ntle= 3 3 3 2 1 1 1 1 1

l augm atocc ptnl corr idmd

0 LOC 2.000 4.950 N 0

0 APW 2.000 5.800 N 0

0 LOC 0.000 6.950 N 1

1 LOC 6.000 4.950 N 0

1 APW 0.000 5.800 N 0

1 LOC 0.000 6.950 N 1

2 LOC 10.000 3.950 N 0

2 APW 0.000 4.800 N 0

2 LOC 0.000 5.950 N 1
 3 APW 0.000 4.800 N 0
 3 LOC 0.000 5.950 N 1
 4 APW 0.000 5.800 N 0
 5 APW 0.000 6.800 N 0
 6 APW 0.000 7.800 N 0
 txtel= Ti z= 22.0 magn_shift= 0.000
 smt= 1.84500 h= 0.0200 nrad= 616 z_dop= 0.0000
 lmb= 5 lmpb= 6
 lim_pb_mt= 10 8 6 6 6 6 6
 ntle= 3 3 2 1 1 1 1 1
 l augm atocc ptnl corr idmd
 0 LOC 2.000 3.950 N 0
 0 APW 2.000 4.800 N 0
 0 LOC 0.000 5.950 N 1
 1 LOC 6.000 3.950 N 0
 1 APW 0.000 4.800 N 0
 1 LOC 0.000 5.950 N 1
 2 APW 2.000 3.800 N 0
 2 LOC 0.000 4.950 N 1
 3 APW 0.000 4.800 N 0
 4 APW 0.000 5.800 N 0
 5 APW 0.000 6.800 N 0
 txtel= _O z= 8.0 magn_shift= 0.000
 smt= 1.84400 h= 0.0200 nrad= 616 z_dop= 0.0000
 lmb= 5 lmpb= 6
 lim_pb_mt= 10 8 6 6 6 6 6
 ntle= 3 2 1 1 1 1 1 1
 l augm atocc ptnl corr idmd
 0 LOC 2.000 2.950 N 0
 0 APW 0.000 3.800 N 0

0 LOC 0.000 4.950 N 1
 1 APW 4.000 2.500 N 0
 1 LOC 0.000 3.950 N 1
 2 APW 0.000 3.500 N 0
 3 APW 0.000 4.800 N 0
 4 APW 0.000 5.800 N 0
 5 APW 0.000 6.800 N 0

II. INPUT FILE DESCRIPTION

First line "TEXT" just gives some idea of what the calculation is going to produce.

Further on all input parameters are explained. Probably the best way to find out the one you need is to do search by its name.

`iter_dft` - number of LDA iterations.

`iter_hf` - number of Hartree-Fock iterations.

`iter_gw` - number of GW iterations.

`iter_qp` - number of Quasiparticle GW iterations.

`admix` - mixing for LDA iterations (charge).

`adspin` - mixing for LDA iterations (spin).

`adm_gw` - initial mixing for HF, QP, GW, or GWG iterations. In all these cases self energy is mixed.

`acc_it_gw` - final mixing for HF, QP, GW, or GWG iterations. Mixing is changed linearly from iteration to iteration from its initial value to its final.

`iexch` - specifies the LDA parametrization for exchange-correlation energy. For details see the file `exhcorr.f`. Only LDA works presently (not GGA).

`nproc_tau` - number of processors for (tau,omega)-parallelization. There are certain requirements. The following numbers: $(n_tau/2+1)/nproc_tau$, $(n_omega_exa+n_omega_asy+1)/nproc_tau$, and $(n_nu_exa+n_nu_asy+1)/nproc_tau$ should all be integer. About the variables (`n_tau`, `n_omega_exa`, `n_omega_asy`, `n_nu_exa`, `n_nu_asy`) see below.

`nproc_k` - number of processors for k-parallelization. Should divide exactly the number of irreducible points in Brillouin zone.

`irel` - takes care of the relativistic effects:

- = 0: nonrelativistic calculation;
- = 1: scalar-relativistic calculation;
- = 2: fully relativistic calculation.

clight - light velocity in a.u. Can be changed if one is interested in the effect or for the debugging purposes.

rel_interst - if =T and **irel**=2, then interstitial region is described fully relativistically (available only for LDA runs). In other situations spin-orbit effect is neglected in interstitial.

irel_core - similar to the parameter **irel** but for core electrons only. Works for pure LDA runs only. In other cases should be set equal to **irel**.

temperature - temperature in K.

allfile - defines where the output goes. Different parts of the code just add their own specifications when perform the output, so a lot of files is formed. The description of output files is going to be written separately.

symgen - generator of the symmetry group. Gives the minimal set of operations which (after all mutual multiplications) produces full set of symmetry operations. In the specific example above: **I** means spatial inversion, **R4Z** - four rotations around Z-axis; **R3D** - three rotations around (111)-axis (main diagonal of the cube for cubic solids).

par - lattice parameter (Bohr radiuses).

natom - number of atoms in the unit cell.

nsort - number of inequivalent atoms.

istruc - It is used mostly to specify the **k**-points of high symmetry. See **k_for_band_plot.f**. The conventions are the following:

- =1 for simple cubic;
- =2 for body-centered cubic;
- =3 for face-centered cubic;
- =4 for hexagonal;
- =5 for simple tetragonal;
- =6 for body-centered tetragonal;

- =7 for simple orthorhombic;
- =8 for body-centered orthorhombic;
- =9 for face-centered orthorhombic;
- =10 for simple monoclinic.

is - specifies the correspondence between full list of atoms and the list of inequivalent atoms. For example for BaFe₂As₂ we have 5 atoms in full list (Ba, Fe, Fe, As, As) and 3 in the list of inequivalent atoms (Ba, Fe, As). So the record in this case should be **is= 1 2 2 3 3**.

b_a - first orthorhombic factor. Scales b-direction.

c_a - second orthorhombic factor. Scales c-direction.

```
a=  -0.500000000000    0.500000000000    0.500000000000
b=   0.500000000000   -0.500000000000    0.500000000000
c=   0.500000000000    0.500000000000   -0.500000000000
```

The above three lines specify vectors of primitive translations measured in lattice parameter units. Orthorhombic scalings can be given here immediately or specified in **b/a;c/a** variables.

tau - gives the atom coordinates in lattice parameter units. Should be repeated for all atoms in the unit cell. The same convention about orthorhombic scalings is applied as in the case of lattice translations.

mdiv - defines the r-mesh in the unit cell (three numbers correspond to the number of divisions along three translation vectors on which the unit cell is built). This mesh is used in electronic density, Hartree potential, and LDA exchange-correlation potential evaluations.

nrdiv - defines the r-mesh in the unit cell which is used in polarizability and self energy calculations.

cut_lapw_ratio - defines the maximal value of $\mathbf{k} + \mathbf{G}$ for LAPW basis in the interstitial region as **cut_lapw_ratio** \times maximal Radius of G-sphere associated with **nrdiv**.

cut_pb_ratio - defines the maximal value of $\mathbf{k} + \mathbf{G}$ for product basis in the interstitial region as **cut_pb_ratio** \times maximal Radius of G-sphere associated with **nrdiv**.

eps_pb - optimization parameter in constructing the product basis inside MT spheres. Usual choice is $10^{-2} \div 10^{-3}$.

nbndf - defines the number of bands to be used in Green's function representation. If **nbndf**=0 then all bands available are used (in this case their number is equal to the number of LAPW+LO basis functions).

emindos - the lowest energy for DOS plotting (relative to chemical potential, in Ry).

emaxdos - the highest energy for DOS plotting (relative to chemical potential, in Ry).

ndos - number of points for DOS plotting (equidistant mesh).

n_cont_frac - defines the number of lowest positive Matsubara frequencies when fitting the continued-fractions approximation for analytical continuation.

e_small - small positive shift when calculating retarded fermionic functions on real axis.(Ry)

ndiv - three numbers which define the k-mesh in Brillouin zone.

metal - when (metal=T) the inverse uniform dielectric constant is enforced to be exactly zero. If (metal=F) there is no such enforcement, which is appropriate for nonmetals. Not particularly important but improves stability when the number of k-points is small.

n_k_div - number of divisions along every line, which connects two k-points of high symmetry. For bands plotting only. The option relevant only for LDA.

k_line - three numbers defying the direction in reciprocal space for certain output purposes.

vv0 - defines the relative volume (V/V_0). V_0 is given by crystal structure and lattice parameter above.

b_extval - Absolute value of external magnetic field (Ry/μ_B).

iter_h_ext - five digits placed together. They are used for initial spin polarization together with variable **magn_shift** (see below about the atom's description). First digit means how many LDA iterations are to be performed with applied field as specified by **magn_shift** for every atom in unit cell. Correspondingly the rest of the digits mean the same for HF, GW, or QP runs. One can start with non-spin-polarized LDA calculation but then switch on the polarization at, for instance, GW level (**iter_h_ext**=00200 if we want to start with two GW iteration with applied field).

b_ext - three numbers, defying the direction of constant external magnetic field, associated with variable **b_extval**.

n_tau - number of points on TAU-mesh (inhomogeneous).

n_tau_int - number of intervals on TAU-mesh to be used in TAU-Frequency transforms.

Not very critical. 1000 is good for many purposes.

n_omega_exa - number of fermionic frequencies on the dense part of the mesh.

n_omega_asy - number of fermionic frequencies on the part of the mesh where we use Chebyshev polynomials (intermediate region).

omega_max - max fermionic frequency (Ry), beyond which we apply asymptotic expansion.

interp_omega_d - number of Matsubara frequencies to be used to find the function at Chebyshev point by interpolation in intermediate region.

n_nu_exa - number of bosonic frequencies on the dense part of the mesh.

n_nu_asy - number of bosonic frequencies on the part of the mesh where we use Chebyshev polynomials.

nu_max - max bosonic frequency (Ry), beyond which we apply asymptotic expansion.

interp_nu_d - number of Matsubara frequencies to be used to find the function at Chebyshev point by interpolation in intermediate region.

Now we input the information for every inequivalent atom in the unit cell.

txtel - this is just symbolic representation of the atom.

z - nuclear charge.

magn_shift - external magnetic field (Ry/ μ_B) for initial spin splitting. Associated with the variable **iter_h_ext**.

smt - MT radius (Bohr radius).

h - defines radial mesh inside MT sphere $r_i = S \frac{e^{hi}-1}{e^{hN}-1}$, $i = 0, N$, where S-MT radius, N-number of points (N=nrad, see next input variable).

nrad - number of points on radial mesh.

z_dop - doping parameter.

lmb - maximal L for LAPW basis.

lmpb - maximal L for product basis.

lim_pb_mt - upper limits for the number of product basis functions for specific L from 0 to lmpb. Acts in compliance with **eps_pb**(see above).

ntle - number of different orbitals for every L from 0 to lmb. Orbitals differ by principal quantum number.

Now for every L and principal quantum number we input the parameters **l**, **augm**, **atocc**, **ptnl**, **corr**, **idmd**.

l - angular momentum;

augm - if (=LOC) than this orbital is local orbital. If (=APW) than it is constructed in accord with standard LAPW procedure.

atocc - initial occupancy of the orbital.

ptnl - potential parameter. $P = N + 1/2 - \arctan(D)/\pi$, where N is the principal quantum number of the orbital, and D is the logarithmic derivative.

corr - specifies whether the orbital is included in correlated set (=L) or not included (=N).

idmd - defines the way we solve the radial equations:

- IDMD = 0 - for the given energy (center of the band);
- IDMD = 1 - for the given potential parameter **ptnl** (see above);
- IDMD = 2 - $\Phi(\text{Smt})=0$; $\Phi'(\text{Smt}) \neq 0$ - bound sol-n, but not deriv;
- IDMD = 3 - $\Phi(\text{Smt})=\Phi'(\text{Smt})=0$ - totally bound sol-n (for deep E);
- IDMD = 4 - for the given energy (equal to the Chemical Potential).

III. DESCRIPTION OF OUTPUT FILES

Besides standard output/error files which are created by the operational system and are useful mostly when something unexpected has happened, there are many other files with useful information. Below we provide the most important of them with brief description. The names of all of them start with the symbols provided by user in the variable **allfile** (see input file description). The rest of the name gives some hint of what is inside in most cases.

allfile.out provides the progression of the calculation. It gives also the time consumed by most relevant subroutines.

allfile_dft.dos provides the spectral function (SF) in LDA approximation. First column in the file is real frequency (eV) measured from chemical potential, second is spin-down SF, third is spin-up SF, and the fourth is the full SF.

`allfile_qp.dos` provides the spectral function (SF) in QP approximation. First column in the file is real frequency (eV) measured from chemical potential, second is spin-down SF, third is spin-up SF, and the fourth is the full SF.

`allfile_dn_qp.dosk` provides the partial spectral function (PSF) in QP approximation for the k-points of high symmetry (spin down). First column in the file is real frequency (eV) measured from chemical potential.

`allfile_up_qp.dosk` provides the partial spectral function (PSF) in QP approximation for the k-points of high symmetry (spin up). First column in the file is real frequency (eV) measured from chemical potential.

`allfile__qp_qp.eig` provides the energies (eV) of band states in QP approximation relative to the chemical potential for all irreducible k-points.

`allfile(ATOM)___sum_qp.pdos` provides the partial density of states (PDOS) in LDA approximation (atom ATOM). First column in the file is real frequency (eV) measured from chemical potential, columns 2-5 correspond to spdf-states of spin-down, columns 6-9 correspond to spdf-states of spin-up. Different file is created for every symmetry-independent sort of atom.

`allfile_Im_sigc_w_band_k.qp` provides the imaginary part of correlation self-energy as a function of Matsubara's frequency in QP approximation for the k-points of high symmetry (spin-down and spin-up). First column in the file is Matsubara's frequency (eV).

`allfile_Re_sigc_w_band_k.qp` provides the real part of correlation self-energy as a function of Matsubara's frequency in QP approximation for the k-points of high symmetry (spin-down and spin-up). First column in the file is Matsubara's frequency (eV).
