WIEN2k 算例

格致斯创 (北京) 科技有限公司　姜骏

北京化工大学

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WIEN2k 算例:Structre

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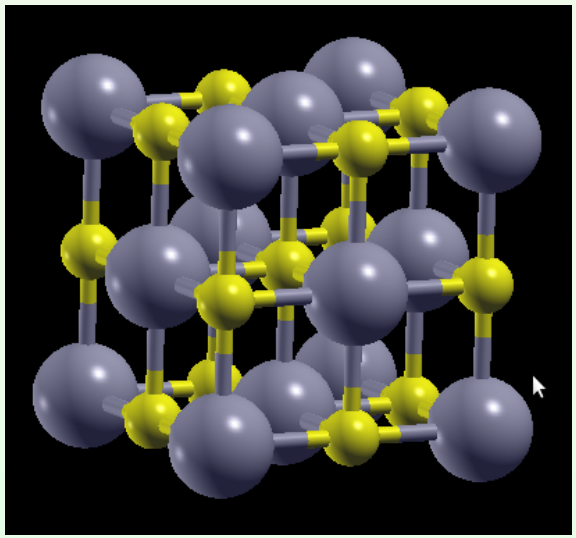

```
1 Title
2 F    LATTICE,NONEQUIV.ATOMS:  225_Fm-3m
3 MODE OF CALC=RELA unit=ang
4   8.178738  8.178738  8.178738 90.000000 90.000000 90.000000
5 ATOM   1: X=0.00000000 Y=0.00000000 Z=0.00000000
6           MULT= 1          ISPLIT= 2
7 Ti         NPT=  781  R0=0.00005000 RMT= 2.24        Z: 22.0
8 LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
9                      0.0000000 1.0000000 0.0000000
10                     0.0000000 0.0000000 1.0000000
11 ATOM   2: X=0.50000000 Y=0.50000000 Z=0.50000000
12          MULT= 1          ISPLIT= 2
13 C         NPT=  781  R0=0.00010000 RMT= 1.83        Z:  6.0
14 LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
15                     0.0000000 1.0000000 0.0000000
16                     0.0000000 0.0000000 1.0000000
17   48      NUMBER OF SYMMETRY OPERATIONS
18  1 0 0 0.00000000
19  0-1 0 0.00000000
20  0 0-1 0.00000000
21        1
22  1 0 0 0.00000000
23  0 0-1 0.00000000
24  0-1 0 0.00000000
25        2
26 -1 0 0 0.00000000
27  0-1 0 0.00000000
28  0 0-1 0.00000000
29        3
30 -1 0 0 0.00000000
31  0 0-1 0.00000000
32  0-1 0 0.00000000
33        4
34  0 1 0 0.00000000
35 -1 0 0 0.00000000
36  0 0-1 0.00000000
37        5
38  0 0 1 0.00000000
39 -1 0 0 0.00000000
40  0-1 0 0.00000000
41        6
42  0 1 0 0.00000000
43  1 0 0 0.00000000
44  0 0-1 0.00000000
45        7
46  0 0 1 0.00000000
47  1 0 0 0.00000000
48  0-1 0 0.00000000
```

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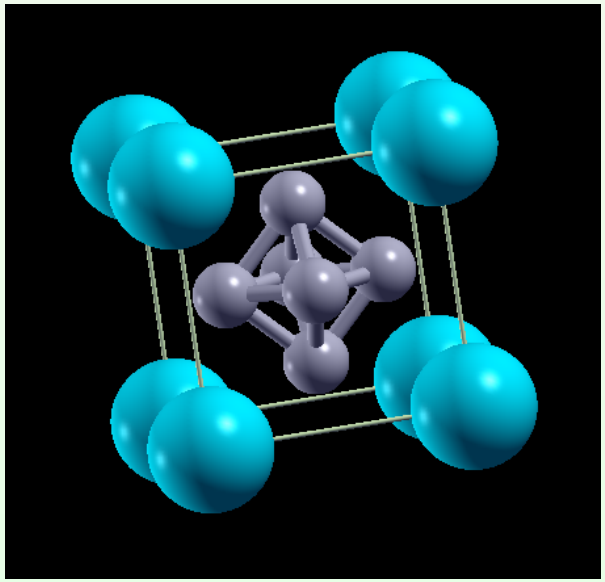

```
CaB6
P   LATTICE,NONEQUIV.ATOMS:  2221_Pm-3m
MODE OF CALC=RELA unit=ang
  7.757329  7.757329  7.757329 90.000000 90.000000 90.000000
ATOM   1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 2
Ca         NPT=  781  R0=0.00010000 RMT= 2.50000      Z: 20.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.20100000
          MULT= 6          ISPLIT=-2
       -2: X=0.50000000 Y=0.50000000 Z=0.79900000
       -2: X=0.20100000 Y=0.50000000 Z=0.50000000
       -2: X=0.79900000 Y=0.50000000 Z=0.50000000
       -2: X=0.50000000 Y=0.20100000 Z=0.50000000
       -2: X=0.50000000 Y=0.79900000 Z=0.50000000
B          NPT=  781  R0=0.00010000 RMT= 1.55         Z:  5.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  48      NUMBER OF SYMMETRY OPERATIONS
-1 0 0 0.00000000
 0-1 0 0.00000000
 0 0-1 0.00000000
       1
-1 0 0 0.00000000
 0-1 0 0.00000000
 0 0 1 0.00000000
       2
-1 0 0 0.00000000
 0 0-1 0.00000000
 0-1 0 0.00000000
       3
-1 0 0 0.00000000
 0 0 1 0.00000000
 0-1 0 0.00000000
       4
-1 0 0 0.00000000
 0 0-1 0.00000000
 0 1 0 0.00000000
       5
-1 0 0 0.00000000
 0 0 1 0.00000000
 0 1 0 0.00000000
       6
-1 0 0 0.00000000
 0 1 0 0.00000000
```

WIEN2k 算例:$CaB6_6$ 的 SCF

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```
 1
 2 Calculating CaB6 in /home/jun_jiang/WORKS/WIEN2k_Cal/CaB6
 3 on jun with PID 6598
 4 using WIEN2k_14.2 (Release 15/10/2014) in /home/jun_jiang/Softs/WIEN2k
 5
 6
 7     start       (Thu Apr 21 15:45:13 CST 2016) with lapw0 (40/99 to go)
 8
 9     cycle 1     (Thu Apr 21 15:45:13 CST 2016)  (40/99 to go)
10
11 >   lapw0 -p    (15:45:13) starting parallel lapw0 at Thu Apr 21 15:45:13 CST 2016
12 -------- .machine0 : 2 processors
13 1.956u 0.080s 0:02.24 90.6%     0+0k 0+1904io 8pf+0w
14 >   lapw1  -p           (15:45:15) starting parallel lapw1 at Thu Apr 21 15:45:15 CST 2016
15 ->  starting parallel LAPW1 jobs at Thu Apr 21 15:45:15 CST 2016
16 running LAPW1 in parallel mode (using .machines)
17 1 number_of_parallel_jobs
18      localhost localhost(56) 32.584u 0.440s 0:17.20 191.9%      0+0k 0+31008io 8pf+0w
19    Summary of lapw1para:
20    localhost     k=0     user=56         wallclock=26.4
21 32.640u 0.452s 0:19.33 171.1%   0+0k 0+31224io 8pf+0w
22 >   lapw2 -p            (15:45:34) running LAPW2 in parallel mode
23       localhost 5.560u 0.212s 0:03.12 184.9% 0+0k 0+1600io 8pf+0w
24    Summary of lapw2para:
25    localhost     user=5.56       wallclock=3.12
26 5.660u 0.236s 0:04.33 136.0%    0+0k 0+2672io 8pf+0w
27 >   lcore       (15:45:39) 0.004u 0.004s 0:00.00 0.0%   0+0k 0+240io 0pf+0w
28 >   mixer       (15:45:39) 0.020u 0.000s 0:00.02 100.0% 0+0k 0+936io 0pf+0w
29 >   mixer       (15:45:39) 0.020u 0.000s 0:00.02 100.0% 0+0k 0+936io 0pf+0w
30 :ENERGY convergence:  0 0 .0000073050000000
31 :CHARGE convergence:  0 0.0001 .0006803
32 ec cc and fc_conv 1 0 1
33
34     cycle 2     (Thu Apr 21 15:45:39 CST 2016)  (39/98 to go)
35
36 >   lapw0 -p    (15:45:39) starting parallel lapw0 at Thu Apr 21 15:45:39 CST 2016
37 -------- .machine0 : 2 processors
38 1.960u 0.072s 0:02.23 91.0%     0+0k 0+1888io 8pf+0w
39 >   lapw1  -p           (15:45:41) starting parallel lapw1 at Thu Apr 21 15:45:41 CST 2016
40 ->  starting parallel LAPW1 jobs at Thu Apr 21 15:45:41 CST 2016
41 running LAPW1 in parallel mode (using .machines)
42 1 number_of_parallel_jobs
43      localhost localhost(56) 32.776u 0.384s 0:17.21 192.6%      0+0k 0+30496io 8pf+0w
44    Summary of lapw1para:
45    localhost     k=0     user=56         wallclock=23.04
46 32.816u 0.412s 0:19.32 171.9%   0+0k 0+30720io 8pf+0w
47 >   lapw2 -p            (15:46:01) running LAPW2 in parallel mode
48       localhost 5.584u 0.216s 0:03.14 184.3% 0+0k 0+1600io 8pf+0w
```

WIEN2k 算例:$CaB6_6$ 的总能

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```
:INFO :  Singular value   5.266E+00 Weight  1.0000E+00 Projections   8.149E-02  3.864E-04
:INFO :  Singular value   1.027E+00 Weight  1.0000E+00 Projections  -8.295E-02 -4.233E-04
:INFO :  Singular value   1.120E-05 Weight  9.5648E-01 Projections   1.941E-03 -1.163E-01

:DIRM :  MEMORY 3/8 RESCALE   1.15 RED 0.799 PRED 0.610 NEXT 0.268
:INFO :  Blimit    3.078E+00  1.223E+00  1.000E+00  4.891E+00
:DIRP :  |MSR1|= 1.463E-04 |PRATT|= 6.351E-04 ANGLE=  23.7 DEGREES
:DIRQ :  |MSR1|= 3.102E-04 |PRATT|= 4.847E-04 ANGLE=  19.8 DEGREES
:DIR  :  |MSR1|= 3.430E-04 |PRATT|= 7.990E-04 ANGLE=  34.2 DEGREES
:MIX  :   MSE1   REGULARIZATION: 2.39E-06  GREED: 0.200  Newton 1.00  0.43

       CHARGES OF MIXED CHARGE DENSITY
:CTO   : INTERSTITIAL CHARGE =    10.309351
:CTO001: CHARGE SPHERE  1    =    18.217757
:CTO002: CHARGE SPHERE  2    =     3.578815

:NEC03: NUCLEAR AND ELECTRONIC CHARGE     50.00000    50.00000

PW CHANGE     H    K    L       Current      Change      Residue
:PTO001:      0    0    0  5.20312320E-02 -7.829E-08 -2.970E-06
:PTO002:     -1    0    0 -3.50091080E-02 -3.278E-06 -1.982E-05
:PTO003:     -1   -1    0  9.89302686E-02 -4.227E-07 -2.578E-05
:PTO004:     -1   -1   -1  6.68682461E-02 -2.179E-06 -1.978E-05
:PTO005:     -2    0    0  3.90826205E-02 -2.061E-06 -1.332E-05
:PTO006:     -2   -1    0  7.26972038E-02 -9.869E-06 -4.877E-05
:PTO007:     -2   -1   -1  2.70950683E-02 -9.111E-06 -4.211E-05
:PTO008:     -2   -2    0  2.25307748E-02 -5.771E-06 -2.006E-05
:PTO009:     -3    0    0  9.59867239E-03 -2.784E-06 -8.422E-06
:PTO010:     -2   -2   -1  2.32953914E-02 -6.898E-06 -3.106E-05
:PTO011:     -3   -1    0  1.57820091E-03 -7.319E-06 -2.896E-05
:PTO012:     -3   -1   -1  3.17852138E-02 -7.805E-06 -2.666E-05

:ENE  : ********** TOTAL ENERGY IN Ry =        -1659.19884293

       TOTAL FORCE IN mRy/a.u. = |F|      Fx             Fy             Fz     with/without FOR in case.in2
:FOR001:   1.ATOM          0.000          0.000          0.000          0.000 partial forces
:FOR002:   2.ATOM          1.600          0.000          0.000          1.600 partial forces
       TOTAL FORCE WITH RESPECT TO GLOBAL CARTESIAN COORDINATES:
:FCA001:   1.ATOM                         0.000          0.000          0.000 partial forces
:FCA002:   2.ATOM                         0.000          0.000          1.600 partial forces
```

WIEN2k 算例:$CaB6_6$ 的能量本征值计算

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```
          ATOMIC SPHERE DEPENDENT PARAMETERS FOR ATOM  Ca
:e__0001: OVERALL ENERGY PARAMETER IS     0.2942
          OVERALL BASIS SET ON ATOM IS LAPW
:E0_0001: E( 0)=     0.2942
             APW+lo
:E0_0001: E( 0)=    -2.5464    E(BOTTOM)=    -2.671    E(TOP)=    -2.421  2  3   162
             LOCAL ORBITAL
:E1_0001: E( 1)=    -1.1618    E(BOTTOM)=    -1.392    E(TOP)=    -0.932  1  2   160
             APW+lo
:E1_0001: E( 1)=     0.6942
             LOCAL ORBITAL

          ATOMIC SPHERE DEPENDENT PARAMETERS FOR ATOM  B
:e__0002: OVERALL ENERGY PARAMETER IS     0.2942
          OVERALL BASIS SET ON ATOM IS LAPW
:E0_0002: E( 0)=     0.2942
             APW+lo
:E1_0002: E( 1)=     0.2942
             APW+lo

          MPI-parallel calculation using     2 processors
          Scalapack processors array (row,col):   2   1

        K=    0.04545    0.04545    0.04545            1
:RKM   : MATRIX SIZE    771LOs:  32  RKM= 6.96  WEIGHT= 8.00  PGR:
          EIGENVALUES ARE:
:EIG00001:       -2.5208063   -1.1232587   -1.1232246   -1.1232246   -0.5716036
:EIG00006:       -0.0377662    0.0006313    0.0006313    0.0370064    0.1189082
:EIG00011:        0.1189082    0.4642867    0.4642867    0.4744986    0.6955540
:EIG00016:        0.6955540    0.7114008    0.7817524    0.7817524    0.8426554
:EIG00021:        0.8570605    0.8570605    0.9357456    1.0481828    1.0481828
:EIG00026:        1.0831291    1.3667560    1.3667560    1.5563634    1.5770406
:EIG00031:        1.5770406    1.6251174    1.7667781    1.8082451    1.8082451
:EIG00036:        1.8131304    1.8281590    1.8281590    1.8519851    1.8519851
:EIG00041:        1.9909394    1.9909394
```

WIEN2k 算例:CaB_6 的 Fermi 能

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```
:KPT    :       NUMBER OF K-POINTS:    56
        Insulator, EF-inconsistency corrected
:GAP    :     0.0068 Ry =      0.093 eV   (provided you have a proper k-mesh)
          Bandranges (emin - emax) and occupancy:
:BAN00004:    4    -1.126173    -1.122149  2.00000000
:BAN00005:    5    -0.571604    -0.505674  2.00000000
:BAN00006:    6    -0.202724    -0.037766  2.00000000
:BAN00007:    7    -0.150839     0.012839  2.00000000
:BAN00008:    8    -0.130821     0.055680  2.00000000
:BAN00009:    9     0.037006     0.214829  2.00000000
:BAN00010:   10     0.118908     0.266602  2.00000000
:BAN00011:   11     0.118908     0.322351  2.00000000
:BAN00012:   12     0.267078     0.464287  2.00000000
:BAN00013:   13     0.304595     0.464287  2.00000000
:BAN00014:   14     0.344830     0.494231  2.00000000
:BAN00015:   15     0.501055     0.839050  0.00000000
:BAN00016:   16     0.667800     0.857437  0.00000000
:BAN00017:   17     0.711401     0.857437  0.00000000
:BAN00018:   18     0.781752     0.866175  0.00000000
:BAN00019:   19     0.781752     0.876549  0.00000000
        Energy to separate low and high energystates:    -0.25272


:NOE    : NUMBER OF ELECTRONS           =   28.000

:FER    : F E R M I - ENERGY(TETRAH.M.)=    0.4942307621
:GMA    : POTENTIAL AND CHARGE CUT-OFF   12.00 Ry**.5
```

WIEN2k 算例:CaB_6 的 DOS

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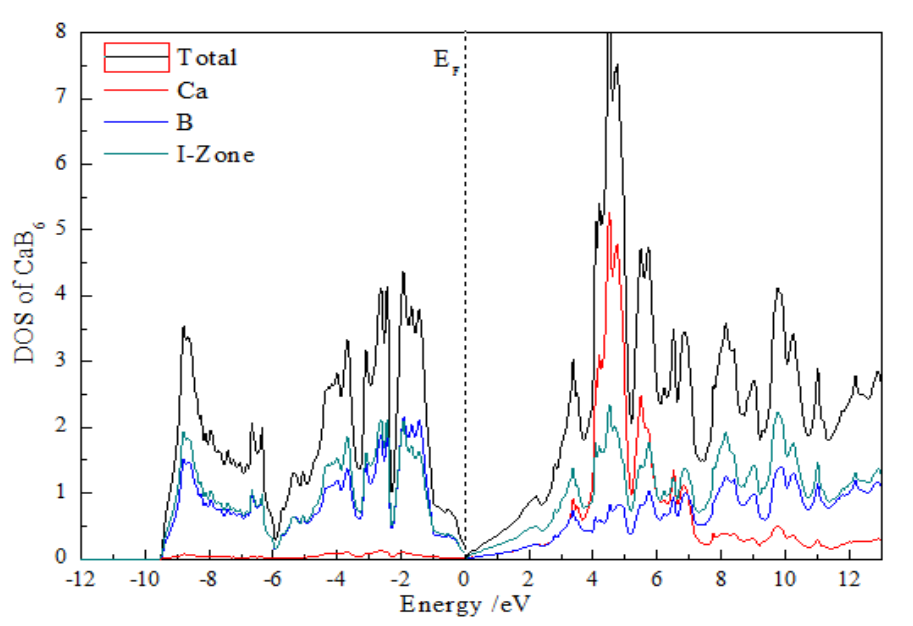
```
1 CaB6
2  -0.50 0.002 1.500 0.003  # EMIN, DE, EMAX, Gauss-broadening(>de)
3   4    N   0.000          # NUMBER OF DOS-CASES below, G/L/B broadening (Ry)
4     0    1   total        # atom, case=column in qtl-header, label
5     1    1   Atom-Ca tot
6     2    1   Atom-B tot
7     3    1   I-Zone
8 SUM: 0 2                      # NUMBER OF SUMMATIONS, max-nr-of summands
9 2 5                         # this sums dos-cases 2+5 from the input above
10
```

Figure: CaB_6.int



WIEN2k 算例:CaB_6 的能带结构

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```
W          40   20    0   40  2.0-0.5 1.5       Template for fcc structure
           39   20    1   40  2.0
           38   20    2   40  2.0
           37   20    3   40  2.0
           36   20    4   40  2.0
           35   20    5   40  2.0
           34   20    6   40  2.0
           33   20    7   40  2.0
           32   20    8   40  2.0
           31   20    9   40  2.0
           30   20   10   40  2.0
           29   20   11   40  2.0
           28   20   12   40  2.0
           27   20   13   40  2.0
           26   20   14   40  2.0
           25   20   15   40  2.0
           24   20   16   40  2.0
           23   20   17   40  2.0
           22   20   18   40  2.0
           21   20   19   40  2.0
L          20   20   20   40  2.0
           19   19   19   40  2.0
           18   18   18   40  2.0
           17   17   17   40  2.0
           16   16   16   40  2.0
           15   15   15   40  2.0
           14   14   14   40  2.0
           13   13   13   40  2.0
           12   12   12   40  2.0
           11   11   11   40  2.0
LAMBDA     10   10   10   40  2.0
            9    9    9   40  2.0
            8    8    8   40  2.0
            7    7    7   40  2.0
            6    6    6   40  2.0
            5    5    5   40  2.0
            4    4    4   40  2.0
            3    3    3   40  2.0
            2    2    2   40  2.0
            1    1    1   40  2.0
GAMMA       0    0    0   40  2.0
            1    0    0   40  2.0
            2    0    0   40  2.0
            3    0    0   40  2.0
            4    0    0   40  2.0
            5    0    0   40  2.0
            6    0    0   40  2.0
            7    0    0   40  2.0
            8    0    0   40  2.0
            9    0    0   40  2.0
```

Figure: CaB_6.klist_band

```
### Figure configuration
 5.0   3.0                          # paper offset of plot
10.0  15.0                          # xsize,ysize [cm]
 1.0   4                            # major ticks, minor ticks
 1.0   1                            # character height, font switch
 1.1   2    4                       # line width, line switch, color switch
### Data configuration
-14.0   8.0   2                     # energy range, energy switch (1:Ry, 2:eV)
1       0.49423                     # Fermi switch, Fermi-level (in Ry units)
1   999                             # number of bands for heavier plotting   1,1
0       1     0.2                   # latom, itypc, size  of heavier plotting


Fermi switch:
  0...no line
  1...solid line
  2...dashed line
  3...dotted line

Line switch:
  0...dots
  1...lines
  2...lines and open circle
  3...lines and filled circles

Color switch (re-define your colors in defins.f)
  0...black
  1...one-color plot
  2...three-color plot
  3...multi-color plot
  4...multi-color plot, one color for each irr. representations

Font switch:
  0...no text
  1...Times and Symbol
  2...Times, Symbol, and Times-Italic
  3...Helvetica, Symbol, and  Helvetica-Italic
  4...(include your own fonts in defins.f)


```

Figure: CaB_6.insp

WIEN2k 算例:CaB_6 的能带结构

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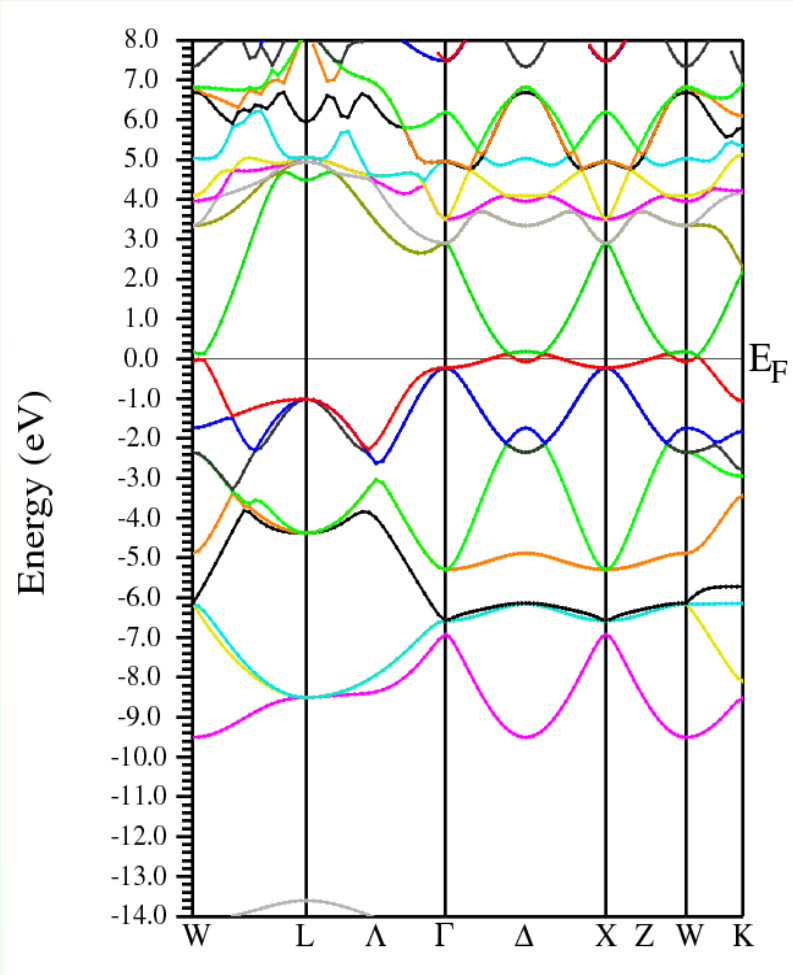

Figure: The Band-structure of CaB_6

WIEN2k 算例:Cr 的反铁磁计算

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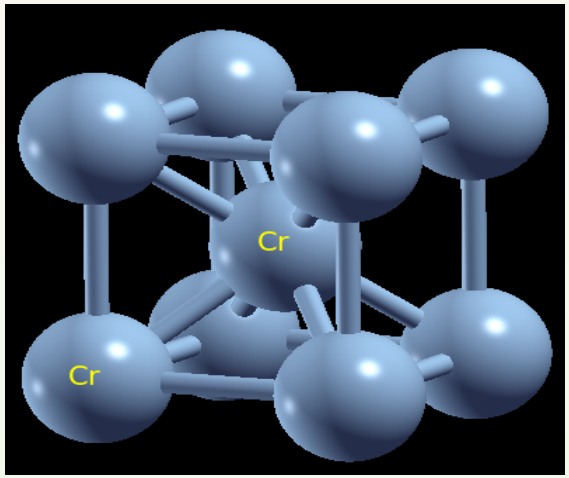
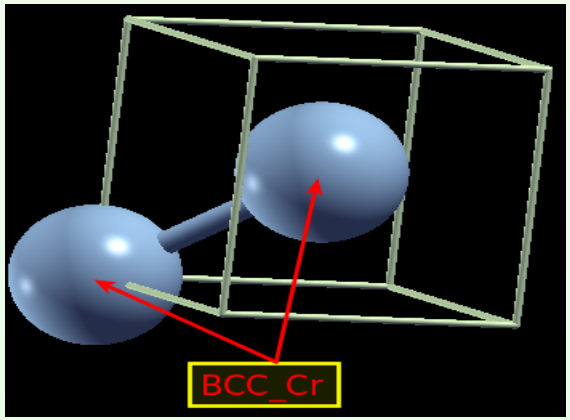
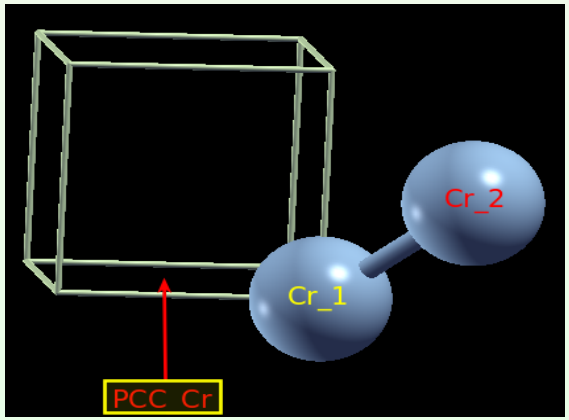


(a) Structure



(b) BCC_Cr



(c) PCC_Cr

WIEN2k 算例:Cr 的反铁磁计算

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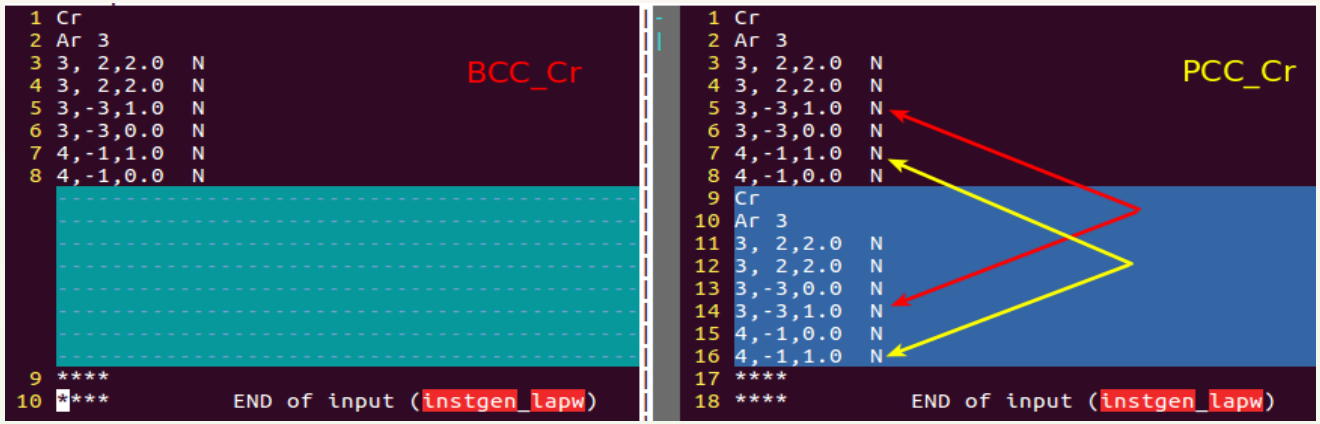

Figure: Cr.inst

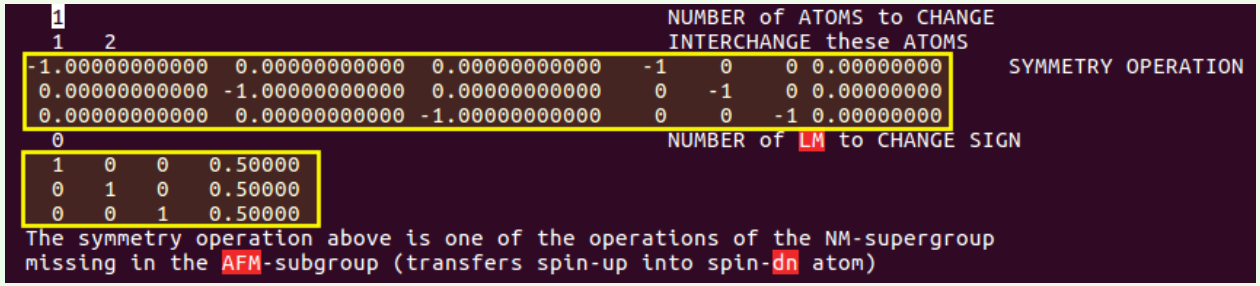

Figure: Cr.inclmcopy

WIEN2k 算例:Cr 的反铁磁计算

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```
      SPIN MAGNETIC MOMENTS OF MIXED CHARGE DENSITY
:MMINT:  MAGNETIC MOMENT IN INTERSTITIAL   =     0.00000
:MMI001: MAGNETIC MOMENT IN SPHERE    1    =     1.22904
:MMI002: MAGNETIC MOMENT IN SPHERE    2    =    -1.22904
:MMTOT:  SPIN MAGNETIC MOMENT IN CELL      =     0.00000

:NEC03: NUCLEAR AND ELECTRONIC CHARGE      48.00000    48.00000

PW CHANGE      H    K    L        Current       Change       Residue
:PUP001:       0    0    0  2.27856834E-02 -3.521E-07 -4.010E-07
:PUP002:      -1    0    0  3.77938878E-03  3.083E-06  9.546E-07
:PUP003:      -1   -1    0  2.36856940E-03 -4.767E-07 -4.462E-07
:PUP004:      -1   -1   -1 -1.68219216E-03 -1.491E-06 -3.919E-07
:PUP005:      -2    0    0 -3.52565081E-03 -6.071E-08 -1.280E-07
:PUP006:      -2   -1    0 -3.32375768E-03 -2.143E-06 -4.851E-07
:PUP007:      -2   -1   -1 -2.54967529E-03  6.288E-08  1.157E-07
:PUP008:      -2   -2    0  2.23109667E-05  3.866E-08  9.231E-08
:PUP009:      -3    0    0 -2.63725738E-04 -9.404E-08 -2.085E-08
:PUP010:      -2   -2   -1  6.86882099E-04  2.653E-07  1.800E-08
:PUP011:      -3   -1    0 -7.32642220E-04 -8.635E-08 -5.311E-08
:PUP012:      -3   -1   -1  2.44655033E-04  1.800E-07  2.605E-08
:PDN001:       0    0    0  2.27856834E-02 -3.521E-07 -4.010E-07
:PDN002:      -1    0    0 -3.77938878E-03 -3.083E-06 -9.546E-07
:PDN003:      -1   -1    0  2.36856940E-03 -4.767E-07 -4.462E-07
:PDN004:      -1   -1   -1  1.68219216E-03  1.491E-06  3.919E-07
:PDN005:      -2    0    0 -3.52565081E-03 -6.071E-08 -1.280E-07
:PDN006:      -2   -1    0  3.32375768E-03  2.143E-06  4.851E-07
:PDN007:      -2   -1   -1 -2.54967529E-03  6.288E-08  1.157E-07
:PDN008:      -2   -2    0  2.23109667E-05  3.866E-08  9.231E-08
:PDN009:      -3    0    0  2.63725738E-04  9.404E-08  2.085E-08
:PDN010:      -2   -2   -1 -6.86882099E-04 -2.653E-07 -1.800E-08
:PDN011:      -3   -1    0 -7.32642220E-04 -8.635E-08 -5.311E-08
:PDN012:      -3   -1   -1 -2.44655033E-04 -1.800E-07 -2.605E-08

:ENE  : ********** TOTAL ENERGY IN Ry =         -4203.54307464
```

```
      SPIN MAGNETIC MOMENTS OF MIXED CHARGE DENSITY
:MMINT:  MAGNETIC MOMENT IN INTERSTITIAL   =    -0.00000
:MMI001: MAGNETIC MOMENT IN SPHERE    1    =    -0.00000
:MMTOT:  SPIN MAGNETIC MOMENT IN CELL      =    -0.00000

:NEC03: NUCLEAR AND ELECTRONIC CHARGE      24.00000    24.00000

PW CHANGE      H    K    L        Current       Change       Residue
:PUP001:       0    0    0  2.28551932E-02 -2.889E-08 -6.221E-08
:PUP002:       0   -1   -1  2.15471373E-03  5.166E-08  6.420E-08
:PUP003:       0    0   -2 -3.61735255E-03  5.110E-08  2.046E-07
:PUP004:       1   -1   -2 -2.49898610E-03  1.709E-08  6.792E-08
:PUP005:       0   -2   -2  5.42938420E-05  7.183E-09  3.225E-08
:PUP006:       0   -1   -3 -6.84043940E-04  1.509E-08  6.716E-08
:PUP007:       2   -2   -2  2.08588729E-04 -1.289E-09 -2.389E-09
:PUP008:       1   -2   -3  4.29655903E-04  1.220E-09  8.107E-09
:PUP009:       0    0   -4 -3.11024995E-07  2.679E-10  7.502E-10
:PUP010:       1   -1   -4  8.46380557E-05  1.784E-10 -2.830E-11
:PUP011:       0   -3   -3  6.02472175E-05  2.004E-10  6.606E-10
:PUP012:       0   -2   -4  7.15481438E-05  6.757E-11 -1.801E-10
:PDN001:       0    0    0  2.28551573E-02  1.206E-08 -4.823E-08
:PDN002:       0   -1   -1  2.15467483E-03 -4.458E-09  2.322E-08
:PDN003:       0    0   -2 -3.61701055E-03 -2.391E-08 -1.300E-07
:PDN004:       1   -1   -2 -2.49902800E-03  2.220E-08  8.362E-08
:PDN005:       0   -2   -2  5.42772376E-05  7.851E-09  3.843E-08
:PDN006:       0   -1   -3 -6.83935454E-04 -1.131E-08 -4.346E-08
:PDN007:       2   -2   -2  2.08580932E-04 -3.173E-10  2.007E-09
:PDN008:       1   -2   -3  4.29643977E-04  9.128E-11  1.167E-08
:PDN009:       0    0   -4 -3.07397481E-07 -6.382E-10 -2.693E-09
:PDN010:       1   -1   -4  8.46390200E-05 -3.095E-10 -7.642E-10
:PDN011:       0   -3   -3  6.02445714E-05  6.382E-10  3.377E-09
:PDN012:       0   -2   -4  7.15469103E-05  2.914E-10  1.392E-09

:ENE  : *WARNING** TOTAL ENERGY IN Ry =         -2101.76951301
```

E_{AFM}:

$$
\begin{aligned}
&-4203.54307464-2\times(-2101.76951301)\\
=&-0.0405\mathrm{Ry}\\
=&-0.11\mathrm{eV}
\end{aligned}
$$

WIEN2k 算例:EuB_6 的 LDA+U

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```
  1  1  0                    nmod, natorb, ipr
PRATT  1.0                   BROYD/PRATT, mixing
  1 1  3                     iatom nlorb, lorb
 1                           nsic 0..AMF, 1..SIC, 2..HFM
 6.32 0.00          U J (Ry)   Note: we recommend to use U_eff = U-J and J=0
```

Figure: EuB_6.inorb

```
-12.                        Emin cutoff energy
 1                         number of atoms for which density matrix is calculated
1  1 3          index of 1st atom, number of L's, L1
0 0             r-index, (l,s)index
```

Figure: EuB_6.indm

WIEN2k 算例:EuB_6 的 LDA+U

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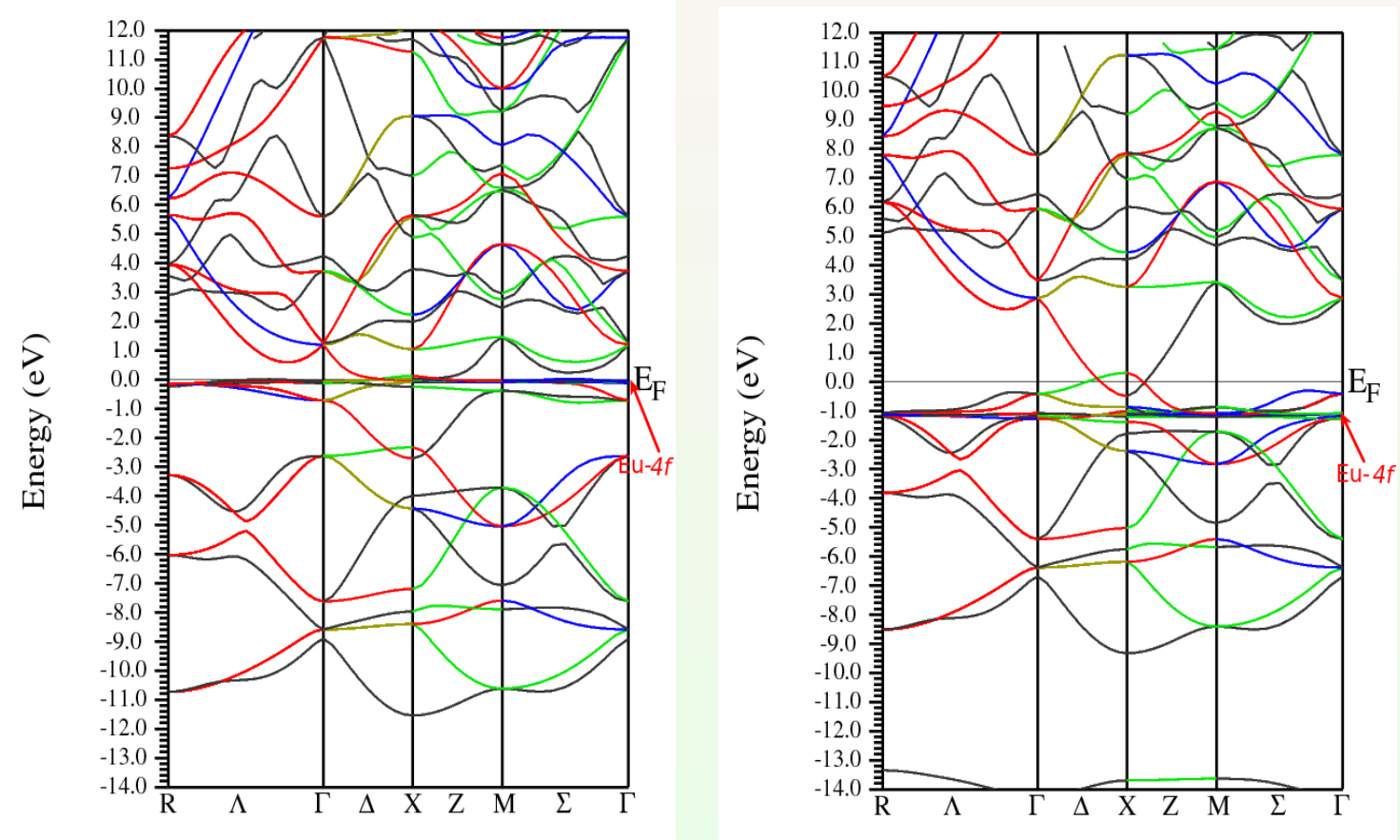

Figure: The spin-up Band-structure of EuB_6.

WIEN2k 算例:EuB_6 的 LDA+U

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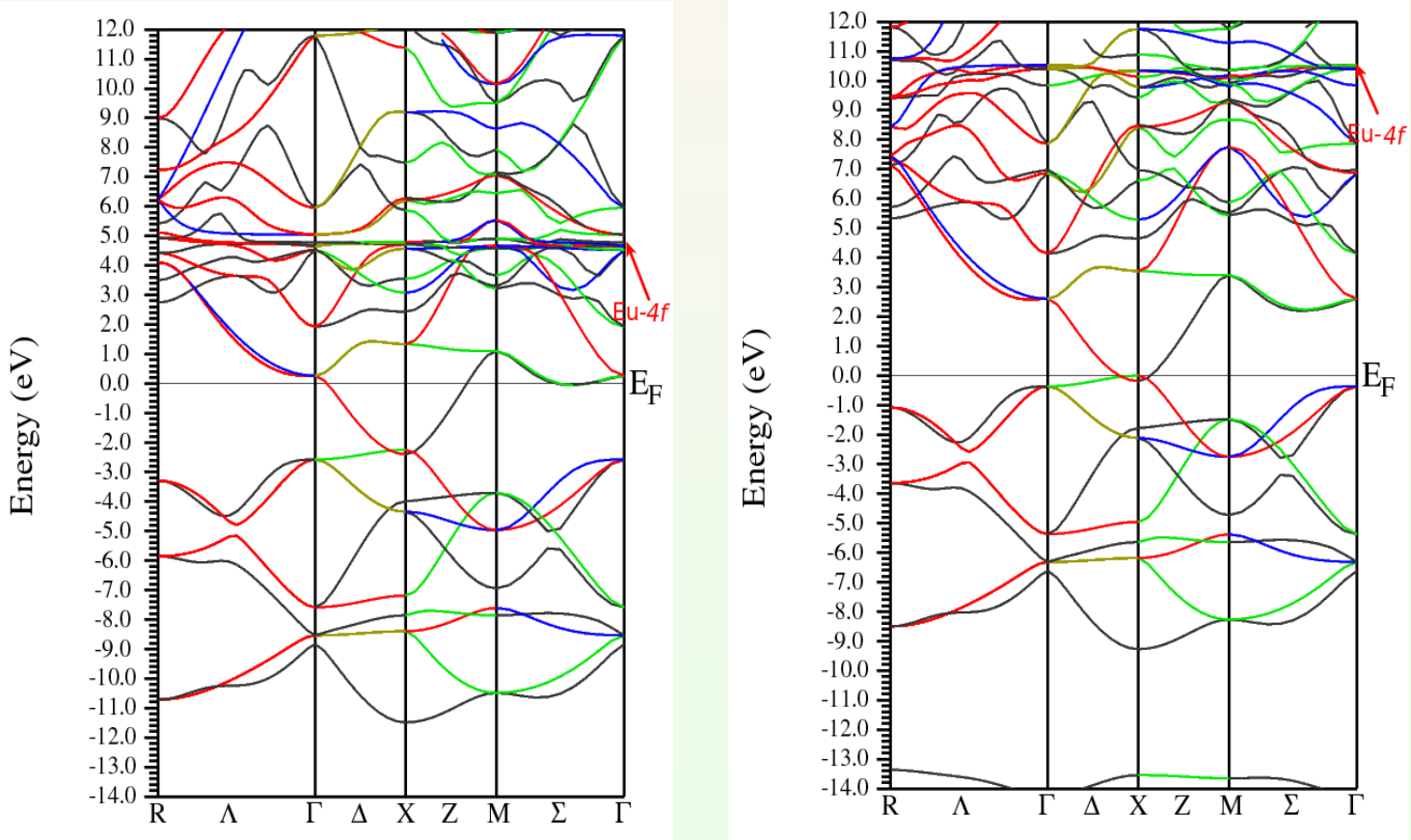

Figure: The spin-dn Band-structure of EuB_6.

WIEN2k 算例:EuB_6 的旋-轨耦合

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```
EuB6
P   LATTICE,NONEQUIV.ATOMS:  2 221_Pm-3m
MODE OF CALC=RELA unit=ang
  7.788320  7.788320  7.788320 90.000000 90.000000 90.000000
ATOM   1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 2
Eu         NPT=  781  R0=0.00001000 RMT= 2.50000     Z: 63.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.20100000
          MULT= 6          ISPLIT= 2
ATOM  -2:X= 0.50000000 Y=0.50000000 Z=0.79900000
ATOM  -2:X= 0.20100000 Y=0.50000000 Z=0.50000000
ATOM  -2:X= 0.79900000 Y=0.50000000 Z=0.50000000
ATOM  -2:X= 0.50000000 Y=0.20100000 Z=0.50000000
ATOM  -2:X= 0.50000000 Y=0.79900000 Z=0.50000000
B          NPT=  781  R0=0.00010000 RMT= 1.56        Z:  5.0
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  48      NUMBER OF SYMMETRY OPERATIONS
-1 0 0 0.00000000
 0-1 0 0.00000000
 0 0-1 0.00000000
       1
-1 0 0 0.00000000
 0-1 0 0.00000000
 0 0 1 0.00000000
       2
-1 0 0 0.00000000
 0 0-1 0.00000000
 0-1 0 0.00000000
       3
-1 0 0 0.00000000
```

```
 1 EuB6                                  s-o calc. M|| 0.00  0.00  1.00
 2 P                          3 221_
 3                RELA
 4   7.788320  7.788320  7.788320 90.000000 90.000000 90.000000
 5 ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
 6           MULT= 1          ISPLIT=-2
 7 Eu         NPT=  781  R0=.000010000 RMT=   2.50000   Z:  63.00000
 8 LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
 9                      0.0000000 1.0000000 0.0000000
10                      0.0000000 0.0000000 1.0000000
11 ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.20100000
12           MULT= 2          ISPLIT=-2
13        -2: X=0.50000000 Y=0.50000000 Z=0.79900000
14 B         NPT=  781  R0=.000100000 RMT=   1.56000   Z:   5.00000
15 LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
16                      0.0000000 1.0000000 0.0000000
17                      0.0000000 0.0000000 1.0000000
18 ATOM  -3: X=0.20100000 Y=0.50000000 Z=0.50000000
19           MULT= 4          ISPLIT= 8
20        -3: X=0.79900000 Y=0.50000000 Z=0.50000000
21        -3: X=0.50000000 Y=0.20100000 Z=0.50000000
22        -3: X=0.50000000 Y=0.79900000 Z=0.50000000
23 B          NPT=  781  R0=.000100000 RMT=   1.56000   Z:   5.00000
24 LOCAL ROT MATRIX:    0.0000000 0.0000000 1.0000000
25                      0.0000000 1.0000000 0.0000000
26                     -1.0000000 0.0000000 0.0000000
27   16      NUMBER OF SYMMETRY OPERATIONS
28 -1 0 0 0.00000000
29  0-1 0 0.00000000
30  0 0-1 0.00000000
31        1  A   1 so. oper.  type  orig. index
32 -1 0 0 0.00000000
```

Figure: EuB_6.structure

WIEN2k 算例:EuB_6 的旋-轨耦合

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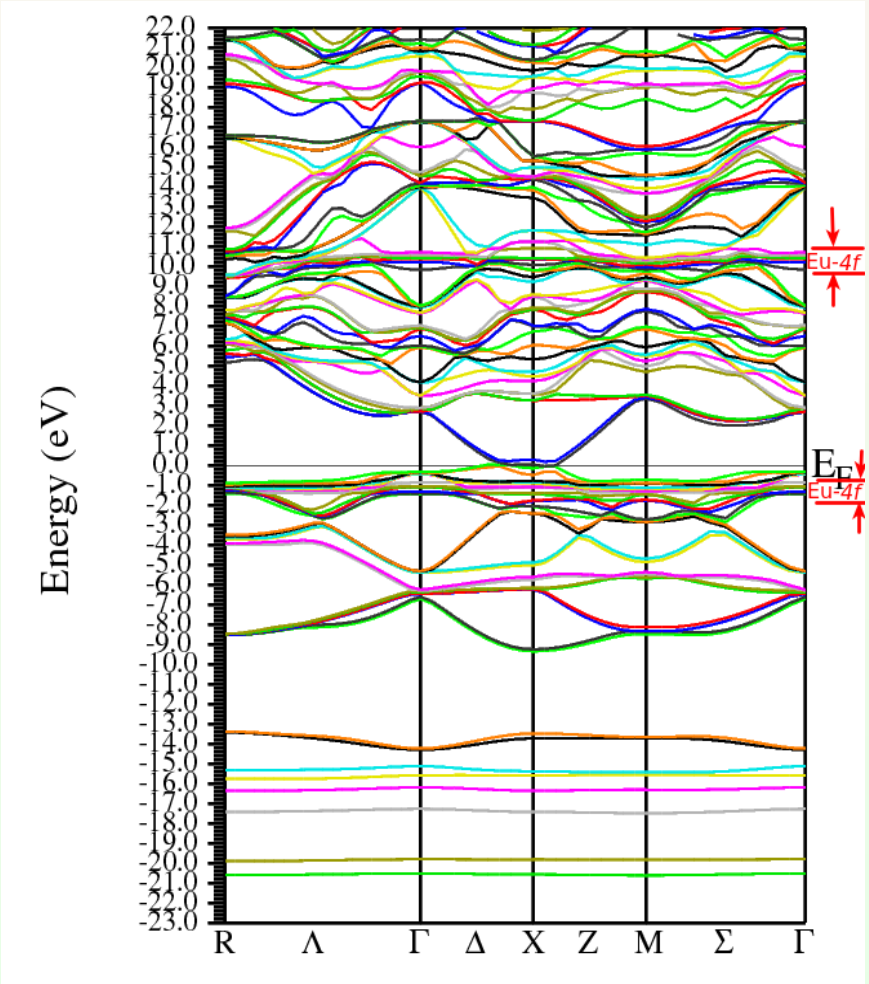
```
WFFIL
4  0  0                    llmax,ipr,kpot
-10  3.5                   Emin, Emax
0 0 1                      h,k,l (direction of magnetization)
 1                         number of atoms with RLO
1 0.30 0.000 CONT          atom-number, E-param for RLO
2 2 3     number of atoms without SO, atomnumbers
```

Figure: EuB_6.inso



WIEN2k 算例: 光学性质计算

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```
99999 1          number of k-points, first k-point
-5.0 3.0 9999    Emin, Emax for matrix elements, NBvalMAX
9                number of choices (columns in *outmat): 2: hex or tetrag. case
1                Re xx
2                Re yy
3                Re zz
4                Re xy
5                Re xz
6                Re yz
7                Im xy
8                Im xz
9                Im yz
OFF              ON/OFF   writes MME to unit 4

Choices:
1......Re <x><x>
2......Re <y><y>
3......Re <z><z>
4......Re <x><y>
5......Re <x><z>
6......Re <y><z>
7......Im <x><y>
8......Im <x><z>
9......Im <y><z>
```

(a) EuB_6.inop

```
   1  9999 9999              : LOWER,UPPER and (optional) UPPER-VAL BANDINDEX
 0.0000    0.00100   1.0000 : EMIN DE EMAX FOR ENERGYGRID IN ryd
eV                          : output units  eV / ryd  / cm-1
 4                          : SWITCH
 2                          : NUMBER OF COLUMNS
 0.1  0.1  0.3              : BROADENING (FOR DRUDE MODEL - switch 6,7 - ONLY)

SWITCH:

   0...JOINTDOS FOR EACH BAND COMBINATION
   1...JOINTDOS AS SUM OVER ALL BAND COMBINATIONS
   2...DOS FOR EACH BAND
   3...DOS AS SUM OVER ALL BANDS
   4...Im(EPSILON)
   5...Im(EPSILON) for each band combination
   6...INTRABAND contributions
   7...INTRABAND contributions including band analysis
```

(b) EuB_6.injoint

```
 0.1    Gamma: broadening of interband spectrum
 0.0    energy shift (scissors operator)
 0      add intraband contributions? yes/no: 1/0
12.60   plasma frequencies  (from joint, opt 6)
 0.20   Gammas for Drude terms
```

(c) EuB_6.inkram

WIEN2k 算例: 光学性质计算

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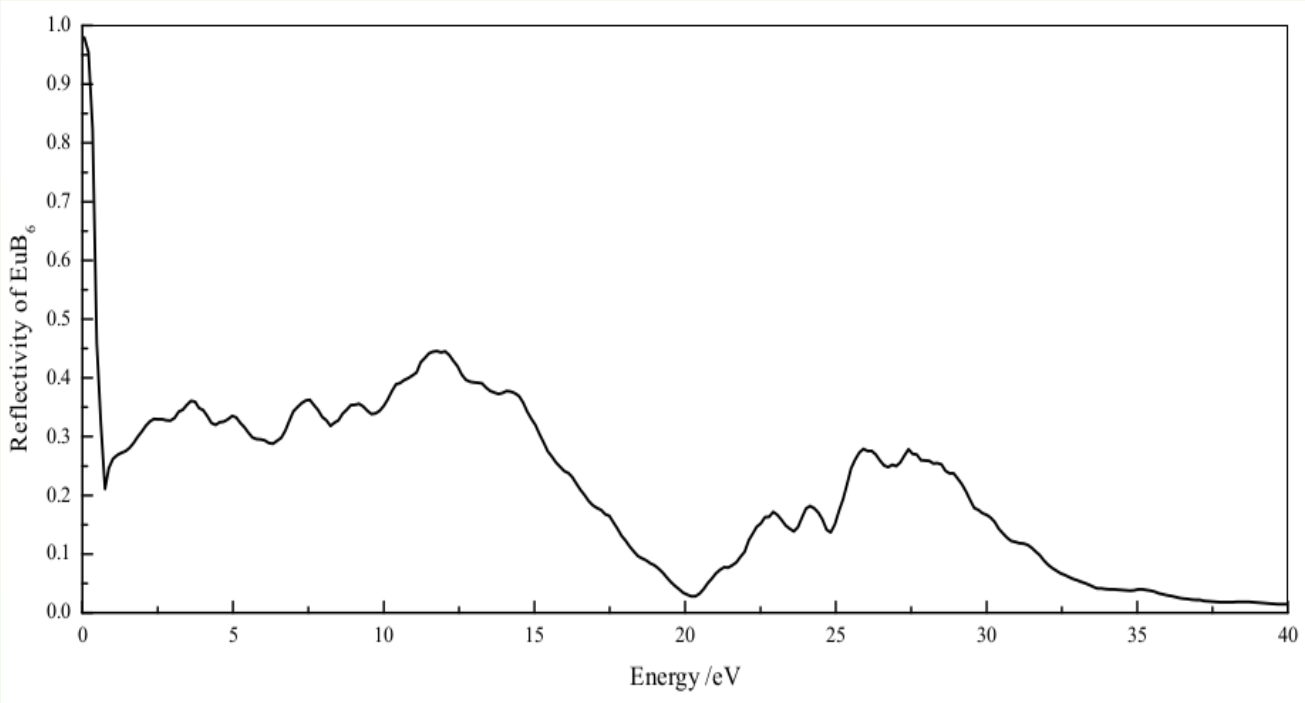

Figure: The Reflectivity of the EuB_6

WIEN2k 算例: 光学性质计算

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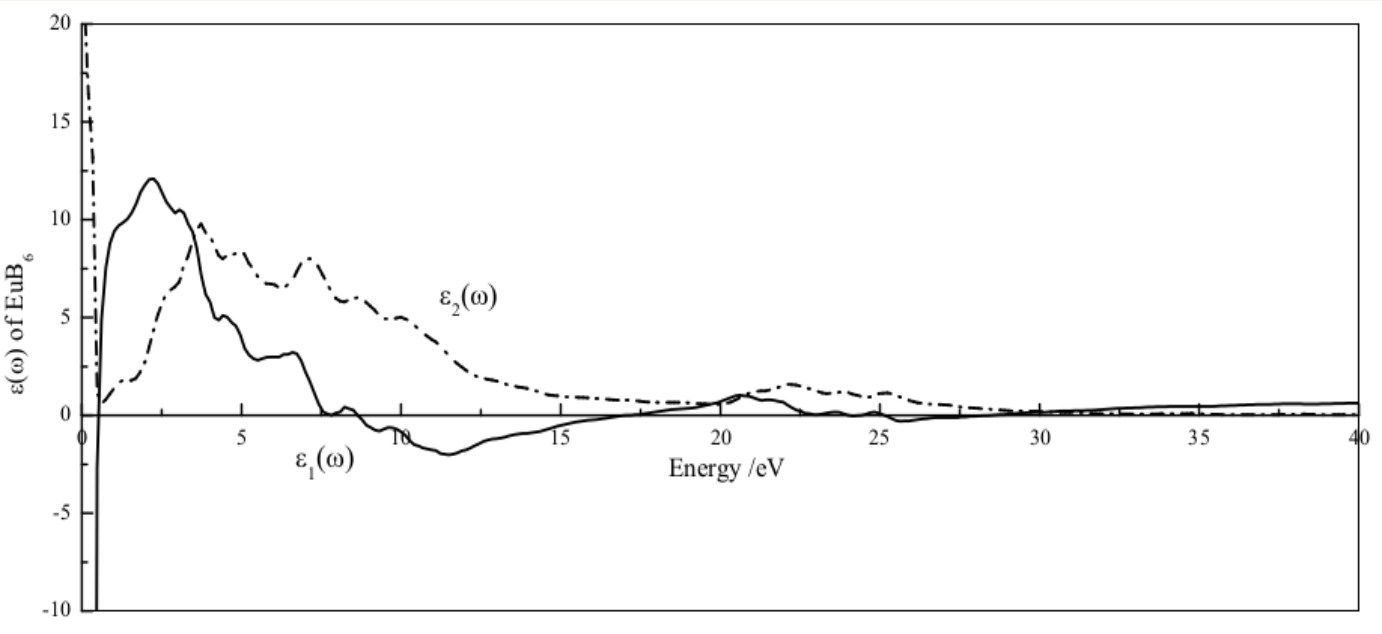

Figure: The dielectric of the EuB_6

WIEN2k 算例: 光学性质计算

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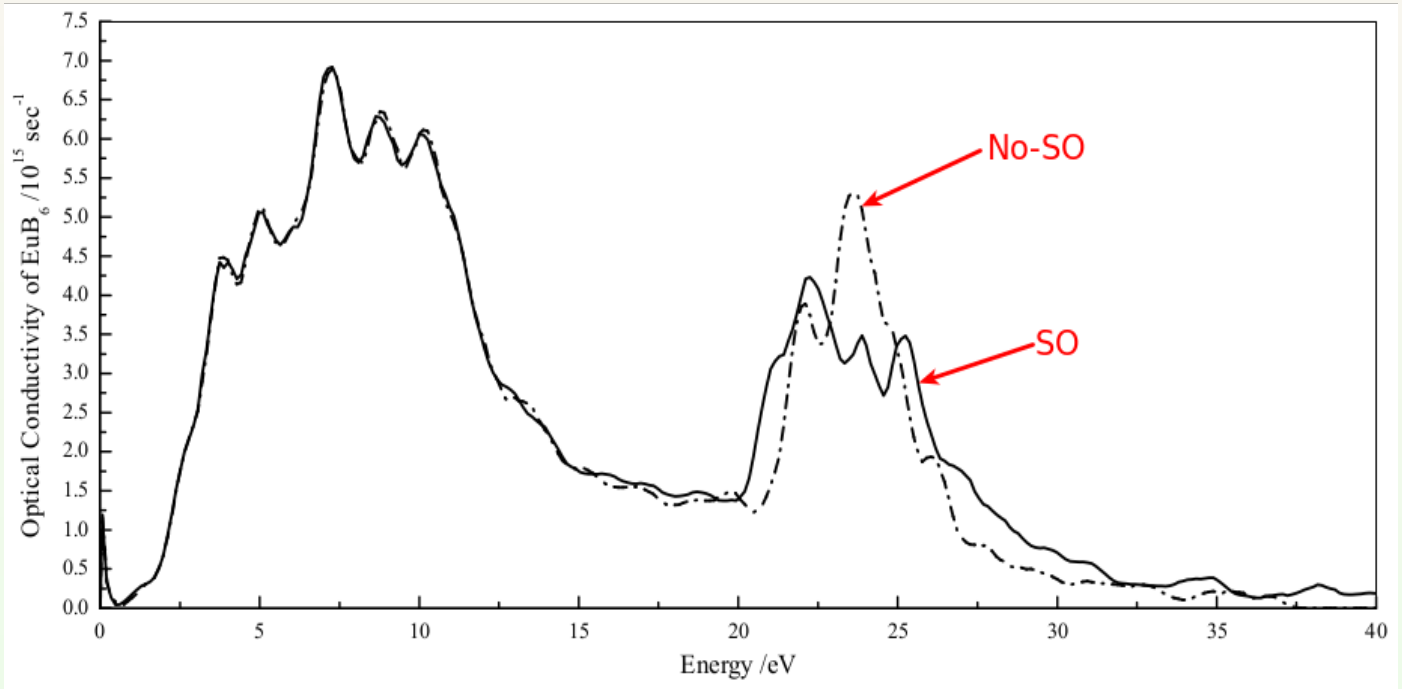

Figure: The R-Conductivity of the EuB_6

WIEN2k 算例: 光学性质计算

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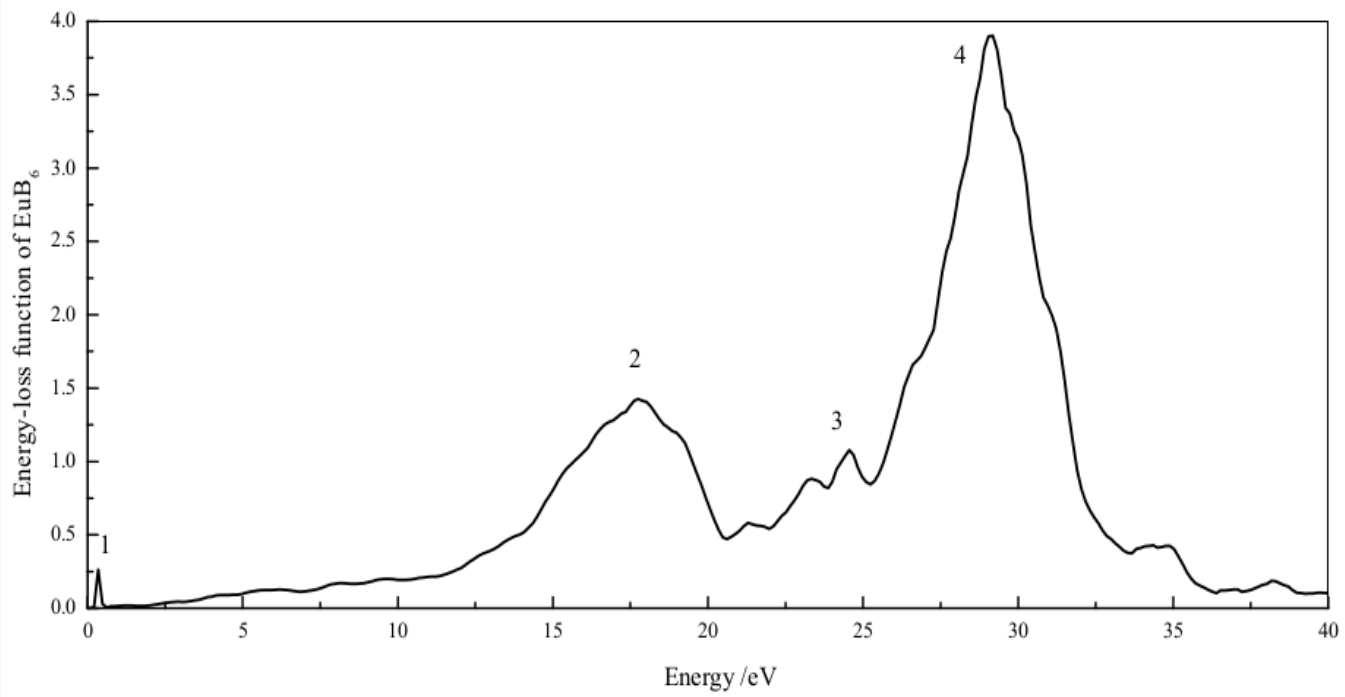

Figure: The E-loss function of the EuB_6

Ubuntu 挂载

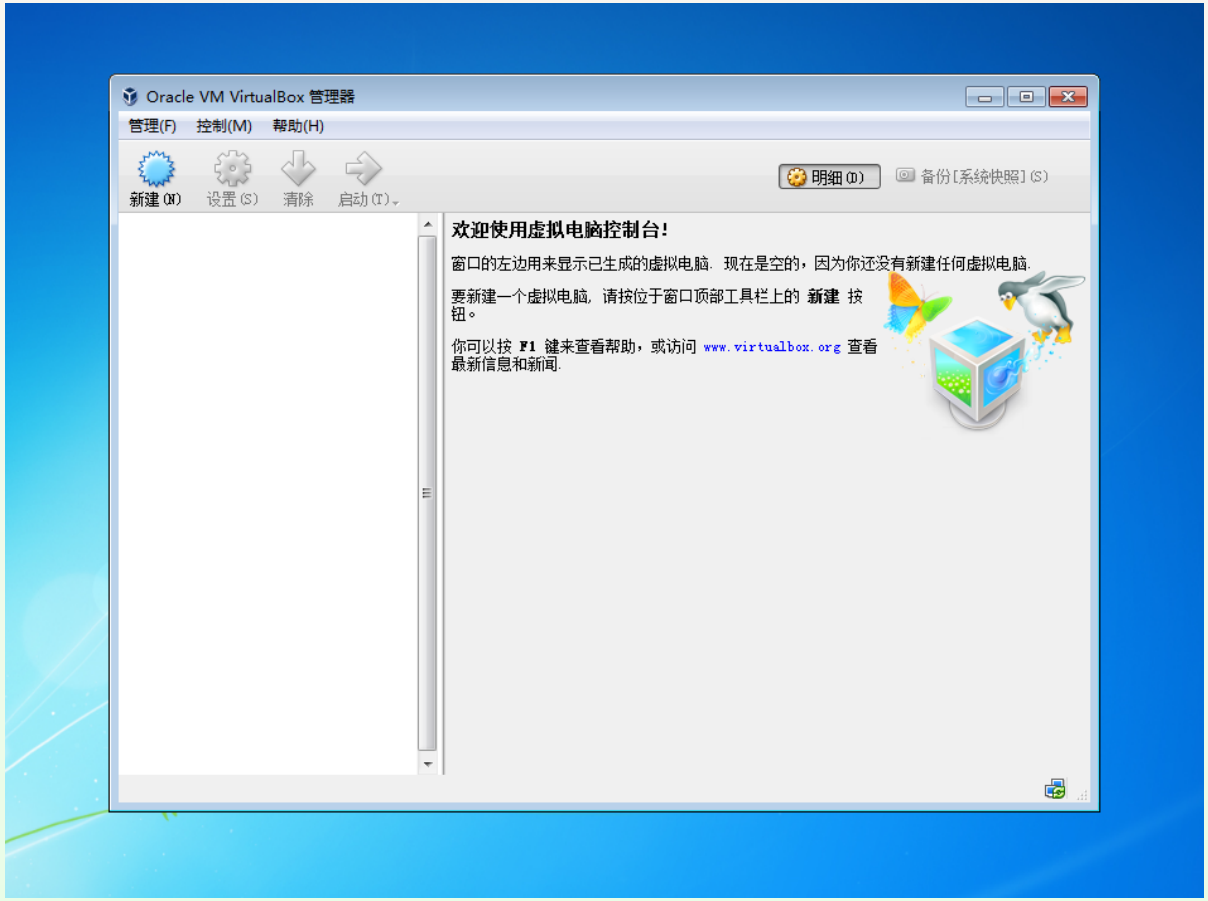

Figure: The step 1 of uploading Ubuntu.

Ubuntu 挂载

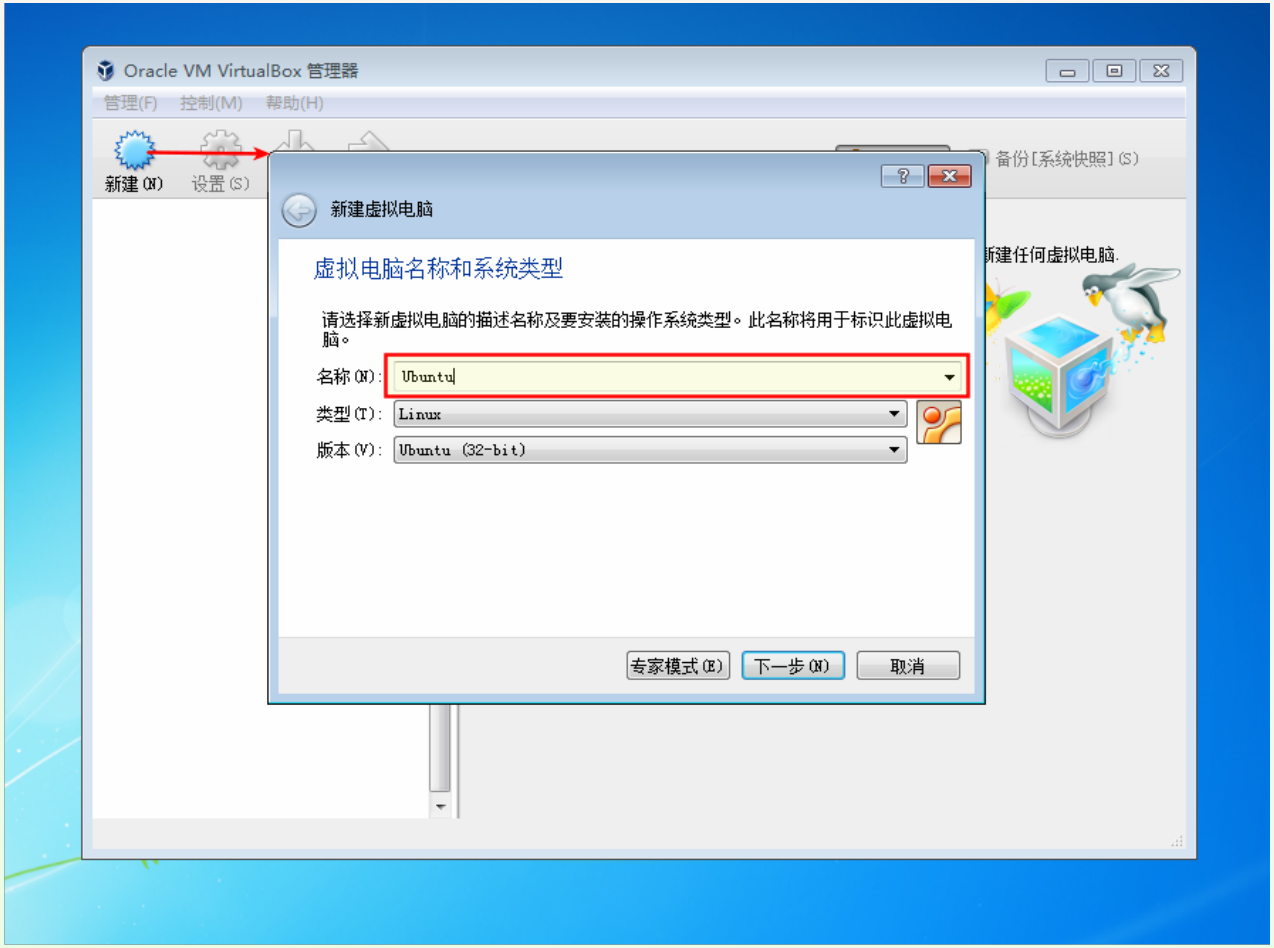

Figure: The step 2 of uploading Ubuntu.

Ubuntu 挂载

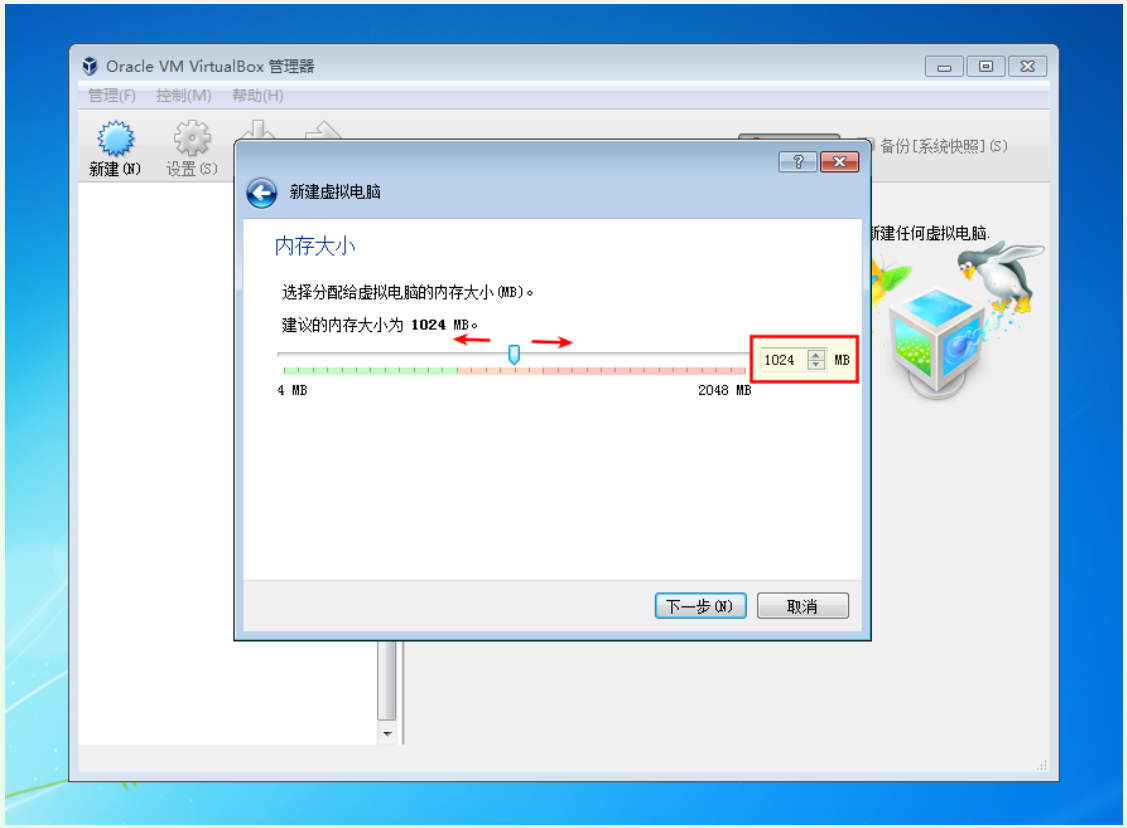

Figure: The step 3 of uploading Ubuntu.

Ubuntu 挂载

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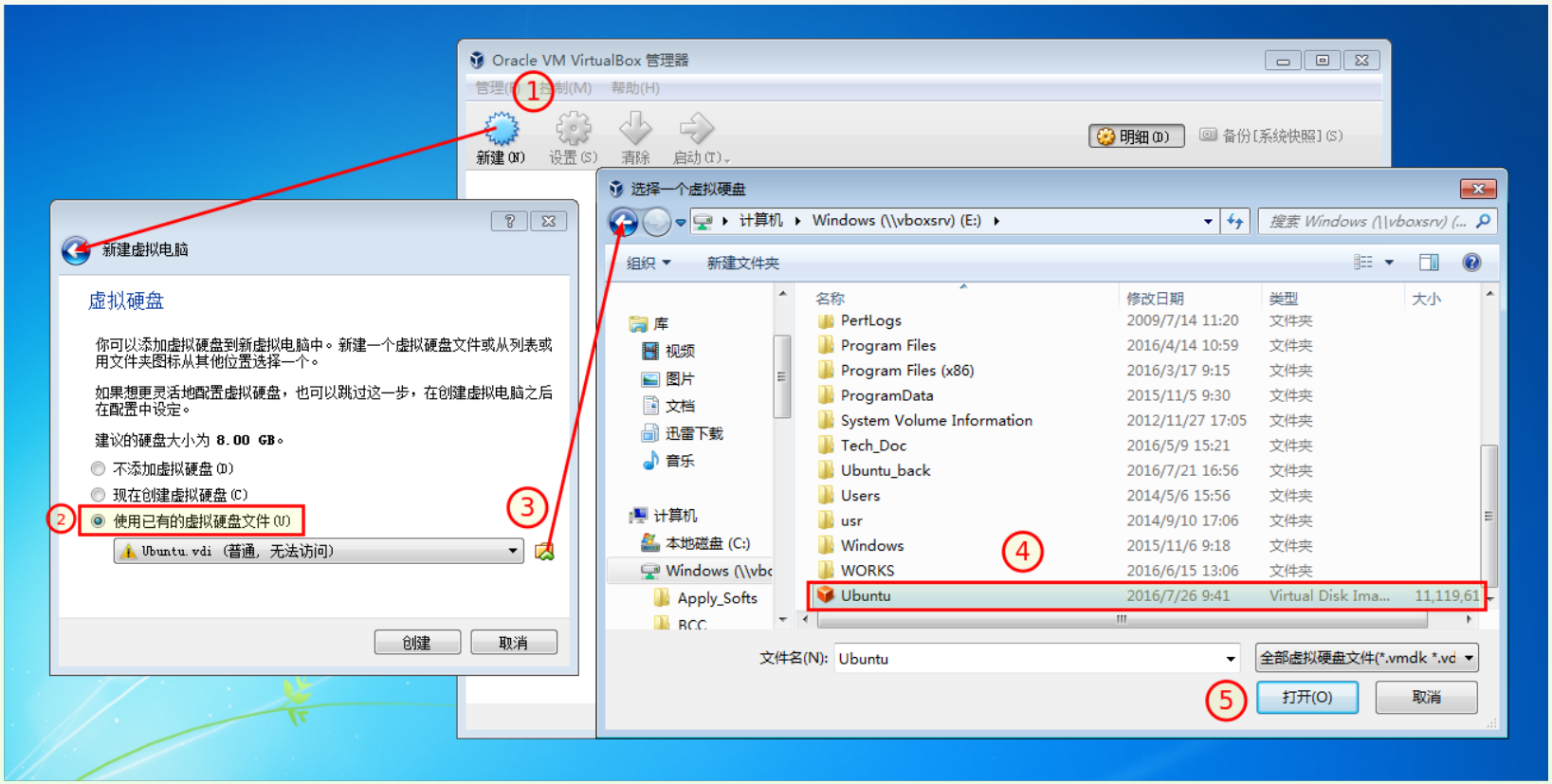

Figure: The step 4 of uploading Ubuntu.

Ubuntu 挂载

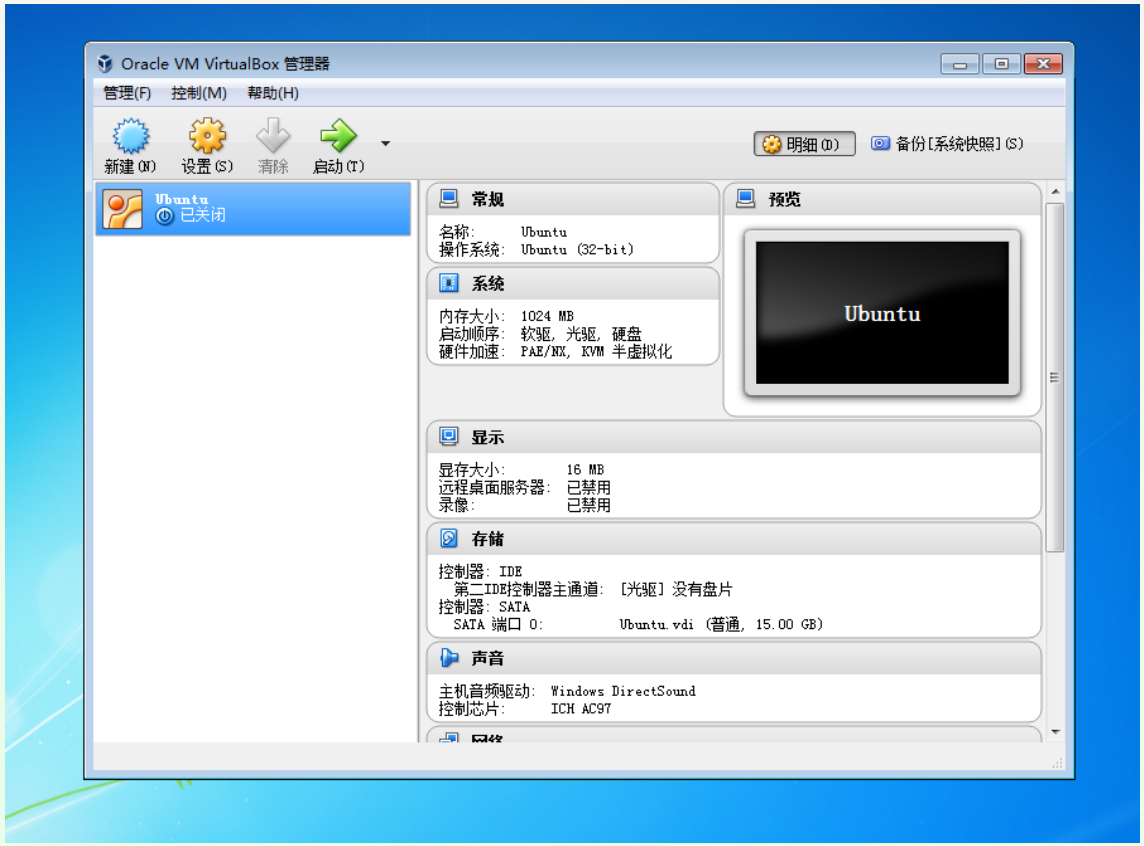

Figure: The step 5 of uploading Ubuntu.