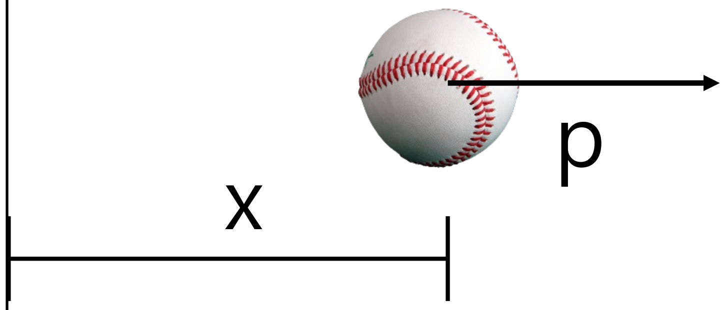
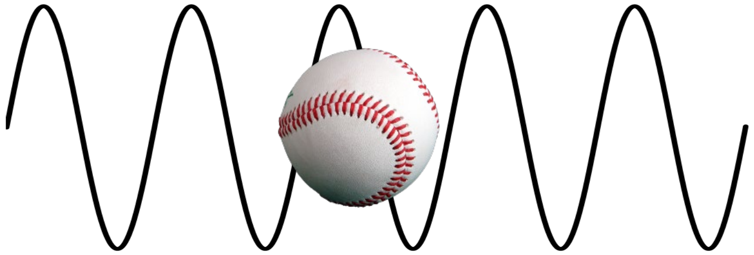
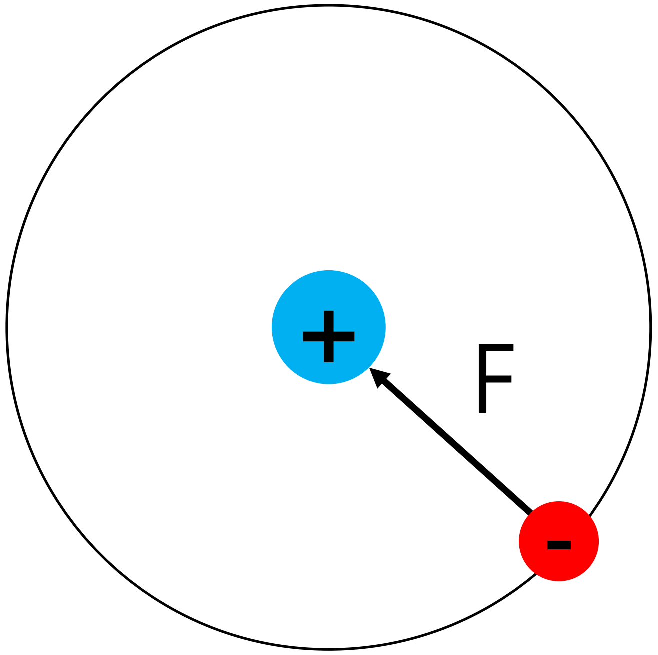
Experiment 3.
Quantum Chemical Calculation:
The Potential Energy Curve and the Orbitals of H_2^+

Theory

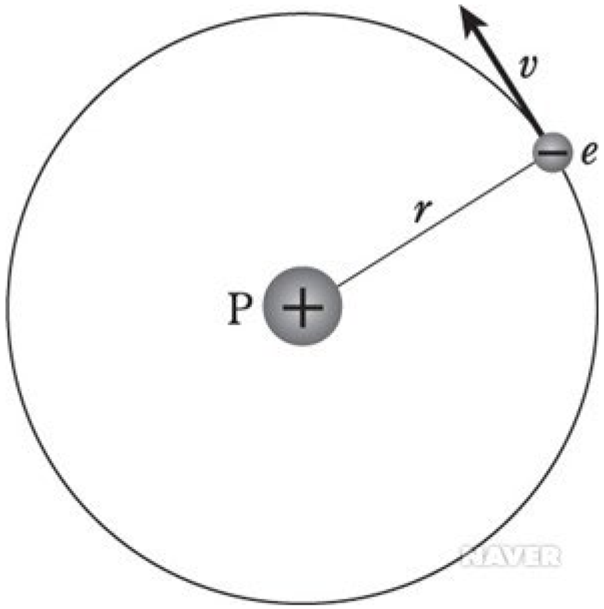
Classical vs Quantum

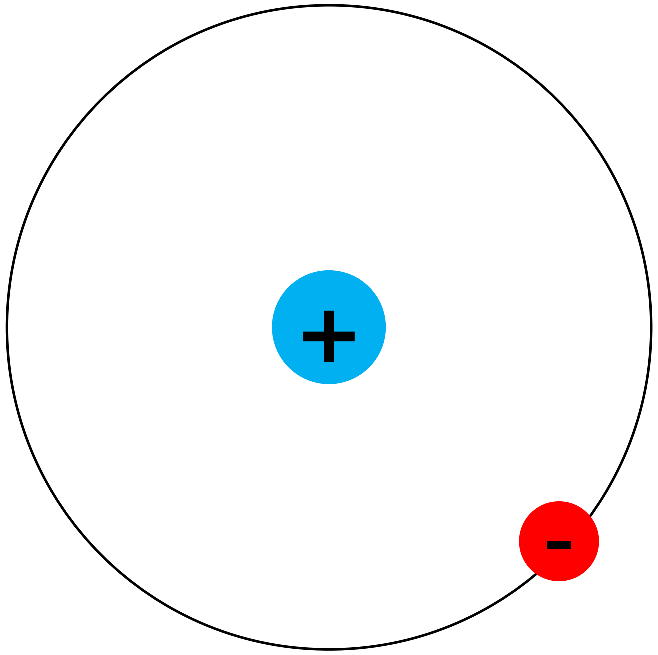
	Classical Mechanics	**Quantum Mechanics**
		
Description of particles	A particle is described as displacement (x) and momentum (p)	A particle is described as wave function ψ(x), square as its probability distribution and energy (E)
Governing equation	Newton Equation (Equation of motion) $F = ma$	Schrödinger Equation $\hat{H}\psi = E\psi$

Example: Hydrogen like Atom



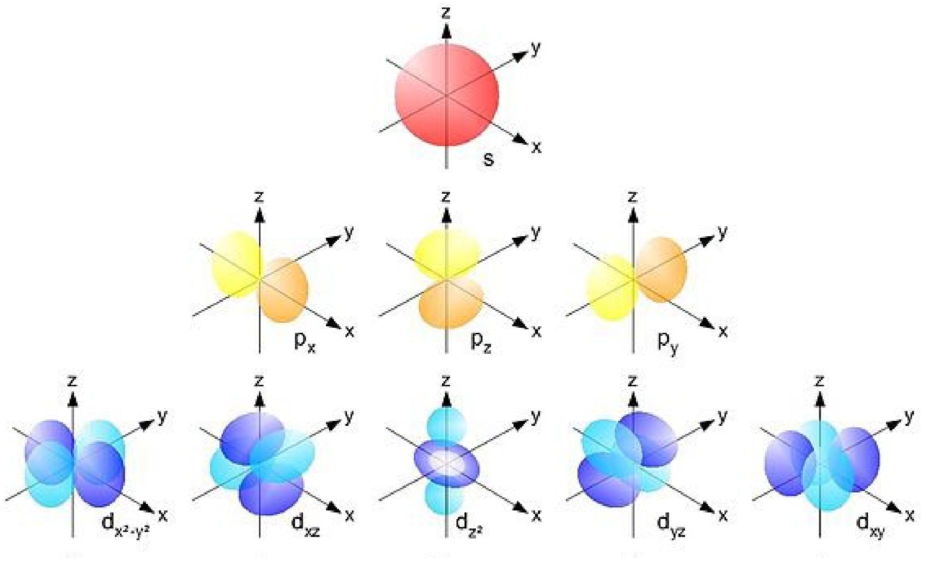
$$F = ma = \frac{Ze^2}{4\pi\epsilon_0 r^2}$$





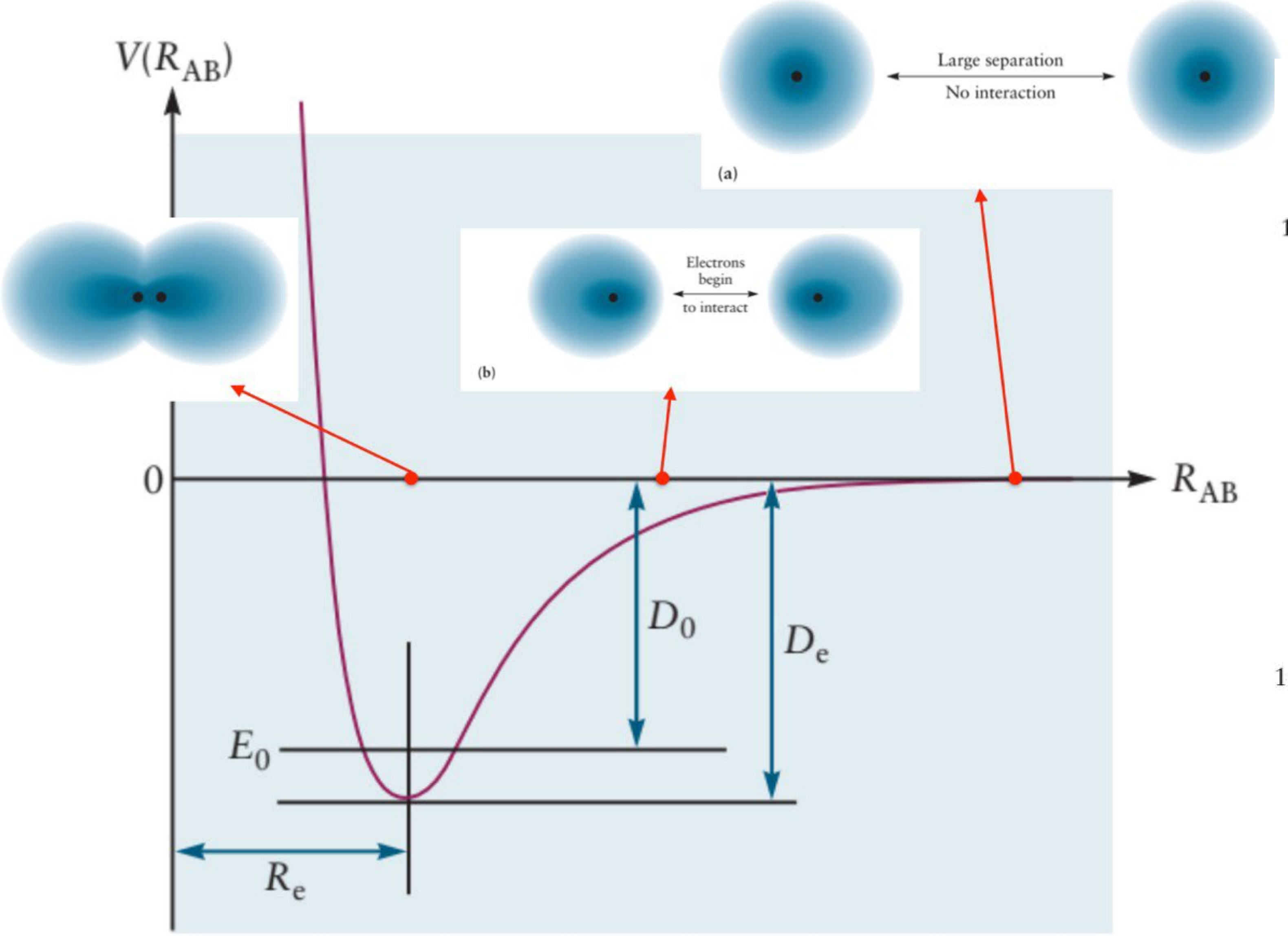
$$V(r) = -\frac{Ze^2}{4\pi\epsilon_0 r}$$

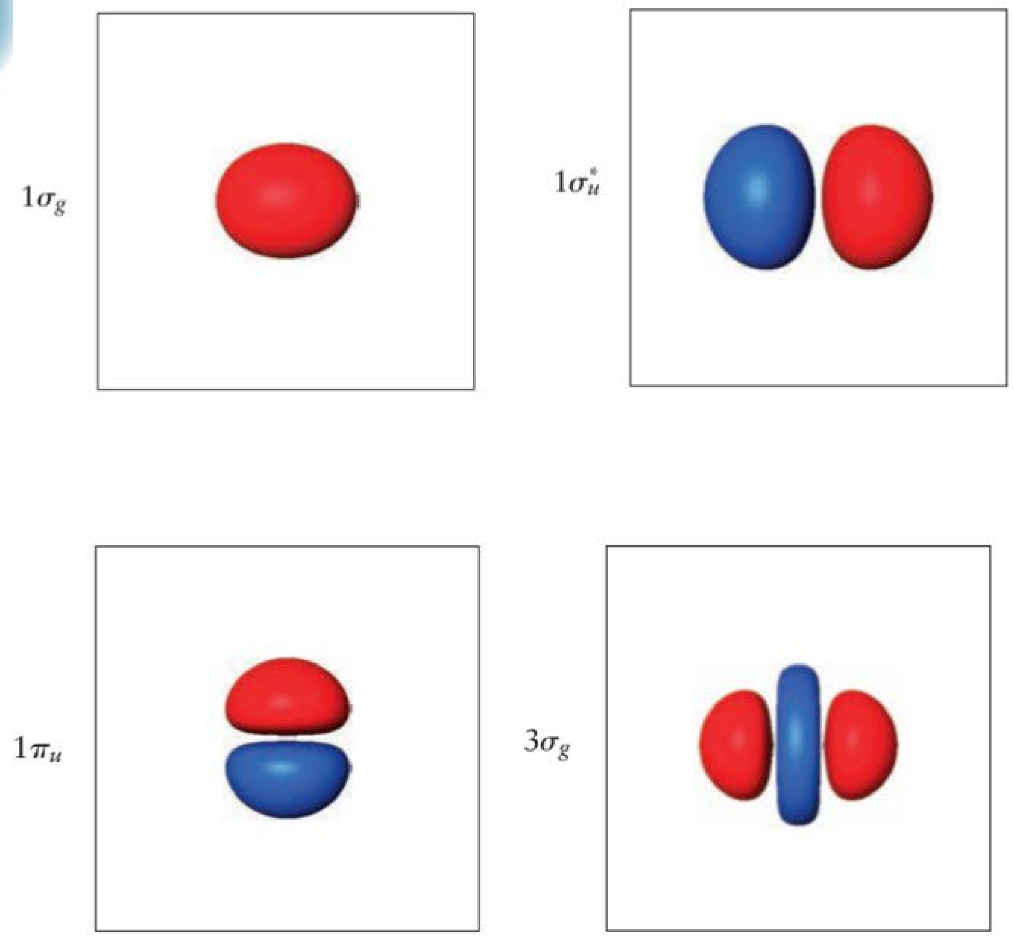
$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(r)\psi = E\psi$$



Goal of the experiment

Schrödinger Equation : $\hat{H}\psi = E\psi$





Schrödinger equation

$$\hat{H}\psi = E\psi$$

Hamiltonian

wave function

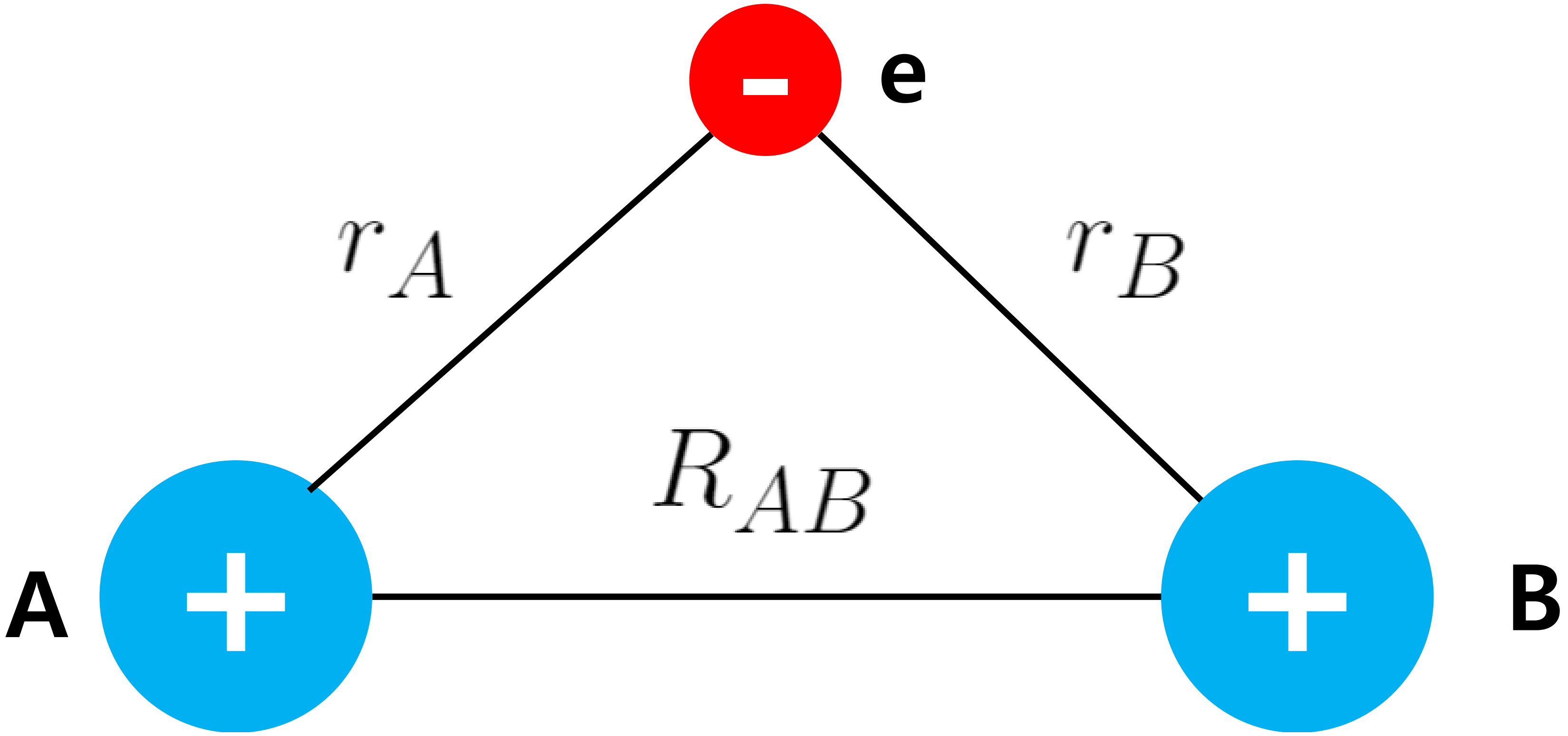
Energy of the state

- Hamiltonian: the operator corresponding to the total energy of a system.

$$\hat{H} = -\sum_{i=1}^{N} \frac{\hbar^2}{2m_i}\nabla_i^2 + \enclose{circle}{V}$$

Potential energy

Schrödinger equation for H_2^+



$$V = -\frac{e^2}{4\pi\epsilon_0 r_A} - \frac{e^2}{4\pi\epsilon_0 r_B} + \frac{e^2}{4\pi\epsilon_0 R_{AB}}$$

$$\hat{H} = -\frac{\hbar^2}{2m_{\mathrm{N}}}(\nabla_A^2\psi + \nabla_B^2\psi) - \frac{\hbar^2}{2m_e}\nabla_e^2\psi + V\psi = E\psi$$

Solving the Schrödinger equation

Born-Oppenheimer approximation:

- Motion of electron is much faster than the motion of nucleus ($m_{nuc} \approx 1820 m_{elec} >>>> m_{elec}$)
- Regard the positions of nuclei as fixed -> Only consider electron wave function
- Since nucleus is fixed, we cannot differentiate

$$\hat{H} = -\sum_{i=1}^{N_{\mathrm{nuc}}} \cancel{\frac{\hbar^2}{2m_{N_i}}\nabla_i^2} - \sum_{j=1}^{N_{\mathrm{elec}}} \frac{\hbar^2}{2m_{e_j}}\nabla_j^2 + V$$

H_2^+ molecule $$\hat{H} \simeq -\frac{\hbar^2}{2m_e}\nabla_e^2 - \frac{e^2}{4\pi\epsilon_0 r_A} - \frac{e^2}{4\pi\epsilon_0 r_B} + \frac{e^2}{4\pi\epsilon_0 R_{AB}}$$

Solving the Schrödinger equation

1. Fix the positions of the nuclei (i.e., fix R_{AB}) and solve the Schrödinger equation for the electronic Hamiltonian $\hat{H}^{elec}(R_{AB})$.

$$\hat{H} \simeq \underbrace{\boxed{-\frac{\hbar^2}{2m_e}\nabla_e^2 - \frac{e^2}{4\pi\epsilon_0 r_A} - \frac{e^2}{4\pi\epsilon_0 r_B}}}_{\hat{H}^{elec}(R_{AB})} + \underbrace{\boxed{\frac{e^2}{4\pi\epsilon_0 R_{AB}}}}_{V_{nn}(R_{AB})}$$

$$\hat{H}^{elec}(R_{AB})\psi = E\psi \xrightarrow{\qquad\qquad} \epsilon_0^{elec}(R_{AB}), \epsilon_1^{elec}(R_{AB}), \epsilon_2^{elec}(R_{AB}), \ldots$$

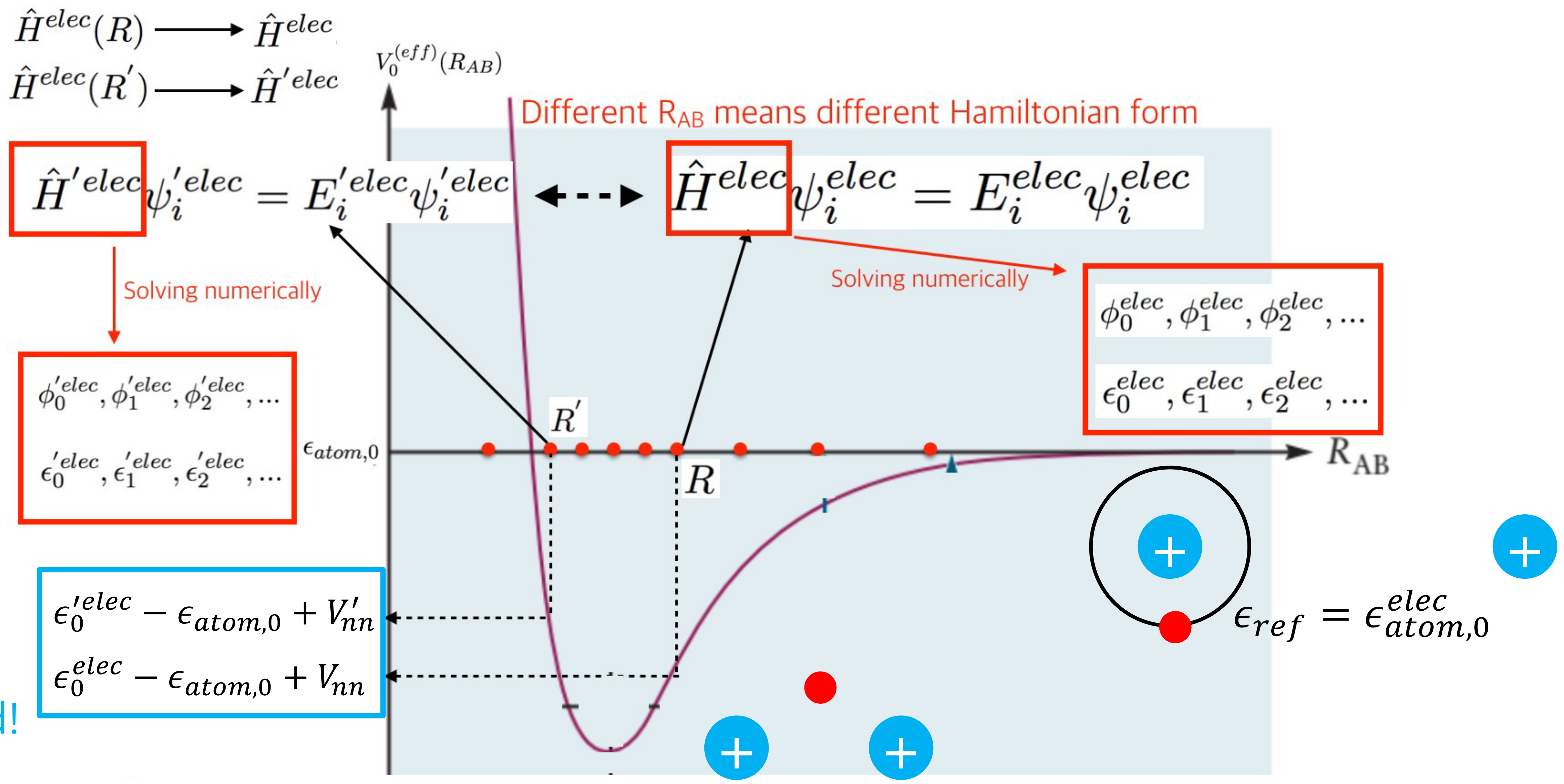
2. For actual energy, add the nuclear-nuclear potential energy $V_{nn}(R_{AB})$.

$$V_i^{(eff)}(R_{AB}) = \epsilon_i^{elec}(R_{AB}) + V_{nn}(R_{AB})$$

"Effective" potential

Solving the Schrödinger equation

3. To obtain potential energy curve, we must consider subtracted energy: $\epsilon_0^{elec}(R_{AB}) - \epsilon_{atom,0}^{elec} + V_{nn}(R_{AB})$



$\hat{H}^{elec}(R) \longrightarrow \hat{H}^{elec}$

$\hat{H}^{elec}(R') \longrightarrow \hat{H}'^{elec}$

Different R_{AB} means different Hamiltonian form

$\hat{H}'^{elec}\psi_i'^{elec} = E_i'^{elec}\psi_i'^{elec}$ ⟵ ⟶ $\hat{H}^{elec}\psi_i^{elec} = E_i^{elec}\psi_i^{elec}$

Solving numerically

$\phi_0'^{elec}, \phi_1'^{elec}, \phi_2'^{elec}, \ldots$

$\epsilon_0'^{elec}, \epsilon_1'^{elec}, \epsilon_2'^{elec}, \ldots$

Solving numerically

$\phi_0^{elec}, \phi_1^{elec}, \phi_2^{elec}, \ldots$

$\epsilon_0^{elec}, \epsilon_1^{elec}, \epsilon_2^{elec}, \ldots$

$\epsilon_{ref} = \epsilon_{atom,0}^{elec}$

Final results that are required!

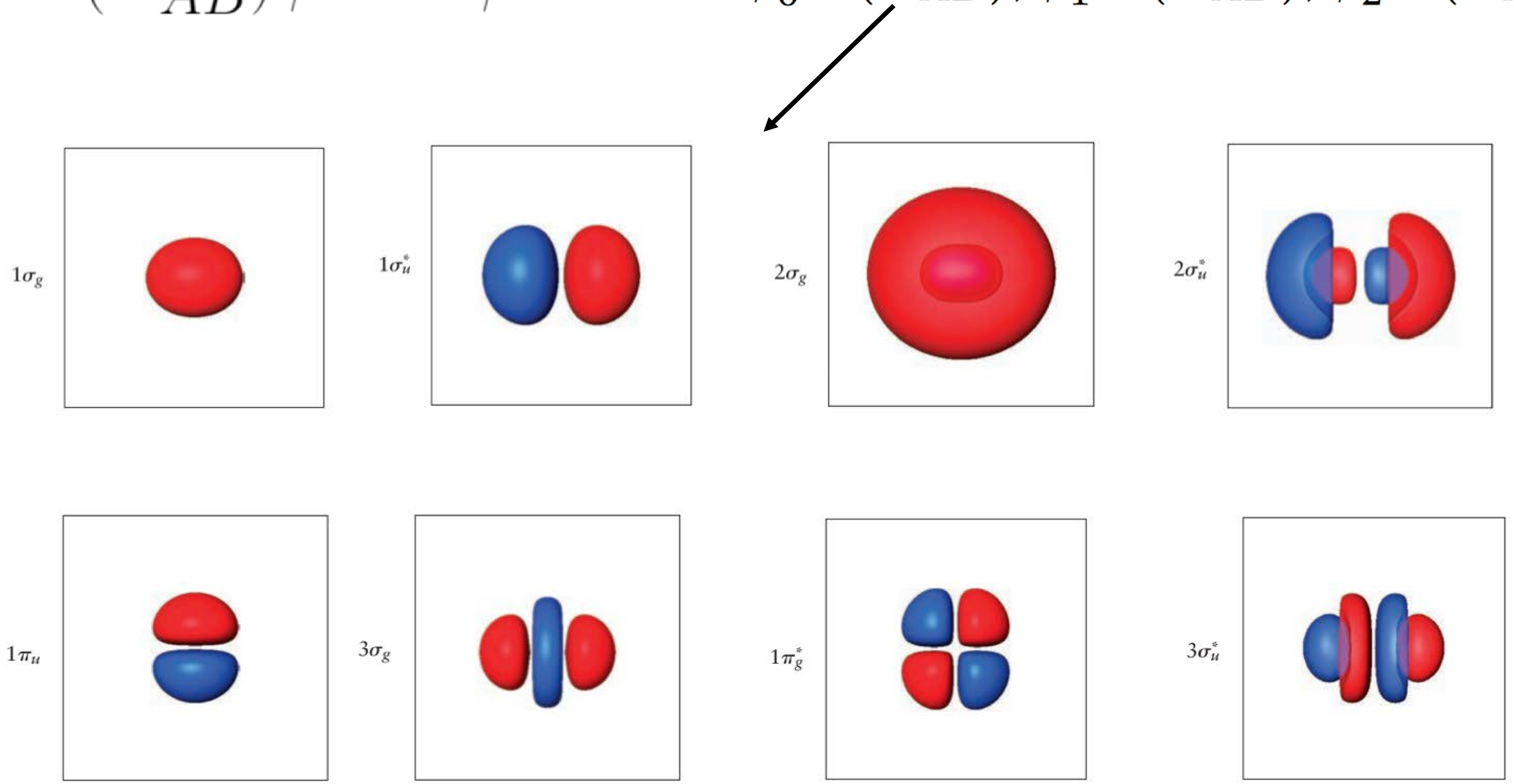
$\epsilon_0'^{elec} - \epsilon_{atom,0} + V_{nn}'$

$\epsilon_0^{elec} - \epsilon_{atom,0} + V_{nn}$

Orbitals

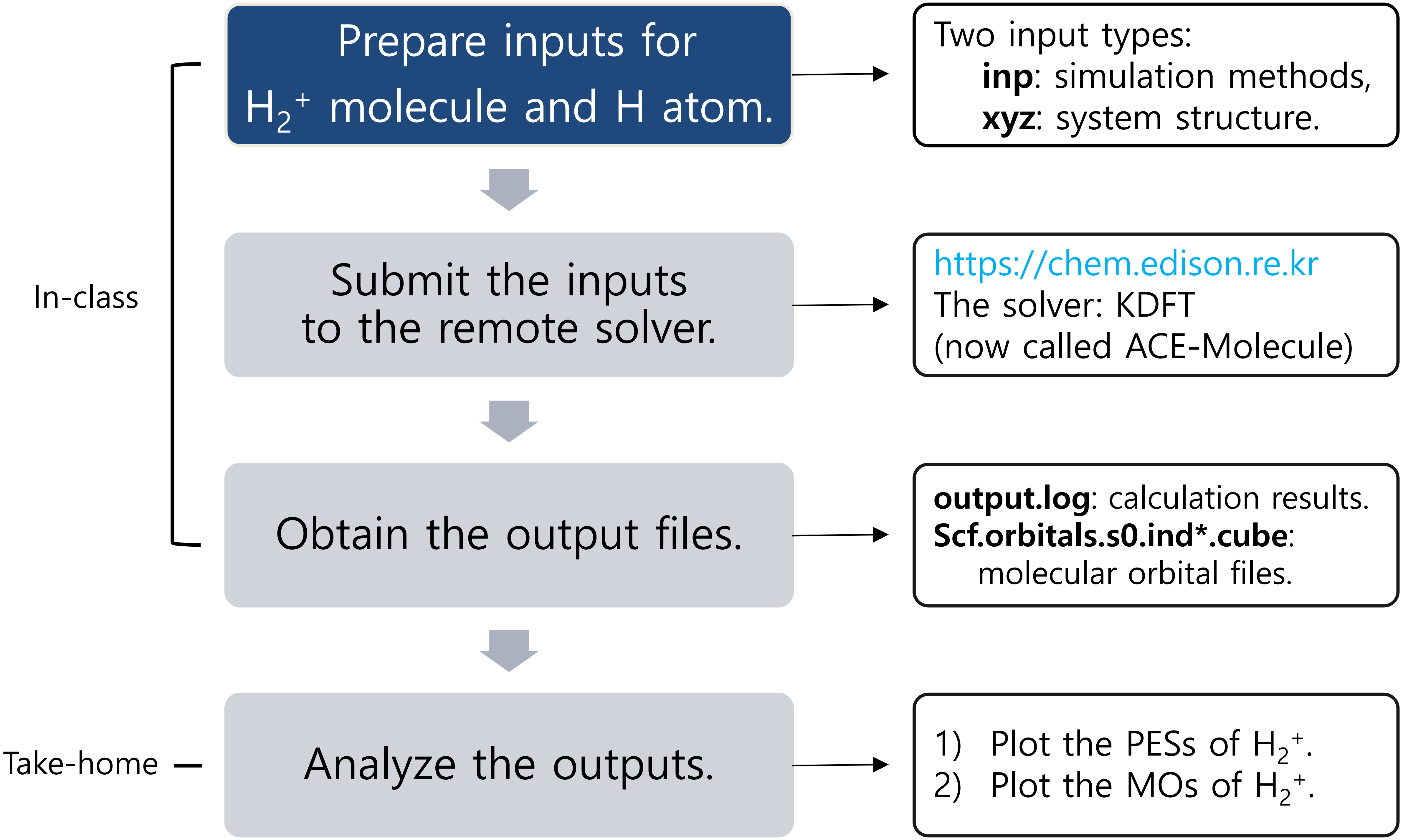
Orbitals = Wave functions of a **single-electron system.**

$$\hat{H}^{elec}(R_{AB})\psi = E\psi \longrightarrow \phi_0^{elec}(R_{AB}), \phi_1^{elec}(R_{AB}), \phi_2^{elec}(R_{AB}), \dots$$



Simulation

Simulation Outline



In-class

Prepare inputs for H_2^+ molecule and H atom.

Two input types:
inp: simulation methods,
xyz: system structure.

Submit the inputs to the remote solver.

https://chem.edison.re.kr
The solver: KDFT
(now called ACE-Molecule)

Obtain the output files.

output.log: calculation results.
Scf.orbitals.s0.ind*.cube:
molecular orbital files.

Take-home

Analyze the outputs.

1) Plot the PESs of H_2^+.
2) Plot the MOs of H_2^+.

1st input needed: **inp**

```
%%BasicInformation
Scaling 0.5
Radius 2.5
NumElectrons 1.0
Centered 1
  %%Pseudopotential
  UsingDoubleGrid 1
  FineDimension 2
  %%End
%%End

%%Scf
NumberOfEigenvalues 9
  %%ExchangeCorrelation
  FunctionalName EXX
  %%End
%%End
```

An **inp** file contains the settings of your simulation, such as the quantities to compute, the accuracy, etc.

In all the simulations required in this experiment, you need not change the **inp** content.

To learn more about the commands, please consult the app manual.

2nd input needed: **xyz**

An **xyz** file contains the coordinates of your molecular system.

Number of atoms in the molecule ->

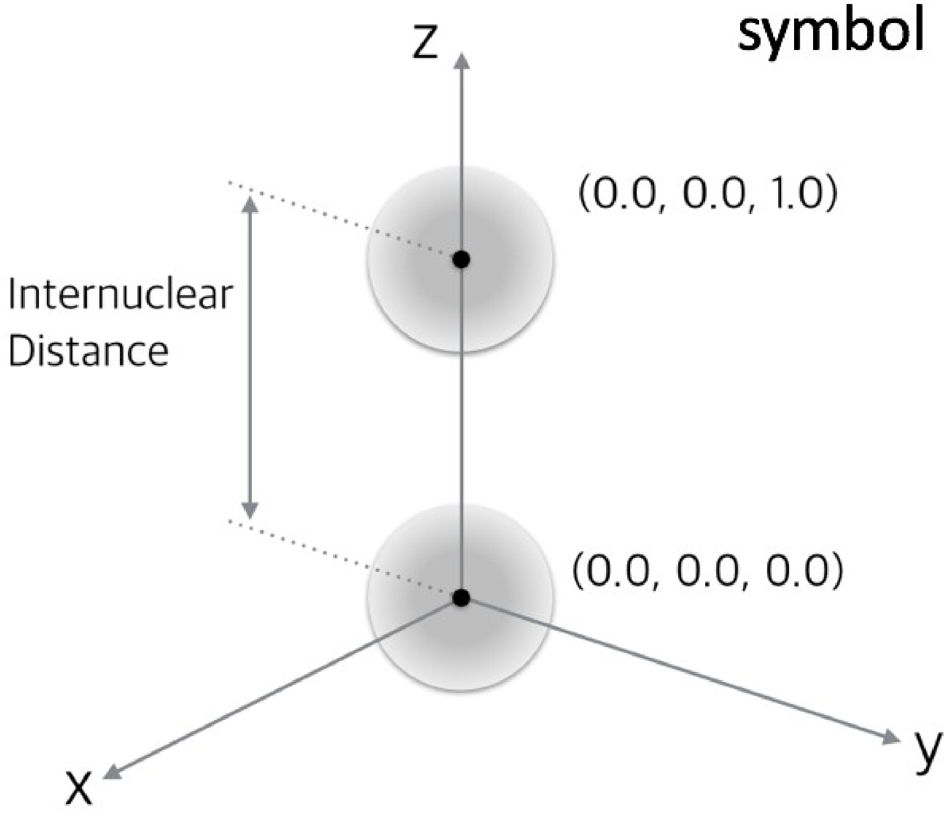
One blank line! ->

```
2

H 0.0 0.0 0.0
H 0.0 0.0 1.0
```

Element symbol

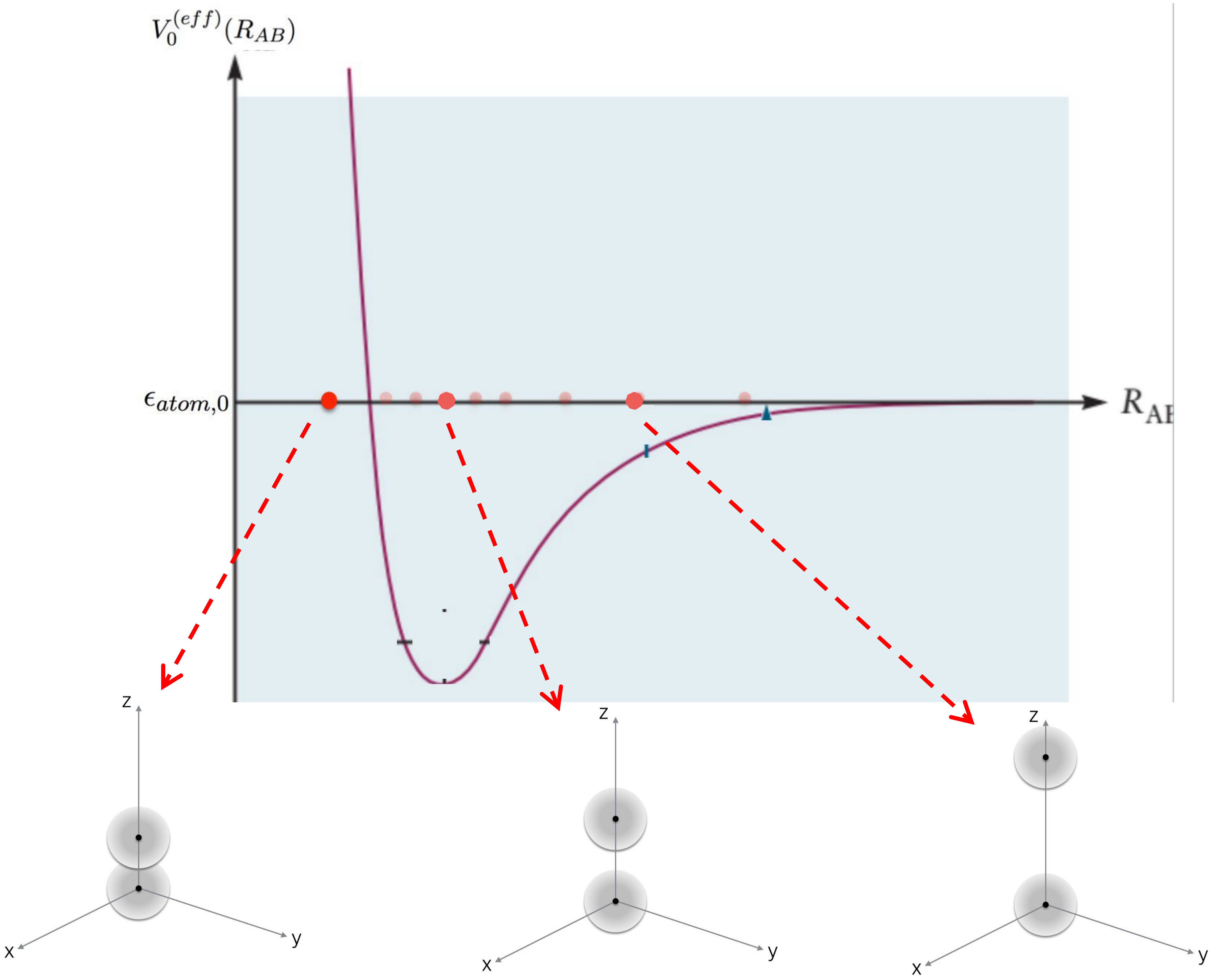
Cartesian coordinate (x, y, z) of each atom (unit : Angstrom)

$1\text{Angstrom} = 1\text{A}^{o} = 10^{-10}\text{m}$



2nd input needed: **xyz**

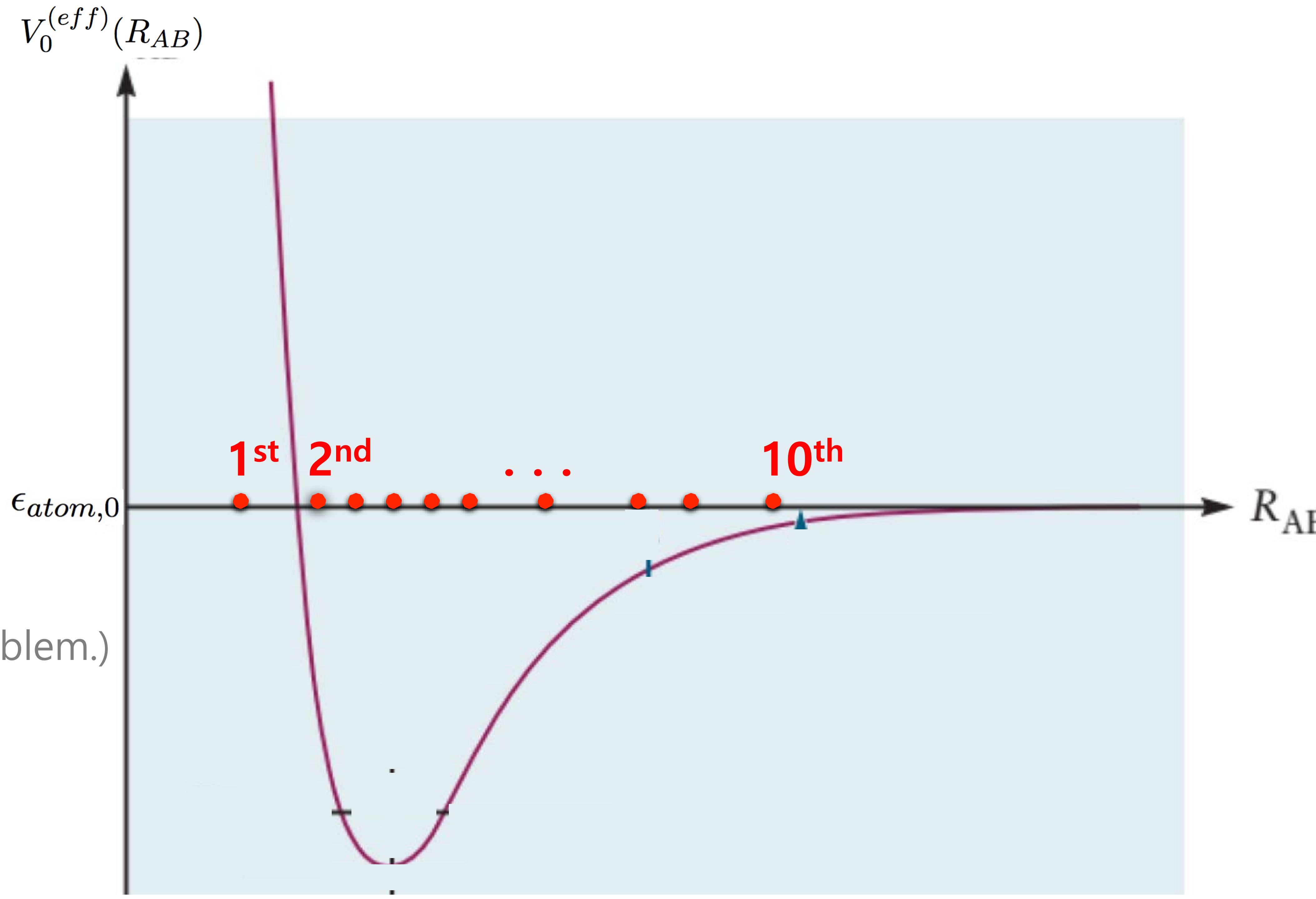
To make a potential-energy curve of H_2^+, we need multiple **xyzs**.



Required inputs in Exp. 3

One **inp**
and the **xyzs**
corresponding to
the 10 different
H–H distances.

(And an additional **xyz** of a single H-atom system, for the optional problem.)



Flow of using a remote solver

Your compute

Prepare inputs

Go to the EDISON site
chem.edison.re.kr
and submit your inputs.

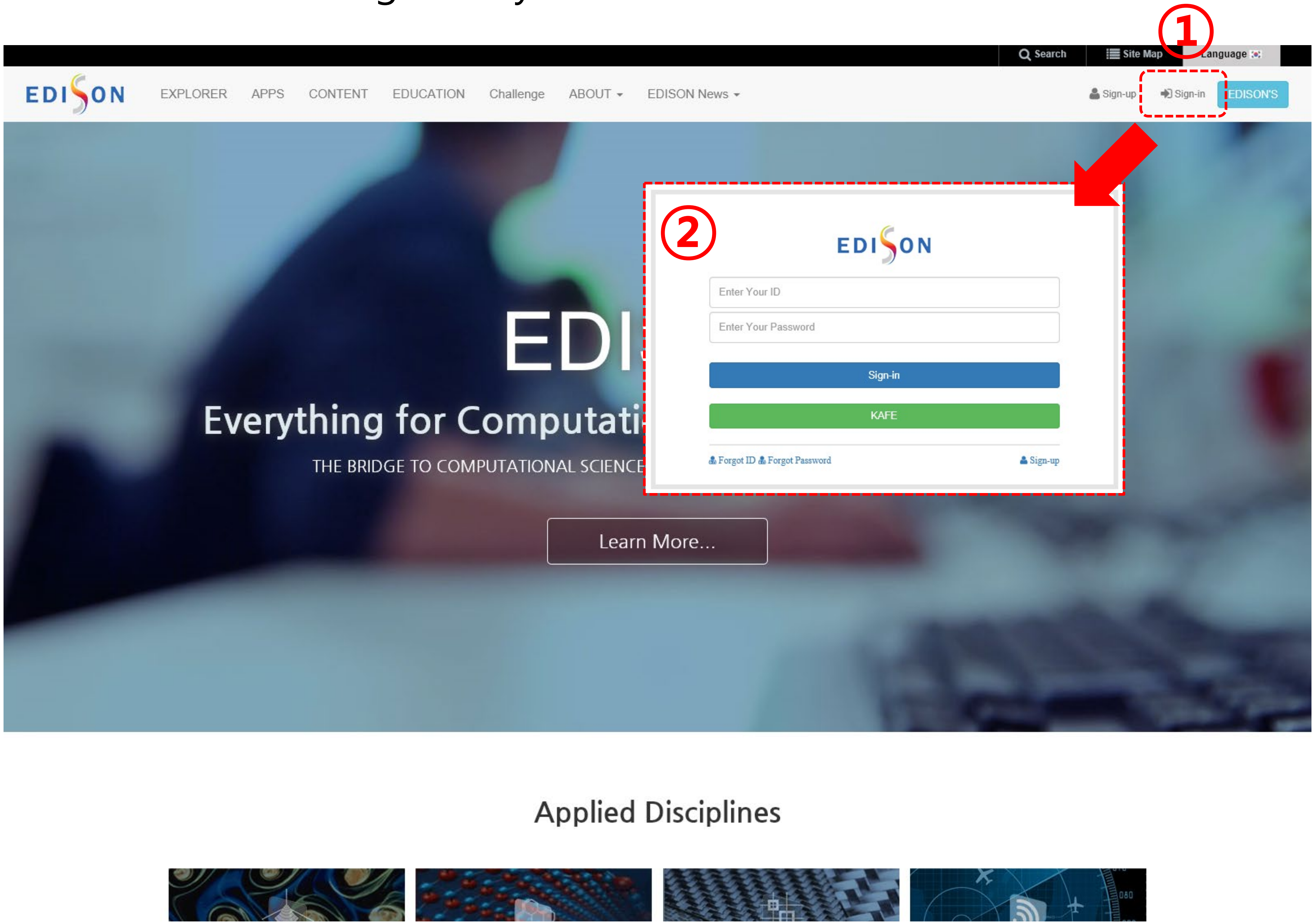
The EDISON server is where your calculation is executed. The server has the solver app with multiple CPUs.

Analyze outputs

Download the output files.

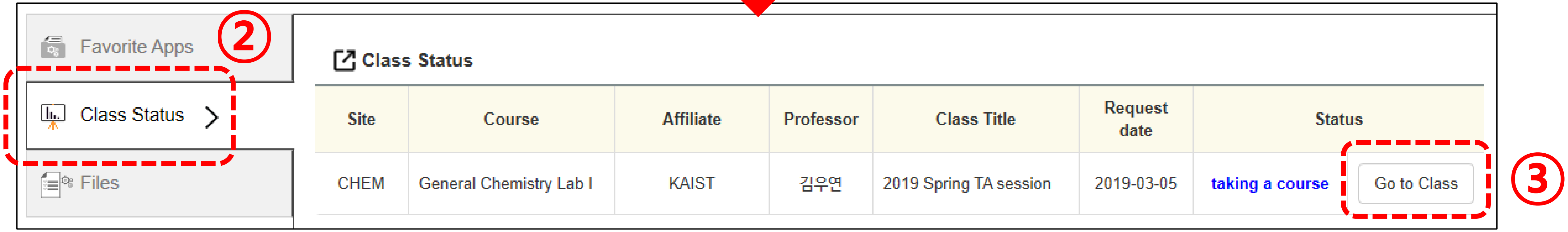
Getting started

Sign in to the EDISON web, chem.edison.re.kr
Account information will be given by TAs.



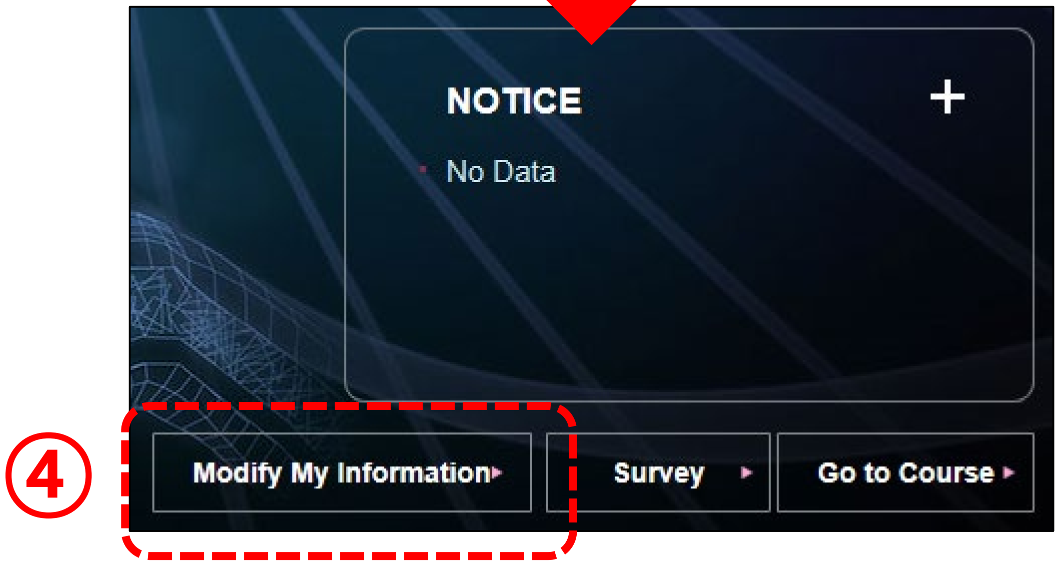
Getting started

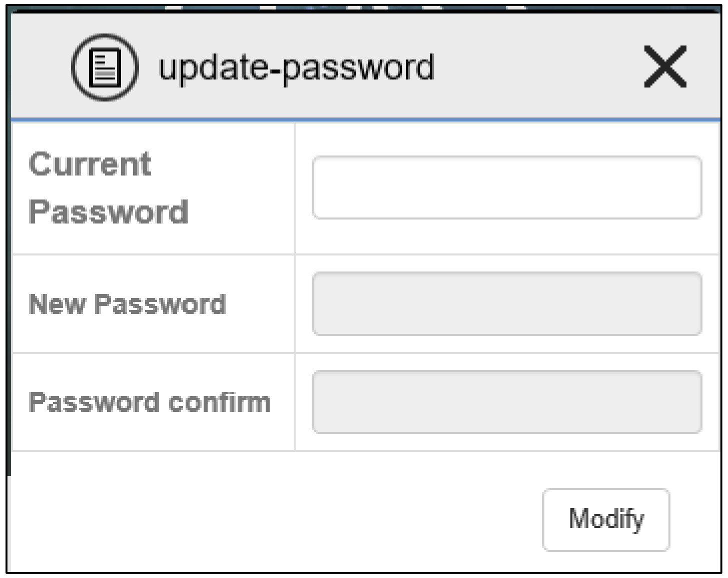
Students are recommended to change their passwords.
Follow what shown below to change your password (Make it simple!)



Class Status

Site	Course	Affiliate	Professor	Class Title	Request date	Status
CHEM	General Chemistry Lab I	KAIST	김우연	2019 Spring TA session	2019-03-05	taking a course Go to Class

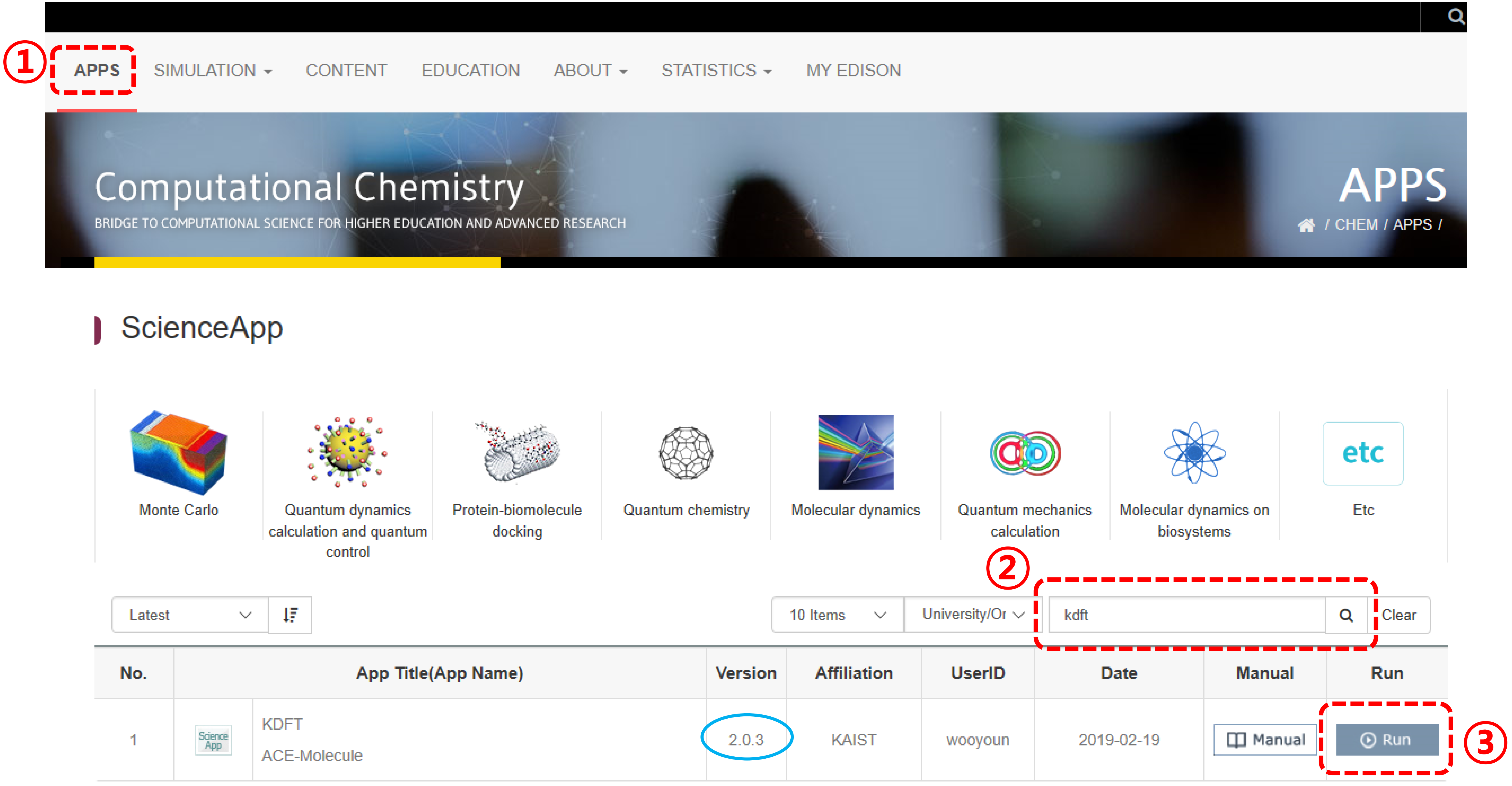




Current Password	
New Password	
Password confirm	

Getting started

Go launch the KDFT app.

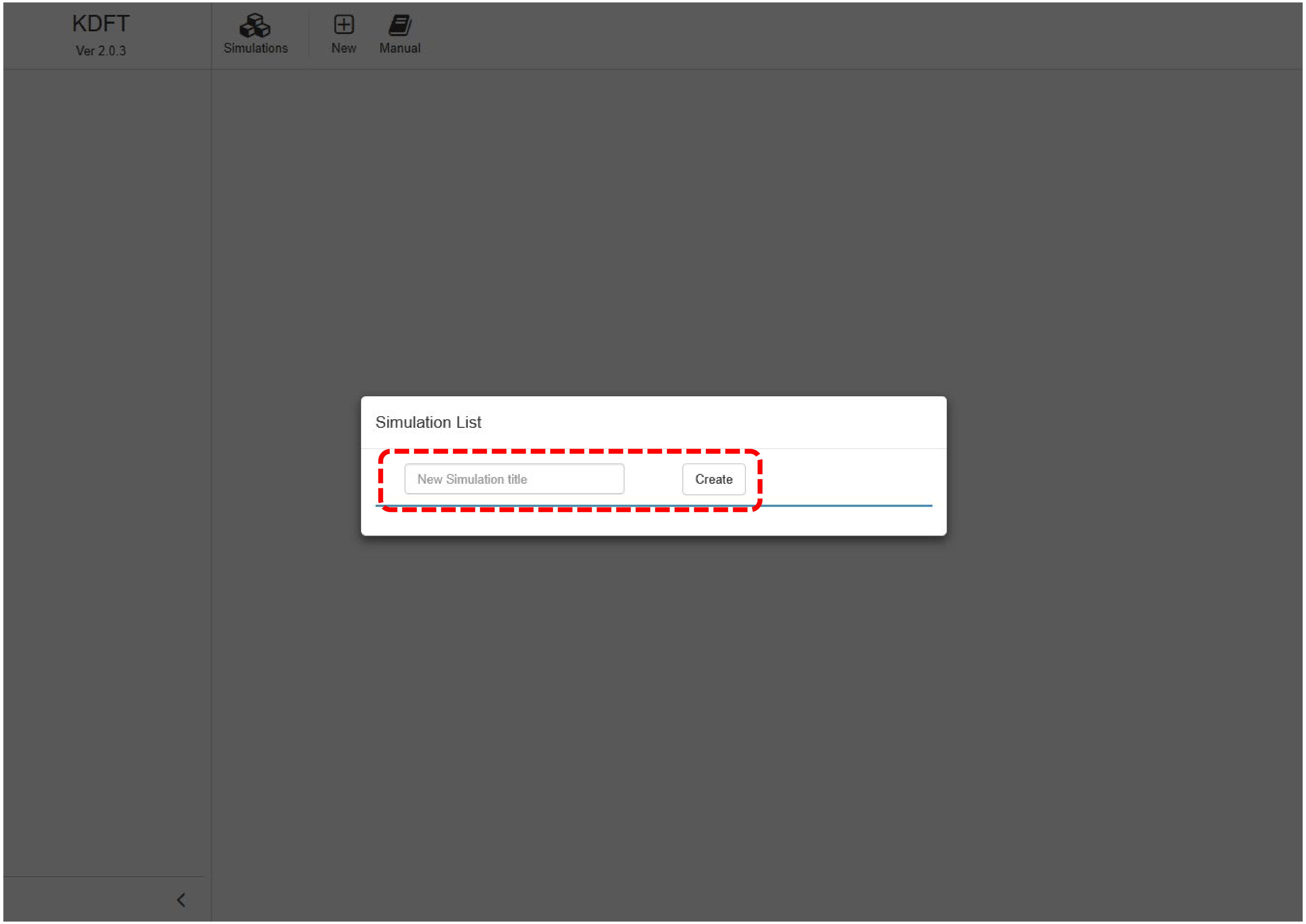


Search: kdft

No.	App Title(App Name)	Version	Affiliation	UserID	Date	Manual	Run
1	KDFT ACE-Molecule	2.0.3	KAIST	wooyoun	2019-02-19	Manual	Run

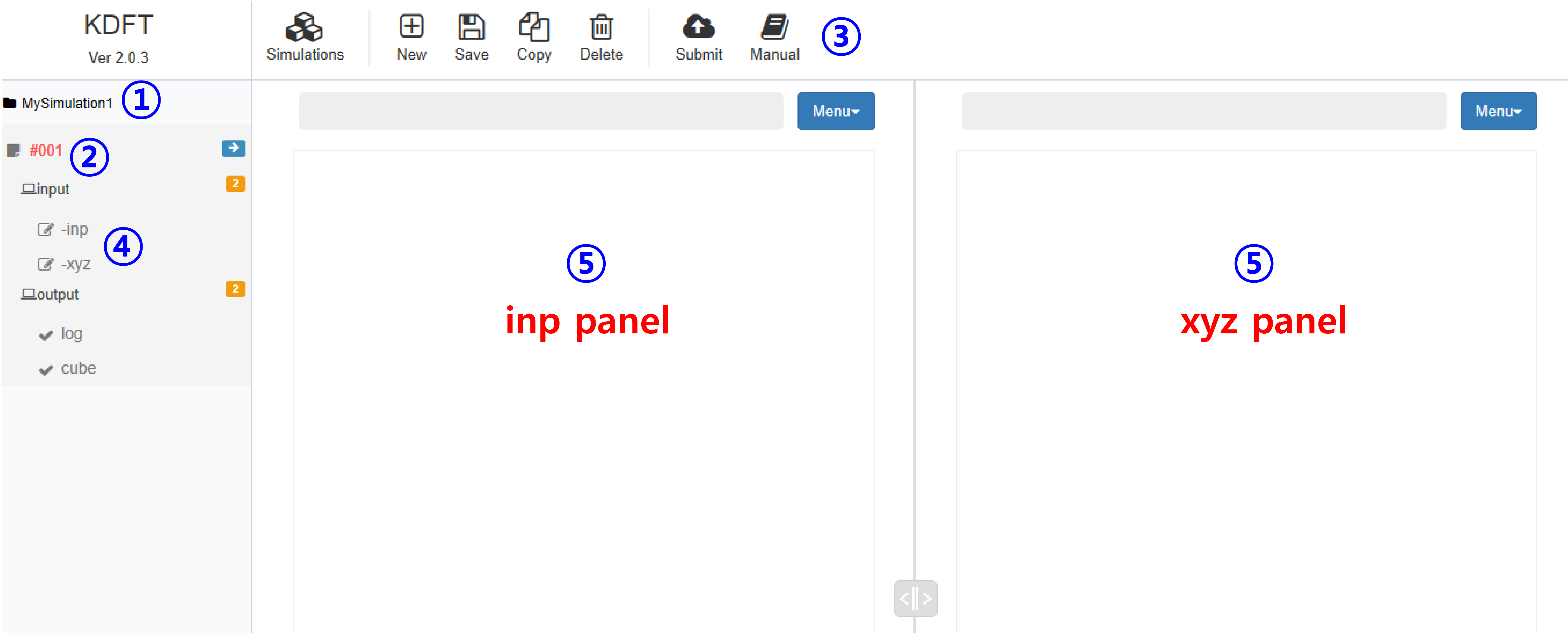
Your first simulation

Name a simulation as you want.



Your first simulation

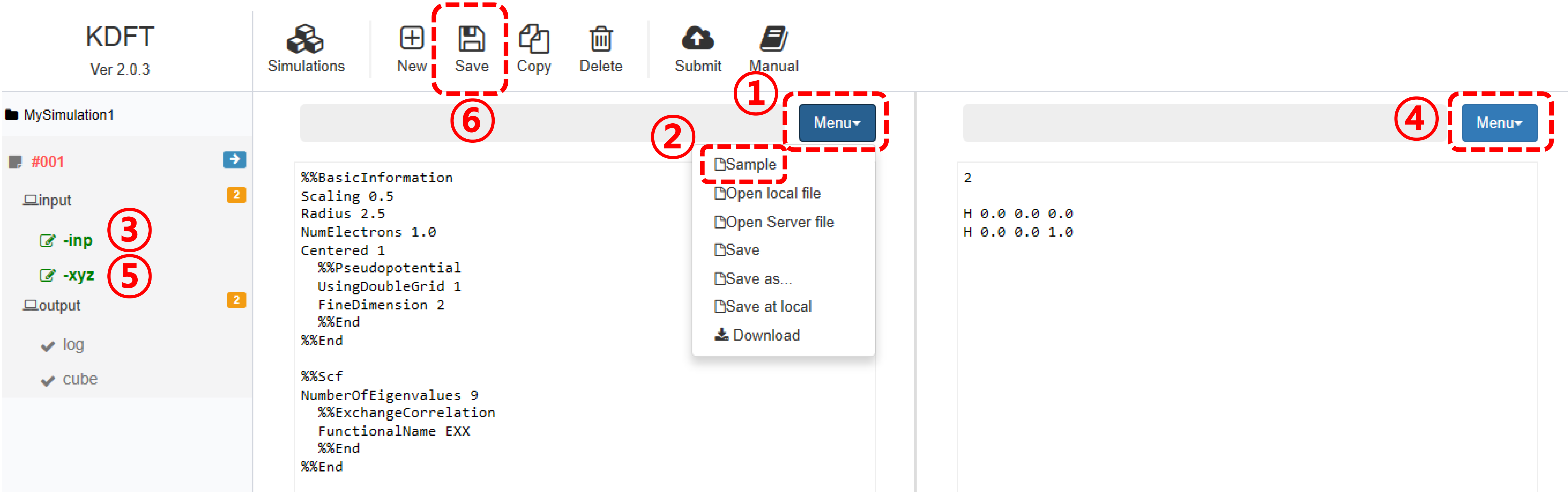
Let's first get familiar with the simulation workspace.



① Your simulation. One "simulation" includes multiple "jobs".
② A job. A job is the specification/management of an actual simulation process.
③ The toolbar for editing and submitting jobs.
④ The input ports for showing your input content and status.
⑤ The panels for editing your two input types **inp** and **xyz**.

Your first simulation

Set up the two inputs: **inp** and **xyz**.



```
%%BasicInformation
Scaling 0.5
Radius 2.5
NumElectrons 1.0
Centered 1
  %%Pseudopotential
  UsingDoubleGrid 1
  FineDimension 2
  %%End
%%End

%%Scf
NumberOfEigenvalues 9
  %%ExchangeCorrelation
  FunctionalName EXX
  %%End
%%End
```

```
2

H 0.0 0.0 0.0
H 0.0 0.0 1.0
```

①→② Click "Menu" and then "Sample" to load a sample **inp** file.

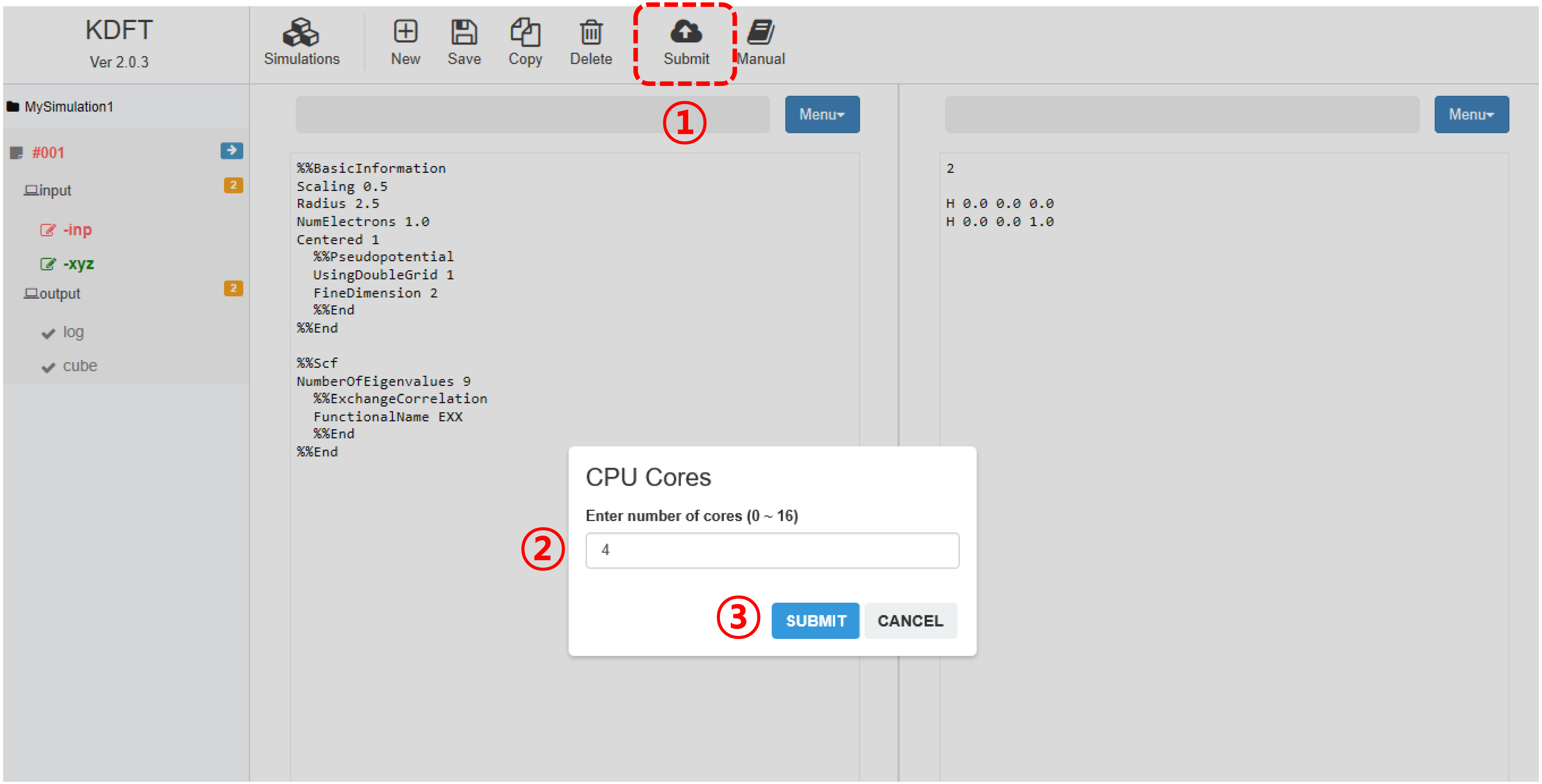
③ Check if the color changes to green.
This indicates that the **inp** is successfully entered.
(Note the problematic indication is gray, not red.
If red, it means the corresponding panel is being active.)

④→⑤ Do similarly for **xyz**.

⑥ After **inp** and **xyz** are entered, click "Save".

Your first simulation

Click “Submit” and set the number of (CPU) cores used.
The default 4 cores will do. Do not use a large number of cores.



```
%%BasicInformation
Scaling 0.5
Radius 2.5
NumElectrons 1.0
Centered 1
  %%Pseudopotential
  UsingDoubleGrid 1
  FineDimension 2
  %%End
%%End

%%Scf
NumberOfEigenvalues 9
  %%ExchangeCorrelation
  FunctionalName EXX
  %%End
%%End
```

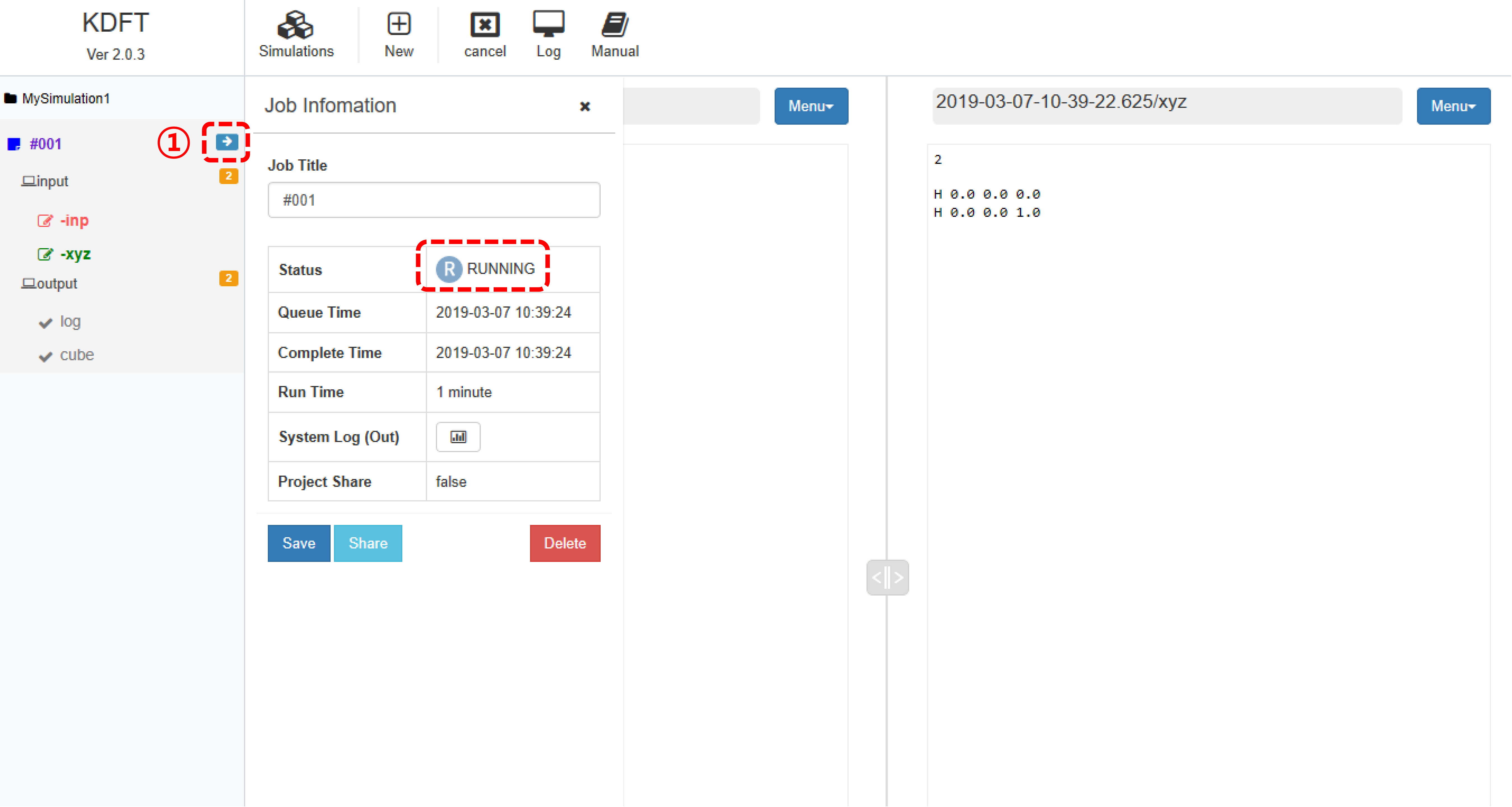
```
2

H 0.0 0.0 0.0
H 0.0 0.0 1.0
```

CPU Cores

Enter number of cores (0 ~ 16): 4

Your first simulation

After submitting the job, you can click ① to monitor the job status.
Note that the "Job Information" panel does not auto-refresh by itself!



Job Infomation

Job Title	#001
Status	R RUNNING
Queue Time	2019-03-07 10:39:24
Complete Time	2019-03-07 10:39:24
Run Time	1 minute
System Log (Out)	
Project Share	false

2019-03-07-10-39-22.625/xyz

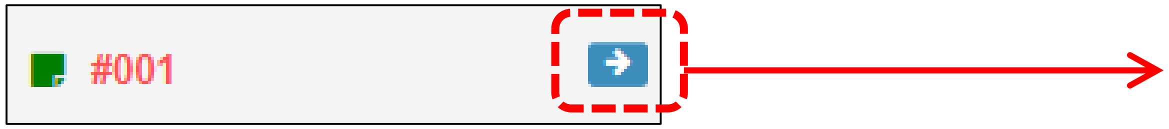
```
2

H 0.0 0.0 0.0
H 0.0 0.0 1.0
```

Monitoring the job status

Monitor whether your job finishes successfully.


#001

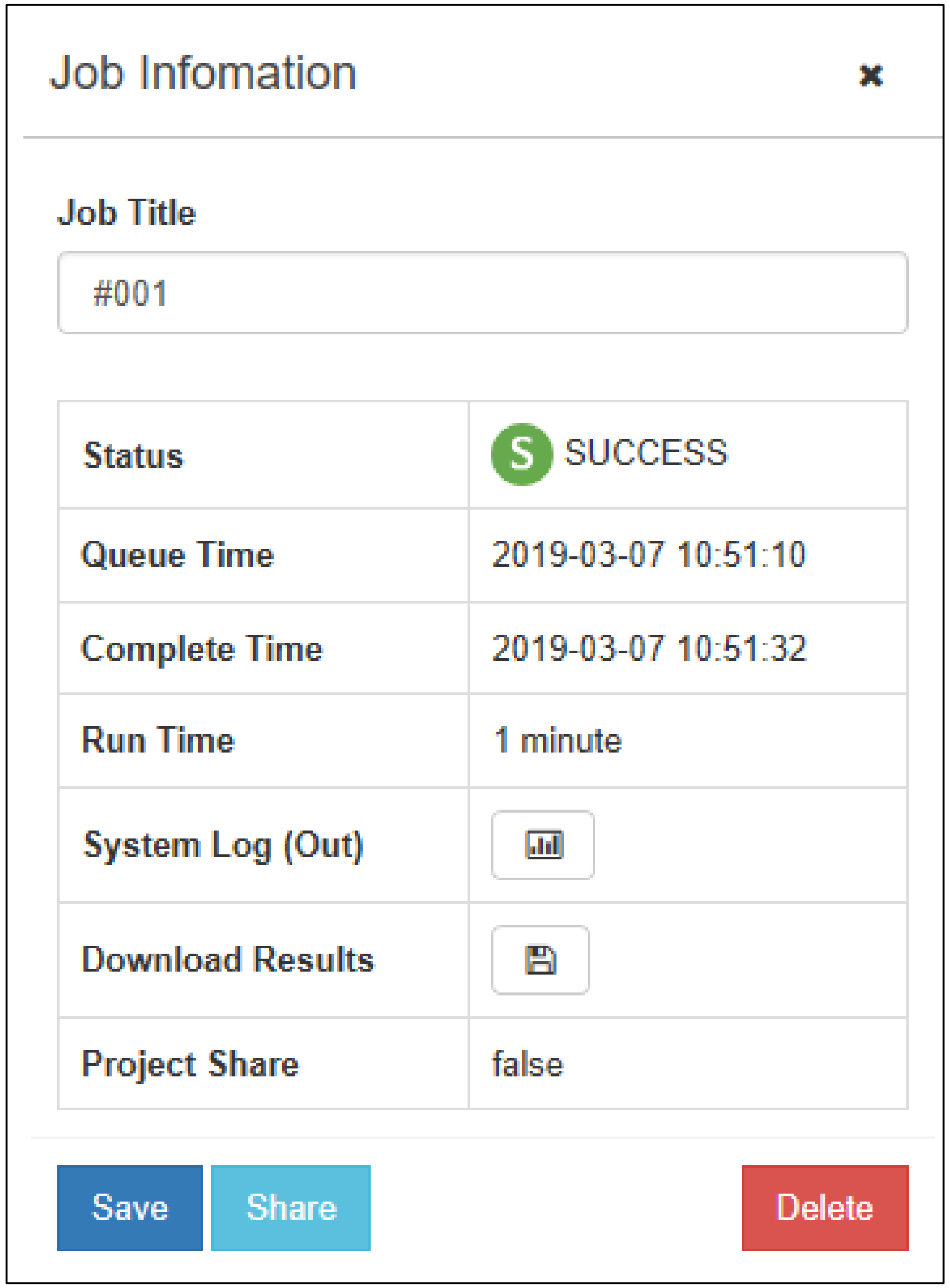
"R" status: job is running
or
"Q" status: job is waiting to be run.


#001

"S" status: job ended normally.


#001

"F" status: job ended w/ errors!
Check the errors in your inputs
and run a *new* job.

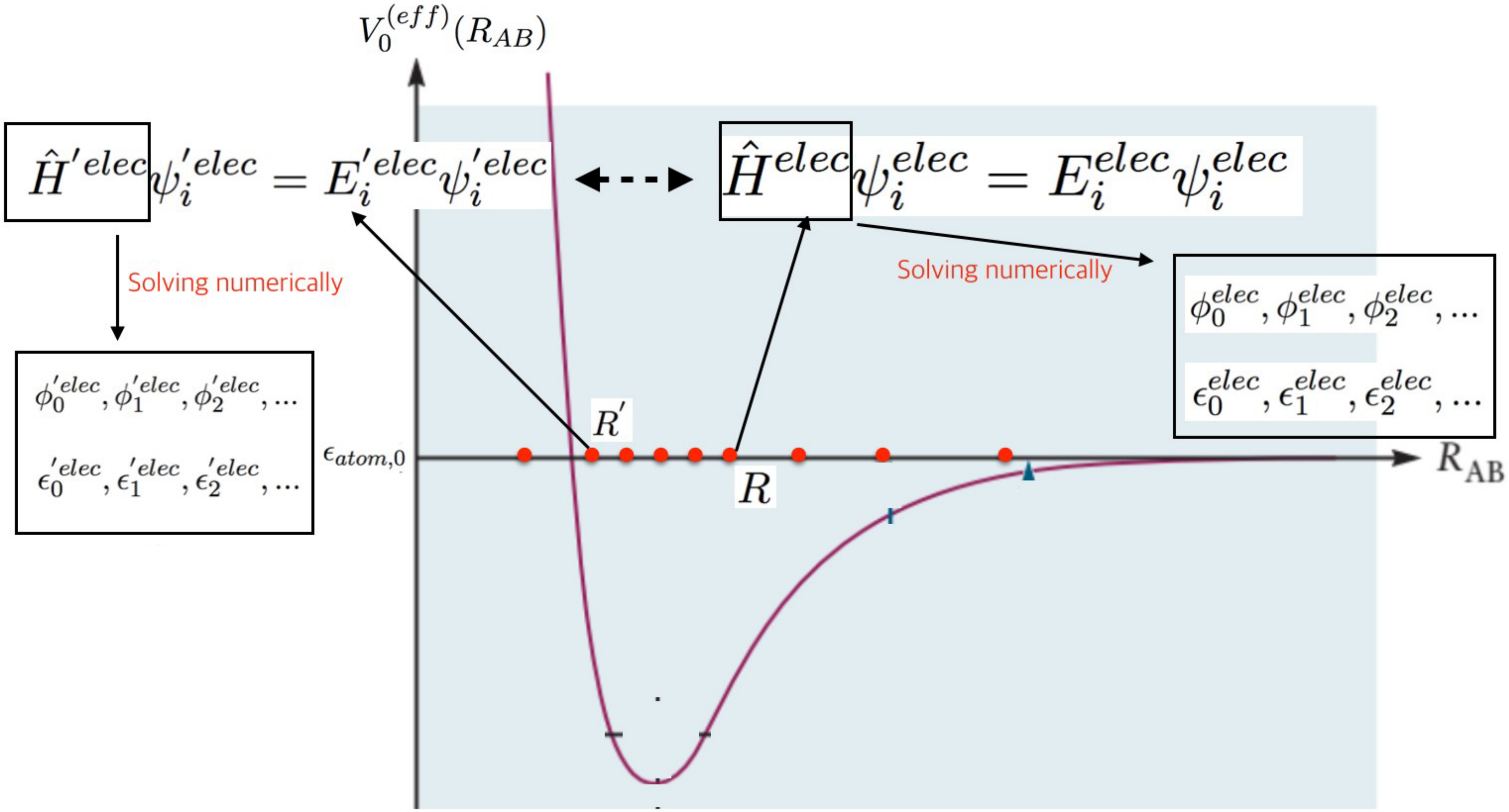

Job Infomation

Job Title: #001

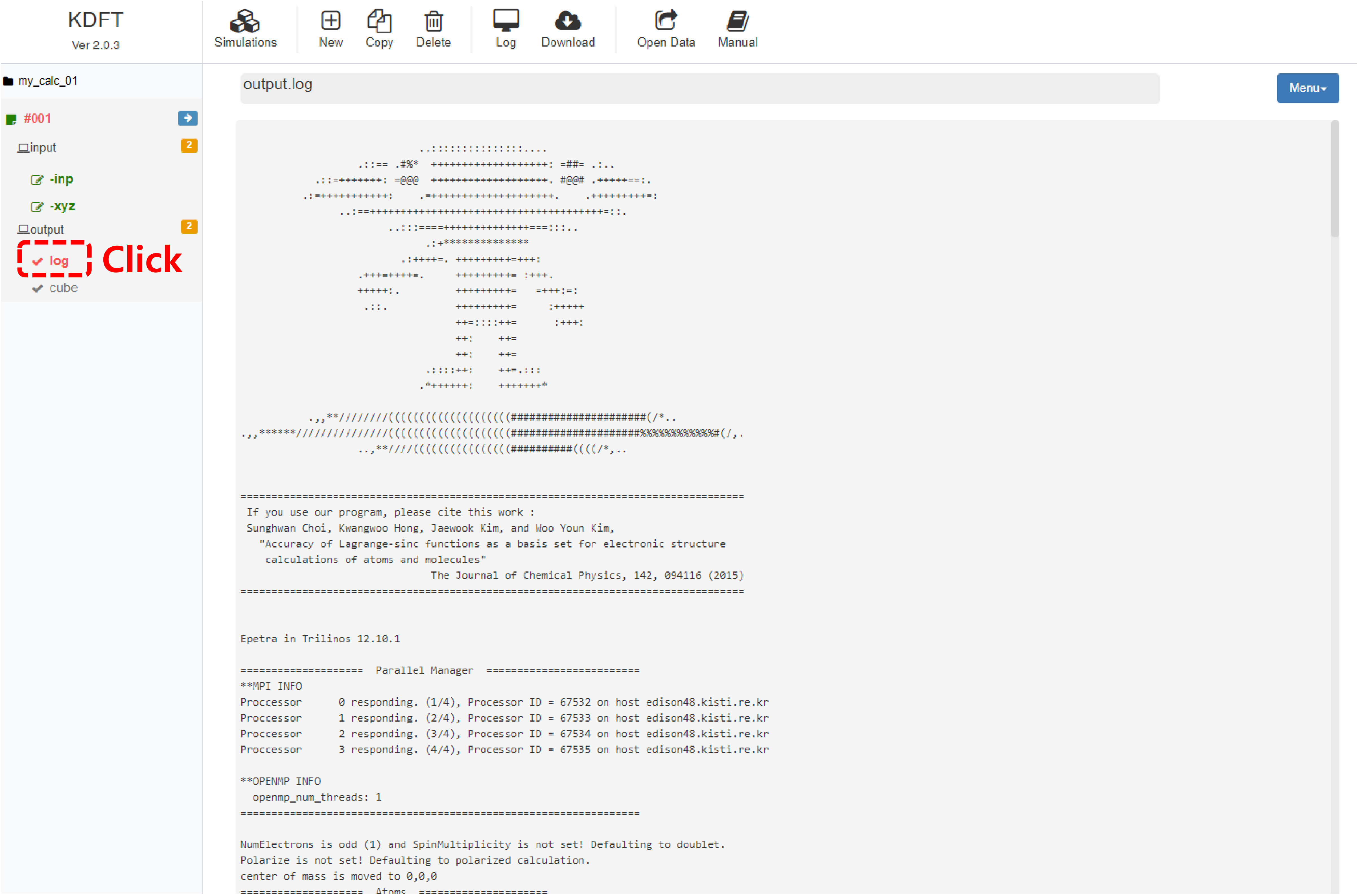
Status	S SUCCESS
Queue Time	2019-03-07 10:51:10
Complete Time	2019-03-07 10:51:32
Run Time	1 minute
System Log (Out)	
Download Results	
Project Share	false

Data in the output files

For each calculation (with a specific R_{AB}),
A **log** file contains ϵ_i^{elec}, V_{nn} and other physical values of the system.
A **cube** file contains the information for drawing the shape of one ϕ_i^{elec}.



1st output: the log file



```
                             ..::::::::::::::::....
                   .::== .#%*  +++++++++++++++++++: =##= .:..
            .::=++++++++: =@@@  +++++++++++++++++++. #@@# .+++++==:.
          .:=++++++++++++:    .=++++++++++++++++++++.    .++++++++++=:
                ..:==+++++++++++++++++++++++++++++++++++++++++=::.
                        ..:::====+++++++++++++++===:::..
                              .:+**************
                          .:+++++=. ++++++++++=++++:
                   .+++=++++=.     ++++++++++= :+++.
                   +++++:.         ++++++++++=   =+++:=:
                    .::.           ++++++++++=     :+++++
                                   ++=::::++=      :+++:
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                                   ++:    ++=
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                             .*++++++:    +++++++*

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==================================================================================
 If you use our program, please cite this work :
 Sunghwan Choi, Kwangwoo Hong, Jaewook Kim, and Woo Youn Kim,
   "Accuracy of Lagrange-sinc functions as a basis set for electronic structure
    calculations of atoms and molecules"
                               The Journal of Chemical Physics, 142, 094116 (2015)
==================================================================================



Epetra in Trilinos 12.10.1

====================  Parallel Manager  ========================
**MPI INFO
Proccessor      0 responding. (1/4), Processor ID = 67532 on host edison48.kisti.re.kr
Proccessor      1 responding. (2/4), Processor ID = 67533 on host edison48.kisti.re.kr
Proccessor      2 responding. (3/4), Processor ID = 67534 on host edison48.kisti.re.kr
Proccessor      3 responding. (4/4), Processor ID = 67535 on host edison48.kisti.re.kr

**OPENMP INFO
  openmp_num_threads: 1
=================================================================

NumElectrons is odd (1) and SpinMultiplicity is not set! Defaulting to doublet.
Polarize is not set! Defaulting to polarized calculation.
center of mass is moved to 0,0,0
====================  Atoms  =====================
```
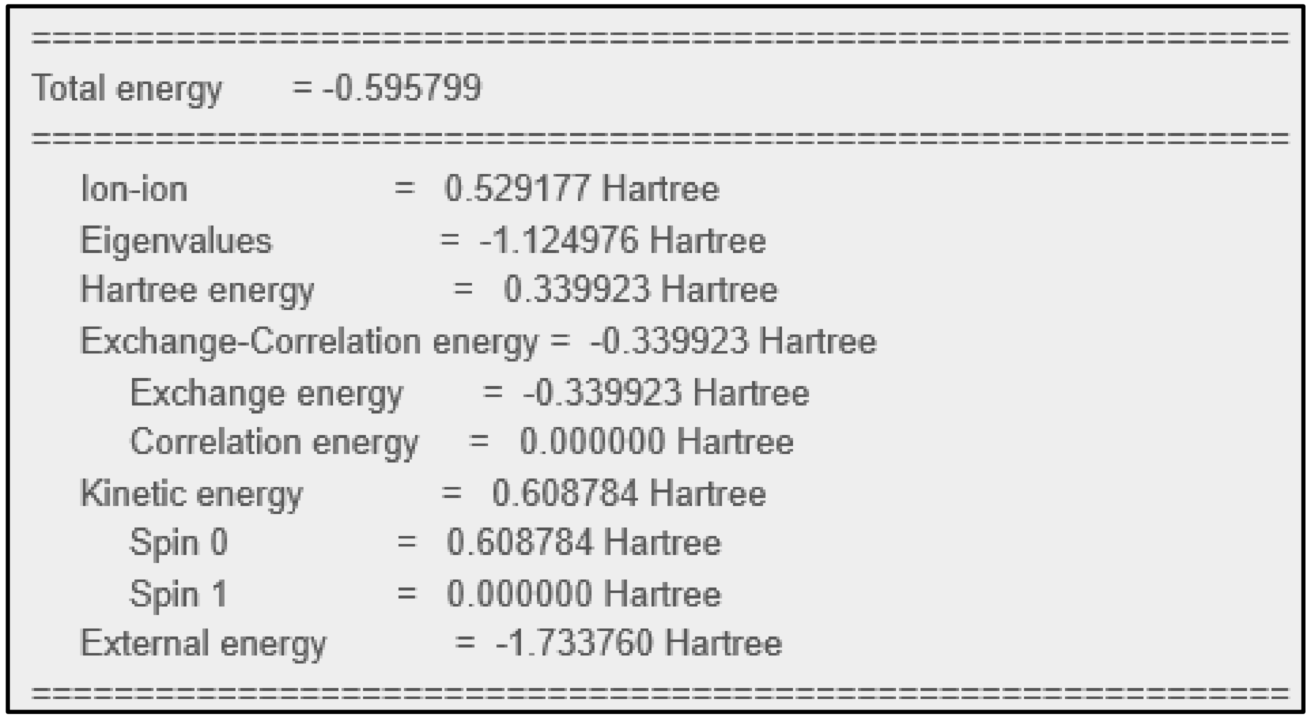

1st output: the log file

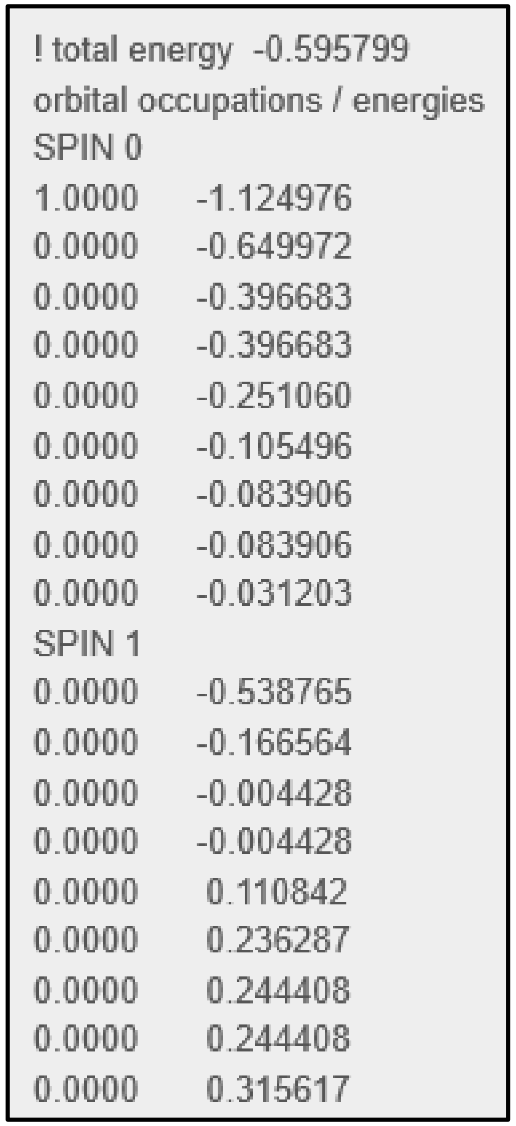
Scroll the log panel down to see the following sections:

The energy information of the system



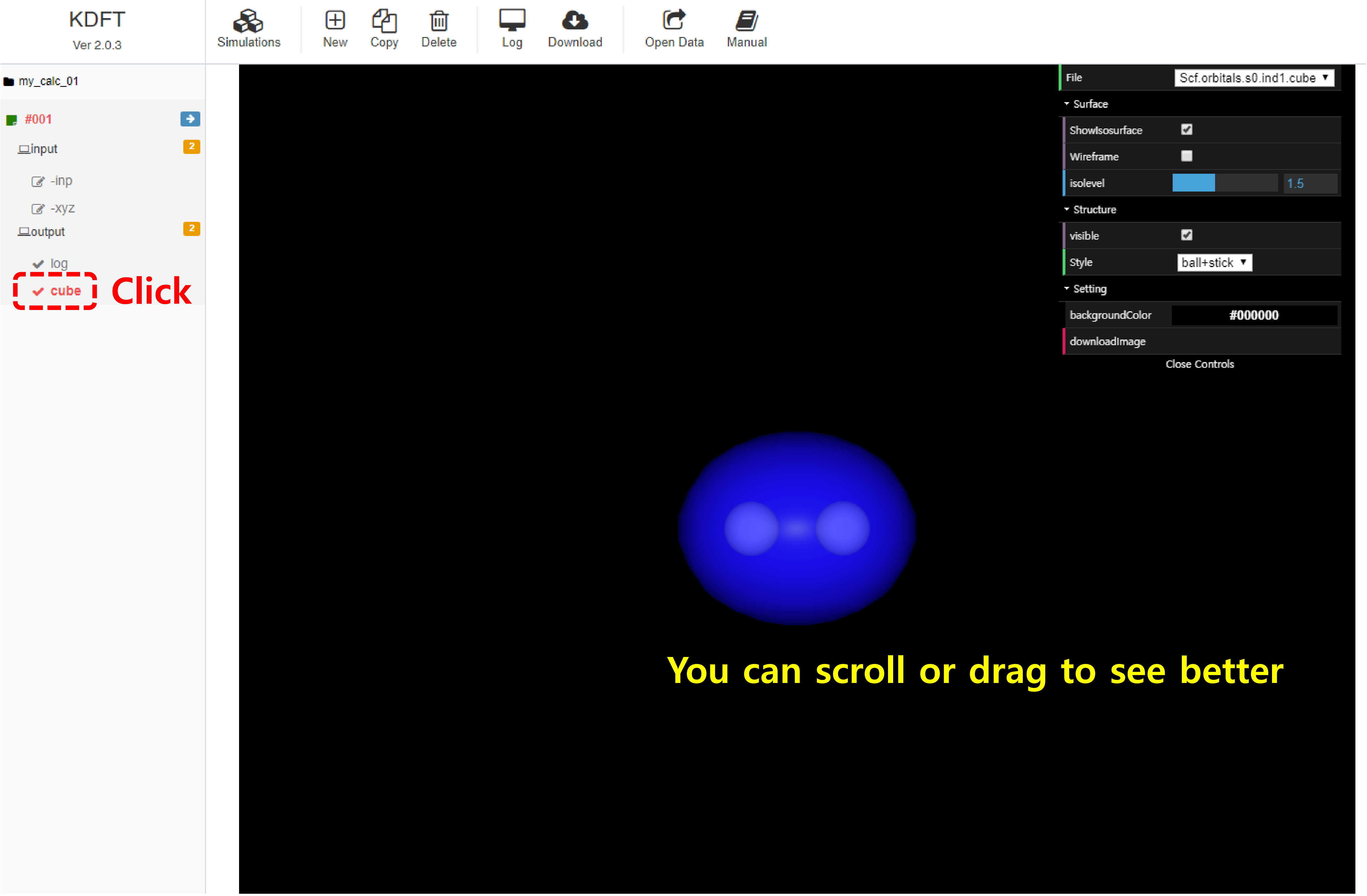
```
==================================================================
Total energy      = -0.595799
==================================================================
   Ion-ion                  =   0.529177 Hartree
   Eigenvalues              =  -1.124976 Hartree
   Hartree energy           =   0.339923 Hartree
   Exchange-Correlation energy =  -0.339923 Hartree
      Exchange energy       =  -0.339923 Hartree
      Correlation energy    =   0.000000 Hartree
   Kinetic energy           =   0.608784 Hartree
      Spin 0                =   0.608784 Hartree
      Spin 1                =   0.000000 Hartree
   External energy          =  -1.733760 Hartree
==================================================================
```

The orbital energies of the system



```
! total energy  -0.595799
orbital occupations / energies
SPIN 0
1.0000     -1.124976
0.0000     -0.649972
0.0000     -0.396683
0.0000     -0.396683
0.0000     -0.251060
0.0000     -0.105496
0.0000     -0.083906
0.0000     -0.083906
0.0000     -0.031203
SPIN 1
0.0000     -0.538765
0.0000     -0.166564
0.0000     -0.004428
0.0000     -0.004428
0.0000      0.110842
0.0000      0.236287
0.0000      0.244408
0.0000      0.244408
0.0000      0.315617
```

2nd output: the cube files



File: Scf.orbitals.s0.ind1.cube

ShowIsosurface ☑

Wireframe ☐

isolevel 1.5

visible ☑

Style ball+stick

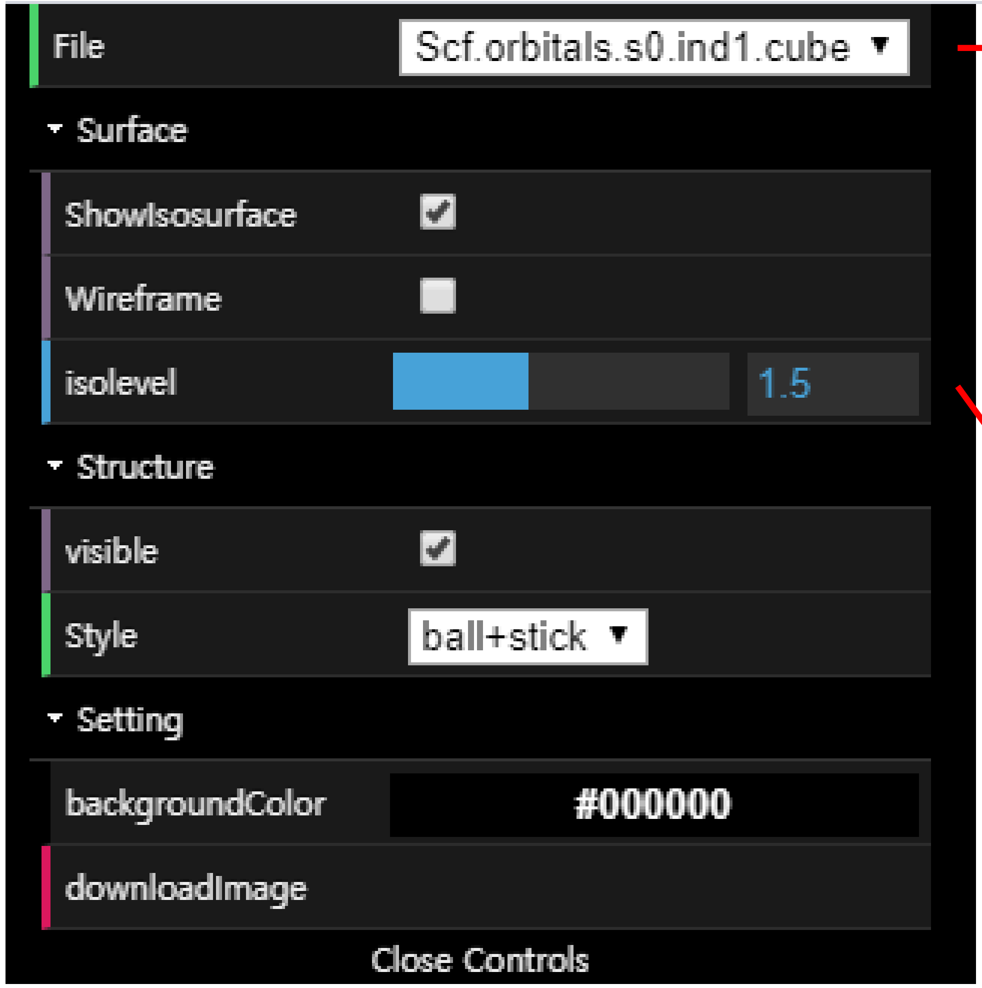
backgroundColor #000000

Click

You can scroll or drag to see better

2nd output: the cube files

Various settings can be changed in the control panel.
The most important things include:



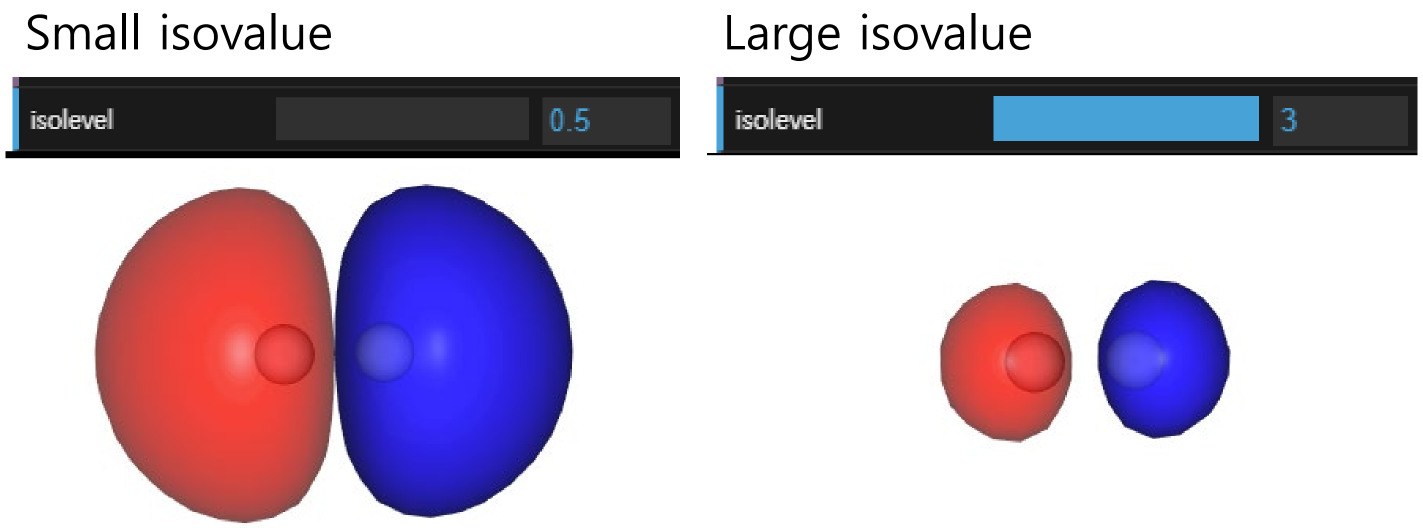
File: Scf.orbitals.s0.ind1.cube ▼
▾ Surface
ShowIsosurface ☑
Wireframe ☐
isolevel 1.5
▾ Structure
visible ☑
Style: ball+stick ▼
▾ Setting
backgroundColor #000000
downloadImage
Close Controls

(1) Cube file names:

Scf.orbitals.s0.ind1.cube
Scf.orbitals.s0.ind2.cube
Scf.orbitals.s0.ind3.cube
⋮

Spin alpha (s0)
Orbital number (3)

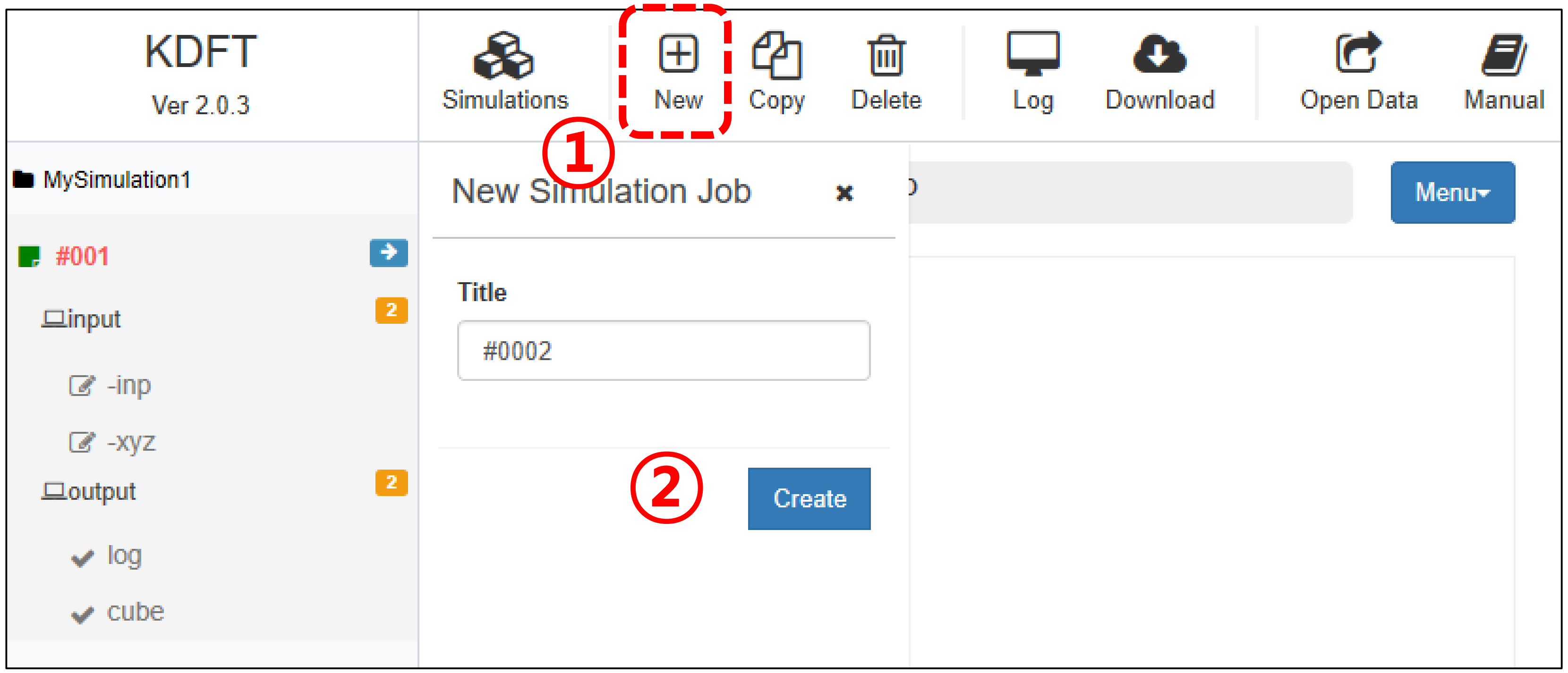
(2) Surface isovalue control:

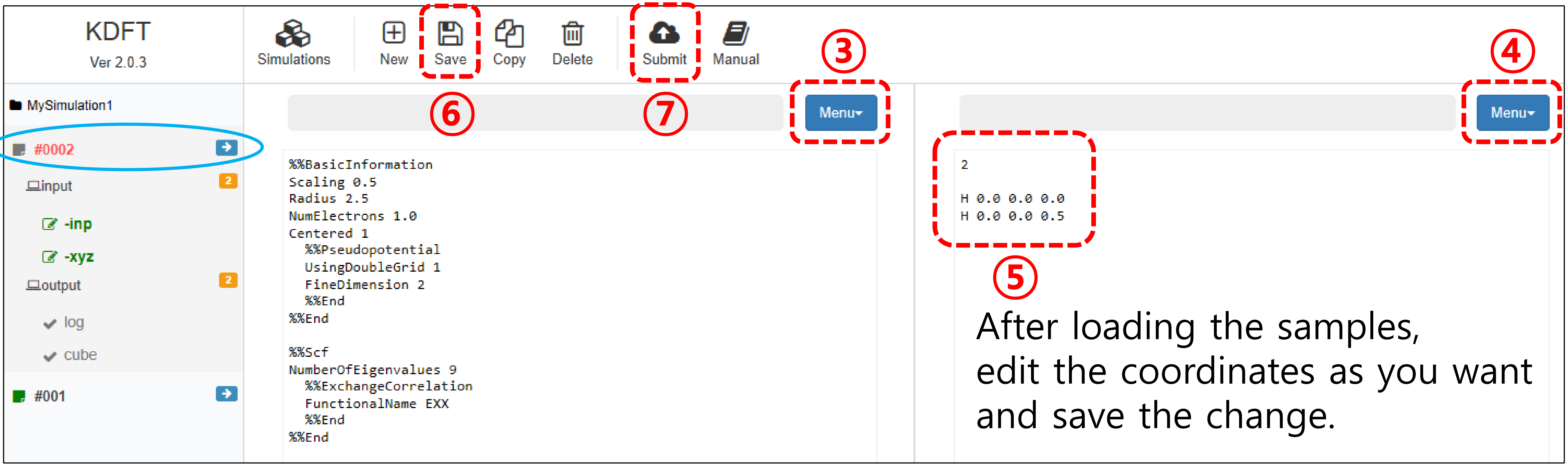


Small isovalue: isolevel 0.5

Large isovalue: isolevel 3

Submitting additional jobs





```
%%BasicInformation
Scaling 0.5
Radius 2.5
NumElectrons 1.0
Centered 1
  %%Pseudopotential
  UsingDoubleGrid 1
  FineDimension 2
  %%End
%%End

%%Scf
NumberOfEigenvalues 9
  %%ExchangeCorrelation
  FunctionalName EXX
  %%End
%%End
```

```
2

H 0.0 0.0 0.0
H 0.0 0.0 0.5
```

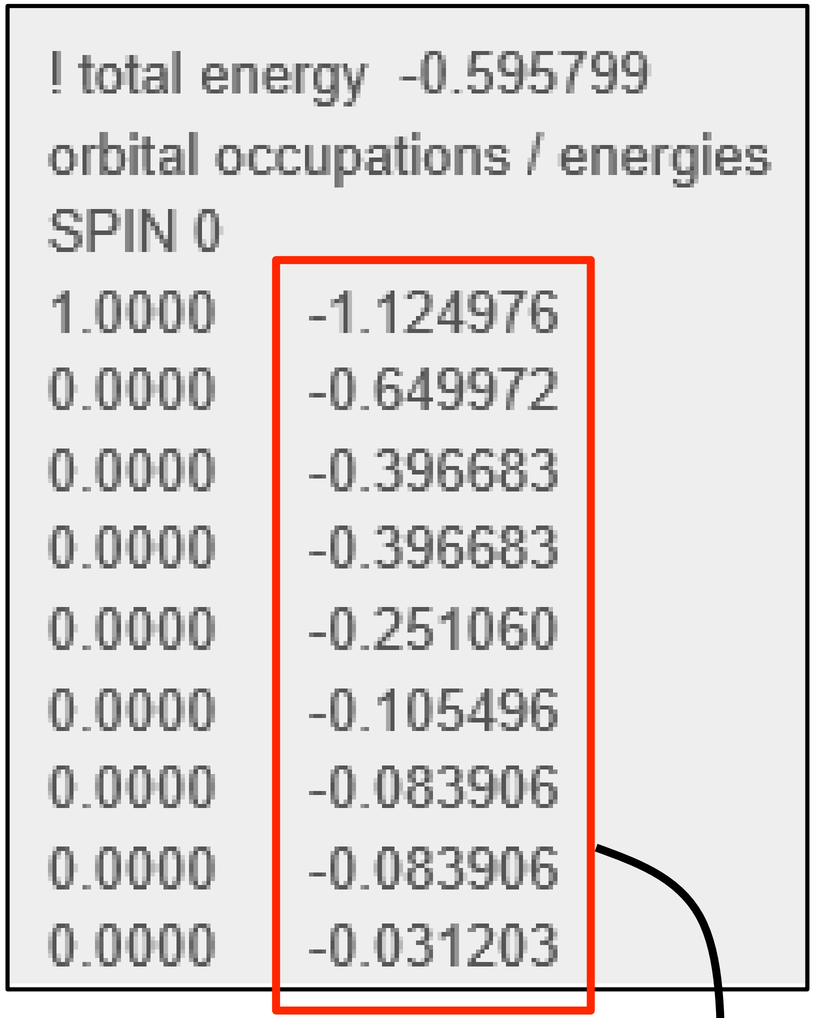
After loading the samples, edit the coordinates as you want and save the change.

Analyses

Analysis 1. Potential energy curve of H_2^+ ground state

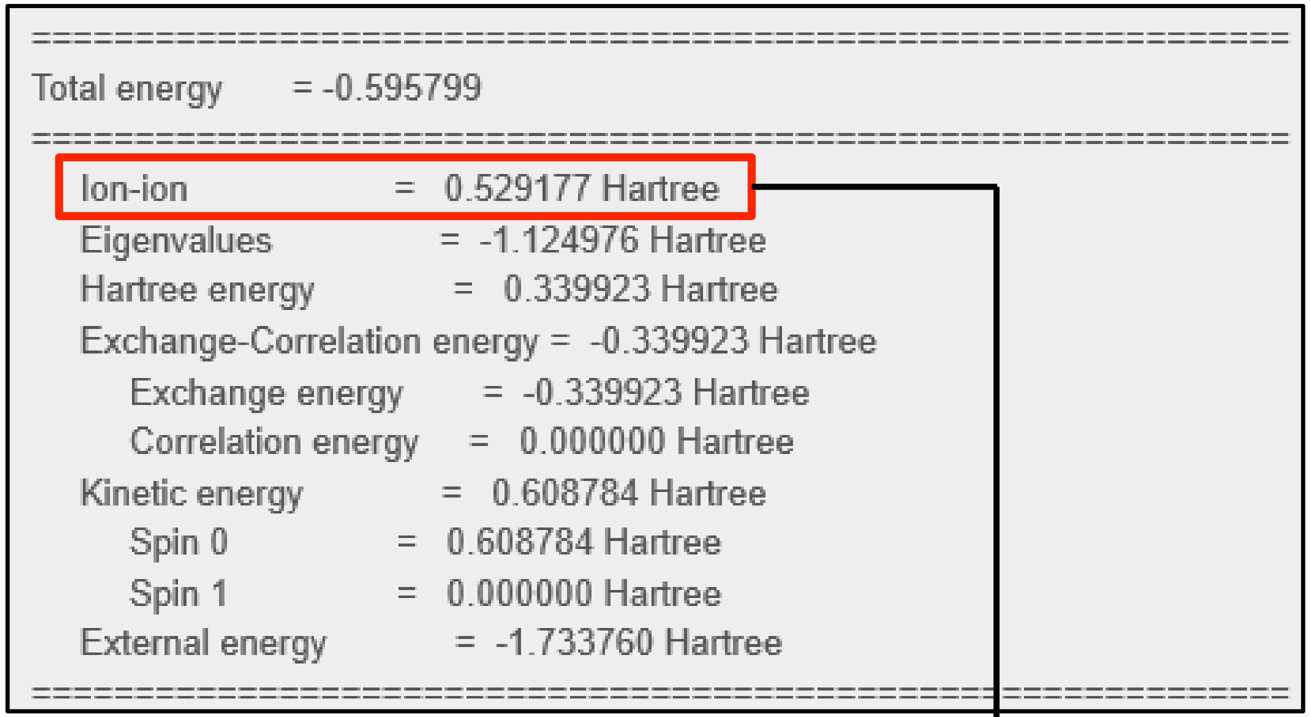
Find the following sections in the log:

[1]



```
! total energy  -0.595799
orbital occupations / energies
SPIN 0
1.0000    -1.124976
0.0000    -0.649972
0.0000    -0.396683
0.0000    -0.396683
0.0000    -0.251060
0.0000    -0.105496
0.0000    -0.083906
0.0000    -0.083906
0.0000    -0.031203
```

[2]



```
=====================================================================
Total energy       = -0.595799
=====================================================================
  Ion-ion                    =   0.529177 Hartree
  Eigenvalues                =  -1.124976 Hartree
  Hartree energy             =   0.339923 Hartree
  Exchange-Correlation energy =  -0.339923 Hartree
      Exchange energy        =  -0.339923 Hartree
      Correlation energy     =   0.000000 Hartree
  Kinetic energy             =   0.608784 Hartree
      Spin 0                 =   0.608784 Hartree
      Spin 1                 =   0.000000 Hartree
  External energy            =  -1.733760 Hartree
=====================================================================
```

V_{nn}

(Often in literatures, "ion" is used for "nucleus".)

-1.124976 = ϵ_0^{elec} = ground-state *electronic* energy = 1st orbital energy

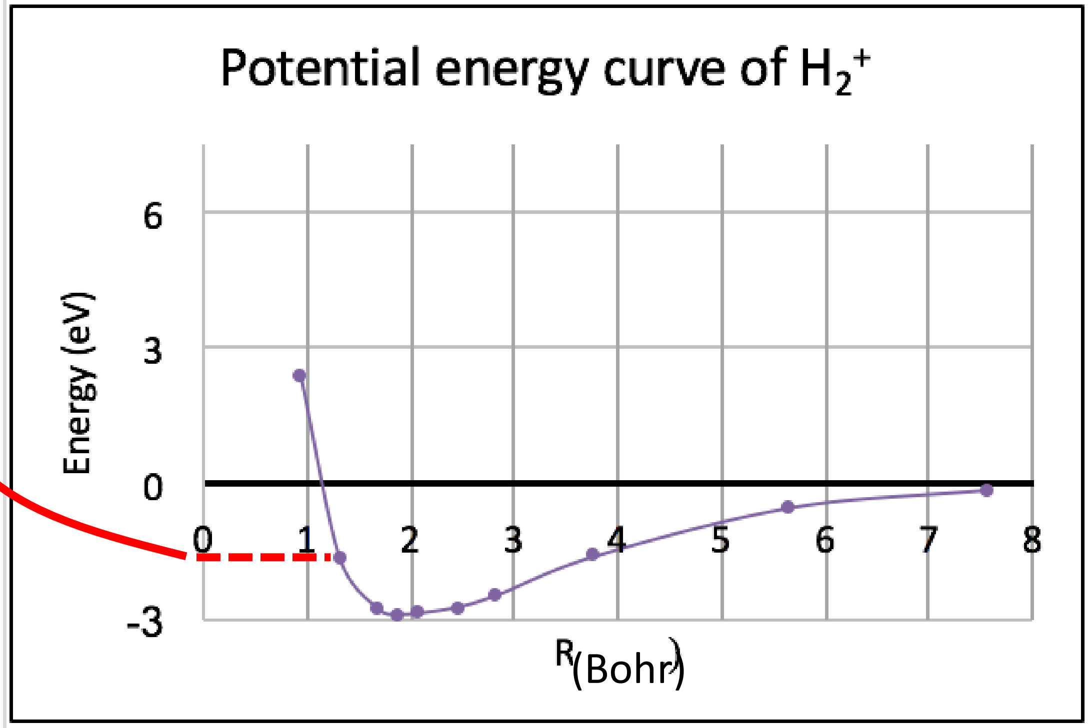
-0.649972 = ϵ_1^{elec} = 1st excited-state *electronic* energy = 2nd orbital energy

. . .

Analysis 1. Potential energy curve of H_2^+ ground state

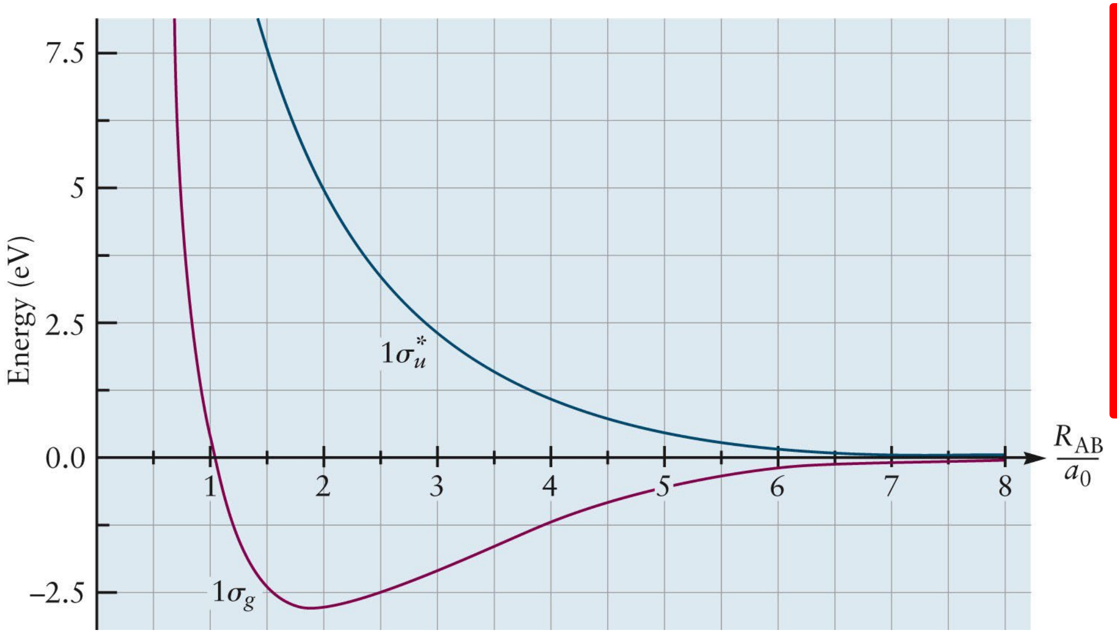
$$\underline{\epsilon_0^{elec}(R) + V_{nn}(R)} - \underline{\epsilon_{atom,0}} =$$

(The ground-state *electronic* energy) + (ion-ion potential of H_2^+ with separation R)



The *total* energy of H_2^+ at *infinite* R

-0.489063 hartree (Provided in the report sheet)

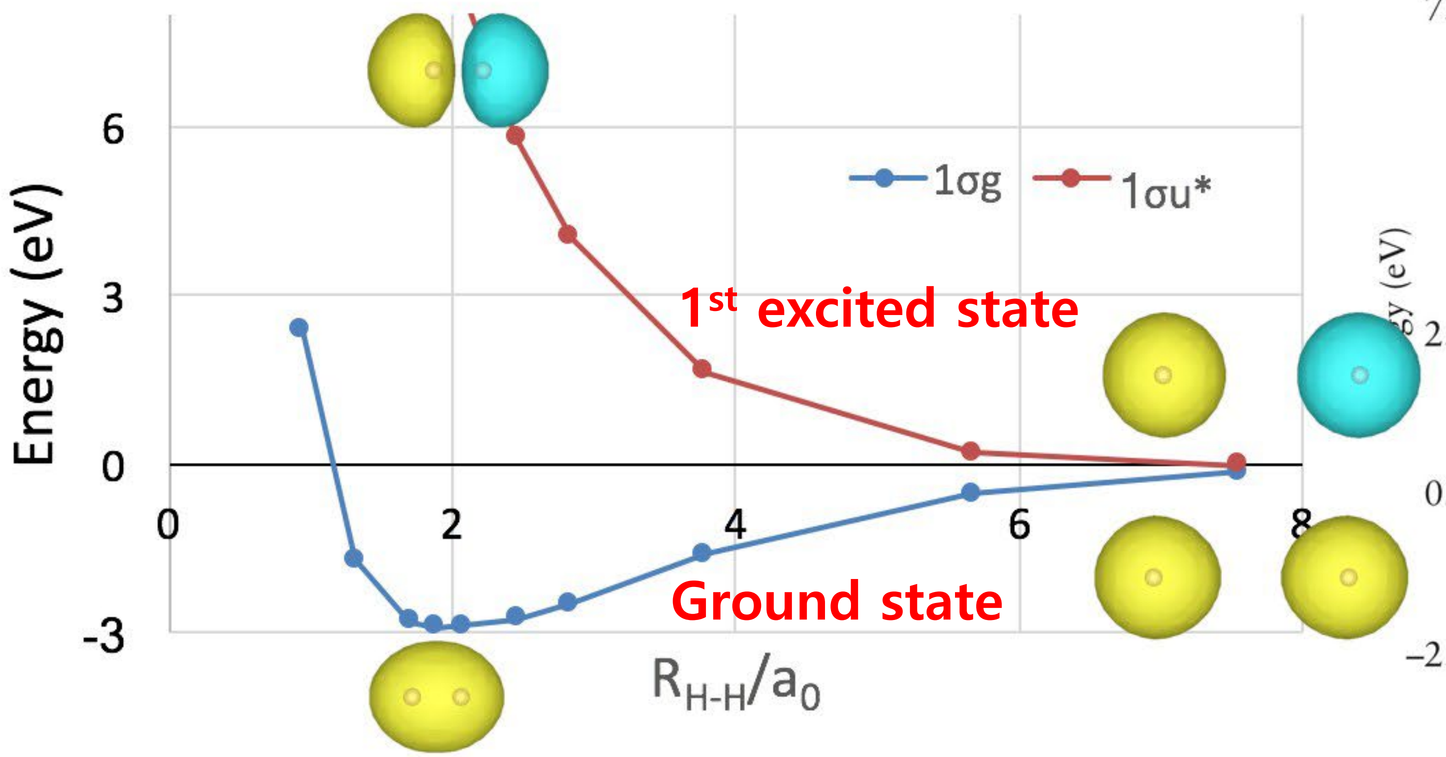


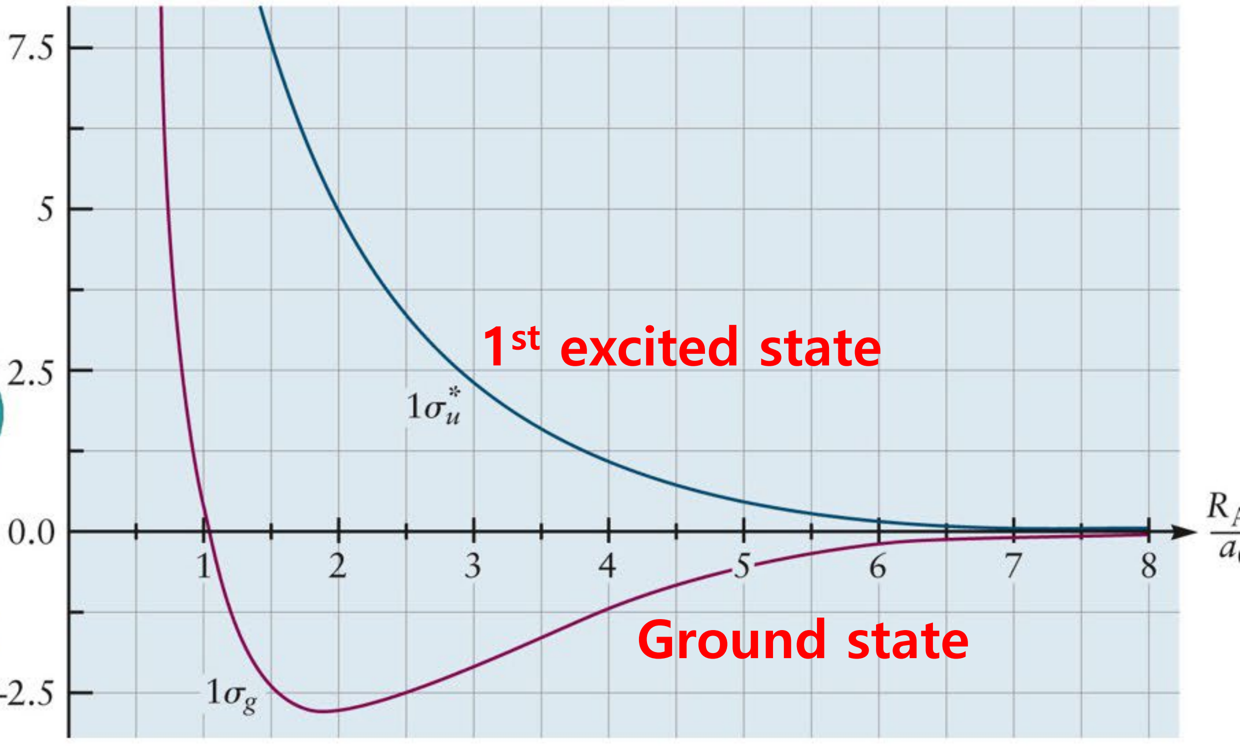
To get a graph as in the text book,

1. Convert the length unit from angstrom to bohr (1 Å ~ 1.889726 bohr).
2. Convert the energy unit from hartree to eV (1 hartree ~ 27.211386 eV).

Ex. If you obtained energy -0.624 hartree at 0.8A°, you should plot (-0.624 x 27.211486eV, 0.8 x 1.889726 Bohr)

Analysis 2. Potential energy curve of H_2^+ first excited state





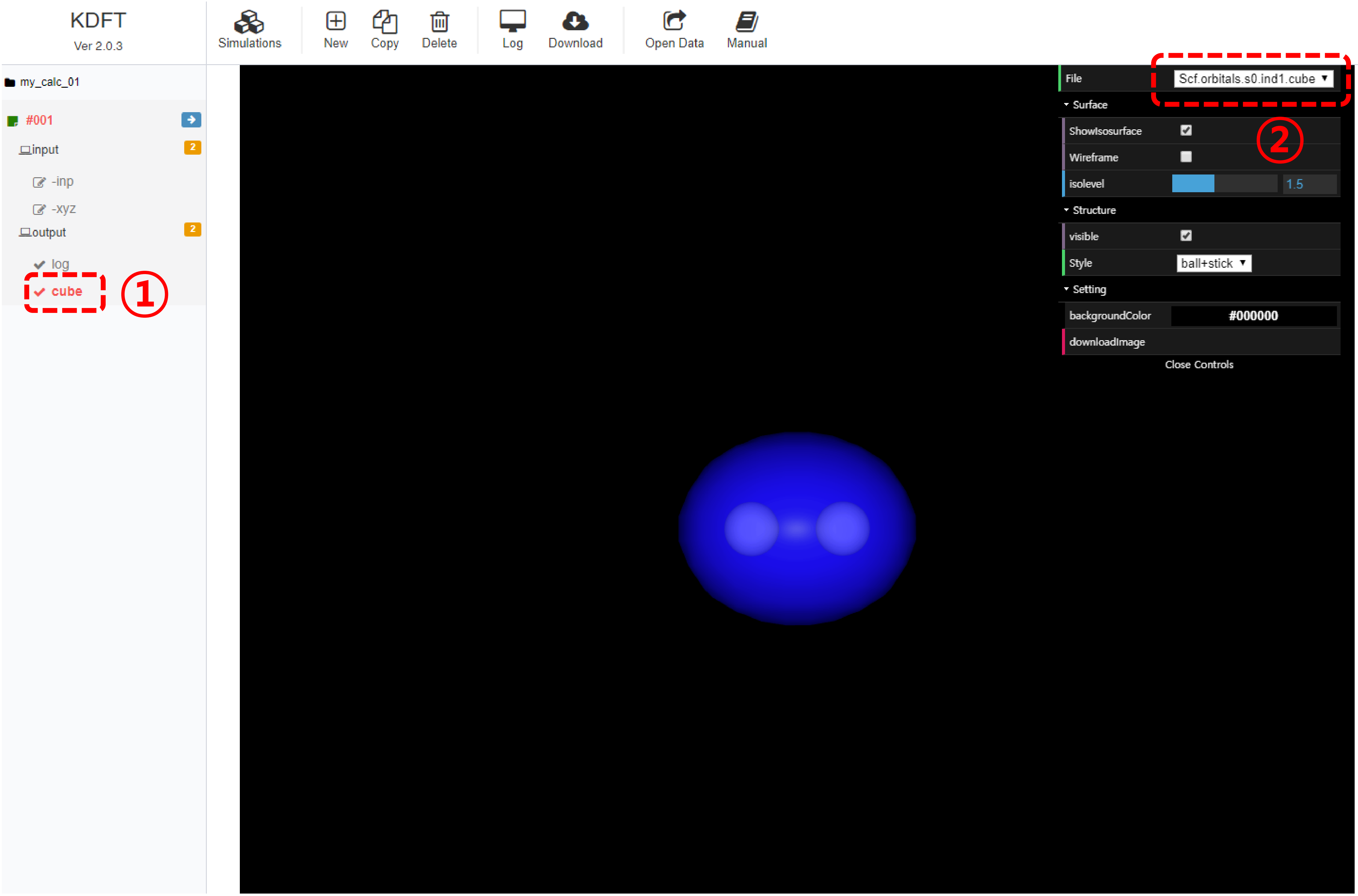
$$\epsilon_{1}^{elec}(R) + \underbrace{V_{nn}(R) - \epsilon_{atom,0}}_{\text{Same as previous}}$$

$\downarrow$

The first excited-state *electronic* energy of H_2^+ with separation R.

Analysis 3. Visualization of orbitals

We will only visualize alpha-spin orbitals ("...**s0**..." cube files).



File: Scf.orbitals.s0.ind1.cube

ShowIsosurface ☑

Wireframe ☐

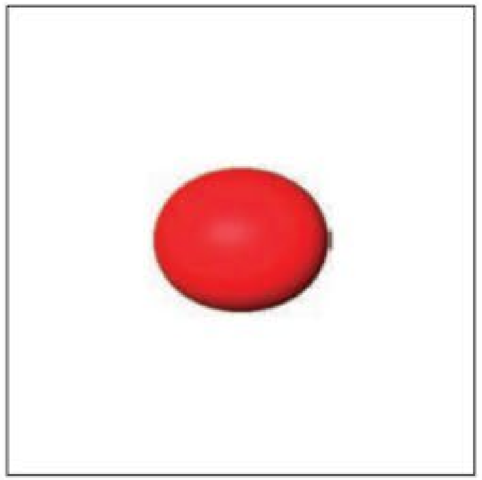
isolevel 1.5

visible ☑

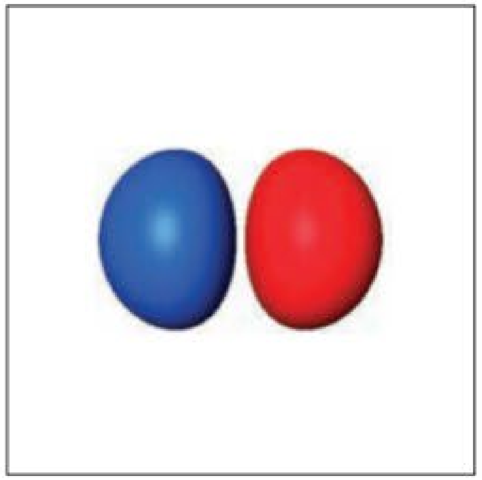
Style: ball+stick

backgroundColor #000000

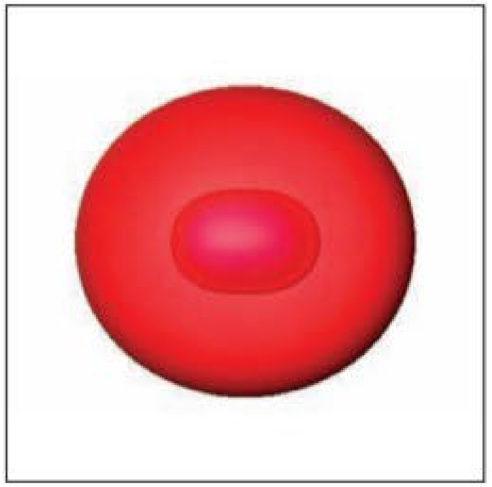
Analysis 3. Visualization of orbitals: Examples



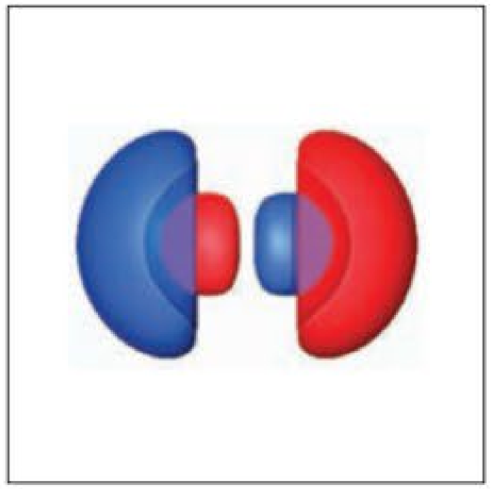
$1\sigma_g$



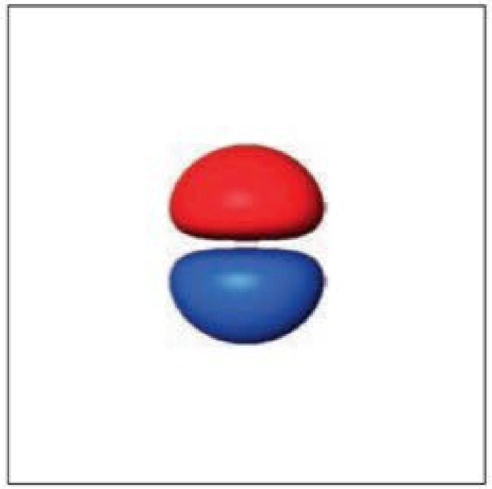
$1\sigma_u^*$



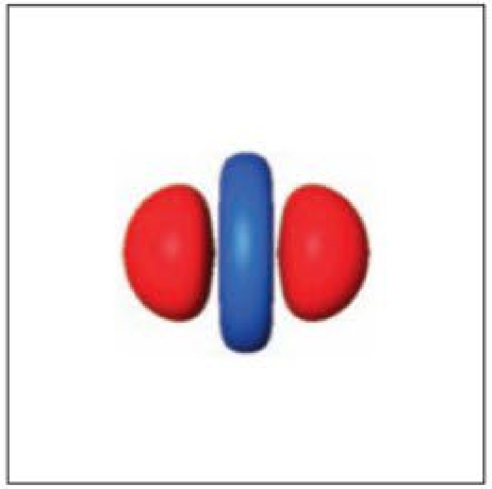
$2\sigma_g$



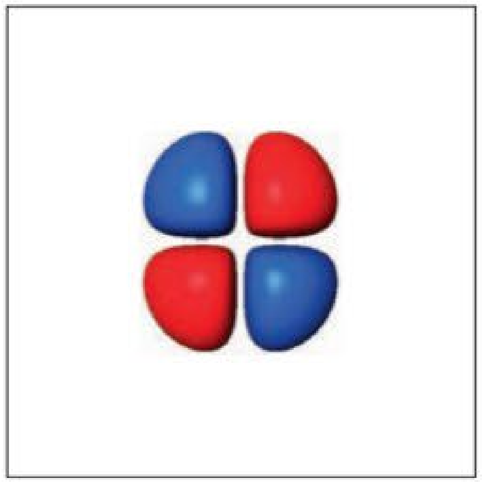
$2\sigma_u^*$



$1\pi_u$



$3\sigma_g$



$1\pi_g^*$

Analysis 3. Visualization of orbitals: **Isosurface setting**

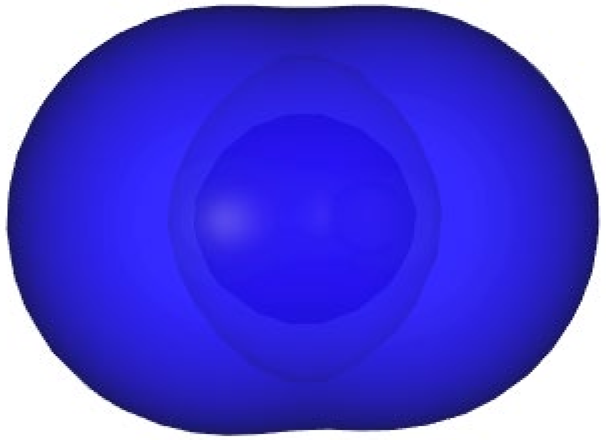
Visualization of a molecular orbital $\phi_i(\mathbf{r})$ is done by plotting the isosurface $S_i(v)$ specified by some value v (the *isovalue*):

$$S_i(v) \coloneqq \{\mathbf{r}: |\phi_i(\mathbf{r})| = v\}.$$

When plotting an orbital, the viewer *automatically* sets some value for v. However, there are some cases where the default value is *not* satisfactory!

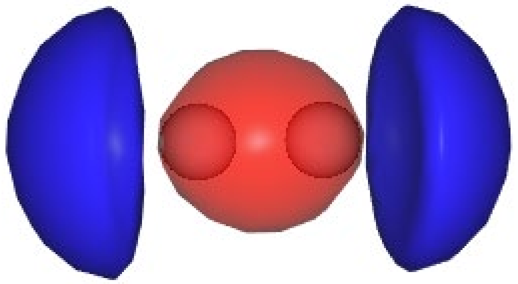
Example of plotting the $2\sigma_g$ orbital of H_2^+:

$S_{2\sigma_g}(v = 0.8)$



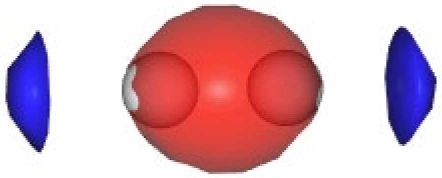
$S_{2\sigma_g}(v = 1.5)$

(default)



The default isosurface does *not* capture the double-shell structure!

$S_{2\sigma_g}(v = 2.0)$

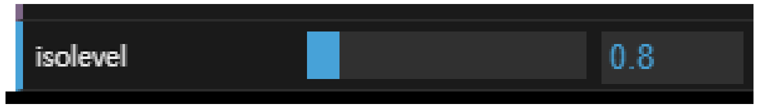


Analysis 3. Visualization of orbitals: **Isosurface setting**

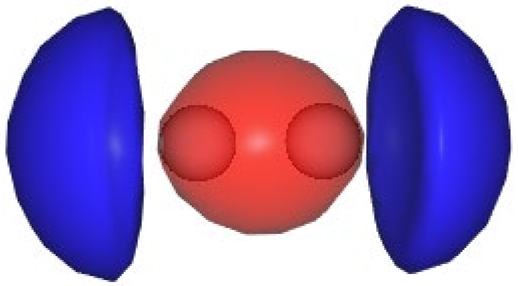
So properly control the isovalue to get a correct view.

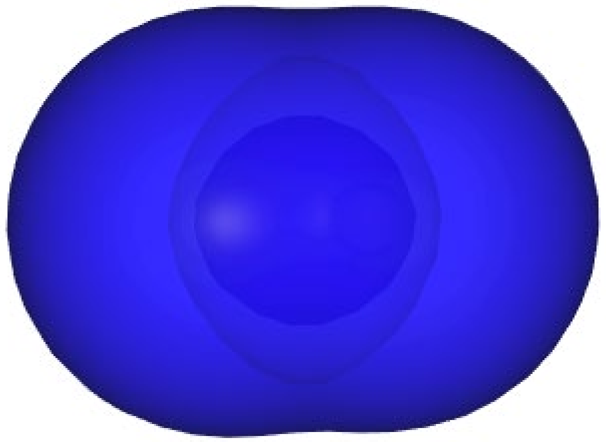
isolevel 1.5

→



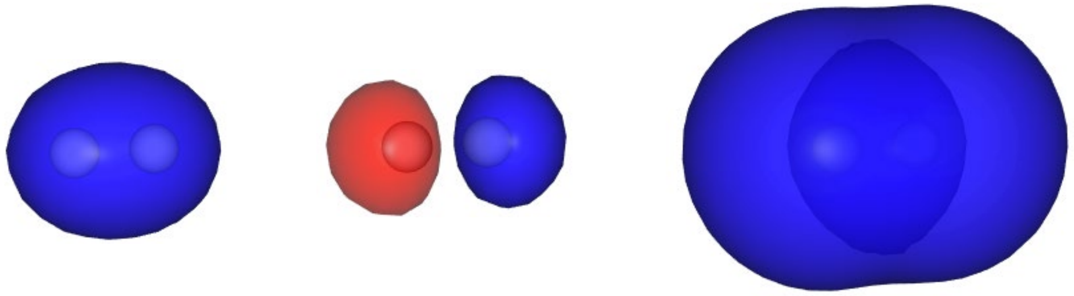
isolevel 0.8





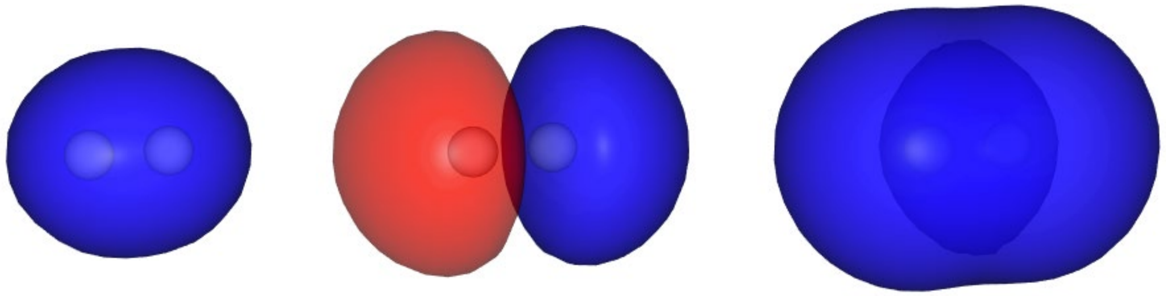
NOTE that when plotting multiple orbitals, use isovalue = 0.8

Incorrect



$v = 1.5$ $v = 3.0$ $v = 0.8$

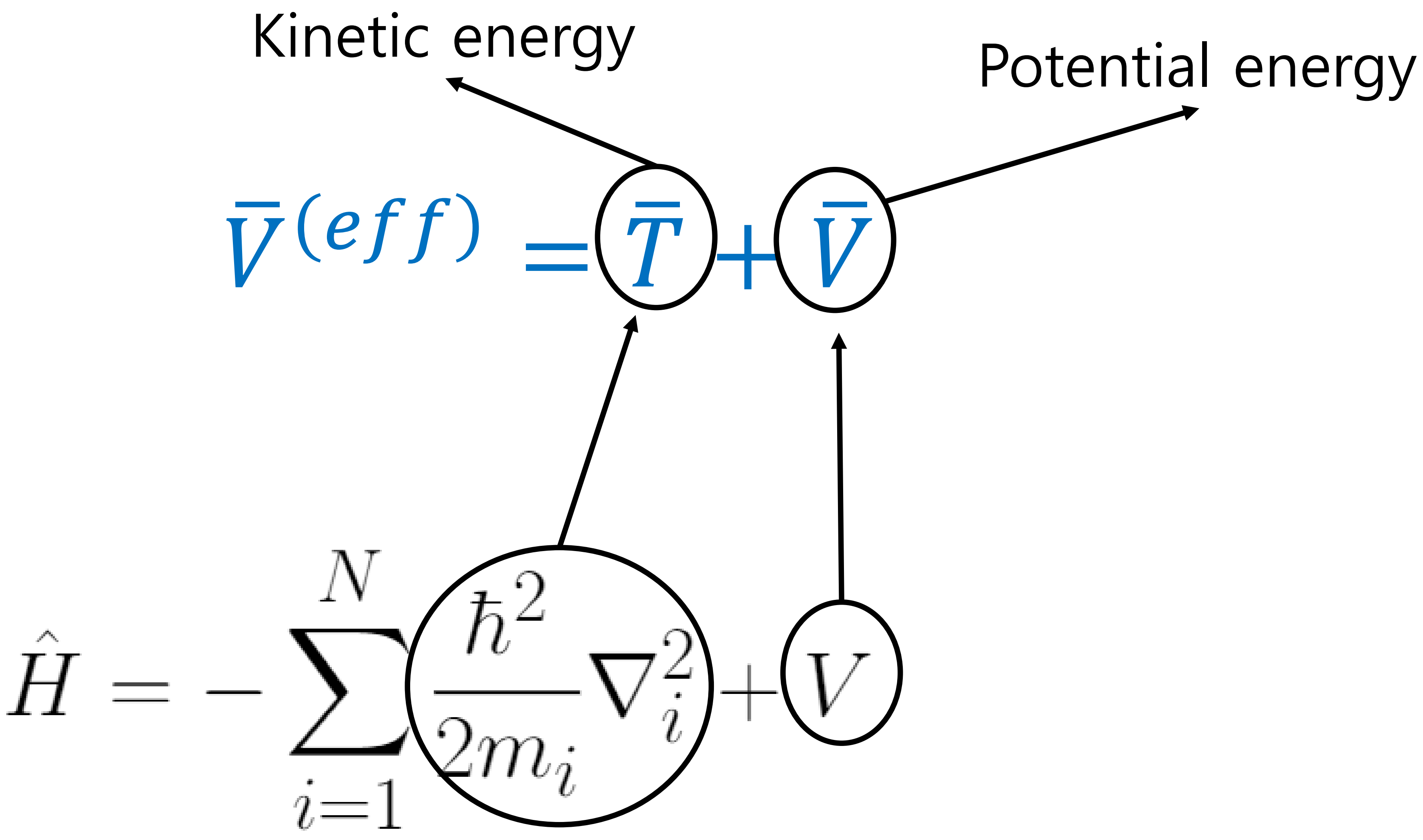
Correct



$v = 0.8$ $v = 0.8$ $v = 0.8$

Analysis 4. (Optional)
Contributions of average potential and kinetic energy

Let’s see how each of the potential energy and kinetic energy contributes to the total energy.



Kinetic energy

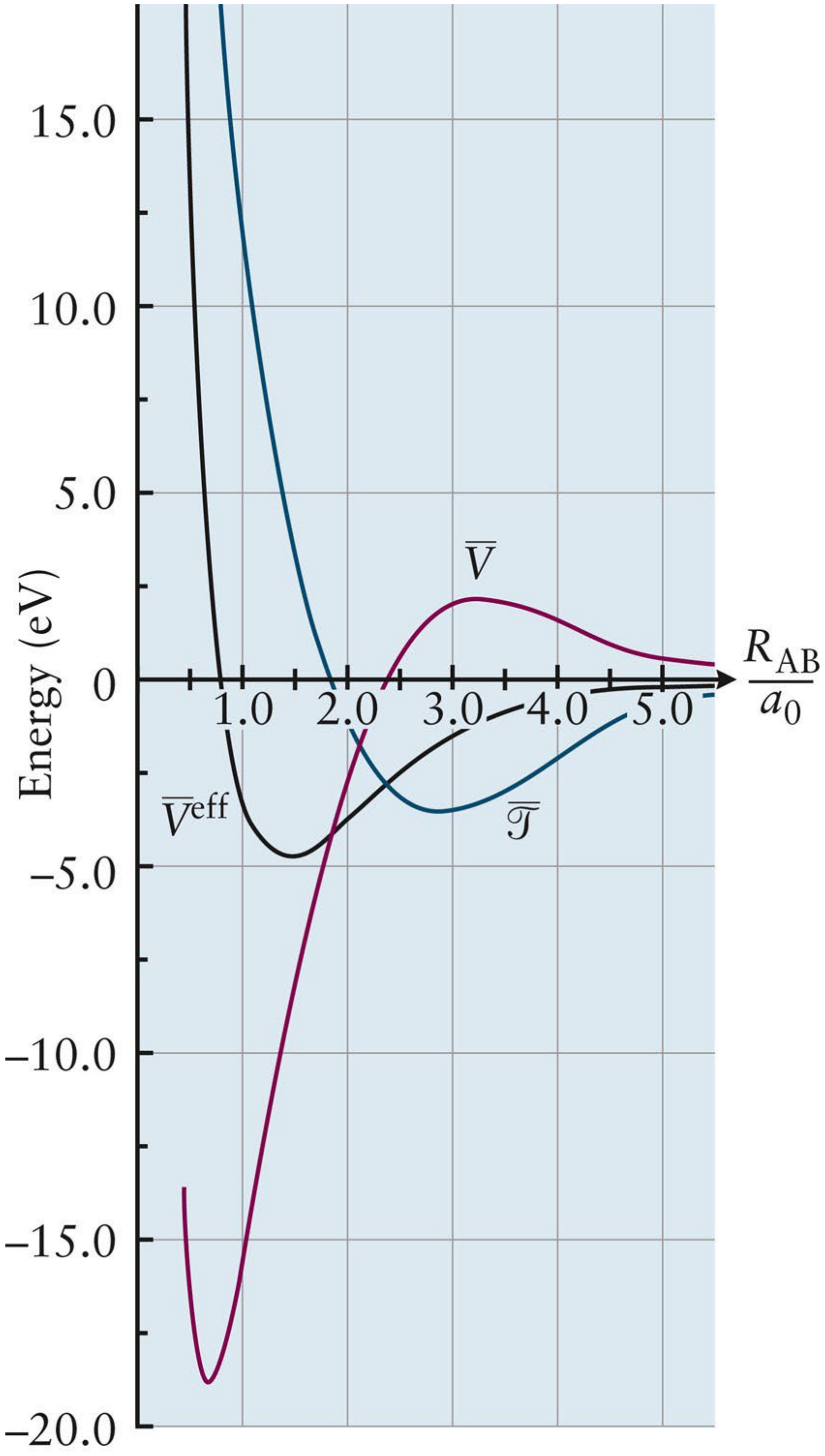
Potential energy

$$\bar{V}^{(eff)} = \bar{T} + \bar{V}$$

$$\hat{H} = -\sum_{i=1}^{N} \frac{\hbar^2}{2m_i}\nabla_i^2 + V$$

Analysis 4. (Optional)
Contributions of average potential and kinetic energy

Let's see how each of the potential energy and kinetic energy contributes to the total energy.



$\bar{V}$ = *total* Coulomb potential energy

= nucleus-nucleus potential energy V_{nn}

\+ nucleus-electron potential energy V_{ne}

\+ electron-electron potential energy V_{ee}

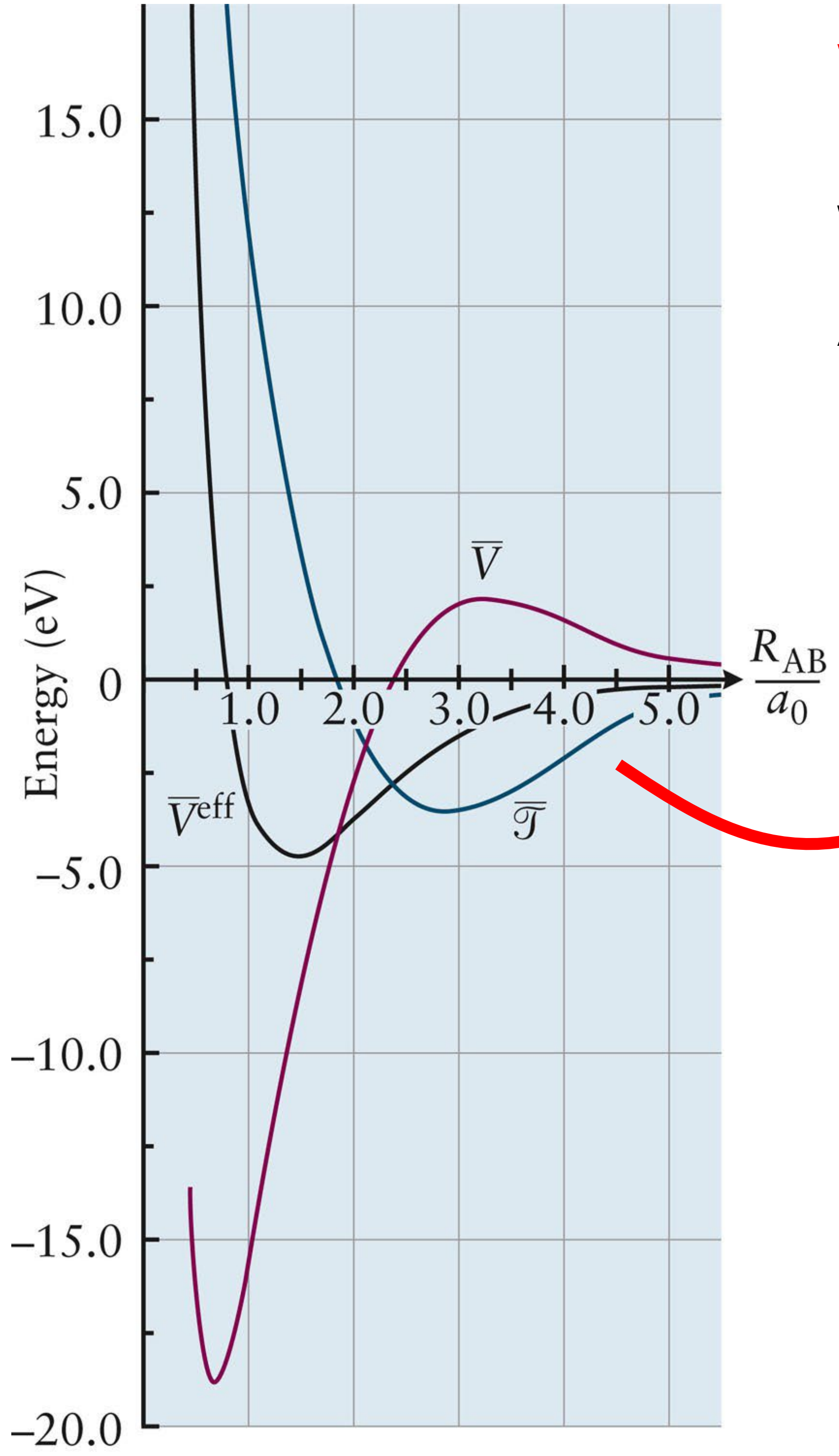
($V_{ee} = 0$ for H_2^+.)

$\bar{T}$ = electronic kinetic energy

$$\bar{V}^{(eff)} = \bar{V} + \bar{T}$$

$\bar{V}^{(eff)}$ is called the effective potential energy, which is actually the total energy that we have calculated.

Analysis 4. (Optional)
Contributions of average potential and kinetic energy



To plot the graph as drawn in the text book, we need to subtract $\bar{V}$ and $\bar{T}$ of **a H atom**.

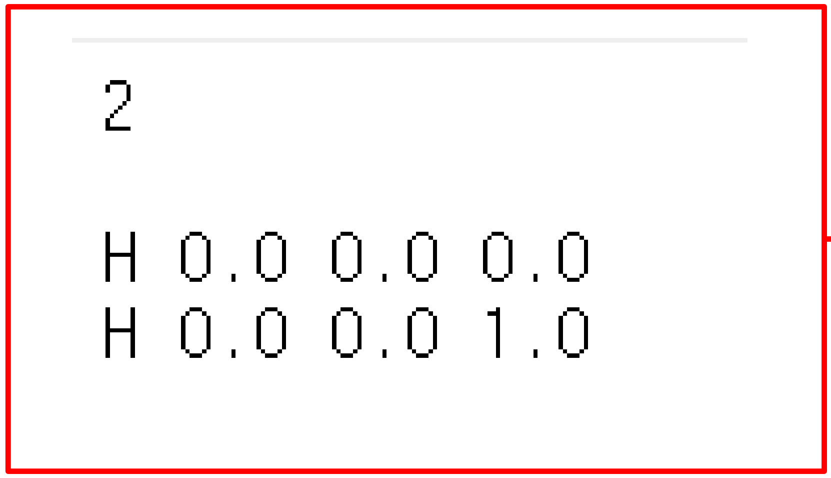
Why?
As said in Theory part, an H^+ ion has no $\bar{V}$ nor $\bar{T}$.
So $\bar{V}$ and $\bar{T}$ of H_2^+ at infinite R equal to
$\bar{V}$ and $\bar{T}$ of a (neutral) H atom.

$$\bar{V}(R) = \bar{V}_{\mathrm{H}_2^+}(R) - \bar{V}_{\mathrm{H\,atom}}(R)$$
$$\bar{T}(R) = \bar{T}_{\mathrm{H}_2^+}(R) - \bar{T}_{\mathrm{H\,atom}}(R)$$

$$\begin{aligned}\bar{V}^{(eff)}(R) &= \bar{V}(R) + \bar{T}(R) \\ &= \bar{V}_{\mathrm{H}_2^+}^{(eff)}(R) - \bar{V}_{\mathrm{H\,atom}}^{(eff)}(R)\end{aligned}$$

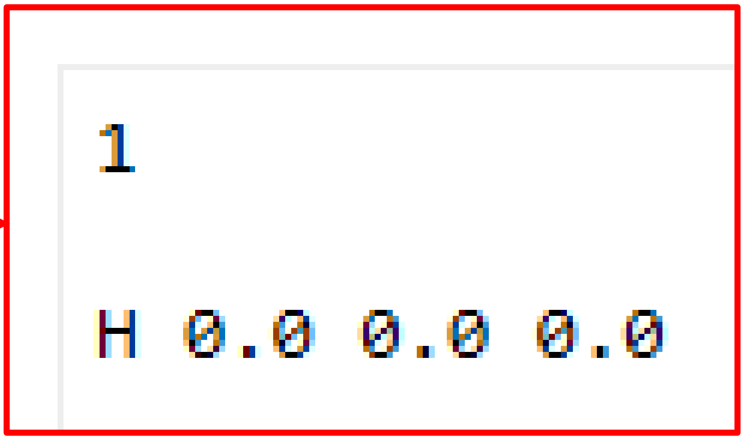
Analysis 4. (Optional)
Contributions of average potential and kinetic energy

To simulate a H atom, run a job with the following **xyz**:



```
2

H 0.0 0.0 0.0
H 0.0 0.0 1.0
```

H_2^+ molecule

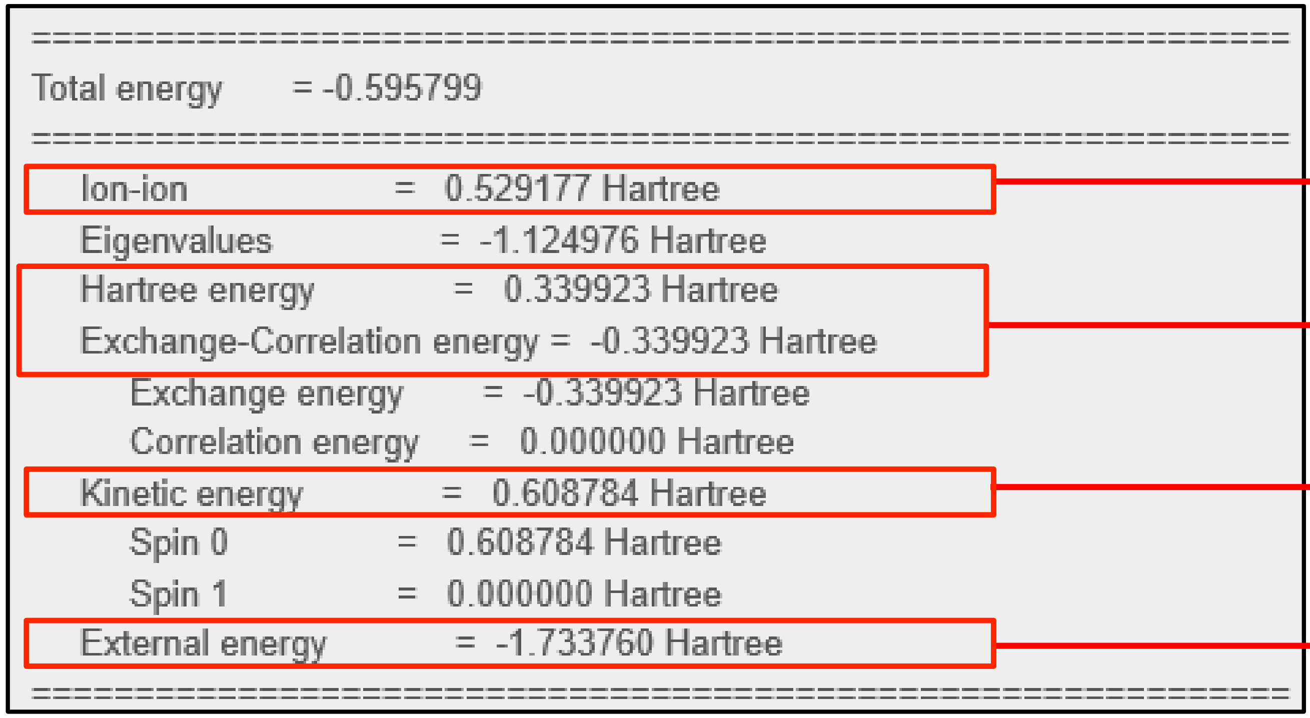


```
1

H 0.0 0.0 0.0
```

H atom

Analysis 4. (Optional)
Contributions of average potential and kinetic energy

Calculation result of 1.0-Å H_2^+:



```
==============================================================
Total energy     = -0.595799
==============================================================
   Ion-ion                =   0.529177 Hartree
   Eigenvalues              = -1.124976 Hartree
   Hartree energy           =   0.339923 Hartree
   Exchange-Correlation energy = -0.339923 Hartree
      Exchange energy        = -0.339923 Hartree
      Correlation energy     =   0.000000 Hartree
   Kinetic energy           =   0.608784 Hartree
      Spin 0               =   0.608784 Hartree
      Spin 1               =   0.000000 Hartree
   External energy          = -1.733760 Hartree
==============================================================
```

V_{nn} of H_2^+

V_{ee} of H_2^+

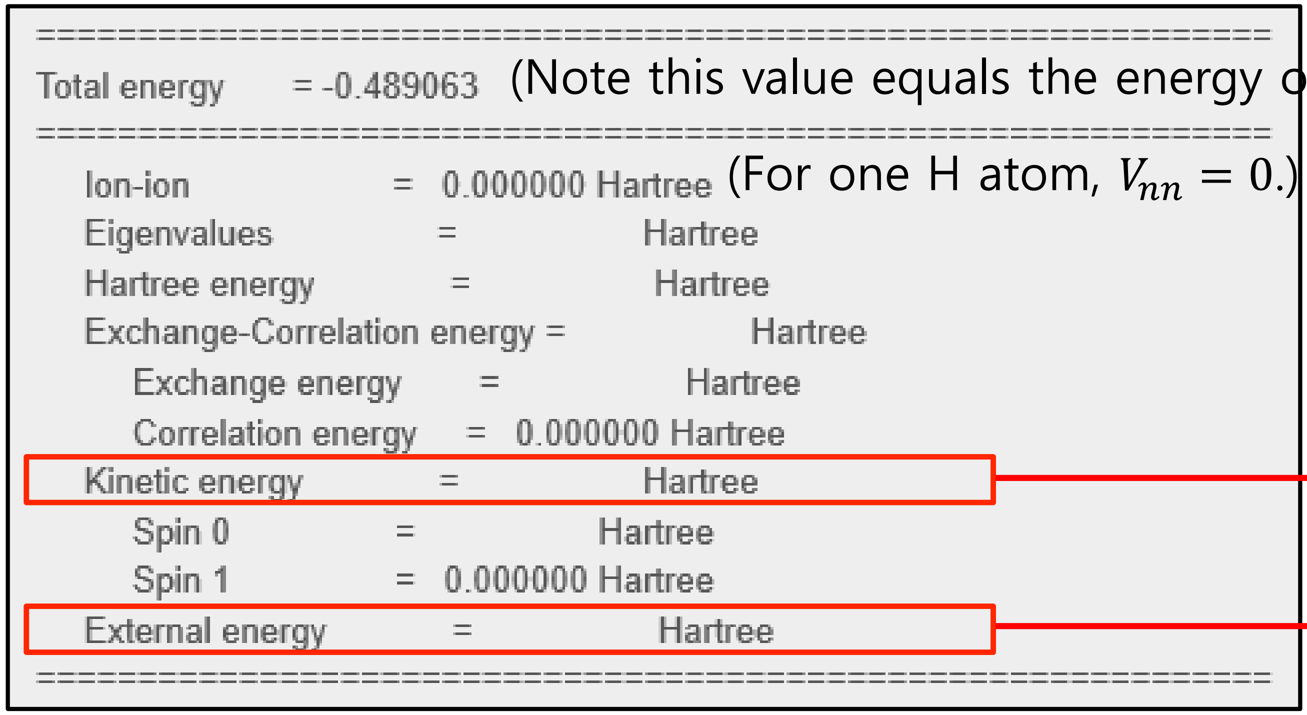
$\bar{T}$ of H_2^+

V_{ne} of H_2^+

$\bar{V}$ of H_2^+

$\bar{V}^{(eff)}$ of H_2^+

Calculation result of a H atom:



```
==============================================================
Total energy     = -0.489063
==============================================================
   Ion-ion                =   0.000000 Hartree
   Eigenvalues              =              Hartree
   Hartree energy           =              Hartree
   Exchange-Correlation energy =              Hartree
      Exchange energy        =              Hartree
      Correlation energy     =   0.000000 Hartree
   Kinetic energy           =              Hartree
      Spin 0               =              Hartree
      Spin 1               =   0.000000 Hartree
   External energy          =              Hartree
==============================================================
```

(Note this value equals the energy of $\mathrm{H_2}(R \rightarrow \infty)$ in the report sheet.)

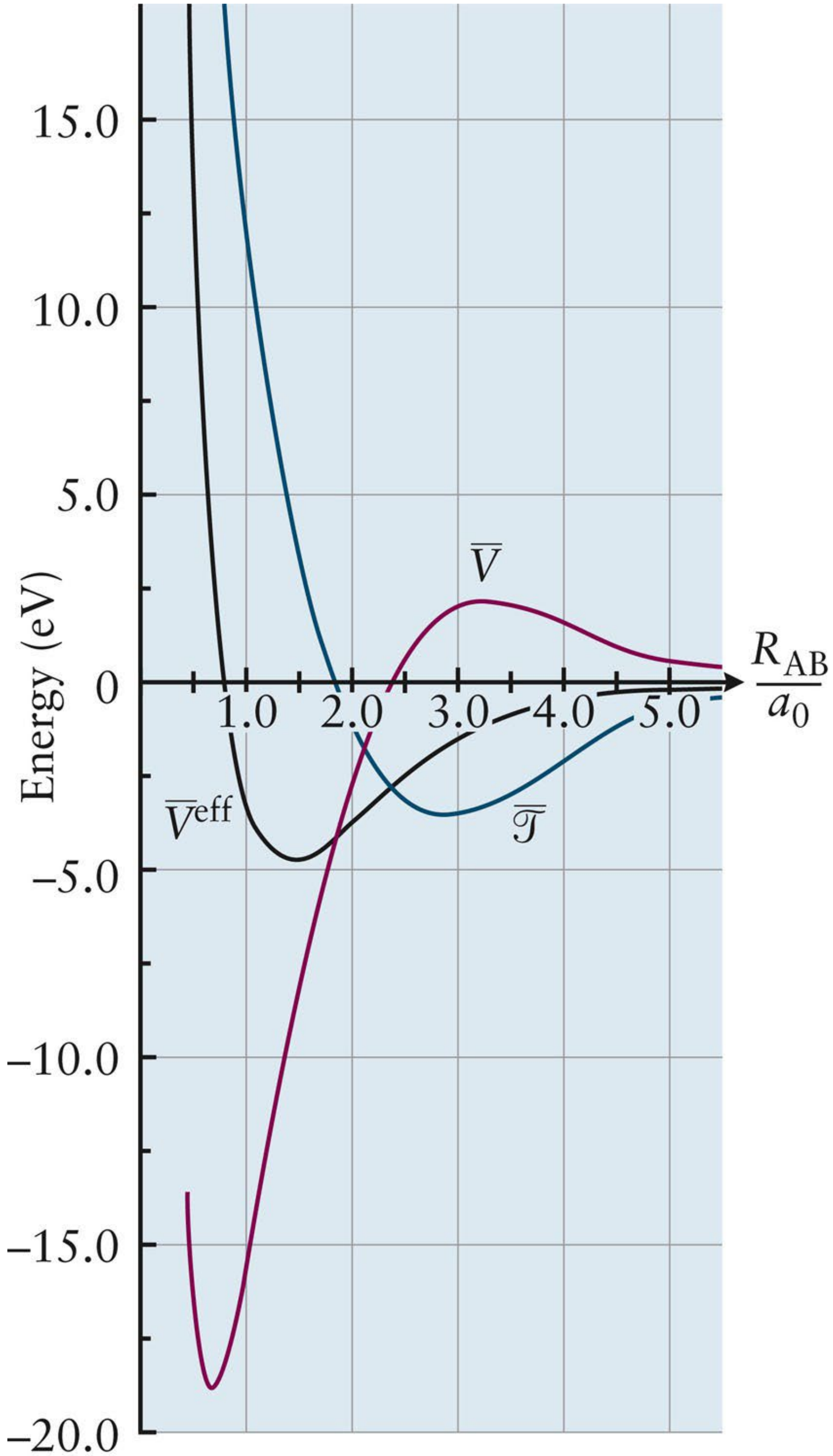
(For one H atom, $V_{nn} = 0$.)

$\bar{V}^{(eff)}$ of a H atom

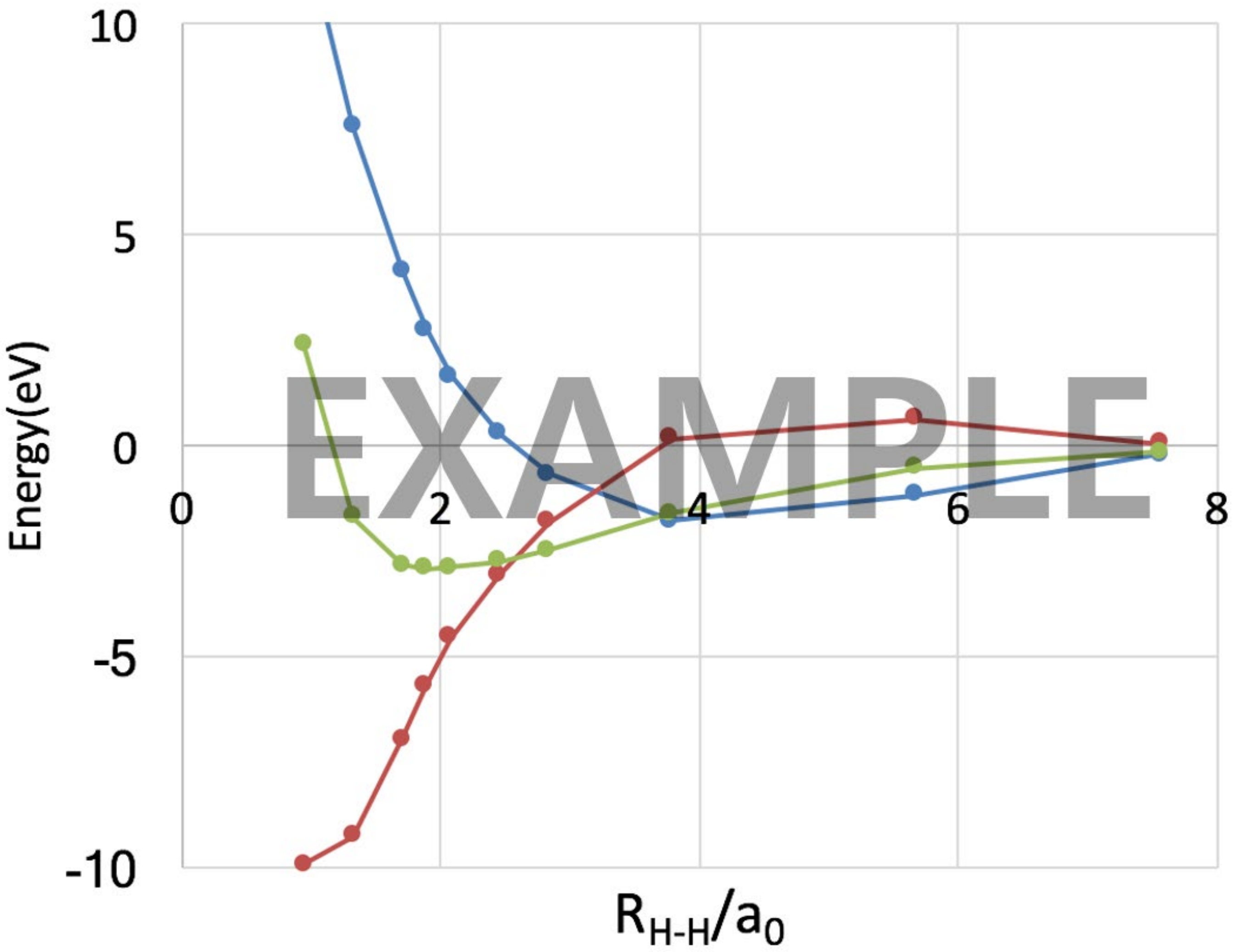
$\bar{T}$ of H atom

V_{ne} of H atom = $\bar{V}$ of H atom

Analysis 4. (Optional)
Contributions of average potential and kinetic energy



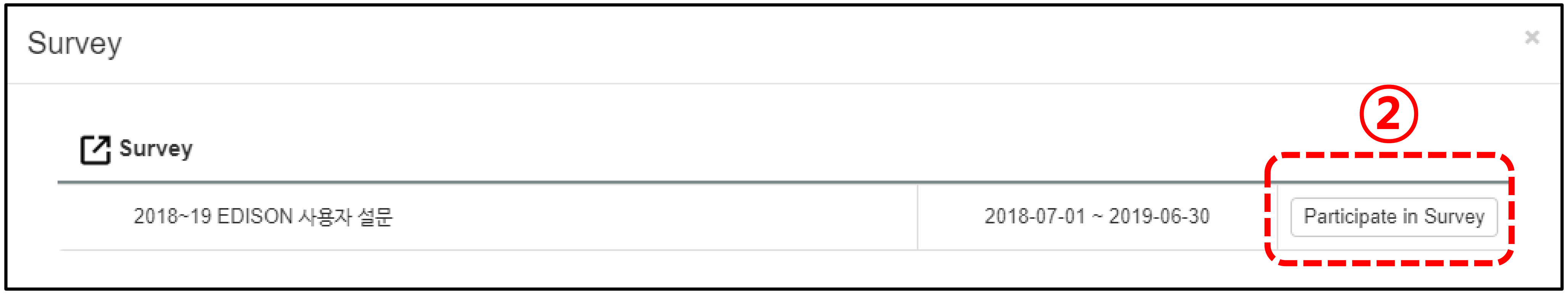
Using your ten H_2^+ simulations
and one single-H-atom simulation,
draw eV-bohr plots of $\bar{V}$, $\bar{T}$ and $\bar{V}^{(eff)}$.



Portal survey

Please answer the survey about your experience of the EDISON portal.
All answers will help improve the portal for better user experience!

NOTE that the questions are provided in **Korean**.



2018~19 EDISON 사용자 설문 2018-07-01 ~ 2019-06-30

You may skip this if there is no Survey button shown!