STATE-Senri

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STATE-Senri

(Simulation Tool for Atom TEchnology)

- Density Functional Theory
  LDA、GGA、GGA+U、vdW-DF
- Ultrasoft pseudopotential
- Plane wave basis set
- Iterative diagonalization
  Davidson method, RMM-DIIS method
- Broyden charge density mixing
- Fortran90+MPI+OpenMP: Very good parallelization efficiency.

--> Applicable to wide range of materials.

STATE-Senri

(Simulation Tool for Atom TEchnology)

- Structure Optimization
- Finite Temperature Molecular Dynamics
- Reaction Path Search
- ESM to calculate electro-cheimcal reactions and electric field effects.
- Vibrational Spectra (IR, HREELS)、Electronic States (XPS, UPS)、STM Image calculations

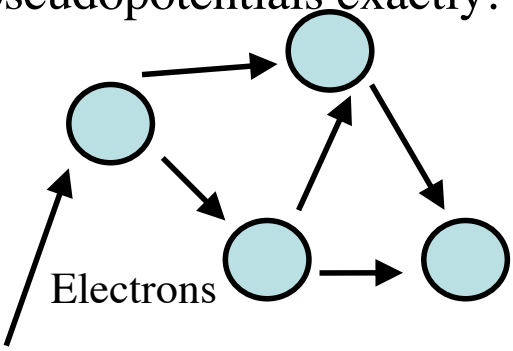
Pseudopotential Method

- Core Electrons: Tightly bound to nuclei
  --> Localized close to nuclei.
- Valence Electrons: Weakly bound to nuclei
  --> Delocalized around neighboring atoms.
- Physical and chemical properties of materials should be mainly governed by the valence electron states.

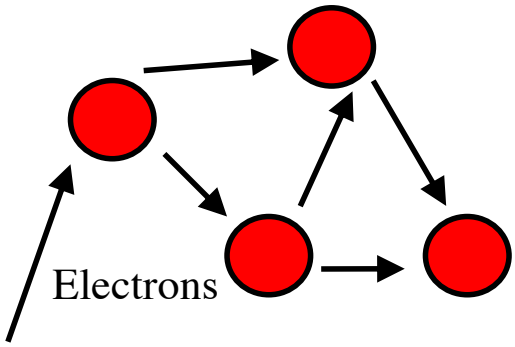
  --> Necessary to reproduce valence electron states accurately.

Concept of Pseudopotential

- Atom : Scattering potential of electrons.
- Core electrons are localized within spheres of radius r_c
- If the scattering properties of pseudopotentials outside of radius r_c are the same as those of true atomic potentials, then the valence electron states should be reproduced by pseudopotentials exactly.



True atomic potentials



Pseudopotentials which have exactly the same scattering properties for valence electrons

Advantages of the pseudopotential method

- It is as accurate as an all-electron full-potential linearized augumented plane wave (FLAPW) method for valence states.
- It is computationally fast because it does not calculate core states explicitly.
- Required number of effective digits can be smaller compared with all-electron methods because it does not treat core states of which energies have large absolute values.
- Pseudopotentials and pseudowave functions are smooth and can be expanded by plane wave basis sets efficiently.

Norm-conserving pseudopotentials

To construct norm-conserving pseudopotentials, we first perform all-electron calculation for an isolated atom and obtain energy eigenvalues ε_l, wave functions $\psi_l(r)$, and, self-consistent effective potential $V^{\mathrm{AE}}(r)$. l is an angular momentum quantum number of a valence state.
satisfies the following Kohn-Sham equation.

$$\left(T + V^{\mathrm{AE}}(r)\right)\psi_l(r) = \varepsilon_l \psi_l(r),$$

$$T = -\frac{1}{2r^2}\frac{d}{dr}r^2\frac{d}{dr} + \frac{l(l+1)}{2r^2},$$

$$\langle \psi_l | \psi_l \rangle = \int_0^\infty \left|\psi_l(r)\right|^2 r^2 dr = 1.$$

Costruction of pseudo wave function

Next, we construct pseudowave function $\varphi_l(r)$ by smoothing true wave function $\psi_l(r)$ inside the cutoff radius of r_{cl}.
Usually, we expand $\varphi_l(r)$ by polynomial functions inside the r_{cl}.

$$\varphi_l(r) = \begin{cases} \psi_l(r) & \text{for } r \geq r_{\mathrm{cl}} \\ \sum_{t=0}^{M} c_{l,2t} r^{2t+l} & \text{for } r \leq r_{\mathrm{cl}} \end{cases}$$

Two more constraints are imposed on $\varphi_l(r)$

- They are nodeless inside r_{cl}.
- The norm-conserving condition:

$$\int_0^{r_{\mathrm{cl}}} \left|\psi_l(r)\right|^2 r^2 dr = \int_0^{r_{\mathrm{cl}}} \left|\varphi_l(r)\right|^2 r^2 dr.$$

The norm-conserving condition is very important to ensure the accuracy of pseudopotentials.

Construction of pseudopotentials

By solving the Kohn-Sham equation inversely, pseudo-potential $V_l(r)$ which acts pseudowave function $\varphi_l(r)$.

$$V_l(r) = \frac{(\varepsilon_l - T)\varphi_l(r)}{\varphi_l(r)}.$$

Pseudopotentials become angular momentum dependent and therefore, they are non-local. Usually, angular momentum dependence are taken into account only up to l=2 and pseudo-potentials for l>2 are replaced by a common potential $V_{\mathrm{loc}}(r)$.

$$V^{\mathrm{ps}} = \sum_{l,m=0}^{l=l_{\max},m=l} |Y_{lm}\rangle (V_l(r) - V_{\mathrm{loc}}(r)) \langle Y_{lm}| + V_{\mathrm{loc}}(r)$$

where, $|Y_{lm}\rangle$ are projectors onto states with angular quantum numbers of l and m momentum.

Norm-conserving Pseudopotential

- The norm-conserving pseudopotentials are constructed by imposing the following three conditions.

1. They reproduce correct eigenenergies ε_l for valence electrons.
2. Pseudo-wave functions coincide with all-electron wave functions outside the cutoff radii r_{cl}.
3. Pseudo-wave functions have correct norm inside the cutoff radii r_{cl}.

$$4\pi \int_0^{r_c} \left|\psi_l^{\mathrm{AE}}(r)\right|^2 r^2 dr = 4\pi \int_0^{r_c} \left|\psi_l^{\mathrm{ps}}(r)\right|^2 r^2 dr$$

$$= -2\pi \left(r\psi_l^{\mathrm{AE}}\right)^2 \frac{d}{d\varepsilon}\frac{d}{dr} \ln \psi_l^{\mathrm{AE}} \Big|_{r_c}$$

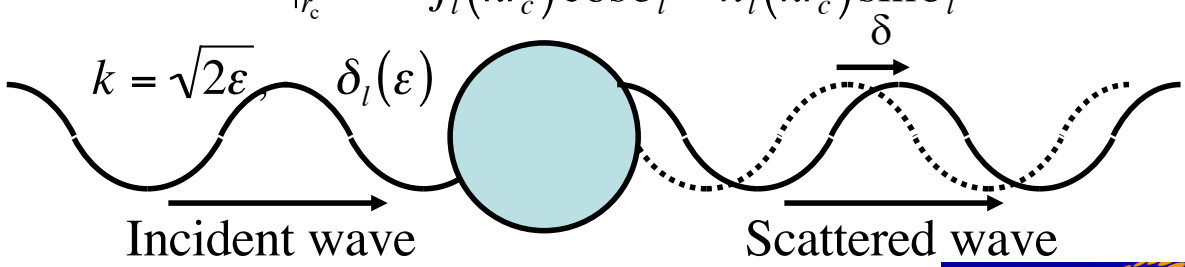
The norm-conserving condition

The norm-conserving condition can be related to logarithmic derivatives of wave functions by the following equation.

$$\int_0^{r_c} |\psi_l(r)|^2 r^2 dr = \int_0^{r_c} |\phi_l(r)|^2 r^2 dr = -\frac{1}{2}(r\phi_l(r))^2 \frac{d}{d\varepsilon}\frac{d}{dr}\ln\phi_l(r)\Big|_{r_c}$$

The logarithmic derivatives of wave functions can be related to phase shifts of scattered wave functions by spherical potentials.

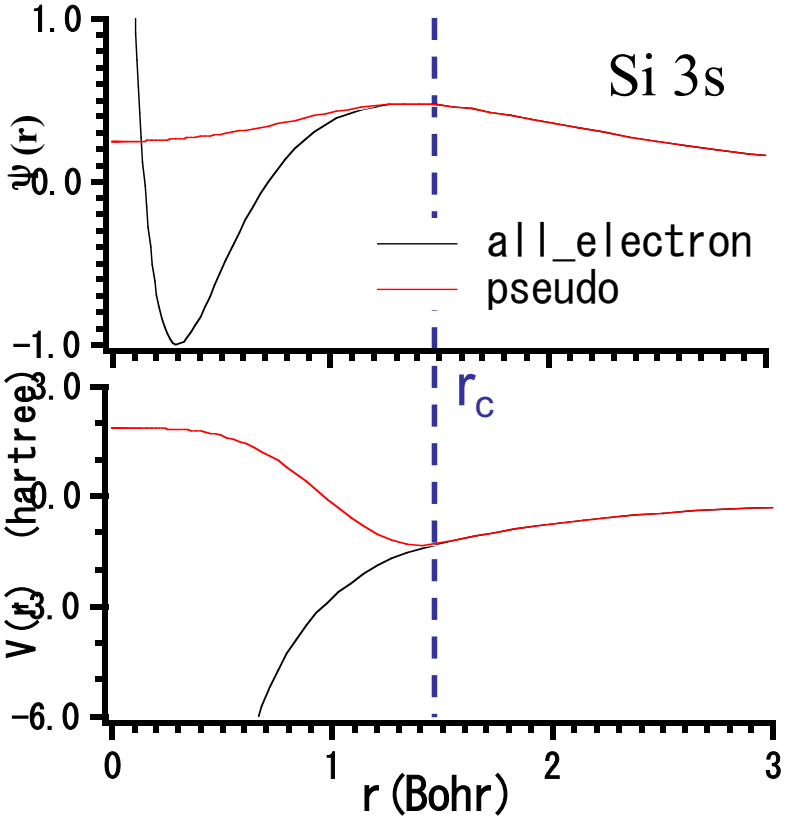
$$\frac{d}{dr}\ln\phi_l(r)\Big|_{r_c} = \frac{k\left[j_l'(kr_c)\cos\delta_l - n_l'(kr_c)\sin\delta_l\right]}{j_l(kr_c)\cos\delta_l - n_l(kr_c)\sin\delta_l},$$



The norm-conserving condition

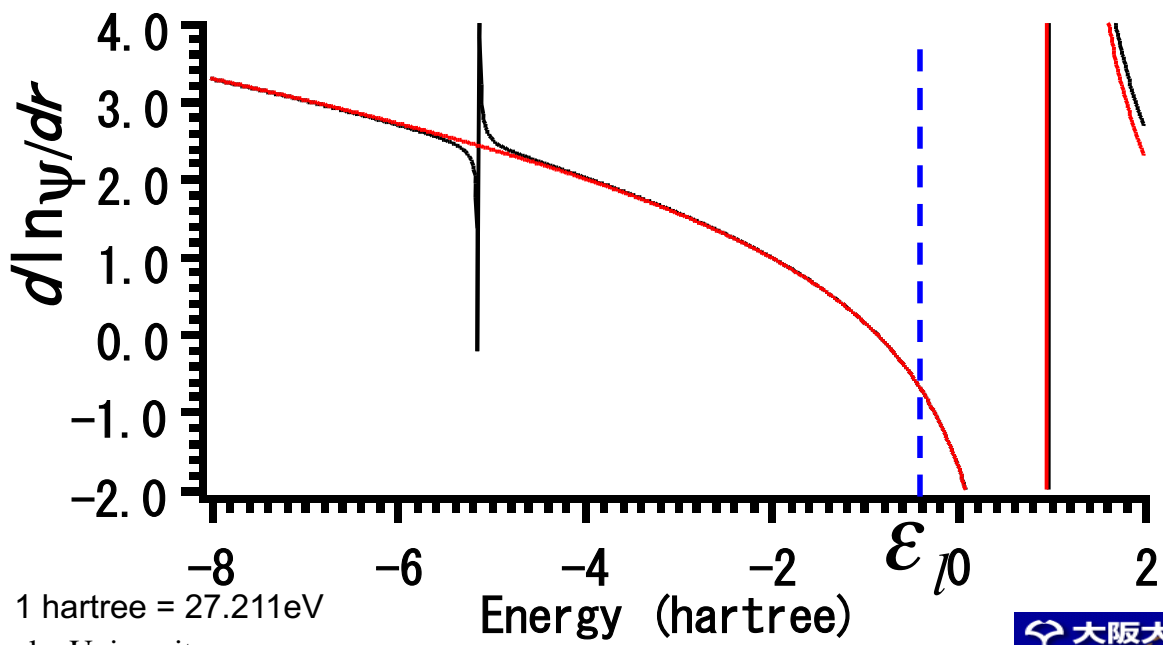
A pseudo-wave function $\varphi_l(r)$ is constructed in such a way that it has the correct scattering property at the eigen energy ε_l outside the cutoff radius r_{cl}. By imposing the norm-conserving condition, the scattering property becomes correct not only at the eigen energy ε_l but also at other energies ε up to the first order of ε-ε_l. Therefore, the norm-conserving condition is very important to ensure the accuracy of pseudopotentials.

Norm-conserving pseudopotential



Norm-conserving pseudopotential

- The logarithmic derivative of pseudo-wave function agrees with that of true wave function in wide range of energy.



1 hartree = 27.211eV

Plane Wave Basis Set

- Pseudopotentials and pseudo-wave functions can be expanded by plane waves efficiently because they are quite smooth.

$$\left|\psi_{i,\mathbf{k}}\right\rangle = \sum_{\mathbf{G}}^{|\mathbf{k}+\mathbf{G}|\le G_{\max}} c_{i,\mathbf{k}+\mathbf{G}}\left|\mathbf{k}+\mathbf{G}\right\rangle,$$

$$\left\langle \mathbf{r}\middle|\mathbf{k}+\mathbf{G}\right\rangle = \frac{1}{\sqrt{\Omega_{\mathrm{a}}}}\exp\left(i\left(\mathbf{k}+\mathbf{G}\right)\bullet\mathbf{r}\right),$$

Ω_{a} : Unit cell volume

$$\left\langle \mathbf{k}+\mathbf{G}\middle|\mathbf{k}'+\mathbf{G}'\right\rangle = \delta_{\mathbf{k}\mathbf{k}'}\delta_{\mathbf{G}\mathbf{G}'}$$

Cutoff Wavenumber (Cutoff Energy)

The number of reciprocal points ***G*** used in plane wave expansion is, in principle, infinite. However, in practice, it should be finite and the summation with respect to ***G*** should be cutoff. Usually, we cutoff ***G*** in such a way that the norm of ***k***+***G*** is smaller than a cutoff wave number $G_{\max}$.

$$\psi_{i\mathbf{k}}\left(\mathbf{r}\right) = \sum_{\mathbf{G}}^{|\mathbf{k}+\mathbf{G}|\le G_{\max}} c_{i\mathbf{k}+\mathbf{G}}\frac{1}{\sqrt{\Omega}}\exp\left(i\left(\mathbf{k}+\mathbf{G}\right)\bullet\mathbf{r}\right),$$

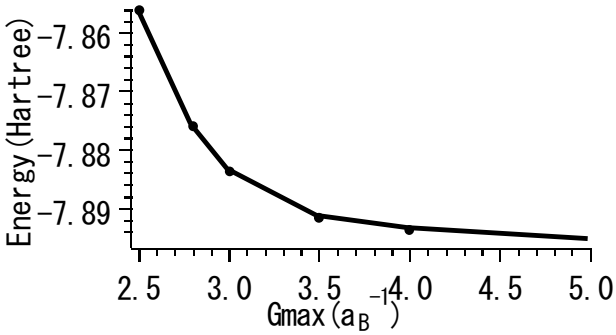
c_{ik} is a Fourier transofrm of $\psi_{ik}(\boldsymbol{r})$.

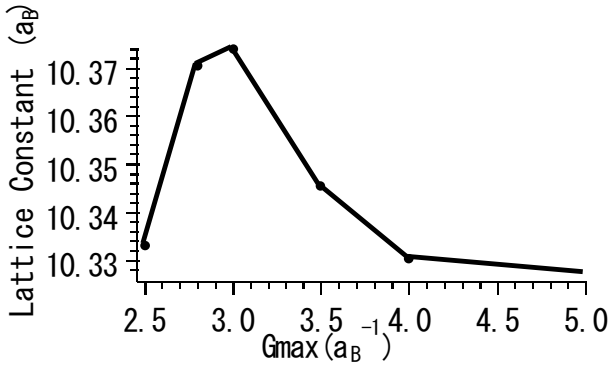
$$c_{i\mathbf{k}+\mathbf{G}} = \frac{1}{\sqrt{\Omega}}\int_{\Omega}\exp\left(-i\left(\mathbf{k}+\mathbf{G}\right)\bullet\mathbf{r}\right)\psi_{i\mathbf{k}}\left(\mathbf{r}\right)d\mathbf{r}.$$

$2\pi/G_{\max}$ corresponds to the spacial resolution of the basis set. Therefore, the required $G_{\max}$ depends on the steepness of pseudo-wave functions.

$G_{\max}^2$ is called "Cutoff Energy".

Cutoff Wavenumber: Example Si





By using G_{max}=3.5 a_B^{-1}, the total energy is converged within 0.1 eV and the lattice constant is within 0.001 nm. In general, energy differences among different structures converge better than the absolute values of total energies.

1 Hartree = 27.2116 eV

Advantages of Plane Wave Basis Set

- The size of a plane wave basis set can be enlarged systematically by increasing the cutoff G_{max}.
  --> No Over Completeness Problem!
- The whole space can be covered with the same accuracy.
  --> No Basis Set Superposition Error!
- Atomic forces can be easily calculated because of the Hellmann-Feynman theorem for the derivative of the total energy with respect to atomic positions.

$$\mathbf{F}_I = -\frac{d}{d\mathbf{R}_I} E_{\mathrm{T}}$$

$$= -\sum_{i\mathbf{k}} f_{i\mathbf{k}} \langle \psi_{i\mathbf{k}} | \frac{\partial}{\partial \mathbf{R}_I} \left(V_{\mathrm{loc}}^{\mathrm{ion}} + V_{\mathrm{NL}} \right) | \psi_{i\mathbf{k}} \rangle - \frac{d}{d\mathbf{R}_I} E_{\mathrm{EW}}$$

- Very efficient FFT can be used.

Problem in Norm Conserving Pseudopotentials

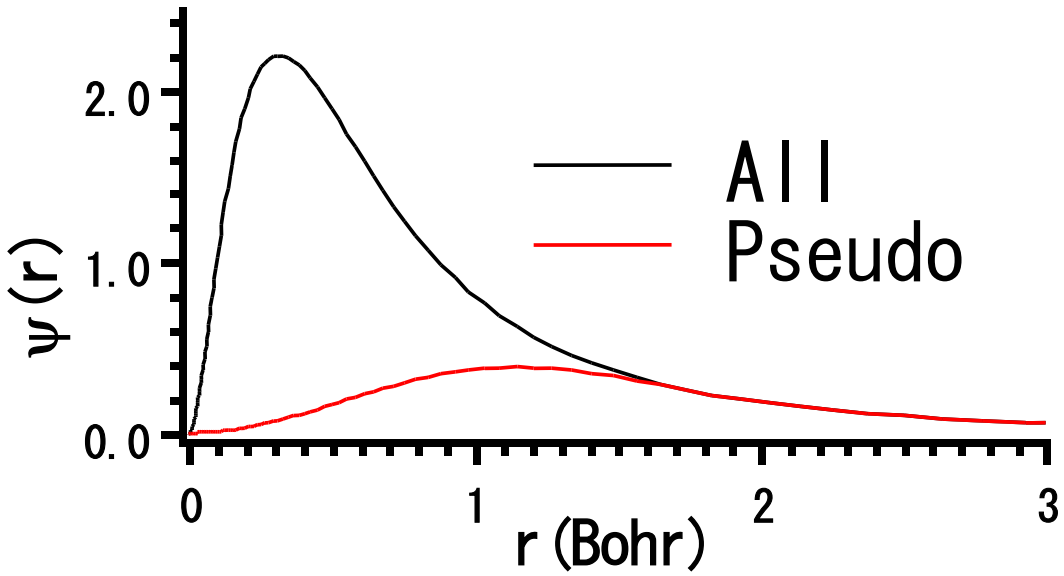
- Nodeless wave functions such as O2*p* and Cu 3*d*.

→Wave functions have large amplitude close to nuclei.

→To satisfy the norm-conserving condition, pseudo-wave functions should also have large amplitude near nuclei.

→The required number of plane waves to expand steep pseudo-wave functions becomes large and calculations become very heavy.

Ultrasoft Pseudopotential



- By removing the norm-conserving condition, pseudo-wave functions can be very smooth.

→ Ultrasoft Pseudopotential

Generalized Norm-conserving Condtion

$$4\pi\int_0^{r_c}\left|\psi_l^{\mathrm{AE}}(r)\right|^2 r^2 dr = \left\langle\psi_l^{\mathrm{AE}}\middle|\psi_l^{\mathrm{AE}}\right\rangle_{r_c} = \left\langle\psi_l^{\mathrm{PS}}\middle|S\middle|\psi_l^{\mathrm{PS}}\right\rangle_{r_c}$$

$$= -2\pi\left(r\psi_l^{\mathrm{PS}}\right)^2 \frac{d}{d\varepsilon}\frac{d}{dr}\ln\psi_l^{\mathrm{PS}}\Big|_{r_c},$$

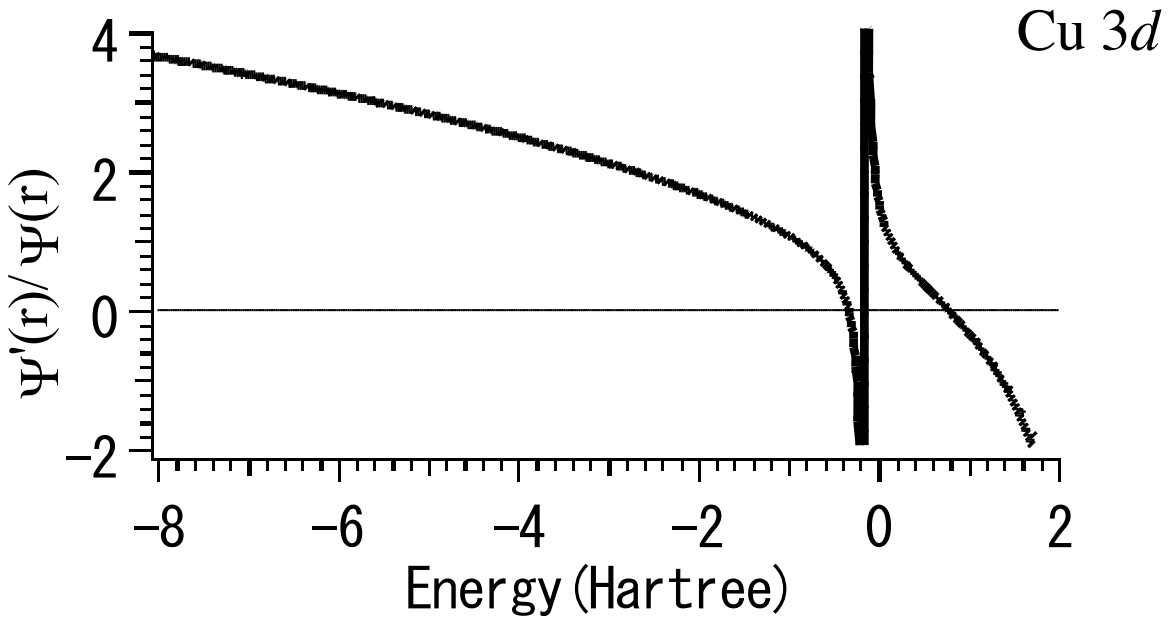
Generalized Norm-conserving Condition

$$S = 1 + \sum_{nm} q_{nm}\left|\beta_n\right\rangle\left\langle\beta_m\right|, \qquad \left\langle\psi_l^{\mathrm{PS}}\middle|\beta_m\right\rangle = \delta_{lm}.$$

$$H\left|\psi_l^{\mathrm{PS}}\right\rangle = \varepsilon_l S\left|\psi_l^{\mathrm{PS}}\right\rangle.$$

Generalized Eigen Value Problem

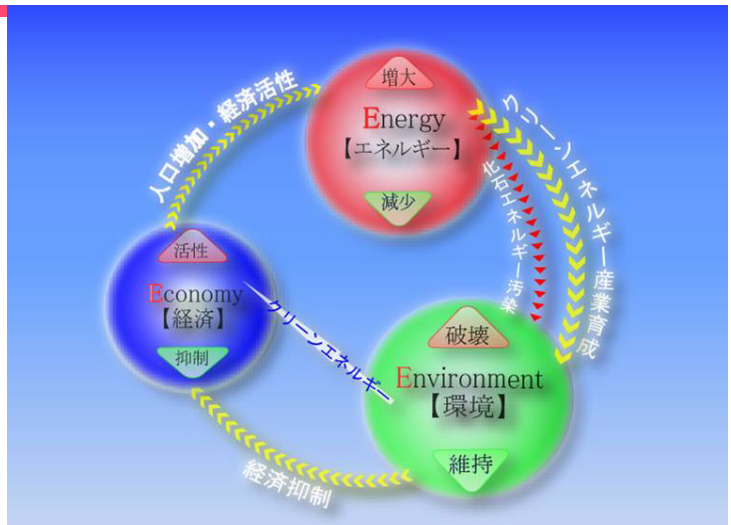
Ultrasoft Pseudopotential



The accuracy of pseudopotentials can be improved further by employing multiple reference states.

3E-trilemma

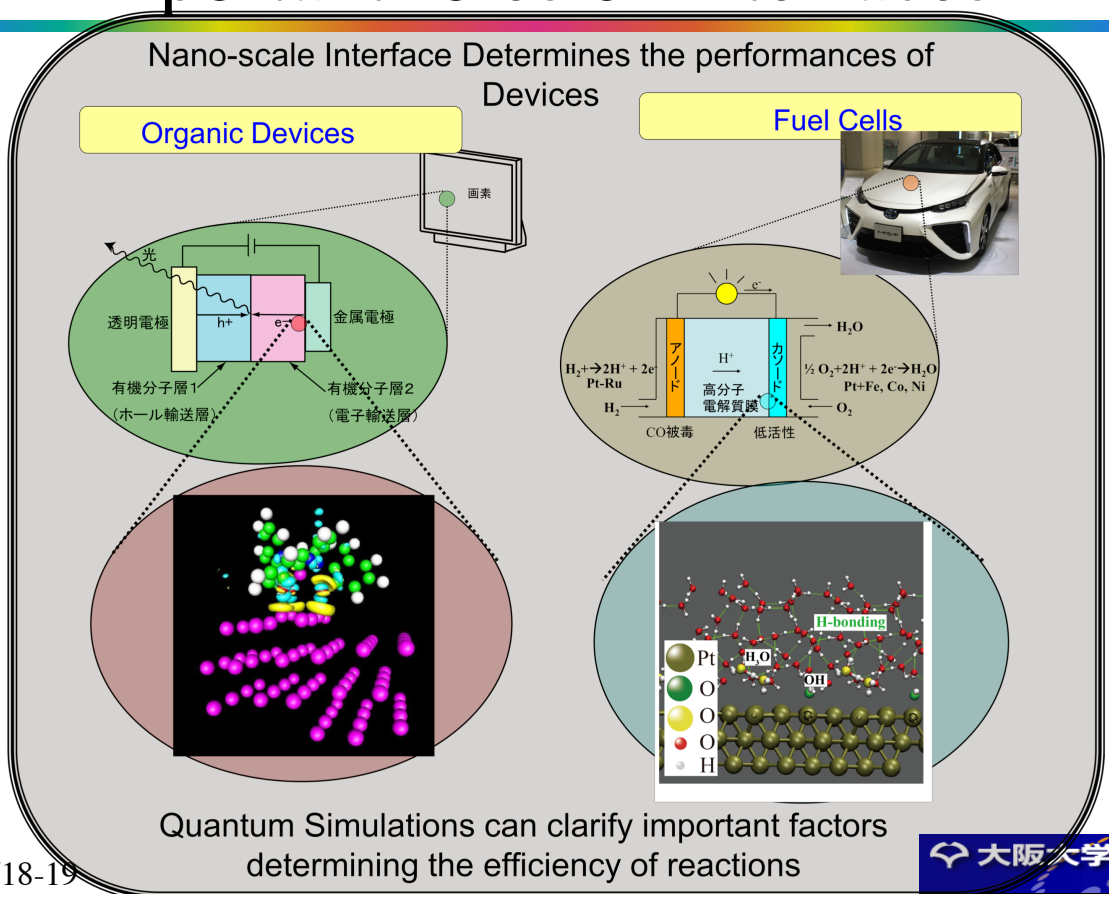
- Economy
- Energy
- Environment



[1]濱川圭弘："太陽光発電ー最新の技術とシステムー", CMC, (2000)

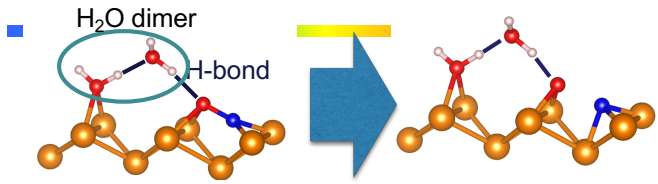
Solve the trilemma by Quantum Simulations.

Important roles of Interfaces

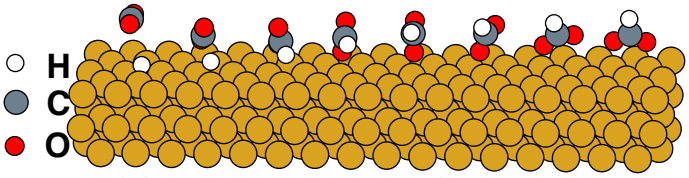


Quantum Simulations can clarify important factors determining the efficiency of reactions

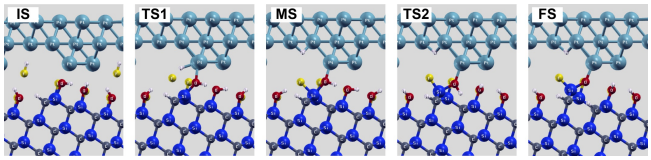
Heterogeneous Catalyst



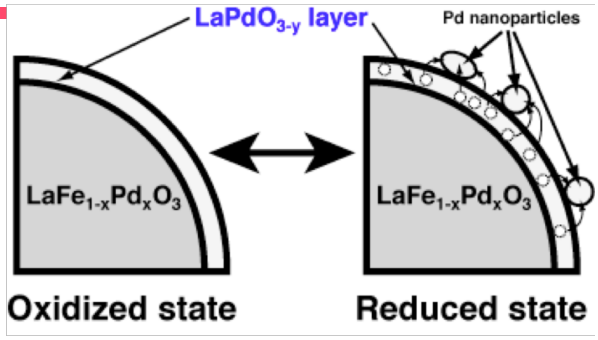
NO dissociation by H_2O
Thanh Ngoc Pham *et al.*,***JPhysChemC.***(2018).



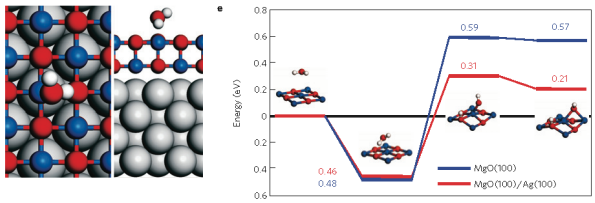
CO_2 hydrogenation on Cu surfaces
G.C. Wang *et al.*,***J. Phys. Chem. B***, (2006).
Fahdzi Muttaqien, *et al.*, ***J. Chem. Phys.*** (2014),
J. Chem. Phys. (2017) , ***Chem. Comm***. (2017).



Etching of SiC by Pt catalyst
Bui Van Pho *et al.*,***Appl. Phys. Lett.***, (2015)
J.J.Appl.Phys (2018).

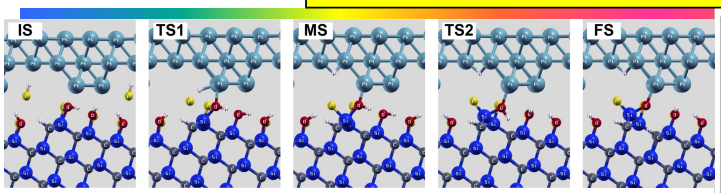


Suppression of Pd Sintering
I. Hamada *et al.*, ***J. Am. Chem. Soc.***, (2011).



H_2O dissociation on MgO/Ag,
H.-J. Shin et al., ***Nature Materials*** (2010).

Heterogeneous Catalyst



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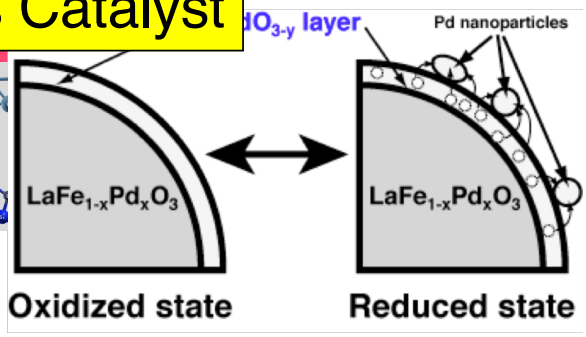

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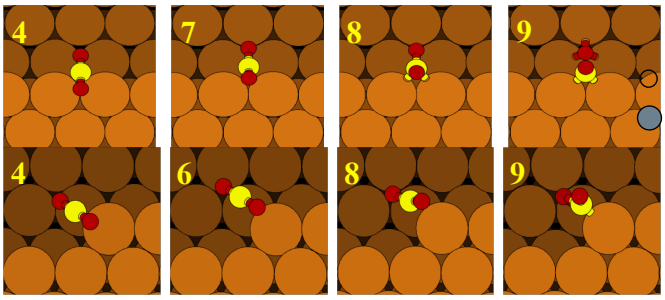
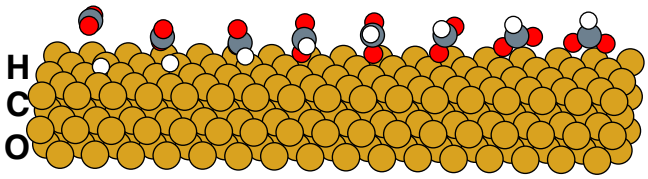
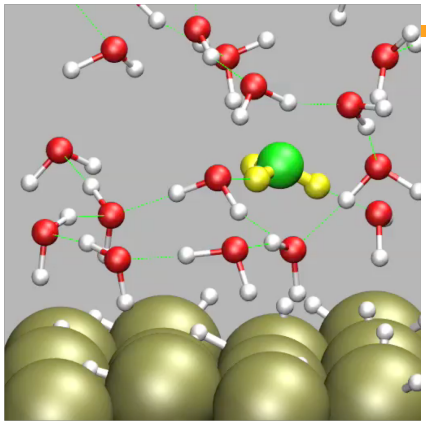


CO_2 adsorption/dissociation on Cu surfaces
Fahdzi Muttaqien, *et al.*,
J. Chem. Phys. (2014), ***J. Chem. Phys.*** (2017).

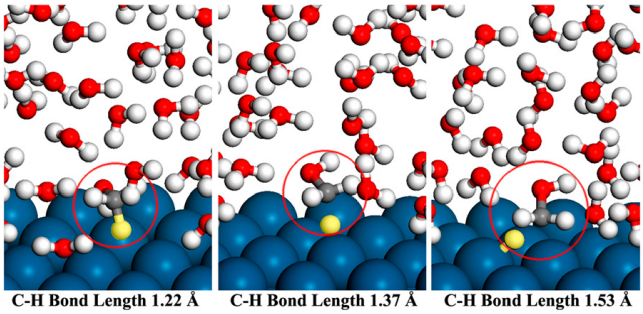


CO_2 hydrogenation/decomposition on Cu
G.C. Wang *et al.*,***J. Phys. Chem. B***, (2006).
Fahdzi Muttaqien *et al.*, ***Chem. Comm***. (2017).

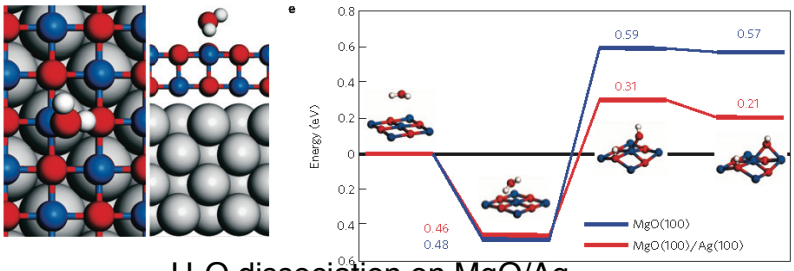
Chemical Reactions at Water/Solid Interfaces



Hydrogen Evolution Reaction
M. Otani *et al.*, ***J. Phys. Soc. Jpn*** (2008).
PCCP (2008), ***JPCC*** (2008).



Methanol Oxidation on Pt Electrode
J. Herron *et al.*, ***PNAS USA*** (2016).



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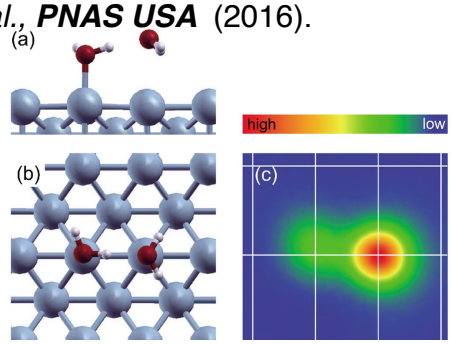

Water Dimer / Cu(110)
T. Kumagai *et al.*,
Phys. Rev. Lett., (2008),
Phys. Rev. B (2009).

Input fil

- Ictrl : Should be always " 0 0
- GMAX

The cutoff wave number of plane

- GMAXP

The cutoff wave number of plane

These cutoff numbers depend on p

Example :

pot.Al_pbe1, pot.Si_pbe1, pot.
pot.Ge_pbe1,

GMAX = 3～4, GMAXP =

pot.H_lda3, pot.C_pbe3, pot.O_

GMAX = 5.0 , GMAXP = 1

pot.H_lda1, pot.C_pbe1, pot.O_

GMAX = 5.5, GMAXP = 2

It is necessary to check the depenc

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  0     0     0     0     0     0  : Ictrl
  5.0000 15.0000   2   6   6   : GMAX, GMAXP, NTYP, NATM, NATM2
  47 0  : number of space group, type of bravis lattice
   22.0000 21.0000  20.0000  90.0   90.0  90.0  : a,b,c,alpha,beta,ga
   1      1       1       1      1     1     : knx,kny,knz, k-point s
   1   0   : NCORD, NINV,   : IWEI, IMDTYP, ITYP
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    2.3483288468    1.7534586685    0.0000000000  1  1  2
    2.3483288468   -1.7534586685    0.0000000000  1  1  2
   -1.2627229833    0.0000000000    0.0000000000  1  1  1
   -2.3483288468    1.7534586685    0.0000000000  1  1  2
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   6   1  : Simple=1,Broyd2=3,Blugel=6,    1:charge, 2:potential mix.
   0    8  0.8 : starting mixing, kbxmix,alpha
  0.60  0.50  0.60  0.70  1.00    : DTIM1, DTIM2, DTIM3, DTIM4, dtim_
 300.00     4     1    0.10D-07  1.d-06  : DTIO ,IMDALG, IEXPL, EDELTA
  0.0010  0.05D-02    0           : WIDTH,FORCCR,ISTRESS
 ggapbe          1                : XCTYPE, nspin
  1.00     3                     : destm, n_stm
 102  : NBZTYP 0-SF, 1-BK, 2-SC, 3-BCC, 4-FCC, 5-DIA, 6-HEX
   0   0   0   : NKX, NKY, NKZ
   0   0   0   : NKX2,NKY2,NKZ2
  10           : NEG
      1        : NonLocalProjection
      0        : 0; random numbers, 1; matrix diagon
  2   0      0      0(MB) : imsd, i_2lm, i_sd2another, wksz for phas
      0        : evaluation of eko difference.0 = no ,1 = yes
      0
      0    0.0
  10                                  : mvelsc
  300.0D0   50.0D0    30       1.0D0  : tempw,tolp,nroll,anneal
  500.0D0    8        15       1      : wnosep,nhc,nosy,ndrt
   5.0D-8                             : frict
   0                                  : mcnstr
   DIST    1    3            1.83401
   DIST    2    3            1.83401
   BEND    1    3    2     104.23195
```

Input file: nfinp_1

- Ictrl : Should be always " 0 0 0 0 0 0 "
- GMAX

The cutoff wave number of plane wave basis set for wave functions.

- GMAXP

The cutoff wave number of plane wave basis set for charge density.

These cutoff numbers depend on pseudopotentials.

Example:

pot.Al_pbe1, pot.Si_pbe1, pot.S_pbe1, pot.Cl_pbe1, pot.Br_pbe1, pot.Ge_pbe1,

GMAX = 3～4, GMAXP = 10

pot.H_lda3, pot.C_pbe3, pot.O_pbe3,

GMAX = 5.0 , GMAXP = 15.0

pot.H_lda1, pot.C_pbe1, pot.O_pbe1,

GMAX = 5.5, GMAXP = 20.0

It is necessary to check the dependence of total energies on cutoff.

Input file: nfinp_1

- **NTYPE :** Number of atomic types in a unit cell
- **NATM = NATM2**

The number of atoms in a unit cell

- **NUM_SPACE_GROUP**

Specify the symmetry of the system by the group space number.

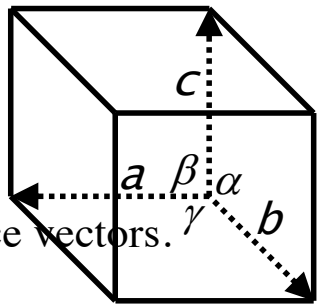
- **TYPE_OF_BRAVAIS_LATTICE**

Specify the type of Bravais lattice.

0 **SIMPLE**
1 **BODY_CENTER**
2 **FACE_CENTER**
3 **A_CENTER**
4 **B_CENTER**
5 **C_CENTER**
6 **RHOMBOHEDRAL_CENTER**

Unit Cell

1）Specify the lengths of the lattice vectors and the angles among them.



a ***b*** ***c*** ***α*** ***β*** ***γ***

2）Specify the Cartesian coordinates of the lattice vectors.

Cartesian

ax ***ay*** ***az***
bx ***by*** ***bz***
cx ***cy*** ***cz***

K-points

kx ky kz 1 1 1 : KNX, KNY, KNZ, K-POINT_SHIFT

Atomic coordinates

NCORD: Unit of coordinates

0 Unit of Primitive Cell

1 Cartesian coordinate in Bohr radius

2 Unit of Conventional Cell

NINV: Obsolete

x y z IWEI IMDTYP ITYP

x y z IWEI IMDTYP ITYP

x y z IWEI IMDTYP ITYP

…

IWEI : Obsolete and should be always 1

IMDTYP = 0 : Fix atomic position

1 : Move atomic position

ITYPE : Atom type number

Input file: nfinp_1

- **IATOMN :** Atomic Number of atom type 1
- **ALFA: Obsolete**
- **AMION:** Atomic Mass
- **ILOC:** Obsolete
- **IVAN**: Obsolete
- **ZETA1:** Initial spin polarization of atom

Input file: nfinp_1

- **ICOND**

  How to prepare the initial wave functions.

  0 : Generate from scratch

  1 : Read from “restart.data” which has the latest date.

- **INIPOS**

  How to prepare the initial atomic positions.

  0 : Read from nfinp_1.

  1 : Read from “restart.data” which has the latet data.

  2 : Read from “GEOMETRY” which can be modified by text editor.

- **INIVEL**

  Specify the atom velocities actually used;

  0 → Initialized, 1→ Read from restart file, 2→ Read from GEOMETRY file

Input file: nfinp_1

- **ININOS**

  Specify the thermostat variables actually used;

  0 : Initialized

  1 : Read from “restart.data” which has the latest date.

- **INIACC**

  Reset accumulators and the counter of MD steps.

  0 : Initialize.

  1 : Read from “restart.data” and continue accumulating.

- **NMD1**

  Maximum number of iterations for SCF calculations.

- **NMD2**

  Maximum number of molecular dynamics steps.

- **CPUMAX**

  Maximum CPU time in seconds.

Input file: nfinp_1

- **Way-of-mix**
  - **1 Simple**
  - **2 BROYD1**
  - **3 BROYD2**
  - **4 DFP**
  - **5 PULAY**
  - **6 BLUGEL**
- **Mix-what: 1 Charge Mixing, 2 Potential Mixing**
- **KBXMIX**

  The maximum total number of iterations to be used for mixing.
- **MIX_ALPHA**

  Fraction of new charge density in charge density mixing. 0.3～0.8.

Structure Optimization and Molecular Dynamics

DTIO:

- Increment of time for each step of molecular dynamics simulation. (1 a.u. =2.4x10^{-17}seconds)
- The time step should be carefully chosen to assure the accuracy of molecular dynamics. It depends on atomic types, maximum forces acting on atoms, and integration scheme of the Newton equation of motion.
- For QUENCHING and NEB schemes, the time step should be 50～300a.u.
- For GDIIS scheme, the time step should be 400～800a.u.
- For NORMAL_MODE, it is not used.
- For FINITE_TEMPERATURE_MD and if the system includes hydrogen, the time step should be about 20a.u. If hydrogen is not included, the time step should be 50～100a.u.

Structure Optimization and Molecular Dynamics

IMDALG: Algorithms of MD

1 Newtonian equations of motion

2 Quenching Molecular Dynamics

This scheme works well when forces acting on atoms are larger than 0.02 hartree/a_B.

3 Vibration normal mode analysis.

4 GDIIS: Generalized Direct Inversion of Iterative Subspace

This scheme becomes efficient when the maximum force is smaller than about 0.02 hartree/a_B.

6 Nudged Elastic Band Method

Method for reaction path search proposed by Mills, Jonsson, Schenter, *Surf. Sci.* 324 305 (1994).

Input file: nfinp_1

- **EDELTA:** Energy criteria for convergence [in Hartree/atom]
  Recommended values: 0.1d-08 ～ 0.1d-09
- **WIDTH: Scheme of Brillouin Zone Sampling**
  WIDTH < -10.0 Tetrahedral scheme
  -10.0 < WIDTH < 10.0 Special k-points scheme is used and the absolute value of WIDTH, namely, |WIDTH| means the energy broadening around the Fermi level
- **FORCCR:** Criterion for force in MD [Hartree/Bohr radius]
  If the maximum force is smaller than FORCCR, the molecular dynamics is terminated.
  Recommended value: 1.d-03 [Hartree/Borh radius]
- **XCTYPE**
  Selection of exchange-correlation function.
  GGAPBE :Generalized Gradient Approximation by Perdew, Burke and Ernzerhof, Phys. Rev. Lett. **77** 3865 (1996). (Recommended)
  LDAPW91 : Local Density Approximation.

Input file: nfinp_1

- **NSPIN**

  0 : No spin polarization.

  1 : Spin polarized calculation.
- **DESTM**

  Energy width for STM-imaging.
- **KEG**

  Number of eigenvalues.

CMD-WS STATE-Senri

Input file: nfinp_1

- **IMSD**

  Choose optimization method.

  2 : Davidson method.

  1 : Residual-vector Minimization Method.

  Davidson scheme is quite stable but computationally less efficient compared with RMM scheme. RMM is very fast but it is less stable compared with Davidson scheme. When you start calculations from scratch wave functions, you should use Davidson scheme for first 5-10 iterations and switch sot RMM scheme.
- **EDELTA**

  Convergence criteria for wave function optimization.

  Recommended values: 0.10D-7～0.10D-8

Osaka University

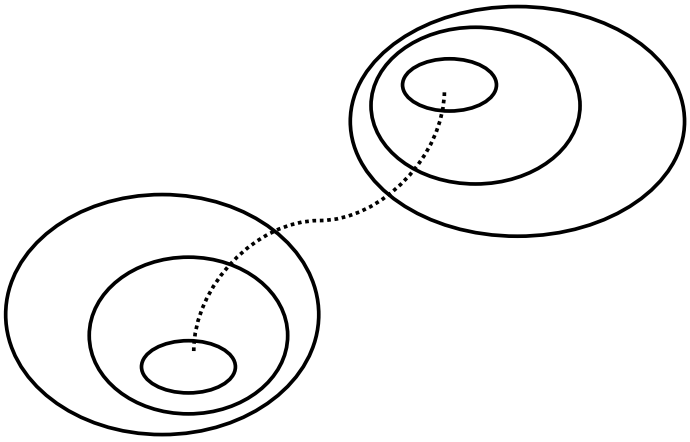
Reaction Path Search

&JOB_TYPE NEB

&END_JOB_TYPE

NEB: Nudged Elastic Band Method

Mills, Jonsson, Schenter, *Surf. Sci.* 324 305 (1994).



CMD-WS STATE-Senri

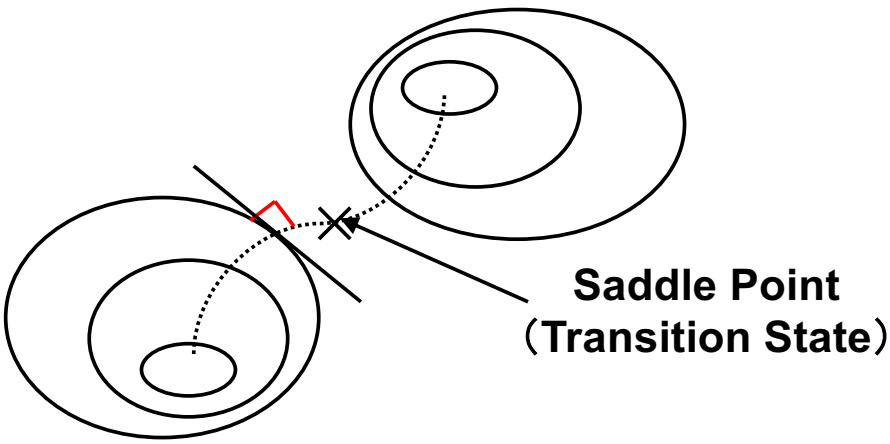
Reaction Path Search

&JOB_TYPE NEB

&END_JOB_TYPE

NEB: Nudged Elastic Band Method

Mills, Jonsson, Schenter, *Surf. Sci.* 324 305 (1994).



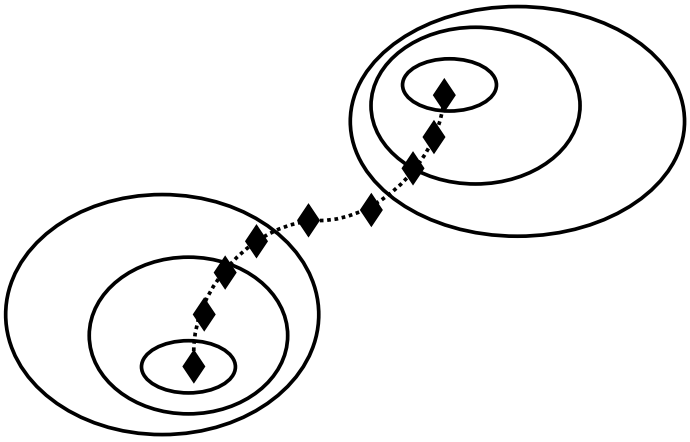
最小エネルギー経路はポテンシャルの等高線の接線に垂直

Reaction Path Search

```
&JOB_TYPE        NEB
&END_JOB_TYPE
```

NEB: Nudged Elastic Band Method

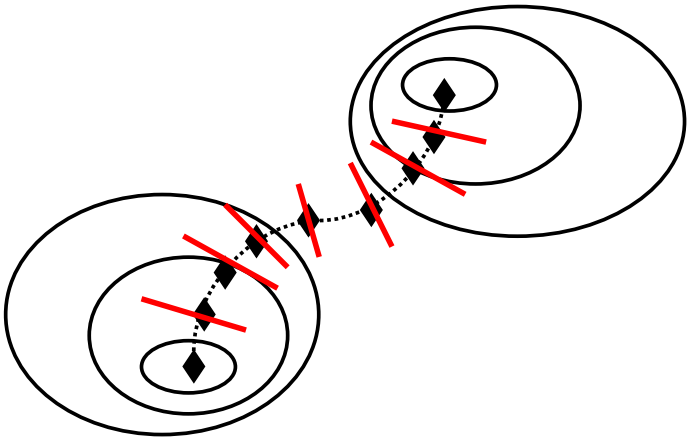
Mills, Jonsson, Schenter, *Surf. Sci.* 324 305 (1994).



CMD-WS STATE-Senri

Reaction Path Search

&JOB_TYPE NEB
&END_JOB_TYPE
NEB: Nudged Elastic Band Method
Mills, Jonsson, Schenter, *Surf. Sci.* 324 305 (1994).



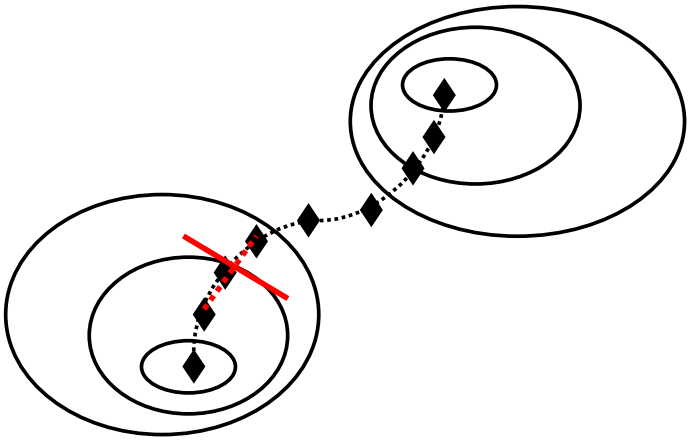
Osaka University

Reaction Path Search

```
&JOB_TYPE        NEB
&END_JOB_TYPE
```

NEB: Nudged Elastic Band Method

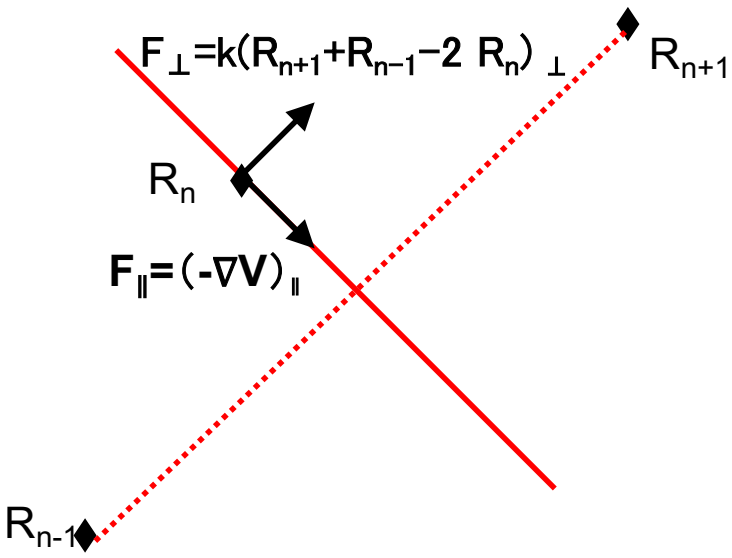
Mills, Jonsson, Schenter, *Surf. Sci.* 324 305 (1994).



各レプリカを両隣のレプリカを結ぶ直線の垂直二等分面内で最適化

CMD-WS STATE-Senri

Reaction Path Search



各レプリカを両隣のレプリカを結ぶ直線の垂直二等分面内で最適化

Untar state files

- ***Copy a state file to your directory.***

```
cp ~localuser/cmd/morikawa/state-senri.tar.gz .
```

- ***Unzip and untar state files.***

```
> gzip –d state-senri.tar.gz
> tar xvf state-senri.tar .
```


Submitting a job

- ***Submit a job***

```
> mpirun –np 1 ./STATE < nfinp_1 > nfout_1 &
```

- ***Plot density of states (DOS)***

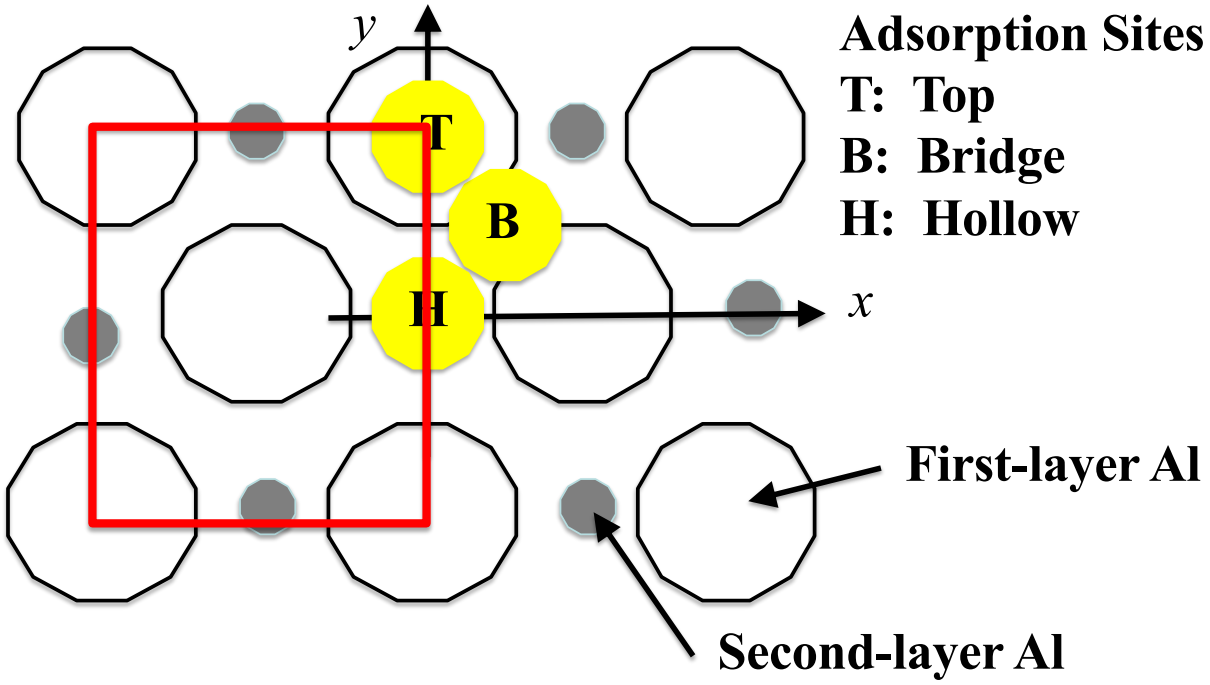
```
> gnuplot
>> plot "dos.data" u 1:2 w l
                            ↑
                            "el"
```

Submitting a job

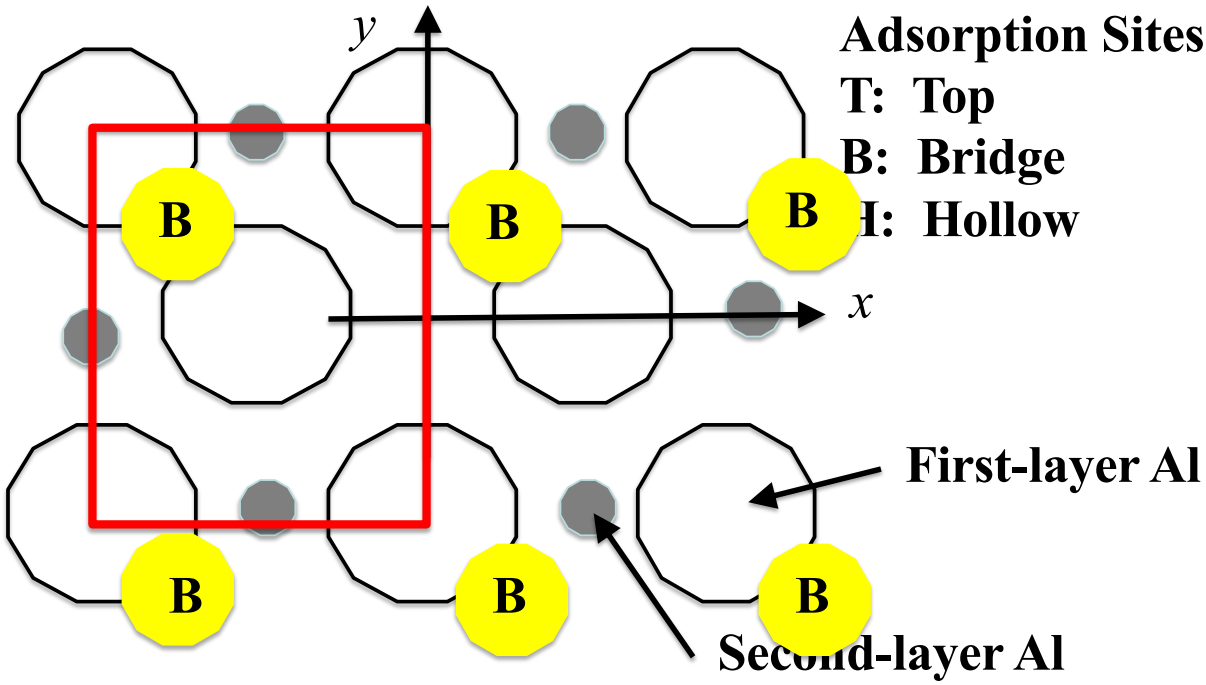
- ***Plot density of states (DOS)***

```
> gnuplot
>> plot "dos.data" u 1:2 w l , "" u 1:3 w l
                                  ↑
                                  "el"
```


Cl on Al(100)



Cl on Al(100)



Loging to cmd2

```
>>  ssh –Y astud??@cmd2.phys.sci.osaka-u.ac.jp

Account ID
   astud??        ?? = 01  ~   24
Password
   cmdaastud??
```

copy state-senri tar file

```
>>  cp /home/CMD/teac04/state.tar.gz .
>>  tar xvfz state.tar.gz
>>  cd STATE
>>  ls –l
>>  example          : example files
>>  external         : external libraries
>>  gncpp            : pseudo-potential database
>>  README      : README file
>>  src              : source codes
>>  test             : test files
>>  tools            : tool programs
```


Installation of mpich and libfftw3-dev

```
>> sudo apt-get install mpich
>> sudo apt-get install libfftw3-dev
```