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Exploration of the energy landscape with ABINIT : String Method, NEB, Free Energy

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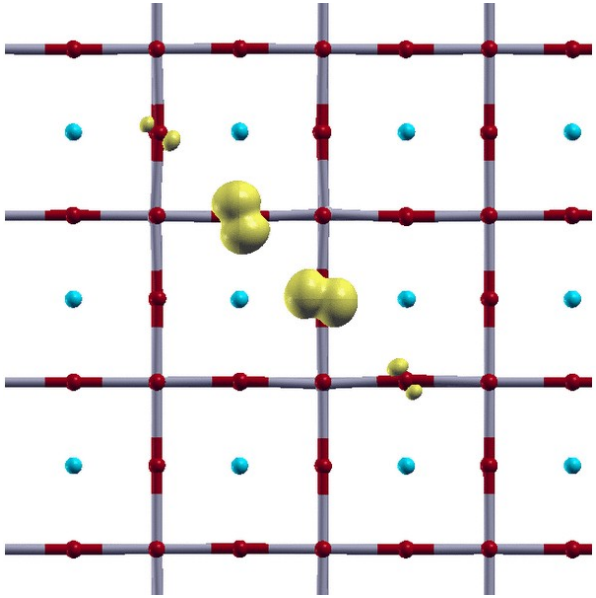
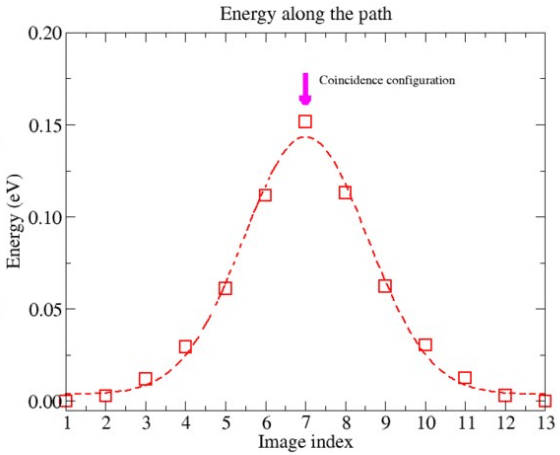
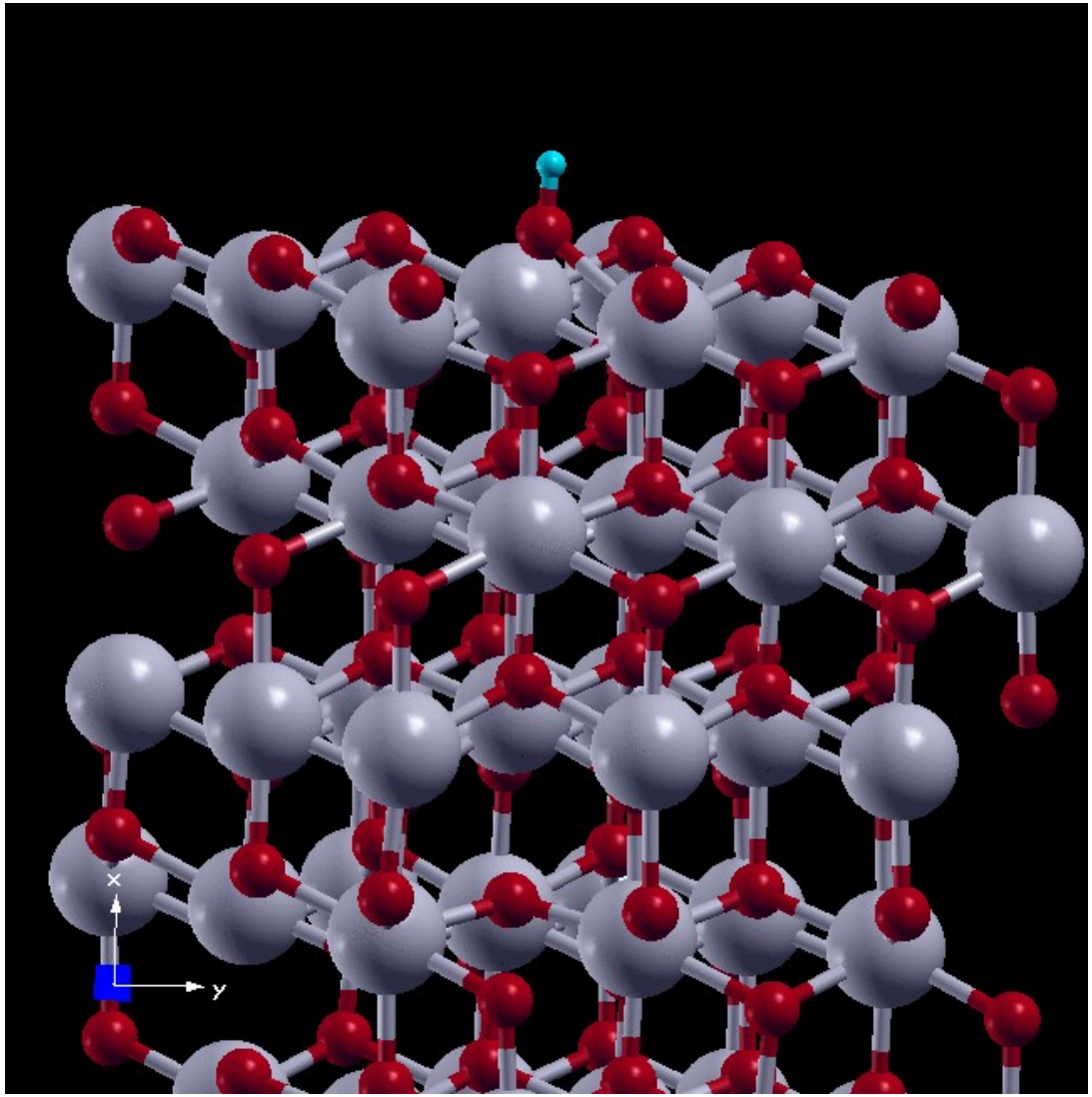




CONTENT



Proton transfer between two O atoms of a O-ZrO2(111) Surface

(String Method)

1 - Introduction

Yesterday, you have learnt how to perform
STRUCTURAL OPTIMIZATIONS with ABINIT
= how to obtain ***(local) minima*** of the ***energy landscape*** in configuration space.

What happens inbetween ?

There are specific physical problems in which the energy landscape between the minima is important and plays a role.

Example : *Transition between two local minima* of the energy landscape
According to **Transition State Theory (TST)**, the transition **rate**,
if the mechanism if **THERMALLY ACTIVATED**
(thermal overbarrier motion),
is controlled by an ENERGY BARRIER

$$k = k_0 e^{-E_a / k_B T}$$

1 - Introduction

TST : activation energy ~ free energy barrier
=> approximated by a static (« T=0K ») barrier ΔE

ΔE can be obtained by **computing the MEP**
ΔE = E(saddle point) – E(Min)

Prefactor ?

Harmonic Transition State Theory :

Classical framework:

$$k_0 = \frac{\prod_{i}^{3N-3} \nu_i^{Min}}{\prod_{i}^{3N-4} \nu_i^{Saddle}}$$

« attempt frequency »

Phonon frequencies in the stable (initial) configuration of the 3N-3 modes (acoustic modes excluded)

Phonon frequencies in the Saddle point configuration of the 3N-4 modes (acoustic modes + imaginary mode excluded)

See e.g. Sundell, Björketun, Wahnstrom, PRB 76, 094301 (2007)

1 - Introduction

Quantum corrections :

$$\Delta E^{qm} = E(saddle) - E(min) + \frac{1}{2}\sum_{i}^{3N-4} h\nu_i^{Saddle} - \frac{1}{2}\sum_{i}^{3N-3} h\nu_i^{Min}$$

$$k_0^{qm} = \frac{k_B T}{h} \frac{\prod_{i}^{3N-3} \left[1 - e^{-h\nu_i^{Saddle}/k_B T}\right]}{\prod_{i}^{3N-4} \left[1 - e^{-h\nu_i^{Min}/k_B T}\right]}$$

Thermal overbarrier regime but quantization of vibration modes taken into account.

See e.g. Sundell, Björketun, Wahnstrom, PRB 76, 094301 (2007)

1 - Introduction

High-temperature limit ($k_B T >> h\nu_i$) :

$$k_0^{qm} \rightarrow k_0$$

Low-temperature limit ($k_B T << h\nu_i$) :

$$k_0^{qm} \rightarrow \frac{k_B T}{h} \qquad k \rightarrow \frac{k_B T}{h} e^{-\Delta E^{qm}/k_B T}$$

NB1 : the regime remains thermal overbarrier (no tunneling)

NB2 : at very low temperature, one might have a quantum tunneling regime (requires specific modeling ! e.g. Flynn-Stoneham formula)
Ex : diffusion of H atoms in metals (e.g. in Nb or Ta below ~ 200 K)

See e.g. Sundell, Björketun, Wahnstrom, PRB 76, 094301 (2007)

CONTENT

2 – Minimum Energy Paths (MEPs)

Path between two local minima (stable or metastable configurations) in configuration space, that involves the smallest possible energy barrier.

There are **two main algorithms** allowing computation of MEPs :
String Method (SM) & **Nudged Elastic Band** (NEB)

Computing a MEP requires to sample the path between the two minima
=> the path is **discretized** : it is approximated by **a finite number of intermediate configurations**

Needs replicas of the system => performed using keyword **imgmov**

String Method : **imgmov** 2 NEB : **imgmov** 5

Number of replicas (intermediate configurations) along the path : **nimage**
Maximal number of steps for SM/NEB : **ntimimage**
Tolerance criterion for convergence : **tolimg**
(energy difference with previous step, per image)

2 – Minimum Energy Paths (MEPs)

String Method & NEB :

Path computed between two local minima =
Two optimized configurations (that have been obtained before, e.g. by a structural optimization !) => **xred_1img** & **xred_lastimg**

Allows determination of **energy barriers**
(fundamental to evaluate rate of thermally-activated mechanisms)

Other keywords :

dynimage(nimage): 0 if fixed image, 1 if evolving
=> 0 for first and last image, 1 for intermediate images
Parallelization over images : **npimage** (recommended = **nimage**)

Precise optionnally
fxcartfactor: « time step »
string_algo : 1 by default, Simplified String Method, 2 (energy-weighted arc length)
neb_algo : 0, 1 (NEB + improved tangent, default), 2 : CI-NEB

The MEP should be CONVERGED with the number of images

CONTENT

2.a The String Method

SM : Iterative procedure in which each iteration consists of two steps:

Step 1: evolution

Positions are modified following the forces:

For image (s): $$x_{i,\alpha}^{(s)}(n+1) = x_{i,\alpha}^{(s)}(n) + fxcartfactor \times f_{i,\alpha}^{(s)}(n)$$

with $$f_{i,\alpha}^{(s)}(n) = -\frac{\partial E_{tot}^{(s)}(n)}{\partial x_{i\alpha}^{(s)}}$$

(present implementation = steepest-descent)

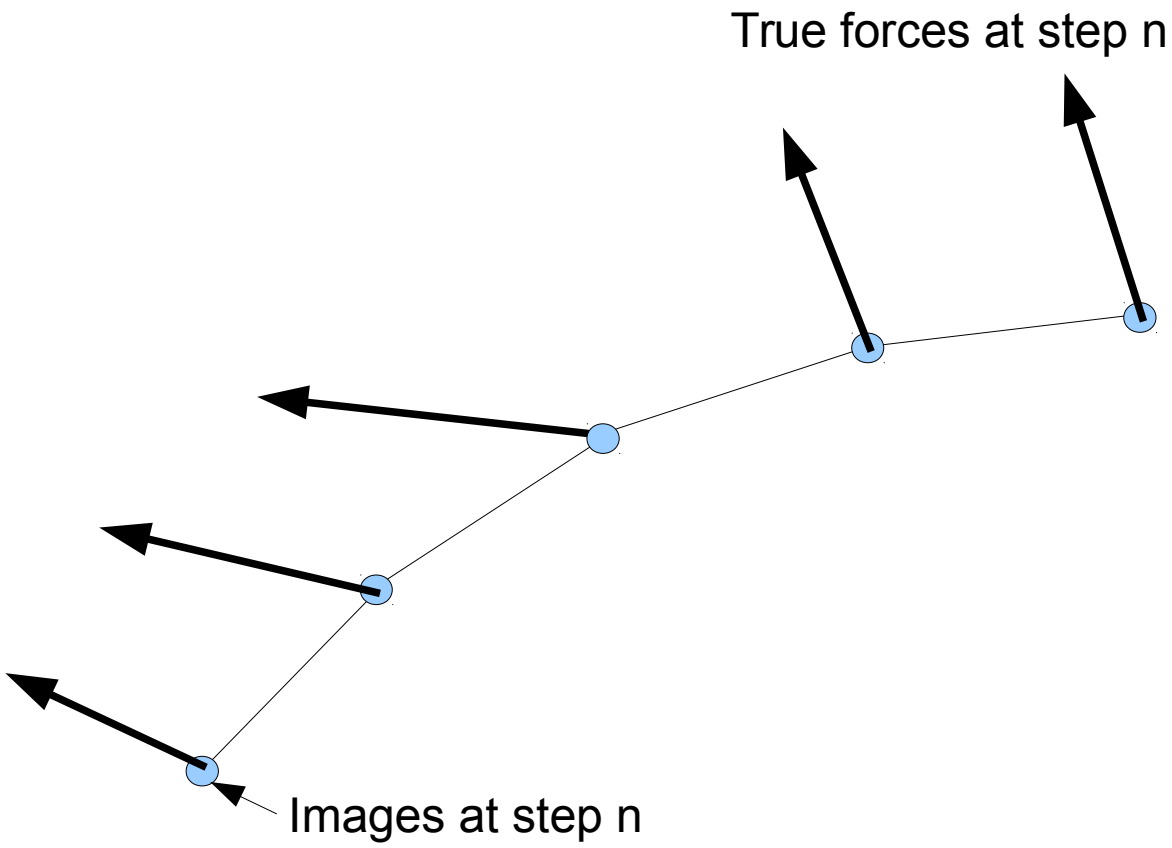
Step 2: reparametrization

The images are equally redistributed along the string

E, Ren, Vanden-Eijnden, The Journal of Chemical Physics 126, 164103 (2007).

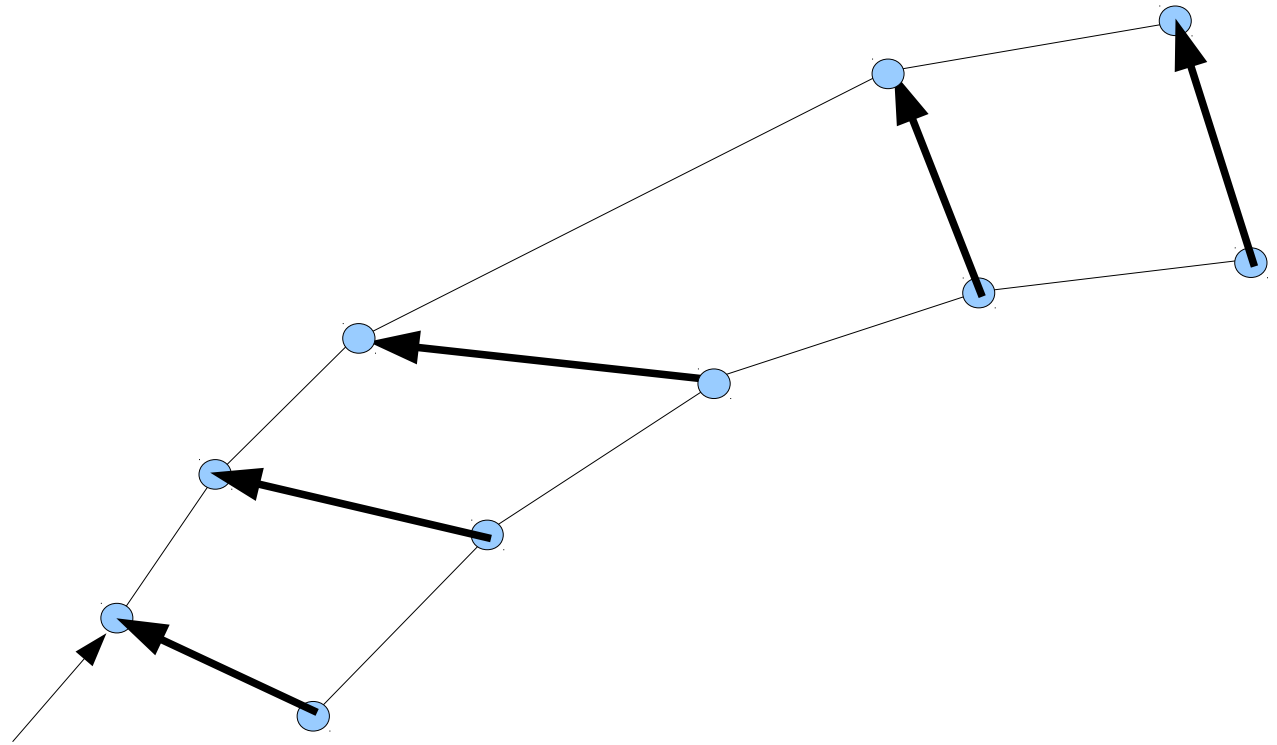
2.a The String Method

Example (2D):



2.a The String Method

Example (2D):

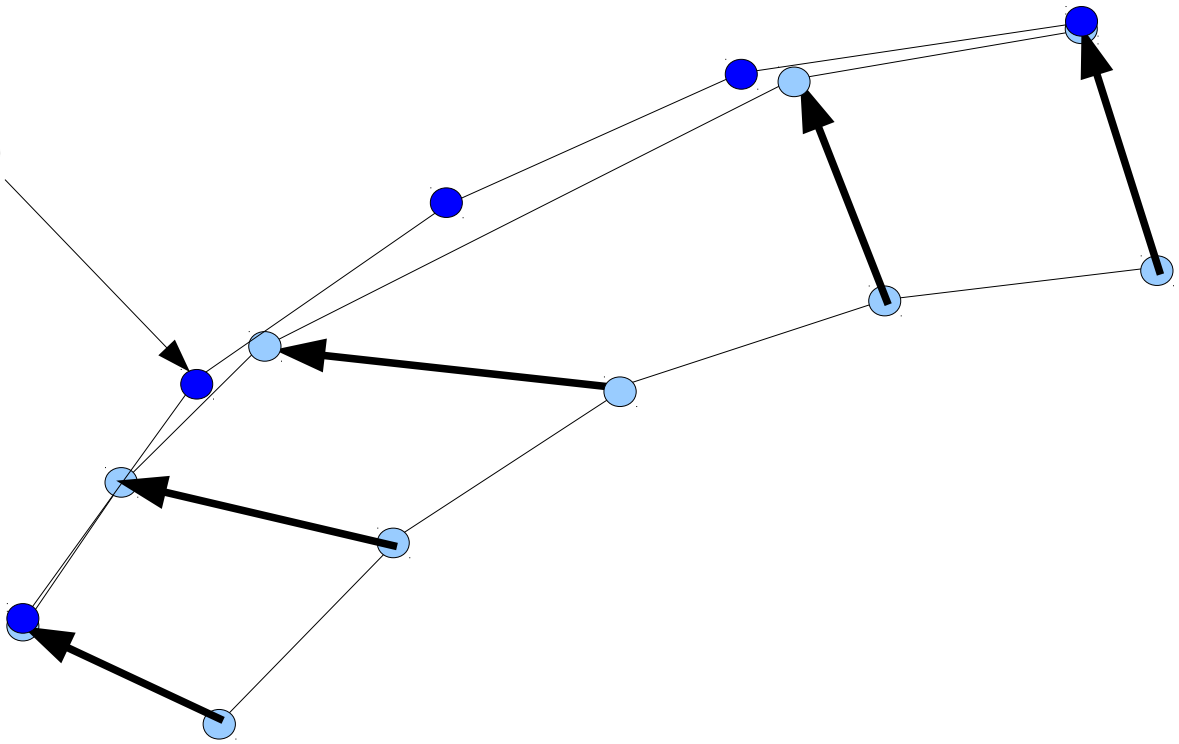


Step n+1: evolution step

2.a The String Method

Example (2D):

Step n+1:
reparametrization step
=> Images at step n+1



2.a The String Method

Example (the one of the Tutorial) : Hopping of a proton between a H2O and a NH3 molecules, supposed at fixed (arbitrary) distance.

```
#Cell and atoms
acell  10.0 5.0 5.0 Angstrom
natom  8                    # Number of atoms
ntypat 3  typat 1 3 3 2 3 3 3 3 # Type of atoms (H2O + NH3 + H)
znucl 8.0 7.0 1.0           # Z of atoms
natfix 2  iatfix 1 4        # Keep O and N atoms fixed

#parallelization
#paral_kgb 1   npimage 10   npband 10 npfft 2  bandpp 1

#options for printing
 prtwf 0                    # Option for WF printing
 prtden 0                   # Option for density printing
 prteig 0                   # Option for eigvalues printing

#ground state
ecut 20    pawecutdg 40
toldff 5.0d-7               # Stopping criterion of SCF cycle
nstep 50
nband  10                   # Number of bands to compute
occopt 1                    # Occupations scheme
kptopt 0                    # Scheme for k-points generation
nkpt 1  kpt 0.0 0.0 0.0  # Explicit k-point (gamma point)

#XC
ixc -001009   # Select LDA XC functional (LDA PZ from LibXC)

nsym 1        # No symmetry
charge 1.0   # Charge of the simulation cell
```

```
#String Method
xangst          0.0000000000E+00  0.0000000000E+00  0.0000000000E+00
                -3.7593832509E-01 -2.8581911534E-01  8.7109635973E-01
                -3.8439081179E-01  8.6764073738E-01 -2.8530130333E-01
                 4.0000000000E+00  0.0000000000E+00  0.0000000000E+00
                 4.3461703447E+00 -9.9808458269E-02 -9.5466143436E-01
                 4.3190273240E+00 -7.8675247603E-01  5.6699786920E-01
                 4.3411410402E+00  8.7383785043E-01  4.0224838603E-01
                 1.0280313162E+00  2.2598784215E-02  1.5561763093E-02

xangst_lastimg      0.0000000000E+00  0.0000000000E+00  0.0000000000E+00
                -3.0400286349E-01 -1.9039526061E-01  9.0873550186E-01
                -3.2251946581E-01  9.0284480687E-01 -1.8824324581E-01
                 4.0000000000E+00  0.0000000000E+00  0.0000000000E+00
                 4.4876385468E+00 -1.4925704575E-01 -8.9716581956E-01
                 4.2142401901E+00 -7.8694929117E-01  6.3097154506E-01
                 4.3498225718E+00  8.7106686509E-01  4.2709343135E-01
                 2.9570301511E+00  5.5992672027E-02 -1.3560839453E-01

nimage 12      # Number of images along the string
imgmov 2       #String Method
ntimimage 100      # Max. number of relaxation steps of the string
tolimg 0.0001   # Tol. criterion (will stop when average energy of cells < tolimg)
dynimage 0 10*1 0     # Keep first and last images fixed
fxcartfactor 1.0       # Time step for evolution  step of string metho
prtvolimg 0       # Printing volume (0=full, 1=intermediate, 2=minimal)
```

2.a The String Method

If no particular assumtpion about symmetries along the MEP :
=> set **nsym** 1

Keywords to atomic positions :
First image : **xred_1img** or simply **xred**
Last image : **xred_lastimg** of **xred_9image** (if nimage=9)

xred can be replaced by **xangst** or **xcart**

You can specify intermediate points

SM performed under FIXED lattice vectors !
(no relaxation fo the cell along the MEP, the cell is fixed ;
It is the same for all the images)

2.a The String Method

First step of SM : ABINIT interpolates linearly between the images specified in the input file

Fixed images :
The first and last images are fixed (do not evolve) and must correspond to optimized configurations previously obtained.
By default :
dynimage 0 1 1 …. 1 1 0

string_algo
1 : default, Simplified String Method,
2 : « energy-weighted arc length », must give a finer distribution of the images near the saddle point

Symmetric path : it's better using an **odd** number of images !

2.a The String Method

Strong point :

string_algo = 1
Images equidistant along the MEP => the index of the image is proportional to the distance along the MEP

=> index of the image = ideal reaction coordinate !

Rq : this si also the case for the NEB using **neb_algo** 1

There is is physical information not only at the saddle point !
(see below polaron and proton transfers)

NB : **in somes favorable cases**, you need not compute the MEP to have the Barrier ! i.e. if you can constrain the saddle point, e.g. with symmetries !
(structural opt with symmetry constraints can give you directly the saddle point)
Unfortunately, this is rarely the case...

CONTENT

2.b The Nudged Elastic Band (NEB)

Nudged Elastic Band method (NEB):

- construct **nimage** images intermediate between the initial and the final configuration (*previously optimized*)

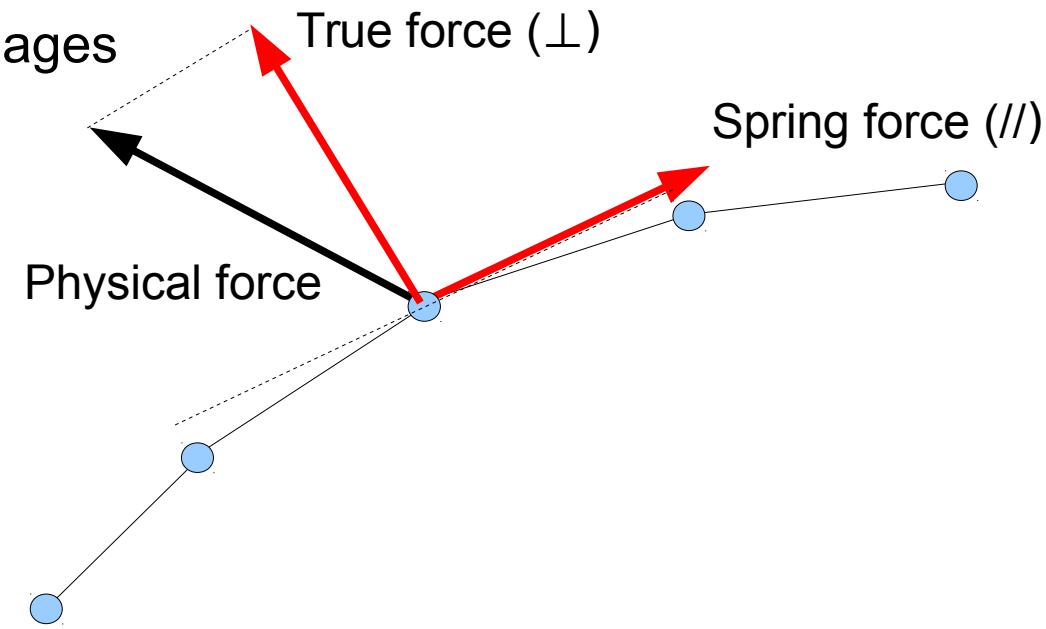
- add spring forces between the images

- evolve images according to

a) projection of spring forces parallel to the tangent

+

b) projection of physical forces perpendicular to the tangent



neb_algo 1 : the spring constant is the same for all images and ensures equal spacing of the images along the MEP.

2.b The Nudged Elastic Band (NEB)

Keywords for NEB :
imgmov 5

neb_algo 0 :original method
1 : NEB + improved tangent* (default value)
(improved calculation of tangent direction, modifies the spring force acting on the images)
2 : CI-NEB : Climbing-image NEB (algo seems to be broken...)

neb_spring : minimal and maximal values of the spring constant connecting images for the NEB method. For **neb_algo** 1, it is constant, for **neb_algo** 2 it can vary.

Related to CI-NEB :
cineb_start : 1st iteration at which the CI-NEB begins (default=7)
(several iterations of standard NEB first performed to find the highest-energy image)

* G. Henkelman and H. Jónsson, "Improved tangent estimate in the nudged elastic band method for finding minimum energy paths and saddle points", The Journal of chemical physics 113, 9978–9985 (2000).

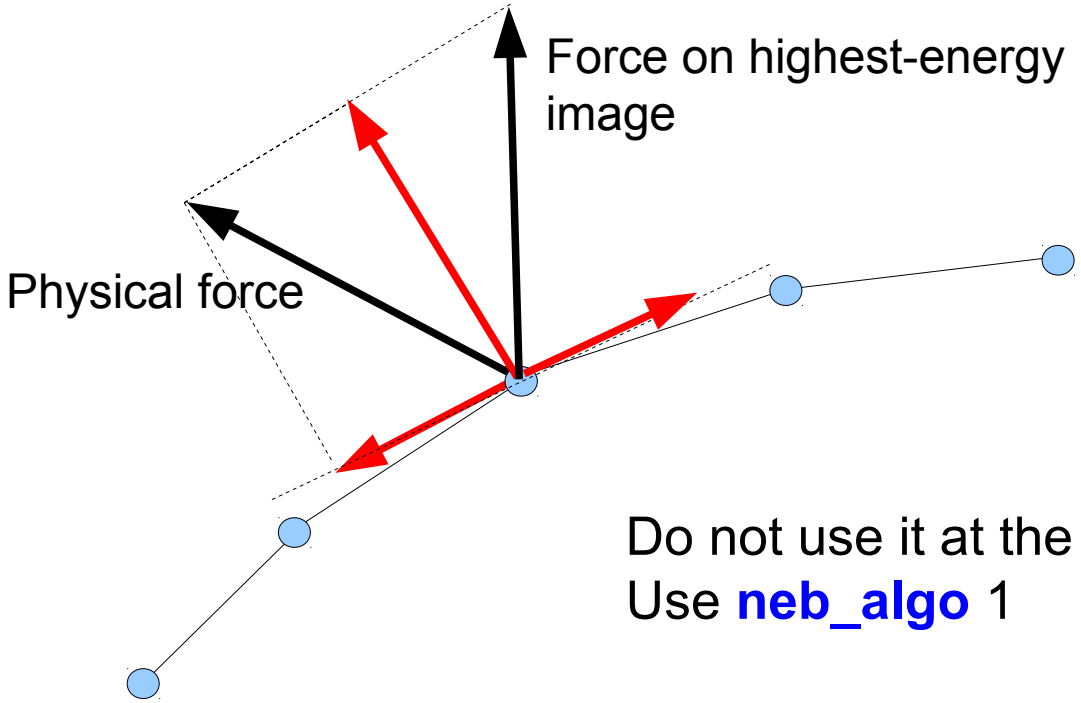
2.b The Nudged Elastic Band (NEB)

Principle of the CI-NEB :

The highest-energy image is forced to come at the saddle point by inverting the // component of the physical force on it.

To identify this image, a number of iterations (**cineb_start**) of standard NEB is first performed. No spring force on this highest-energy image.

Spring constants are variable.



Do not use it at the moment !

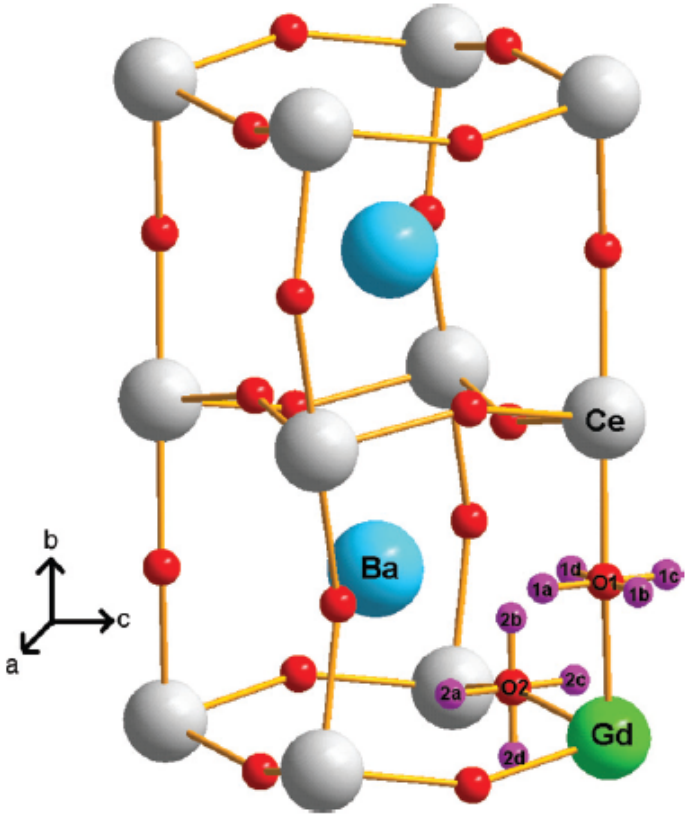
Use **neb_algo** 1

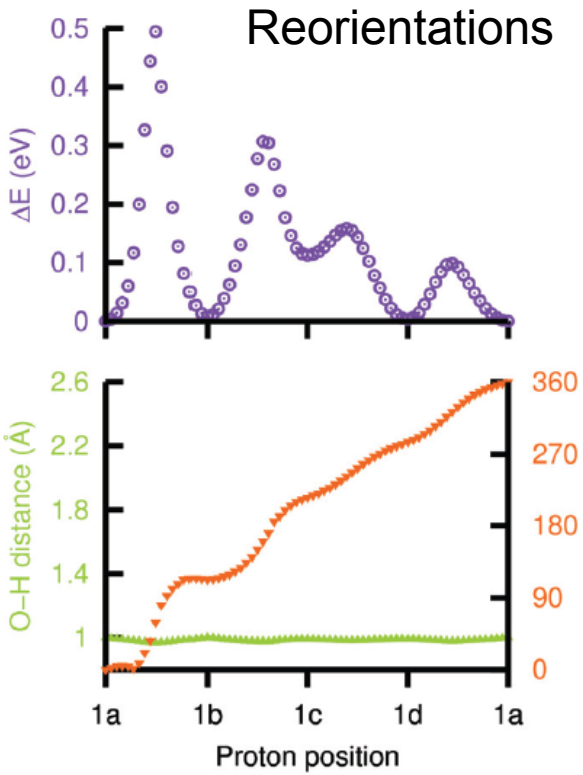
* G. Henkelman, B. P. Uberuaga, H. Jonsson The Journal of chemical physics 113, 9901 (2000).

CONTENT

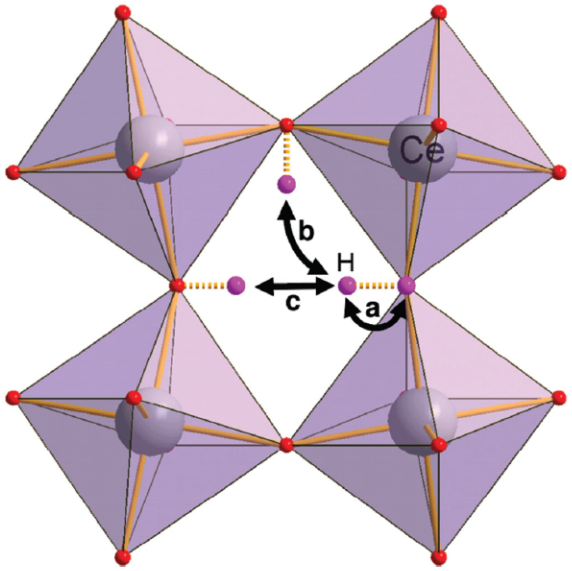
3.a Hopping of a defect in a solid

Hoppings and reorientations of protons in $Gd:BaCeO_3$





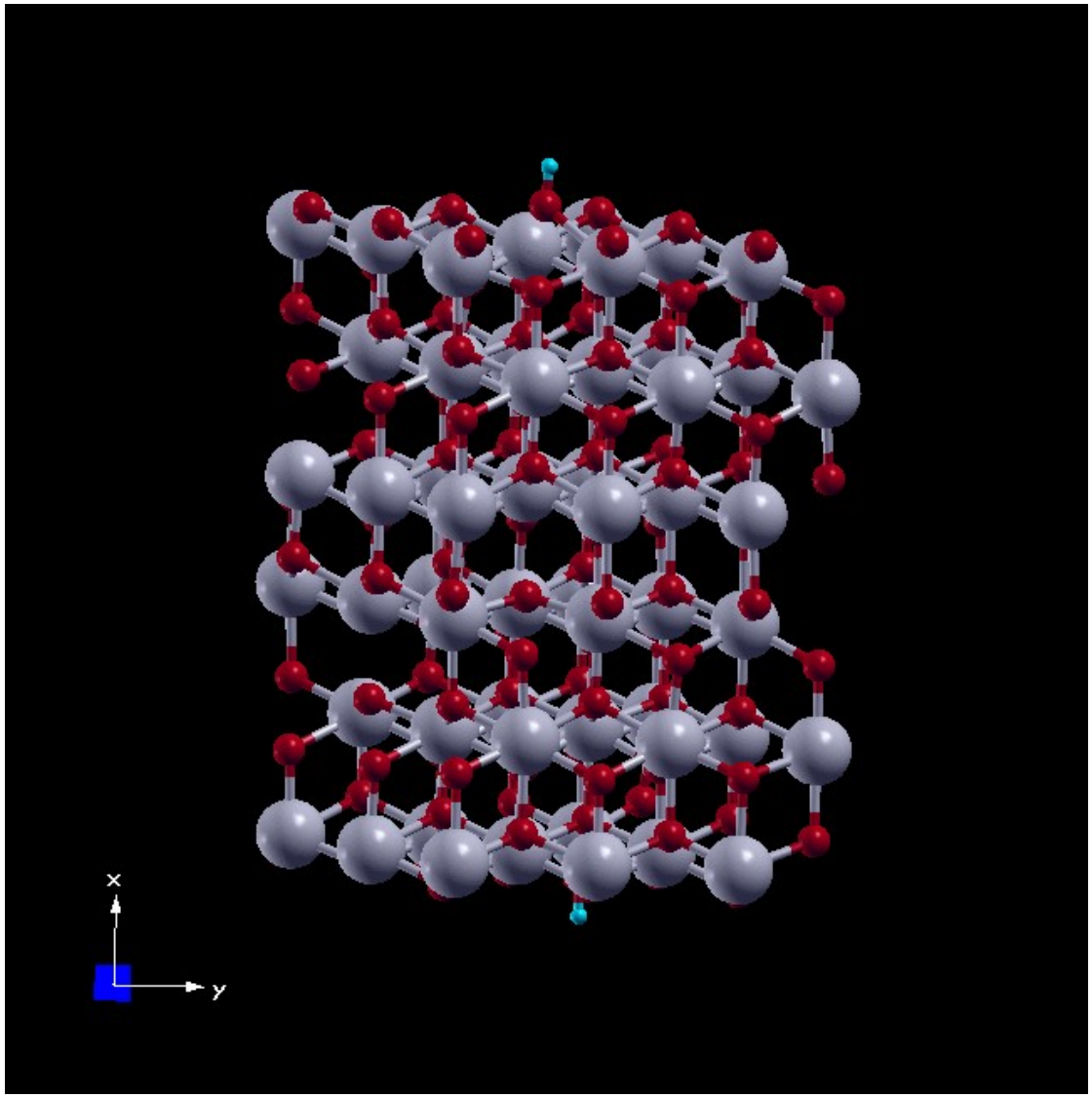
PhD J. Hermet



J. Hermet, M. Torrent, F. Bottin, G. Dezanneau, G. Geneste, PRB **87**, 104303 (2013)

3.a Hopping of a defect in a solid

Proton transfer on the O-ZrO2(111) surface



nimage 11
(9 evolving)

motions of the two oxygens

Proton transfer made possible by « cooperative » motion of the two oxygens

CONTENT

3.b Hopping of a small polaron

When an electron or a hole is released in the lattice of an insulator (e.g. by a point defect), it may localize on a single atom, instead of staying in a Bloch like delocalized band state = small polaron.

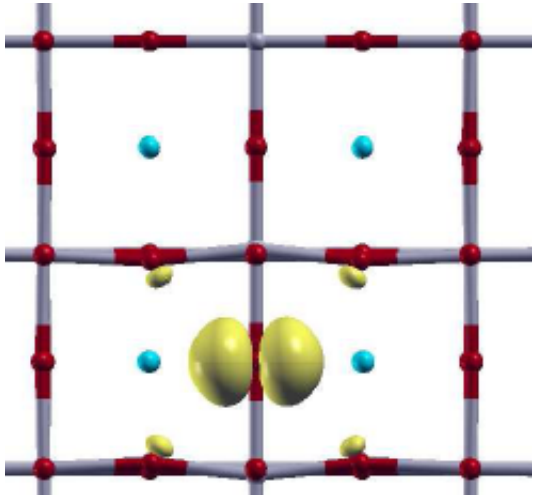
=> the crystal around is distorted (polarized), which in return creates a potential favorable to the localization of the electron(or hole)

= **SELF-TRAPPING**

Energy of the relaxed polaronic configuration minus energy of the configuration with perfet crystal and delocalized electron/hole = **self-trapping energy**
The small polaron is stable if the self-trapping energy is negative.

Ex : oxygen-type hole polaron in $BaSnO_3$

(DFT+U with
U on oxygen p)



3.b Hopping of a small polaron

Small polarons may diffuse in the lattice, by hopping from an atom onto another ; their hopping rate is usually **thermally activated**.

$$r = r_0 e^{-E_a / k_B T}$$

=> Hopping requires to overcome an energy barrier ; which one ?

It is not the electron/hole that overcomes an energy barrier (the electron gas is supposed to stay in its ground state, thus no thermal agitation for the electron gas) => tunneling ?

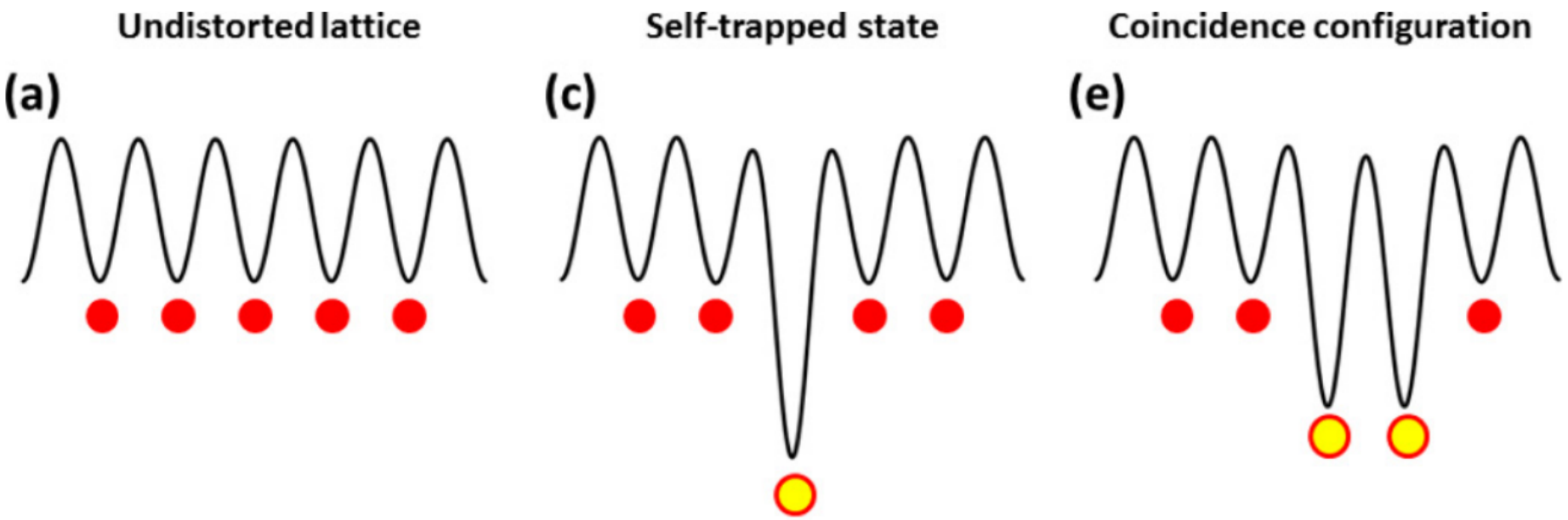
Self-trapped configuration : tunneling impossible !

Resonant tunneling possible in specific configurations
in which the levels on either side of the electronic barrier are in coincidence
= coincidence configurations (CC).

These configurations have energy ~ **Ec** and occur by the thermal fluctuations of the lattice atoms

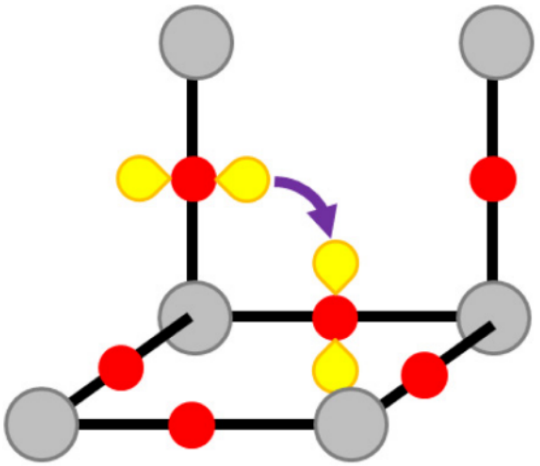
$$r \sim r_0 e^{-E_c / k_B T}$$

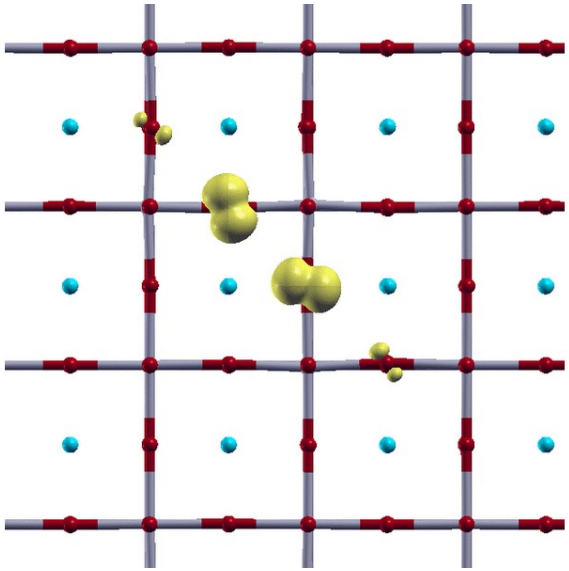
3.b Hopping of a small polaron

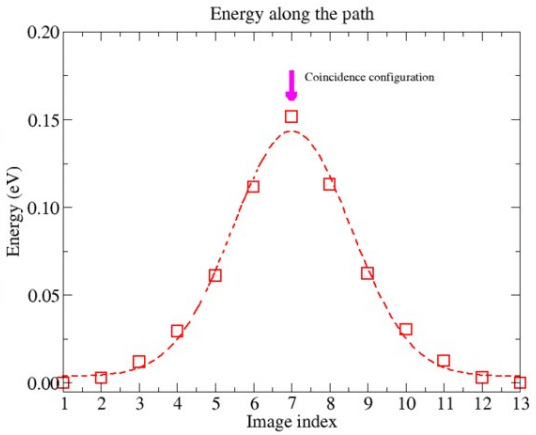


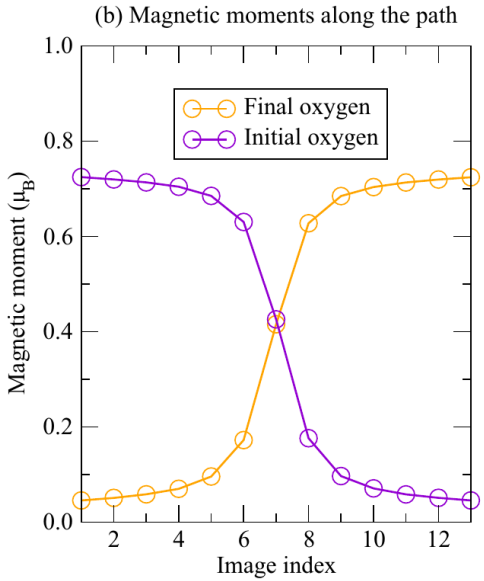
3.b Hopping of a small polaron

Case of the oxygen-type hole polaron in BaSnO3









Warning :

- DFT calculation assumes the polaron in its ground state all along the path
- this may not be the case in reality
- because the tunneling transfer in the CC can be long (if electronic coupling is weak)

G. Geneste, B. Amadon, M. Torrent, G. Dezanneau, PRB 96, 134124 (2017)

3.b Hopping of a small polaron

If the polaron **has the time to adjust** to the lattice configuration (i.e. adiabatic approximation OK along the MEP)

=> adiabatic transfer

$$r \sim r_0 e^{-E_c / k_B T}$$

Controlled by lattice vibrations

If the polaron **has the NOT time** to adjust to the lattice configuration (i.e. adiabatic approximation not valid anymore near the CC)

=> non-adiabatic transfer :

- the polaron may not have the time to cross, and remains on the starting site
- many occurrences of the CC are necessary before transfer occurs
- at CC, the polaron is not in an (adiabatic) eigenstate
- prefactor controlled by tunneling of the hole at CC (usually << that of lattice vibrations)

Requires to know the electronic coupling at CC (not provided by NEB)
= [E(1st excited state) – E(GS)]/2 at CC

CONTENT

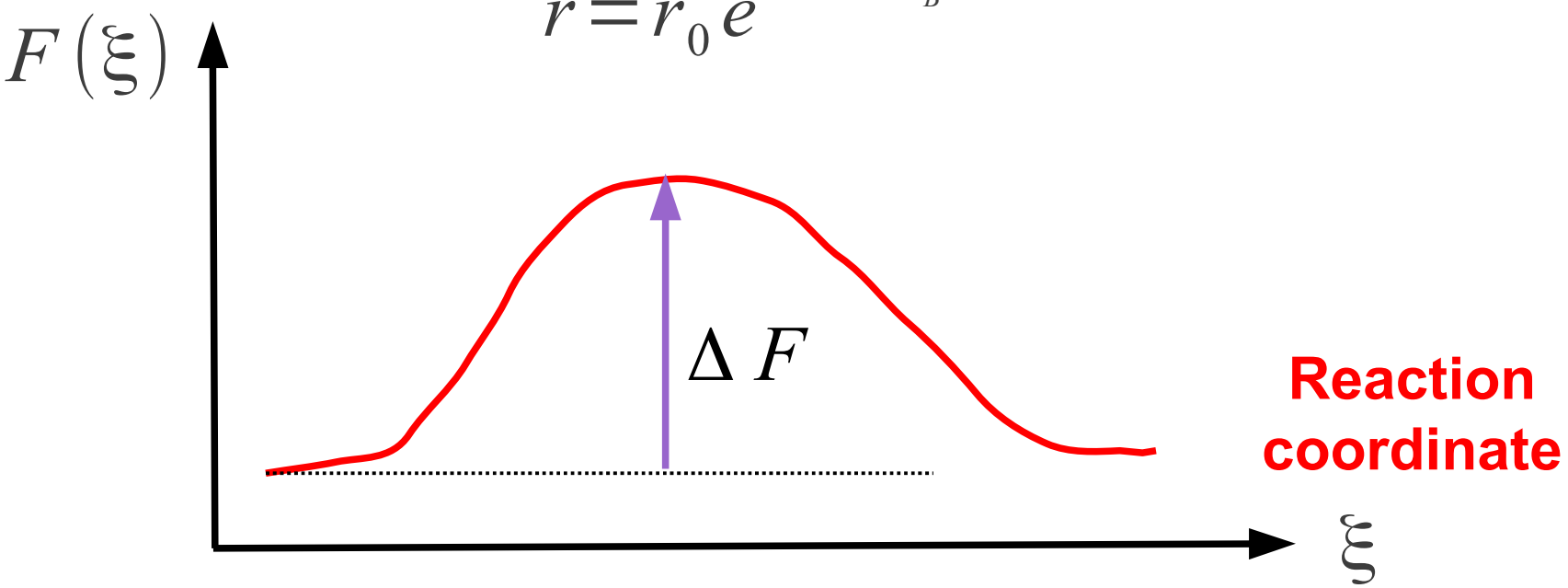
4 – Thermal effects : free energy landscape

MEPs (String Method, NEB) provide a **« static » barrier.**

This static barrier is free of thermal and/or quantum effects.

=> TST normally involves a « free energy » barrier in the expression of the **transition rate** :

$$r = r_0 e^{-\Delta F / k_B T}$$



4 – Thermal effects : free energy landscape

How to obtain this free energy barrier ?

Remember that the free energy as a function a reaction coordinate ξ is related to the density of probability of this reaction coordinate ξ, as

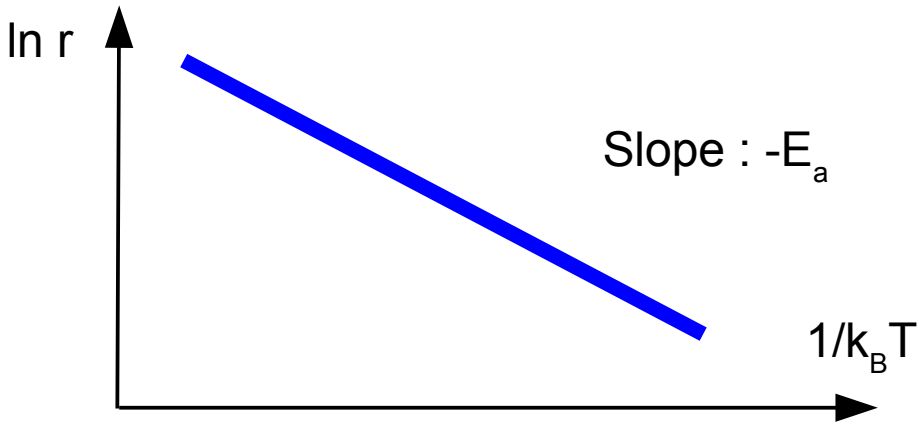
$$F(\xi) - F(\xi_0) = -k_B T \ln \frac{P(\xi)}{P(\xi_0)}$$

With P(ξ) the density of probability of ξ at thermodynamic equilibrium :

$$P(\xi) \propto C \int \dots \int_{\{x_{i\alpha}\}} \delta(\xi(\{x_{i\alpha}\}) - \xi) e^{-V(\{x_{i\alpha}\})/k_B T} dX$$

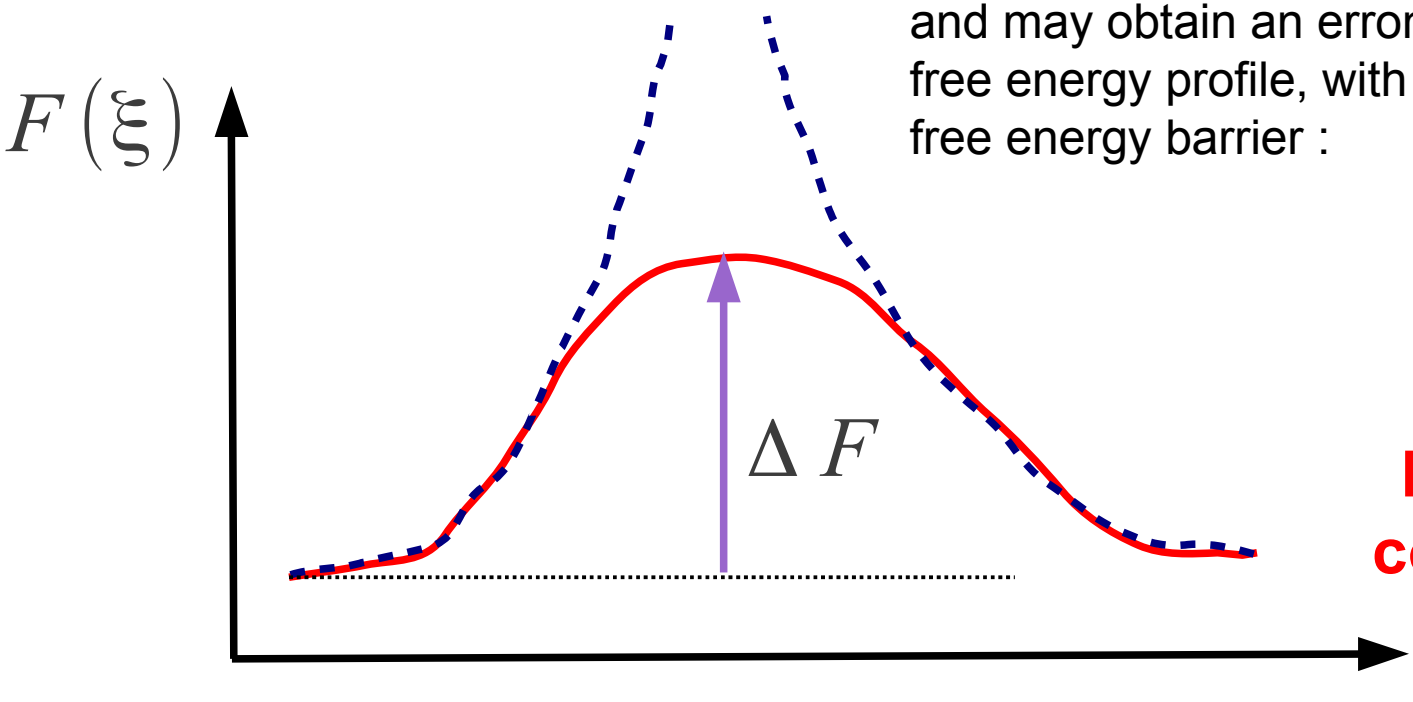
1st possibility : make very long MD runs, at various temperatures, and count the events ! Then plot the log of the rate as a function of 1/T : The slope should be minus the activation energy !

4 – Thermal effects : free energy landscape



Unfortunately, this is rarely POSSIBLE because the statistics will be too bad, especially if the barrier is large w/r to kT !

You will not sample correctly the high free energy (=low proba) regions and may obtain an erroneous free energy profile, with a wrong free energy barrier :



Reaction coordinate

4 – Thermal effects : free energy landscape

Chemists have treated and solved this problem since a long time !
« Blue-Moon » ensemble : Method to simulate the **occurrence of RARE events** within Molecular Dynamics (MD)

- simulate each step of the event by **« forcing » ξ to take a chosen value :**

=> MD under (holonomic) constraint of FIXED ξ

Method of Lagrange multipliers

- Obtain for each value of ξ the derivative of the free energy
« mean force » on the constraint : $-\frac{dF}{d\xi}$

- recover the (free) energy profile by (thermodynamic) integration :

$$\Delta F = F(\xi) - F(\xi_0) = \int_{\xi_0}^{\xi} \frac{dF}{d\xi}(\xi')\, d\xi'$$

Sprik, Cicotti, J. Chem. Phys. ***109****, 7737, (1998)*

4 – Thermal effects : free energy landscape

General case :

$$\xi\left(\{x_{i\alpha}\}\right)$$

$$\frac{dF}{d\xi}=\frac{\langle Z^{-1/2}\left(-\lambda+k_B T\, G\right)\rangle_\xi}{\langle Z^{-1/2}\rangle_\xi}$$

with :

$$Z=\sum_{i=1}^{N}\frac{1}{m_i}\left(\frac{\partial\xi}{\partial\vec{r}_i}\right)^2$$

$$G=\frac{1}{Z^2}\sum_{i=1}^{N}\sum_{j=1}^{N}\frac{1}{m_i m_j}\frac{\partial\xi}{\partial\vec{r}_i}\frac{\partial^2\xi}{\partial\vec{r}_i\partial\vec{r}_j}\frac{\partial\xi}{\partial\vec{r}_j}$$

Time average under fixed ξ (constrained MD)
= « *blue-moon* » *ensemble average*

$$F(\xi_2)-F(\xi_1)=\int_{\xi_1}^{\xi_2}\frac{dF}{d\xi}(\xi')\,d\xi'$$

Sprik, Cicotti, J. Chem. Phys. ***109****, 7737, (1998)*

4 – Thermal effects : free energy landscape

Implementation **in ABINIT of the LINEAR constraint**
i.e. linear combination between atomic positions

$$\xi\left(\{x_{i\alpha}\}\right)=\sum_{i\alpha} a_{i\alpha} x_{i\alpha}$$

Real coefficients

1) *Lagrangian* with *constraints*

$$L=[T\left(\{\dot{x}_{i\alpha}\}\right)-V\left(\{x_{i\alpha}\}\right)]-\lambda[\sum_{i\alpha} a_{i\alpha} x_{i\alpha}-\xi]$$

2) Apply *Euler-Lagrange equations* :

$$m_i \frac{d^2 x_{i\alpha}}{dt^2}=f_{i\alpha}-\lambda a_{i\alpha}$$

Lagrange multiplier computed at each step as $\lambda(t)=\dfrac{\sum_{i\alpha} a_{i\alpha}\dfrac{f_{i\alpha}(t)}{m_i}}{\sum_{i\alpha}\dfrac{a_{i\alpha}^2}{m_i}}$

3) *Derivative of the free energy* :

$$\frac{dF}{d\xi}=-\langle\lambda\rangle_\xi=-\frac{\sum_{i\alpha}\dfrac{a_{i\alpha}}{m_i}\langle f_{i\alpha}\rangle_\xi}{\sum_{i\alpha}\dfrac{a_{i\alpha}^2}{m_i}}$$

4 – Thermal effects : free energy landscape

- **Physically acceptable** linear constraints satisfy : $\sum_{i\alpha} a_{i\alpha} = 0$

- However, even if $\sum_{i\alpha} a_{i\alpha} \neq 0$, a supplemental constraint has been added to ensure that center of mass does not move.

- Value of the constraint ξ : **FIXED** by **INITIAL** set of positions.

- Initialization of the velocities :

The initial velocities must be modified to ensure that the constraint is obeyed, i.e.

$$\sum_{i\alpha} a_{i\alpha} \frac{d x_{i\alpha}}{dt} = 0$$

- Implemented in the routine **pimd_apply_constraint** (m_pimd.F90).

- PIMD : the constraint is applied on the centroid.

4 – Thermal effects : free energy landscape

- The constraint is STRICTLY obeyed all along the MD trajectory (at EACH step, NOT on average)

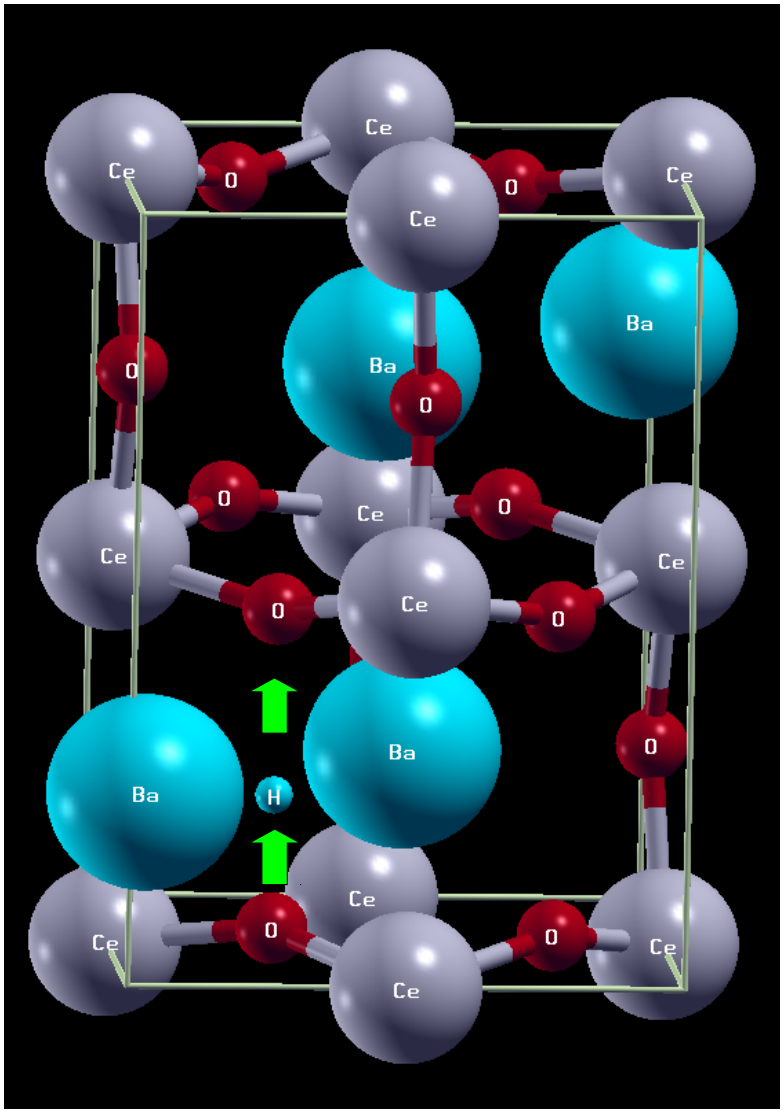
Ex :

- Reaction coordinate = -36.5852098477
- Reaction coordinate = -36.5852098477
- Reaction coordinate = -36.5852098477
- Reaction coordinate = -36.5852098477
- Reaction coordinate = -36.5852098477
- Reaction coordinate = -36.5852098477
- Reaction coordinate = -36.5852098477

- the Center of mass is also strictly FIXED

Center of mass:
4.6876358799 6.5991695708 4.6808066009
Center of mass:
4.6876358799 6.5991695708 4.6808066009
Center of mass:
4.6876358799 6.5991695708 4.6808066009

4 – Thermal effects : free energy landscape



Example :

$BaCeO_3$: orthorhombic perovskite

Pnma space group

Excellent protonic conductor

Inter-octahedral transfer of H^+

Cell = 20 atoms

Reaction coordinate : $(O_1H)_y$ - $(O_2H)_y$

$= y(H)-y(O_1) – [y(O_2) – y(H)]$

PIMD, T=200 K

P=32 beads

4 – Thermal effects : free energy landscape

Example of input file of constrained PIMD

```
# PARALLELIZATION
          # => 864 procs
paral_kgb 1
npkpt 9
npband 3
npfft 1
npimage 32

# PIMD/MD
optcell 0
irandom 3
restartxf -1
imgmov 9   # langevin PIMD
ntimimage 10000
nimage 32
mdtemp 400 200
vis 5d-05
dynimage 32*1
nsym 1
pitransform 0
amu      140 16 138 1 # ce o ba h
pimass  140 16 138 1
dtion 10
```

```
# CONSTRAINTS
pimd_constraint 1
nconeq 1
natcon 3
iatcon 5 20 1 #ox1 ox2 hydrogen
wtatcon
0.0 -1.0 0.0 0.0 -1.0 0.0 0.0 2.0 0.0

# ground state
nband 111
occopt 3
tsmear 0.001
pawovlp -1
ixc 11
ecut 18.0
pawecutdg 25.0
kptopt 1
ngkpt 3 2 3
nstep 100
toldff 1.0d-05
prtden 0
prtwf 0

charge 1.0
```

```
# atoms
znucl  58 8 56 1
ntypat 4
natom 21
typat
4 3 1 2 2 3 2 2 3 3 1 1 1 2 2 2 2 2 2 2 2

# cell and atomic positions
acell 11.941471  16.813056  11.913748

xred
  0.279                 0.216                 0.723  #yH to be varied
  2.5108646807E-02  2.5000000000E-01 -8.0469316958E-03
 -1.3877787808E-17 -9.7144514655E-17  5.0000000000E-01
  4.8011508619E-01  2.5000000000E-01  7.9658009587E-02
  2.7974388262E-01  4.3160947462E-02  7.2102708776E-01 #ox1
  9.7489135319E-01  7.5000000000E-01  1.0080469317E+00
  5.1988491381E-01  7.5000000000E-01  9.2034199041E-01
  7.2025611738E-01  9.5683905254E-01  2.7897291224E-01
  5.2510864681E-01  2.5000000000E-01  5.0804693170E-01
  4.7489135319E-01  7.5000000000E-01  4.9195306830E-01
  5.0000000000E-01  5.0000000000E-01 -6.9388939039E-17
 -1.3877787808E-17  5.0000000000E-01  5.0000000000E-01
  5.0000000000E-01 -9.7144514655E-17 -6.9388939039E-17
  9.8011508619E-01  2.5000000000E-01  4.2034199041E-01
  1.9884913809E-02  7.5000000000E-01  5.7965800959E-01
  7.7974388262E-01  4.5683905254E-01  7.7897291224E-01
  7.2025611738E-01  5.4316094746E-01  2.7897291224E-01
  2.2025611738E-01  9.5683905254E-01  2.2102708776E-01
  2.2025611738E-01  5.4316094746E-01  2.2102708776E-01
  2.7974388262E-01  4.5683905254E-01  7.2102708776E-01 #ox2
  7.7974388262E-01  4.3160947462E-02  7.7897291224E-01
```

Thanks for your attention !