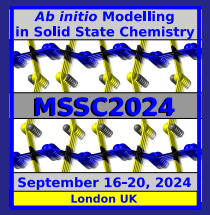
CRYSTAL input/output.

Giuseppe Mallia
g.mallia@imperial.ac.uk

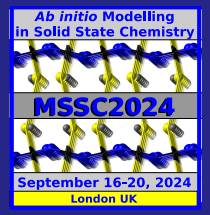
Imperial College London - Chemistry Department
Thomas Young Centre:
the London Centre for Theory and Simulation of Materials

16th September 2024

Imperial College London



Outline



CRYSTAL executables

CRYSTAL executables

The CRYSTAL package consists of two executables:

- **crystal**
  - performs integrals calculation and SCF part
  - computes total energy and wavefunction
  - performs geometry optimization
  - calculates vibrational frequencies
  - computes total energy and wavefunction in the presence of an external electric field

CRYSTAL executables

The CRYSTAL package consists of two executables:

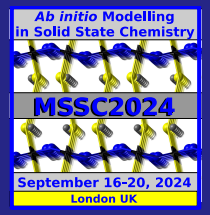
- **crystal**
  - performs integrals calculation and SCF part
  - computes total energy and wavefunction
  - performs geometry optimization
  - calculates vibrational frequencies
  - computes total energy and wavefunction in the presence of an external electric field
- **properties**
  - performs the wavefunction analysis (e. g. one electron properties)

CRYSTAL parallel executables

- **Pcrystal**
  - Medium systems
- **MPPcrystal**
  - Large systems

From CRYSTAL14

- **Pproperties**



CRYSTAL inputs

crystal input

- The executable **crystal** requires an input file
- The input is an ASCII text file.
- If you are an experimentalist, you can imagine that

$$input = sample$$

- The conventional extention of the file is .d12 (e.g. MgO.d12)
- The input is read by executing the following command

crystal $<$ MgO.d12

Pcrystal and MPPcrystal input

Pcrystal

- The keyword SCFDIR is strongly recommended to decrease the I/O operations during the execution;
- The input is read by executing the following command:
  Examples:
  aprun -np 32 **Pcrystal**
  mpirun -np 32 **Pcrystal**
  mpiexec **Pcrystal**
  poe **Pcrystal**
- The executable is looking for a file: INPUT
  Example:
  cp MgO.d12 INPUT
  this is performed by means of a script

MPPcrystal

- The keyword MPP was mandatory before CRYSTAL14.

properties input

- The executable **properties** requires an independent input file
- The input is an ASCII text file.
- The conventional extention of the file is **.d3** (e.g. band_structure.d3)
- The input is read by executing the following command

$$\textbf{properties} < \text{band\_structure.d3}$$

- The wave function file, obtained at the end of the execution of the **crystal** program, is necessary to run the executable **properties**.

properties input (wave function)

- The executable **properties** can read either fort.9 or fort.98.
  - fort.9: binary wave function (smaller size : $<$ 50Mb)
  - fort.98: formatted wave function ($\approx$ 2.5 $\times$)

properties input (wave function)

- The executable **properties** can read either fort.9 or fort.98.
  - fort.9: binary wave function (smaller size : $<$ 50Mb)
  - fort.98: formatted wave function ($\approx 2.5\times$)
- The keyword RDFMWF is necessary to read the wave function from fort.98.
- The keyword FMWF generates a fort.98 from a fort.9. WHY? If it is necessary to change platform.

properties input (missing wave function)


```
*******************************************************************************
*                                                                             *
*                                CRYSTAL23                                    *
*                          public : 1.0.1 - October 2022                      *
*                           HTTP://WWW.CRYSTAL.UNITO.IT                       *
*                                                                             *
*                                MAIN AUTHORS                                 *
*                                                                             *
*  R. DOVESI(1,11), V.R. SAUNDERS(2), C. ROETTI(1,11), R. ORLANDO(1,11),      *
*  C.M. ZICOVICH-WILSON(1,3), F. PASCALE(4), B. CIVALLERI(1,11),              *
*  K. DOLL(5), N.M. HARRISON(6), I.J. BUSH(7), Ph. D'ARCO(8),                 *
*  M. LLUNELL(9), M. CAUSA'(10), Y. NOEL(8), L. MASCHIO(1,11), A. ERBA(1,11)  *
*  M. RE'RAT(14), S. CASASSA(1,11), B.G. SEARLE(2), J.K. DESMARAIS(1)         *
*                                                                             *
*        CONTRIBUTIONS TO THE CODE HAVE ALSO BEEN GIVEN BY                    *
*                                                                             *
*  M. FERRABONE(1,11), M. DE LA PIERRE(1,11), M. FERRERO(1,11),               *
*  J. BAIMA(1,11), E. ALBANESE(1,11), M.F. PEINTINGER(12), R. BAST(13),       *
*  B. KIRTMAN(15), V. LACIVITA(1,11), R. DEMICHELIS(1,16)                     *
*  G. BRANDEBURG(17), S. SALUSTRO(1,11), G. SANSONE(1,11)                     *
*  M.T. RUGGIERO(18), L.E. DAGA(1), L. DONA'(1), A. COSSARD(1)                *
 .................
*******************************************************************************
EEEEEEEEEE STARTING  DATE 09 09 2024 TIME 10:10:10.0
ERROR **** init_properties_io **** Wavefunction file can not be found
TTTTTTTTTTTTTTTTTTTTTTTTTTTTT ERR         TELAPSE        0.00 TCPU        0.00
```

Pproperties input

- The input is read by executing the following command:
  Examples:
  mpirun -np 32 **Pproperties**
  mpiexec **Pproperties**
- The executable is looking for a file: INPUT
  Example:
  cp BAND.d3 INPUT
  this is performed by means of a script

crystal input

crystal input scheme

CRYSTAL input is given by keywords.
It consists of three sections:

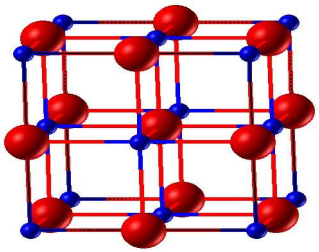
0. Title
1. Geometry input section
2. Basis set input section
3. Method and SCF input section

crystal input structure

Each sections ends with the keyword END.
Optional keywords can be specified for each sections.

0. Title
1. Geometry input section
   - standard geometry input
   - geometry editing keywords (optional)
   - geometry optimization and vibrational frequencies calculation (optional)
   - external electric field (optional)
2. Basis set input section
   - standard basis set input
   - optional basis set related keywords
3. Method and SCF input section
   - Reciprocal space integration parameters
   - Hamiltonian related keywords (optional)
   - SCF related keywords (optional)

crystal input example: MgO crystal - fcc cell



The basis set adopted is STO-3G.

The default hamiltonian is RHF.

```
Title
Geometry section
Optional keywords
→
Basis set section
Optional keywords
→
Method/SCF section
Optional keywords
→
```

```
MgO bulk: exp geom
CRYSTAL
0 0 0
225
4.21
2
12 0. 0. 0.
8 0.5 0.5 0.5
END
12 3
1 0 3 2. 0.
1 1 3 8. 0.
1 1 3 2. 0.
8 2
1 0 3 2. 0.
1 1 3 6. 0.
99 0
END
SHRINK
8 8
END
```

crystal input example geometry (I): MgO crystal - fcc cell


```
MgO: exp geom
CRYSTAL
0 0 0
225
4.21
2
12 0. 0. 0.
8 0.5 0.5 0.5
END
```

Title
Dimensionality of the system
Crystallographic information (3D only)
Space Group (Fm3m - 225)
Lattice parameters (cubic)
Number of non equivalent atoms
Atomic number and fractional coordinates
End of geometry input section

- The atom positions are expressed in fractionary coordinates.
- The atoms given in input belong to the asymmetric unit of the conventional(or crystallographic) unit cell. (e.g. 8 atoms in the conventional cell, 2 atoms in the input file)

crystal input example geometry (II): MgO crystal - fcc cell

- Several optional keywords are available for geometry editing:
  - modification of the symmetry
  - manipulation of atoms (displacement, rotation, insertion, ...)
  - reduction of the periodicity (3D→ 2D, 2D→ 1D, 3D→ 0D, . . .)

  Geometry tutorial
- Geometry optimization and vibrational frequencies calculation are sub-blocks of this section. Each of this sub-block requires an END keyword.

  Geometry optimization and vibrational frequencies tutorials
- Applied electric field

crystal input example basis set (I): MgO crystal - fcc cell


```
12 3
1 0 3 2. 0.
1 1 3 8. 0.
1 1 3 2. 0.
8 2
1 0 3 2. 0.
1 1 3 6. 0.
99 0
END
```

Atomic number and number of shells
Basis set input: code, type, nr. of primitive, formal charge and scale factor of the shell:
0. indicates standard Pople STO-nG value

Here, Mg and O have been described with a minimal STO-3G basis set
End of basis set input section

- Basis set and initial electronic configuration are mandatory for each atom with different atomic number;

crystal input example basis set (II): MgO crystal - fcc cell

- Different basis can be defined for atom with the same atomic number; (e.g. Fe^{2+} and Fe^{3+}, O^{2-} and O^{-})

O^{2-}	O^{-}
8 2 1 0 3 2. 0. 1 1 3 **8.** 0.	8 2 1 0 3 2. 0. 1 1 3 **7.** 0.

- Effective Core Potential must be inserted along with the valence-only basis set;
- Optional keywords are related to:
  - modification of the electronic configuration
  - use of ghost functions
- **Basis set tutorial**

crystal input example method/SCF (I): MgO crystal - fcc cell


```
SHRINK
8 8
END
```

Reciprocal space integration parameters

End of SCF input section

- Reciprocal space integration parameters are the so-called shrinking factors and must be specified for periodic calculations (3D, 2D and 1D).
- This section specifies the adopted theoretical method (default: RHF)
- and controls the SCF part of the calculation

crystal input example method/SCF (II): MgO crystal - fcc cell

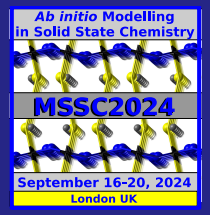
- The type of run can be choosen, for example:
  - Standard SCF (default before CRYSTAL14)
  - SCFDIR (default)
  - MPP
- The computational conditions on integrals calculation can be set.
- The convergence criteria can be modified.
- The convergence tools can be selected.
- The options for spin-polarized systems can be activated.
- **Hamiltonian and SCF tutorial**

crystal input example DFT


```
DFT
EXCHANGE
LDA
CORRELAT
VWN
ENDDFT
SHRINK
8 8
END
```

DFT input block
Keyword to define the exchange functional
Selected exchange functional
Keyword to define the correlation functional
Selected correlation functional
End of the DFT input block
Reciprocal space integration parameters
End of the Method/SCF input section

- Keywords are available to modify accuracy in DFT calculations (e.g. integration grid)
- The keyword SPIN must be specified for spin-polarized systems



crystal output

crystal output example: Header

CRYSTAL header

```
*******************************************************************************
*                                                                             *
*                                  CRYSTAL23                                  *
*                          public : 1.0.1 - October 2022                      *
*                           HTTP://WWW.CRYSTAL.UNITO.IT                       *
*                                                                             *
*                                MAIN AUTHORS                                 *
*                                                                             *
*  R. DOVESI(1,11), V.R. SAUNDERS(2), C. ROETTI(1,11), R. ORLANDO(1,11),      *
*  C.M. ZICOVICH-WILSON(1,3), F. PASCALE(4), B. CIVALLERI(1,11),              *
*  K. DOLL(5), N.M. HARRISON(6), I.J. BUSH(7), Ph. D'ARCO(8),                 *
*  M. LLUNELL(9), M. CAUSA'(10), Y. NOEL(8), L. MASCHIO(1,11), A. ERBA(1,11)  *
*  M. RE'RAT(14), S. CASASSA(1,11), B.G. SEARLE(2), J.K. DESMARAIS(1)         *
*                                                                             *
*        CONTRIBUTIONS TO THE CODE HAVE ALSO BEEN GIVEN BY                    *
*                                                                             *
*  M. FERRABONE(1,11), M. DE LA PIERRE(1,11), M. FERRERO(1,11),               *
*  J. BAIMA(1,11), E. ALBANESE(1,11), M.F. PEINTINGER(12), R. BAST(13),       *
*  B. KIRTMAN(15), V. LACIVITA(1,11), R. DEMICHELIS(1,16)                     *
*  G. BRANDEBURG(17), S. SALUSTRO(1,11), G. SANSONE(1,11)                     *
*  M.T. RUGGIERO(18), L.E. DAGA(1), L. DONA'(1), A. COSSARD(1)                *
 ................
*******************************************************************************
```

It reports the CRYSTAL version and the main authors of the code.

Date and time

crystal output example: Geometry section – conventional cell

Title
Periodicity

Crystallo-graphic information.

Lattice parameters

Atomic positions in the asymmetric unit.

```
MgO bulk: exp geom

CRYSTAL CALCULATION
(INPUT ACCORDING TO THE INTERNATIONAL TABLES FOR X-RAY CRYSTALLOGRAPHY)
CRYSTAL FAMILY                          :  CUBIC
CRYSTAL CLASS  (GROTH - 1921)           :  CUBIC HEXAKISOCTAHEDRAL

SPACE GROUP (CENTROSYMMETRIC)           :  F M 3 M

LATTICE PARAMETERS  (ANGSTROMS AND DEGREES) - CONVENTIONAL CELL
       A            B            C         ALPHA         BETA         GAMMA
    4.21000      4.21000      4.21000     90.00000     90.00000     90.00000

NUMBER OF IRREDUCIBLE ATOMS IN THE CONVENTIONAL CELL:    2

INPUT COORDINATES

ATOM  AT. N.                  COORDINATES
  1   12     0.000000000000E+00  0.000000000000E+00  0.000000000000E+00
  2    8     5.000000000000E-01  5.000000000000E-01  5.000000000000E-01
```

This corresponds to the crystal structure given as input.

crystal output example: Geometry section – primitive cell

Primitive cell

Lattice parameters

Atomic positions

Symmetry

Size of the direct lattice

```
**********************************************************************

<< INFORMATION >>: FROM NOW ON, ALL COORDINATES REFER TO THE PRIMITIVE CELL

**********************************************************************

LATTICE PARAMETERS  (ANGSTROMS AND DEGREES) - PRIMITIVE CELL
      A          B          C          ALPHA      BETA       GAMMA          VOLUME
   2.97692    2.97692    2.97692    60.00000   60.00000   60.00000      18.654615

COORDINATES OF THE EQUIVALENT ATOMS (FRACTIONARY UNITS)

N. ATOM EQUIV AT. N.           X                   Y                   Z

  1   1   1   12 MG    0.00000000000E+00  0.00000000000E+00  0.00000000000E+00

  2   2   1    8 O    -5.00000000000E-01 -5.00000000000E-01 -5.00000000000E-01

NUMBER OF SYMMETRY OPERATORS          :   48
**********************************************************************
* GEOMETRY EDITING - INPUT COORDINATES ARE GIVEN IN ANGSTROM
**********************************************************************

GEOMETRY NOW FULLY CONSISTENT WITH THE GROUP

GCALCO - MAX INDICES DIRECT LATTICE VECTOR    14    14    14
NO.OF VECTORS CREATED 6999 STARS  105 RMAX    59.53536 BOHR
```

crystal output example: Geometry section – Final geometry printing

Lattice parameters Atomic positions

If the initial geometry is not primitive, the transformation matrix from the primitive to the crystallographic cell is given with the lattice parameters and the atomic positions in the conventional unit cell.

Irreducible atoms are labelled by T

```
GEOMETRY FOR WAVE FUNCTION - DIMENSIONALITY OF THE SYSTEM     3
(NON PERIODIC DIRECTION: LATTICE PARAMETER FORMALLY SET TO 500)
*******************************************************************************
LATTICE PARAMETERS (ANGSTROMS AND DEGREES) - BOHR = 0.5291772083 ANGSTROM
PRIMITIVE CELL - CENTRING CODE 5/0 VOLUME=    18.654615 - DENSITY  3.559 g/cm^3
        A              B              C           ALPHA      BETA       GAMMA
    2.97691955     2.97691955     2.97691955    60.000000  60.000000  60.000000
*******************************************************************************
ATOMS IN THE ASYMMETRIC UNIT    2 - ATOMS IN THE UNIT CELL:     2
    ATOM              X/A                 Y/B                 Z/C
*******************************************************************************
  1 T  12 MG    0.000000000000E+00  0.000000000000E+00  0.000000000000E+00
  2 T   8 O    -5.000000000000E-01 -5.000000000000E-01 -5.000000000000E-01

TRANSFORMATION MATRIX PRIMITIVE-CRYSTALLOGRAPHIC CELL
-1.0000   1.0000   1.0000   1.0000  -1.0000   1.0000   1.0000   1.0000  -1.0000

*******************************************************************************
CRYSTALLOGRAPHIC CELL (VOLUME=         74.61846100)
        A              B              C           ALPHA      BETA       GAMMA
    4.21000000     4.21000000     4.21000000    90.000000  90.000000  90.000000

COORDINATES IN THE CRYSTALLOGRAPHIC CELL
    ATOM              X/A                 Y/B                 Z/C
*******************************************************************************
  1 T  12 MG    0.000000000000E+00  0.000000000000E+00  0.000000000000E+00
  2 T   8 O    -5.000000000000E-01 -5.000000000000E-01 -5.000000000000E-01

T = ATOM BELONGING TO THE ASYMMETRIC UNIT
```

crystal output example: Geometry section – Final geometry symmetry

The symmetry operators are printed at the end of the geometry editing.

```
****  48 SYMMOPS - TRANSLATORS IN FRACTIONARY UNITS
 V INV                        ROTATION MATRICES                          TRANSLATOR
 1   1  1.00  0.00  0.00  0.00  1.00  0.00  0.00  0.00  1.00    0.00  0.00  0.00
 2   2  0.00  1.00  0.00  1.00  0.00  0.00 -1.00 -1.00 -1.00    0.00  0.00  0.00
 3   3 -1.00 -1.00 -1.00  0.00  0.00  1.00  0.00  1.00  0.00    0.00  0.00  0.00
 4   4  0.00  0.00  1.00 -1.00 -1.00 -1.00  1.00  0.00  0.00    0.00  0.00  0.00
 5   6  0.00  0.00  1.00  1.00  0.00  0.00  0.00  1.00  0.00    0.00  0.00  0.00
 6   5  0.00  1.00  0.00  0.00  0.00  1.00  1.00  0.00  0.00    0.00  0.00  0.00
 7   8  1.00  0.00  0.00  0.00  0.00  1.00 -1.00 -1.00 -1.00    0.00  0.00  0.00
 8   7  1.00  0.00  0.00 -1.00 -1.00 -1.00  0.00  1.00  0.00    0.00  0.00  0.00
 9  10 -1.00 -1.00 -1.00  0.00  1.00  0.00  1.00  0.00  0.00    0.00  0.00  0.00
10   9  0.00  0.00  1.00  0.00  1.00  0.00 -1.00 -1.00 -1.00    0.00  0.00  0.00
11  12  0.00  1.00  0.00 -1.00 -1.00 -1.00  0.00  0.00  1.00    0.00  0.00  0.00
12  11 -1.00 -1.00 -1.00  1.00  0.00  0.00  0.00  0.00  1.00    0.00  0.00  0.00

.....................................................................................

36  35  1.00  1.00  1.00 -1.00  0.00  0.00  0.00  0.00 -1.00    0.00  0.00  0.00
37  37  0.00  1.00  0.00  1.00  0.00  0.00  0.00  0.00  1.00    0.00  0.00  0.00
38  38  1.00  0.00  0.00  0.00  1.00  0.00 -1.00 -1.00 -1.00    0.00  0.00  0.00
39  40  0.00  0.00  1.00 -1.00 -1.00 -1.00  0.00  1.00  0.00    0.00  0.00  0.00
40  39 -1.00 -1.00 -1.00  0.00  0.00  1.00  1.00  0.00  0.00    0.00  0.00  0.00
41  41  1.00  0.00  0.00  0.00  0.00  1.00  0.00  1.00  0.00    0.00  0.00  0.00
42  42  0.00  0.00  1.00  0.00  1.00  0.00  1.00  0.00  0.00    0.00  0.00  0.00
43  45  0.00  0.00  1.00  1.00  0.00  0.00 -1.00 -1.00 -1.00    0.00  0.00  0.00
44  46 -1.00 -1.00 -1.00  1.00  0.00  0.00  0.00  1.00  0.00    0.00  0.00  0.00
45  43  0.00  1.00  0.00 -1.00 -1.00 -1.00  1.00  0.00  0.00    0.00  0.00  0.00
46  44  0.00  1.00  0.00  0.00  0.00  1.00 -1.00 -1.00 -1.00    0.00  0.00  0.00
47  47 -1.00 -1.00 -1.00  0.00  1.00  0.00  0.00  0.00  1.00    0.00  0.00  0.00
48  48  1.00  0.00  0.00 -1.00 -1.00 -1.00  0.00  0.00  1.00    0.00  0.00  0.00
```

crystal output example: Geometry section – Final geometry vectors

The translational lattice vectors and the cartisian coordinate of the atoms are printed out.

```
DIRECT LATTICE VECTORS CARTESIAN COMPONENTS (ANGSTROM)
          X                  Y                  Z
  0.000000000000E+00   0.210500000000E+01   0.210500000000E+01
  0.210500000000E+01   0.000000000000E+00   0.210500000000E+01
  0.210500000000E+01   0.210500000000E+01   0.000000000000E+00


CARTESIAN COORDINATES - PRIMITIVE CELL
*********************************************************************************
*      ATOM          X(ANGSTROM)          Y(ANGSTROM)          Z(ANGSTROM)
*********************************************************************************
  1    12 MG    0.000000000000E+00   0.000000000000E+00   0.000000000000E+00
  2     8 O     2.105000000000E+00   2.105000000000E+00   2.105000000000E+00
```

crystal output example: Basis set section

Basis set functions of each non equivalent atom

Atom type and cartesian coordinates (Bohr)

Shell type, gaussian exponents and coefficients

```
**********************************************************************
LOCAL ATOMIC FUNCTIONS BASIS SET
**********************************************************************
  ATOM   X(AU)   Y(AU)   Z(AU)    NO. TYPE  EXPONENT  S COEF   P COEF   D/F/G COEF
**********************************************************************
  1 MG  0.000  0.000  0.000
                                     1 S
                                          2.992E+02 1.543E-01 0.000E+00 0.000E+00
                                          5.451E+01 5.353E-01 0.000E+00 0.000E+00
                                          1.475E+01 4.446E-01 0.000E+00 0.000E+00
                                   2-    5 SP
                                          1.512E+01-9.997E-02 1.559E-01 0.000E+00
                                          3.514E+00 3.995E-01 6.077E-01 0.000E+00
                                          1.143E+00 7.001E-01 3.920E-01 0.000E+00
                                   6-    9 SP
                                          1.395E+00-2.196E-01 1.059E-02 0.000E+00
                                          3.893E-01 2.256E-01 5.952E-01 0.000E+00
                                          1.524E-01 9.004E-01 4.620E-01 0.000E+00
  2 O   3.978  3.978  3.978
                                    10 S
                                          1.307E+02 1.543E-01 0.000E+00 0.000E+00
                                          2.381E+01 5.353E-01 0.000E+00 0.000E+00
                                          6.444E+00 4.446E-01 0.000E+00 0.000E+00
                                  11-   14 SP
                                          5.033E+00-9.997E-02 1.559E-01 0.000E+00
                                          1.170E+00 3.995E-01 6.077E-01 0.000E+00
                                          3.804E-01 7.001E-01 3.920E-01 0.000E+00
```

crystal output example: General information (I)

This section gives computational information concerning

1) the studied system

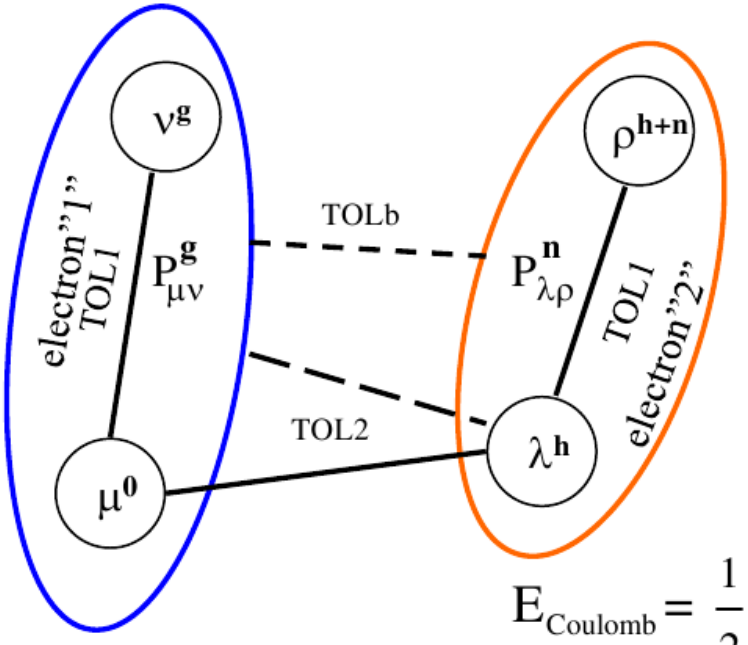
2) the tolerances for the integrals evaluation

3) the theoretical method

4) the computational conditions for the SCF iteration procedure (convergence criteria, shrinking factors and number of k points)

```
N. OF ATOMS PER CELL         2  COULOMB OVERLAP TOL          (T1) 10** -6
NUMBER OF SHELLS             5  COULOMB PENETRATION TOL      (T2) 10** -6
NUMBER OF AO                14  EXCHANGE OVERLAP TOL         (T3) 10** -6
N. OF ELECTRONS PER CELL    20  EXCHANGE PSEUDO OVP (F(G))   (T4) 10** -6
CORE ELECTRONS PER CELL     12  EXCHANGE PSEUDO OVP (P(G))   (T5) 10**-12
N. OF SYMMETRY OPERATORS    48  POLE ORDER IN MONO ZONE                 4
*******************************************************************************
TYPE OF CALCULATION :  RESTRICTED CLOSED SHELL
HARTREE-FOCK HAMILTONIAN

*******************************************************************************
MAX NUMBER OF SCF CYCLES      50  CONVERGENCE ON DELTAP        10**-16
NO MIXING OF F MATRICES           CONVERGENCE ON ENERGY        10**- 6
SHRINK. FACT.(MONKH.)    8  8  8  NUMBER OF K POINTS IN THE IBZ     29
SHRINKING FACTOR(GILAT NET)    8  NUMBER OF K POINTS(GILAT NET)     29
*******************************************************************************
```

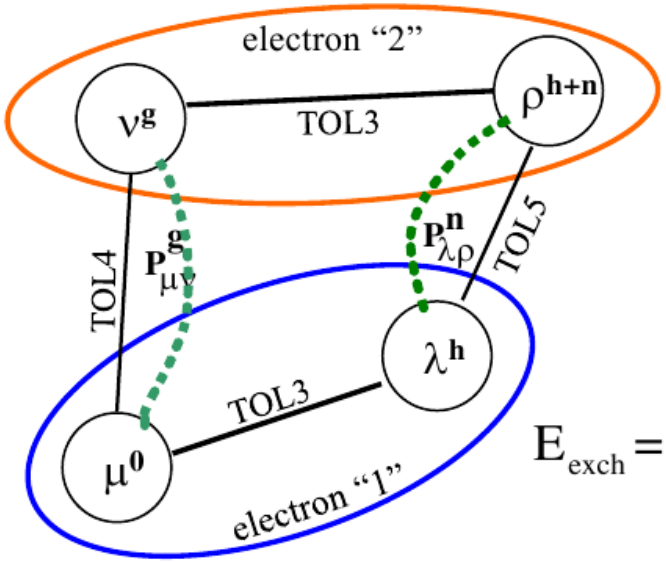
CRYSTAL main computational parameters: TOLINTEG



$$E_{Coulomb} = \frac{1}{2}\sum_{\mu,\nu}^{m}\sum_{g}^{\infty} P^{g}_{\mu,\nu}\sum_{\lambda,\rho}^{m}\sum_{n}^{\infty} P^{n}_{\lambda,\rho}\sum_{h}^{\infty}[(\chi^{0}_{\mu}\chi^{g}_{\nu}|\chi^{h}_{\lambda}\chi^{h+n}_{\rho})]$$

TOL2

TOL1



$$E_{exch} = \frac{1}{4}\sum_{\mu,\nu}^{m}\sum_{g}^{\infty} P^{g}_{\mu,\nu}\sum_{\lambda,\rho}^{m}\sum_{n}^{\infty} P^{n}_{\lambda,\rho}\sum_{h}^{\infty}[(\chi^{0}_{\mu}\chi^{h}_{\lambda}|\chi^{g}_{\nu}\chi^{h+n}_{\rho})]$$

TOL3

crystal output example: General information (II)

Coordinates of the k-points used in the IBZ sampling

Information on the direct and reciprocal space

Information about the resource usage:
1) Dimensions of density

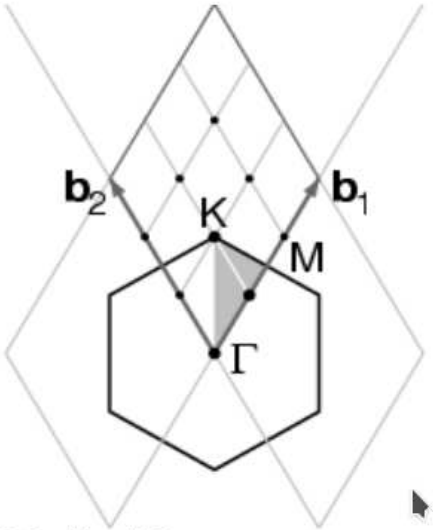
2) Fock matrix in direct space

3) integrals storage

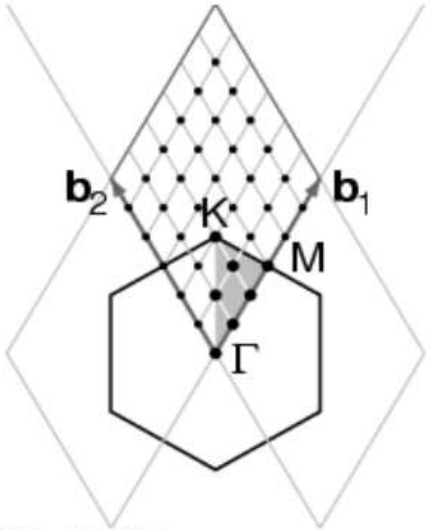
4) memory usage

```
*** K POINTS COORDINATES (OBLIQUE COORDINATES IN UNITS OF IS =  8)
  1-R(  0  0  0)   2-C(  1  0  0)   3-C(  2  0  0)   4-C(  3  0  0)
  5-R(  4  0  0)   6-C(  1  1  0)   7-C(  2  1  0)   8-C(  3  1  0)
  9-C(  4  1  0)  10-C(  5  1  0)  11-C(  6  1  0)  12-C(  7  1  0)
 13-C(  2  2  0)  14-C(  3  2  0)  15-C(  4  2  0)  16-C(  5  2  0)
 17-C(  6  2  0)  18-C(  3  3  0)  19-C(  4  3  0)  20-C(  5  3  0)
 21-R(  4  4  0)  22-C(  3  2  1)  23-C(  4  2  1)  24-C(  5  2  1)
 25-C(  4  3  1)  26-C(  5  3  1)  27-C(  6  3  1)  28-C(  5  4  1)
 29-C(  6  4  2)

DIRECT LATTICE VECTORS COMPON. (A.U.)     RECIP. LATTICE VECTORS COMPON. (A.U.)
       X             Y             Z            X             Y             Z
   0.0000000     3.9778735     3.9778735     -0.7897669     0.7897669     0.7897669
   3.9778735     0.0000000     3.9778735      0.7897669    -0.7897669     0.7897669
   3.9778735     3.9778735     0.0000000      0.7897669     0.7897669    -0.7897669

DISK SPACE FOR EIGENVECTORS (FTN 10)      10780 REALS

SYMMETRY ADAPTION OF THE BLOCH FUNCTIONS ENABLED

MATRIX SIZE: P(G)   13898, F(G)    2820, P(G) IRR     666, F(G) IRR     346
MAX G-VECTOR INDEX FOR 1- AND 2-ELECTRON INTEGRALS 319

INFORMATION **** GENBUF **** COULOMB BIPO BUFFER LENGTH (WORDS) =       66150
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTT INPUT       TELAPSE        0.01 TCPU         0.00
```

Sampling of k points Monkhorst net



2D Graphite - IS=3



2D Graphite - IS=6

```
*** K POINTS COORDINATES (OBLIQUE COORDINATES IN UNITS OF IS =  3)
  1-R(  0  0  0)   2-C(  1  0  0)   3-C(  1  1  0)
```

```
*** K POINTS COORDINATES (OBLIQUE COORDINATES IN UNITS OF IS =  6)
  1-R(  0  0  0)   2-C(  1  0  0)   3-C(  2  0  0)   4-R(  3  0  0)
  5-C(  1  1  0)   6-C(  2  1  0)   7-C(  2  2  0)
```

crystal output example: Neighbors Analysis

Label, atomic type, distance and neighbors position in terms of the direct lattice cell for each non-equivalent atom. (default: 6)

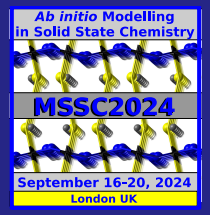
Number of internal degrees of freedom of the system (special positions).

```
 ATOM   N      R/ANG       R/AU    NEIGHBORS (ATOM LABELS AND CELL INDICES)
1 MG    6      2.1050      3.9779    2 O   -1 0 0    2 O    0-1 0    2 O    0 0-1
                                       2 O   -1-1 0    2 O   -1 0-1    2 O    0-1-1
1 MG   12      2.9769      5.6256    1 MG  -1 0 0    1 MG   1 0 0    1 MG  -1 0 1
                                       1 MG   1 0-1    1 MG  -1 1 0    1 MG   1-1 0
                                       1 MG   0-1 0    1 MG   0 1 0    1 MG   0-1 1
                                       1 MG   0 1-1    1 MG   0 0-1    1 MG   0 0 1
1 MG    8      3.6460      6.8899    2 O    0 0 0    2 O   -1-1 1    2 O   -1 1-1
                                       2 O    1-1-1    2 O   -2 0 0    2 O    0-2 0
                                       2 O    0 0-2    2 O   -1-1-1
1 MG    6      4.2100      7.9557    1 MG  -1-1 1    1 MG   1 1-1    1 MG  -1 1-1
                                       1 MG   1-1 1    1 MG  -1 1 1    1 MG   1-1-1
.....................................................................................
2 O     6      2.1050      3.9779    1 MG   1 0 0    1 MG   0 1 0    1 MG   0 0 1
                                       1 MG   1 1 0    1 MG   1 0 1    1 MG   0 1 1
2 O    12      2.9769      5.6256    2 O   -1 0 0    2 O    1 0 0    2 O   -1 0 1
                                       2 O    1 0-1    2 O   -1 1 0    2 O    1-1 0
                                       2 O    0-1 0    2 O    0 1 0    2 O    0-1 1
                                       2 O    0 1-1    2 O    0 0-1    2 O    0 0 1
2 O     8      3.6460      6.8899    1 MG   0 0 0    1 MG   1 1-1    1 MG   1-1 1
                                       1 MG  -1 1 1    1 MG   2 0 0    1 MG   0 2 0
                                       1 MG   0 0 2    1 MG   1 1 1
2 O     6      4.2100      7.9557    2 O   -1-1 1    2 O    1 1-1    2 O   -1 1-1
                                       2 O    1-1 1    2 O   -1 1 1    2 O    1-1-1
.....................................................................................

THERE ARE NO SYMMETRY ALLOWED DIRECTIONS
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SYMM        TELAPSE        0.01 TCPU        0.00
```

crystal output example: Integrals calculation

This section reports more information on the integrals evaluation and concludes the first part of a traditional SCF procedure: the integrals calculation.

```
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTT INT_SCREEN  TELAPSE        0.02 TCPU        0.01
INFORMATION **** GENBUF **** COULOMB BIPO BUFFER LENGTH (WORDS) =       66150
INFORMATION **** EXCBUF **** EXCH. BIPO BUFFER: WORDS USED =       97362
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MONIRR      TELAPSE        0.04 TCPU        0.03

 GAUSS70 FOR COULOMB   GAUSS70 FOR EXCHANGE
**SHELL_ORTHODOX** SPACE FOR BIEL. INTEGRALS     1 BUFFERS
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SHLC        TELAPSE        1.05 TCPU        1.04
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MONMAD      TELAPSE        1.10 TCPU        1.09
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTT INT_CALC    TELAPSE        1.10 TCPU        1.09
EEEEEEEEEE INT_CALC TERMINATION  DATE 09 09 2009 TIME 09:09:10.9
```



crystal output example: SCF start

The SCF begins by defining the initial guess of the density matrix.

The default guess for the wave function evaluation is a superposition of atomic densities.

```
********************************************************************************
MgO bulk: exp geom
CRYSTAL - SCF - TYPE OF CALCULATION :  RESTRICTED CLOSED SHELL
********************************************************************************

TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SDIK        TELAPSE        1.20 TCPU        1.10

AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA
        ATOMIC WAVEFUNCTION(S)


NUCLEAR CHARGE 12.0  SYMMETRY SPECIES            S    P
N. ELECTRONS   12.0  NUMBER OF PRIMITIVE GTOS    9    6
                     NUMBER OF CONTRACTED GTOS   3    2
                     NUMBER OF CLOSED SHELLS     3    1
                     OPEN SHELL OCCUPATION       0    0

 ZNUC SCFIT  TOTAL HF ENERGY   KINETIC ENERGY   VIRIAL THEOREM ACCURACY
 12.0   4   -1.970073545E+02  1.945732082E+02 -2.012510183E+00  2.9E-06

NUCLEAR CHARGE  8.0  SYMMETRY SPECIES            S    P
N. ELECTRONS    8.0  NUMBER OF PRIMITIVE GTOS    6    3
                     NUMBER OF CONTRACTED GTOS   2    1
                     NUMBER OF CLOSED SHELLS     2    0
                     OPEN SHELL OCCUPATION       0    4

 ZNUC SCFIT  TOTAL HF ENERGY   KINETIC ENERGY   VIRIAL THEOREM ACCURACY
  8.0   1   -7.380415026E+01  7.344496710E+01 -2.004890507E+00  0.0E+00

AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA
```

crystal output example: SCF Initial Iterations

For each SCF cycle, total charge of the atoms (Mulliken scheme), total energy and values of the convergence criteria are printed.

The insulating or conducting state is given.

```
CHARGE NORMALIZATION FACTOR    1.00000000
TOTAL ATOMIC CHARGES:
 12.0000000    8.0000000
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTT QGAM         TELAPSE         0.75 TCPU         0.44
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTT BIEL         TELAPSE         0.98 TCPU         0.45
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTT TOTENY       TELAPSE         1.02 TCPU         0.45
CYC   0 ETOT(AU) -2.706739657077E+02 DETOT -2.71E+02 tst  0.00E+00 PX  1.00E+00
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTT DIIS         TELAPSE         1.05 TCPU         0.45
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTT FDIK         TELAPSE         1.14 TCPU         0.45
INSULATING STATE
TOP OF VALENCE BANDS -    BAND     10; K    12; EIG -2.0823120E-01 AU
TOP OF VALENCE BANDS -    BAND     10; K     1; EIG -2.0986026E-01 AU
BOTTOM OF VIRTUAL BANDS - BAND     11; K     1; EIG -2.0214157E-02 AU
INDIRECT ENERGY BAND GAP:   5.1162 eV
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTT PDIG         TELAPSE         1.29 TCPU         0.46
CHARGE NORMALIZATION FACTOR    1.00000000
TOTAL ATOMIC CHARGES:
 10.9720640    9.0279360
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTT QGAM         TELAPSE         1.29 TCPU         0.46
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTT BIEL         TELAPSE         1.32 TCPU         0.46
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTT TOTENY       TELAPSE         1.32 TCPU         0.46
CYC   1 ETOT(AU) -2.711666822111E+02 DETOT -4.93E-01 tst  0.00E+00 PX  1.00E+00
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTT DIIS         TELAPSE         1.35 TCPU         0.46
DIIS TEST: 0.12746E-01 AT SCF   CYCLE    1 - MIX   30 %
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTT FDIK         TELAPSE         1.40 TCPU         0.46
INSULATING STATE
TOP OF VALENCE BANDS -    BAND     10; K    12; EIG -1.0524839E-01 AU
TOP OF VALENCE BANDS -    BAND     10; K     1; EIG -1.1016867E-01 AU
BOTTOM OF VIRTUAL BANDS - BAND     11; K     1; EIG  2.1942560E-01 AU
INDIRECT ENERGY BAND GAP:   8.8348 eV
```

crystal output example: SCF Final Iterations

At the end of the SCF, the final energy, the number of cycles and the convergence criteria are printed out.

Energy contributions.

The time is given in seconds.

```
CHARGE NORMALIZATION FACTOR    1.00000000
TOTAL ATOMIC CHARGES:
 11.2227092    8.7772908
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTT QGAM        TELAPSE        2.53 TCPU        0.53
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTT BIEL        TELAPSE        2.53 TCPU        0.53
+++ ENERGIES IN A.U. +++
::: EXT EL-POLE : L =  0                          -4.6909140273412E+02
::: EXT EL-POLE : L =  1                          -1.2059033205648E-21
::: EXT EL-POLE : L =  2                          -6.2702983366010E-20
::: EXT EL-POLE : L =  3                          -4.1667424606656E-22
::: EXT EL-POLE : L =  4                          -1.0938442645678E-04
::: EXT EL-SPHEROPOLE                              3.9644228426855E+00
::: BIELET ZONE E-E                                5.1161989807269E+02
::: TOTAL E-E                                      4.6492808796833E+01
::: TOTAL E-N + N-E                               -5.1175574976429E+02
::: TOTAL N-N                                     -7.3084276676762E+01
::: KINETIC ENERGY                                 2.6712907389490E+02
::: TOTAL    ENERGY                               -2.7121814374932E+02
::: VIRIAL COEFFICIENT                             9.9240440050511E-01
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTT TOTENY      TELAPSE        2.53 TCPU        0.53
CYC   7 ETOT(AU) -2.712181437493E+02 DETOT -4.93E-09 tst  3.48E-10 PX  3.62E-04

== SCF ENDED - CONVERGENCE ON ENERGY      E(AU) -2.7121814374932E+02 CYCLES   7

TOTAL ENERGY(HF)(AU)(   7) -2.7121814374932E+02 DE-4.9E-09 tst 3.5E-10 PX 3.6E-04
EIGENVECTORS IN FORTRAN UNIT 10
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTT END         TELAPSE        2.64 TCPU        0.54
EEEEEEEEEE TERMINATION  DATE 06 07 2017 TIME 19:44:09.9
```

crystal output example: DFT: pure

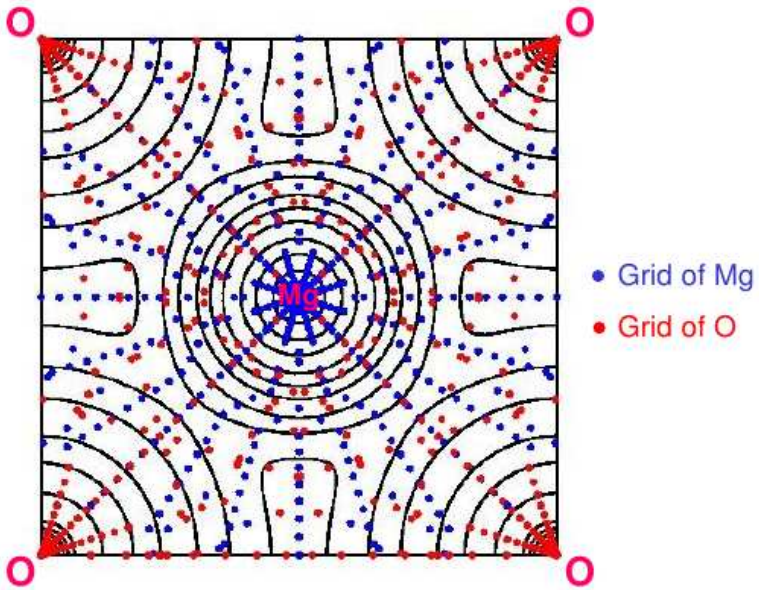
The DFT theoretical method is indicated.

```
********************************************************************************
TYPE OF CALCULATION :  RESTRICTED CLOSED SHELL
KOHN-SHAM HAMILTONIAN

(EXCHANGE)[CORRELATION] FUNCTIONAL:(DIRAC-SLATER LDA)[PERDEW-ZUNGER]
```

DFT computational parameters on the numerical integration scheme (atomic radii, weights, thresholds and grid information)

```
.....................................................................
DFT PARAMETERS

     ATOM        ELECTRONS    NET CHARGE    R(ANGSTROM)
  1   12  MG      12.0000       0.0000      1.60000000
  2    8  O        8.0000       0.0000      0.74000000

SIZE OF GRID=       1292
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MAKE_GRID2  TELAPSE        0.84 TCPU        0.61
BECKE WEIGHT FUNCTION
RADSAFE =     2.00
TOLERANCES - DENSITY:10**- 6; POTENTIAL:10**- 9; GRID WGT:10**-14

RADIAL INTEGRATION  - INTERVALS (POINTS,UPPER LIMIT):            1( 75,  4.0*R)

ANGULAR INTEGRATION - INTERVALS (ACCURACY LEVEL [N. POINTS] UPPER LIMIT):
 1(  4[  86]   0.2)  2(  8[ 194]   0.5)  3( 12[ 350]   0.9)  4( 16[ 974]   3.5)
 5( 12[ 350]9999.0)
```

Integration of the exchange-correlation density functional



001 plane of a unit cell of MgO

The exchange-correlation density functional is integrated numerically on a mesh of points in atomic domains.

Radial points:
Gauss formula
(n_r=number of radial points)

Angular points:
Lebedev distribution
(L=Lebedev accuracy parameter)

crystal output example: DFT: hybrid

The B3LYP functional has been selected

The percentage of fock exchange is reported.

```
********************************************************************************
TYPE OF CALCULATION :  RESTRICTED CLOSED SHELL
KOHN-SHAM HAMILTONIAN

(EXCHANGE)[CORRELATION] FUNCTIONAL:(BECKE)[LEE-YANG-PARR]

NON-LOCAL WEIGHTING FACTOR (EXCHANGE) =           0.9000
NON-LOCAL WEIGHTING FACTOR [CORRELATION] =        0.8100

HYBRID EXCHANGE - PERCENTAGE OF FOCK EXCHANGE    20.0000
```

crystal output example: DFT: pure - SCF Final Iterations

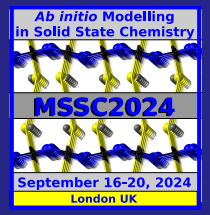
At the end of the SCF, the final DFT energy, the number of cycles and the convergence criteria are printed out.

```
CHARGE NORMALIZATION FACTOR   1.00000000
TOTAL ATOMIC CHARGES:
 11.4794677   8.5205323
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MOQGAD      TELAPSE        3.29 TCPU        1.68
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SHELLXN     TELAPSE        3.40 TCPU        1.79
+++ ENERGIES IN A.U. +++
::: EXT EL-POLE                                -4.8821772815712E+02
::: EXT EL-SPHEROPOLE                           4.1919197072099E+00
::: BIELET ZONE E-E                             5.5399116511276E+02
::: TOTAL E-E                                   6.9965356662852E+01
::: TOTAL E-N + N-E                            -5.0951805771653E+02
::: TOTAL N-N                                  -7.3084276676762E+01
::: KINETIC ENERGY                              2.6580241766248E+02
::: PSEUDO TOTAL   ENERGY                      -2.4683456006795E+02
::: VIRIAL COEFFICIENT                          1.0370005645681E+00
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MONMO3      TELAPSE        3.40 TCPU        1.80
NUMERICALLY INTEGRATED DENSITY     20.0000155038
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTT NUMDFT      TELAPSE        3.45 TCPU        1.84
CYC   6 ETOT(AU) -2.705350949836E+02 DETOT -3.86E-08 tst  3.79E-09 PX  2.94E-04

== SCF ENDED - CONVERGENCE ON ENERGY      E(AU) -2.7053509498361E+02 CYCLES   6


ENERGY EXPRESSION=HARTREE+FOCK EXCH*0.00000+(LDA        EXCH)*1.00000+PZ


TOTAL ENERGY(DFT)(AU)(  6) -2.7053509498361E+02 DE-3.9E-08 tester 3.8E-09
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTT EDFT        TELAPSE        3.45 TCPU        1.84
```

crystal output example: DFT: hybrid - SCF Final Iterations

At the end of the SCF, the final hybrid DFT energy, the number of cycles and the convergence criteria are printed out.

```
CHARGE NORMALIZATION FACTOR   1.00000000
TOTAL ATOMIC CHARGES:
 11.3814866   8.6185134
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MOQGAD      TELAPSE        6.37 TCPU        4.37
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTT SHELLXN     TELAPSE        6.77 TCPU        4.77
+++ ENERGIES IN A.U. +++
::: EXT EL-POLE                                -4.8089797576501E+02
::: EXT EL-SPHEROPOLE                           4.1021905460823E+00
::: BIELET ZONE E-E                             5.4230176472309E+02
::: TOTAL E-E                                   6.5505979504157E+01
::: TOTAL E-N + N-E                            -5.1039972787588E+02
::: TOTAL N-N                                  -7.3084276676762E+01
::: KINETIC ENERGY                              2.6632915753038E+02
::: PSEUDO TOTAL   ENERGY                      -2.5164886751810E+02
::: VIRIAL COEFFICIENT                          1.0283415305329E+00
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTT MONMO3      TELAPSE        6.78 TCPU        4.78
NUMERICALLY INTEGRATED DENSITY     20.0000148330
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTT NUMDFT      TELAPSE        6.91 TCPU        4.91
CYC   7 ETOT(AU) -2.719432579213E+02 DETOT -1.85E-09 tst  1.29E-10 PX  9.09E-05

== SCF ENDED - CONVERGENCE ON ENERGY      E(AU) -2.7194325792131E+02 CYCLES   7


ENERGY EXPRESSION=HARTREE+FOCK EXCH*0.20000+(BECKE      EXCH)*0.80000+LYP


TOTAL ENERGY(DFT)(AU)(  7) -2.7194325792131E+02 DE-1.8E-09 tester 1.3E-10
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTT EDFT        TELAPSE        6.91 TCPU        4.91
```



CRYSTAL scripts

CRYSTAL scripts: runcry17


```
./runcry17
Usage:

./runcry17 inpfilename [filename_restart_data (r-filename)]

inpfilename.d12          CRYSTAL input deck for wave function
                         calculation
   optional files

[inpfilename.gui]        geometry input file
                         (EXTERNAL or DLVINPUT in geometry input)

   optional files - SCF guess from previous run density matrix
   or RESTART in geometry optimization and frequency calculation

[r-filename.f9]          fort.9 written by a previous run
                         (GUESSP or GUESSF in SCF input)
[r-filename.f13]         fort.13 reducible density matrix written
                         by a previous run (RESTART in FREQCALC)
```

CRYSTAL scripts: runcry17


```
Results are written in current directory, in file:
inpfilename.out (default suffix)

The following files, if present and not empty, are moved
from scratch directory to current directory:

scratch            current                  content

fort.9             inpfilename.f9           binary wave function
fort.98            inpfilename.f98          formatted wave function
optc* or opta*     inpfilename.optstory/    history of geometry opt
SCAN*              inpfilename.scanstory/   geometries of scanned
                                            modes
HESSOPT.DAT (66)   inpfilename.hessopt      formatted hessian
HESSFREQ.DAT (66)  inpfilename.hessfreq     formatted hessian
OPTINFO.DAT (68)   inpfilename.optinfo      complete info
                                            for opt restart
```

CRYSTAL scripts: runcry17 - example 1


```
mssc@pc3:~/test> ls
MgO.d12

mssc@pc3:~/test> runcry17 MgO
mssc@pc3:~/test> ls -rtl
-rw-r--r-- 1 mssc  mssc     887 Sep  9 09:00 MgO.d12
-rw-rw-r-- 1 mssc  mssc  117940 Sep  9 09:09 MgO.f9
-rw-rw-r-- 1 mssc  mssc  291818 Sep  9 09:09 MgO.f98
-rw-rw-r-- 1 mssc  mssc   32229 Sep  9 09:09 MgO.out


mssc@pc3:~/test> grep -A2 "SCF E" MgO.out
 == SCF ENDED - CONVERGENCE ON ENERGY      E(AU) -2.7121814374931E+02 CYCLES   7

 TOTAL ENERGY(HF)(AU)(   7) -2.7121814374931E+02 DE-4.9E-09 tst 3.5E-10 PX 3.6E-04
```

CRYSTAL scripts: runcry17 - example 2 - GUESSP


```
mssc@pc3:~/test> grep -A2 "SCF E" MgO_MAXCYCLE4.out
 == SCF ENDED - TOO MANY CYCLES           E(AU) -2.7121814186767E+02 CYCLES   4

 TOTAL ENERGY(HF)(AU)(   4) -2.7121814186767E+02 DE-1.1E-03 tst 1.6E-04 PX 8.9E-02

mssc@pc3:~/test> ls -rt
MgO_MAXCYCLE4.d12                MgO_MAXCYCLE4.f98
MgO_MAXCYCLE4.f9                 MgO_MAXCYCLE4.out
```

Create an input with the GUESSP directive: MgO_GUESSP.d12

```
mssc@pc3:~/test> runcry17 MgO_GUESSP MgO_MAXCYCLE4
...
mssc@pc3:~/test> grep -A2 "SCF E" MgO_GUESSP.out
 == SCF ENDED - CONVERGENCE ON ENERGY     E(AU) -2.7466415303345E+02 CYCLES   3

 TOTAL ENERGY(HF)(AU)(   3) -2.7466415303345E+02 DE 6.0E-09 tst 1.1E-09 PX 3.1E-04
```

CRYSTAL scripts: runcry17 - example 2 - GUESSP

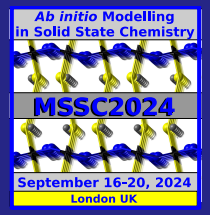

```
...
RESTART FROM A PREVIOUS DENSITY MATRIX - DEP ACTIVE
...
CYC   0 ETOT(AU) -2.746641528970E+02 DETOT -2.75E+02 tst  0.00E+00 PX  1.00E+00
CHARGE NORMALIZATION FACTOR   1.00000000
TOTAL ATOMIC CHARGES:
 11.2219078   8.7780922
TTTTTTTTTTTTTTTTTTTTTTTTTTTTT MOQGAD      TELAPSE         0.29 TCPU        0.03
TTTTTTTTTTTTTTTTTTTTTTTTTTTTT SHELLXN     TELAPSE         0.72 TCPU        0.43
TTTTTTTTTTTTTTTTTTTTTTTTTTTTT MONMO3      TELAPSE         0.72 TCPU        0.43
CYC   0 ETOT(AU) -2.712181418677E+02 DETOT -2.71E+02 tst  0.00E+00 PX  1.00E+00
```

Please note: The script runcry17 copies MgO_MAXCYCLE4.f9 into **fort.20** in the temporary directories.
The keyword GUESSP activates the reading of the file **fort.20**.
If the fort.20 does not exist, this is the error message printed by crystal:

```
ERROR **** GUESSP **** COPY OF WAVEFUNCTION FILE fort.20 CAN NOT BE FOUND
TTTTTTTTTTTTTTTTTTTTTTTTTTTTT ERR         TELAPSE         0.01 TCPU        0.01
```

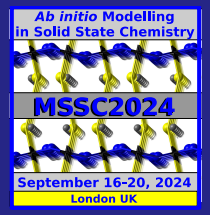
CRYSTAL scripts: runprop17


```
/runprop17
Usage:

./runprop17 inpfilename wf-filename [f80-filename]

inpfilename.d3      input deck for properties
wf-filename.f9      fort.9 written by a previous crystal run
                    (binary)

   optional files

[wf-filename.f98]   fort.98 written by a previous crystal run
                    input must begin with RDFMWF

Results are written in current directory, in file:
inpfilename_wf-filename.outp (default suffix)
```



CRYSTAL scripts: runprop17


```
The following files, if present and not empty, are moved
from scratch directory to current directory:

scratch     current                    content

fort.98     inpfilename.f98            formatted wavefunction (FMWF)
FINDSYM.DAT inpfilename.FINDSYM
fort.80     inpfilename.f80            Wannier functions (LOCALWF)
fort.33     inpfilename.xyz            atoms coordinates (COORPRT)
fort.34     inpfilename.gui            GUI - geometry input (EXTPRT)
PPAN.DAT    inpfilename.ppan           Mulliken population analysis
BAND.DAT    inpfilename_dat.BAND       band structure (BAND)
DIEL.DAT    inpfilename_dat.DIEL       dielectric constant
DOSS.DAT    inpfilename_dat.DOSS       density of states (DOSS)
RHOLINE.DAT inpfilename_dat.RHOLINE    data for 1D charge (or spin)
fort.31     inpfilename_dat.prop3d     data for 3D charge (or spin)

inpfilename.f98
inpfilename_wf-filename.f98
```



CRYSTAL tutorials

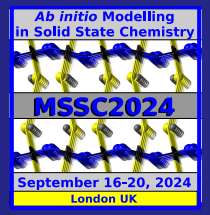
CRYSTAL tutorial project

Development of the CRYSTAL tutorials

R.Dovesi, R.Orlando, S.Casassa, Y.Noel, F.Pascale, G.Mallia, M.Ferrero, I.P.R Moreira, M.Llunell, M.Rerat, C.Darrigan, A.Damin, A.M.Ferrari, K.Doll, L.Valenzano, L. Maschio, A.Erba, M.De La Pierre, M.Ferrabone, J.Baima, E. Albanese, V.Lacivita, M. Halo, ...

with contributions by P. Ugliengo and N.M. Harrison

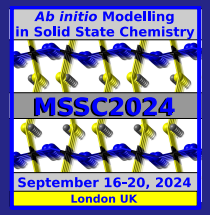
CRYSTAL tutorial project: webpage



Acknoledgement to Dr B. Civalleri

The structure of this talk is based on a previous one given by

Dr Bartolomeo (Mimmo) Civalleri
Dipatimento di Chimica IFM
Universita' di Torino
Via P. Giuria 7, I-10125 Torino, Italy
bartolomeo.civalleri@unito.it


Ab initio Modelling
in Solid State Chemistry
MSSC2024
September 16-20, 2024
London UK

THANK YOU!!!