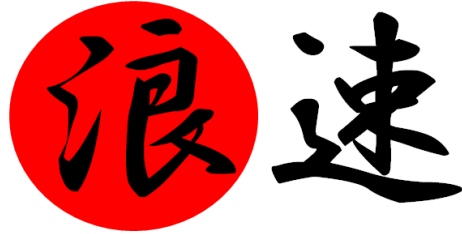


The fastest wave



Naniwa

User's manual

Version 2017.03.03

Code name: BlueSKY

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In your future publications of academic work performed using NANIWA, the use of the software shall be properly acknowledged, e.g. in the form: "The calculations have been performed using the NANIWA codes developed at Osaka University & National Institute of Technology, Akashi College, Japan [1,2]."

[1] Hiroshi Nakanishi, 2016. Ch.6 Quantum adsorption states of small mass atoms on solid surfaces. In: H. Kasai, M. C. S. Escaño, ed. Physics of Surface, Interface and Cluster Catalysis. Bristol, UK, IOP Publishing.

[2] Hiroshi Nakanishi, "Quantum States of the Hydrogen Isotope in Solid Materials and on Their Surfaces", J. Comput. Chem. Jpn., Vol. 15, No. 5, pp. 124–135 (2016).

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Naniwa programs are protected by Japanese Patent 4774523 & 5902495 and US Patent 8,140,467. Additional patents may be pending in Japan and elsewhere.

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1. Introduction

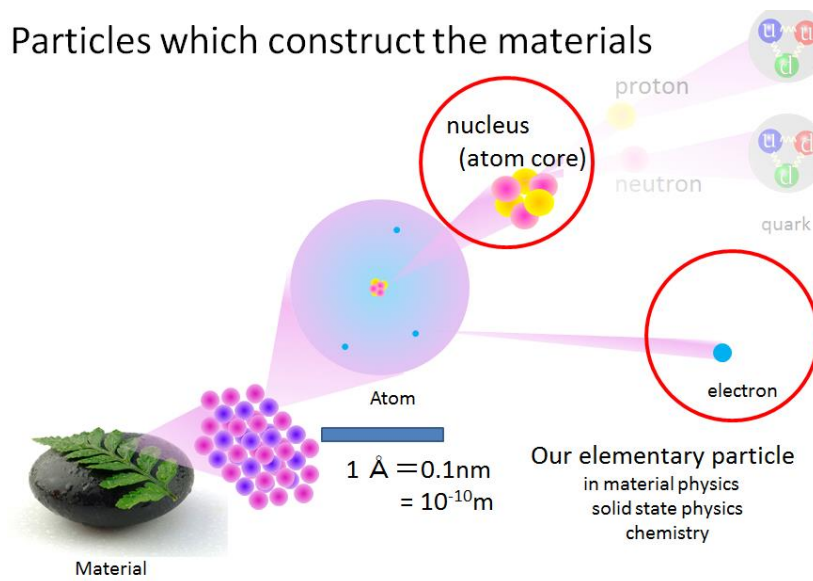
The first principles calculation based on the density functional theory is one of the most successful and powerful methods in the materials physics. And also the first principles molecular dynamics methods have been used for various dynamical behaviors which are from vibrational motions to chemical or biochemical reactions. In the case of small mass atoms like hydrogen atoms, we should treat their nuclei in a quantum-mechanical manner, in addition to the electrons. The quantum behaviors of the nuclei have crucial roles to play in the materials related to today's energy technology: fuel cell and lithium-ion rechargeable battery, and also various catalytic reactions to produce hydrogen fuel, not only from their academic interests.

We have been developing the quantum simulation code for the small mass atoms motion in materials, "Naniwa" [1-15].

"NANIWA" series codes are computational codes for performing first principles quantum mechanical calculations, which were developed at Kasai laboratory (-2015) in Osaka University and have been developed at Nakanishi laboratory in NITAC (2016-). This document describes about the *Naniwa-K* [3,4], which is a nucleus version of the first principles quantum state calculations [5-15]. You can solve the eigenvalue problem and obtain the eigenstates and their eigenenergies for atom (nuclear) motion in the materials by this code.

1.1 Naniwa formulation

We consider that kinds of particles which construct the material are electron and nucleus. If we know how these particles behave, we can know the material properties.



Total Hamiltonian of the electrons and nuclei in material is given by

$$H = \sum_{I=1}^{N_{\text{nc}}} \left(-\frac{\hbar^2}{2M_I} \right) \nabla_I^2 + \sum_{i=1}^{n_e} \left(-\frac{\hbar^2}{2m_e} \right) \nabla_i^2 + V(\vec{r}, \vec{R}) \quad (1)$$

where M_I and m_e are masses of electron and nucleus I , and \hbar is the Dirac constant. Numbers of nucleus and electron are N_{nc} and n_e . Potential energy is given by the coulomb interaction between all particles;

$$V(\vec{r}, \vec{R}) = \sum_{i=1}^{n_e} \sum_{I=1}^{N_{\text{nc}}} \frac{-Z_I e^2}{|\vec{r}_i - \vec{R}_I|} + \sum_{i=1}^{n_e} \sum_{j=1}^{i-1} \frac{e^2}{|\vec{r}_j - \vec{r}_i|} + \sum_{I=1}^{N_{\text{nc}}} \sum_{J=1}^{I-1} \frac{Z_J Z_I e^2}{|\vec{R}_J - \vec{R}_I|} \quad (2)$$

where Z_I is atomic number of nucleus I , and e is elementary charge.

The positions of the electrons and nuclei are indicated by

$$\vec{r} = (\vec{r}_1, \vec{r}_2, \vec{r}_3, \dots, \vec{r}_i, \dots, \vec{r}_{n_e}), \quad (3.1)$$

$$\vec{R} = (\vec{R}_1, \vec{R}_2, \vec{R}_3, \dots, \vec{R}_I, \dots, \vec{R}_{N_{\text{nc}}}). \quad (3.2)$$

Total Schrödinger equation is

$$H \Psi(\vec{r}, \vec{R}) = E \Psi(\vec{r}, \vec{R}), \quad (4)$$

where E and Ψ are the total energy and wave function describing the state of this material system.

Within the adiabatic approximation, we can divide the wave function Ψ into two parts;

$$\Psi_{n,\omega}(\vec{r}, \vec{R}) = \psi_{n;\vec{R}}(\vec{r}) \cdot \phi_{\omega;n}(\vec{R}), \quad (5)$$

Where $\psi_{n;\vec{R}}(\vec{r})$ is the n -th electron wave function in the case of the fixed nucleus position \vec{R} and

$\phi_{\omega;n}(\vec{R})$ is the ω -th nucleus motion wave function in the case of the electron state n .

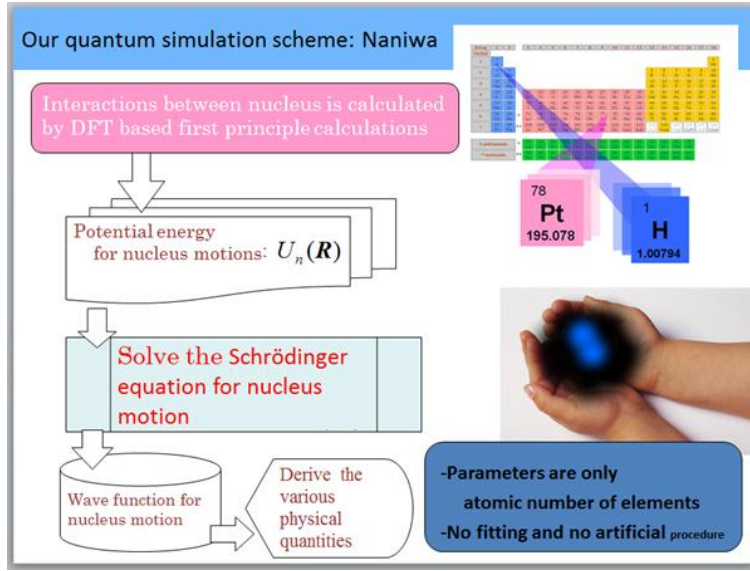
Then, we can divide the total Schrödinger equation into two equations. One is for electrons,

$$\left[\sum_{i=1}^{n_e} \left(-\frac{\hbar^2}{2m_e} \right) \nabla_i^2 + V(\vec{r}, \vec{R}) \right] \psi_{n;\vec{R}}(\vec{r}) = U_n(\vec{R}) \psi_{n;\vec{R}}(\vec{r}) \quad (6)$$

Another is for nuclei

$$\left[\sum_{I=1}^{N_{\text{nc}}} \left(-\frac{\hbar^2}{2M_I} \right) \nabla_I^2 + U_n(\vec{R}) \right] \phi_{\omega;n}(\vec{R}) = E_{\omega;n} \phi_{\omega;n}(\vec{R}). \quad (7)$$

From Schrödinger equation for electron system with fixed R , we can obtain the eigenenergies and eigenstates with the aid of the conventional first principles (*electron states*) calculation. The eigenenergies, $U_n(\vec{R})$ of electron state as a function of R can be considered as the adiabatic potential energy surface for nucleus motion. Eigenenergy of nuclei corresponds to the total energy, E , appeared in the Schrödinger equation for total system. Naniwa series codes solve this equation.



Naniwa-SKY code solves the Schrödinger equation for a single atom motion in the material.;

$$\left[-\frac{\hbar^2}{2M} \left(\frac{\partial^2}{\partial X^2} + \frac{\partial^2}{\partial Y^2} + \frac{\partial^2}{\partial Z^2} \right) + U_0(X, Y, Z) \right] \phi_{\omega,0}(X, Y, Z) = E_{\omega,0} \phi_{\omega,0}(X, Y, Z). \quad (8)$$

The wave function for atom motion in the material has rather position localized character. Then we described it by linear combination of the 3D-Gauss functions located at grid points,

$$\phi_{\omega}(X, Y, Z) = \sum_{\ell=1}^{N_G} C_{\omega,\ell} G_{\ell}(X, Y, Z), \quad (9)$$

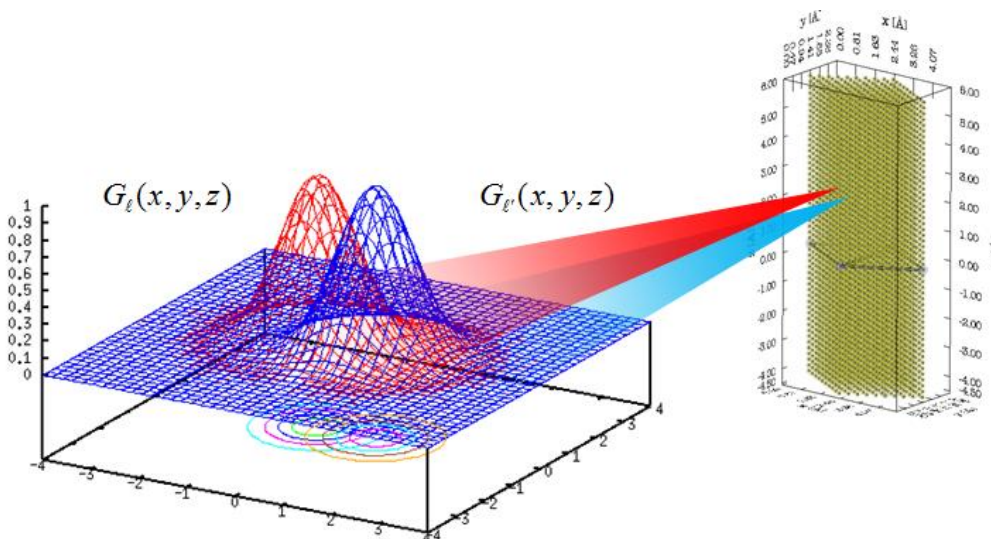
where $G_{\ell}(X, Y, Z)$ is the ℓ -th 3D-Gauss function located at the ℓ -th grid point $\vec{R}_{\ell}(X_{\ell}, Y_{\ell}, Z_{\ell})$,

$$G_{\ell}(X, Y, Z) = \left(\frac{8\alpha_x\alpha_y\alpha_z}{\pi^3} \right)^{1/4} \exp\{ -\alpha_x(X - X_{\ell})^2 - \alpha_y(Y - Y_{\ell})^2 - \alpha_z(Z - Z_{\ell})^2 \}, \quad (10)$$

Factors $\alpha_x, \alpha_y, \alpha_z$ indicate the decays of Gauss function along the X, Y, Z directions

$$G_{\ell}(X, Y, Z; \vec{k}) = \left(\frac{8\alpha_x\alpha_y\alpha_z}{\pi^3} \right)^{1/4} \exp\{ -\alpha_x(X - X_{\ell})^2 + ik_x X - \alpha_y(Y - Y_{\ell})^2 + ik_y Y - \alpha_z(Z - Z_{\ell})^2 + ik_z Z \}$$

The nearest neighbor 3D-Gauss functions have to be overlapped.



Naniwa code use the variation method with the trial function (9) to solve the Schrödinger equation (8). And Naniwa code solves the following equation instead of eq (8).

$$\sum_{\ell'} [H_{\ell\ell'} - E_{\omega,0} S_{\ell\ell'}] C_{\omega,\ell} = 0 \quad (11.0)$$

$$H_{\ell\ell'} = K_{\ell\ell'} + U_{\ell\ell'} \quad (11.1)$$

$$K_{\ell\ell'} = \iiint_{-\infty}^{+\infty} G_{\ell}(X,Y,Z) \left[-\frac{\hbar^2}{2M} \left(\frac{\partial^2}{\partial X^2} + \frac{\partial^2}{\partial Y^2} + \frac{\partial^2}{\partial Z^2} \right) \right] G_{\ell'}(X,Y,Z) dXdYdZ, \quad (11.2)$$

$$U_{\ell\ell'} = \iiint_{-\infty}^{+\infty} G_{\ell}(X,Y,Z) U_0(X,Y,Z) G_{\ell'}(X,Y,Z) dXdYdZ \quad (11.3)$$

$$S_{\ell\ell'} = \iiint_{-\infty}^{+\infty} G_{\ell}(X,Y,Z) G_{\ell'}(X,Y,Z) dXdYdZ \quad (11.4)$$

Here, we can integrate K and S , analytically. On Naniwa-K code, the special routines are installed to integrate U in an efficient way [Japanese Paten No.5902495]. From eq.11.0, secular equation is written by

$$\begin{vmatrix} H_{11} - E S_{11} & H_{12} - E S_{12} & \cdots & H_{1N_G} - E S_{1N_G} \\ H_{21} - E S_{21} & H_{22} - E S_{22} & \cdots & H_{2N_G} - E S_{2N_G} \\ \vdots & \vdots & \ddots & \vdots \\ H_{N_G1} - E S_{N_G1} & H_{N_G2} - E S_{N_G2} & \cdots & H_{N_GN_G} - E S_{N_GN_G} \end{vmatrix} = 0 \quad (12)$$

We solve the secure eq.(12) and obtain eigenenergy $E_{\omega,0}$, $\omega = 0,1,2 \dots$. Then, we can solve eq.(11.0) for all obtained $E_{\omega,0}$, and get the corresponding eigenvectors $(C_{\omega,1}, C_{\omega,2}, C_{\omega,3}, \dots, C_{\omega,N_G})$.

You should check the convergence of these numerical results by the some trial runs for various Gaussian decay factors $\alpha_x, \alpha_y, \alpha_z$ and number of grid point, N_G .

The expectation value of an observable, O , at ω th state is given by

$$\begin{aligned} \langle O \rangle_{\omega} &= \iiint \phi_{\omega}^*(X,Y,Z) \hat{O} \phi_{\omega}(X,Y,Z) dXdYdZ \\ &= \sum_{q=1}^{N_G} \sum_{q'=1}^{N_G} C_{\omega,q}^* C_{\omega,q'} \iiint G_q(X,Y,Z) \hat{O} G_{q'}(X,Y,Z) dXdYdZ \end{aligned} \quad (13)$$

It is easy to calculate $\langle O \rangle_{\omega}$ from obtained eigenvectors $(C_{\omega,1}, C_{\omega,2}, C_{\omega,3}, \dots, C_{\omega,N_G})$.

2. System Requirements

Hardware

Recommended

Computer Processor: 3.0GHz Intel Core i7 or better

Computer Memory: 8 GB/core or more

Operating System: 64-bit Linux distribution

Software

(1) Naniwa package file : NaniwaSKYXXXXXXXXX.tar.gz

XXXXXXXXX is version number. (ex. NaniwaSKY20160817.tar.gz)

(2) ab initio electronic state calculation package

For install

(1) Compiler: Intel® Fortran compiler [16]

(2) Math library: Intel ® Math Kernel Library (MKL) [17]

For use

(1) Text editor: vi , mule ... (as you like)

(2) C shell: csh or tcsh

(When you use other Unix shell, you must rewrite the script files by yourself.)

(3) Visualization tool: gnuplot and OpenDX, XCrySDen, or VESTA.

“**gnuplot**” is a command-line program that can make 2- and/or 3-dimensional plots of functions and data. [18]

“**OpenDX**” is IBM Visualization Data Explorer program. [19]

“**XCrySDen**” is a crystalline and molecular structure visualization program. [20]

“**VESTA**” is a Visualization program for Electronic and STructural Analysis.

3. How to install

(1) Copy the package file “NaniwaSkyXXXXXXXXX.tar.gz” to your home directory.

XXXXXXXXX is version number. (ex. NaniwaSky20160817.tar.gz)

(2) Decompress the package file.

Type following command lines:

```
gzip -d NaniwaSkyXXXXXXXXX.tar.gz [Enter]
```

```
tar xvf NaniwaSkyXXXXXXXXX.tar [Enter]
```

You can get following directory on your home directory.

Installed directory structure

~+ : your home directory

| -- naniwa +

| -- doc: documents

| -- SRC : source codes

| -- bin: :you will install the execution programs into this directory

| -- work: working directory

| -- qs : script for Grid Engine (Job scheduler)

| -- etc +

| -- OpenDX: files for Visualization software OpenDX®

| -- charge: files for BADER CHARGE ANALYSIS

| -- potential: files for making potential data

| -- example: input data examples

| -- results: some simulation results

(3) Move to SRC directory

Type :

```
cd ./naniwa/SRC [Enter]
```

(4) Compile the source codes

Type :

```
make all [Enter]
```

The compilation must finish without errors, although warnings may be possible.

If you get error message, you must modify following values in “Makefile” file under SRC directory.

(A) Error message

```
make: ifort: Command not found
make: *** [naniwa] Error 127
```

Please ask to your system administrator to install Intel Fortran.

If you use older Intel Fortran, please change the compiler name in "Makefile"

From

```
FC = ifort
```

To

```
FC = ifc
```

(B) Error message:

```
/tmp/fortzvGoSf.o: In function `MAIN_':
NaniwaSYMk.f(.text+0x40fb): undefined reference to `dfti_create_descriptor_highd'
NaniwaSYMk.f(.text+0x410f): undefined reference to `dfti_set_value_intval'
NaniwaSYMk.f(.text+0x4123): undefined reference to `dfti_set_value_intval'
NaniwaSYMk.f(.text+0x4137): undefined reference to `dfti_set_value_intvec'
NaniwaSYMk.f(.text+0x414b): undefined reference to `dfti_set_value_intvec'
NaniwaSYMk.f(.text+0x4155): undefined reference to `dfti_commit_descriptor_external'
NaniwaSYMk.f(.text+0x416d): undefined reference to `dfti_compute_forward_zz'
NaniwaSYMk.f(.text+0x41a0): undefined reference to `dfti_free_descriptor_external'
NaniwaSYMk.f(.text+0x6fb2): undefined reference to `zhegv_'
make: *** [naniwa] Error 1
```

If you see the above-mentioned errors, you must change the path of Intel MKL installed directory in Makefile

From

```
LIB = /opt/intel/mkl/lib/intel64
```

```
INC= -I/opt/intel/mkl/include
```

To

```
LIB = /opt/intel/mkl/lib/em64t
```

```
INC= -I/opt/intel/mkl/include
```

or

```
LIB = /opt/intel/mkl/XXXXXX/lib/em64t
```

```
INC = -I/opt/intel/mkl/XXXXXX/include
```

here, XXXXXXXX is version of the Intel MKL installed on your computer.

(C) Error message:

```
fastDFT3D_MKL.f(5): error #7002: Error in opening the compiled module file. Check INCLUDE paths. [MKL_DFTI]

    Use MKL_DFTI
-----^
fastDFT3D_MKL.f(10): error #6457: This derived type name has not been declared. [DFTI_DESCRIPTOR]

    type(DFTI_DESCRIPTOR), POINTER :: hand
-----^
compilation aborted for fastDFT3D_MKL.f (code 1)
make: *** [naniwa] Error 1
```

If you see the above-mentioned errors, you should ask to your system administrator to compile mkl_dfti.f90.

Please do followings as root (super user).

```
cd /opt/intel/mkl/include
ifort -c mkl_dfti.f90
```

* You can find some hints to solve your problem in Makefile.

(5) Move the execution file to binary directory

Type:

```
make all-install [Enter]
```

Check the execution files under bin directory

Type :

```
ls ../bin [Enter]
```

You can see following files:

```
BandStructure  cellexpander  chkPOTENG  makeBHGCAR  naniwaSS_run  state2dx
BHGCAR2DX      ChargeState  eigen2spec  makePOTENG  poteng2dx     state2xsf
```

(6) test run.

Move to work directory.

```
cd [Enter]
```

```
cd ./naniwa/work [Enter]
```

Copy the test data.

```
cp -r ../etc/example/test ./ [Enter]
```

```
cd ./test [Enter]
```

If necessary, change the "LD_LIBRARY_PATH" value in "run.csh" file by text editor :

```
setenv LD_LIBRARY_PATH LD_LIBRARY_PATH:'/opt/intel/mkl/lib/em64t'.
```

or

```
setenv LD_LIBRARY_PATH LD_LIBRARY_PATH:'/opt/intel/mkl/XXXXXXXXX/lib/em64t'.
```

here, XXXXXXXX is version of the Intel MKL installed on your computer.

Execute the program

```
csh ./run.csh [Enter]
```

```
machine name
Job start date & time
Naniwa start date & time
finish naniwa
Naniwa terminate date & time
```

Check output files

```
ls [Enter]
```

If successful, you can get the following LOG file:

```
*****
*           Naniwa code           *
*****
NaniwaSky Version 2012.11.22
created by NAKANISHI, Hiroshi
OSAKA UNIVERSITY

-----
INSET title :
*

Calculaton mode :           0
*** Full calculation

-----
Atomic Mass =  1.000000000000000    (proton)
              = 1.672621637000000E-027 (kg)

-----
Number of node index (No1,No2,No3)
           9           9           9
Gaussian decay factors (1/Angstrom Angstrom)
SigmaX=  5.000000000000000
SigmaY=  5.000000000000000
SigmaZ=  5.000000000000000

-----
** No correction by symmetry.

-----
- Lattice vector (A)
  3.000000000000000           0.000000000000000
0.000000000000000E+000
  0.000000000000000E+000           3.00000000
0.000000000000000E+000
  0.000000000000000E+000           0.000000000000000
3.000000000000000

- Lattice unit volume (A^3)
  27.0000000000000

-----
Reciprocal lattice vector (/A)
  2.09439510239320           0.000000000000000
0.000000000000000E+000
  0.000000000000000E+000           2.0943951
0.000000000000000E+000
  0.000000000000000E+000           0.000000000000000
2.09439510239320

-----
wave00005.xsf was created.
WAVE function
  Max value=  1.68540114820597
  Min value= -1.84336513692804
  probability= 0.999869835826559

-----
wave00006.xsf was created.
WAVE function
  Max value=  1.93274716286747
  Min value= -1.03123097291435
  probability= 0.999869796584020

-----
wave00007.xsf was created.
WAVE function
  Max value=  1.72099225797871
  Min value= -1.72768364358320
  probability=  1.00175769772228

-----
wave00008.xsf was created.
WAVE function
  Max value=  1.00317921937198
  Min value= -1.96774733538390
  probability=  1.00175785191399

-----
wave00009.xsf was created.
WAVE function
  Max value=  0.825426714232840
  Min value= -2.44372845893816
  probability=  1.00175785169862

-----
wave00010.xsf was created.
WAVE function
  Max value=  1.64599264710982
  Min value= -1.54178274285677
  probability= 0.999839014572012
```

4. Program codes and files

4.1 Programs

(1) naniwaSS_run : main simulation execution file to calculate eigenstates and eigenenergies

Input files: INSET : simulation setting information

POTENG : Potential energy surface for atom motion

KPOINTS (option): for dispersion [Under construction, Coming soon]

Output files: LOG : run time information

EIGEN: Eigenenergy for atom motion

stateXXXXX: information about eigenstate for atom motion

(2) Tools for getting potential energy surface for atom motion

(2.1) auto.csh: automatic launcher for ab initio electronic state calculation VASP

(2.2) collect.csh: to make POTDAT from many OSZICAR files of VASP

(2.3) makePOTENG: to make POTENG from POTDAT and POTDAT.cfg

(2.4) chkPOTENG: checking the max and min values in POTENG file.

(3) Tools for visualization of results

(3.1) poteng2dx: to make input file for WaveViewer3D in order to see the potential energy surface

input file: POTENG, POTDAT.cfg (option)

output file: PES.dat, PES3D.general

(3.2) state2dx: to make input file for WaveViewer3D in order to see the wave function

input files: stateXXXXX, POTDAT.cfg (option)

output files: waveXXXX.dat, waveXXXX.general

usage : state2dx [start state number] [end state number]

example: state2dx 1 10 *[Enter]*

(3.3) WaveViewer3D_XXX (Visual program for OpenDX (<http://www.opendx.org/>))

WaveViewer3D_XXX.cfg, WaveViewer3D_XXX.net

(3.4) state2xsf: to make input file for XcrySDen in order to see the wave function

input files: stateXXXXX, POTDAT.cfg (option)

output files: waveXXXX.xsf

usage : state2xsf [start state number] [end state number]

example: state2xsf 1 10 *[Enter]*

(4) Band structure builder

(4.1) BandStructure: [Under construction, coming soon]

4.2 files

4.2.1 List of important files

INPUT files:

INSET : Calculation setting about basis function and particle mass, etc.
POTENG : Super cell geometry and potential energy surface
KPOINTS : [Under construction, coming soon]

OUTPUT files:

LOG : calculation information

under the directory of "kpoint0000"

EIGEN : Eigenenergy set
state00000 : Eigenstate information of the ground state
stateXXXXX : Eigenstate information of the XXXXXX th excited state

4.2.2 INSET

Example

```
* Naniwa Sky test / Hydrogen
* Calculation mode
* 0: full calculation, 1: parameter-check only (1)
*
0 (2)
* Mass of your quantum particle (/proton mass)
* 0:muon, 1:proton, 2: deuterium, 3: tritium,4: quadrium, n: Hydrogen-n
1
c Number of nodes for the 3D Gaussian functions (No1 x No2 x No3) (3)
9 9 35
c Gaussian decay factor (SigmaX, SigmaY SigmaZ) (1/Angstrom Angstrom)
10.18 10.18 10.6
c number of output eigen states (4)
20
c correction by Symmetry: E, C3v, C4v
C3v (5)
(6)
```

Contents

(0) Comment lines

The lines that begin with with a "c" or "*" (asterisk) are comment line. In comment lines, you can write something as you like in these lines, but don't change the number of all comment lines and their positions in INSET.

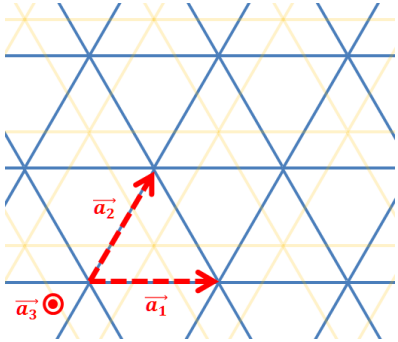
(1) Calculation mode in the 5th line

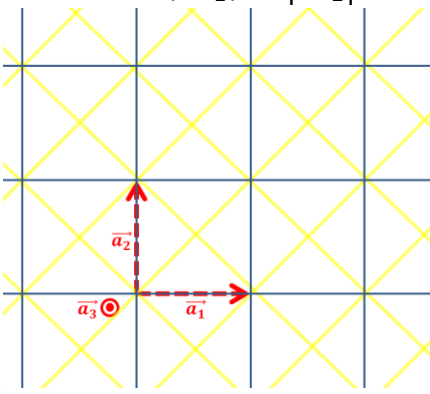
0; full calculation mode.

- 1: parameter check mode. (no calculation)
- (2) Mass of the target quantum particle, which unit is that of a proton.
 1: proton, 2: deuterium, 3: tritium, 4: quadrium, n: Hydrogen-n
 if you input 0, program will replace it by the mass value of the (Anti)muon.
- (3) Number of nodes for the 3D Gaussian functions (No1 x No2 x No3) in the 8th line
 Please input 3 positive integer numbers which are numbers of nodes for 3D Gaussian functions, No1, No2, No3. They correspond to the numbers of partitions of primitive vectors: $\vec{La}_1, \vec{La}_2, \vec{La}_3$ (See next section 4.2.3)
- (4) Gaussian decay factor (SigmaX, SigmaY SigmaZ) in the 10th lines
 Please input 3 positive floating-point type data which are Gaussian decay factors along the directions of x, y and z-axis, $\sigma_x, \sigma_y, \sigma_z$. Their unit is 1/(Angstrom·Angstrom). (If you put 0, 0, 0, then these values are automatically reset by default values.)
- (5) Number of output eigen states in the 12th line
 Please input a positive integer number of output eigen states which you request.
- (6) Correction by crystal structure symmetry
- (6)-1. Correction by rotational symmetry around z-axis
 Please input one rotational symmetry symbol.
 Supported symbols: C1, C3v, C4v (Schönflies notation)
 for surfaces perpendicular to Z-axis
- (6)-2. Correction by Crystal structure symmetry
 Supported symbols: Oh, Td², Oh⁷ (Schönflies notation)
 graphene (special)
-

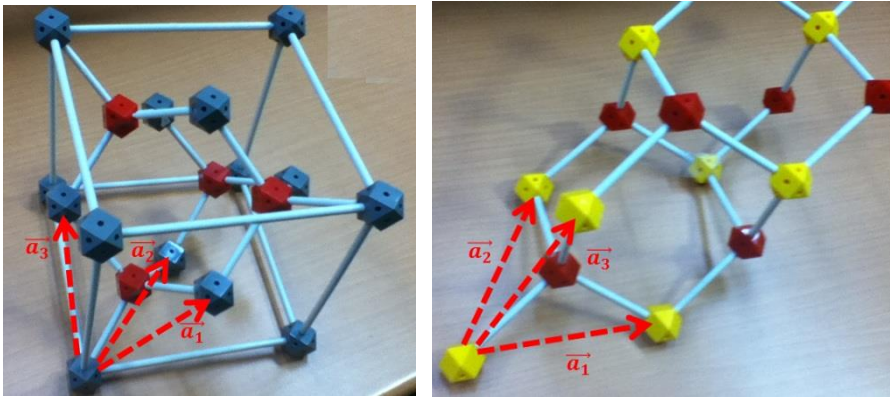
Supported symmetry symbols.

(i)	
Symbol	E
Symmetry	1-fold rotation
Requirement	non

(ii)	
Symbol	C3v
Symmetry	3-fold rotation symmetry with 3 mirror planes containing the z-axis (vertical planes).
Requirement	$No1=No2$, $ \overline{La_1} = \overline{La_2} $, $2\overline{a_1} \cdot \overline{a_2} = \overline{a_2} ^2$, $\sigma_x = \sigma_y$
	

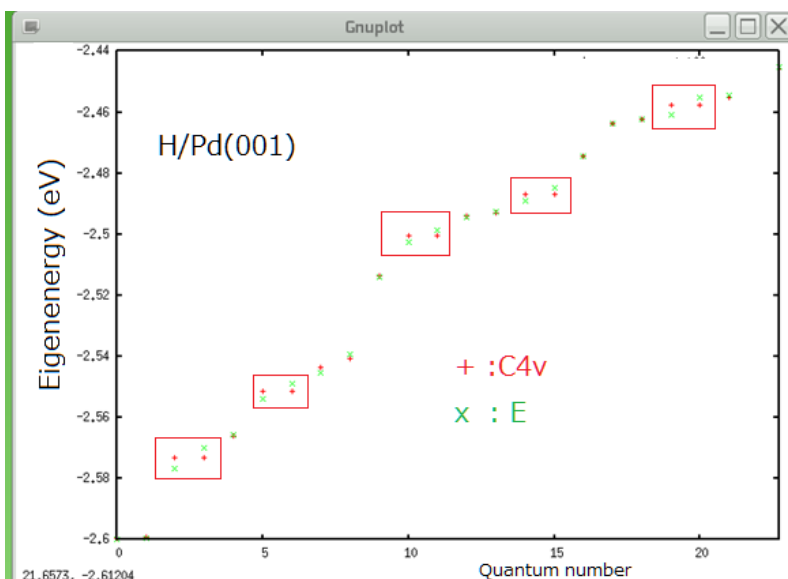
(iii)	
Symbol	C4v
Symmetry	4-fold rotation symmetry with 4 mirror planes containing the z-axis (vertical planes).
Requirement	$No1=No2$, $ \overline{La_1} = \overline{La_2} $, $\sqrt{2}\overline{a_1} \cdot \overline{a_2} = \overline{a_2} ^2$, $\sigma_x = \sigma_y$
	

(iv)	
Symbol	Oh
Symmetry	The rotation axes of an octahedron or cube (three 4-fold axes, four 3-fold axes, and 6 diagonal 2-fold axes) with a mirror plane perpendicular to the z-axis (horizontal plane).
Requirement	$No_1=No_2=No_3$, $ L\vec{a}_1 = L\vec{a}_2 = L\vec{a}_3 $, $\sqrt{2} \vec{a}_1 \cdot \vec{a}_2 = \sqrt{2} \vec{a}_1 \cdot \vec{a}_3 = \sqrt{2} \vec{a}_2 \cdot \vec{a}_3 = \vec{a}_2 ^2$, $\sigma_x = \sigma_y = \sigma_z$

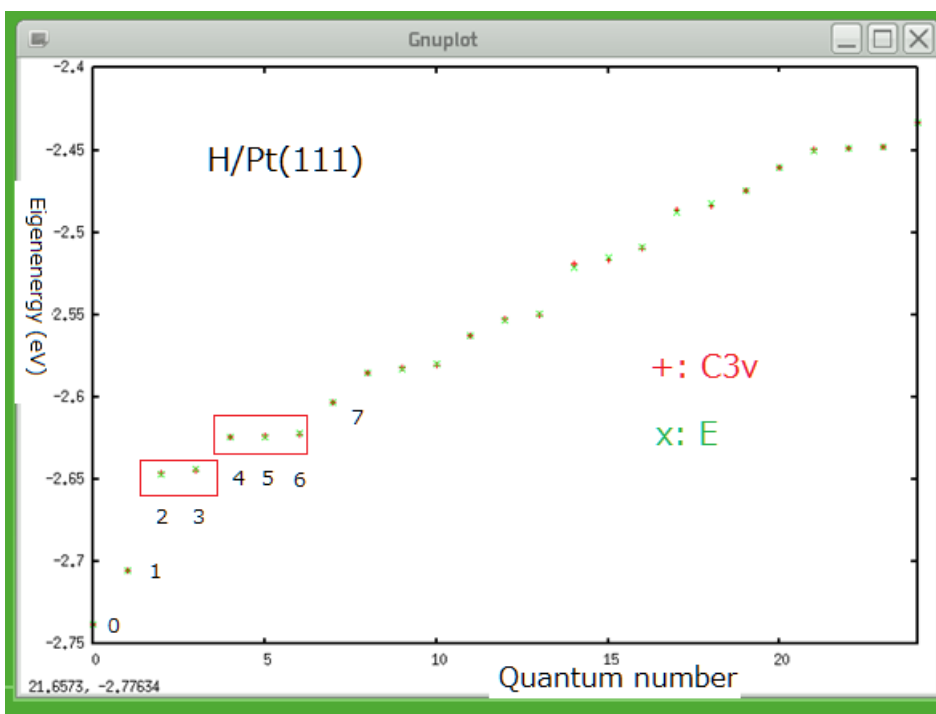
(v)	
Symbol	Td ² , F ⁻⁴ 3m, 216
Symmetry	Zinc Blend crystal structure.
Requirement	$No_1=No_2=No_3$, $ L\vec{a}_1 = L\vec{a}_2 = L\vec{a}_3 $, $2 \vec{a}_1 \cdot \vec{a}_2 = 2 \vec{a}_1 \cdot \vec{a}_3 = 2 \vec{a}_2 \cdot \vec{a}_3 = \vec{a}_1 ^2$, $\sigma_x = \sigma_y = \sigma_z$
	

(vi)	
Symbol	Oh ⁷ , F ^{d-3} m, 227
Symmetry	Diamond crystal structure.
Requirement	$No_1=No_2=No_3$, $ L\vec{a}_1 = L\vec{a}_2 = L\vec{a}_3 $, $2 \vec{a}_1 \cdot \vec{a}_2 = 2 \vec{a}_1 \cdot \vec{a}_3 = 2 \vec{a}_2 \cdot \vec{a}_3 = \vec{a}_1 ^2$, $\sigma_x = \sigma_y = \sigma_z$ $No_1 \bmod 4 = 0$

When you use this function, you can get accurate degenerate eigen values.
 In the case of hydrogen atom in Pd(001), which has C4v symmetry, you can get following eigenvalues:



And in the case of hydrogen atom in Pt(111), which has C3v symmetry, you can get following eigenvalues:



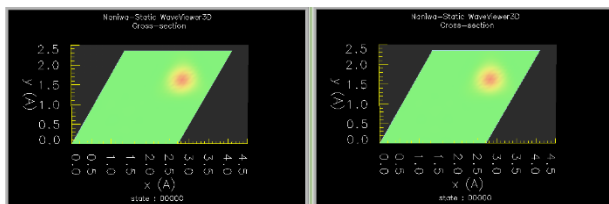
Green: no correction

and their wave functions:

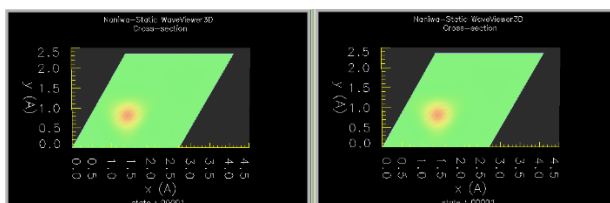
E (no use)

C3v

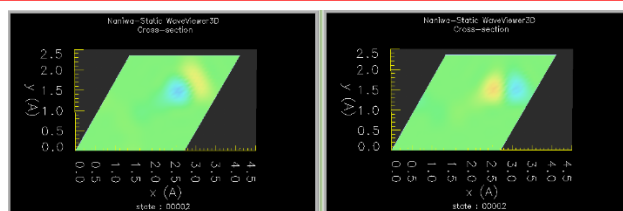
the ground state



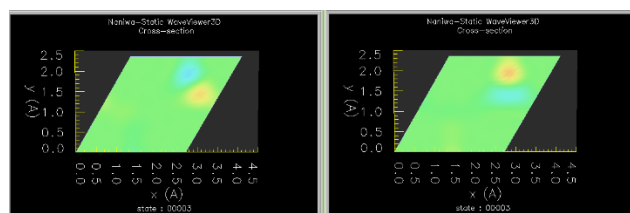
the 1st excited state



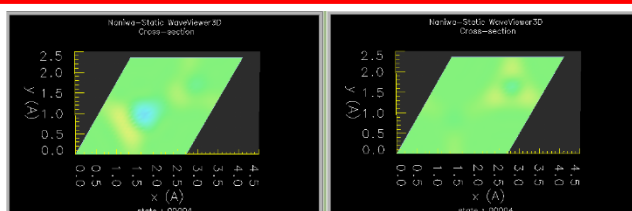
the 2nd excited state



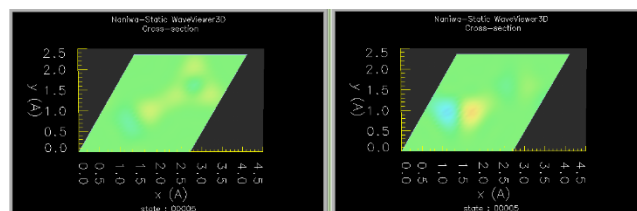
the 3rd excited state



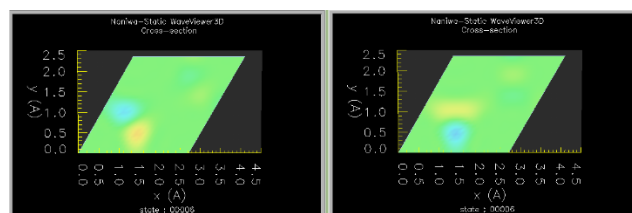
the 4th excited state

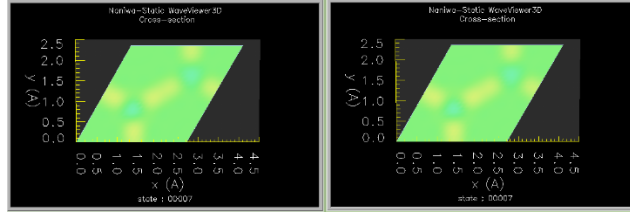


the 5th excited state



the 6th excited state





the 7th excited state

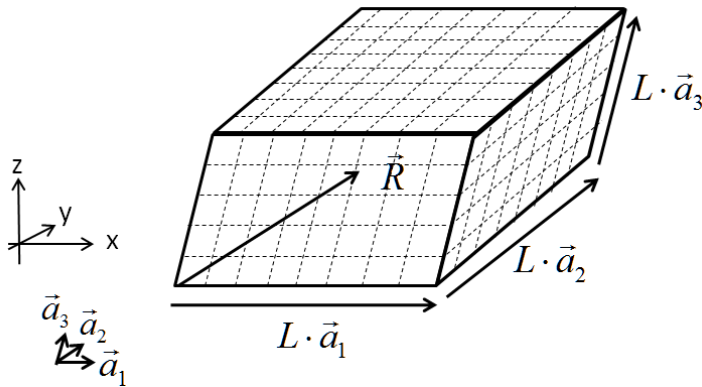
4.2.3 POTENG

The first line is a comment line. The second line provides a universal scaling factor L (Angstrom), which is used to scale the primitive vectors in the simulation system. On the following three lines, the three primitive vectors, $L\vec{a}_1$, $L\vec{a}_2$, $L\vec{a}_3$, defining the supercell of the simulation material system are given. Each line has the x, y, z components of Cartesian coordinate system, whose unit is L . The sixth line supplies the numbers, N_1, N_2, N_3 , of the potential energy calculation point along the primitive vectors, $\vec{a}_1, \vec{a}_2, \vec{a}_3$. The lines from seventh provide the potential energy values (eV) and its particle positions. Each line has $n_1, n_2, n_3, U(R_{n_1, n_2, n_3})$.

$$\text{Here, } R_{n_1, n_2, n_3} = L \left(\frac{n_1}{N_1} \vec{a}_1 + \frac{n_2}{N_2} \vec{a}_2 + \frac{n_3}{N_3} \vec{a}_3 \right),$$

where

$$\begin{aligned} n_1 &= 0, 1, 2, \dots, N_1 - 1 \\ n_2 &= 0, 1, 2, \dots, N_2 - 1 \\ n_3 &= 0, 1, 2, \dots, N_3 - 1 \end{aligned}$$



```

* POTENG: POTENTIAL ENERGY for H on Pd(111)
  2.820295
  1.000000      0.0000000E+00  0.0000000E+00
  0.5000000      0.8660254      0.0000000E+00
  0.0000000E+00  0.0000000E+00      3.81165754909725
    12          12          44
    1           1           1 -8.7710377E-04
    2           1           1 -6.4631744E-04
    3           1           1 -3.8508927E-03
    4           1           1 -1.8527496E-03
    5           1           1 -2.3826952E-03
    6           1           1 -4.5110146E-03
    7           1           1 -6.5468652E-03
    ~           ~           ~

    ~           ~           ~
   11          2           1 -1.1861493E-03
   12          2           1 -6.4631744E-04
    1           3           1 -3.8508927E-03
    2           3           1 -1.2586723E-03
    3           3           1 -1.6357267E-03
    4           3           1 -2.8395073E-03
    5           3           1 -5.4807067E-03
    6           3           1 -8.3559640E-03
    2          12          44 -1.732900
    3          12          44 -0.2266000
    4          12          44  1.000000
    5          12          44  1.000000
    6          12          44  1.000000
    7          12          44  1.000000
    8          12          44  1.000000
    9          12          44  1.000000
   10         12          44  1.000000
   11         12          44  1.000000
   12         12          44 -0.2266000

* END of POTENG

```

4.2.4 LOG

It gives you the information about your simulation situation.
 When the simulation is executing, you can check it by following command.

```
tail -f LOG [Enter]
```

Following is the example of LOG file.

```

*****
*           Naniwa code           *
*****
mode: NaniwaSSk Version 2012.02.10
      created by NAKANISHI, Hiroshi
      OSAKA UNIVERSITY

-----
Calculaton mode :           0
*** Full calculation
-----

```

Atomic Mass = 1.00000000000000 (proton)
= 1.672621637000000E-027 (kg)

Number of node index (No1,No2,No3)
9 9 35

Gaussian decay factors (1/Angstrom Angstrom)
SigmaX= 5.09173682192627
SigmaY= 5.09173682192627
SigmaZ= 8.55607353478694

- Lattice vector (A)
3.98849944000000 0.00000000000000E+000 0.00000000000000E+000
0.00000000000000E+000 3.98849944000000 0.00000000000000E+000
0.00000000000000E+000 0.00000000000000E+000 11.9654983200000

- Lattice unit volume (A^3)
190.348676260400

Reciprocal lattice vector (1/A)
1.57532565230225 0.00000000000000E+000 0.00000000000000E+000
0.00000000000000E+000 1.57532565230225 0.00000000000000E+000
0.00000000000000E+000 0.00000000000000E+000 0.525108550767416

Reciprocal lattice unit volume (1/A^3)
1.30313611328161

MSG: reading POTENG
MSG: finish reading POTENG
MSG: start FFT of POTENG data
MSG: finish FFT
I cannot find KPOINTS file.
I will set single k-point calculation.

K-sampling point information.

Number of K-points: 1

fractional of reciprocal lattice vector
(unit : b1/2, b2/2, b3/2)

1 : 0.000000E+00 0.000000E+00 0.000000E+00

kx,ky,kz vector (1/A)

1 : 0.000000E+00 0.000000E+00 0.000000E+00

MSG: start k-loop

+++++

MSG: k-loop: 1

MSG: POTMTX file is created

MSG: start diagonalization

MSG: end diagonalization

MSG: info from ZHEGV = 0

Eigen energy value (eV)

0 -2.738340
1 -2.705202
2 -2.647121
3 -2.643604
4 -2.624361
5 -2.624101
6 -2.622245

```

7 -2.603370
8 -2.585140
9 -2.583143
10 -2.579886
11 -2.563037
12 -2.553304
13 -2.549820
14 -2.521095
15 -2.514894
16 -2.509215
17 -2.488150
18 -2.482372
19 -2.474471

```

MSG:checking the probality of each eigenstates
All k-point calculation, which you requested,are done.

```

*****
* Naniwa code is terminated *
*****

```

44.2.5. EIGEN

It gives you the information about quantum number and eigenenergies (eV)

0	-2.738340
1	-2.705202
2	-2.647118
3	-2.643600
4	-2.624484
5	-2.624043
6	-2.622192
7	-2.603305
8	-2.585474
9	-2.583032
10	-2.579732
11	-2.562970
~	~
~	~
2828	1.397943
2829	1.401005
2830	1.405767
2831	1.427601
2832	1.433854
2833	1.451622
2834	1.454133

4.2.6 stateXXXXX

It gives you the information about the XXXXXth eigenstate.


```

stateXXXXX
  0
-2.73834024018558
  2.82029500000000    0.000000000000000E+000  0.000000000000000E+000
  1.41014750000000    2.44244710549300    0.000000000000000E+000
0.000000000000000E+000  0.000000000000000E+000  10.7499987274312
  9          9          35
10.1834736495052    10.1834736495052    10.6003270094309
  0          0          0
(-1.777456224903666E-006,-4.974294848068331E-007)
  1          0          0
(7.765809220410138E-007,4.430627433556088E-007)
  2          0          0
(1.439251475885052E-006,-2.545852331603858E-007)
  ~          ~          ~
~          ~          ~
(-5.370729930410416E-006,5.895488939631636E-007)
  5          8          34
(-5.362392471165102E-006,2.837122256840745E-007)
  6          8          34
(3.192389365300413E-006,-2.070464429167339E-007)
  7          8          34
(-2.748703204133705E-006,1.452834001927643E-007)
  8          8          34
(2.221894867527162E-006,0.000000000000000E+000)

```

state file name

quantum number, ω

eigenenergies (eV)

$(\overline{La}_1)_x$ $(\overline{La}_1)_y$ $(\overline{La}_1)_z$ (Å)

$(\overline{La}_2)_x$ $(\overline{La}_2)_y$ $(\overline{La}_2)_z$ (Å)

$(\overline{La}_3)_x$ $(\overline{La}_3)_y$ $(\overline{La}_3)_z$ (Å)

n_{g1} n_{g2} n_{g3} : Numbers of Gaussian grid along \overline{a}_1 , \overline{a}_2 , \overline{a}_3 , where $n_{g1} \times n_{g2} \times n_{g3} = N_G$

σ_x σ_y σ_z : Gaussian decay factors

i_{g1}^1 i_{g2}^1 i_{g3}^1 : 1st grid point indicators along \overline{a}_1 , \overline{a}_2 , \overline{a}_3 .

(Re $C_{\omega,1}$, Im $C_{\omega,1}$): corresponding coefficient of eigenvector

i_{g1}^2 i_{g2}^2 i_{g3}^2 : 2nd grid point indicators along \overline{a}_1 , \overline{a}_2 , \overline{a}_3 .

(Re $C_{\omega,2}$, Im $C_{\omega,2}$): corresponding coefficient of eigenvector

:

$i_{g1}^{N_G}$ $i_{g2}^{N_G}$ $i_{g3}^{N_G}$: N_G -th grid point indicators along \overline{a}_1 , \overline{a}_2 , \overline{a}_3 .

(Re C_{ω,N_G} , Im C_{ω,N_G}): corresponding coefficient of eigenvector

5. How to use (minimum)

5.1 Making 3D-potential energy surface for quantum particle in material.

You must make the potential energy surface for your quantum particle motion in materials by ab initio electron state calculation.

Calculate the total energy : $E(X,Y,Z)$ of electron system as a function of quantum particle position (X,Y,Z) . Use it as adiabatic potential energy: $U(X,Y,Z)$.

Save these potential energy information into POTENG file. (See the section 4.2 files section)

5.2 Making the simulation setting

Make the setting file: INSET (See the section 4.2 files section).

Copy the input file: INSET, POTENG on your working directory.

5.3 Executing the simulation program.

Type following command line on your working directory.

```
~/naniwa/bin/naniwaSS_run [Enter]
```

If successful, you can obtain the LOG file and the kpoint0000 directory.

Please check the contents in the LOG files.

You can find the simulation results under the kpoint0000 directory.

If “Oracle Grid Engine” is installed on your computer, you can submit your simulation by following command line:

```
qsub run.csh [Enter]
```

```
qstat [Enter]
```

5.4 Check simulation results

Move to sub-directory: “kpoint0000”

```
cd ./kpoint0000 [Enter]
```

```
ls [Enter]
```

```
cat EIGEN [Enter]
```

5.4.1 How to see the Eigenenergies as a function of quantum number.

```
gnuplot [Enter]
```

```
GNUPLOT
Version 4.0 patchlevel 0

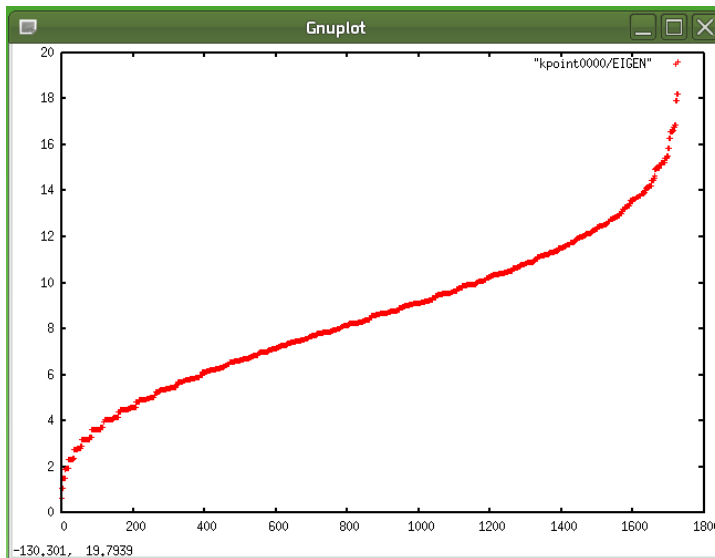
....

....

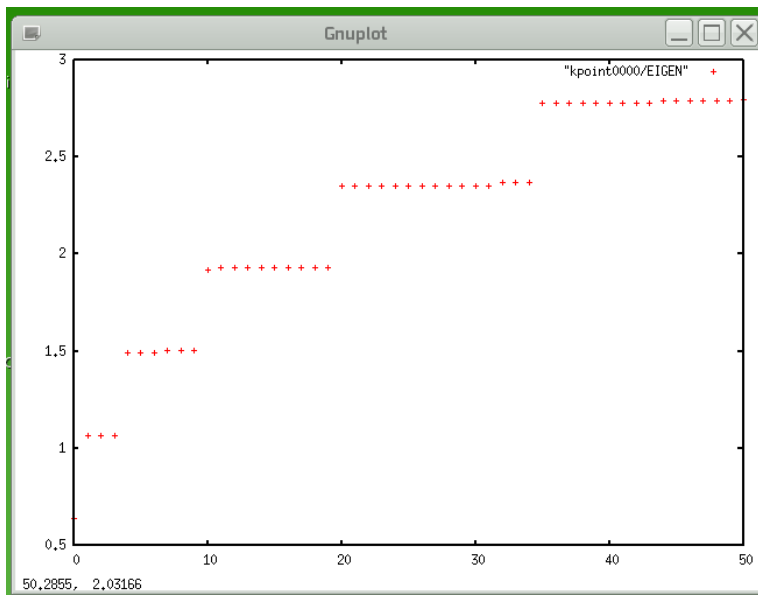
Send bugs, suggestions and mods to
  <gnuplot-bugs@lists.sourceforge.net>

Terminal type set to 'x11'
```

```
gnuplot> plot "EIGEN" [Enter]
```



```
gnuplot> set xrange [0:50] [Enter]
gnuplot> replot [Enter]
```



Quit the gnuplot

```
gnuplot> quit [Enter]
```

5.4.2 How to see the Wave functions

5.4.2.1 OpenDX case

Naniwa package includes the “WaveViewer3D”, which is Visual Program running on the OpenDX.

(1) Convert the eigenstate data for OpenDX

Make the OpenDX data from the ground state to 10th excited state.

```
cp ../INSET ./ [Enter]
../../bin/state2dx 0 10 [Enter]
```

```
stat2dx
I create the files for Opndx from          0 to          10
-----
I got the following data from INSET file.
(n1,n2,n3)=          9          9          9
I set (n1,n2,n3)=          27          27          27
-----
=====
POTDAT.cfg is not found.
Position origine is reset to
0.0000000E+00 0.0000000E+00 0.0000000E+00
=====
wave00000.dat was created.
WAVE function
  Max value=  2.219193
  Min value= -4.8887818E-03
  probability= 0.9999163

wave00000.general was created.gnuplot>
...
wave00010.dat was created.
WAVE function
  Max value=  1.522613
  Min value= -1.618646
  probability= 0.9998179

wave00010.general was created.
```

(2) Convert the potential energy surface (PES) data for OpenDX

```
cp ../POTENG ./ [Enter]
../../bin/poteng2dx [Enter]
```

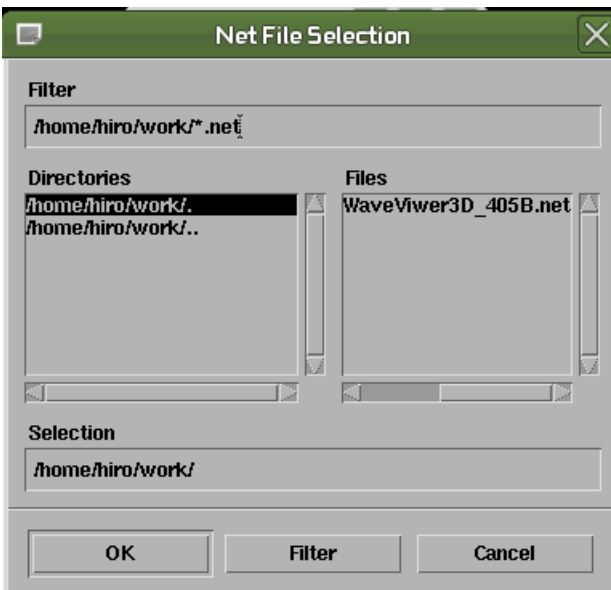
```
=====
POTDAT.cfg is not found.
Position origine is reset to
0.0000000E+00 0.0000000E+00 0.0000000E+00
=====
"PES3D.dat" file was created.
Umax=  1.393875
Umin= 0.0000000E+00
"PES3D.general" file was created.
```

(3) Execute the OpenDX

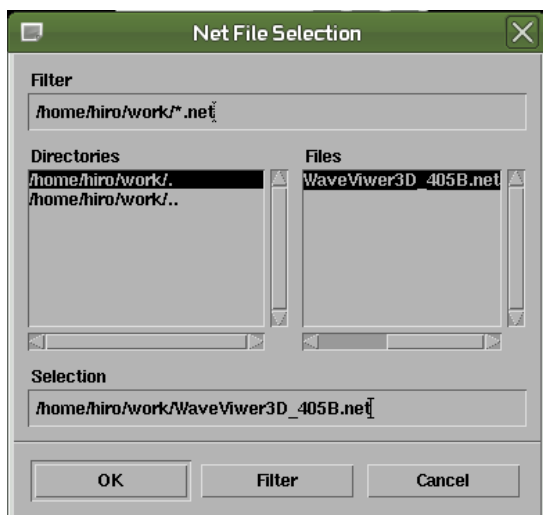
```
cp ../../etc/OpenDX/WaveViwer3D_405B* ./ [Enter]
dx [Enter]
```



Click "Run Visual Programs"



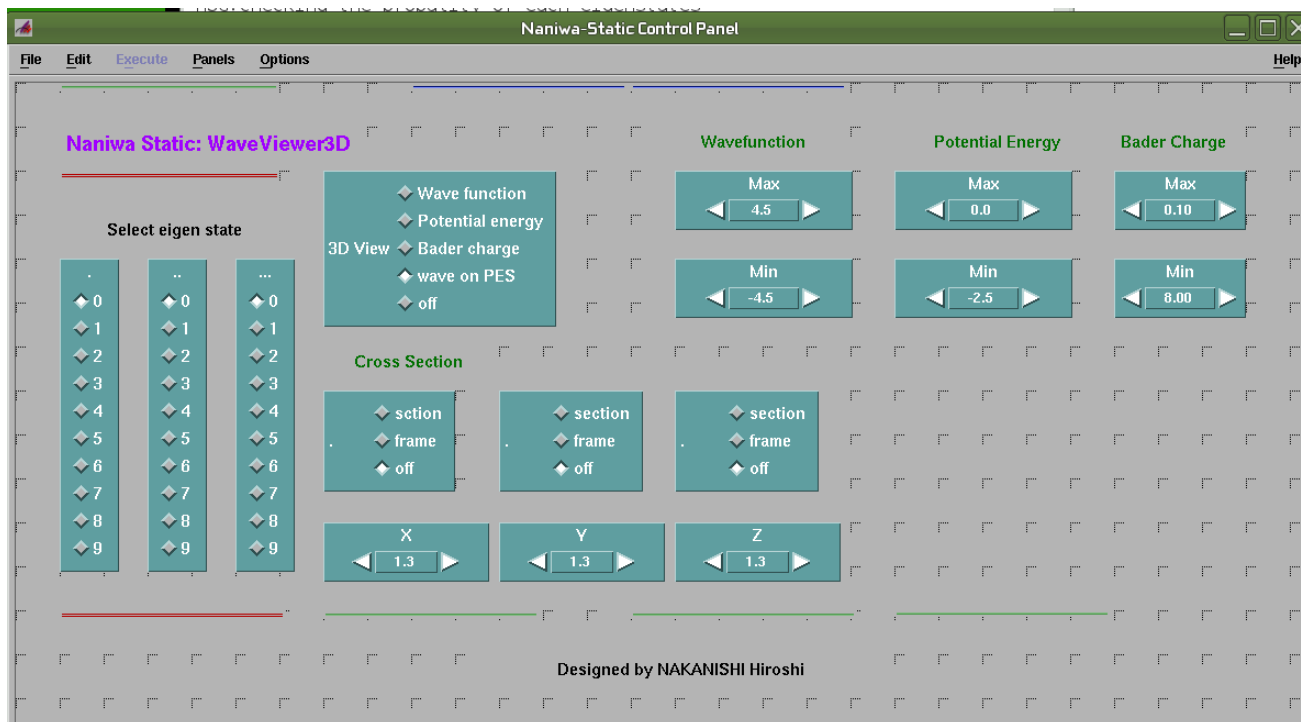
(4) Select the "WaveViewer3D_405B.net in right hand window.



Click “OK” button.

(5) Operate the “WaveViewer3D”,

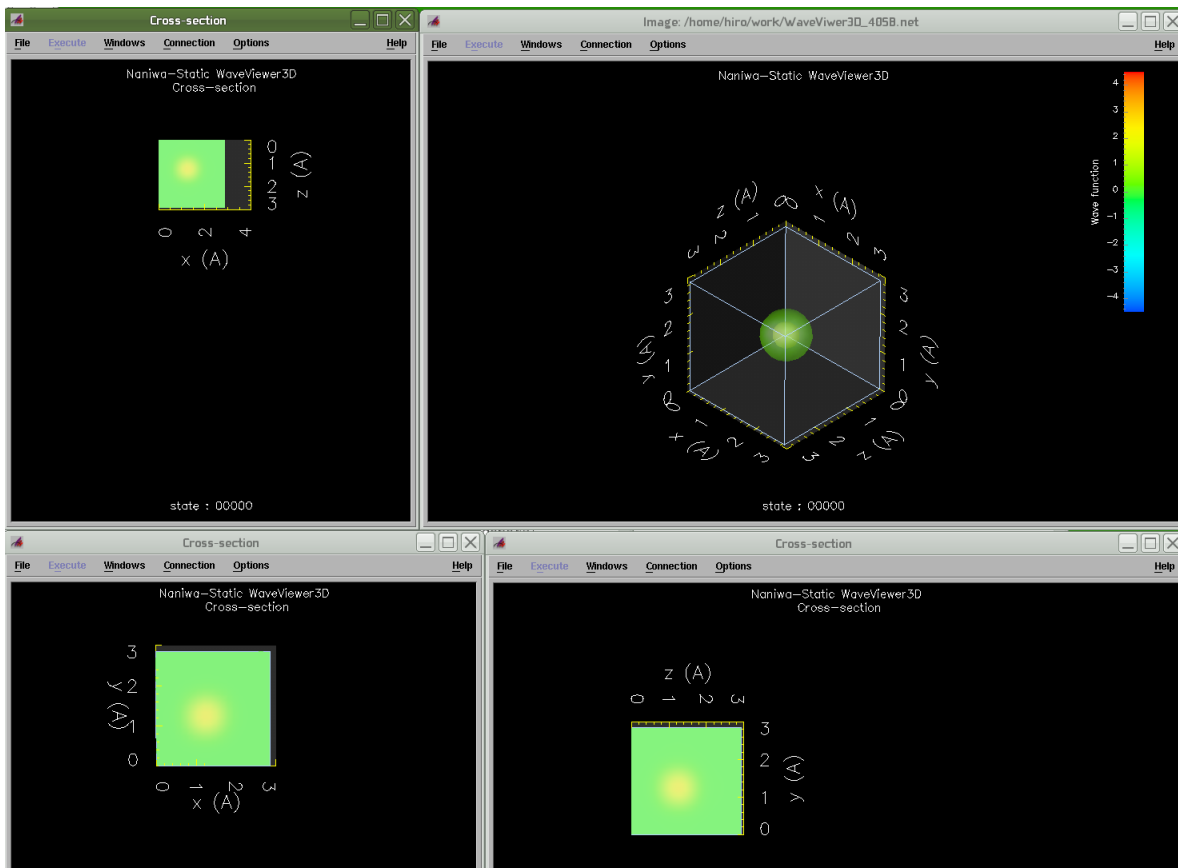
You can control it from Control panel.



(6) See the visualized results

You can see the 3-dimensional model in 4 Visualization windows;

top view, bird view, side view and bottom view.



(7) Quit the OpenDX



Click "Quit" button.

5.4.2.2 XcrySDen case

Naniwa package includes the Output file converter for XCrySDen.

(1) Convert the eigenstate data for XCrySDen.

Make the XCrySDen data from the ground state to 10th excited state.

```
cd ~/naniwa/work/test/kpoint0000 [Enter]
../../bin/state2xsf 0 10 [Enter]
```

```
stat2xsf
I create the files for XCrySDen from          0 to          10
-----
ERROR no INSET file :reset
n1 = 30
n2 = 30
n3 = 90
-----
=====
POTDAT.cfg is not found.
Position origine is reset to
  0.0000000E+00  0.0000000E+00  0.0000000E+00
=====
wave00000.xsf  was created.
WAVE function
  Max value=    2.18718407153673
  Min value= -4.841641351593371E-003
  probability=  0.999931342158014

wave00001.xsf  was created.
WAVE function
  Max value=    2.02312748202589
  Min value= -1.86989237272753
  probability=  0.999900567109712

wave00002.xsf  was created.
WAVE function
  Max value=    1.94090713382515
  Min value= -1.94489431345728
  probability=  0.999900392093716
```

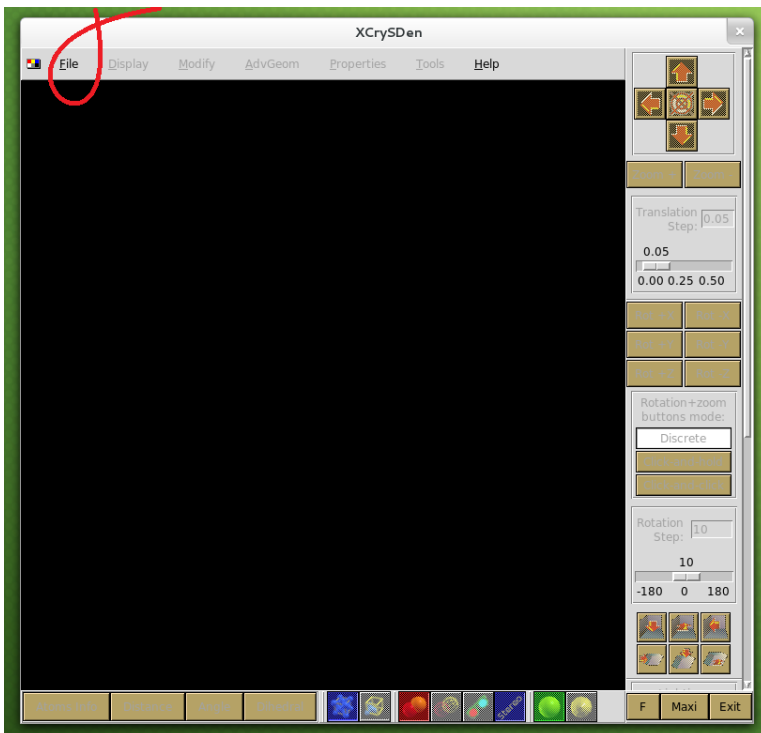
(2) Convert the potential energy surface (PES) data for XCrySDen

```
cp ../POTENG ./ [Enter]
cp ../INSET ./ [Enter]
../../bin/poteng2xsf [Enter]
```

```
*****
PES data  converter for XCrySDen
*****
"PES3D.xsf" file was created.
Umax=    1.393875
Umin=    0.0000000E+00
```

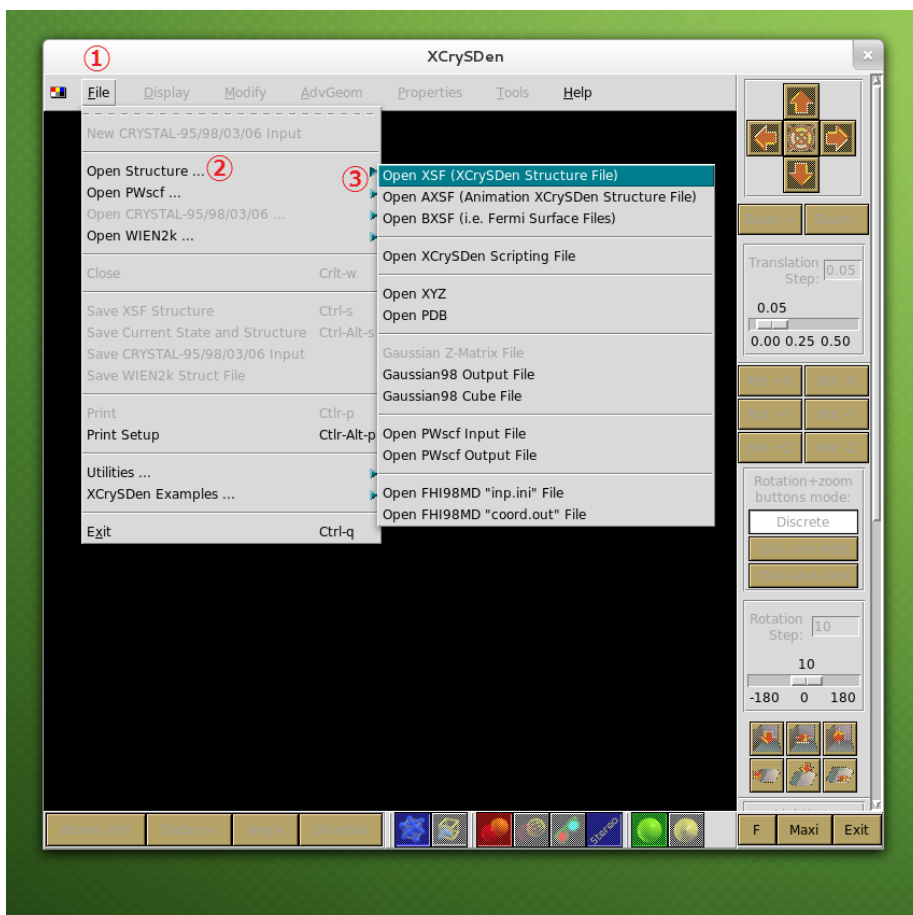
(3) Execute the XCrySDen

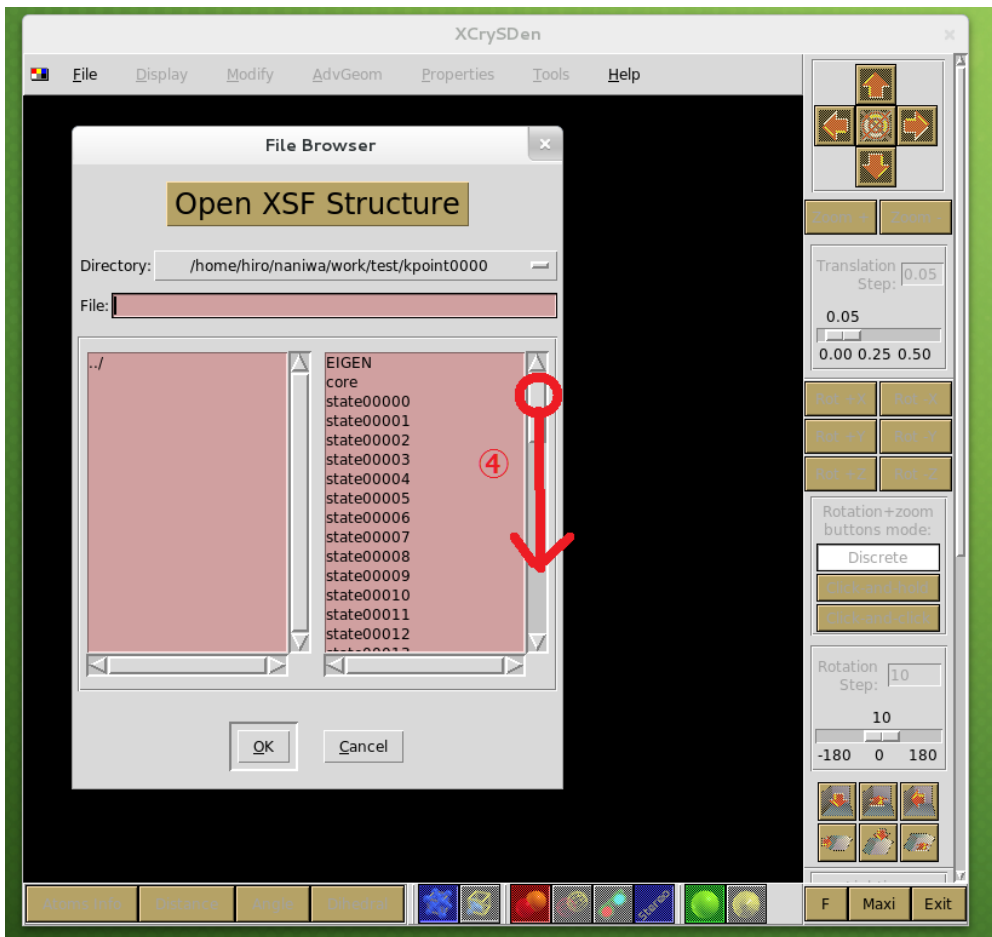
```
xcrysdn [Enter]
```

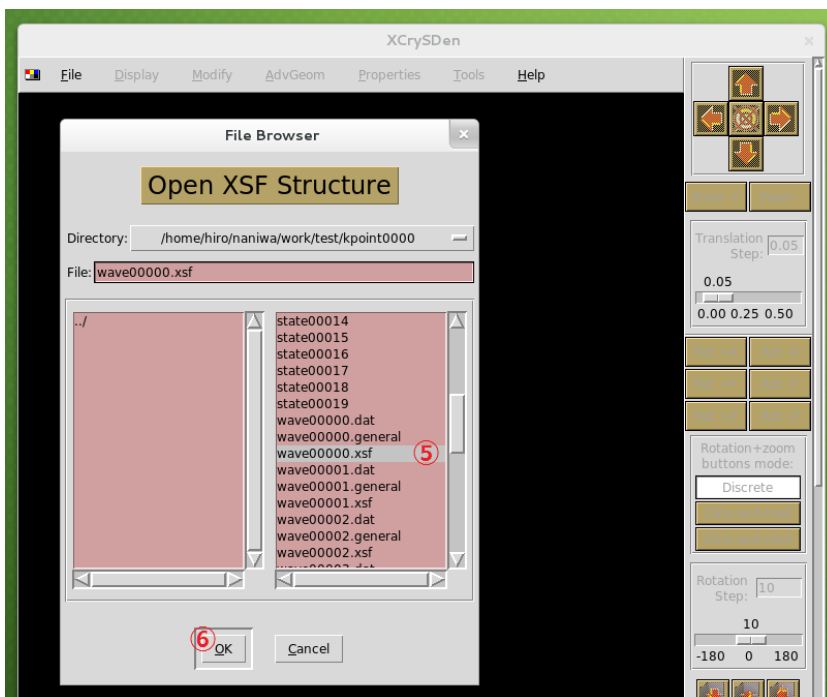
(4) Open the file wave00000.xsf

- ① Click "File"
- ② Click "Open Structure"
- ③ Click "Open XSF (XCrySDen Structure file)"





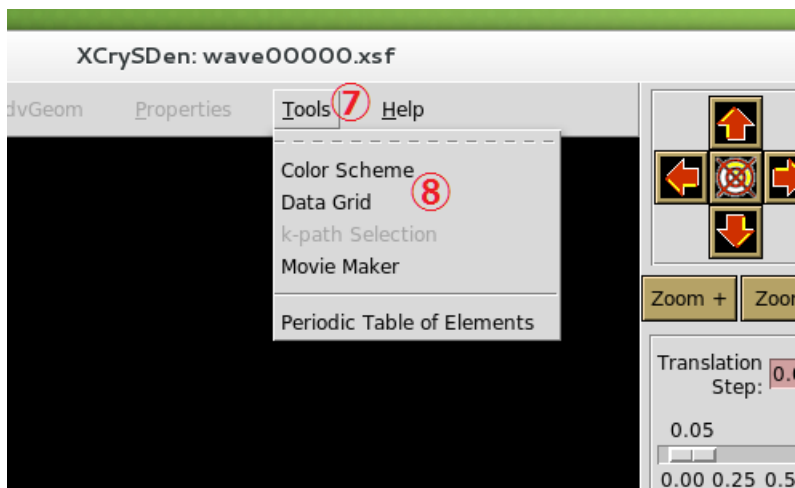
④ Drag down the thumb in 2nd vertical scrollbar.



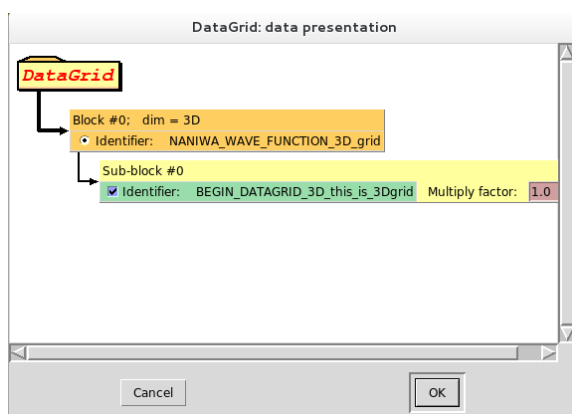
⑤ Select the file “wave00000.xsf”

⑥ Click “OK”

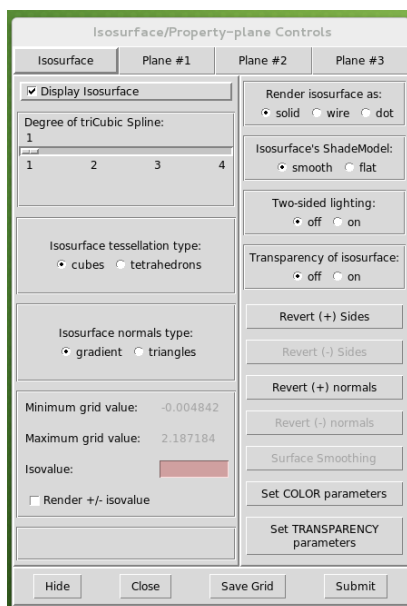
5) Set the view status.



⑦ Click “Tools” ⑧ Click “Data Grid”

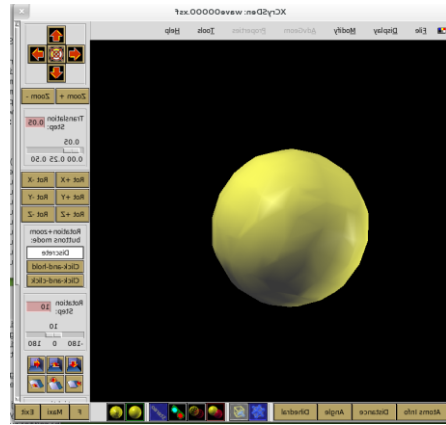
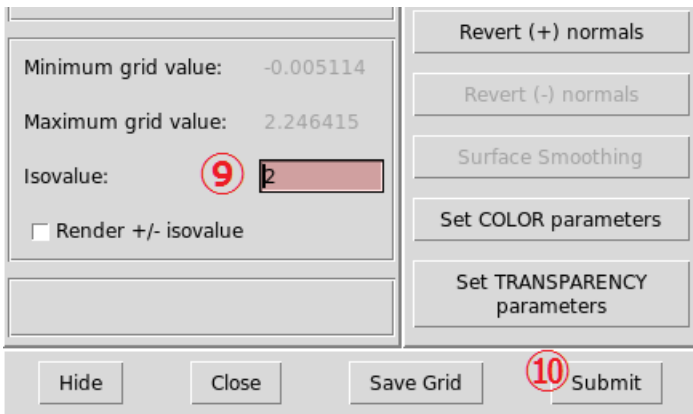


Click ”OK” button.

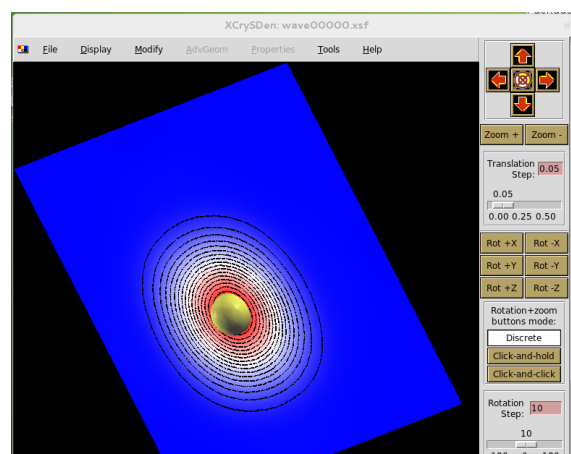
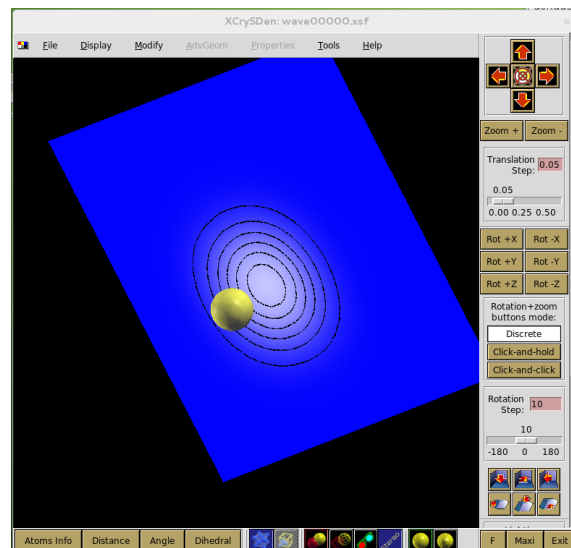
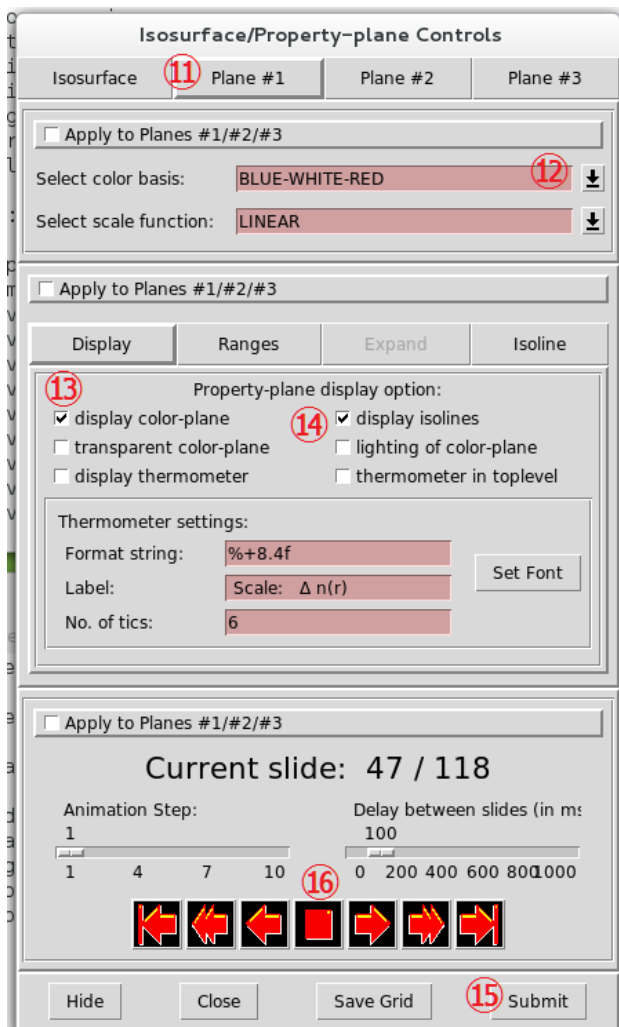


Then, you can see this “Isosurface/Property-plane Controls”

(6) Set adequate Isovalue ⑨ and click “Submit” button ⑩. You can see its isosurface,

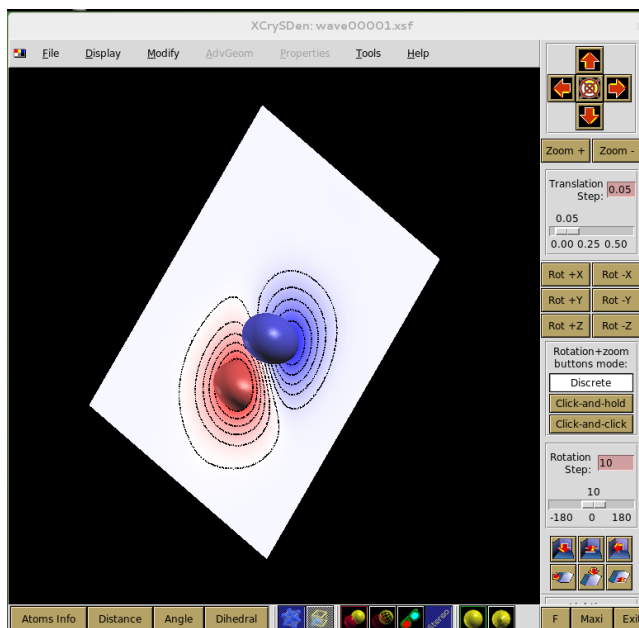
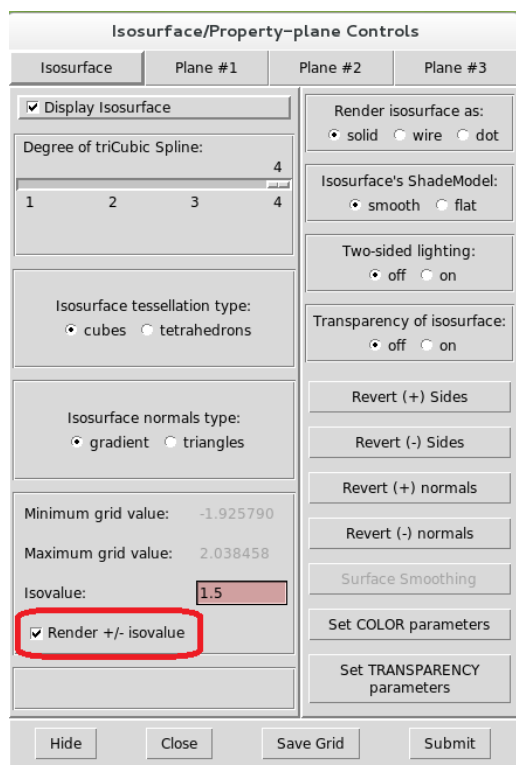


(7) Select “Plane #1” **11** and choose select color basis **12**. And check boxes of display color-plane **13** and display isolines **14**. Click submit button **15** and you can see the isoline on a cross section, which can be moved by arrows **16**.



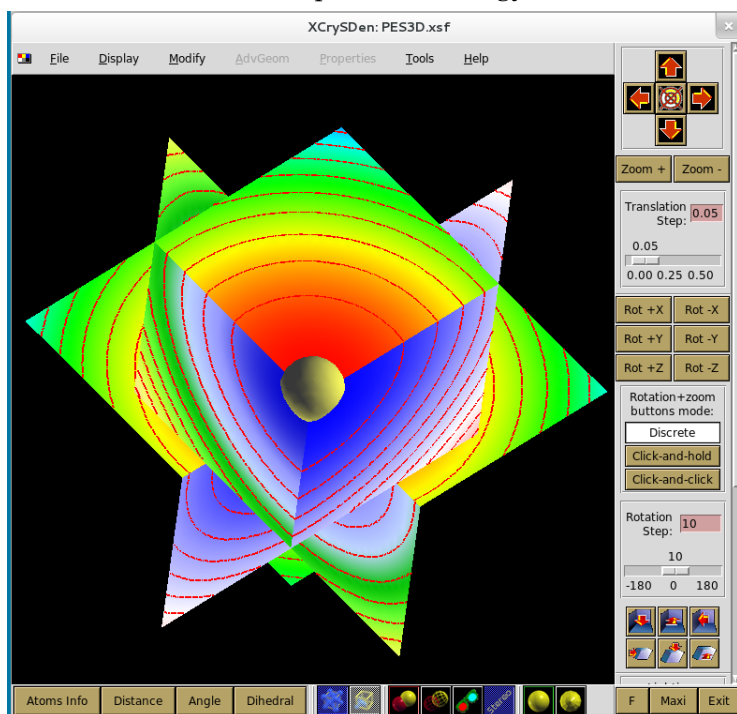
“wave00000.xsf” case

(8) You can also see the excited states whose wave function has node.



“wave00001.xsf” case

(6) You can also see the potential energy surface



“PES3D.xsf” case

(7) Quit the XCRYSDen

Click “File” and “Exit”

And click “Yes”

5.4.2.3 VESTA case

VESTA can read xsf files to show the wavefunctions

(1) Make xsf files.

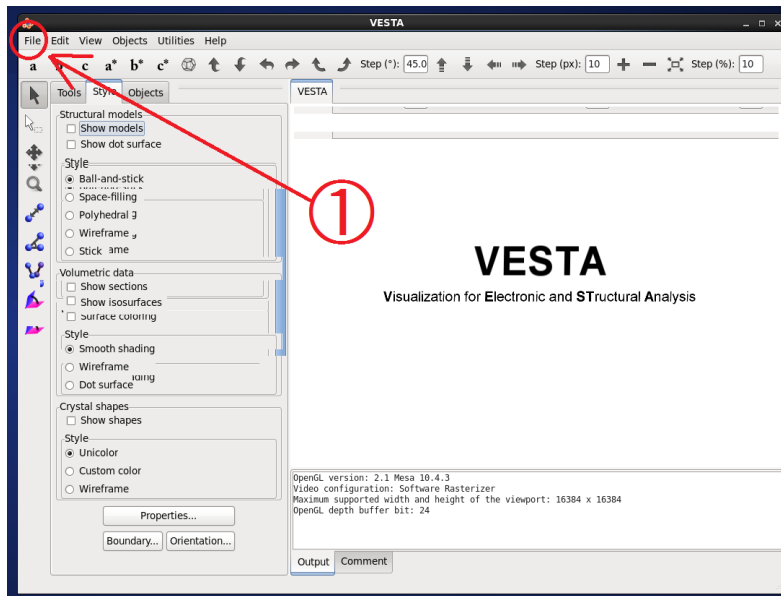
Do the same procedures from (1) to (2) in section 5.4.2.2.

(2) Execute the VESTA

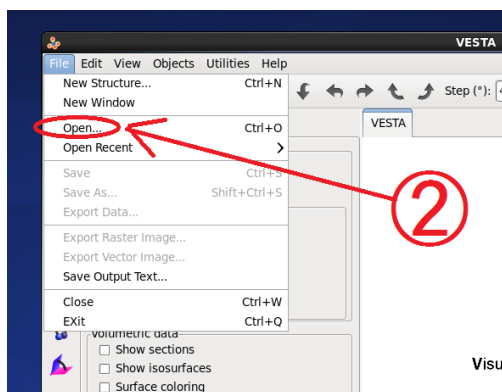
VESTA [Enter]

(3) Open the file wave00000.xsf

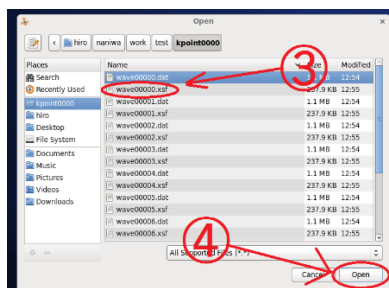
① Click “File”



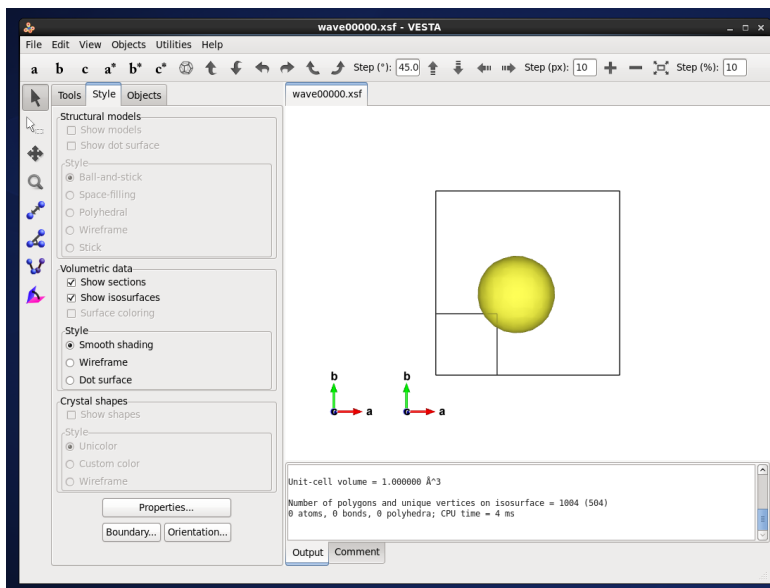
② Click “Open”



③ Select the file “wave00000.xsf” . ④ Click “OK”

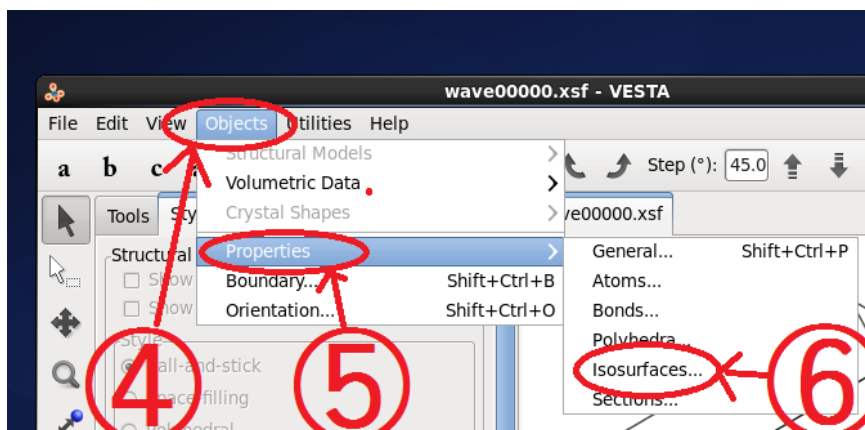


(4) You can see the ground state wave function.

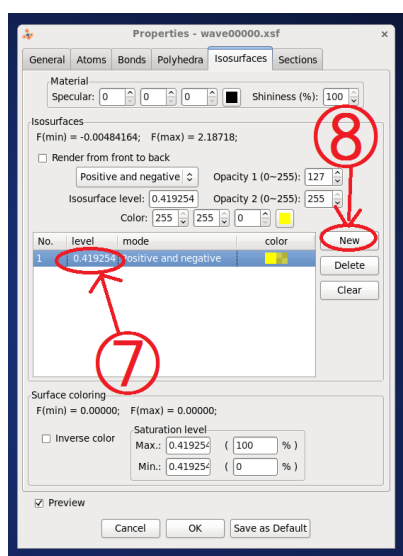


(5) You can control the setting of isosurface.

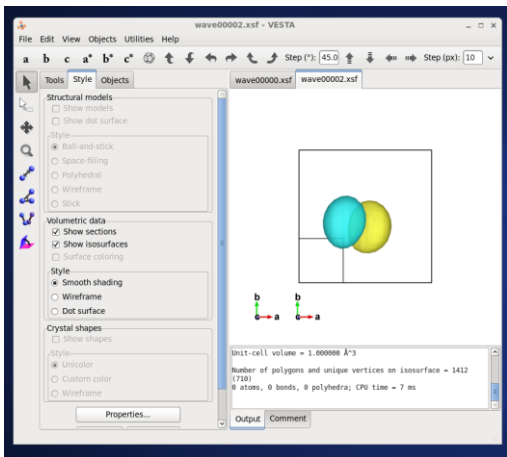
- ④ Click “Object” ⑤ Select “Property” ⑥ Click “Isosurface...”



⑦ You can change the level of isosurface and ⑧ add the other levels.



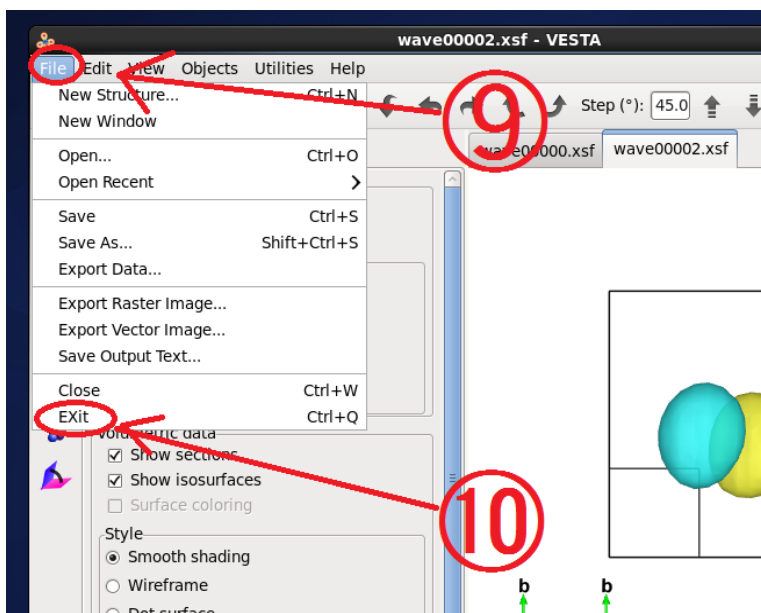
(6) You can also see the excited states whose wave function has node.



“wave00001.xsf” case

(7) Quit the VESTA

- ⑨ Click “File” and ⑩ “Exit”



References

- [1] Hideaki Kasai and Ayao Okiji, *Progress in Surface Science*, Vol. 44, No. 2, pp. 101-183 (1993).
- [2] Wilson Agerico Diño, Hideaki Kasai and Ayao Okiji, *Progress in Surface Science*, Vol. 63, No. 3-5, pp. 63-134 (2000).
- [3] Japanese Patent No. 4774523.
- [4] Japanese patent application 2012-16133.
- [5] Kunihiro Nobuhara, Hiroshi Nakanishi, Hideaki Kasai and Ayao Okiji, *Surface Science*, Vol. 493, No. 1-3, pp. 271-277 (2001).
- [6] Kunihiro Nobuhara, Hiroshi Nakanishi, Hideaki Kasai and Ayao Okiji, *Surface Science*, Vol. 493, No. 1-3, pp. 271-277 (2001).
- [7] Kunihiro Nobuhara, Hideaki Kasai, Hiroshi Nakanishi and Ayao Okiji, *Surface Science*, Vol. 507-510, pp. 82-86 (2002).
- [8] Kunihiro Nobuhara, Hideaki Kasai, Hiroshi Nakanishi and Ayao Okiji, *Journal of Applied Physics* Vol. 92, No. 10, pp. 5704-5706 (2002).
- [9] Kunihiro Nobuhara, Hideaki Kasai, Hiroshi Nakanishi and Wilson Agerico Diño, *Journal of Applied Physics* Vol. 96, No. 9, pp. 5020-5025 (2004).
- [10] Nobuki Ozawa, Tanglaw Abat Roman, Hiroshi Nakanishi, Hideaki Kasai, *Surface Science*, Vol. 600, No. 18, pp. 3550-3554 (2006).
- [11] Tanglaw Roman, Wilson Agerico Diño, Hiroshi Nakanishi, Hideaki Kasai, *e-Journal of Surface Science and Nanotechnology*, Vol. 4, pp. 619-623 (2006).
- [12] Nobuki Ozawa, Tanglaw Roman, Hiroshi Nakanishi, Wilson Agerico Diño, Hideaki Kasai, *Physical Review B* Vol.75, No.11, pp. 115421 (2007).
- [13] Nobuki Ozawa, Tanglaw Roman, Nelson Buntimil Arboleda Jr., Wilson Agerico Diño, Hiroshi Nakanishi, Hideaki Kasai, *Journal of Physics: Condensed Matter*, Vol. 19, No. 48, pp. 365214 (2007).
- [14] Nobuki Ozawa, Nelson Buntimil Arboleda Jr., Hiroshi Nakanishi, Hideaki Kasai, *Surface Science*, Vol. 602, No. 4, pp. 859-863 (2008).
- [15] Nobuki Ozawa, Nelson Buntimil Arboleda Jr., Hiroshi Nakanishi, Nobuaki, Shimoji, Hideaki Kasai, *Surface and Interface Analysis*, Vol. 40, Issue 6-7, pp. 1108-1112 (2008).
- [16] <https://software.intel.com/en-us/intel-parallel-studio-xe>
- [17] <https://software.intel.com/en-us/intel-mkl>
Intel-MKL is included in Intel-Composer-XE [16]
- [18] <http://www.gnuplot.info/>
- [19] <http://www.opendx.org/> (dead link)
- [20] <http://www.xcrysden.org/>
- [21] <http://jp-minerals.org/vesta/en/>

Appendix

A Porting

Naniwa standard version uses the following system-dependent subroutines.

- (1) Intel Fortran built-in subroutine: SYSTEM
- (2) Lapack subroutine: ZHEGV
- (3) Intel MKL procedure: MKL_DFTI

If you want to port Naniwa to other system, you must replace these routines. Please rewrite the (1) UNIXcommand_intel.f, (2) diagonalize_lapack.f and (3) fastDFT3D_MKL.f in SRC directory.

And also you must replace Fortran compiler name and its options.

These are defined in Makefile

```
##      for intel FORTRAN & MKL
##
#
ASR = diagonalize_lapack.f  UNIXcommand_intel.f  fastDFT3D_MKL.f
LIB = /opt/intel/mkl/lib/intel64
INC = -I/opt/intel/mkl/include

##Compiler name and option
FC = ifort
OPT = -O3 -mkl -lpthread
```

A-1. Porting to Hitachi SR16000 with optimized FORTRAN90, MATRIX/MPP and LAPACK

We provide the necessary interface to Hitachi SR16000. You only have to modify the following parts in Makefile.

Comment out part:

```
##      for intel FORTRAN & MKL
##
#
#ASR = diagonalize_lapack.f  UNIXcommand_intel.f  fastDFT3D_MKL.f
#LIB = /opt/intel/mkl/lib/intel64
#INC = -I/opt/intel/mkl/include

##Compiler name and option
#FC = ifort
#OPT = -O3 -mkl -lpthread
```

Please insert mentioned-above red # in Makefile.

Uncommented part:

```

#*      for Hitachi Optimizing FORTRAN90
#*          LAPACK  & MATRIX/MPP
#*
#*          KEK SYSTEM A
#*
#ASR = diagonalize_lapack.f UNIXcommand_hitachi.f fastDFT3D_MPP.f
#LIB = /opt/hitachi/matmpp/lib -lmatmpp -L/srhome/.tools/lib -llapack_sc -lblas_sc
#INC =

#* Compiler name and option
#FC = f90
#OPT = -Os -64 -model=M1 -parallel

```

Please remove the mentioned-above blue # in Makefile.

These procedure replaces SYSTEM and MKL_DFTI to HF_SH and HZFT6M. Later subroutine restricts the value of n_1, n_2, n_3 in POTENG. These integer values must be not less than 8 and power of 2. Please see the naniwa/etc/example/testSR.

B Making 3D-potential energy surface by VASP

example: H in Si bulk

See the directory: `~/naniwa/etc/potentials/SiBulk`

under `~/naniwa/etc/potentials/SiBulk`

host : getting the total energy of host material without hydrogen atom

particle: getting the total energy of hydrogen atom without host material

scan: getting the total energy in the case of hydrogen atom in host material as a function of hydrogen atom position

(1) `cd ~/naniwa/etc/potentials/SiBulk/host/`

`qsub run.csh`

After the calculation, getting the energy `E_host` from last `E0` value in `OSZCAR`

(2) `cd ~/naniwa/etc/potentials/SiBulk/particle/`

`qsub run.csh`

After the calculation, getting the energy `E_particle` from last `E0` value in `OSZCAR`

(3) `cd ~/naniwa/etc/potentials/SiBulk/scan/`

`csh ./auto.csh`

After all calculations, ..

`csh ./collect.csh`

`cp POTDAT ./POTDAT2POTENG`

`cd ./POTDAT2POTENG`

`ifort makePOTENG.f -o makePOTENG`

`vi POTDAT.cfg`

Edit the configuration file: `POTDAT.cfg`

input the value of `E_host` and `E_particle` into this file

```
*title: Potential energy for H in Si bulk
*lattice information
3.83958982184
1.00000000000 0.0 0.0
0.50000000000 0.86602540378 0.0
0.50000000000 0.28867513459 0.81649658092
* data mesh numbers
20 20 20
*origine of positioni (fractional)
0.00000000 0.00000000 0.00000000
*isolated particle energy (eV)
-.11089857E+01
*isolated slab (host) energy (eV)
-.86414775E+02
*cut of energy (eV)
2.00
```

`./makePOTENG`

Then you can obtain the `POTENG` file

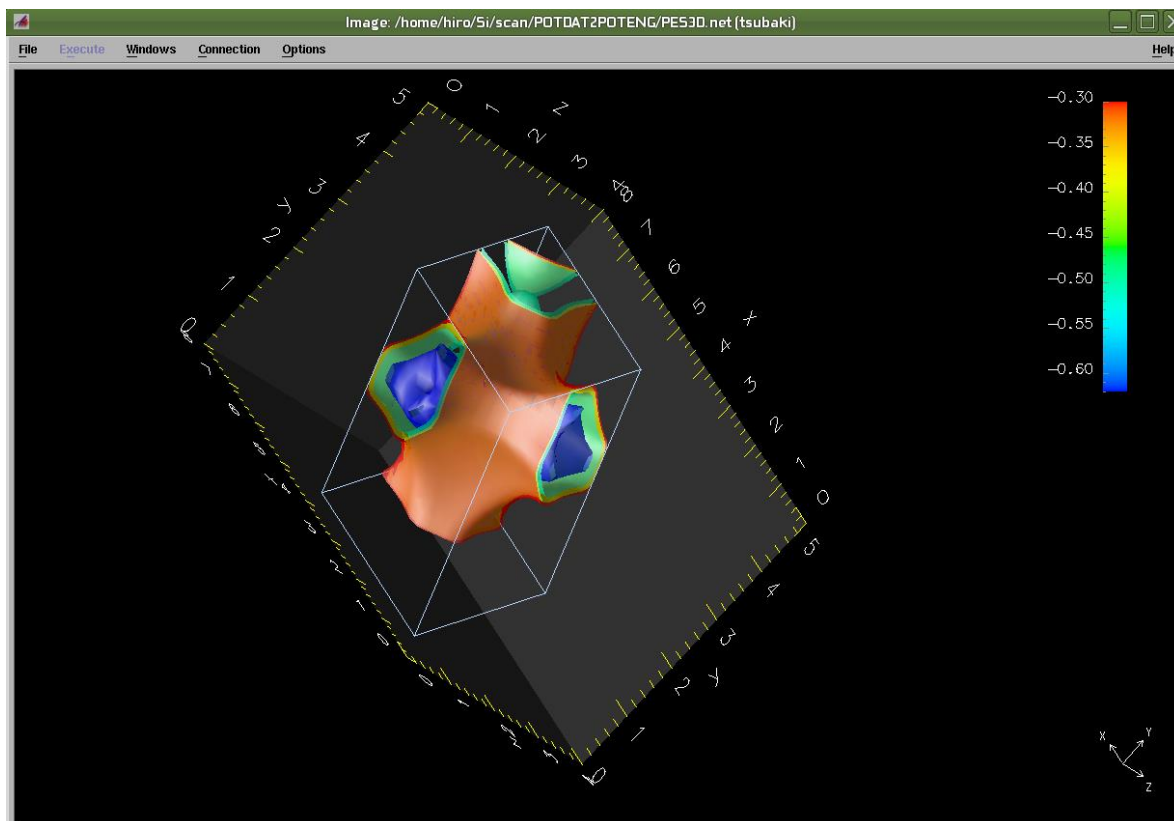
For checking the POTENG file.

```
ifort POTENG2DX.f -o POTENG2DX
dx
```

Click “Run Visual Programs”

Select the “PES3D.net in right hand winodw.

Click “OK” button.

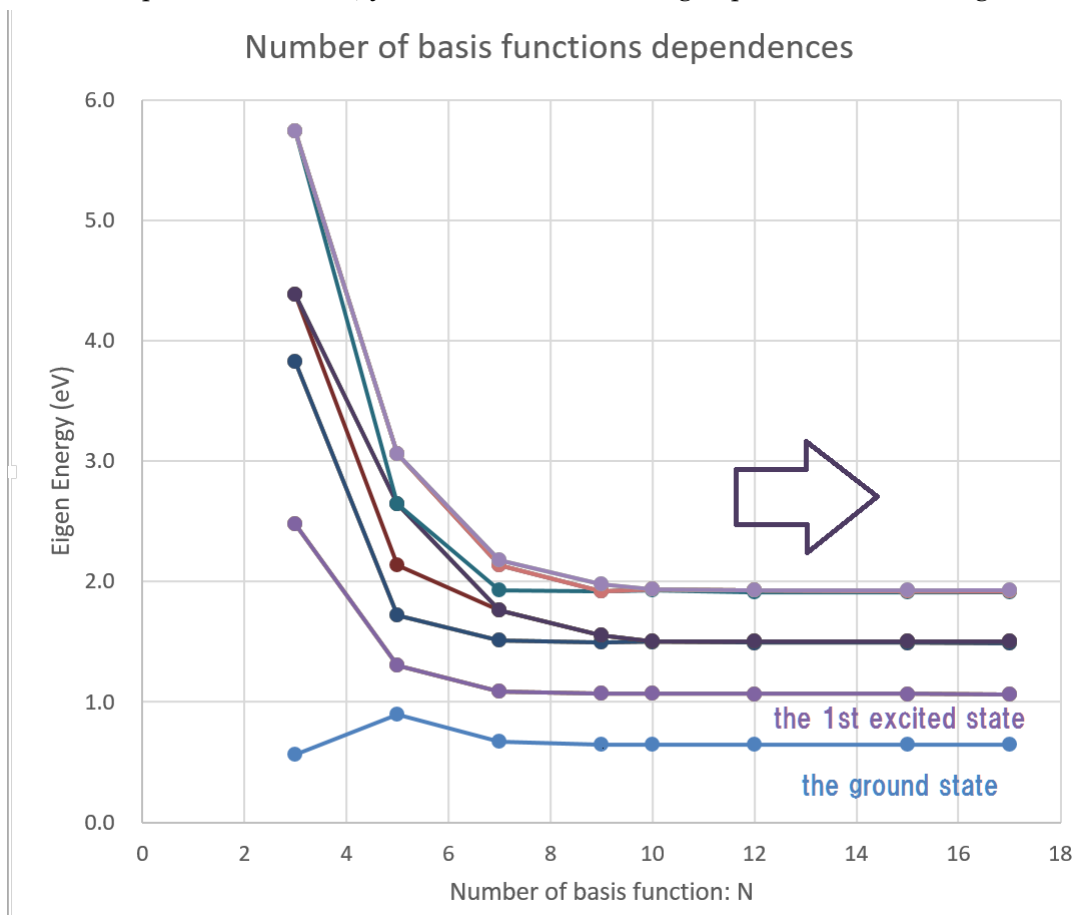


C Required parameters for convergence

In order to get the reliable results, you should try the various parameters and check the convergence of their results.

C.1 Number of nodes for the 3D Gaussian functions

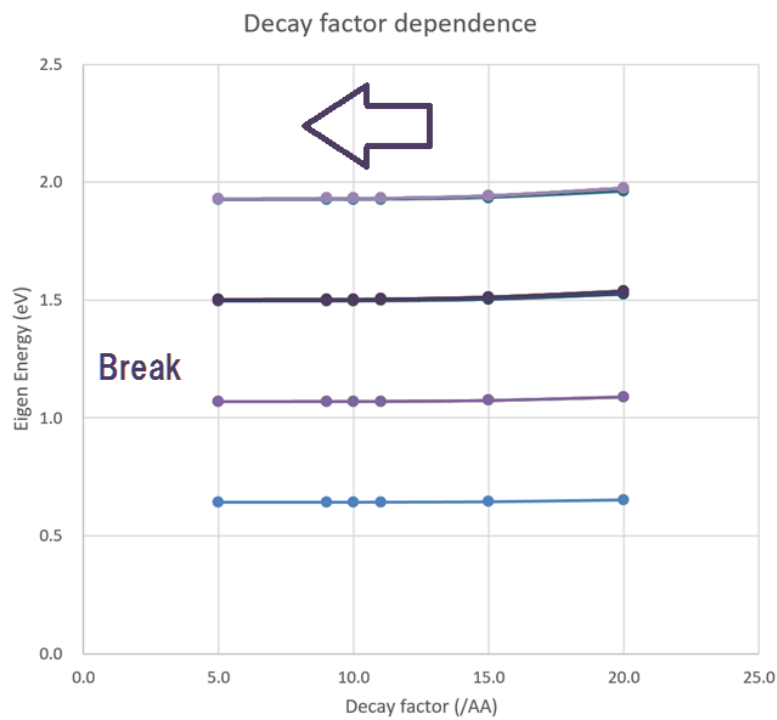
Here we show the Eigenenergy convergency as a function of the number of nodes for the 3D Gaussian functions. When only the number of the nodes are changed in the test program: naniwa/etc/example/Harmonic3D, you can see the following dependences in the figure.



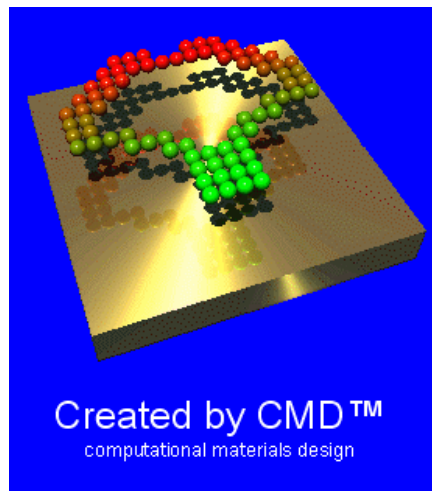
As the numbers of the grid increase, the eigen energies converge and you can get reliable results.

C.2 Gaussian decay factor (SigmaX, SigmaY SigmaZ)

Here we show the Eigenenergy convergency as a function of the decay factor of basis Gaussian functions. When only the decay factors are changed in the test program: naniwa/etc/example/Harmonic3D with fixed numbers of the grids: 10x10x10, you can see the following dependences in the figure.



As the decay factors decrease, the calculated Eigen energies converge, and you can get reliable results. But the decay factors decrease less than certain value, the calculations are suddenly broken. You must also check their wave function shapes.



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