WienJ Documentation

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(Dated: November 13, 2022)

Contents

WienJ: an open-source software package for magnetic materials

Source: https://ourwebsiteXXX

You can find more useful information on website ourwebsiteXXX.

Aiming to investigate magnetic interactions of magnetic materials.

Version 1.0

I. INSTALLATION OF WIENJ (LINUX)

A. Prerequisites

The following packages need to be installed in your working environment first:

Fortran compiler
MPICH

(1) Fortran compiler. Here we recommend ifort and have prepared the Makefile which supports ifort.

(2) MPICH. Version higher than 2.1.5 is recommended.

B. Compilation

First download the .zip file directly from https://ourwebsiteXXX, then uncompress it.

Go into WienJ/src/ directory, and edit Makefile. At present, we prepared Makefile which is mpi+ifort.

If you use gfotran or any other fortran compilers, please edit the definition of "F90" in Makefile. And if you do not need the mpi compiler, you could switch off the compile flag "-DMPI" in Makefile.

After editing Makefile, you can easily use

```
make
```

to compile the WienJ code. After the compilation, the binary "WienJ" is automatically copied to WienJ/bin/ (XXX), you can put this path to the system PATH using

```
export PATH=...(where you install WienJ)/BIN:$PATH
```

to the .bashrc file in your home directory. There is another binary "prepare_wienj.sh" in WienJ/bin/, which is a shell to help prepare the working directory and input files for calculating magnetic interactions.

We also suggest to add your install directory to your .bashrc like that

```
export WIENJROOT=...(where you install WienJ)/BIN
```

Then the shell "prepare_wienj.sh" could also copy the typical input file "dat.in" to your working directory automatically.

II. CAPABILITIES OF WIENJ

Based on combining magnetic force theorem and linear-response approach, we present a computationally efficient method of calculating anisotropic spin Hamiltonian parameters, including Heisenberg interaction, antisymmetric DM interaction and symmetric Γ term. This method is applied in Wien2k, where the linearized augmented plane wave (LAPW) method is used. Meanwhile, using perturbation theory by treating the SOC Hamiltonian as the perturbation, we can get the associated first-order and second-order SOC corrections of the anisotropic exchange couplings. [ref]

For WienJ Version 1.0, we can calculate Heisenberg interaction and antisymmetric DM interaction at this moment, while the calculation module of the symmetric Γ term is under testing and will be added soon.

III. USAGE

Now you can enjoy your exploration for magnetic materials with WienJ.

It will takes you several steps to calculate the Heisenberg interaction J and the antisymmetric Dzyaloshinskii-Moriya (DM) interaction using WienJ. Firstly, we give the introduction of input files which you should prepare or modify.

A. Introduction of input files

There are two kinds of input files you should prepare

Required output data from Wien2k
Main input file dat.in

To calculate the magnetic interactions, many output files from Wien2k are needed, including case.struct, case.klist, case.almblmup/dn, case.r2v/r2vdn, case.radwfup/dn, and case.vorbup/dn. But there is no need to manually prepare them. Usually, they can be prepared by "prepare_wienj.sh" automatically (see steps of running code below). Meanwhile, the prepare_wienj.sh would copy the dat.in file in the directory WienJ/bin to your working directory by your own necessary. All the control and user specified parameters are included in this file.

The input file dat.in is structured in a number of parameters and the format is

```
————————- top of file: dat.in ————————
1 1 (first atom: index and multiplicity index)
1 1 (second atom: index and multiplicity index)
1 (1: FM; 0: AFM. the magnetic configuration you set in first-principles calculation)
1 (1: with SOC; 0: without SOC)
1 (1: J; 2: DM; 3: Both)
5.0 (Rmax)
————————- end of file: dat.in ————————
```

line 1: free format

Any magnetic interaction one want to estimate is between two selected magnetic atoms. The first line is the index and multiplicity index of first atom, which could be found in case.struct of Wien2k.

line 2: free format

The second line is the index and multiplicity index of second magnetic atom.

line 3: free format

The magnetic configuration you set in first-principles calculation. If the selected two magnetic atoms are set to couple ferromagnetically, the parameter should be 1. If the selected two magnetic atoms are set to have opposite spin orientations, the parameter should be 0.

line 4: free format

The parameter whether spin-orbit coupling (SOC) is considered. Note that only when SOC is added, DM interaction will exist and can be calculated.

line 5: free format

The parameter to choose which kind of interaction to be calculated. Here 1 represents Heisenberg interaction J and 2 represents the DM interaction, while 3 represents that both J and DM interaction will be calculated.

line 6: free format

The distance range of magnetic interactions will be printed (the unit: A).

There is a typical example input file "dat.in" in WienJ/bin.

B. calculate J

Before running WienJ, one needs a converged WIEN2k calculation. Usually "runsp_lapw -orb" option is used to consider the spin-polarized case with Coulomb correction.

Then one can obtain the output data from Wien2k via the following steps:

```
x kgen -fbz
edit "NR2V" in case.in0 to "R2V"
x lapw0
x lapw1 -orb -up & x lapw1 -orb -dn
x lapw2 -almd -up & x lapw2 -almd -dn
```

Here we use "x kgen -fbz" to generate the k-mesh for calculating magnetic interactions. Note that do not use the "shifted" k-mesh without Gamma-point in Wien2k. Usually the exchange parameters are short range and decrease quickly with the distance. Therefore these short ranged interactions are converged quickly and a relatively small k-mesh is usually enough. The aim of last steps is to generate the output data such as case.r2v/r2vdn and case.almblmup/dn.

Then you can prepare to calculate magnetic interactions using WienJ. First you can create a subdirectory with the necessary files using:

```
prepare_wienj.sh TARGET
```

which copy the necessary data from Wien2k and the example of main input file "dat.in" into this new directory TARGET. All the control and user specified parameters are included in this file, and you can edit "dat.in" at this moment. The details of this input file are introduced before.

After the preparation of these input files, you can just run WienJ in the same folder

```
wienj
```

or if you want to run using MPICH in multi-cores

```
mpirun -np NC wienj
```

here NC is the number of multi-cores.

The output information during the running are written in j.output and the calculated results are summarized in j.txt (see details below).

C. calculate DM

In general, the process of calculating DM interaction is not much different from calculating Heisenberg J. However, there is still a little difference, since the isotropic Heisenberg Hamiltonian is the scalar term while the antisymmetric DM interaction is the vector term. Note that any DM term $\mathbf{D_{ij}}$ could be written as $\{D_x, D_y, D_z\}$, and WienJ could calculate these three components of the vector $\mathbf{D_{ij}}$ term respectively.

Similarly, before running WienJ, one needs a converged WIEN2k calculation. Usually "runsp_lapw -orb" option is used to consider the spin-polarized case with Coulomb correction.

Then one can obtain the output data from Wien2k via the following steps:

```
initso
x kgen -fbz
edit "NR2V" in case.in0 to "R2V"
x lapw0
x lapw1 -up & x lapw1 -dn
x lapwso -orb -up
x lapw2 -so -almd -up & x lapw2 -so -almd -dn
```

Note that there are two differences compared with the previous steps of calculating Heisenberg J. First, one should run "initso" to generate "case.inso", in which the fourth line describes the direction of magnetization. Here the direction of magnetization also describes the direction of calculating component of DM interactions and one can run three times to calculate the DM components Dx, Dy and Dz respectively. For example, one can set "1 0 0", "0 1 0" and "0 0 1" in cubic, tetragonal or orthorhombic lattices to estimate Dx, Dy and Dz respectively. Secondly, we should run "lapwso" to take SOC into consideration.

The next steps are the same as before:

You can prepare to calculate magnetic interactions using WienJ. First you can create a subdirectory with the necessary files using:

```
prepare_wienj.sh TARGET
```

which copy the necessary data from Wien2k and the example of main input file "dat.in" into this new directory TARGET. All the control and user specified parameters are included in this file, and you can edit "dat.in" at this moment. The details of this input file are introduced before. Note that SOC is considered now and the line 4 in "dat.in" should be set to 1.

After the preparation of these input files, you can just run WienJ in the same folder

```
wienj
```

or if you want to run using MPICH in multi-cores

```
mpirun -np NC wienj
```

here NC is the number of multi-cores.

Similarly, the output information during the running are written in j.output and the calculated results are summarized in j.txt (see below).

D. Introduction of output files

The information during running WienJ would save in output file "j.output" and the calculated results are summarized in "j.txt". This output file "j.txt" is structured in a number of parameters and the format is such as

```
————————- top of file: j.txt ————————————

   R                 distance     J         DM

-1.0 -1.0  0.0        4.27       20.31      3.54

-1.0  0.0  0.0        4.27       20.31     -3.54

 0.0 -1.0  0.0        4.27       20.31     -3.54

 0.0  1.0  0.0        4.27       20.31      3.54

 1.0  0.0  0.0        4.27       20.31      3.54

 1.0  1.0  0.0        4.27       20.31     -3.54

————————- end of file: j.txt ————————————
```

Usually the magnetic properties of crystal materials can be well described by a general pairwise magnetic model

$$H = \sum_{l,n,\alpha,l',n',\beta} J^{\alpha,\beta}_{\mathbf{R}_l+\boldsymbol{\tau}_n,\mathbf{R}_{l'}+\boldsymbol{\tau}_{\boldsymbol{n'}}} S^{\alpha}_{ln} S^{\beta}_{l'n'} \tag{1}$$

where $J^{\alpha,\beta}_{\mathbf{R}_l+\boldsymbol{\tau}_n,\mathbf{R}_{l'}+\boldsymbol{\tau}_{\boldsymbol{n'}}}$, a 3×3 tensor, represents the spin exchange parameter. Here $\mathbf{R}_l$ and $\boldsymbol{\tau}_n$ represent the lattice translation vector and the position of magnetic ions in the lattice basis, while α and β denote x, y or z the cartesian components. As a 3×3 real tensor, $\mathbf{J}_{\mathbf{R}_l+\boldsymbol{\tau}_n,\mathbf{R}_{l'}+\boldsymbol{\tau}_{\boldsymbol{n'}}}$ could be expanded as three terms, and Eq. (1) could be written as

$$\begin{aligned} H = & \sum_{l,n,l',n'} J_{\mathbf{R}_l+\boldsymbol{\tau}_n,\mathbf{R}_{l'}+\boldsymbol{\tau}_{\boldsymbol{n'}}} \mathbf{S}_{ln} \cdot \mathbf{S}_{l'n'} \\ & + \sum_{l,n,l',n'} \mathbf{D}_{\mathbf{R}_l+\boldsymbol{\tau}_n,\mathbf{R}_{l'}+\boldsymbol{\tau}_{\boldsymbol{n'}}} \cdot [\mathbf{S}_{ln} \times \mathbf{S}_{l'n'}] \\ & + \sum_{l,n,l',n'} \mathbf{S}_{ln} \cdot \Gamma_{\mathbf{R}_l+\boldsymbol{\tau}_n,\mathbf{R}_{l'}+\boldsymbol{\tau}_{\boldsymbol{n'}}} \cdot \mathbf{S}_{l'n'} \end{aligned} \tag{2}$$

Here the first term describes the isotropic Heisenberg Hamiltonian with the scalar term $J_{\mathbf{R}_l+\boldsymbol{\tau}_n,\mathbf{R}_{l'}+\boldsymbol{\tau}_{\boldsymbol{n'}}}$, the second one represents the antisymmetric Dzyaloshinskii-Moriya (DM) interactions with the vector term $\mathbf{D}_{\mathbf{R}_l+\boldsymbol{\tau}_n,\mathbf{R}_{l'}+\boldsymbol{\tau}_{\boldsymbol{n'}}}$, and the third one is the rest of anisotropic terms with the symmetric tensor term $\Gamma_{\mathbf{R}_l+\boldsymbol{\tau}_n,\mathbf{R}_{l'}+\boldsymbol{\tau}_{\boldsymbol{n'}}}$.

Note that Translation symmetry will restrict $J_{\mathbf{R}_l+\boldsymbol{\tau}_n,\mathbf{R}_{l'}+\boldsymbol{\tau}_{\boldsymbol{n'}}}$ to be only related to $\boldsymbol{\tau}_n$, $\boldsymbol{\tau}_{n'}$ and $\mathbf{R} = \mathbf{R}_l - \mathbf{R}_{l'}$, irrespective of the starting unit cell. $\boldsymbol{\tau}_n$ and $\boldsymbol{\tau}_{n'}$ are set in line 1 and 2 of "dat.in", and we will print all the $J_{\boldsymbol{\tau}_n,\mathbf{R}+\boldsymbol{\tau}_{\boldsymbol{n'}}}$ with different $\mathbf{R}$, in which the distance of the magnetic interaction agrees the limit set in line 5 of "dat.in".

As shown above, each line in "j.txt" is summarized as $\mathbf{R}$, the distance, and calculated J or DM parameters respectively. Here $\mathbf{R}$ is expressed in terms of lattice vectors, while the distance is in A. Note that S is considered as the unit vectors in the direction of local magnetic moments, and the

calculated interaction parameters such as J and DM parameters are in meV.

IV. TUTORIAL: LEARNING WIENJ THROUGH EXAMPLES

A. Transition-metal ferromagnet Co

Transition-metal ferromagnet Co

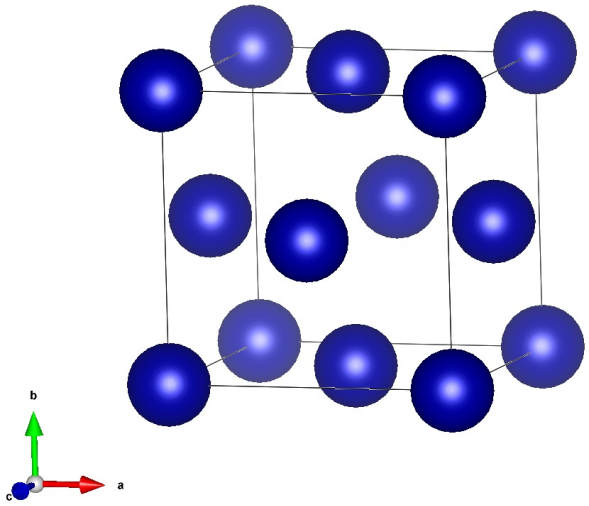

FIG. 1: crystal structure of fcc Co.

Firstly, we show you how to use WienJ to study the magnetic interactions in transition-metal ferromagnet fcc Co. As shown in Fig. 1, fcc Co crystallizes in the cubic structure (space group FM3-M) and the lattice constant a = 3.54 A. Run a converged WIEN2k calculation using "runsp_lapw" option (k-mesh is set to be 20*20*20) and obtain the output data from Wien2k via the following steps:

```
x kgen -fbz
edit "NR2V" in case.in0 to "R2V"
x lapw0
x lapw1 -up & x lapw1 -dn
x lapw2 -almd -up & x lapw2 -almd -dn
```

Here the k-mesh for calculating magnetic interactions is set to be 10*10*10. The input file

"dat.in" is set as

```
————————- top of file: dat.in ————————

1 1 (first atom: index and multiplicity index)

1 1 (second atom: index and multiplicity index)

1 (1: FM; 0: AFM. the magnetic configuration you set in first-principles calculation)

0 (1: with SOC; 0: without SOC)

1 (1: J; 2: DM; 3: Both)

10.0 (Rmax)

————————- end of file: dat.in ————————
```

After running WienJ, we can get the output file "j.txt" shown as

```
————————- top of file: j.txt ————————————

XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX

    R                distance      J

  0.0 -0.5 -0.5        2.51      -26.66

0.5 0.0 -0.5         2.51      -26.66

0.5 -0.5 0.0         2.51      -26.66

-0.5 0.0 -0.5        2.51      -26.66

0.0 0.5 -0.5         2.51      -26.66

-0.5 -0.5 0.0        2.51      -26.66

0.5 0.5 0.0         2.51      -26.66

0.0 -0.5 0.5         2.51      -26.66

0.5 0.0 0.5         2.51      -26.66

-0.5 0.5 0.0         2.51      -26.66

-0.5 0.0 0.5         2.51      -26.66

0.0 0.5 0.5         2.51      -26.66

0.0 0.0 -1.0         3.54       -3.60

0.0 -1.0 0.0         3.54       -3.60

1.0 0.0 0.0         3.54       -3.60

-1.0 0.0 0.0         3.54       -3.60

0.0 1.0 0.0         3.54       -3.60

0.0 0.0 1.0         3.54       -3.60

.....

————————- end of file: j.txt ————————————
```

Here we can see that there are 12 first nearest neighbor (NN) bonds and the 1st NN exchange

interaction is estimated to be -26.6 meV (line 2-13). Meanwhile, there are 6 second nearest neighbor (NN) bonds and the 2nd NN exchange interaction is estimated to be -3.6 meV (line 14-19). The longer magnetic interactions are also print in the file "j.txt". The calculated spin exchange parameters for fcc Co are presented in Table. I. Besides our results, the calculated spin exchange parameters from different groups are also shown for comparison[1][2]. Our calculation quantitative values are in excellent agreement with those calculations of S. Frota-Pessoa and M. Pajda. There are several characteristic features which can be easily observed in these results. The 2nd NN exchange interaction is an order of magnitude smaller than 1st NN exchange interaction, while the change from ferromagnetic to antiferromagnetic spin exchange couplings appears in the 4th nearest neighbours. Such characteristic features are in a quantitative agreement with the others' results.

TABLE I: Effective Heisenberg exchange parameters J (in mRy) for ferromagnetic fcc Co between the first 10 neighbors.

fcc Co			
$2R$	Ref.[1]	Ref.[2]	Calc.
(110)	−1.00	−1.085	−0.978
(200)	−0.091	−0.110	−0.132
(211)	−0.126	−0.116	−0.111
(220)	0.118	0.090	0.105
(310)	−0.026	−0.026	−0.032
(222)	−0.041	−0.043	−0.038
(321)	0.021	0.024	0.019
(400)	−0.016	−0.012	−0.013
(330)	−0.028	−0.026	−0.024
(411)	−0.004	−0.006	−0.001

B. La_2CuO_4

La_2CuO_4

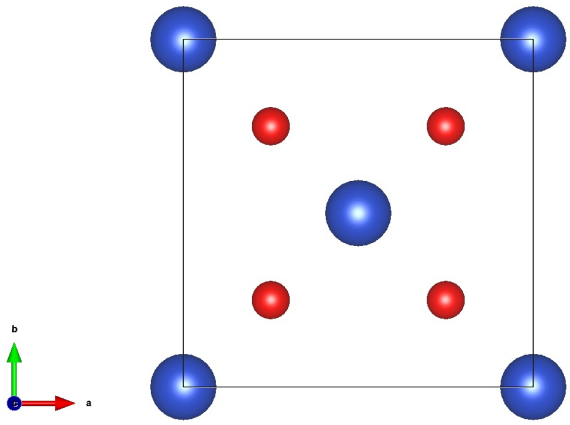

FIG. 2: crystal structure of CuO_2 plane of La_2CuO_4 in the view along z-direction.

As a sanity check on the accuracy of our first-principles method, we first study the magnetic exchange interactions for well-known $3d$ transition metal oxides La_2CuO_4 as an example of the weak ferromagnetism system, which have been studied in a number of theoretical work [3, 4]. The crystal structure of CuO_2 plane of La_2CuO_4 in the view along z-direction is shown in Fig. 2, and we also give the case.struct for reference here.

The LSDA + U (U = 7 eV) calculation is applied since Coulomb U usually imposes significant influences on the electronic structure of strongly correlated systems. The k-mesh of electronic calculation is set to 4*12*12. The calculated value of energy gap of 2.0 eV agrees well with experimental data of about 2 eV, while the calculated magnetic moment on Cu atom is 0.64 μB, which is also in good agreement with the experimental value [5].

Then one can obtain the output data from Wien2k via the following steps:

```
blebleble                                   s-o calc. M||   0.00   1.00   0.00
P                                  14 10 P
                  RELA
  24.764861 10.228332 10.072240 90.000000 90.000000 90.000000
ATOM   -1: X=0.63790000 Y=0.99220000 Z=0.00000000
               MULT= 2              ISPLIT= 8
         -1: X=0.36210000 Y=0.00780000 Z=0.00000000
La1            NPT=   781   R0=.000010000 RMT= 2.37          Z:   57.00000
LOCAL ROT MATRIX:     1.0000000 0.0000000 0.0000000
                      0.0000000 1.0000000 0.0000000
                      0.0000000 0.0000000 1.0000000
.....
.....
.....
ATOM -11: X=0.00000000 Y=0.00000000 Z=0.00000000
               MULT= 1              ISPLIT= 8
Cu1            NPT=   781   R0=.000050000 RMT= 1.92          Z:   29.00000
LOCAL ROT MATRIX:     1.0000000 0.0000000 0.0000000
                      0.0000000 1.0000000 0.0000000
                      0.0000000 0.0000000 1.0000000
ATOM -12: X=0.50000000 Y=0.00000000 Z=0.50000000
               MULT= 1              ISPLIT= 8
Cu2            NPT=   781   R0=.000050000 RMT= 1.92          Z:   29.00000
LOCAL ROT MATRIX:     1.0000000 0.0000000 0.0000000
                      0.0000000 1.0000000 0.0000000
                      0.0000000 0.0000000 1.0000000
ATOM -13: X=0.50000000 Y=0.50000000 Z=0.00000000
               MULT= 1              ISPLIT= 8
Cu3            NPT=   781   R0=.000050000 RMT= 1.92          Z:   29.00000
LOCAL ROT MATRIX:     1.0000000 0.0000000 0.0000000
                      0.0000000 1.0000000 0.0000000
                      0.0000000 0.0000000 1.0000000
ATOM -14: X=0.00000000 Y=0.50000000 Z=0.50000000
               MULT= 1              ISPLIT= 8
Cu4            NPT=   781   R0=.000050000 RMT= 1.92          Z:   29.00000
LOCAL ROT MATRIX:     1.0000000 0.0000000 0.0000000
                      0.0000000 1.0000000 0.0000000
                      0.0000000 0.0000000 1.0000000
.....
.....
.....
```

FIG. 3: case.struct of La_2CuO_4 in Wien2k.

```
initso

x kgen -fbz

edit "NR2V" in case.in0 to "R2V"

x lapw0

x lapw1 -up & x lapw1 -dn

x lapwso -orb -up

x lapw2 -so -almd -up & x lapw2 -so -almd -dn
```

Here we use "x kgen -fbz" to generate the k-mesh for calculating magnetic interactions and the k-mesh is set to 2*6*6. The weak ferromagnetism of La_2CuO_4 is originated from the canting of the magnetic moments, which can be descried by the competition of isotropic Heisenberg interaction and the DM interaction. Since the strength of the DM interaction is proportional to the corresponding J, we calculate only nearest neighbor DM interaction. The input file "dat.in" is set as

```
————————- top of file: dat.in ————————

11 1 (first atom: index and multiplicity index)

14 1 (second atom: index and multiplicity index)

0 (1: FM; 0: AFM. the magnetic configuration you set in first-principles calculation)

1 (1: with SOC; 0: without SOC)

3 (1: J; 2: DM; 3: Both)

5.0 (Rmax)

————————- end of file: dat.in ————————
```

Note that the first and second line depend on your own case.struct file. The output file "j.txt" with the spin direction "1 0 0" is shown as

```
————————- top of file: j.txt ————————————

   R                distance     J          DM

0.0 -1.0 -1.0        3.80       25.76       0.00

0.0 -1.0  0.0        3.80       25.76       0.00

0.0  0.0 -1.0        3.80       25.76       0.00

0.0  0.0  0.0        3.80       25.76       0.00

.....

————————- end of file: j.txt ————————————
```

The output file "j.txt" with the spin direction "0 1 0" is shown as

```
————————- top of file: j.txt ————————————

   R                distance     J          DM

0.0 -1.0 -1.0        3.80       25.76       0.14

0.0 -1.0  0.0        3.80       25.76      -0.14

0.0  0.0 -1.0        3.80       25.76      -0.14

0.0  0.0  0.0        3.80       25.76       0.14

.....

————————- end of file: j.txt ————————————
```

The output file "j.txt" with the spin direction "0 0 1" is shown as

```
————————- top of file: j.txt ————————————

   R                distance     J         DM

0.0 -1.0 -1.0        3.80       25.76     -0.09

0.0 -1.0  0.0        3.80       25.76     -0.09

0.0  0.0 -1.0        3.80       25.76     -0.09

0.0  0.0  0.0        3.80       25.76     -0.09

.....

————————- end of file: j.txt ————————————
```

It can be seen from our results that there are 4 first nearest neighbor bonds and the calculated Heisenberg magnetic coupling for nearest neighbor is 25.76 meV. The three components $\{D_x, D_y, D_z\}$ of nearest neighbor DM interaction could be obtained in spin direction "0 0 1", "0 1 0" and "1 0 0" respectively. The calculated Heisenberg magnetic couplings are summarized in the Table II while the calculated nearest neighbor DM parameters are presented in Table III

TABLE II: The calculated Heisenberg exchange parameters J (in meV) for La_2CuO_4. The calculated spin exchange parameters in the previous theoretical work are also shown for comparison.

	La_2CuO_4		
J	Ref. [4]	Ref. [3]	This work
J_1	27.2	29.2	25.76
J_2	-3.00	-4.1, -3.9	-3.80, -3.38
J_3	-0.05	0	-0.11

The calculated nearest neighbor magnetic coupling J_1 are in very good agreement with the previous theoretical and experimental work. We can find that the spin exchange coupling parameters decrease rapidly with the increasing distance between two Cu ions. The next nearest neighbor magnetic

TABLE III: The calculated first NN DM interaction parameters (in meV) for La_2CuO_4 from directly LSDA+U+SOC calculations.

R	D
(0.5, −0.5, 0)	(−0.09, −0.14, 0)
(−0.5, −0.5, 0)	(−0.09, 0.14, 0)
(−0.5, 0.5, 0)	(−0.09, −0.14, 0)
(0.5, 0.5, 0)	(−0.09, 0.14, 0)

coupling J_2 shows ferromagnetic behavior and is one order of magnitude smaller than J_1. The third nearest neighbor J_3 is antiferromagnetic and almost negligible. The results agree well with the previous theoretical work [3, 4]. Meanwhile, the calculated nearest neighbor DM parameters are presented in Table III. Since SOC in $3d$ orbital is small, the DM interactions proportional to λ^2 are negligible, and the DM interactions proportional to λ are almost the same as the directly calculated DM parameters from LSDA+U+SOC calculations. Thus we only present the directly calculated DM interactions in Table III here. Summarizing the DM parameters of all nearest neighbors, we can evaluate the canting angle by

$$\delta\theta = \frac{\left|\sum_j \overrightarrow{D}_{1j}\right|}{2\sum_j J_{1j}} \tag{3}$$

This equation can be easily obtained where total energy has a minimum. Considering our calculated results, we can see that the sum of $\overrightarrow{D}_{1j}$ has the direction along x-axis, which is in agreement with the previous work. We can estimate the value of the canting angle as 1.7×10^{-3}, which is in a good agreement with the experimental value of 2.2-2.9$\times10^{-3}$. For previous theoretical works, Anisimov et al. [3] proposed the angle value of 0.7×10^{-3} using Green's function technique. With the construction of a reliable tight-binding parametrization of the Hamiltonian with SOC, Lichtenstein

et al. [6] calculated canting angle to be 5.0×10^{-3}. Comparatively our results agree well with the experiment and quite promising.

---

[1] S. Frota-Pessôa, R. Muniz, and J. Kudrnovskỳ, Physical Review B **62**, 5293 (2000).

[2] M. Pajda, J. Kudrnovskỳ, I. Turek, V. Drchal, and P. Bruno, Physical Review B **64**, 174402 (2001).

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[4] X. Wan, T. A. Maier, and S. Y. Savrasov, Physical Review B **79**, 155114 (2009).

[5] K. Yamada, E. Kudo, Y. Endoh, Y. Hidaka, M. Oda, M. Suzuki, and T. Murakami, Solid state communications **64**, 753 (1987).

[6] M. Katsnelson, Y. Kvashnin, V. Mazurenko, and A. Lichtenstein, Physical Review B **82**, 100403 (2010).

v. CITATION

Please cite this paper when using WienJ for your research. :)

XXX

VI. CORRESPONDENCE

Please report bugs to diwang0214@nju.edu.cn.

VII. AUTHORS AND CONTRIBUTIONS

XXX: XXX

XXX: XXX

XXX: XXX