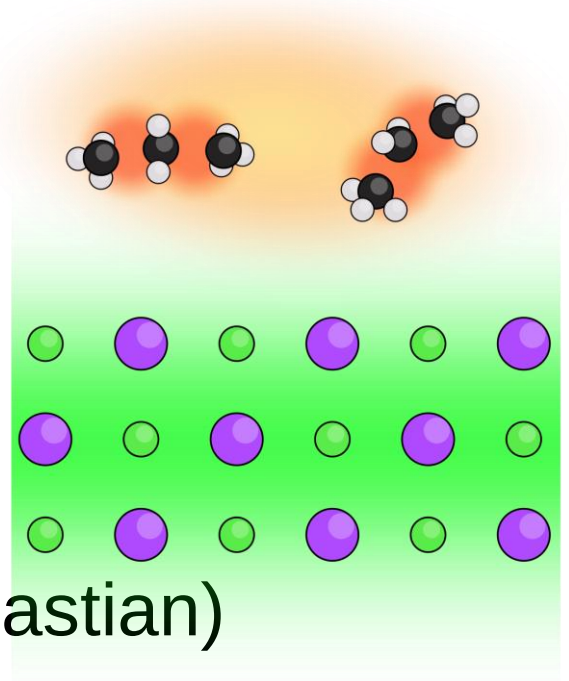
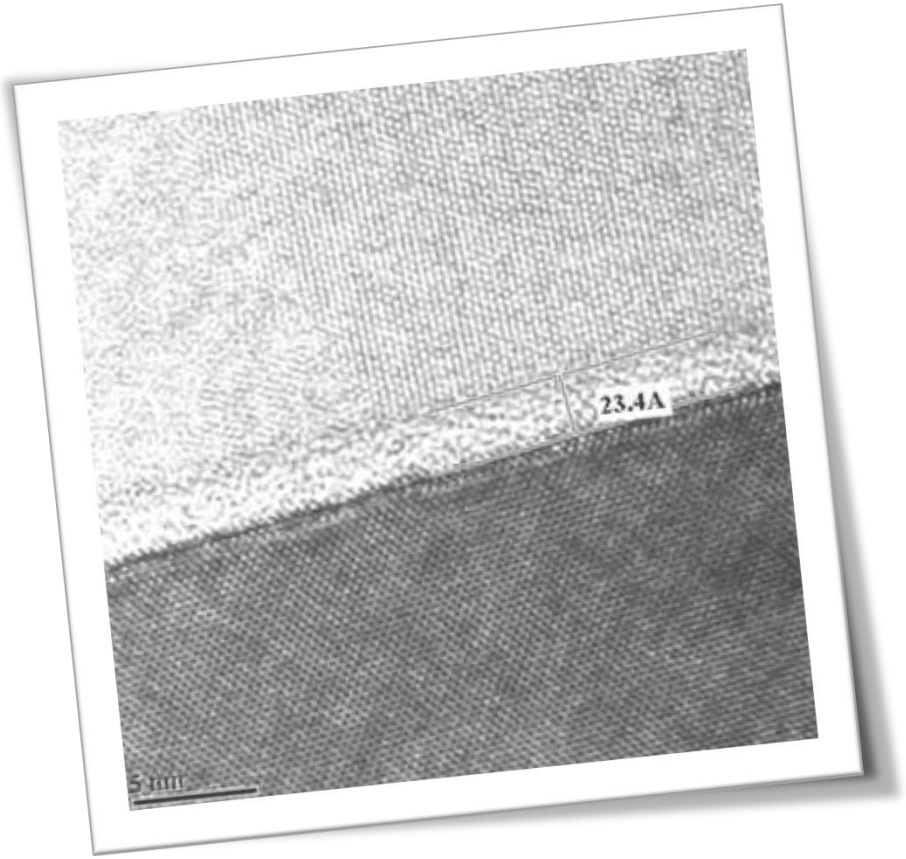
"'Real' world problems"

Some uses of cp2k in our* group



Matt Watkins

- David Gao
- Francisco Lopez (now in San Sebastian)
- Tassem Sayed
- Sanliang Ling (now in chemistry)
- Alex Shluger*



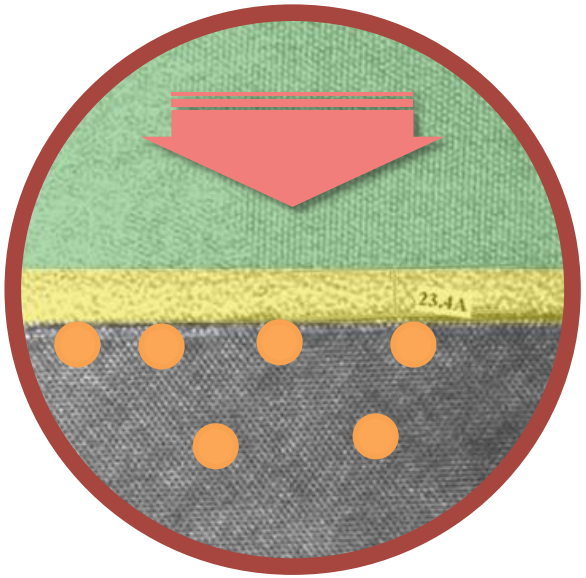
Modeling the Si/SiO_2 system

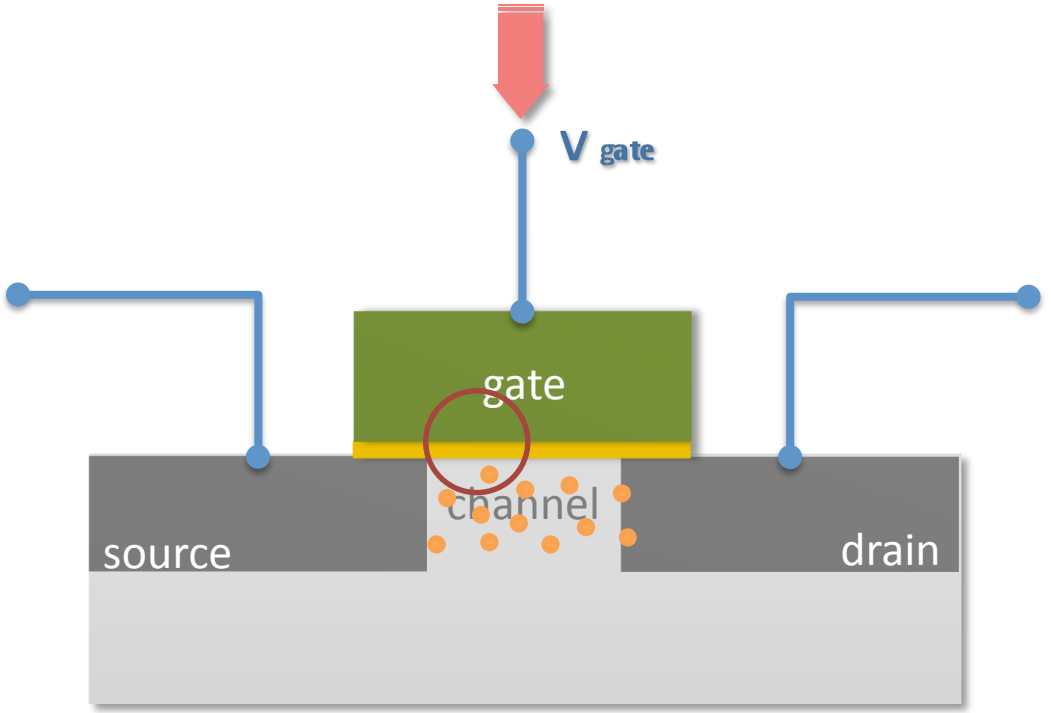
Role of disorder

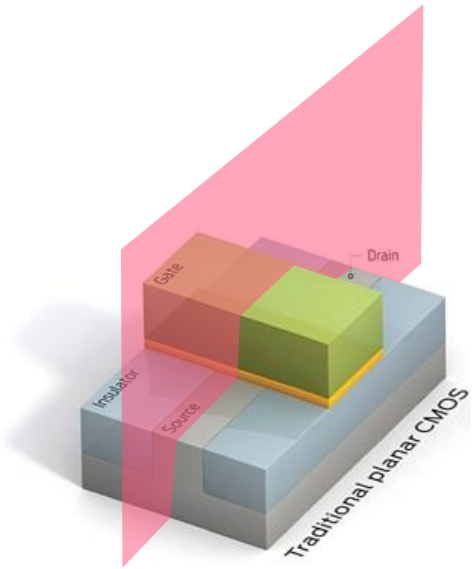
Tassem Sayed

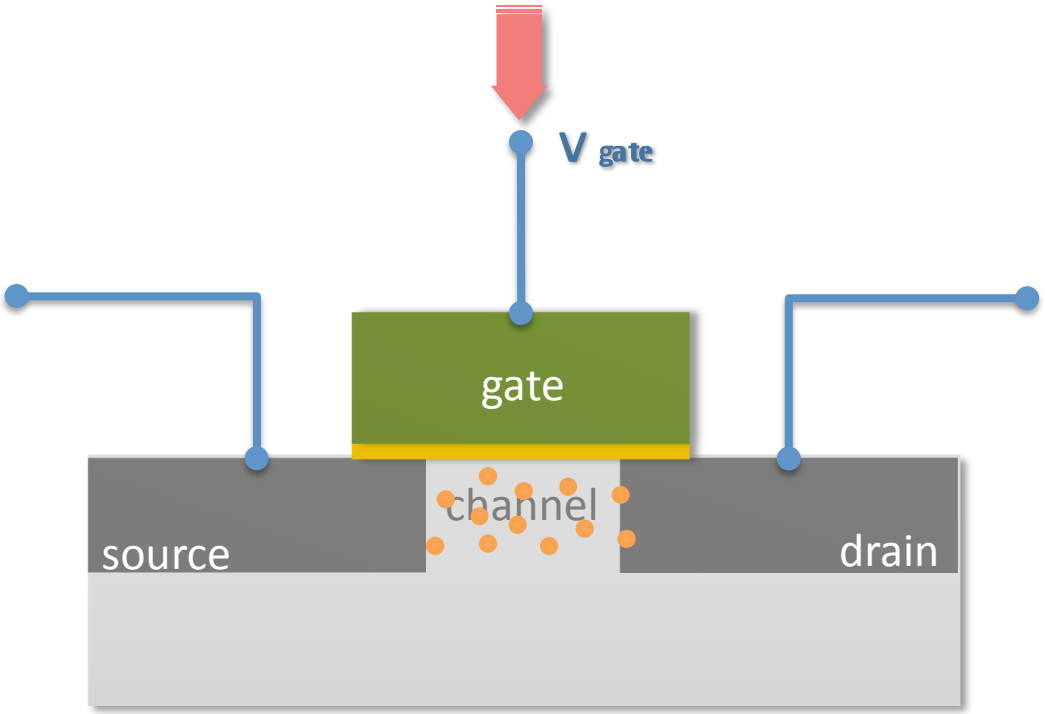
Francisco Lopez El-Gejo

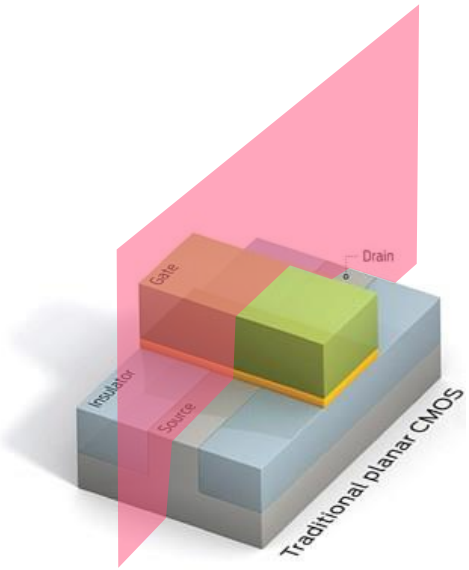
Sanliang Ling

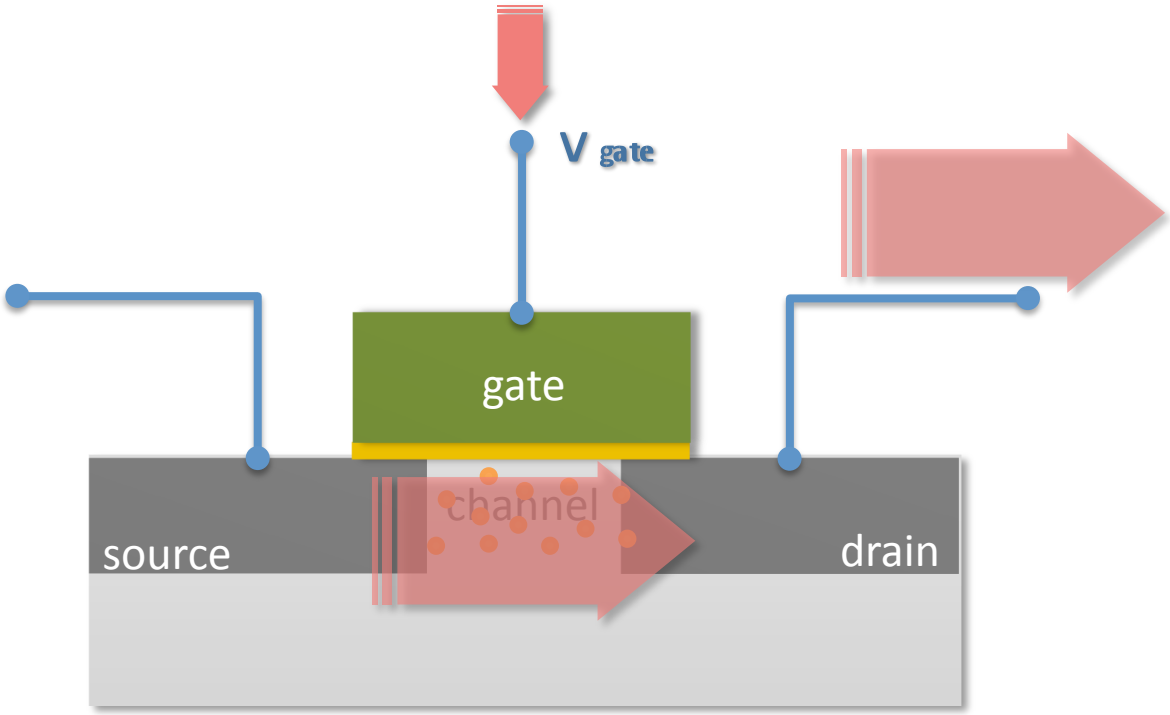


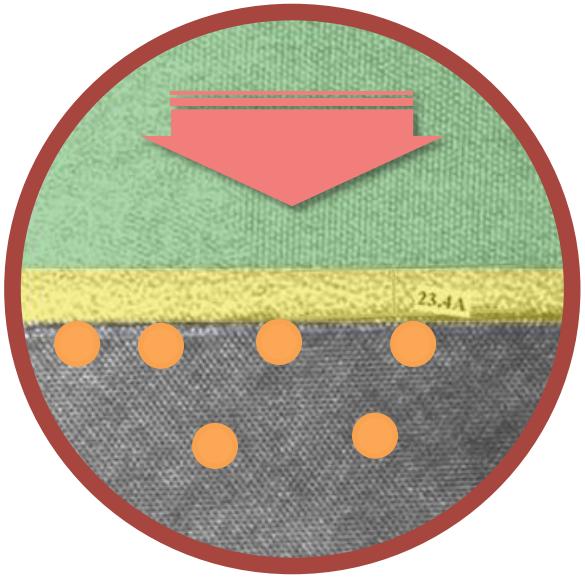

V gate
gate
channel
source
drain

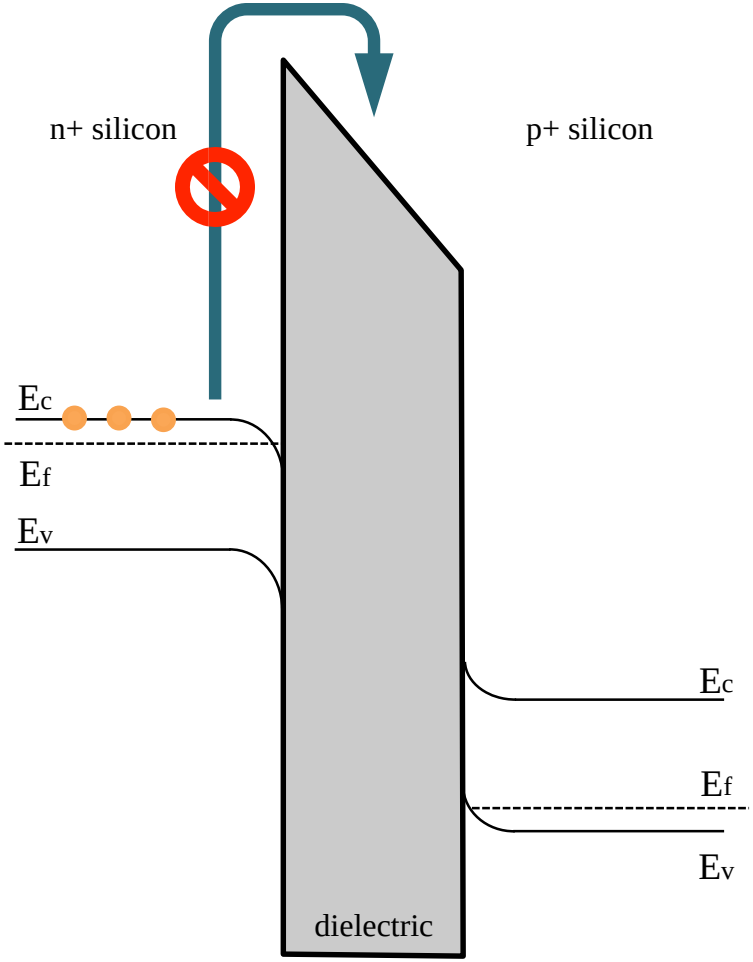

Drain
Gate
Insulator
Source
Traditional planar CMOS


V gate
gate
channel
source
drain

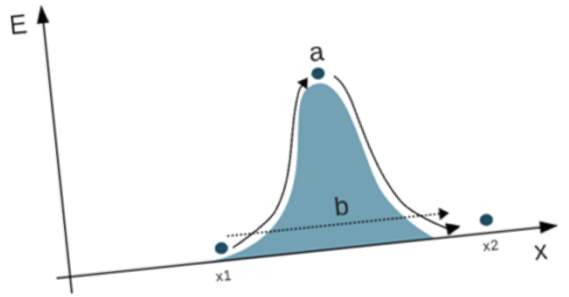

Drain
Gate
Insulator
Source
Traditional planar CMOS

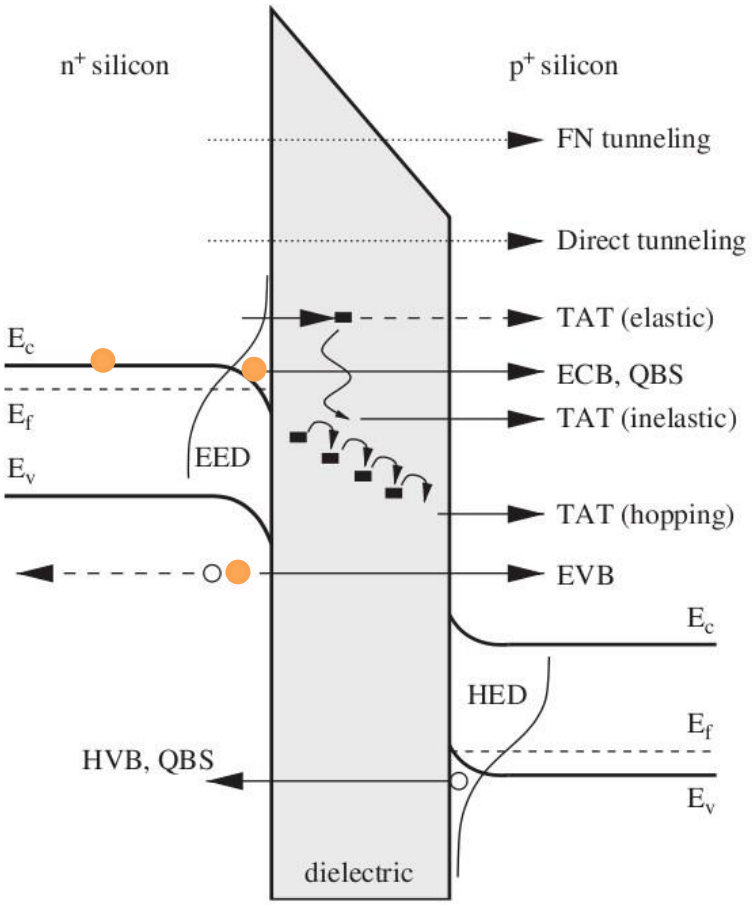

V gate
gate
channel
source
drain




n+ silicon
p+ silicon
Ec
Ef
Ev
Ec
Ef
Ev
dielectric

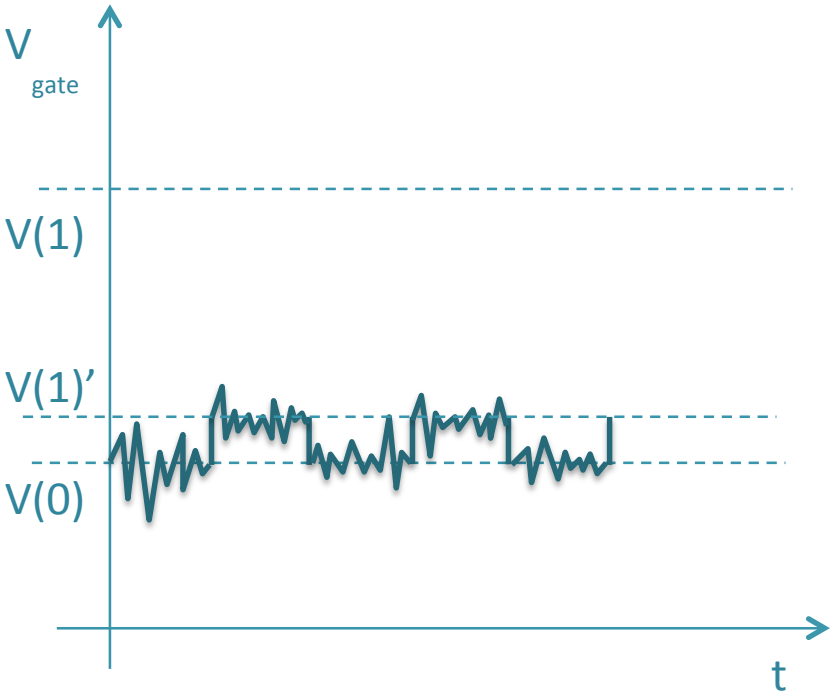
$$T = \frac{e^{-2\int_{x_1}^{x_2} dx \sqrt{\frac{2m}{\hbar^2}(V(x)-E)}}}{\left(1+\frac{1}{4}e^{-2\int_{x_1}^{x_2} dx \sqrt{\frac{2m}{\hbar^2}(V(x)-E)}}\right)^2}$$

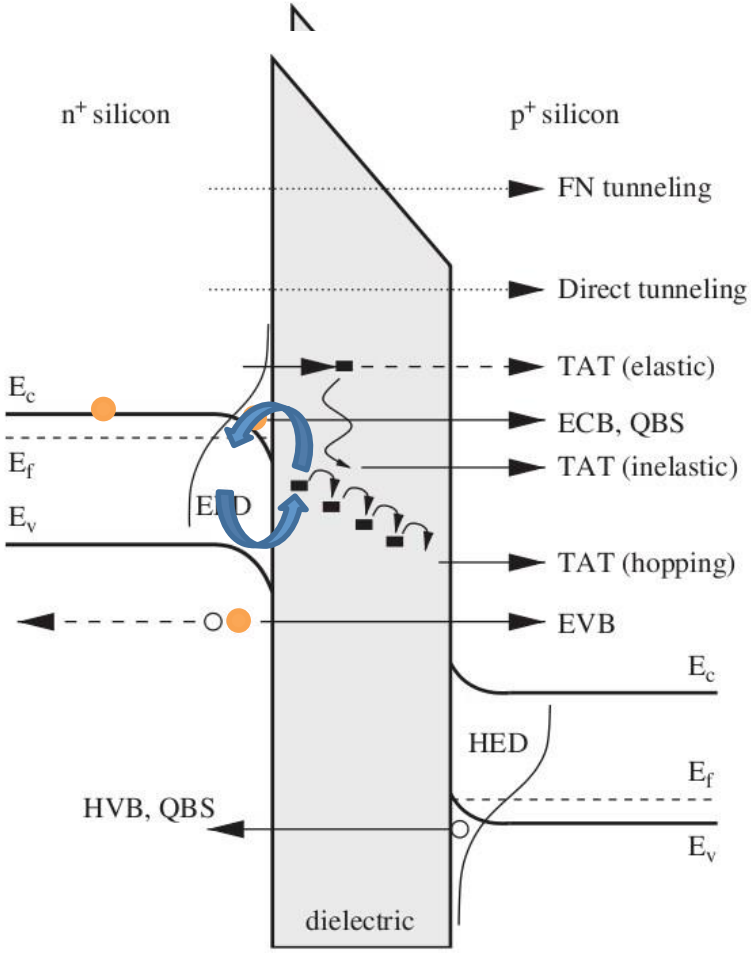




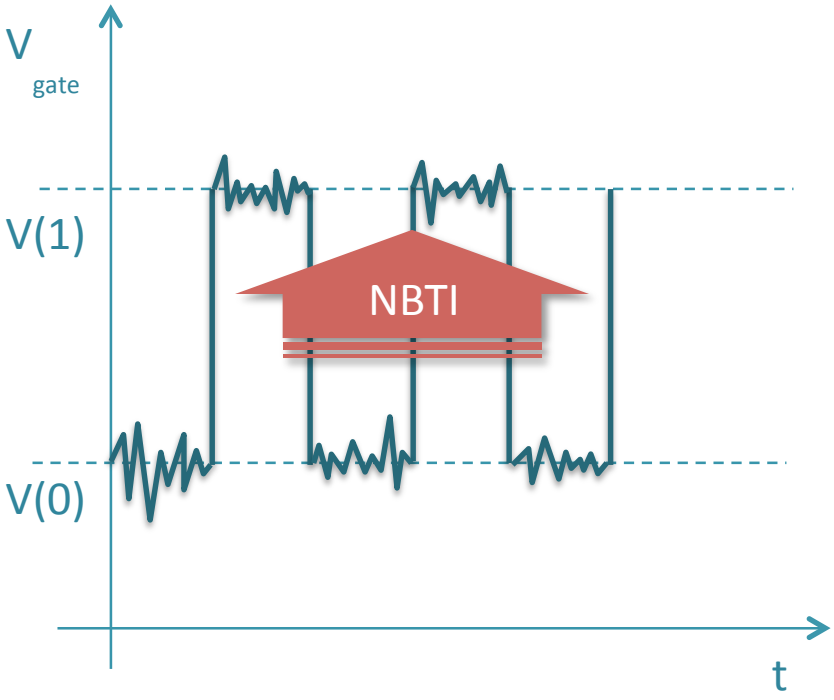
As the width of the dielectric layer is scaled down, Quantum Effects become dominant.

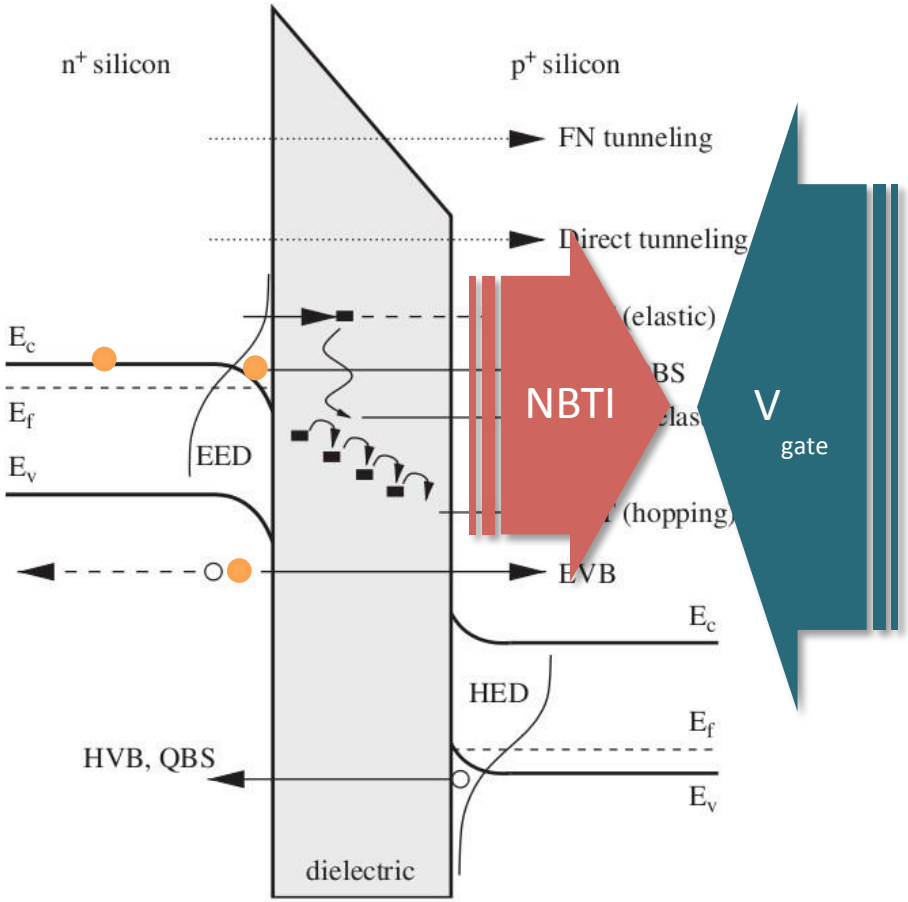
Tunneling allows carriers to transit between the channel and the gate electrode without gaining energy.





Random Telegraph Noise (RTN) is caused by tunneling of carriers back and forth between conduction band of Si at channel and defect levels.



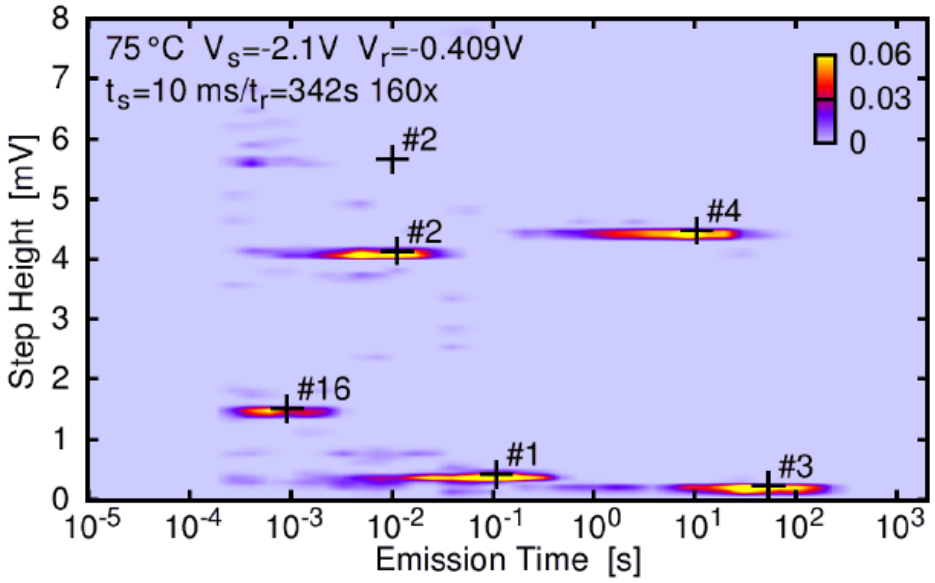


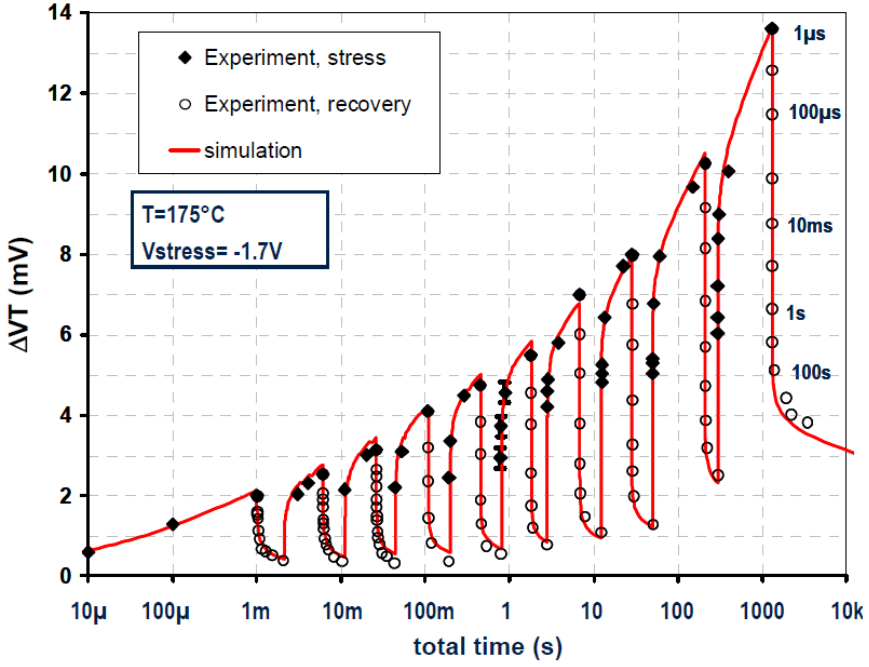
Negative Bias Temperature Instability causes gate voltage to drift, thus preventing from reaching lower operational voltages.

Defects responsible for Reliability Issues

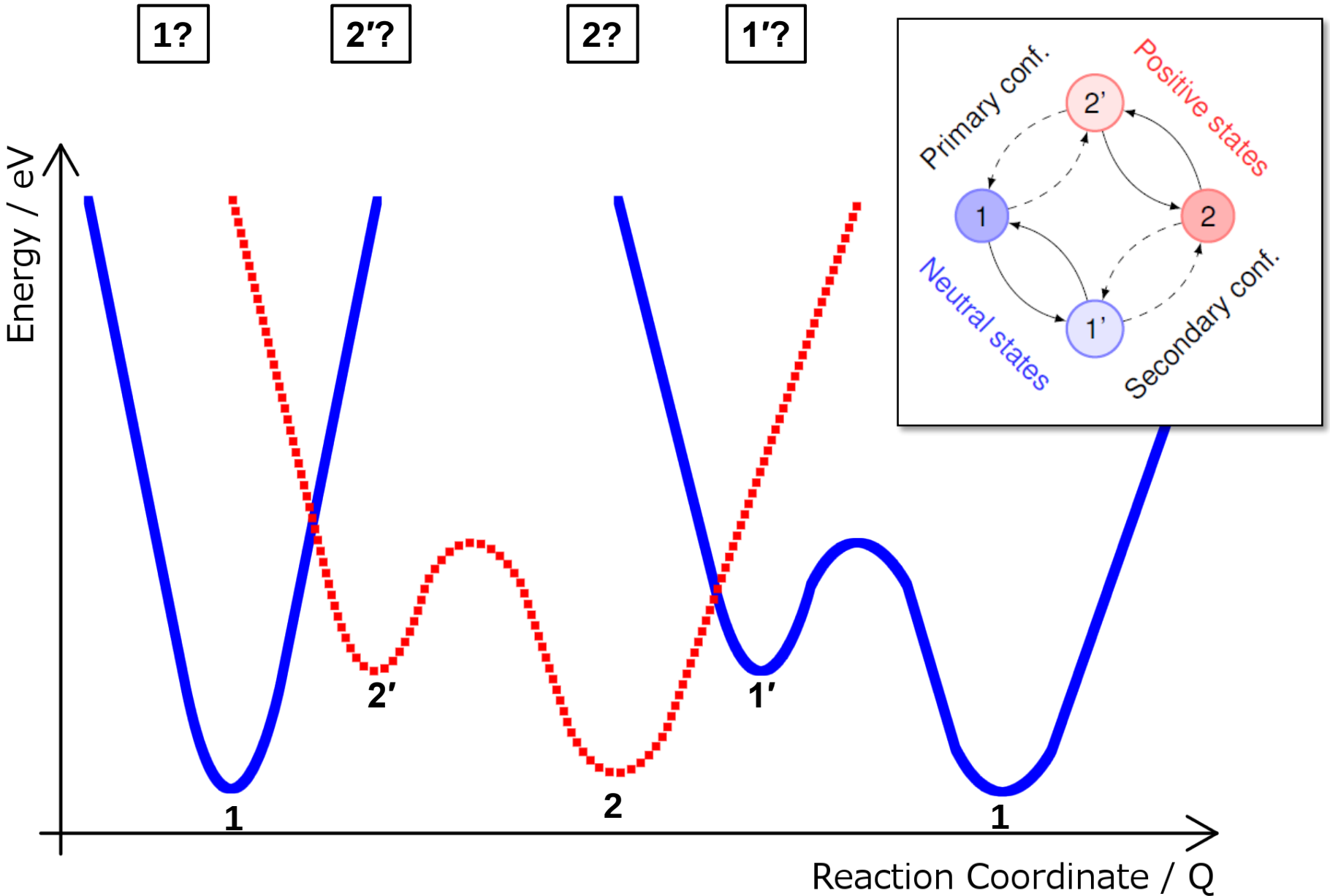
Negative Bias Temperature Instability (NBTI)

- Characterised by shift in threshold voltage over time at high temperatures and high voltages
- Experimental data reveals charge trapping and emission time constants
- Phenomenological model matches experimental data



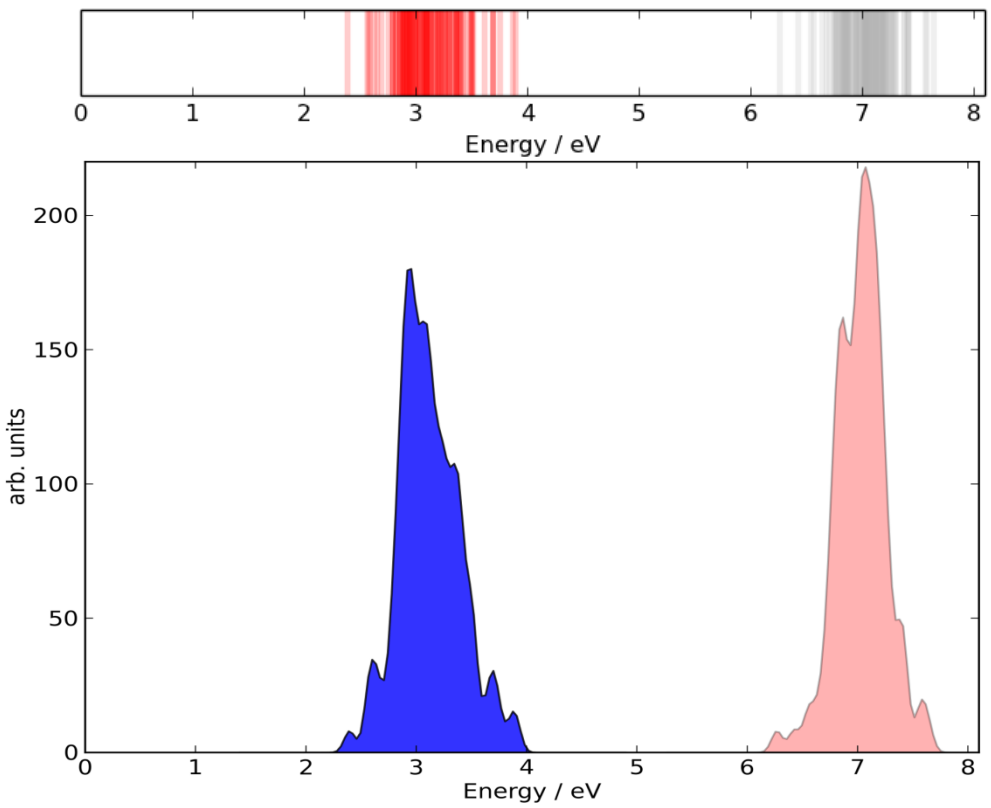


Defects responsible for Reliability Issues

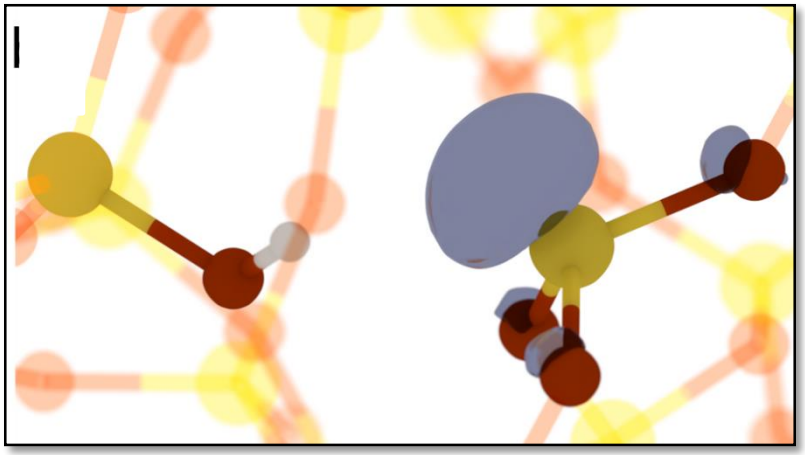


Defects responsible for Reliability Issues

- Hydrogen implicated in NBTI
- Find point defects in a-SiO_2 which interact with H
- 116 Configurations of hydroxyl E' center
- This is lowest energy configuration by ~ 1.2 eV. Other configurations are overlapping in energy
- Defect level 2.4 to 3.9 eV above SiO_2 VB, almost resonant with Si CB



- Barrier to H binding calculated using Nudged elastic band: <1.01 eV>, 0.49 – 1.29 eV



Defects responsible for Reliability Issues

- Hydrogen implicated in NBTI
- Find point defects in a-SiO_2 which interact with H
- 116 Configurations of hydroxyl E' center

```
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  PROGRAM FARMING
  RUN_TYPE NONE
&END GLOBAL
&FARMING
NGROUP 324

&JOB
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  OUTPUT_FILE_NAME a_sio2.out
&END JOB
&JOB
  DIRECTORY run167/dft/neutral/
  INPUT_FILE_NAME a_sio2.inp
  OUTPUT_FILE_NAME a_sio2.out
&END JOB
&JOB
  DIRECTORY run352/dft/neutral/
  INPUT_FILE_NAME a_sio2.inp
  OUTPUT_FILE_NAME a_sio2.out
&END JOB
&JOB
  DIRECTORY run005/dft/neutral/
  INPUT_FILE_NAME a_sio2.inp
  OUTPUT_FILE_NAME a_sio2.out
&END JOB
&JOB
```

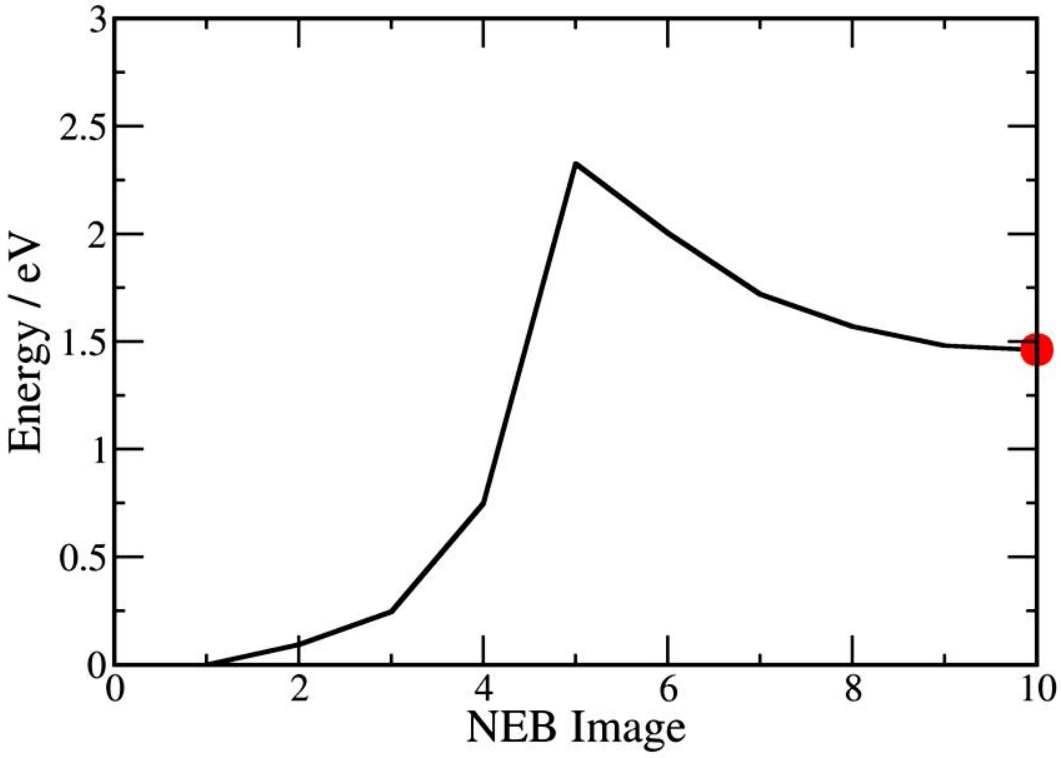
CP2K has built in task farming
Simplest version looks similar to NEB – just splits the job into X separate runs

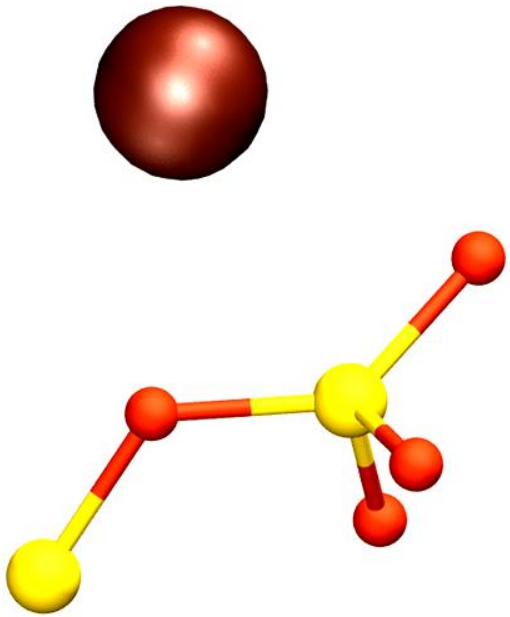
Can also use some simple logic to run sequences of jobs

Examples in tests/FARMING too

Defects responsible for Reliability Issues

- Defect is generated by H interaction w/ bridging O. Caclulate barrier of H binding to O using nudged elastic band method.
- Forward barrier (H binding) averages 0.94 eV, 0.49 – 1.71 eV
- Reverse barrier (H interstitial) averages 1.83 eV, 1.23 – 3.34 eV
- Highest energy as H approaches bridging O



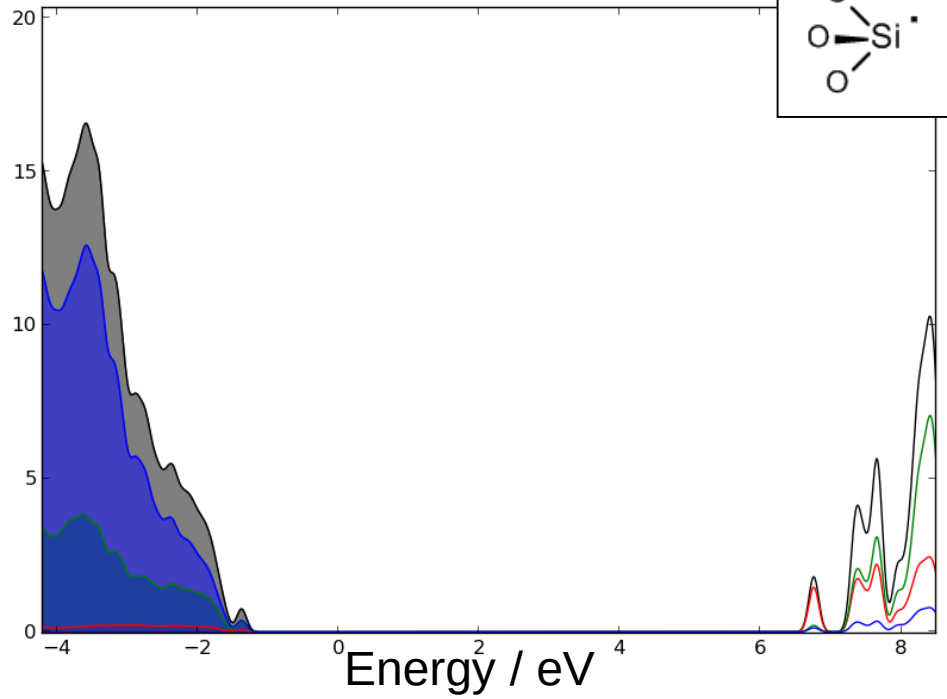


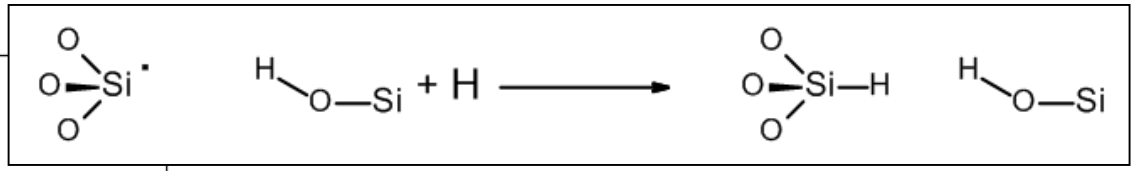
Defects responsible for Reliability Issues

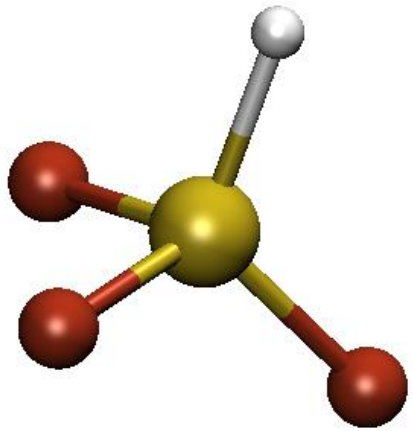
- This defect can be passivated by a neutral H atom
- No states appear in band gap after passivation
- Binding energy of Si-H bond will be calculated as:

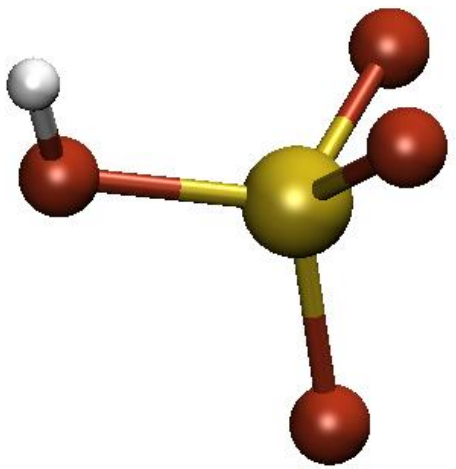
$$E_{Binding} = E^{Tot}_{Interstitial} - E^{Tot}_{Si-H}$$

- $E_{Binding[Si-H]}$ averages at 4.2 eV, ranging from 4.0 to 4.3 eV



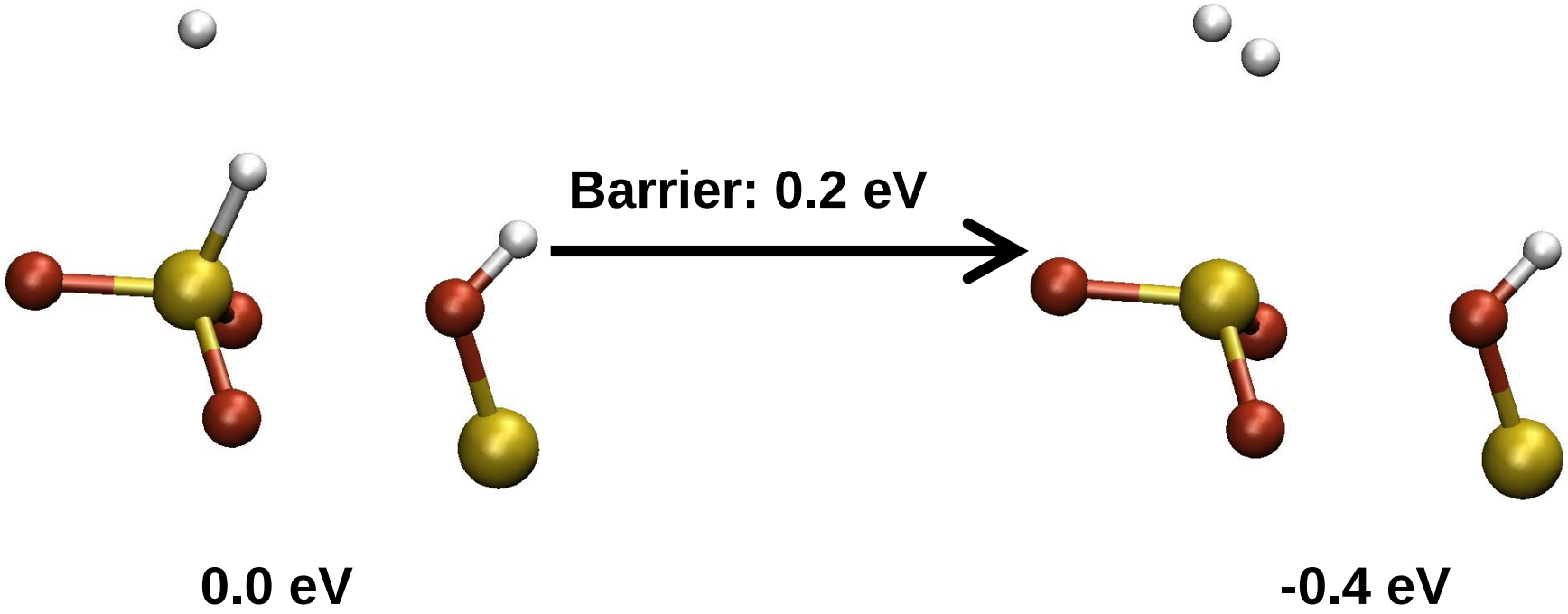






Defects responsible for Reliability Issues

- After H-passivation, the defect can be reactivated by interaction w/ a neutral H atom
- A neutral H atom can remove H from the Si-H so that the defect is reactivated and leaves behind a H_2 interstitial molecule
- Barrier to depassivation: 0.2 eV
- Depassivated state lower in energy by 0.4 eV, 0.2 – 0.7 eV more stable



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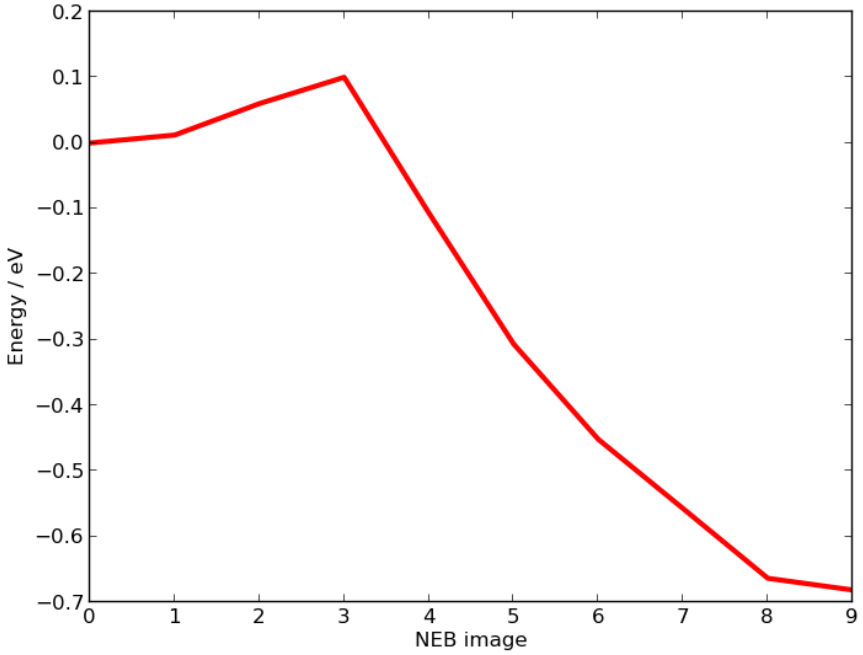
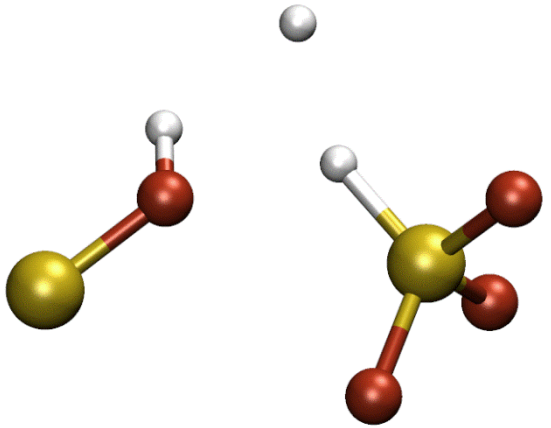
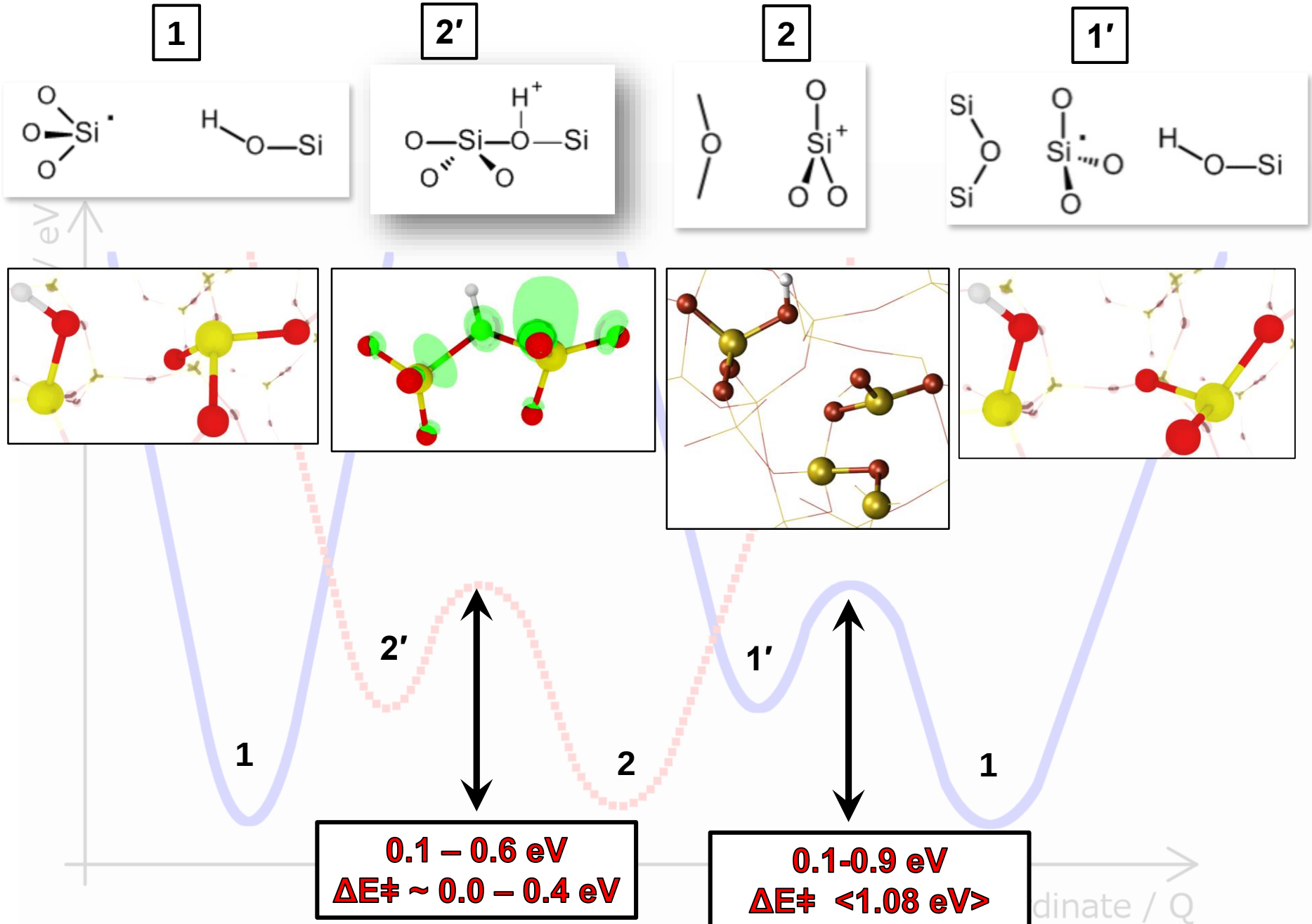
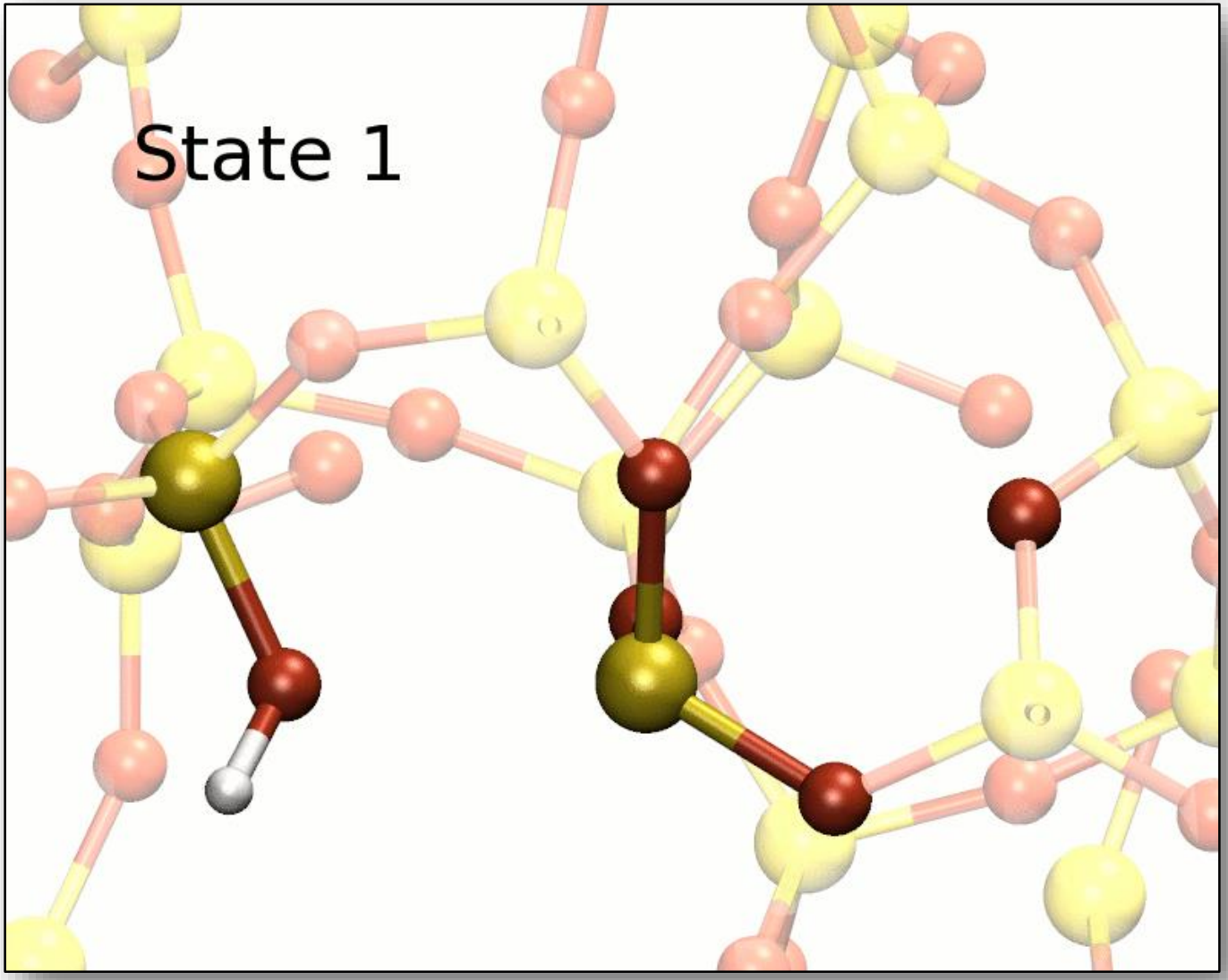




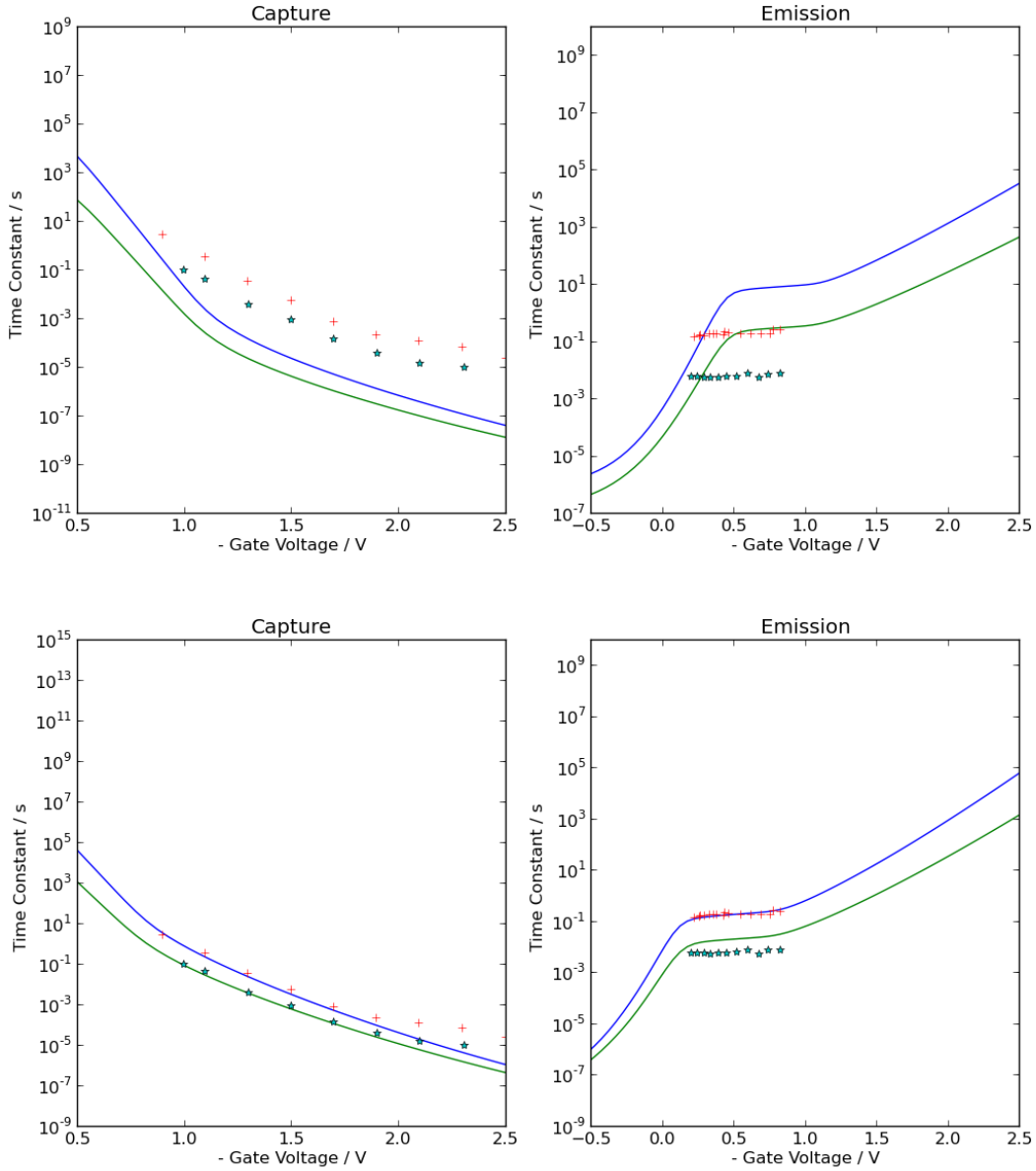
Defects responsible for Reliability Issues



Defects responsible for Reliability Issues

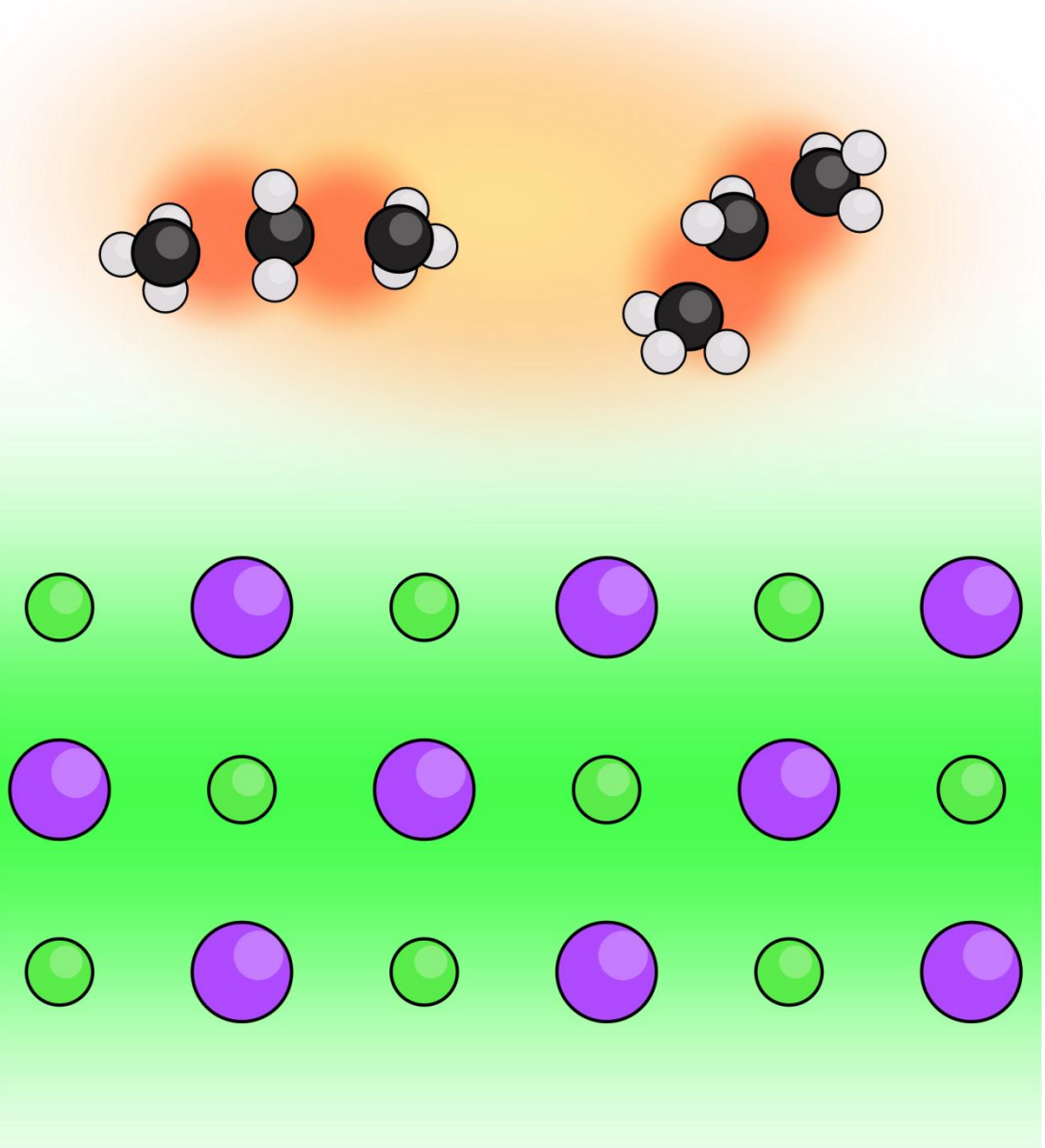


Defects responsible for Reliability Issues



Atomistic data combined with device modelling (hole wavefunctions) and “simple” tunnelling expressions to determine rate constants for charge trapping – experimental observable

Surfaces, molecules and other thingies

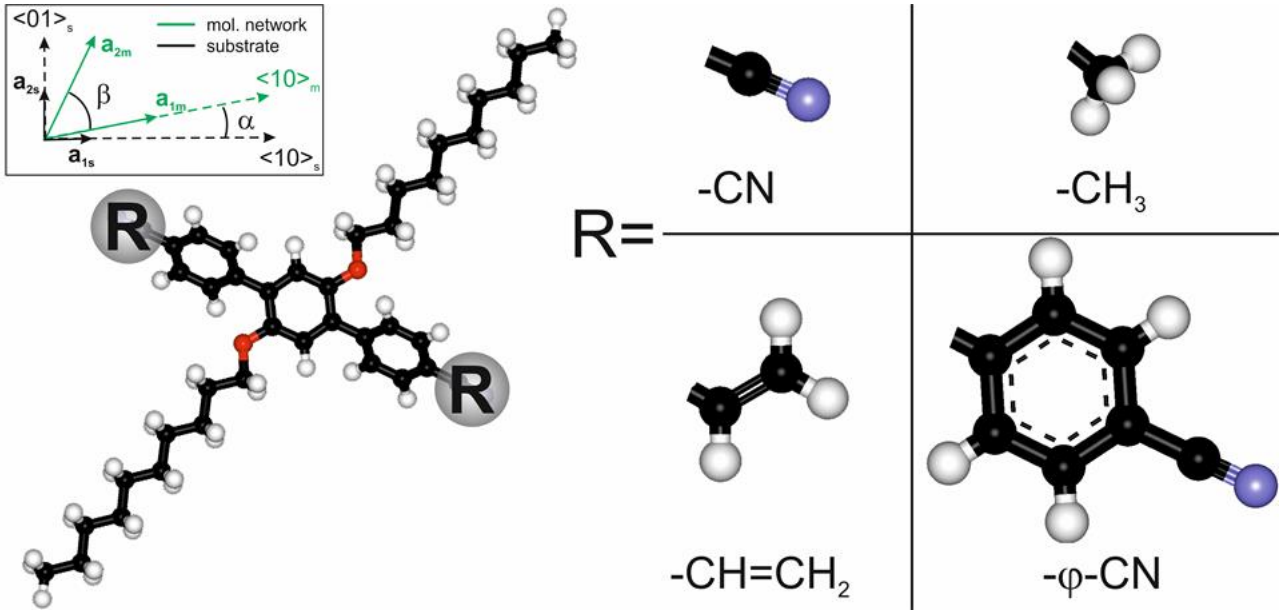


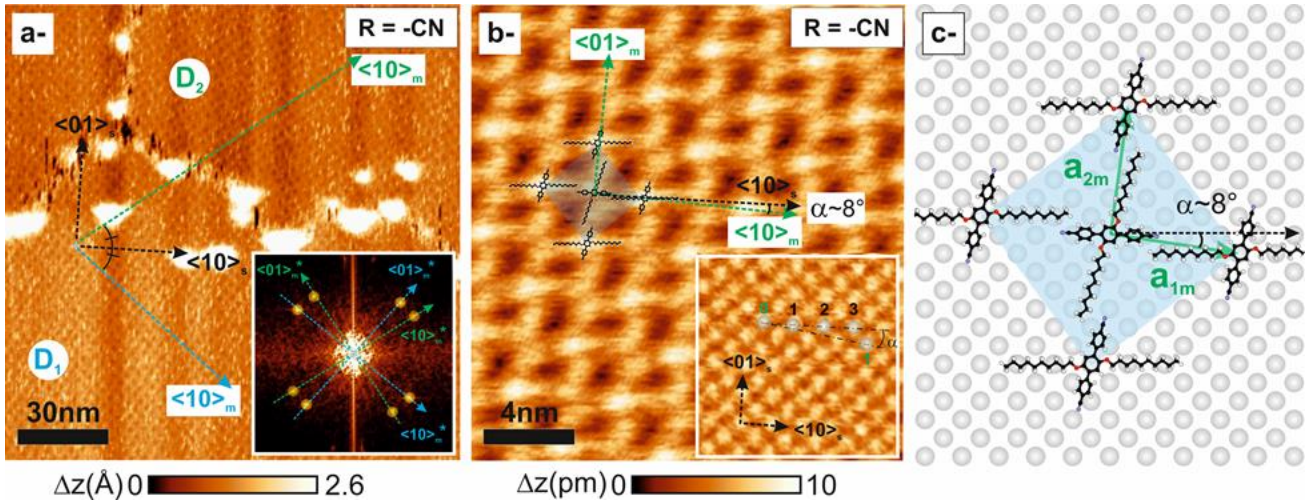
Self assembly at surfaces

Molecule-Surface? These are missing…

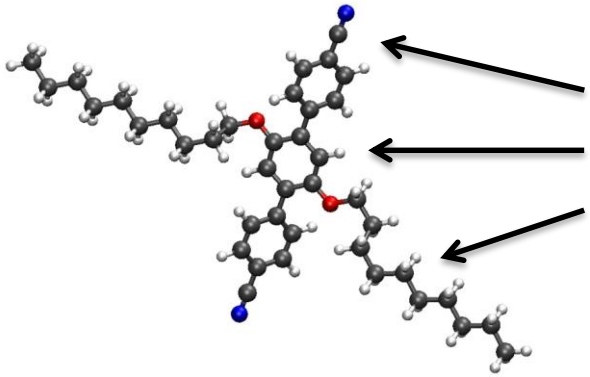
David Gao
Filippo Federici-Canova

Experiments by:
Christian Loppacher,
Laurent Nony;
Université Aix-Marseille


<01>s
mol. network
substrate
a2m
a2s
β
a1m
<10>m
α
a1s
<10>s
R
R
R=
-CN
-CH3
-CH=CH2
-φ-CN

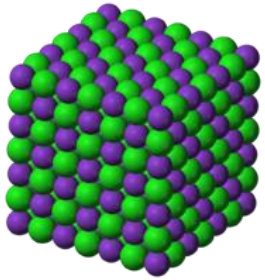

a-
R = -CN
D2
<10>m
<01>s
<10>s
D1
<10>m
30nm
b-
<01>m
R = -CN
<10>s
α~8°
<10>m
4nm
<01>s
<10>s
c-
a2m
α~8°
a1m
Δz(Å) 0
2.6
Δz(pm) 0
10

Introduction to the System (The Blocks)



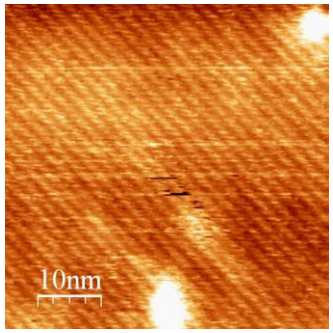
The CDB molecule
- CN anchoring groups
- Central rings
- Hydrocarbon chains

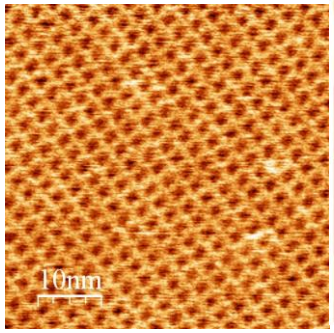
(and some variations)

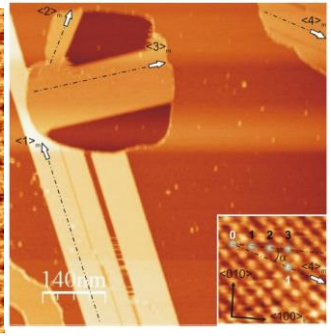


1. **Surfaces with the same crystal structure:**

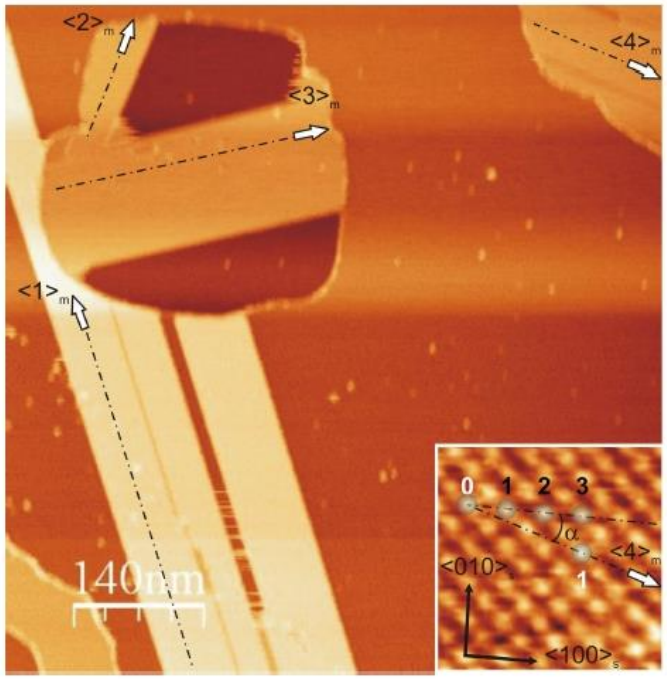
- NaCl with a 5.65 Å unit cell
- KCl with a 6.30 Å unit cell
- RbCl with a 6.58 Å unit cell

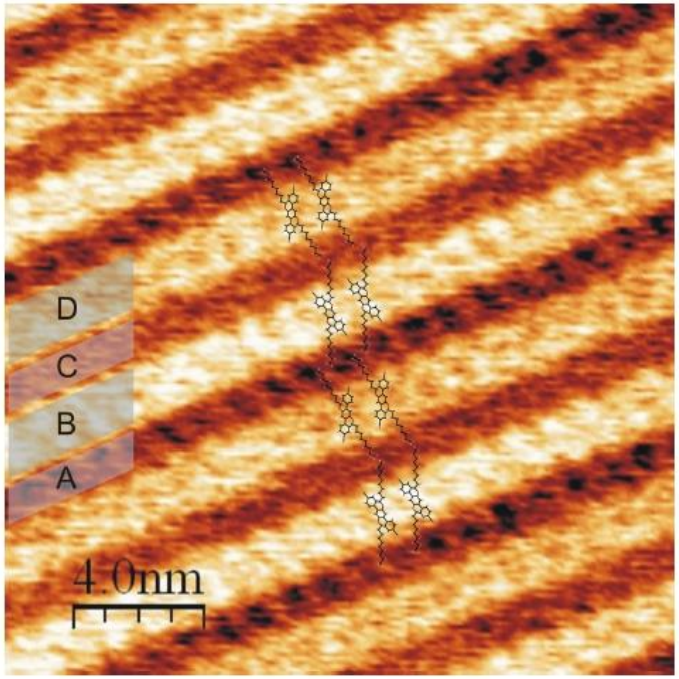




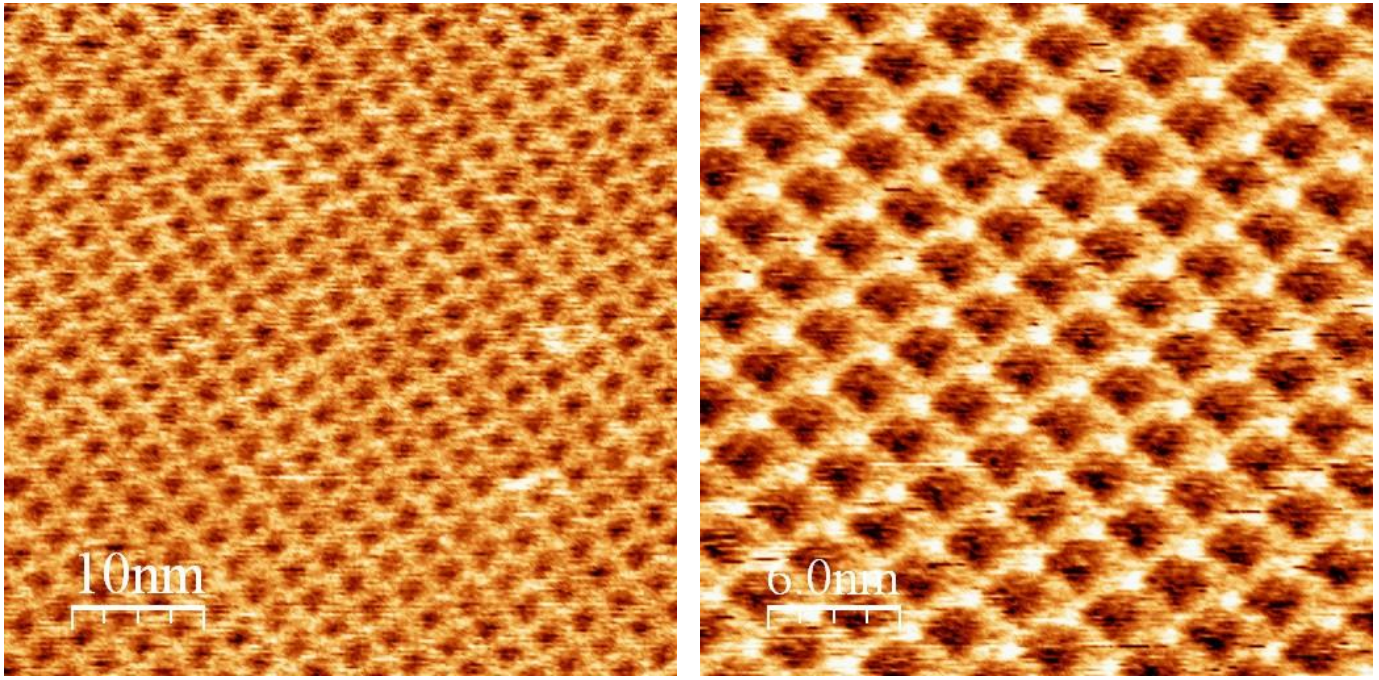


Imaged as:
Bright Spots
Dark Spots
Patterns





- Clearly different patterning from NaCl and RbCl
- Assign another geometry and study the differences via DFT



- Clearly different geometry in comparison to NaCl
- Propose a model for these bright and dark spots and check with DFT

Investigate the adsorption of CDB molecules with the surface and other CDB molecules

The quick details:

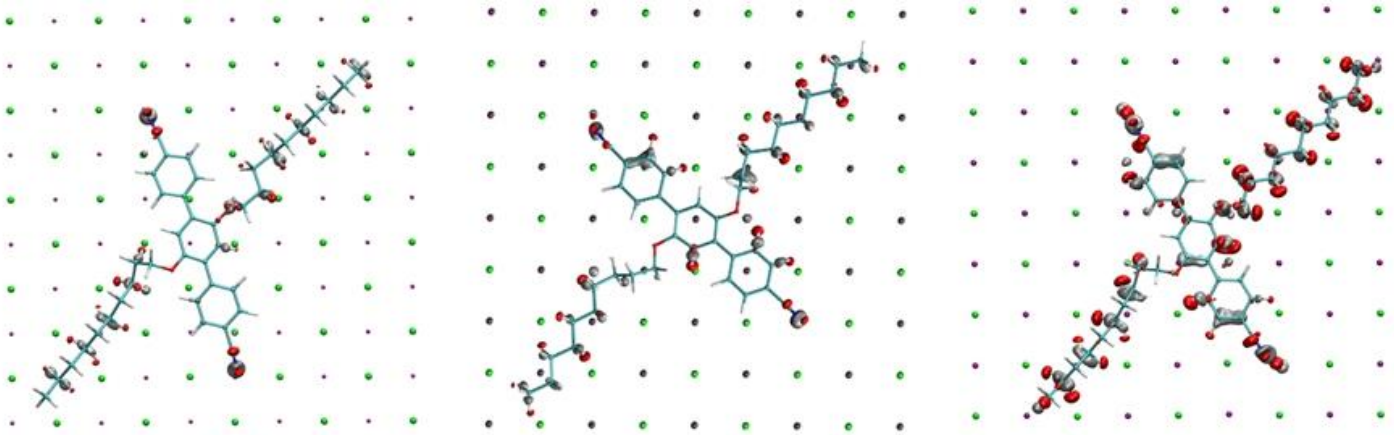
- CP2K GPW
- PBE/GGA
- 3 Atomic Layers of the Substrate
- MOLOPT basis set with GTH pseudopotentials
- Long range dispersion corrections DFT-D2

The Strategy:

- Study the interactions between molecule and surface
- Study the interactions between molecules
- Come up with some models that can explain and predict the structures observed

DFT/QMMM	*Molecular Dynamics*	*vAFM*

CP2K with mixed Gaussian and plane wave (GPW) approach
GGA/PBE with the MOLOPT basis set
DFT-D2 dispersion corrections



A) NaCl(100) B) KCl(100) C) RbCl(100)

The molecule prefers to sit in different geometries on each surface…

Mulliken and Bader analysis indicate no charge transfer occurs…

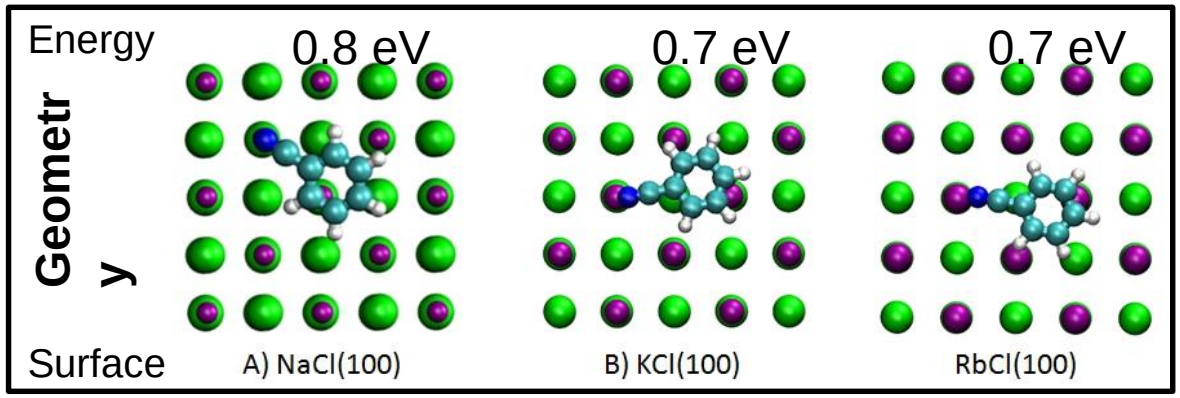
Main interaction appears to be between CN and the surface cations

DFT/QMMM	*Molecular Dynamics*	*vAFM*

The Full Molecule is primarily anchored with 0.4-0.7 eV from DFT

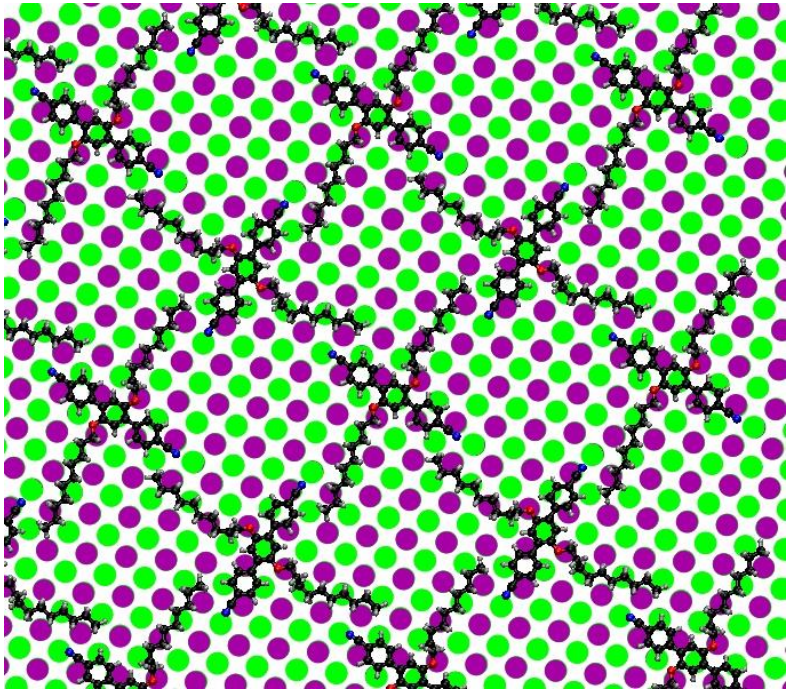
	NaCl(100)	KCl(100)	RbCl(100)
Adsorption Energy	3.69 eV	3.12 eV	3.85 eV
DFT Contribution	0.39 eV	0.70 eV	0.70 eV
Dispersion Contribution	3.30 eV	2.42 eV	3.15 eV

This is accounted for by the CN groups (physisorbed rings on metal: 0.4 eV)

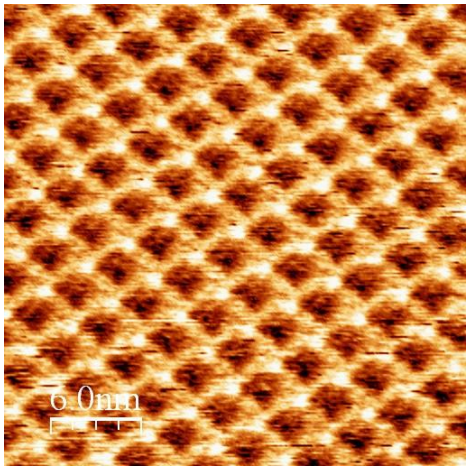


vdW interactions between the rings and chains are relatively uniform

Structure is consistent with experiment



~0.2 eV energy gain per molecule over isolated monomers…

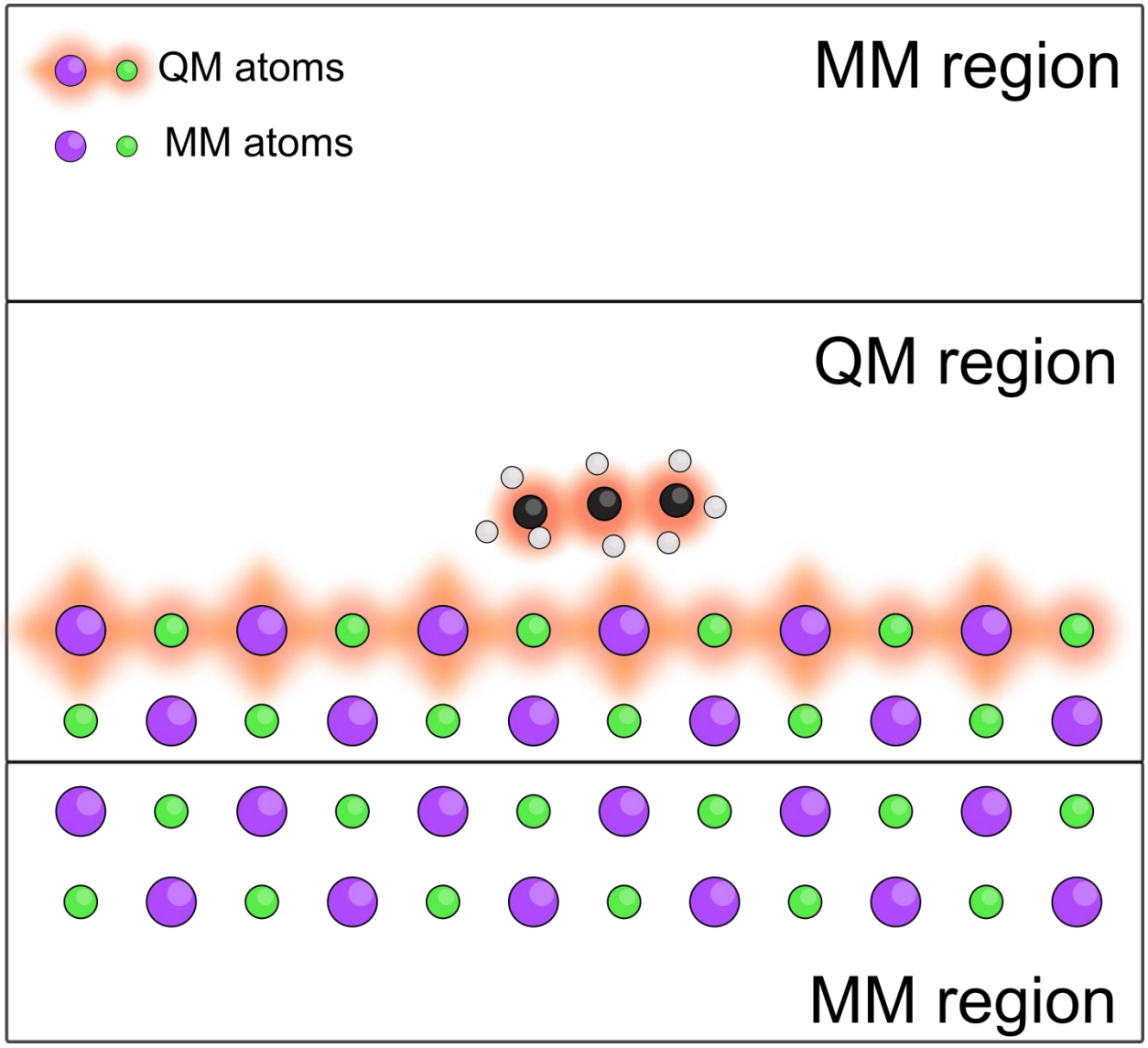


Full DFT system (4 Layers QM)
>700 Atoms – ‘hard’ to do systematic search / MD

QM/MM System (1 Layer QM 3 Layers MM)
~500 QM atoms + 1000 MM atoms to study monolayers
~250 QM atoms + 450 MM atoms to generate force data

Dewetting Movie (4 Layers MM)
~20,000 Atoms

CP2K: Embedded Slab Model – 2D embedding



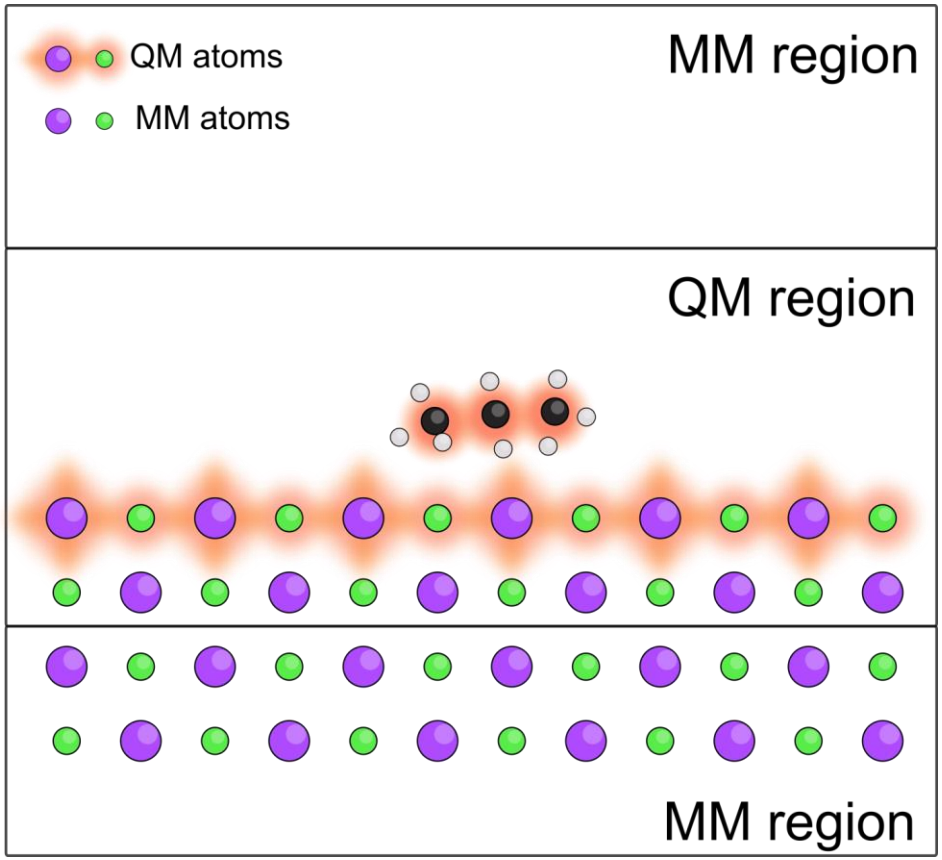
QM-QM is treated normally

QM-MM is treated using Gaussian smeared MM atoms:

1) Short range coarse grids
2) Long range sparse grids

MM-MM is treated classically

CP2K: Embedded Slab Model – 2D embedding



Standard MM setup

```
&QMMM
  &CELL
    ABC 12.6 8.0 12.6
    PERIODIC XYZ
  &END CELL
  ECOUPL GAUSS
  USE_GEEP_LIB 12
  &PERIODIC
  &END PERIODIC

&SUBSYS
  &CELL
    ABC 12.6 50.00 12.6
  &END CELL
  &TOPOLOGY
```

With one layer of alkali halide, we can get away with something like But check convergence!

QMMM Contribution Breakdown

$$E^{\mathrm{MM}} = \frac{1}{2}\int\int \mathrm{d}r\mathrm{d}r' \frac{(\rho^{\mathrm{MM}}(r) + \rho^{\mathrm{B,MM}})(\rho^{\mathrm{MM}}(r') + \rho^{\mathrm{B,MM}})}{|r - r'|} \tag{2}$$

$$E^{\mathrm{QM}} = \frac{1}{2}\int\int \mathrm{d}r\mathrm{d}r' \frac{(\rho^{\mathrm{QM}}(r) + \rho^{\mathrm{B,QM}})(\rho^{\mathrm{QM}}(r') + \rho^{\mathrm{B,QM}})}{|r - r'|} \tag{3}$$

$$E^{\mathrm{QM/MM}} = \int\int \mathrm{d}r\mathrm{d}r' \frac{(\rho^{\mathrm{QM}}(r) + \rho^{\mathrm{B,QM}})(\rho^{\mathrm{MM}}(r') + \rho^{\mathrm{B,MM}})}{|r - r'|} \tag{4}$$

QMMM coupling

$$E_{\mathrm{TOT}}(\mathbf{r}_\alpha,\mathbf{r}_\mathrm{a}) = E^{\mathrm{QM}}(\mathbf{r}_\alpha) + E^{\mathrm{MM}}(\mathbf{r}_\mathrm{a}) + E^{\mathrm{QM/MM}}(\mathbf{r}_\alpha,\mathbf{r}_\mathrm{a}) \quad (1)$$

$$E^{\mathrm{QM/MM}}(\mathbf{r}_\alpha,\mathbf{r}_\mathrm{a}) = \sum_{\mathrm{a}\in\mathrm{MM}} q_\mathrm{a} \int \frac{\rho(\mathbf{r},\mathbf{r}_\alpha)}{|\mathbf{r}-\mathbf{r}_\mathrm{a}|} d\mathbf{r} + \sum_{\substack{\mathrm{a}\in\mathrm{MM}\\ \alpha\in\mathrm{QM}}} v_{\mathrm{VdW}}(\mathbf{r}_\alpha,\mathbf{r}_\mathrm{a}) \quad (2)$$

Adding effect to 1e integrals scales as N_{mm}*$N_{basisfunctions}$^2

$$H^{\mu\nu}_{\mathrm{QM/MM}} = -\int \phi_\mu(\mathbf{r},\mathbf{r}_\alpha) \sum_{\mathrm{a}\in\mathrm{MM}} \frac{q_\mathrm{a}}{|\mathbf{r}_\mathrm{a}-\mathbf{r}|} \phi_\nu(\mathbf{r},\mathbf{r}_\alpha) d\mathbf{r} \quad (4)$$

Directly mapping onto the grid used for the QM calculations is prohibitive – N_{mm}*N_{grid} - because N_{grid} gets very large

An Efficient Real Space Multigrid QM/MM Electrostatic Coupling
Teodoro Laino, Fawzi Mohamed, Alessandro Laio, and Michele Parrinello
J. Chem. Theory Comput. 2005, 1, 1176-1184

QMMM coupling

Replace point charges with Gaussians

$$\rho(|\mathbf{r}-\mathbf{r}_a|) = \left(\frac{1}{\sqrt{\pi} r_{c,a}}\right)^3 \exp\left(-\frac{|\mathbf{r}-\mathbf{r}_a|^2}{r_{c,a}^{\ 2}}\right)$$

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2}\, \mathrm{d}t.$$

$$v_{\mathrm{a}}(\mathbf{r},\mathbf{r}_{\mathrm{a}}) = \frac{\mathrm{Erf}\left(\dfrac{|\mathbf{r}-\mathbf{r}_{\mathrm{a}}|}{r_{\mathrm{c,a}}}\right)}{|\mathbf{r}-\mathbf{r}_{\mathrm{a}}|}$$

"Guassian expansion of electrostatic potential"

Long range part – gives Madelung potential

$$v_{\mathrm{a}}(\mathbf{r},\mathbf{r}_{\mathrm{a}}) = \frac{\mathrm{Erf}\left(\dfrac{|\mathbf{r}-\mathbf{r}_{\mathrm{a}}|}{r_{\mathrm{c,a}}}\right)}{|\mathbf{r}-\mathbf{r}_{\mathrm{a}}|} = \sum_{N_{\mathrm{g}}} A_{\mathrm{g}} \exp\left(-\left(\frac{|\mathbf{r}-\mathbf{r}_{\mathrm{a}}|}{G_{\mathrm{g}}}\right)^2\right) + R_{\mathrm{low}}(|\mathbf{r}-\mathbf{r}_{\mathrm{a}}|) \quad (5)$$

An Efficient Linear-Scaling Electrostatic Coupling for Treating Periodic Boundary Conditions in QM/MM Simulations, Teodoro Laino, Fawzi Mohamed, A. Laio, M. Parrinello, JCTC, 2, 1370 (2006)

“Collocating” the potential:Multi-grids

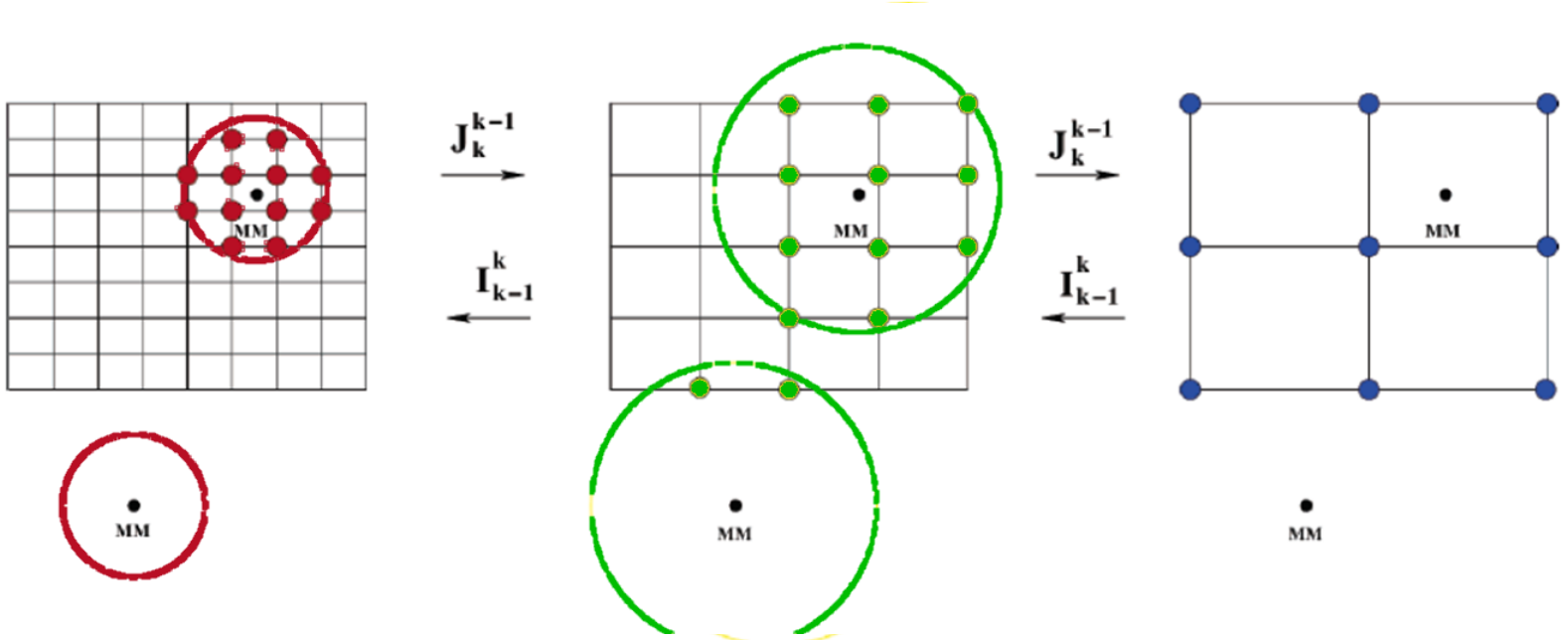


Figure 2. Schematic representation of the collocation procedure. Two MM atoms and three grid levels have been depicted. The circles (in the first and second grid levels) are the collocation regions of the Gaussian centered on the two MM atoms. Atoms whose distance from the QM box is greater than the Gaussian collocation radius do not contribute to the potential on that grid level. However, all atoms contribute to the coarsest grid level through the long-range R_{low} part.

$$V^{\mathrm{QM/MM}}(\mathbf{r},\mathbf{r}_a) = \sum_{i=\mathrm{coarse}}^{\mathrm{fine}} \prod_{k=i}^{\mathrm{fine}-1} I_{k-1}^{k}\, V_i^{\mathrm{QM/MM}}(\mathbf{r},\mathbf{r}_a) \qquad (11)$$

However, overcounting?
decouple artificial QM – QM interactions

$$E = \frac{1}{2}\int_V d\mathbf{r} \int d\mathbf{r}' \frac{\rho(\mathbf{r},\mathbf{r}_\alpha)\rho(\mathbf{r}',\mathbf{r}_\alpha)}{|\mathbf{r}-\mathbf{r}'|} \qquad (26)$$

Let us introduce a new model charge density $\hat{\rho}(\mathbf{r},\mathbf{r}_\alpha)$, which is localized within the same volume V as $\rho(\mathbf{r},\mathbf{r}_\alpha)$ and which reproduces the multipole moments of the correct charge distribution. The representation adopted in ref 32 is given as a sum

$$\hat{\rho}(\mathbf{r},\mathbf{r}_\alpha) = \sum_\alpha q_\alpha g_\alpha(\mathbf{r},\mathbf{r}_\alpha) \qquad (27)$$

of atom-centered spherical Gaussians, which are normalized such that they possess a charge of one

$$g_i(\mathbf{r},\mathbf{r}_\alpha) = \frac{1}{(\sqrt{\pi} r_{c,\alpha})^3} \exp\left(-\frac{|\mathbf{r}-\mathbf{r}_\alpha|^2}{r_{c,\alpha}^{\ 2}}\right) \qquad (28)$$

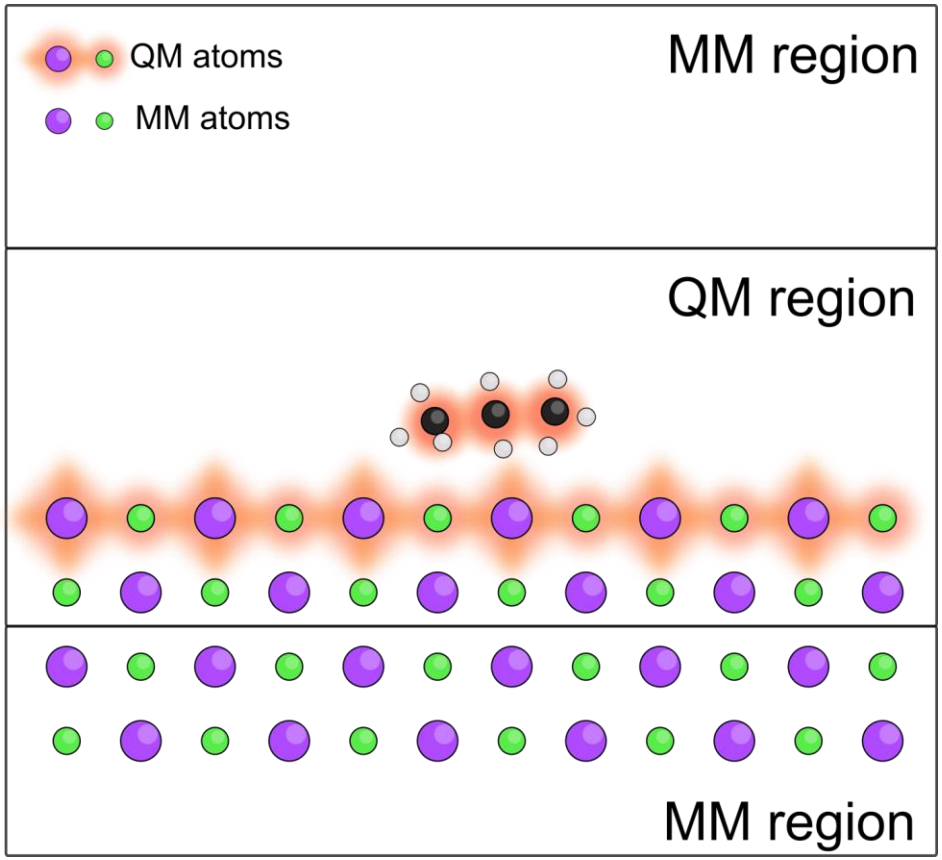
QM calculation carried out in smaller box than the full system – need to add back QM-QM interactions

Use artificial density based on atom centred Gaussian expansion

Calculate artificial QM-QM interactions then subtract and add back in real ones

Details to do this in : Blochl, P. E. J. Chem. Phys. 1995, 103, 7422

CP2K: Embedded Slab Model – 2D embedding



Standard MM setup

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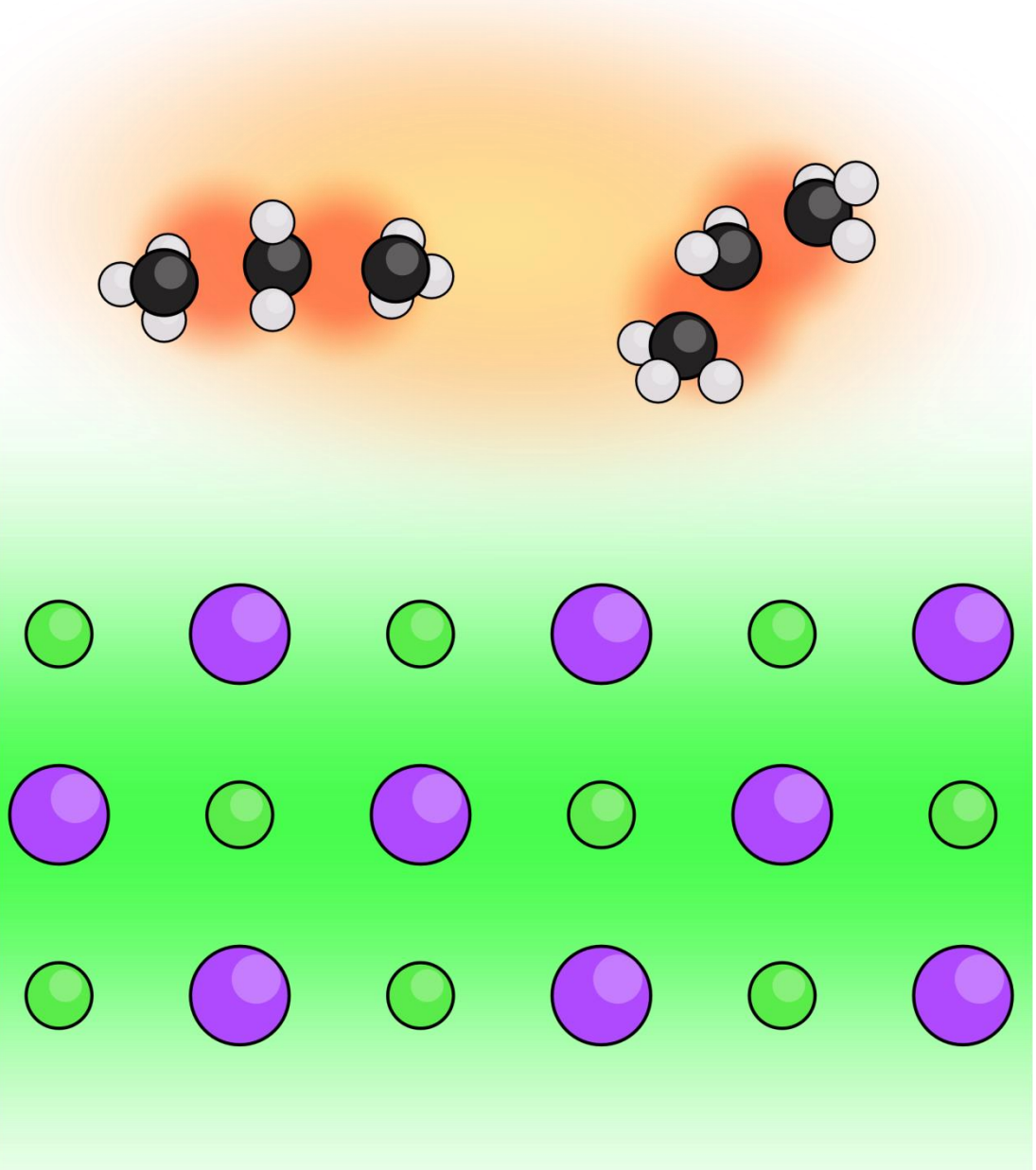
  ECOUPL GAUSS
  USE_GEEP_LIB 12
  &PERIODIC
  &END PERIODIC

&SUBSYS
  &CELL
    ABC 12.6 50.00 12.6
  &END CELL
  &TOPOLOGY
```

Three Main Interactions Within the System



Intramolecular+Intermolecular

CHARMM Forcefield

Charges fit to DFT Mulliken Analysis

Molecule-Surface?
These are missing…

Surface Interactions

C R A Catlow *et al* 1977 *J. Phys. C: Solid State Phys.* **10** 1395

CP2K Shells not implemented,
*fix shells to cores

Check vDOS, bond lengths, rumpling

Molecule-Surface Interactions

Coulomb interactions are already included…

But in a nonphysical way!

CHARMM DFT Mulliken + Catlow Whole Numbers

Another contribution is needed to…

- correct any errors in Coulomb interactions
- Represent short range interactions
- Represent vdW long range interactions

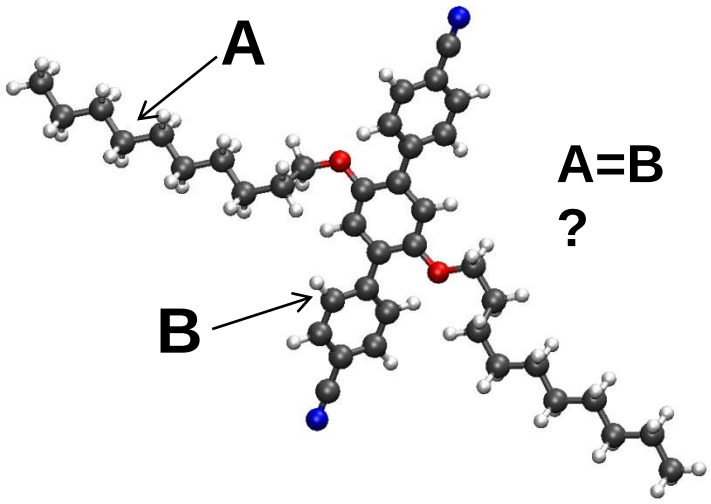
***(Simply analytical, no physical meaning)**

$$V(r) = D_e(1 - e^{-a(r-r_e)})^2$$

$$V_{LJ} = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]:$$

Try Morse or Lennard-Jones

Complex Systems



Many Pairwise Interactions!
Atoms are not all the same…
13 atom types within CDB
(according to CHARMM)

13 molecule atoms
2 surface atoms (KCl)
Several parameters per pair

How do we optimize so many parameters at the same time?
Difficult with the usual methods, lets try Genetic Algorithms

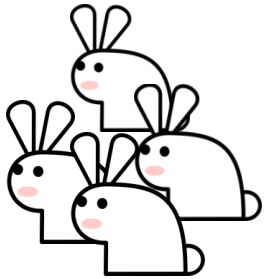
ε1
ε2
ε3
ε4
σ1
σ2
σ3
etc

Lets use **evolution**

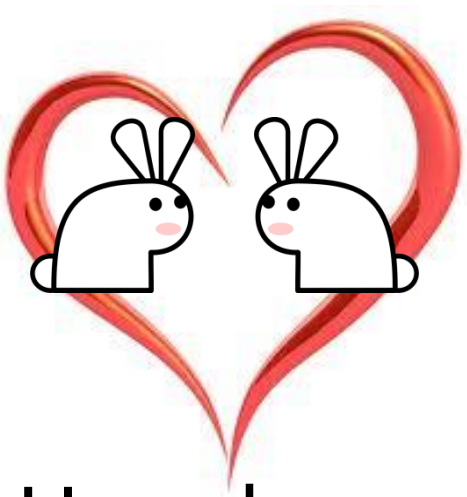
Each parameter becomes a gene…
The set of parameters defines a member

Fitness (f) is how well this set of parameters reproduces DFT data (forces and adsorption energy)

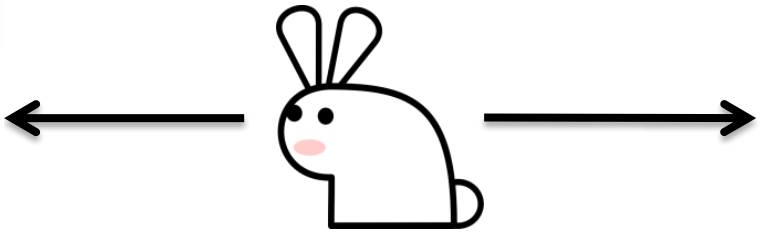
A set of many members represents some population



Fitness governs survival:



Need to decide the fate of each parameter set



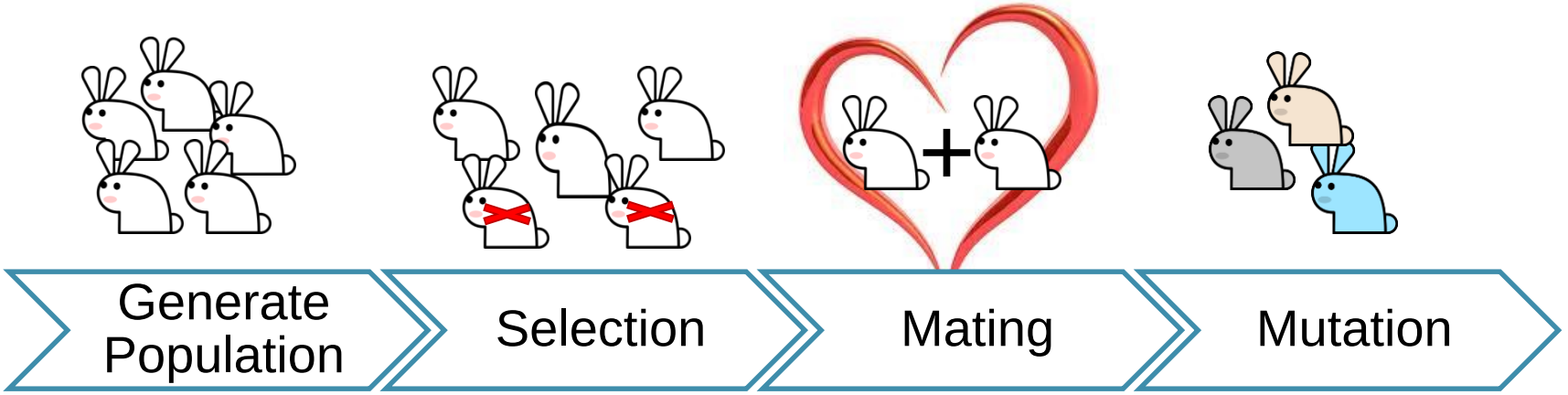
How do we calculate Fitness?

$$Fitness = \sum_{frames} \sum_{atoms} |f_{DFT} - f_{LAMMPS}| + (EA_{DFT} - EA_{LAMMPS})$$

A) Calculate difference in forces on each atom (within the CDB molecule!)

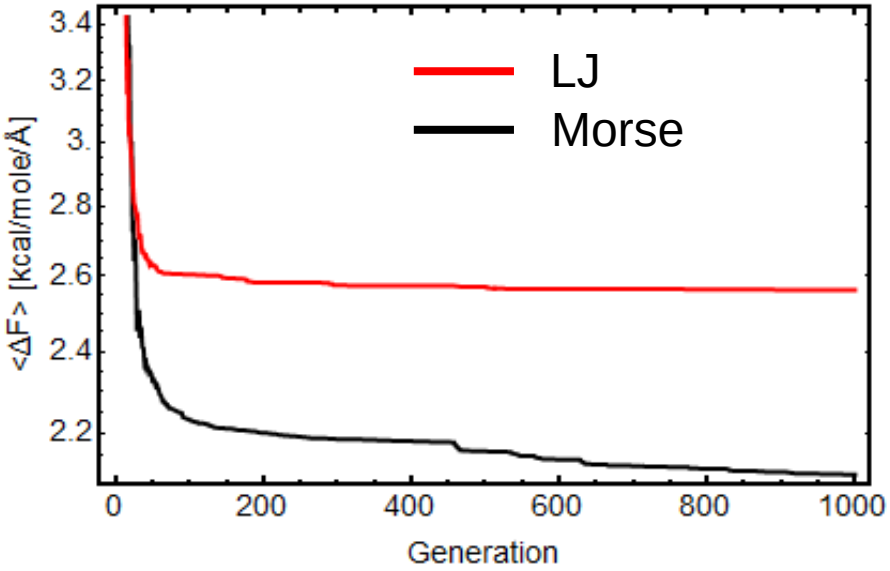
B) Sum up all these differences over all the MD frames used for fitting

How do we evolve the parameter sets?



A) Randomly generate 1024 sets of parameters
B) Calculate the forces on each atom for each frame of DFT data
   - Compute the difference between DFT forces and classical forces
   - Delete the worst members of the population
C) Generate new members up to 1024 by breeding the survivors
D) Introduce random mutations within the population

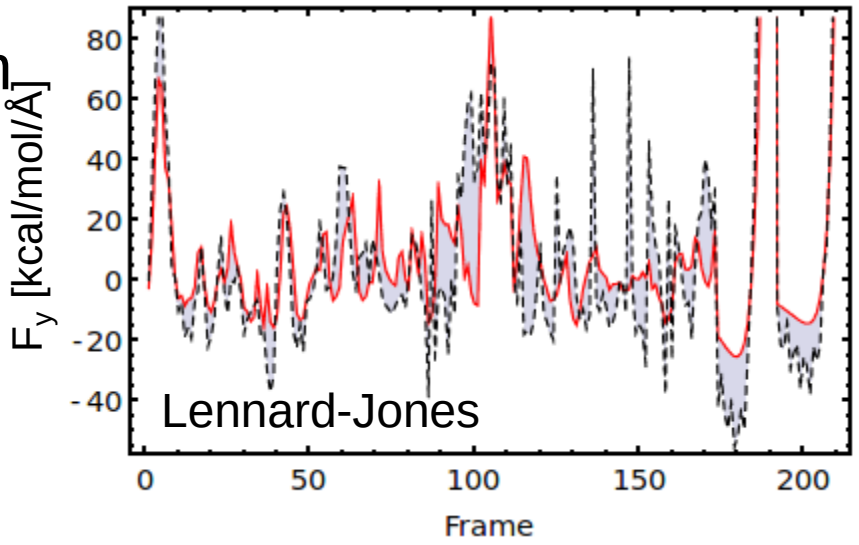
Average force mismatch per atom

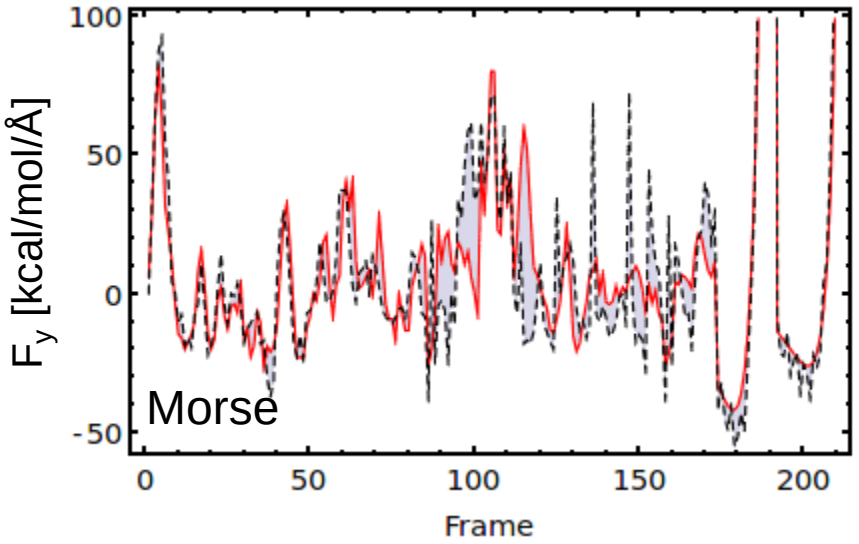


Within our fitting frames
Average force per atom :
38.1 Kcal/mol/Å (DFT)

- both models give around 5% mismatch on average
- Morse is slightly better for this system

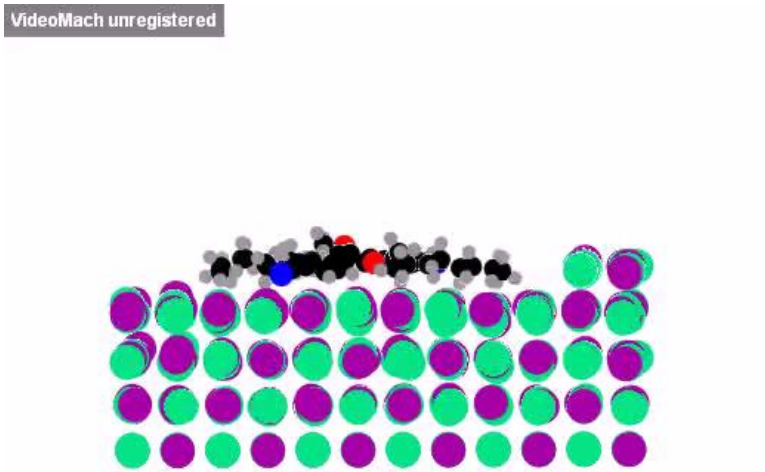
Total molecular force

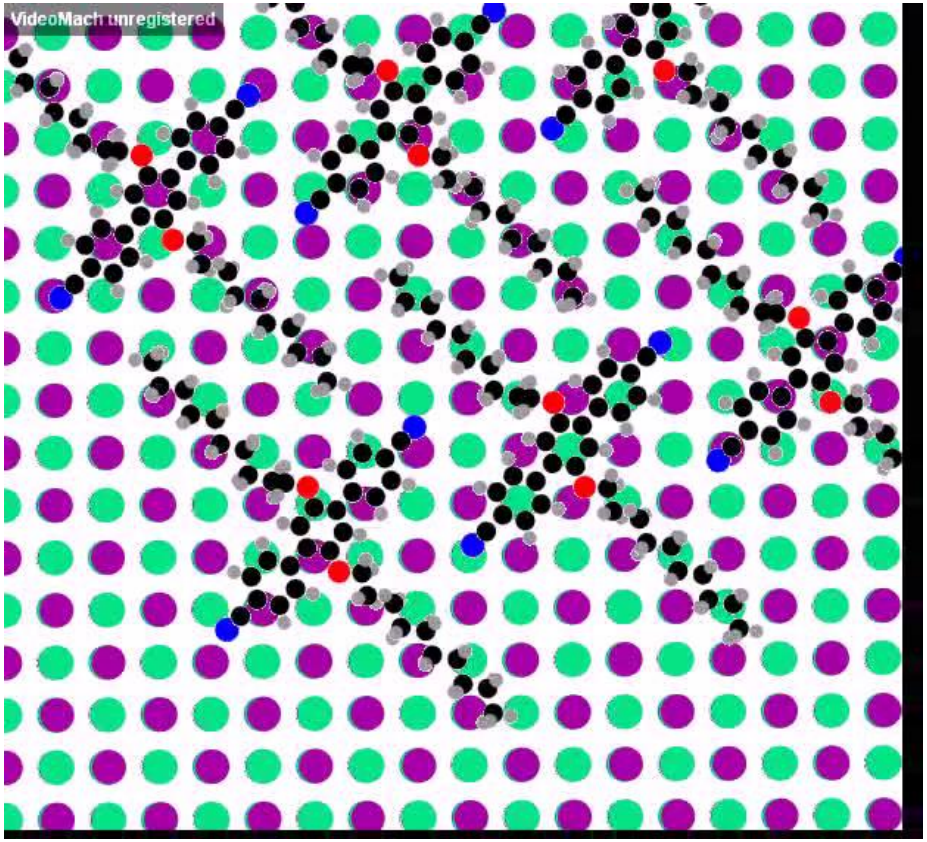




DFT
Classical

Forcefield fitting + MD + collective behaviour

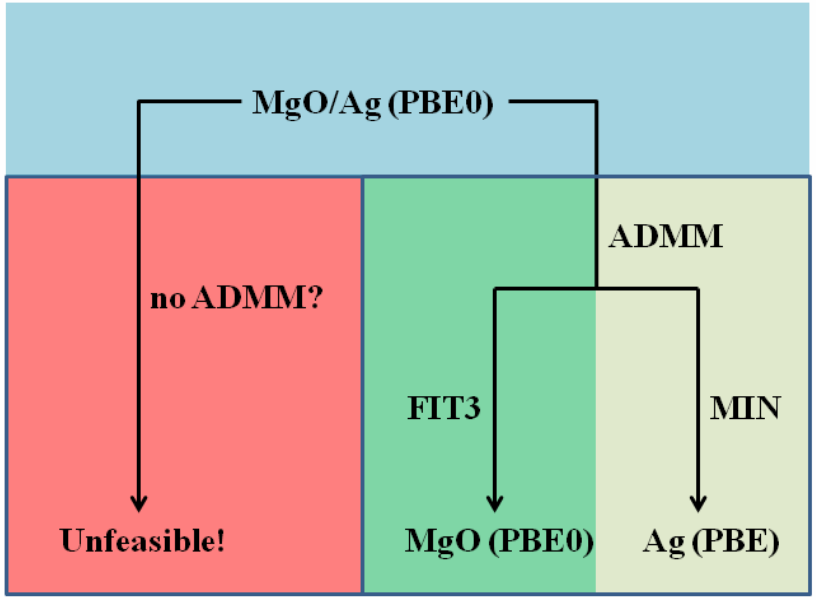


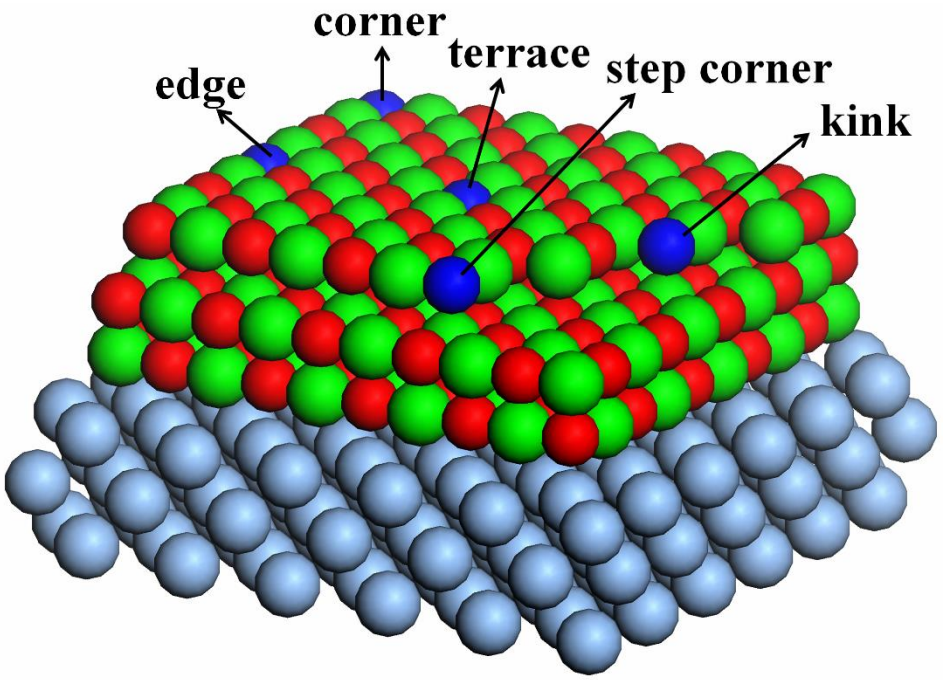


Force matching also implemented in CP2K – Powell algorithm – 2007 Flo

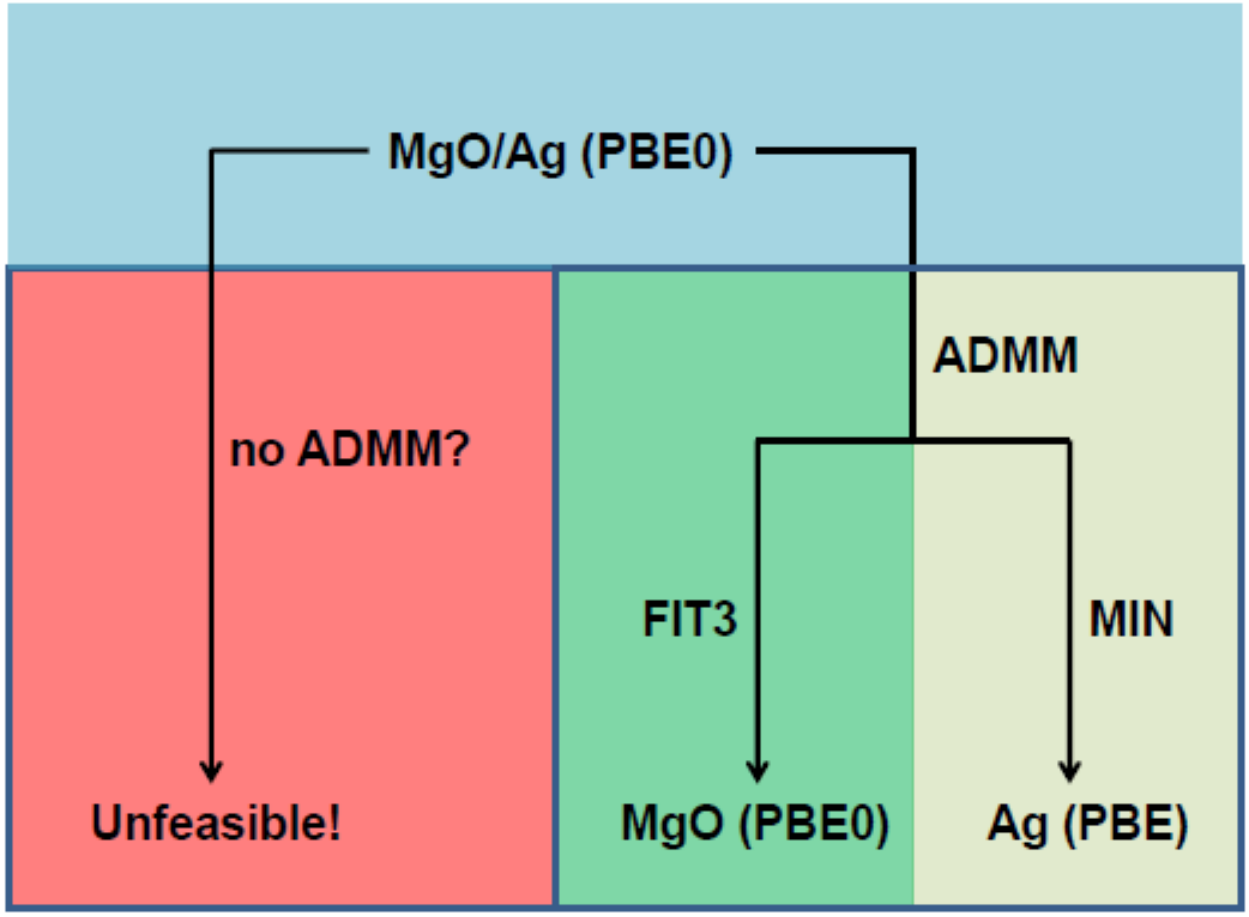
Metal/metal oxides
- hacking ADMM methods

Sanliang Ling





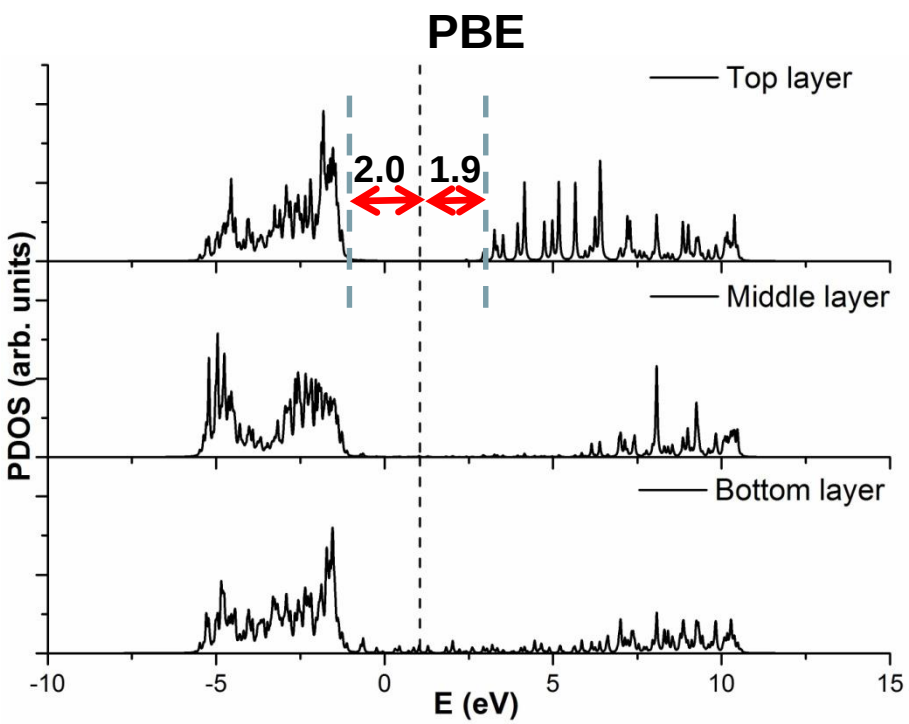
Band offset at Metal/Insulator Interface

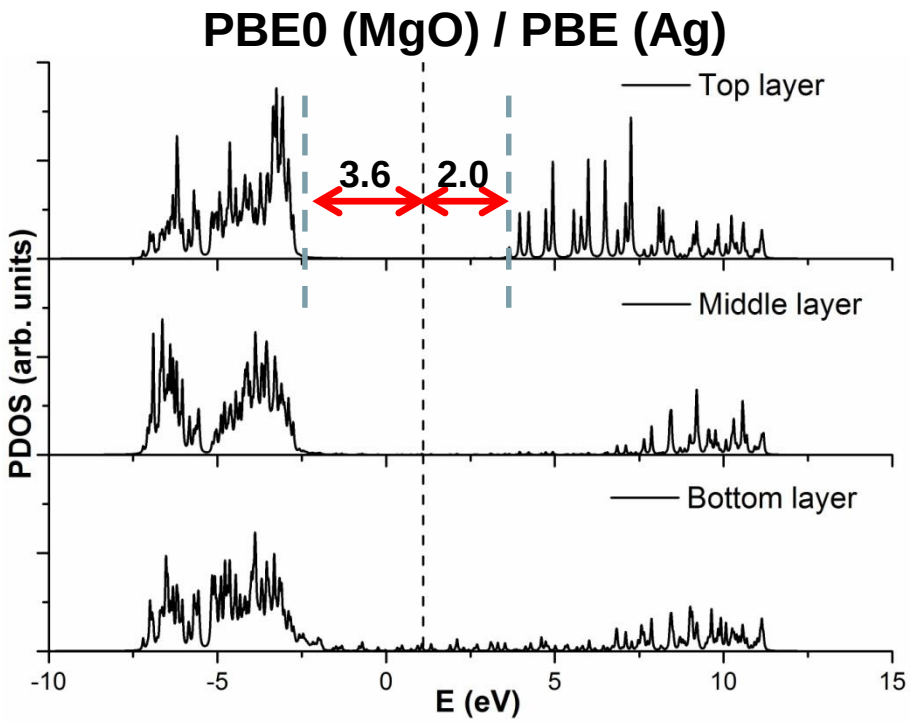


A hybrid approach using auxiliary density matrix method with CP2K

Ling et al. JPCC, 117, 5075 (2013)

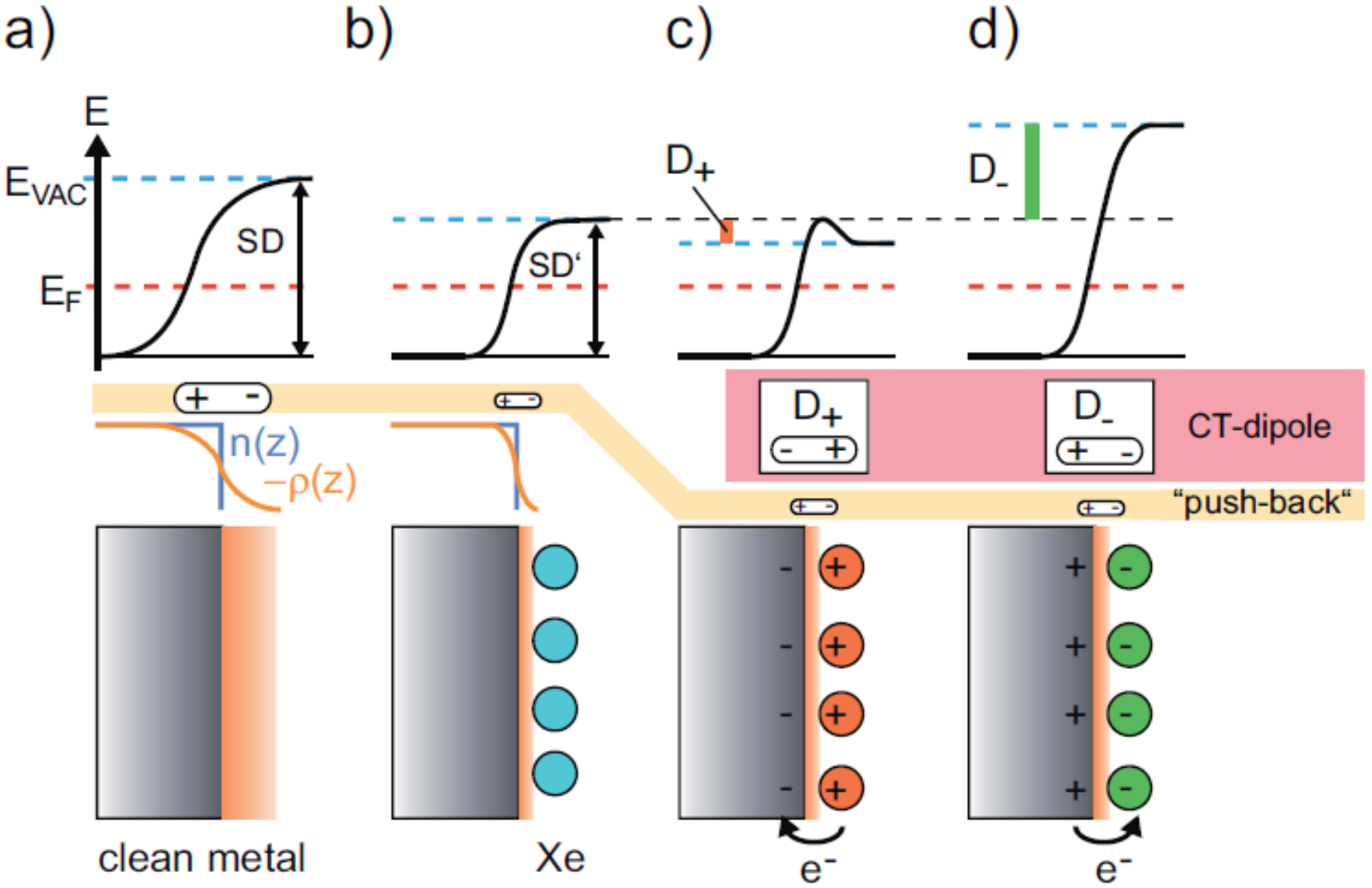
Band offsets at MgO/Ag(001) Interface





Much better band offsets with a non-local hybrid functional for MgO!

Shift of metal work function due to insulator thin film

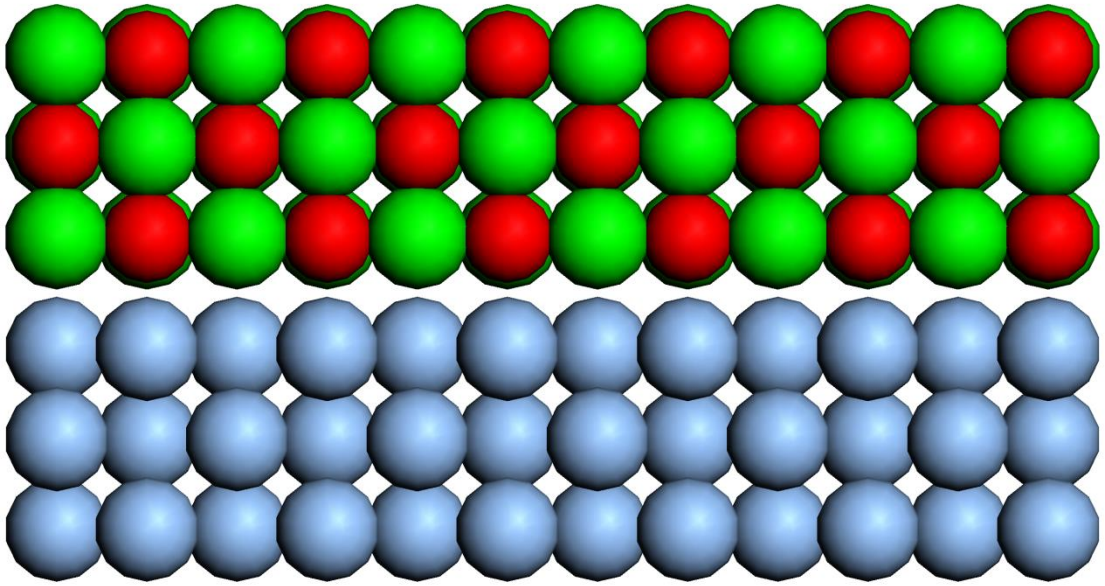


Broker Ph.D. thesis (2010)

Shift of Ag work function due to MgO thin film

MgO (ionic)

Ag (neutral)

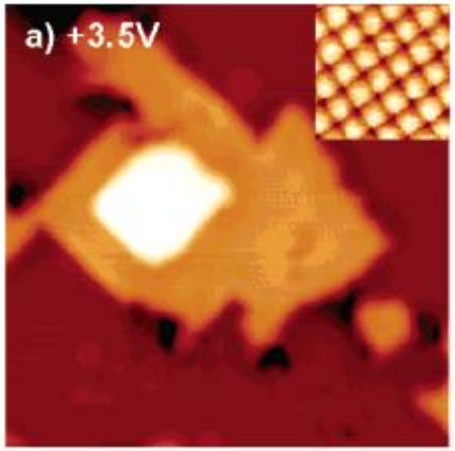


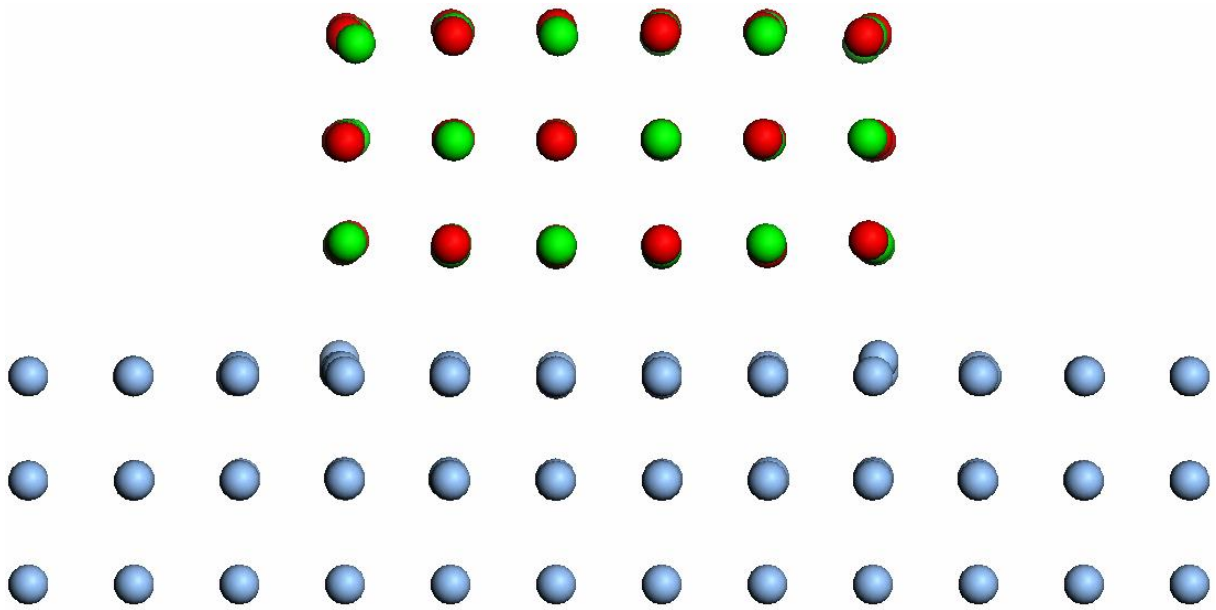
non-reactive weakly bound interface

Method	Interface Ag-O distance (Å)	Shift of work function (eV)
CP2K	2.58	1.78
VASP	2.73	1.2
Expt	~2.5	1.4
CP2K	2.78	1.4

Ling et al. JPCC, 117, 5075 (2013)

Shift of Ag work function due to MgO thin film

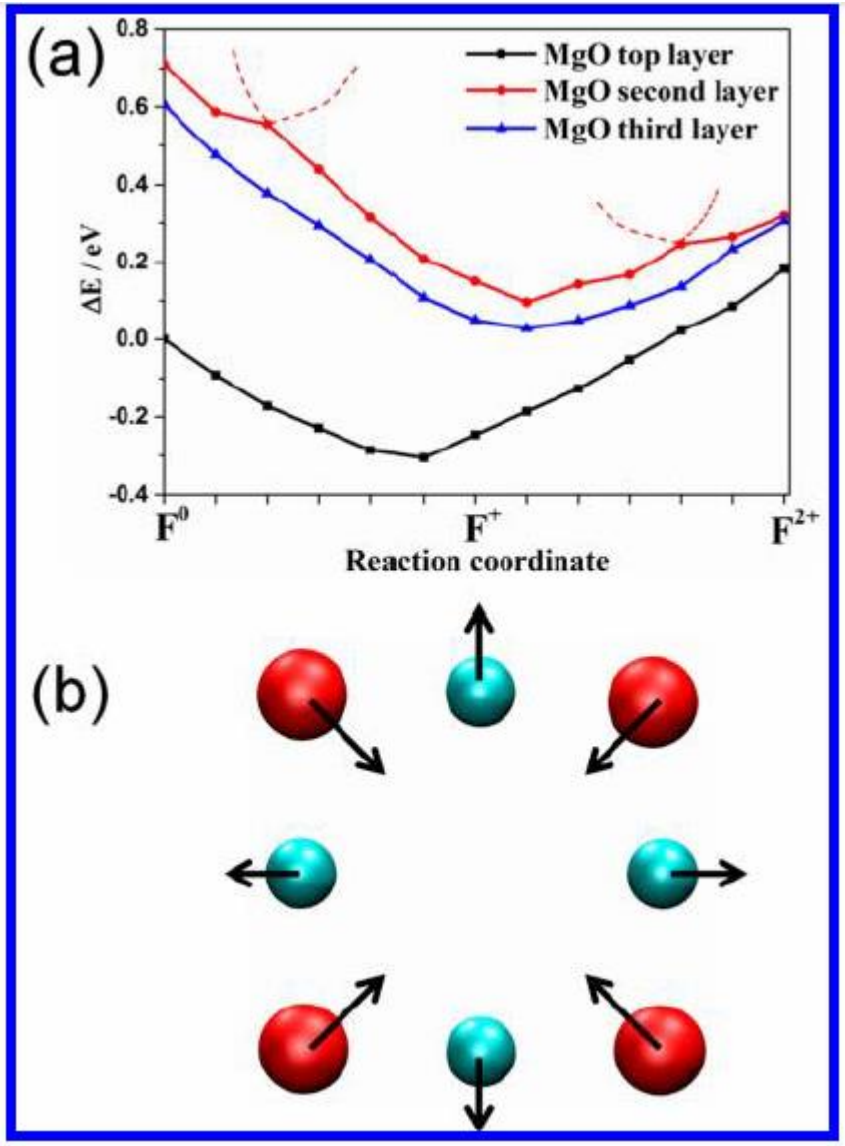




coverage	ϕ	$\Delta\phi$	$d_{\mathrm{Ag-O}}$
17%	3.36	1.00	2.50
34%	3.19	1.17	2.53
56%	2.86	1.49	2.54
100%	2.57	1.78	2.58

Experimentally measured $\Delta\phi$ is an averaged quantity

Controlling charge states?



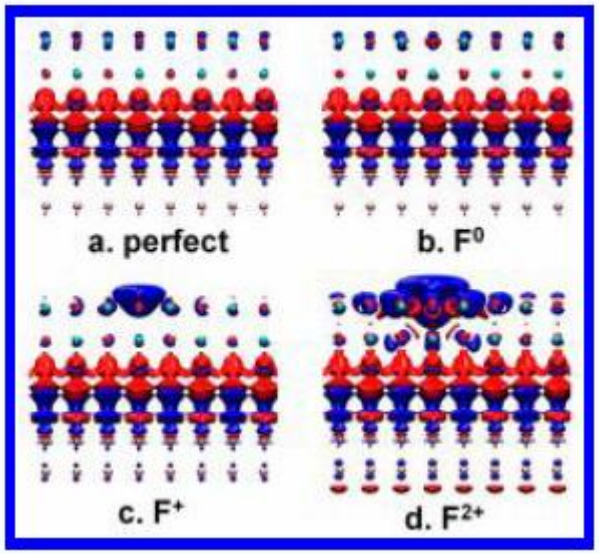
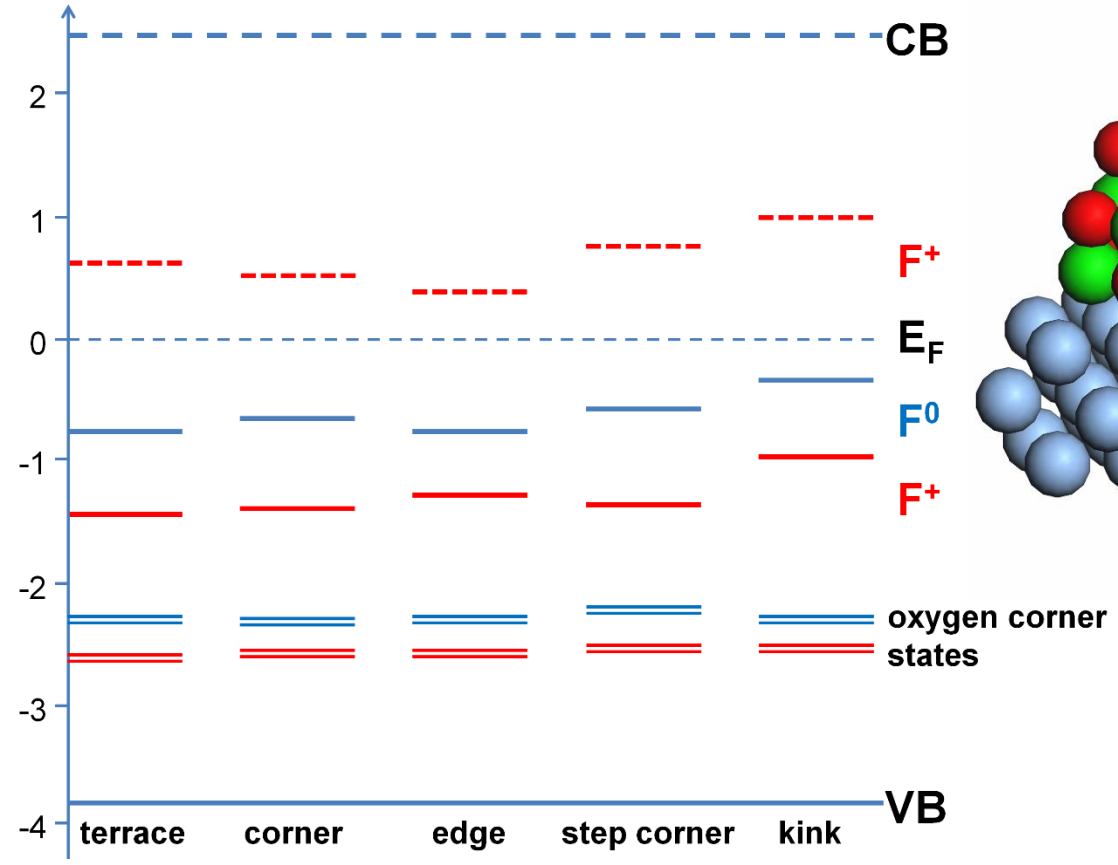
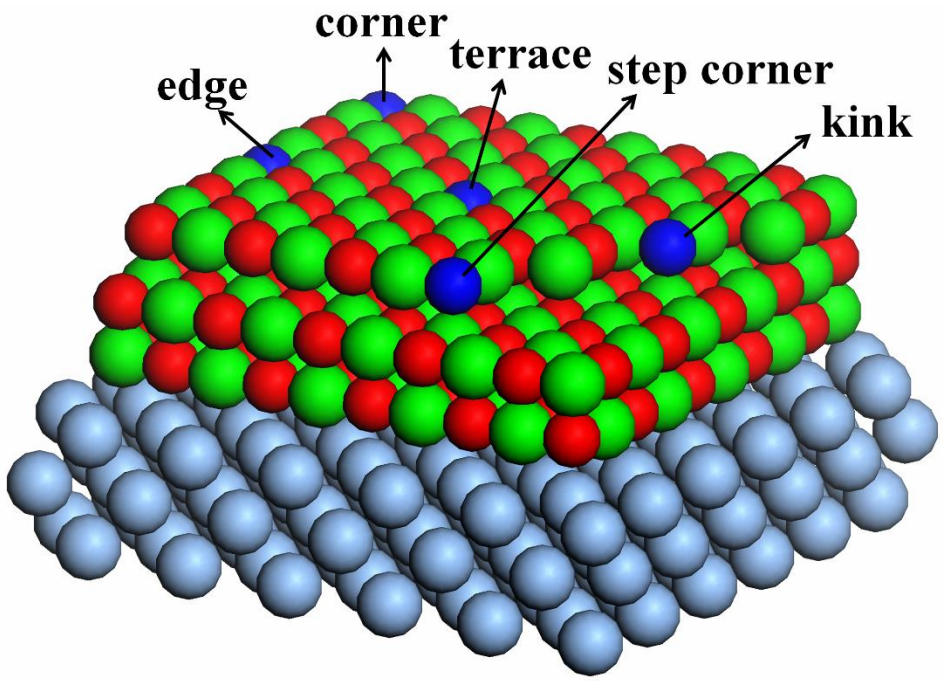


Table 4. Relative Stabilities of F Centers at Different Sites of an MgO Cluster Supported on Ag(001)[a]

size	type	terrace	corner	edge	step corner	kink
3 × 3	F^0	0.18	0.02	0	0.20	–
	F^+	0	0	0.05	0	–
	F^{2+}	0.31	0.62	0.63	0.57	–
5 × 5	F^0	0	0	0	0.09	0.42
	F^+	0.05	0.09	0.16	0	0
	F^{2+}	0.64	1.03	1.05	0.52	0.25

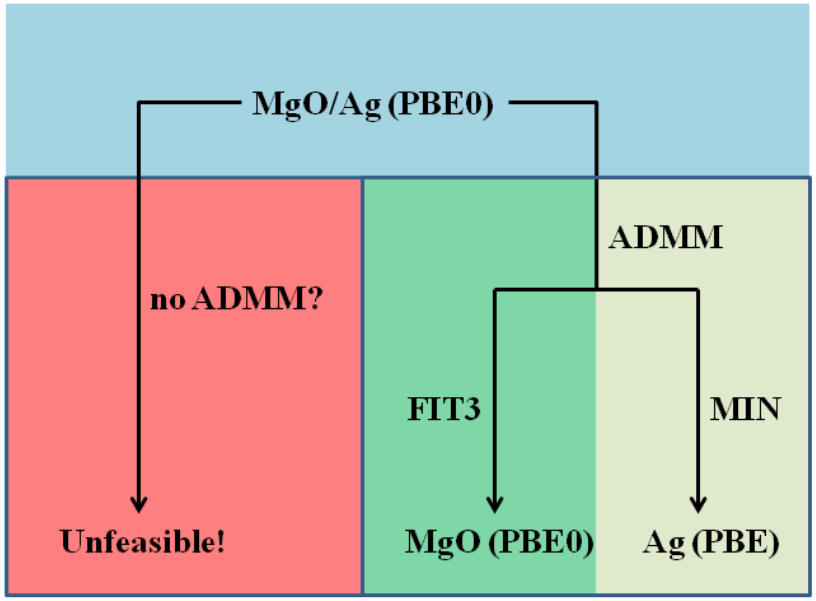
Oxygen vacancies at MgO/Ag(001) Interface

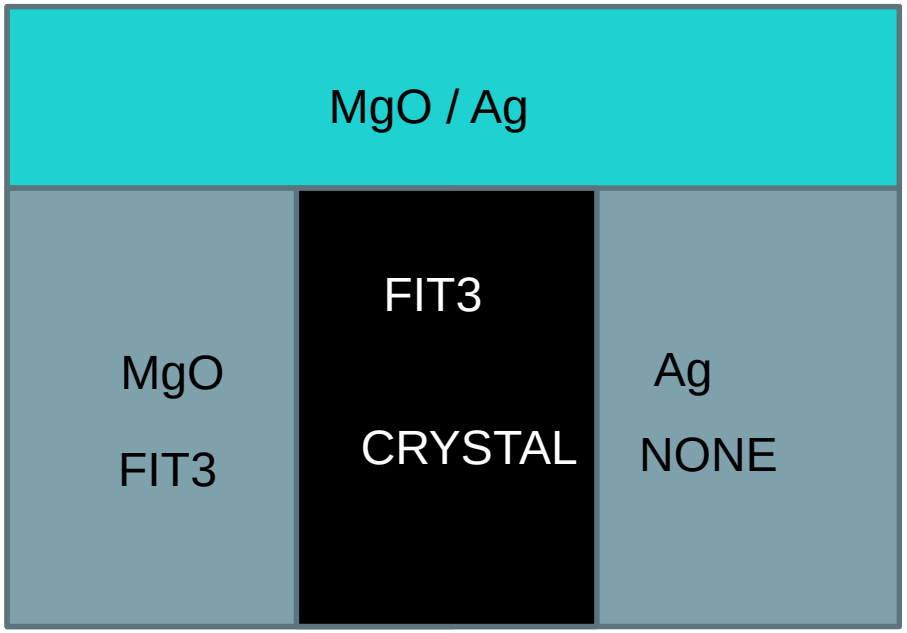




Ling et al. JPCC, 117, 5075 (2013)

“Embedding metal oxides into metals”





Original scheme

New scheme

Integral screening – $$(\mu\nu|\lambda\sigma) = \int\int \phi_\mu(\mathbf{r}_1)\,\phi_\nu(\mathbf{r}_1)\,g(|\mathbf{r}_2 - \mathbf{r}_1|)\,\phi_\lambda(\mathbf{r}_2)\,\phi_\sigma(\mathbf{r}_2)\,d\mathbf{r}_1\mathbf{r}_2$$

If atom i and atom j are both Ag then these integrals are screened (before calculation)

Overlap matrices also hacked $$\hat{S}_{nn'} = \int \hat{\phi}_n(\mathbf{r})\,\hat{\phi}_{n'}(\mathbf{r})\,d\mathbf{r} \text{ and } Q_{nm} = \int \hat{\phi}_n(\mathbf{r})\,\phi_m(\mathbf{r})\,d\mathbf{r}$$

Summary

- A new hybrid PBE/PBE0 approach has been developed to calculate the band offsets at metal/insulator interfaces
- Applicable to large systems
- Can get away from ideal periodically replicated surfaces
- ADMM flexible in choice of basis sets
- More work to be done to smooth transition from hybrid to semi-local functional
- Extend to MIM interfaces – inclusion of bias potential
- Add deltaSCF ability by manipulation of MO occupation numbers