Large-Scale First Principles Calculations of Future Nano-Devices

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and

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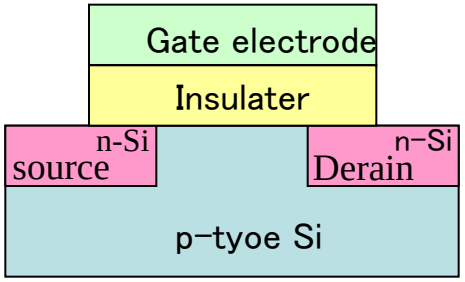
Contents

- Large Scale First Principles Calculations of Si Nanowire by Real Space Density Functional Theory (RSDFT)
- Realization of Mass Production of Modern Nano Devices Based on First Principles Calculations
  - ・MONOS memory (Memory for Automobile)
  - ・High-k LSI (Modern LSI (very common)
- Summary

1. Si Nanowire (The future technology)

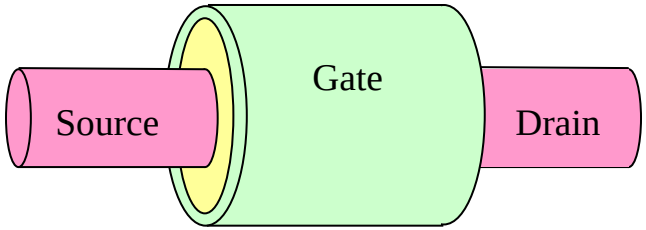
Conventional Planer MOSFET



Development of electric circuit on LSI is governed by the downsizing of MOSFET
(Gate length is less than 50nm)
However, downscaling will end during 2020 and 2030

Downscaling → Serious increase in leakage current

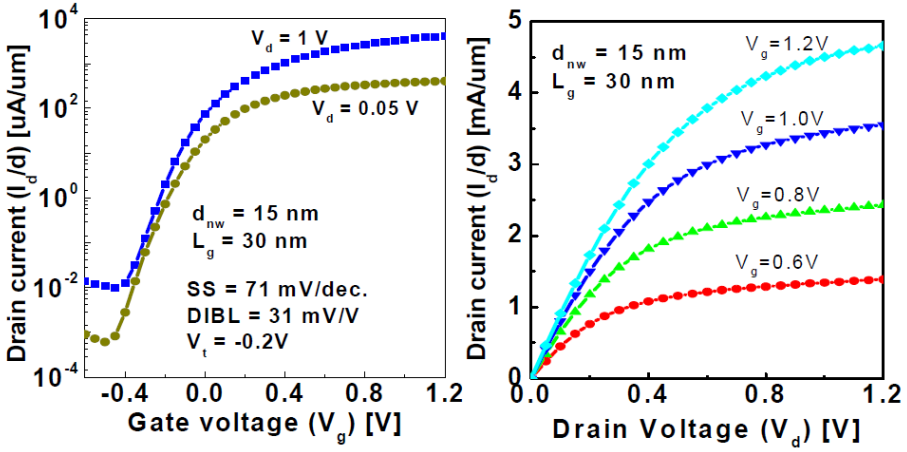
To suppress leakage current, Si nanowire FET is ideal structure.
Due to the electromagnetic analysis



Nano: Quantum Mechanics is inevitable

First principles electronic structure calculations are necessary for designing Si nanowire FET

Experiment of Si nanowire FET



(Samsung, IEDM Technical Digest 2005)

Actually, suppressing leakage current is realized

Next generation MOSFET

However, quantum mechanical designing is necessary for development of Si nanowire FET

First principles device design is inevitable for Si nanowire FET

Large-scale first principles calculation is the key method!

To realize large scale first principles program code

Collaboration with Computer Science Group

Is necessary!!

Density functional theory with real space calculation suited for super parallel machine (to avoid FFT which need all to all communication)

New Algorism for super parallel machine (PACS-CS)

Massive Pararel algorism of Gram-Schmit Orthogonalization
(with High Performance Computation Group)
J-I. Iwata et al. J. Comp. Phys. 2010.

	Time (sec)	GFLOPS/node
Old algorithm	661	0.70
New algorithm	111	4.30

Peak of PACS-CS = 5.6 GFLOPS/node

80%～90% of PACS-CS Peak

New Algorism

$$\psi_1' = \psi_1$$
$$\psi_2' = \psi_2 - \psi_1' \langle \psi_1' | \psi_2 \rangle$$
$$\psi_3' = \psi_3 - \psi_1' \langle \psi_1' | \psi_3 \rangle - \psi_2' \langle \psi_2' | \psi_3 \rangle$$
$$\psi_4' = \psi_4 - \psi_1' \langle \psi_1' | \psi_4 \rangle - \psi_2' \langle \psi_2' | \psi_4 \rangle - \psi_3' \langle \psi_3' | \psi_4 \rangle$$
$$\psi_5' = \psi_5 - \psi_1' \langle \psi_1' | \psi_5 \rangle - \psi_2' \langle \psi_2' | \psi_5 \rangle - \psi_3' \langle \psi_3' | \psi_5 \rangle - \psi_4' \langle \psi_4' | \psi_5 \rangle$$
$$\psi_6' = \psi_6 - \psi_1' \langle \psi_1' | \psi_6 \rangle - \psi_2' \langle \psi_2' | \psi_6 \rangle - \psi_3' \langle \psi_3' | \psi_6 \rangle - \psi_4' \langle \psi_4' | \psi_6 \rangle - \psi_5' \langle \psi_5' | \psi_6 \rangle$$

Matrix Products
Blass 3 is available

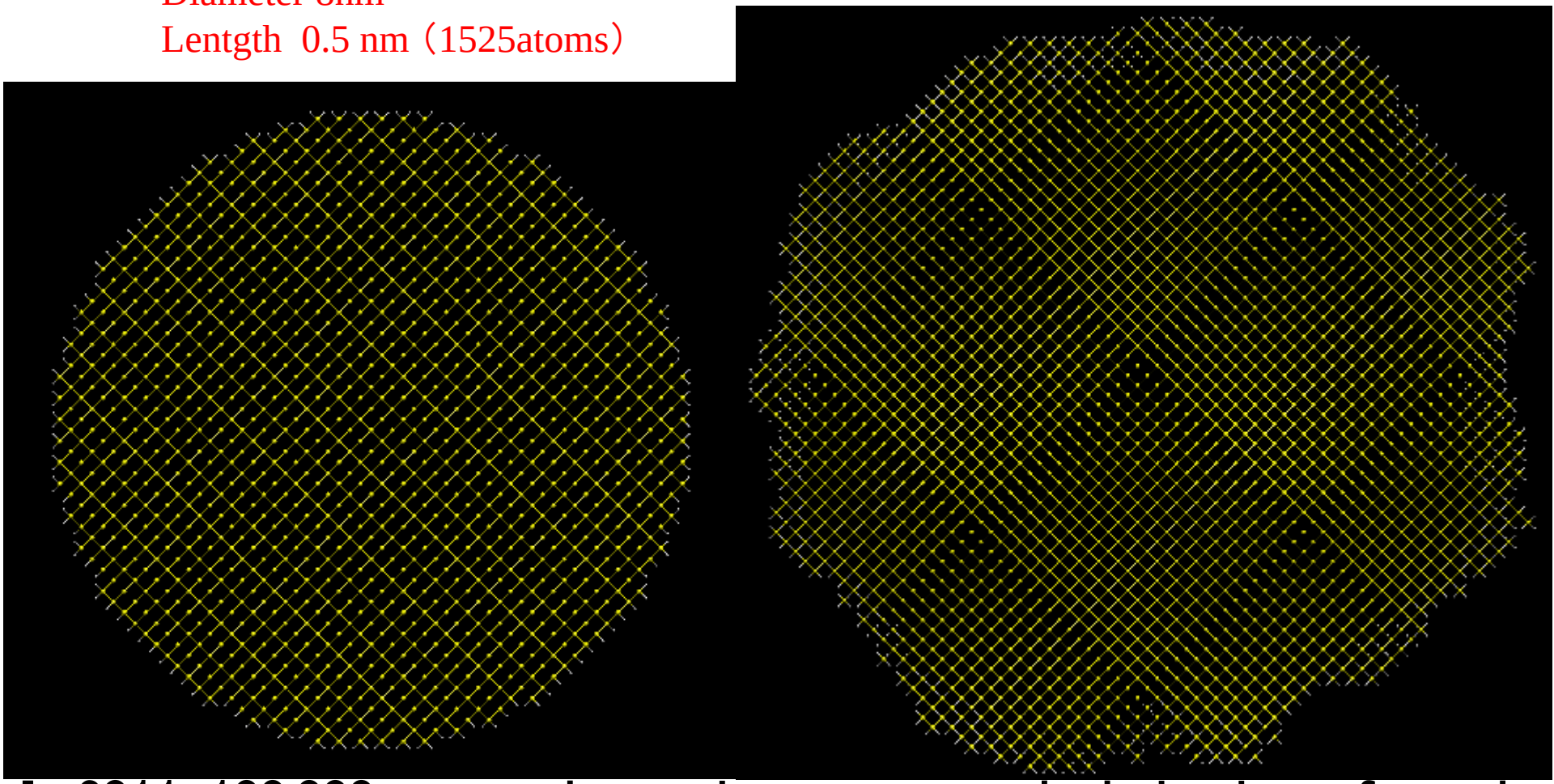
T. Yokozawa, D. Takahashi, T. Boku and M. Sato, (PMAA'06), (2006)

Electronic Structures of Si Nanowires

J-I. Iwata et al. J. Comp. Phys. (2010)

Diameter 8nm
Lentgth 0.5 nm（1525atoms）

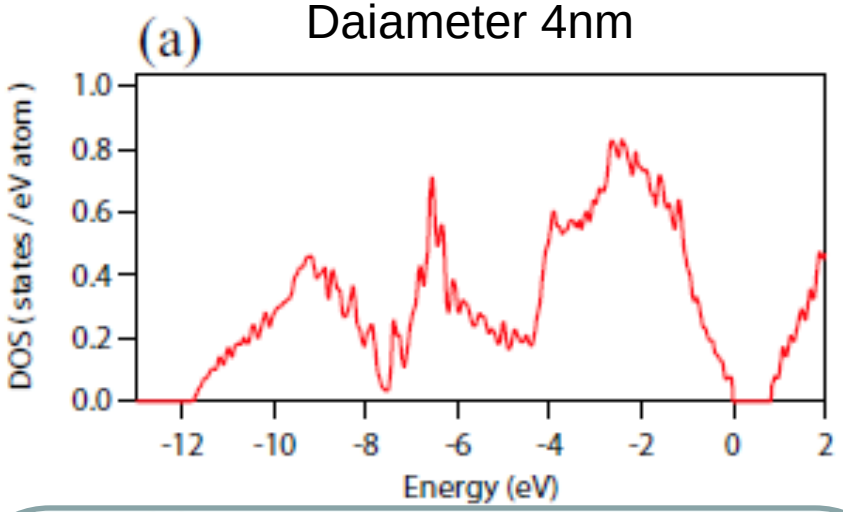
Average daiameter10nm＋randumness
length 3 nm（14,366 atoms）



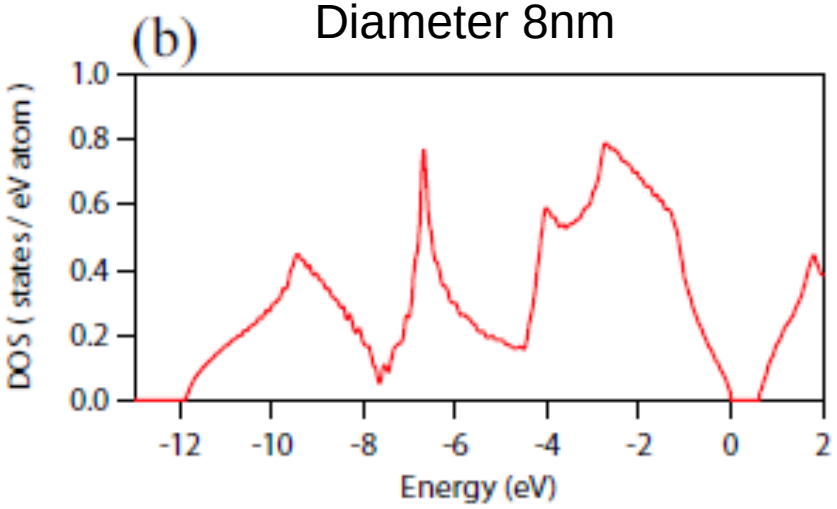
In 2011, 100,000 atoms electronic structure calculation is performed by K computer → Gordon Bell prize (2011)

Density of States obtained by large scale RSDFT calculations

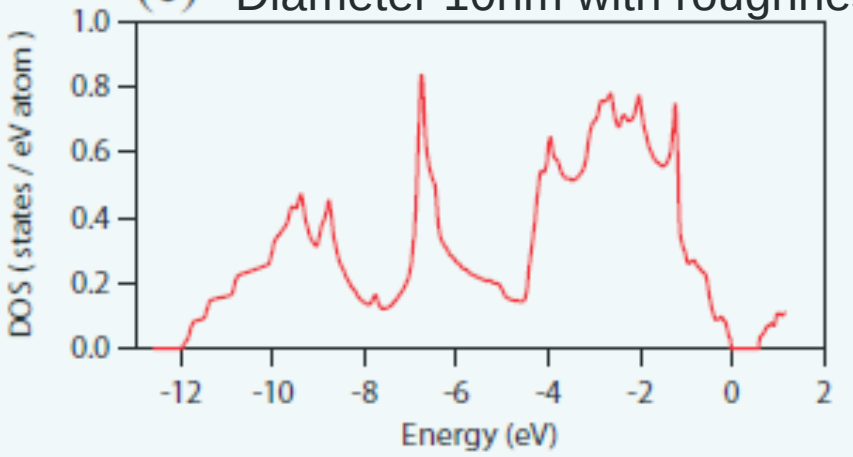
Daiameter 4nm



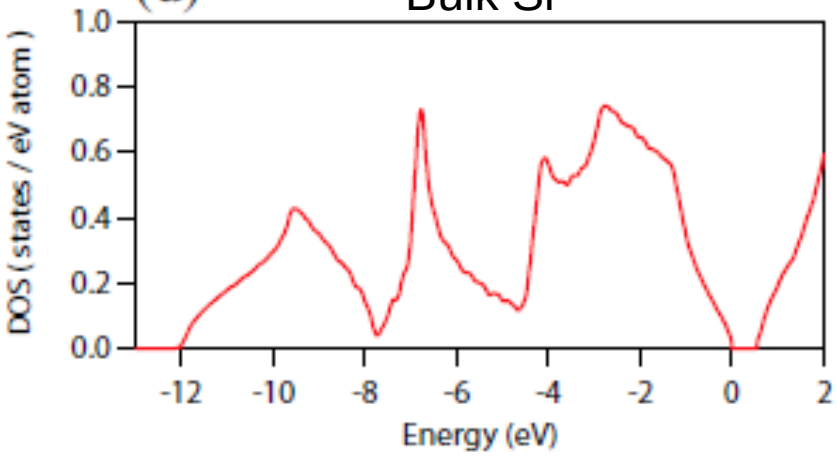
Diameter 8nm



Diameter 10nm with roughness



Bulk Si



Iwata et al. J. Comp. Phys. 2010

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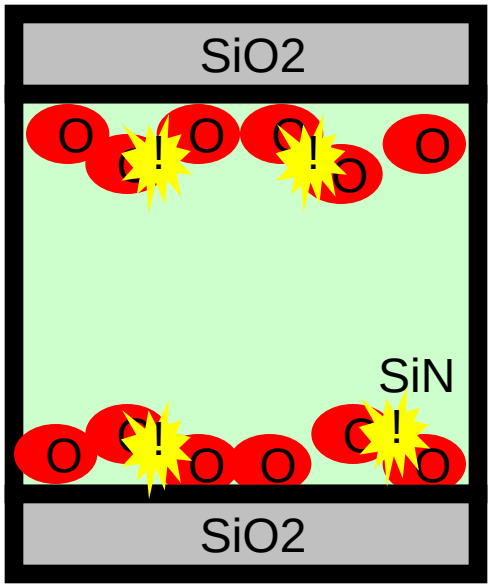
- Interdisiplinary Collaboration toward New Astrobiology

MONOS-type Memories

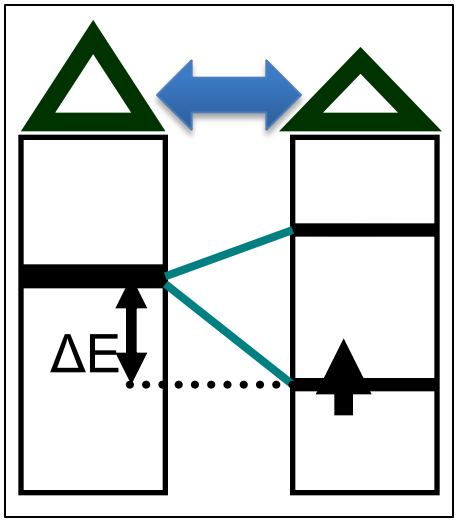
(K. Yamaguchi et al. IEDM 2009, IEDM 2010, JJAP 2011, etc)

Message



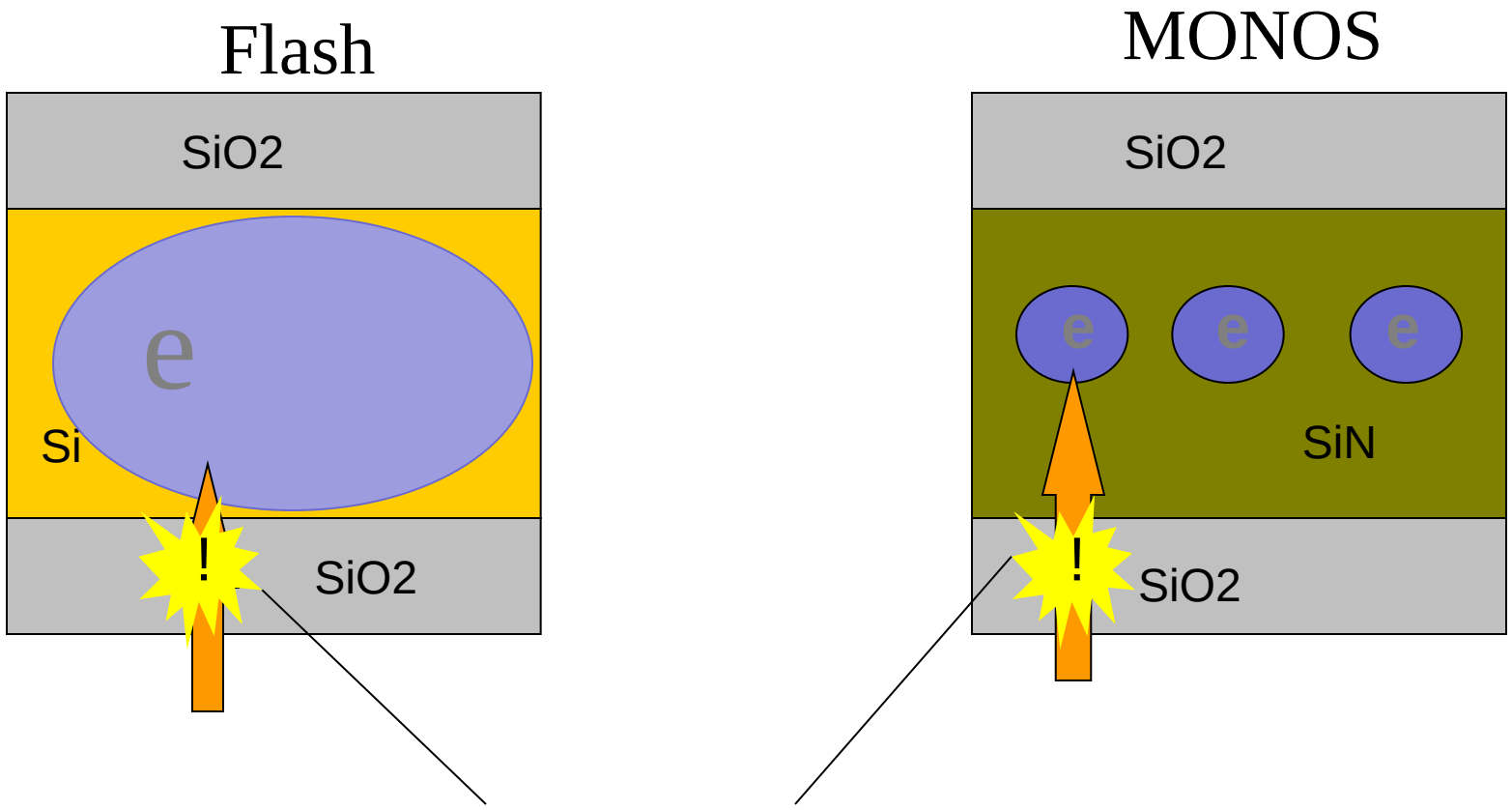
- We have clarify the detailed atomistic behavior of defects of MONOS memory by the *ab initio* calculation.
- The excess O atoms cause an irreversible structural change in the SiN layer.

→The suppression of excess O atoms is effective to improve the MONOS characteristic.



- Defects with Jahn-Teller effect are the most suitable for charge-trap memories.

Conventional Flash memory and MONOS memory

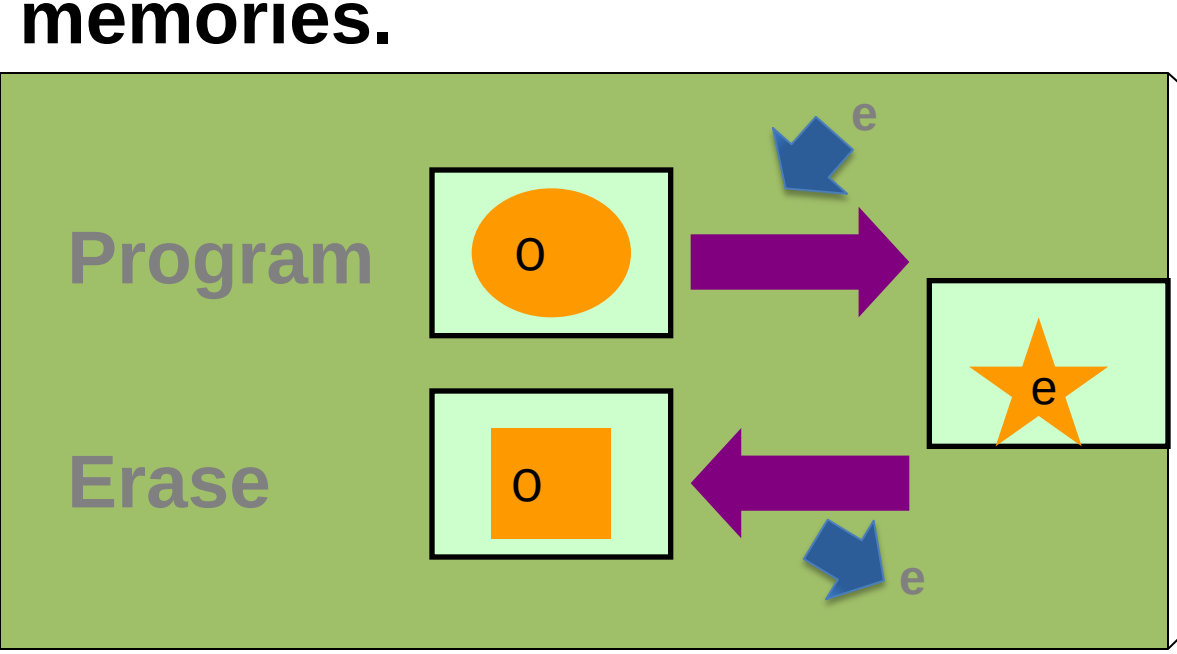


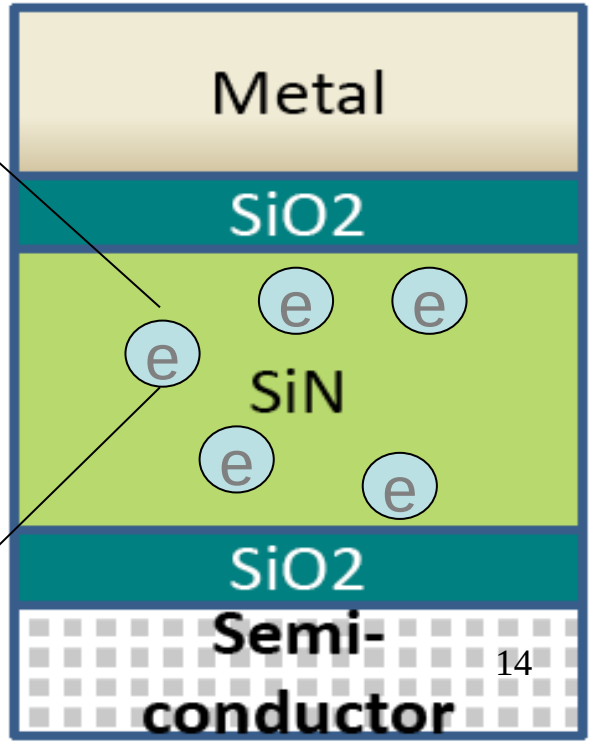
Dielectric breakdown

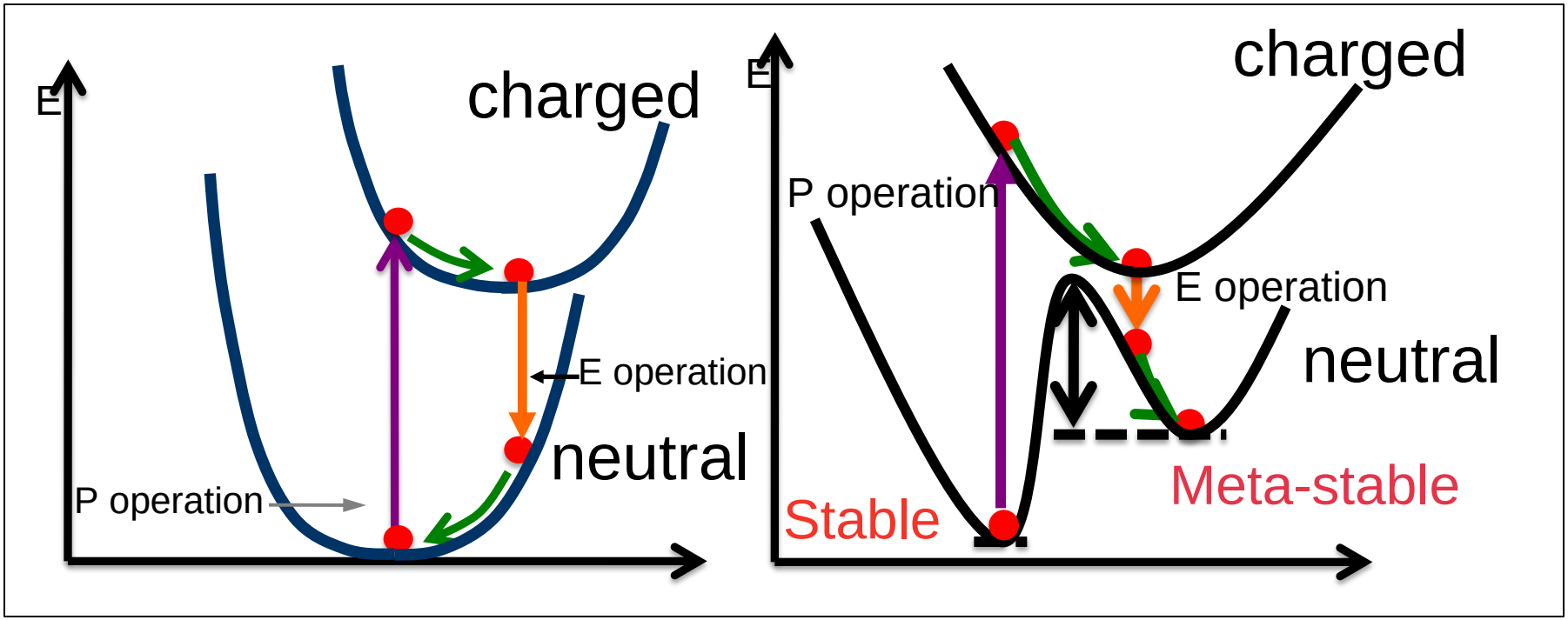
Purpose of our studies

We studied atomistic structural change of defects in SiN layers during Program/Erase cycles using first principles calculations.

We design defects which are suitable for charge trap memories.





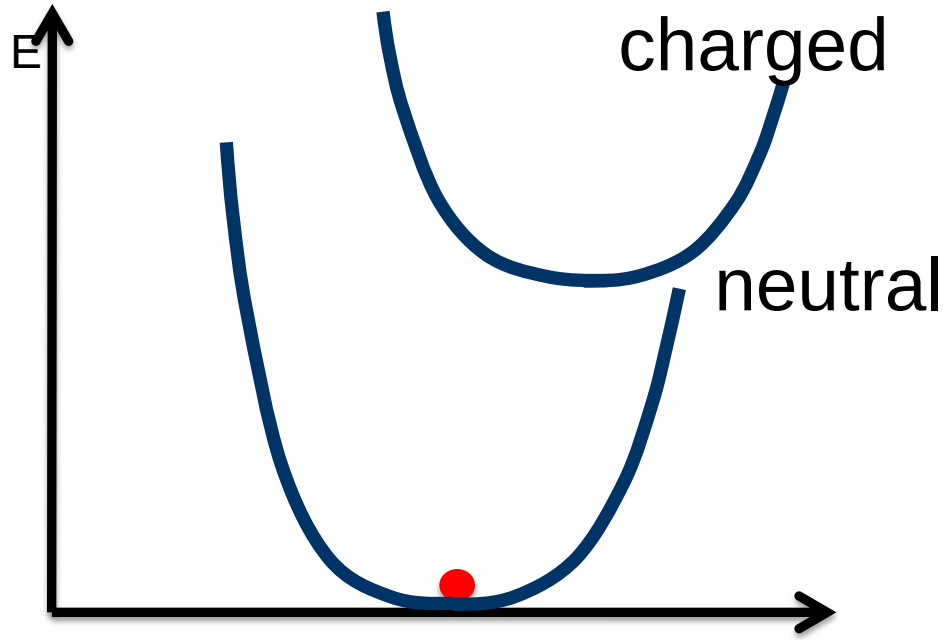


Reversible (suitable)

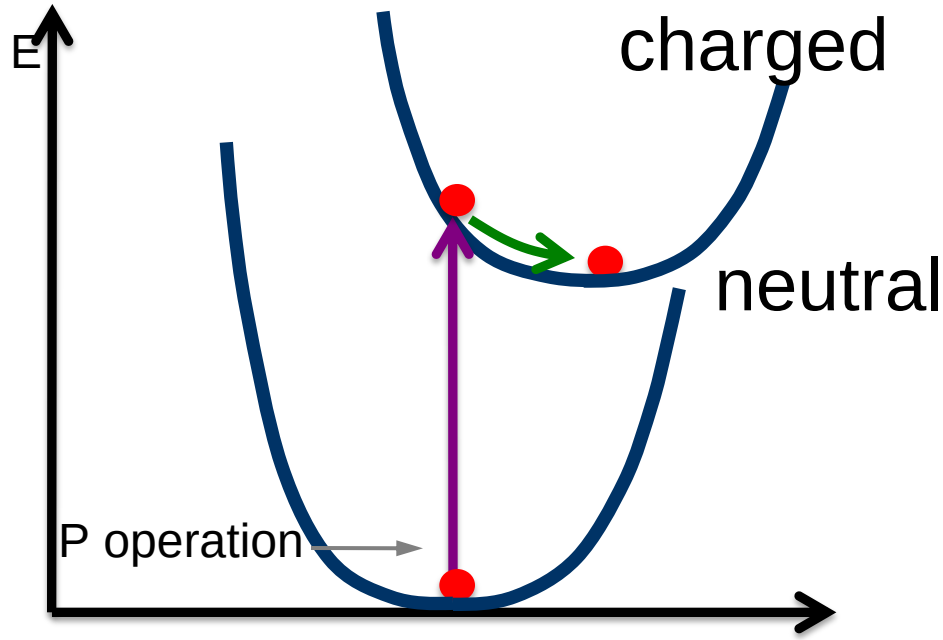
Irreversible (not suitable)

There are two type structural change during P/E cycles.

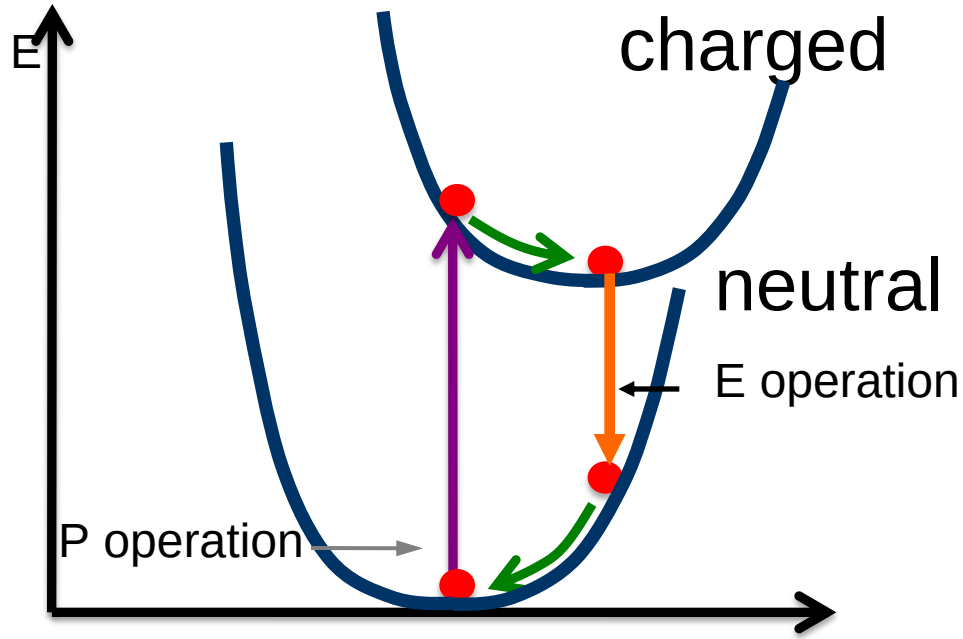
Reversible structural change



Reversible structural change



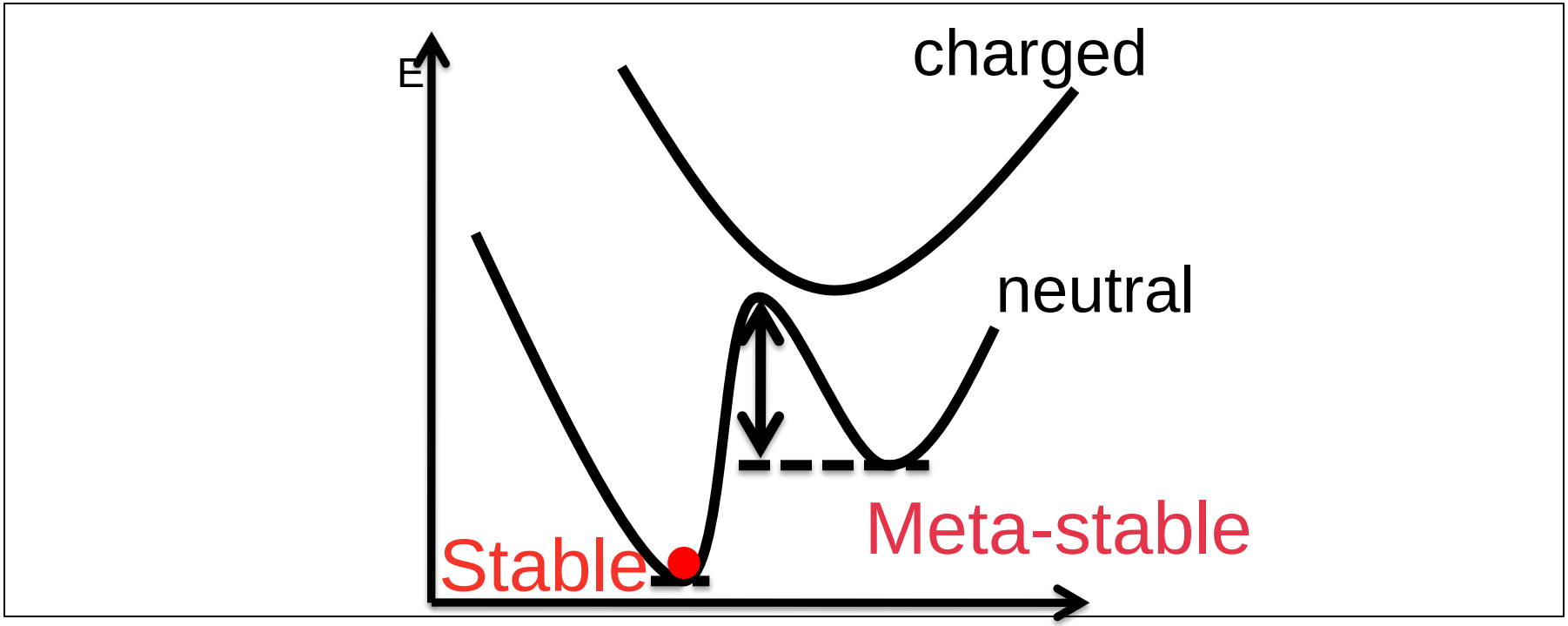
Reversible structural change



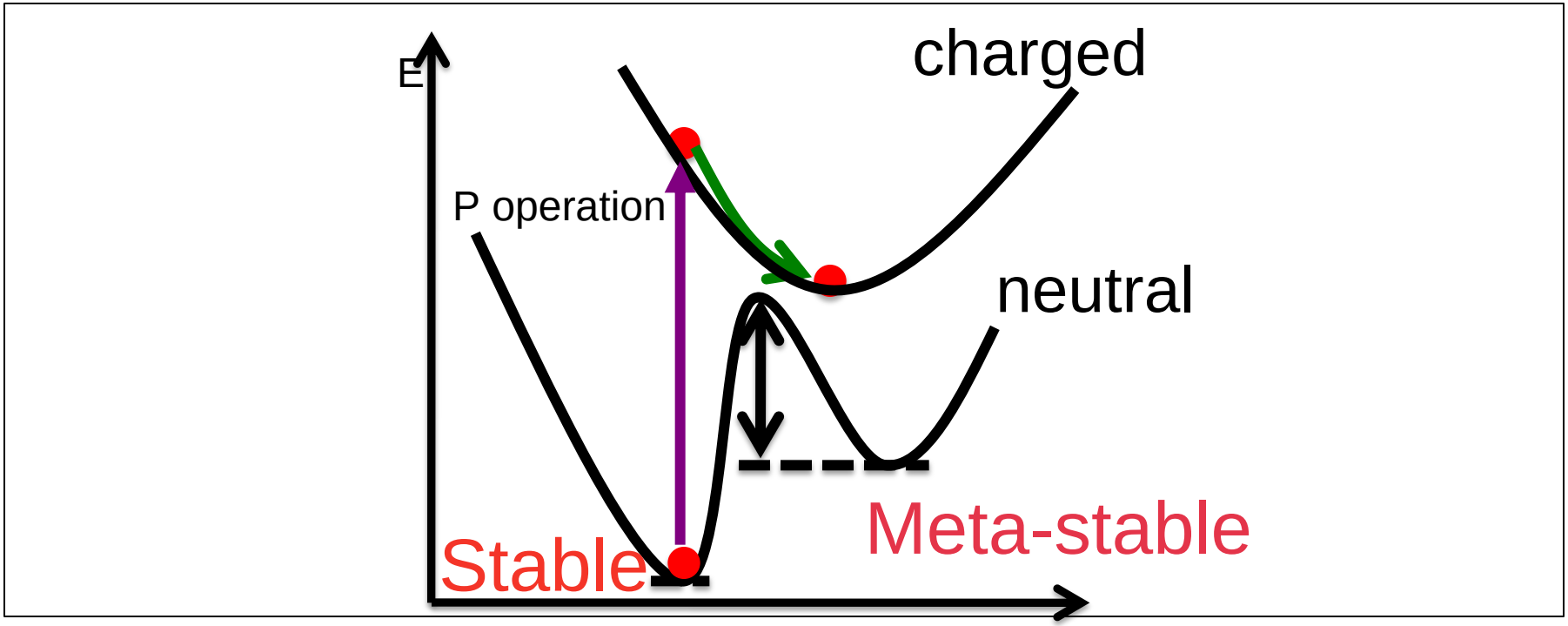
This structural change is reversible during P/E cycles

→ No degradation of memory

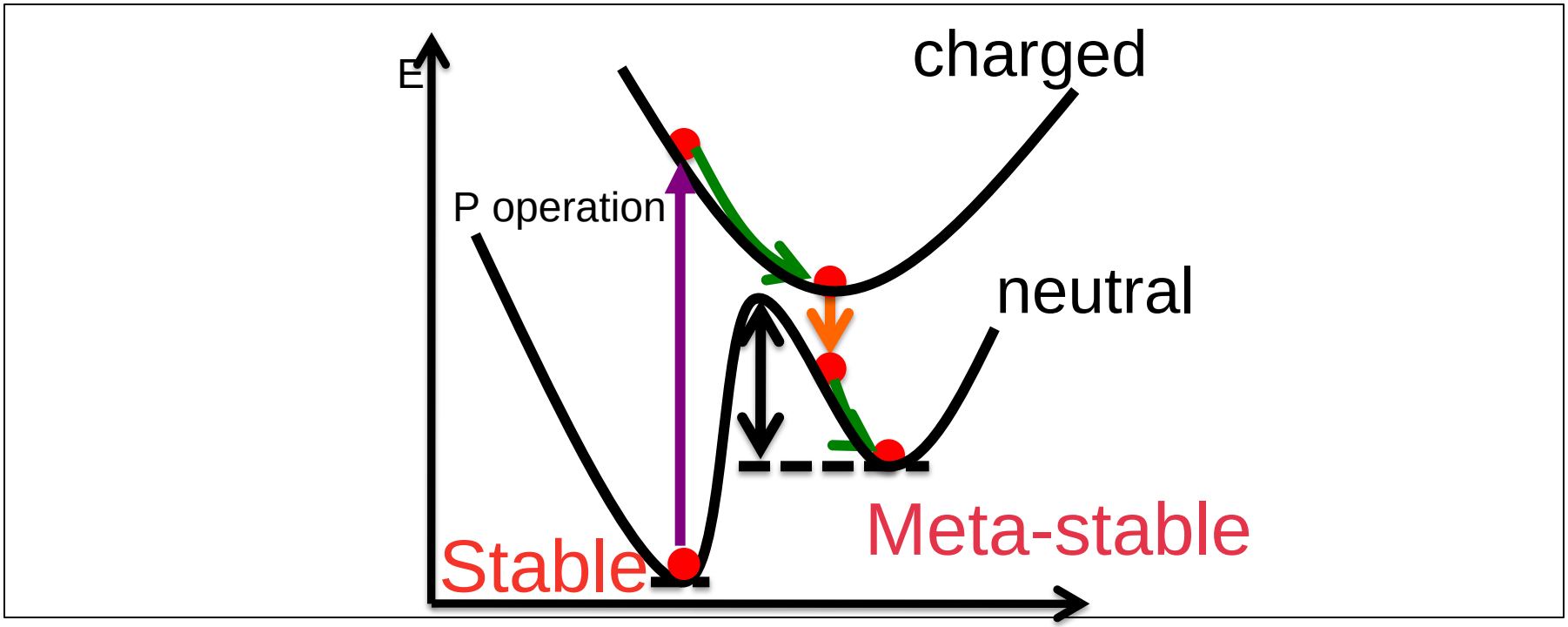
Irreversible structural change



Irreversible structural change



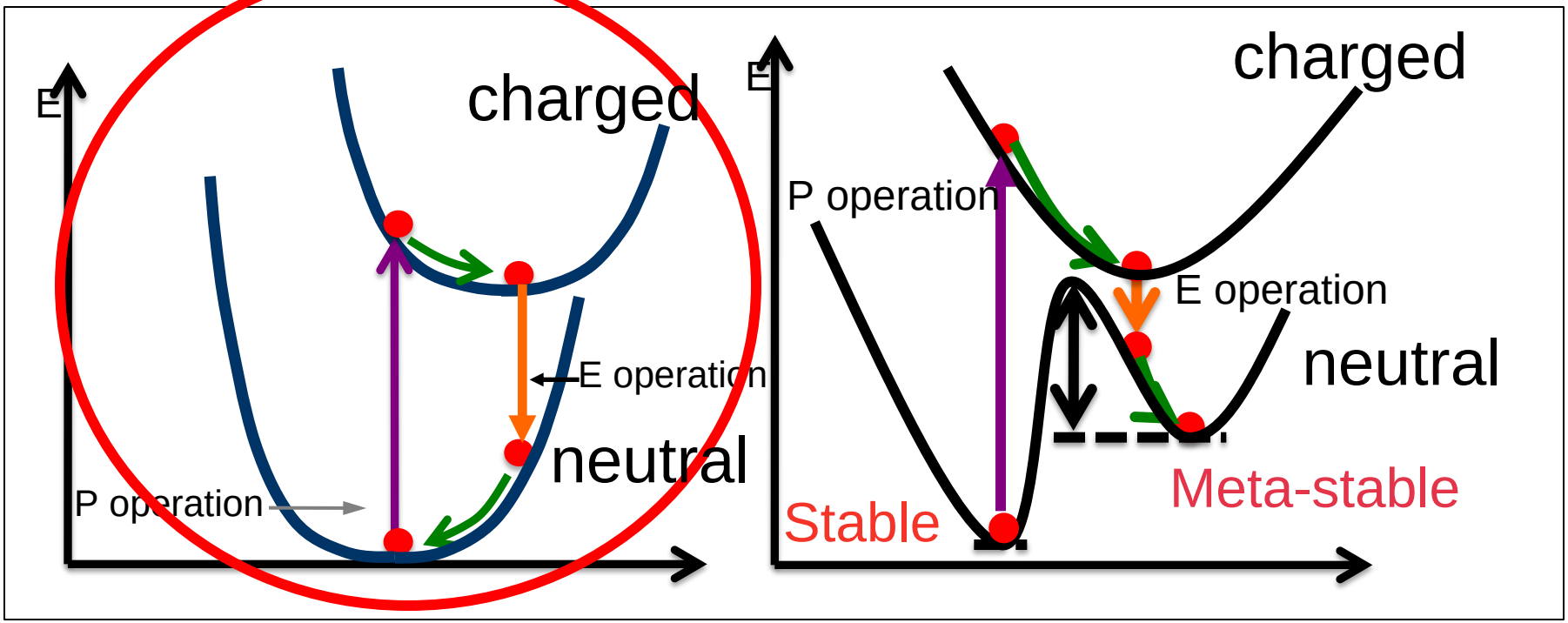
Irreversible structural change



This structural change is irreversible during P/E cycles.

→ Memory degradation

Two-types of structural change



Reversible (suitable)

Irreversible (not suitable)

We investigated how to design reversible type defects.

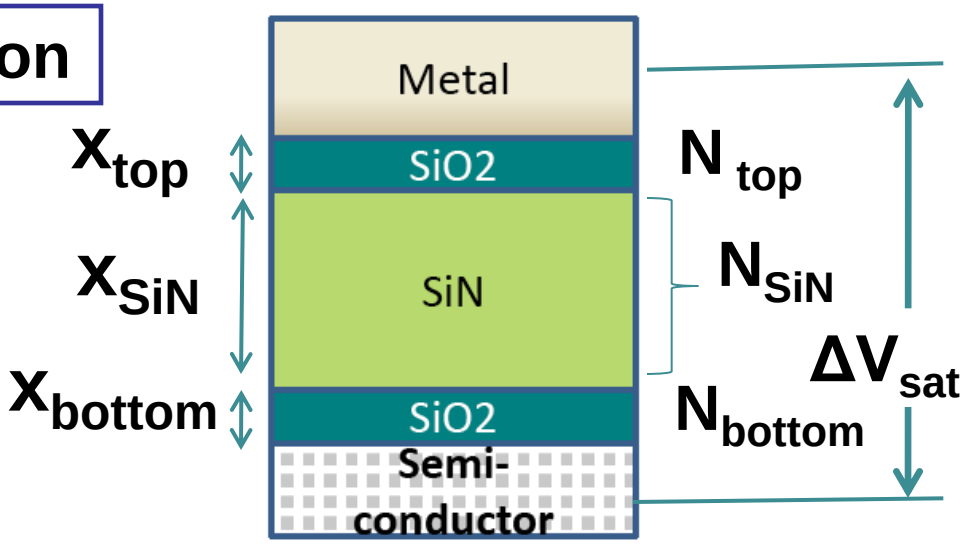
Experimental knowledge

Density of charge trap in SiN layer

Changing x_{SiN} & carrier injection

Measure ΔV_{sat}

Charge trap distribution



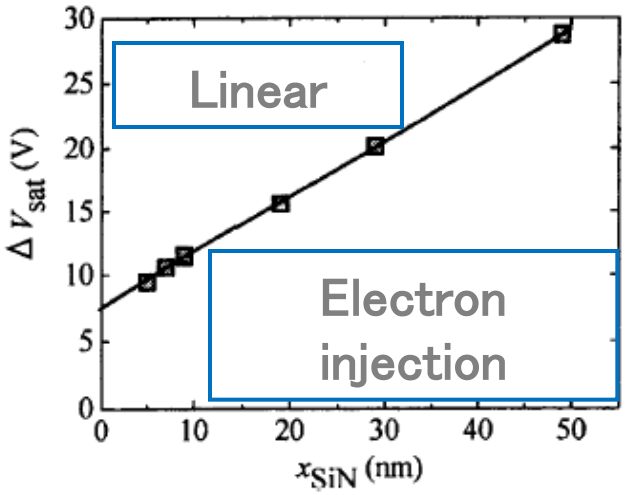
N_{top}, N_{SiN}, N_{bottom} : Charge trap density

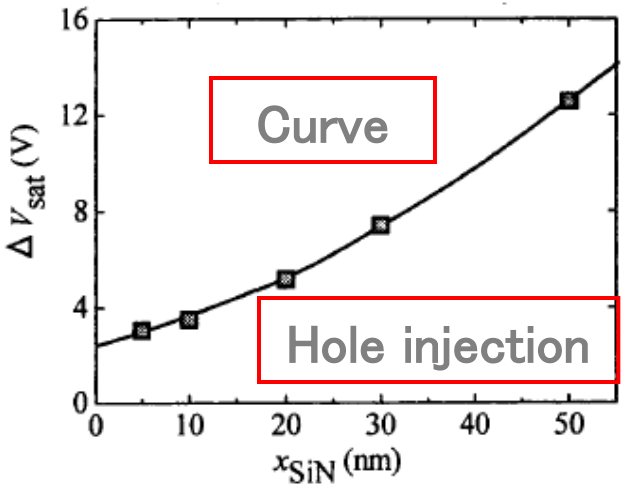
- Saturation voltage
- Each layer thicknesses
- Charge trap density

$$\Delta V_{sat} = \frac{qN_{SiN}}{2\epsilon_{SiN}\epsilon_0} x_{SiN}^2 + \left(\frac{qx_{top}N_{SiN}}{\epsilon_{SiO_2}\epsilon_0} + \frac{qN_{bottom}}{\epsilon_{SiN}\epsilon_0} \right) x_{SiN} + \frac{qx_{top}N_{top}}{\epsilon_{SiO_2}\epsilon_0} + \frac{qx_{top}N_{bottom}}{\epsilon_{SiO_2}\epsilon_0}$$

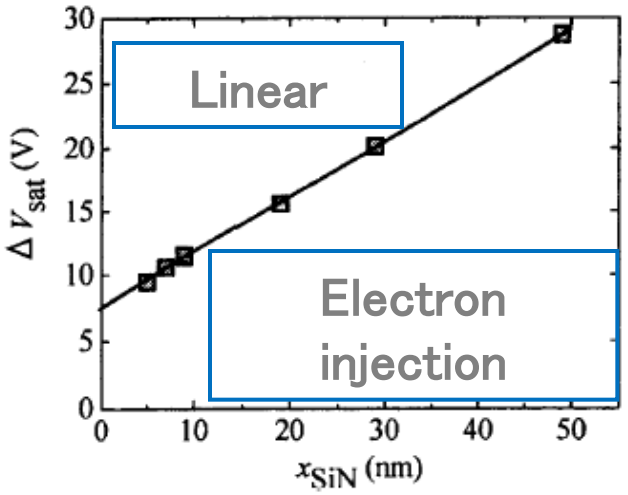
T. Ishida, et al., Proc. IRPS, 2006

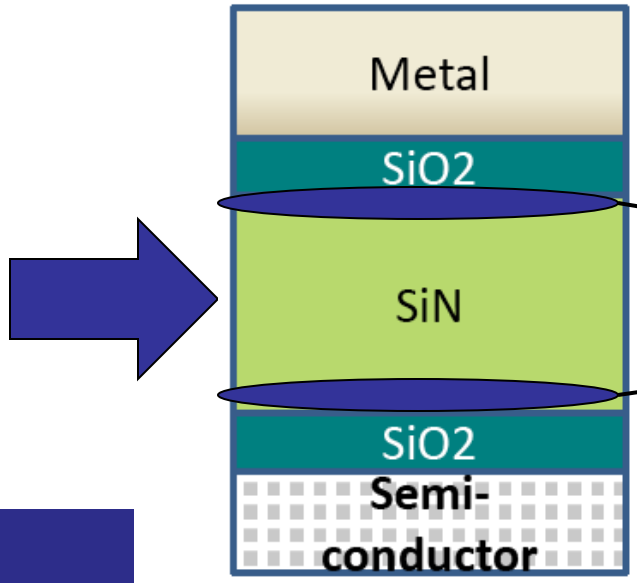
Density of charge trap in SiN layer





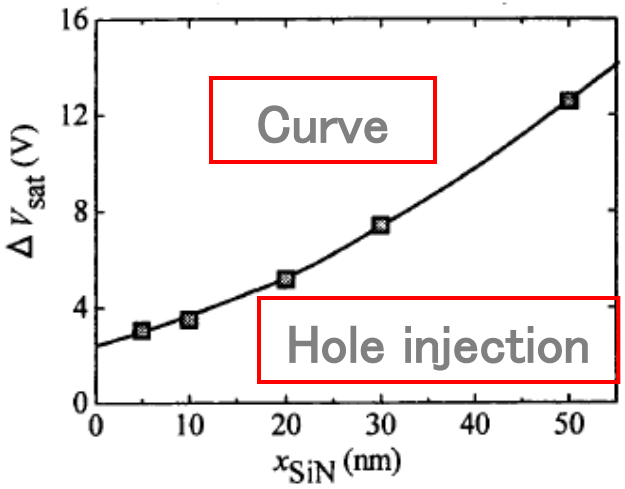
Density of charge trap in SiN layer



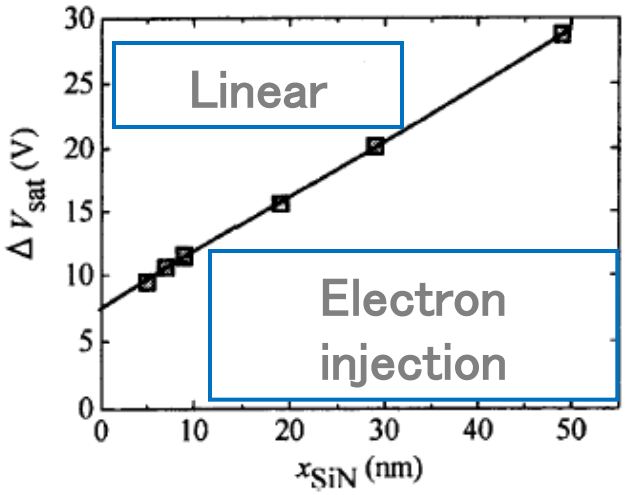


Electron trap distribution

Only SiN/SiO2 interfaces



Density of charge trap in SiN layer



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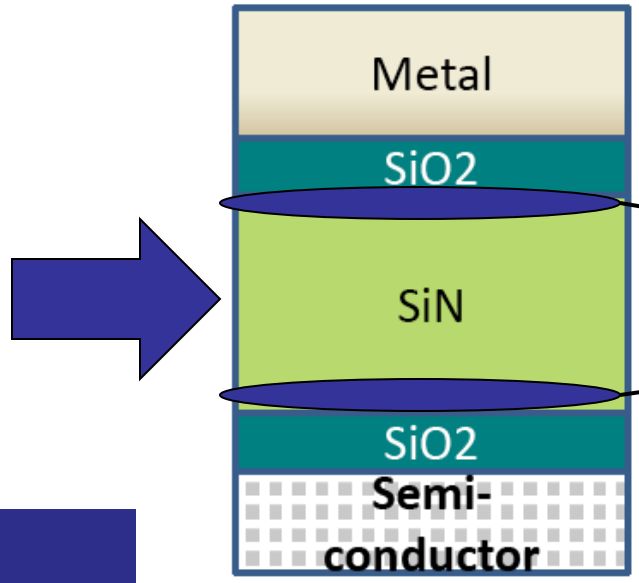

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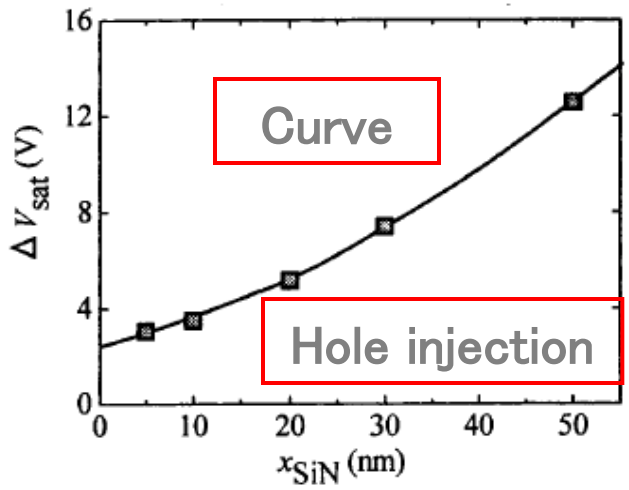
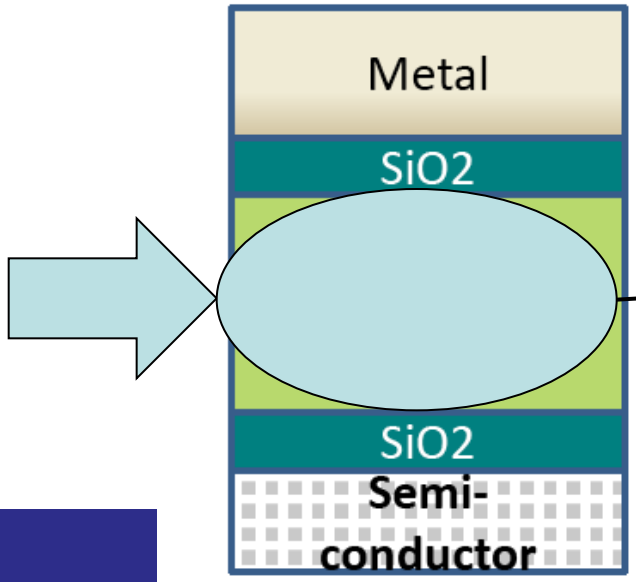
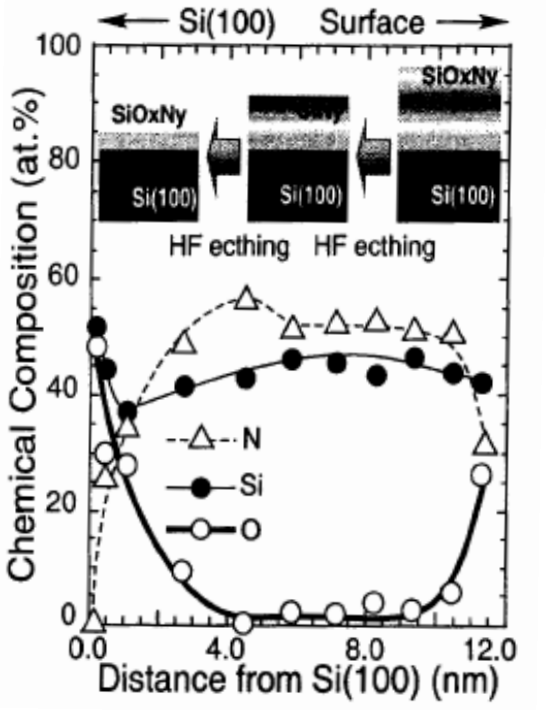


Interface and central part



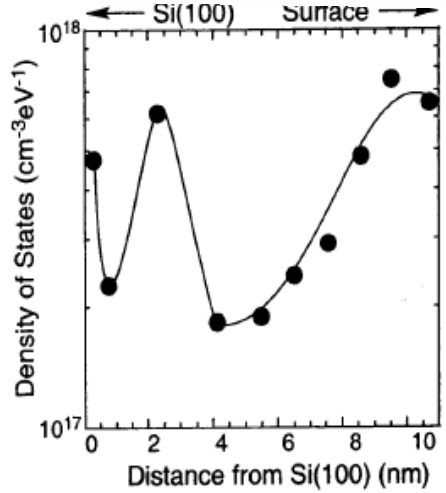
Hole trap distribution

Chemical composition and electronic occupation defect density for the depth direction of the SiN film



Chemical composition

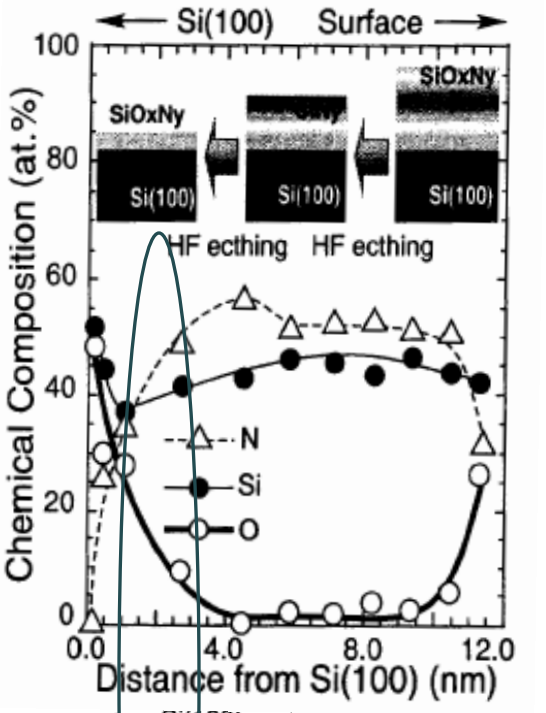
A lot of O atoms are in SiO2/SiN interfaces



Electronic occupation defect density

M. Miura, et al., IEICE Technical Report SDM2007-34

Chemical composition and electronic occupation defect density for the depth direction of the SiN film



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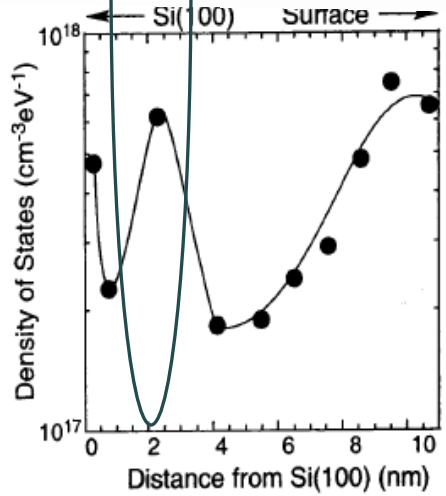
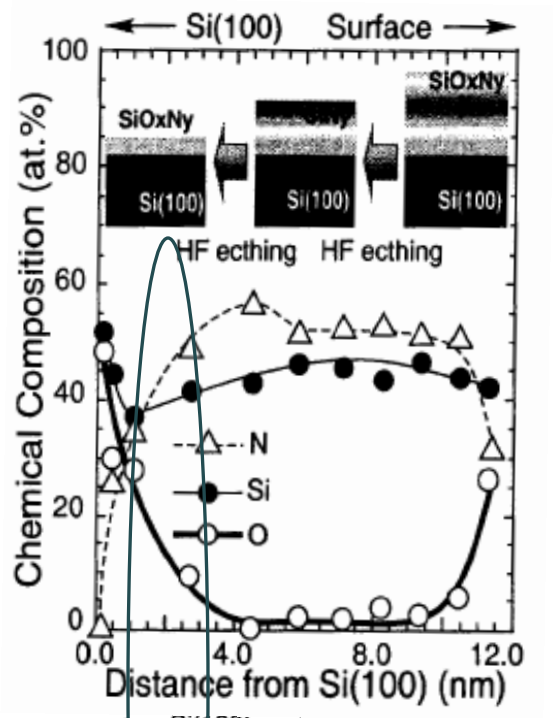


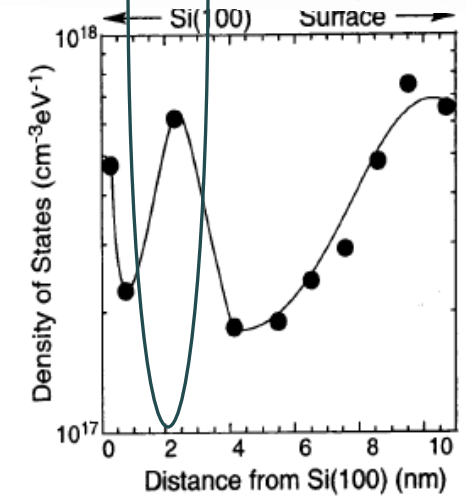
Electronic occupation defect density

Occupation defects exist in same region with O atoms

M. Miura, et al., IEICE Technical Report SDM2007-34

Chemical composition and electronic occupation defect density for the depth direction of the SiN film





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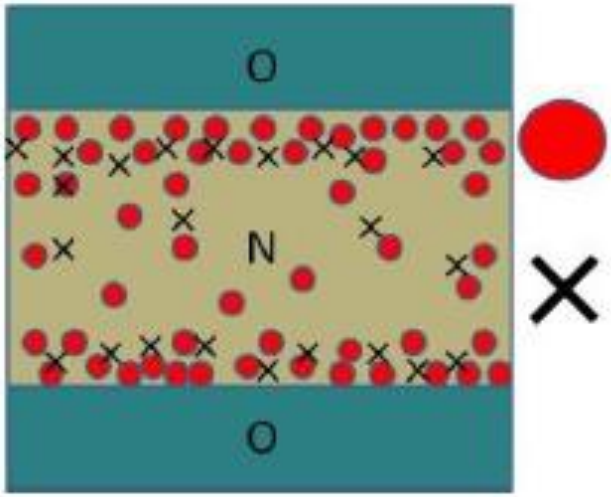


O atoms

Defects

Electronic occupation defect density

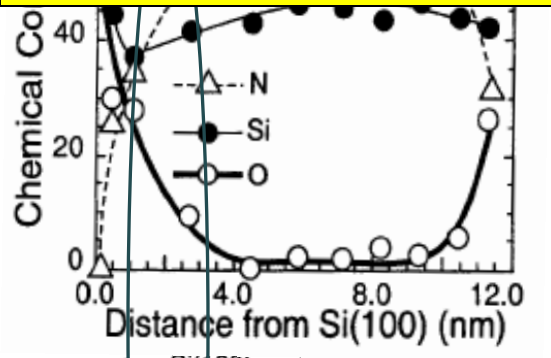
Occupation defects exist in same region with O atoms

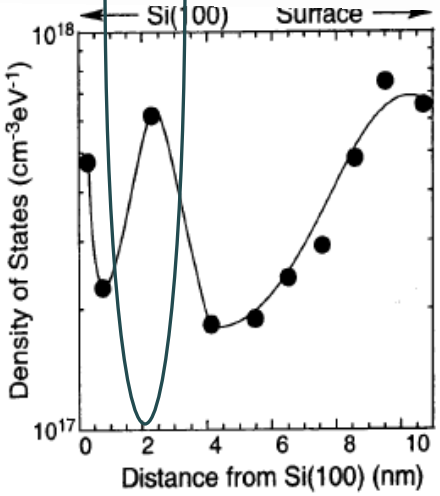
M. Miura, et al., IEICE Technical Report SDM2007-34

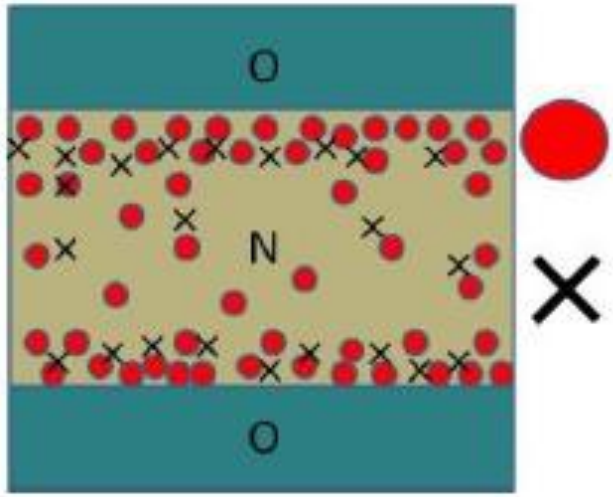
Much of charge traps is necessary for charge trap memory.

O atoms make charge traps in SiN.

O atoms are important in MONOS







O atoms

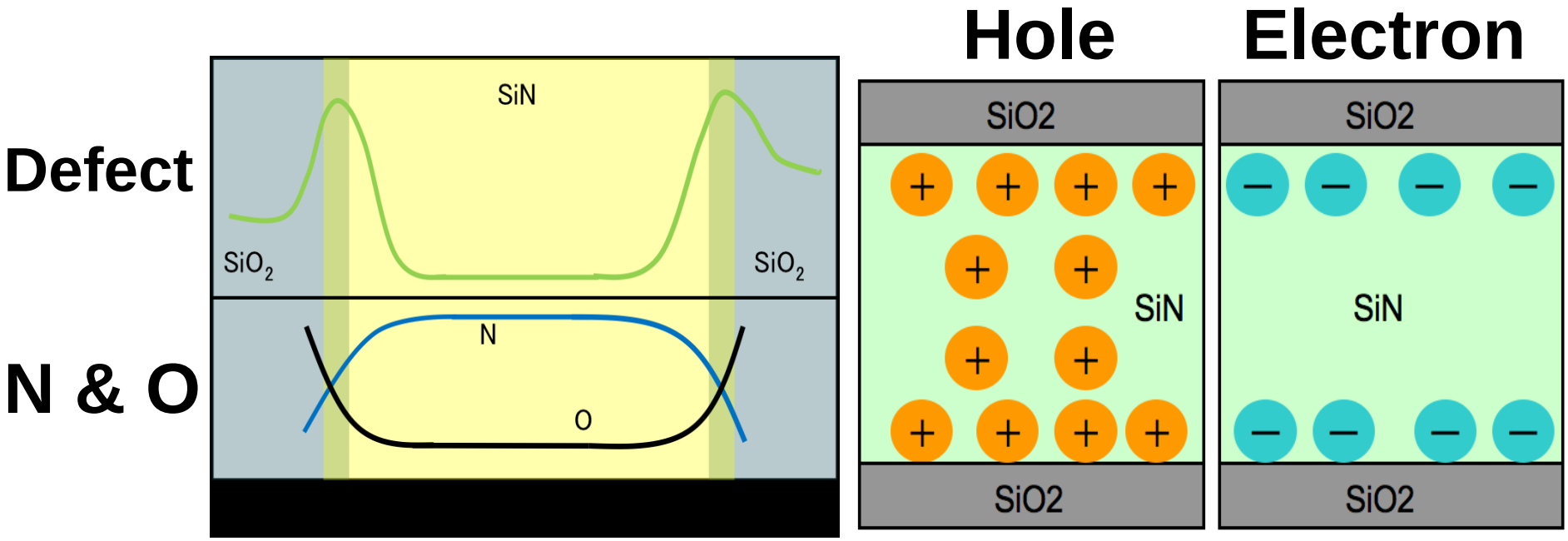
Defects

Electronic occupation defect density

Occupation defects exist in same region with O atoms

M. Miura, et al., IEICE Technical Report SDM2007-34

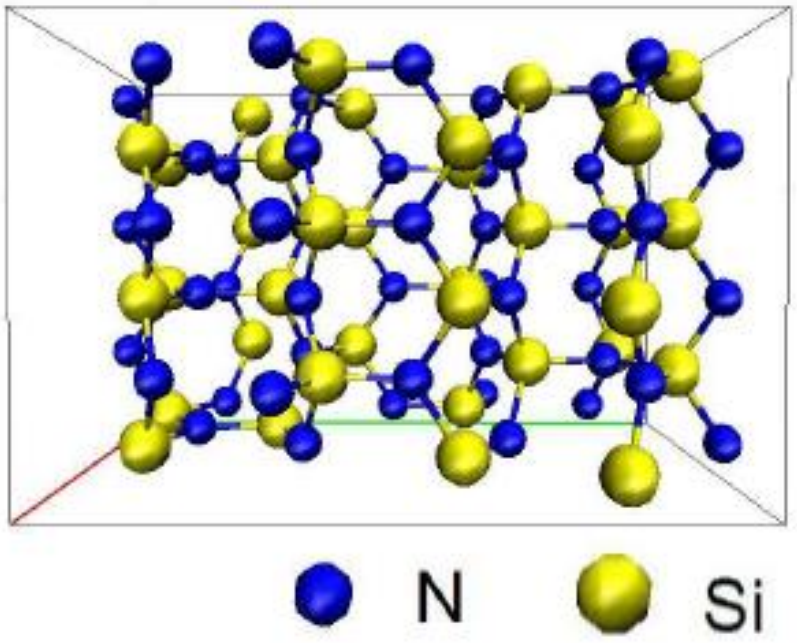
Summary of experimental report



1. O inter-diffusion is observed at SiN/SiO_2 interfaces.
2. Lots of defects are located in the O containing interfacial SiN regions.
3. Electron traps are localized near SiN/SiO2 interfaces. But hole traps are distributed both interface and the central part

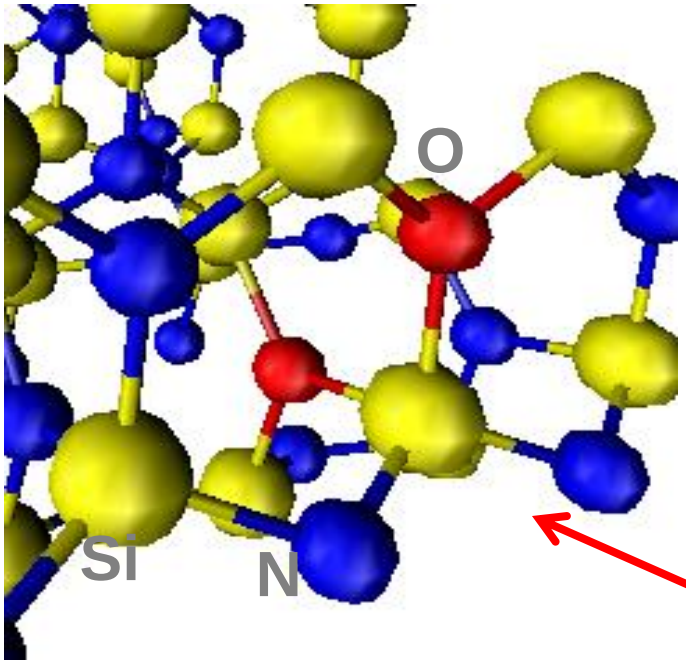
Calculation Model

84 atoms



We prepare the calculation models that Si3N4 84 atoms cell.

Calculation Model 1

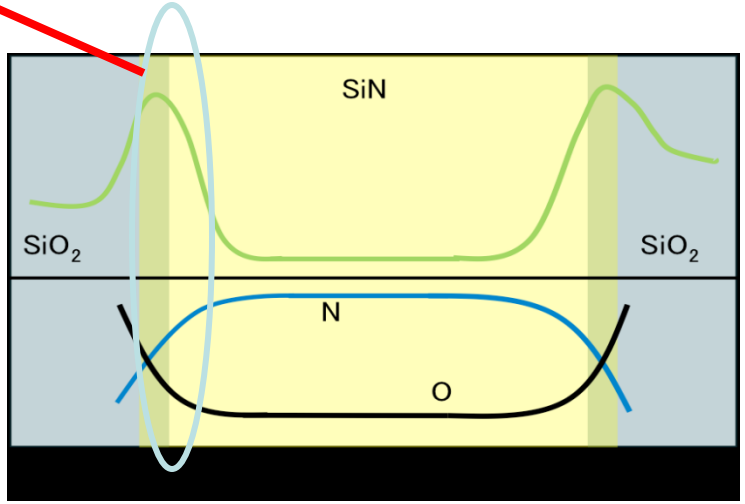


A defect with two substitutional O atoms at N sites.

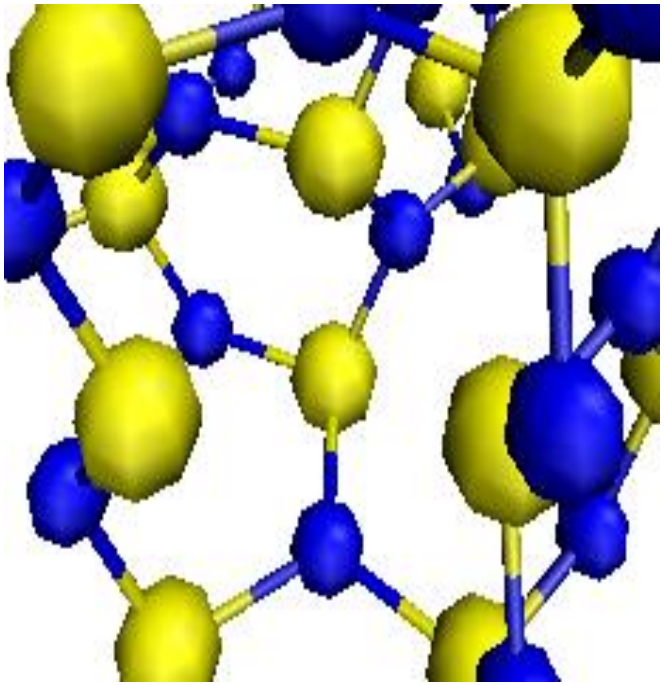
This is the model of excess O atoms in SiN.

Defect

N & O

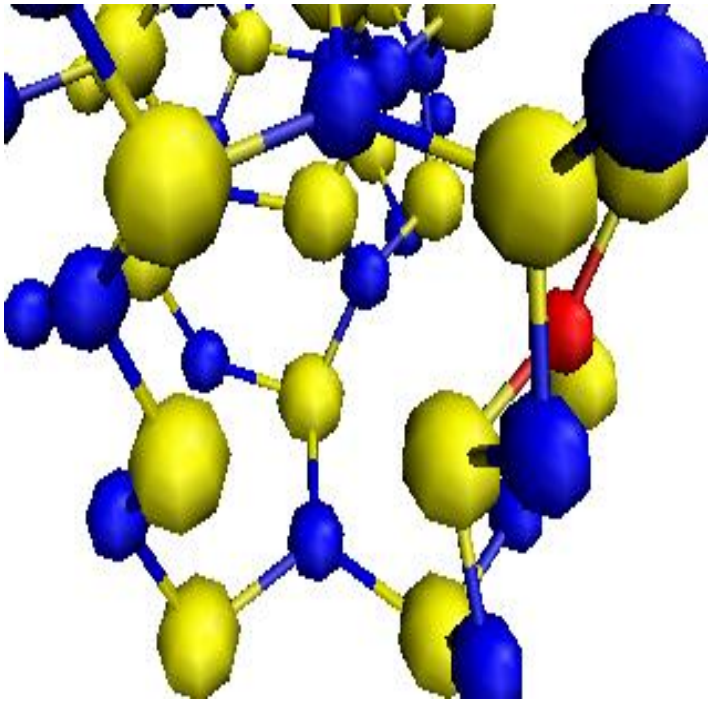


Calculation Model 2



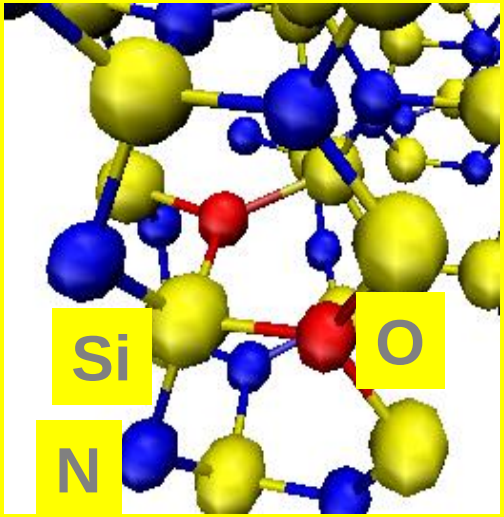
A defect with a N vacancy.

Calculation Model 3



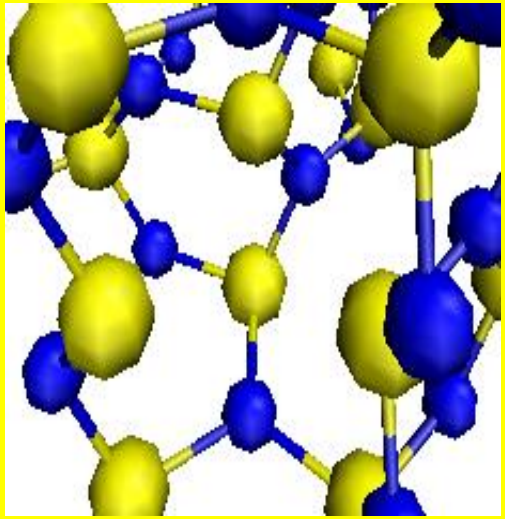
A defect with a N vacancy with one O atom.

Three Calculation Models

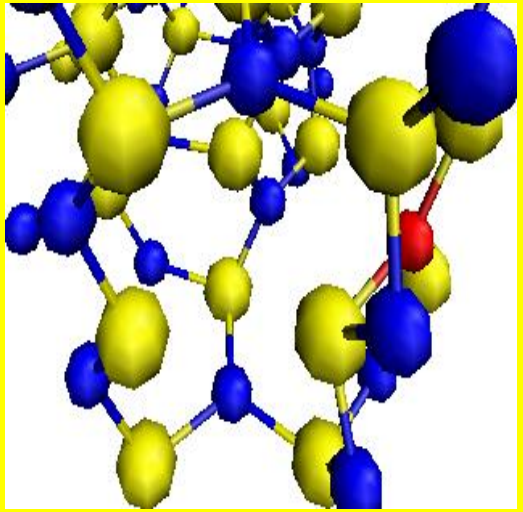


A defect with two substitutional O atoms at N sites.

This is the model of excess O atoms in SiN.

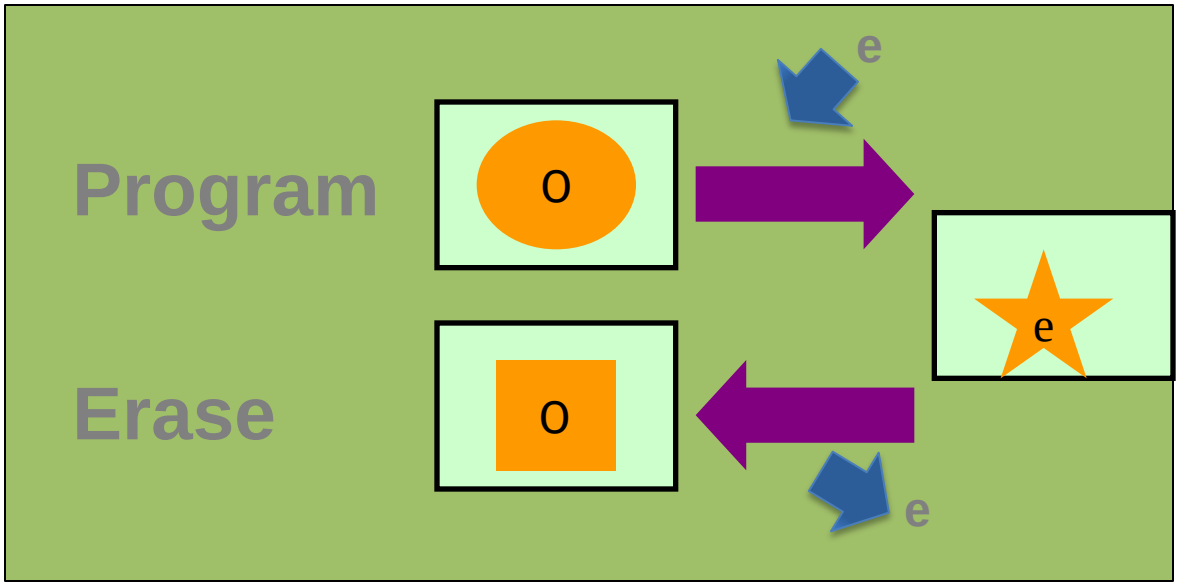


A defect with a N vacancy.



A defect with a N vacancy with one O atom.

The calculation of P/E operation

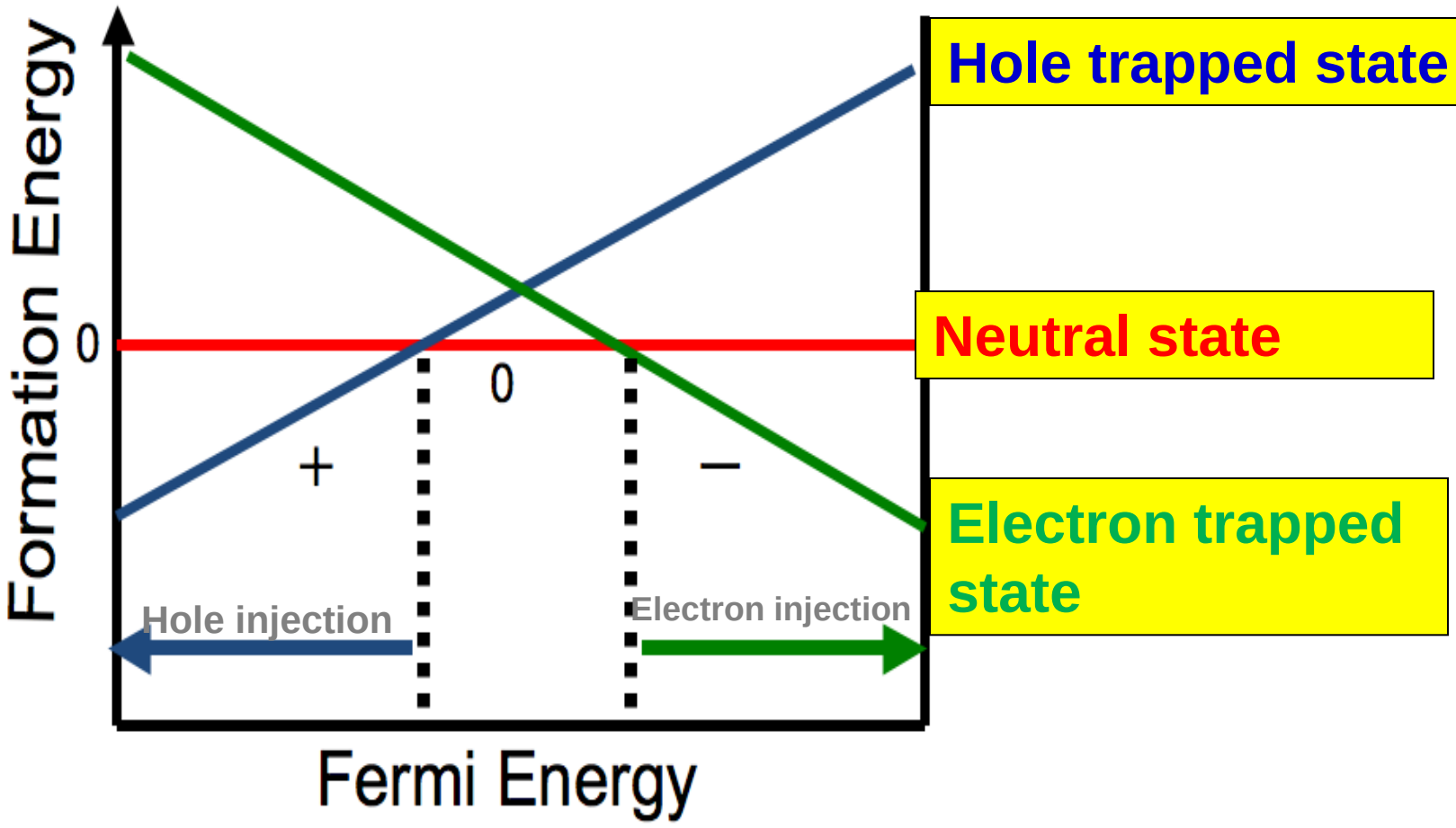


We investigated atomic and electronic structural change during Program/Erase operations (carrier injection & removal).

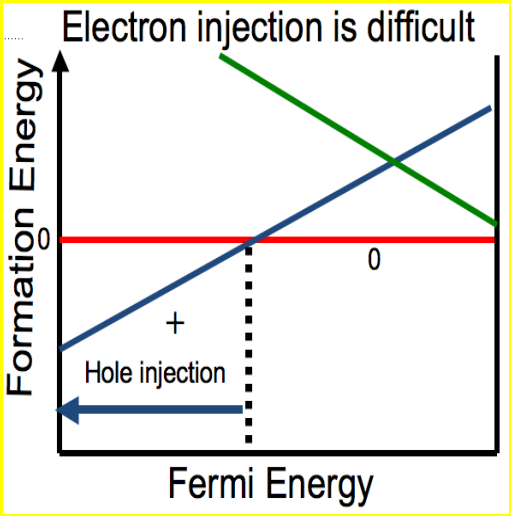
Calculation Method

- First principle calculation
- Generalized gradient approximation
- Ultra-soft pseudo-potential

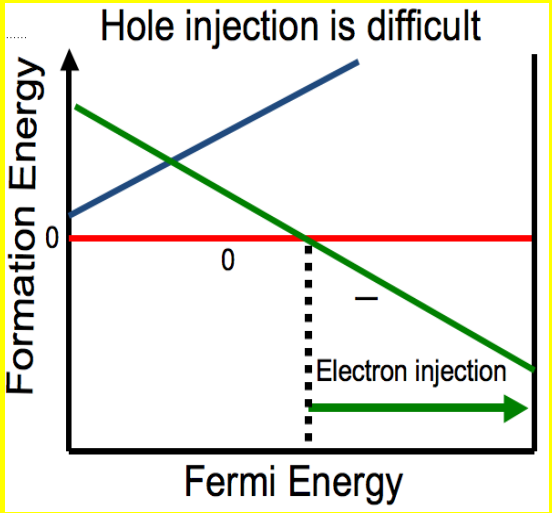
Formation Energy Diagram (example)



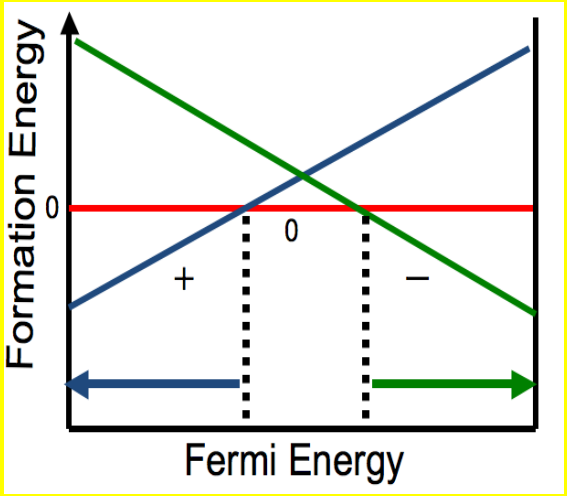
The charged state with the lowest energy is the optimal state at each Fermi energy.



Only hole trapped state is possible



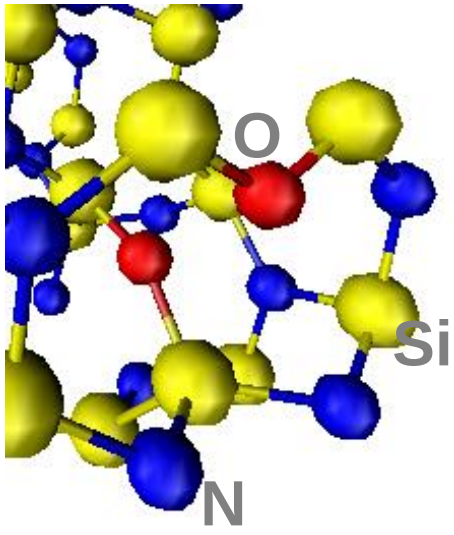
Only electron trapped state is possible



Both electron and hole trapped states are possible

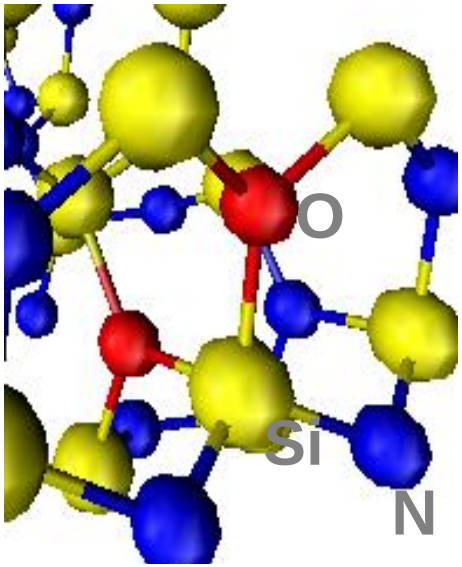
Formation energy diagram corresponds to memory characteristic.

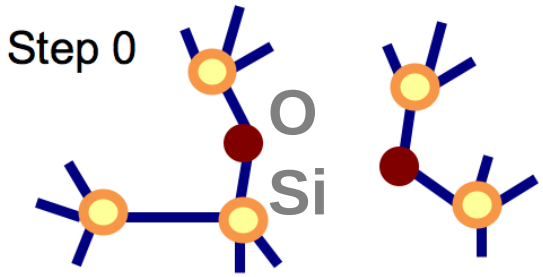
3.1 Result for excess O model

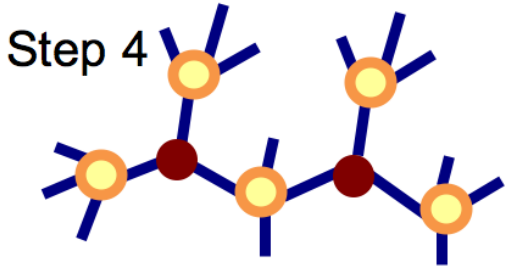


Hole

Program





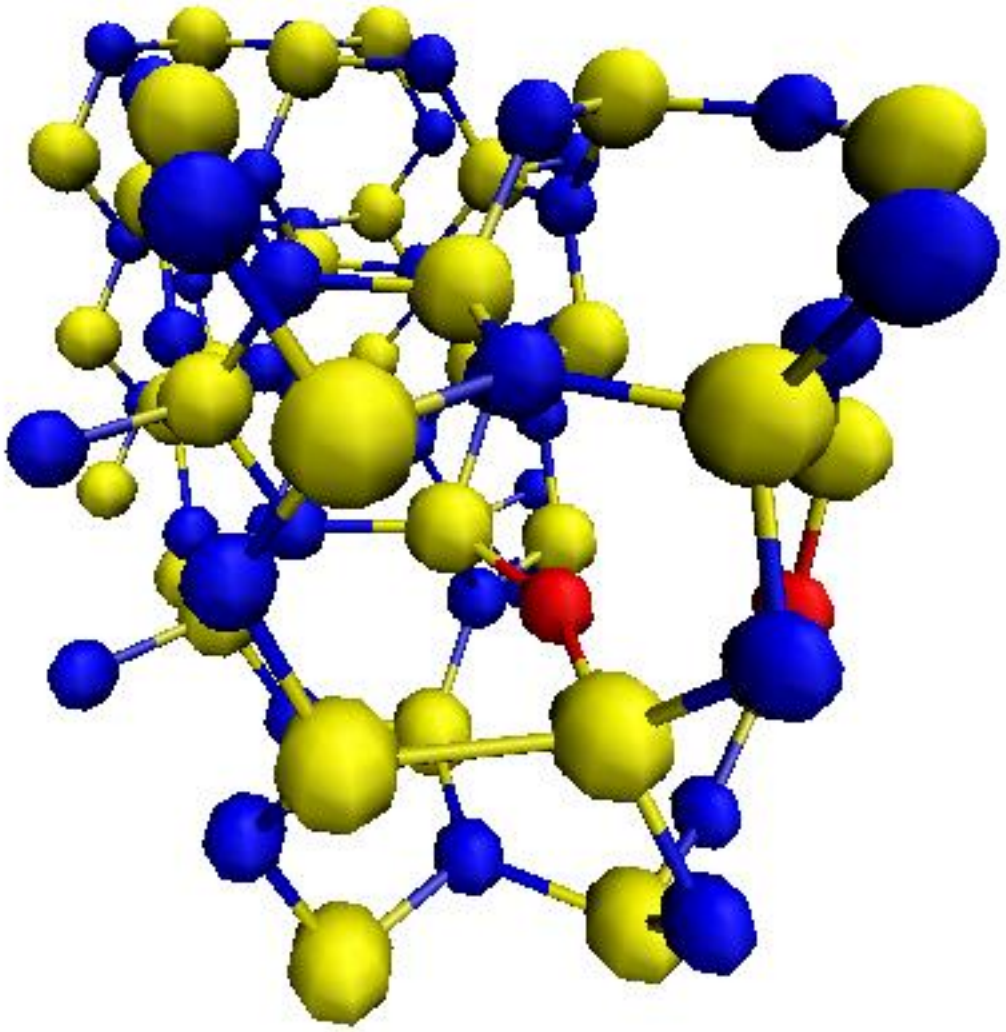


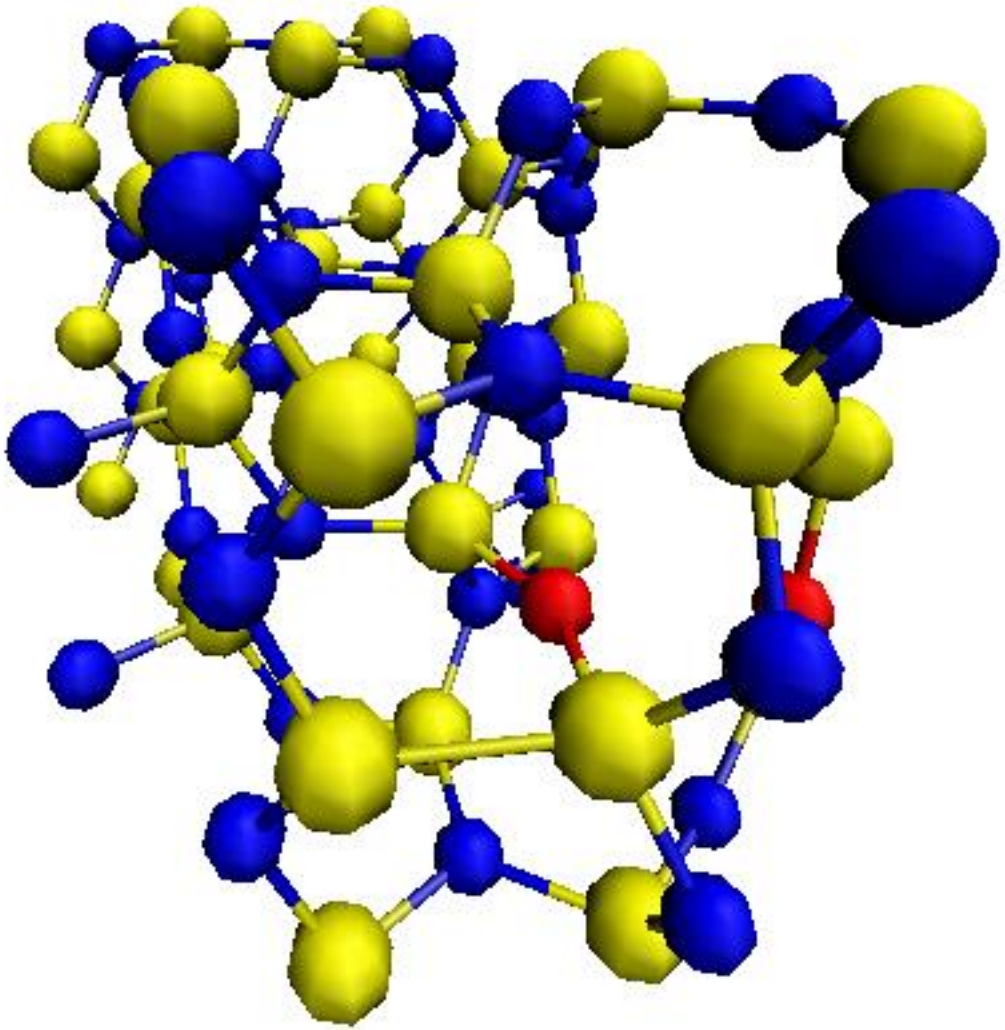
Initial

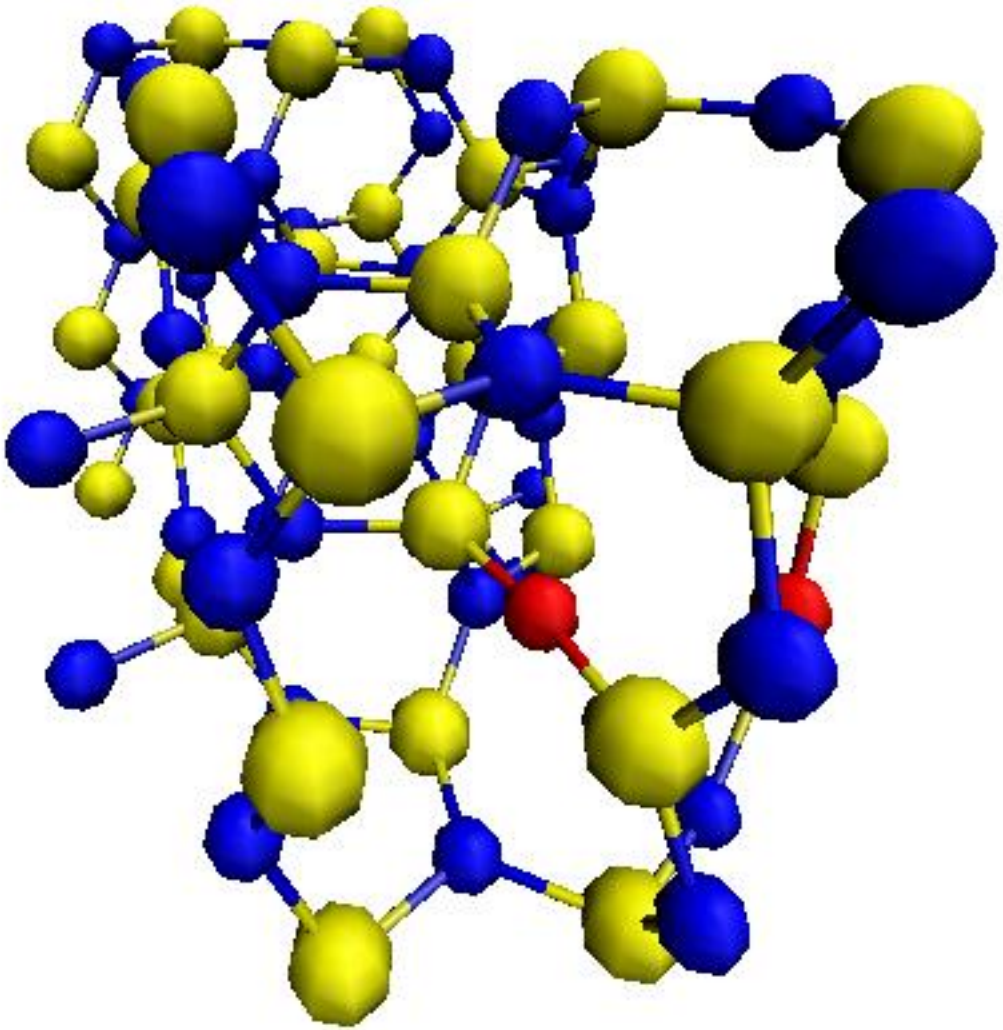
After program operation

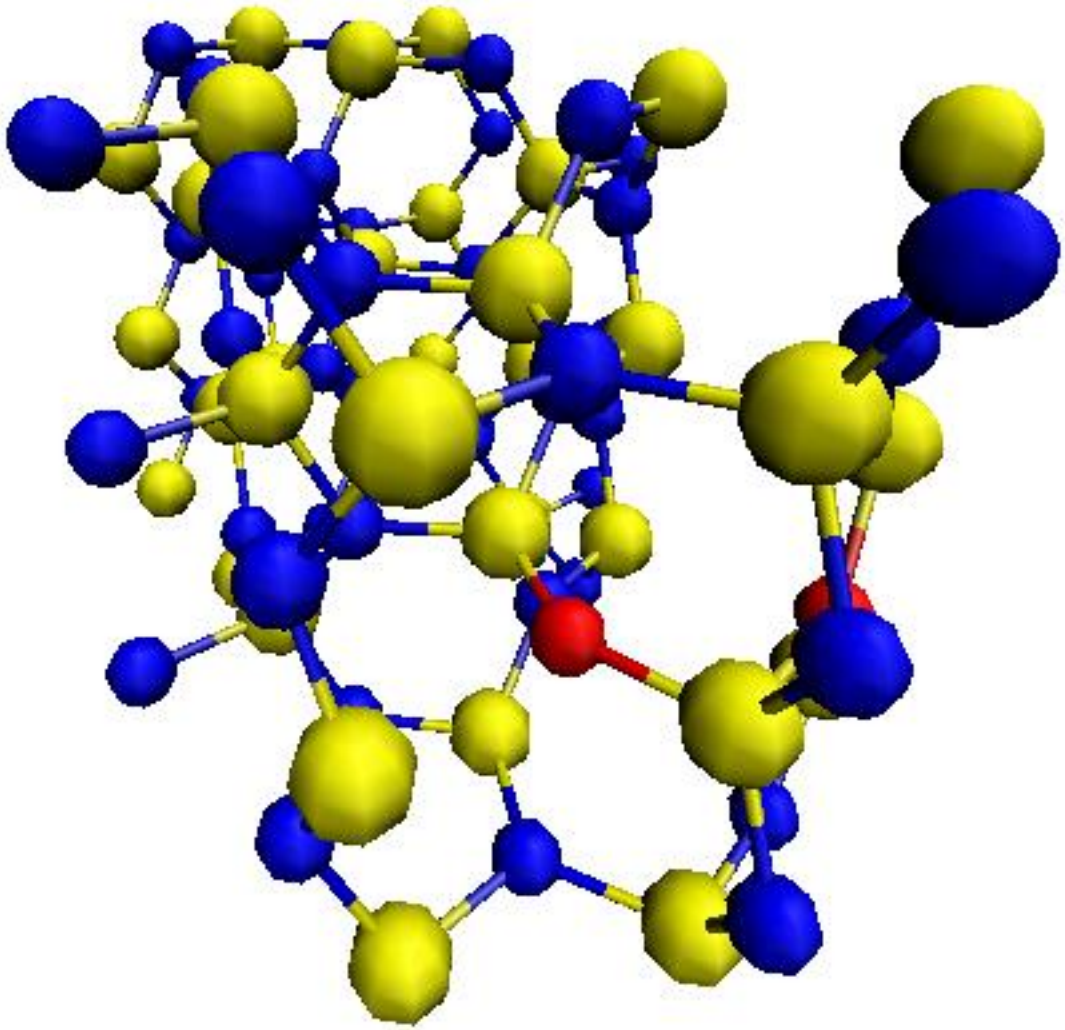
Atomistic structures before and after program operation.

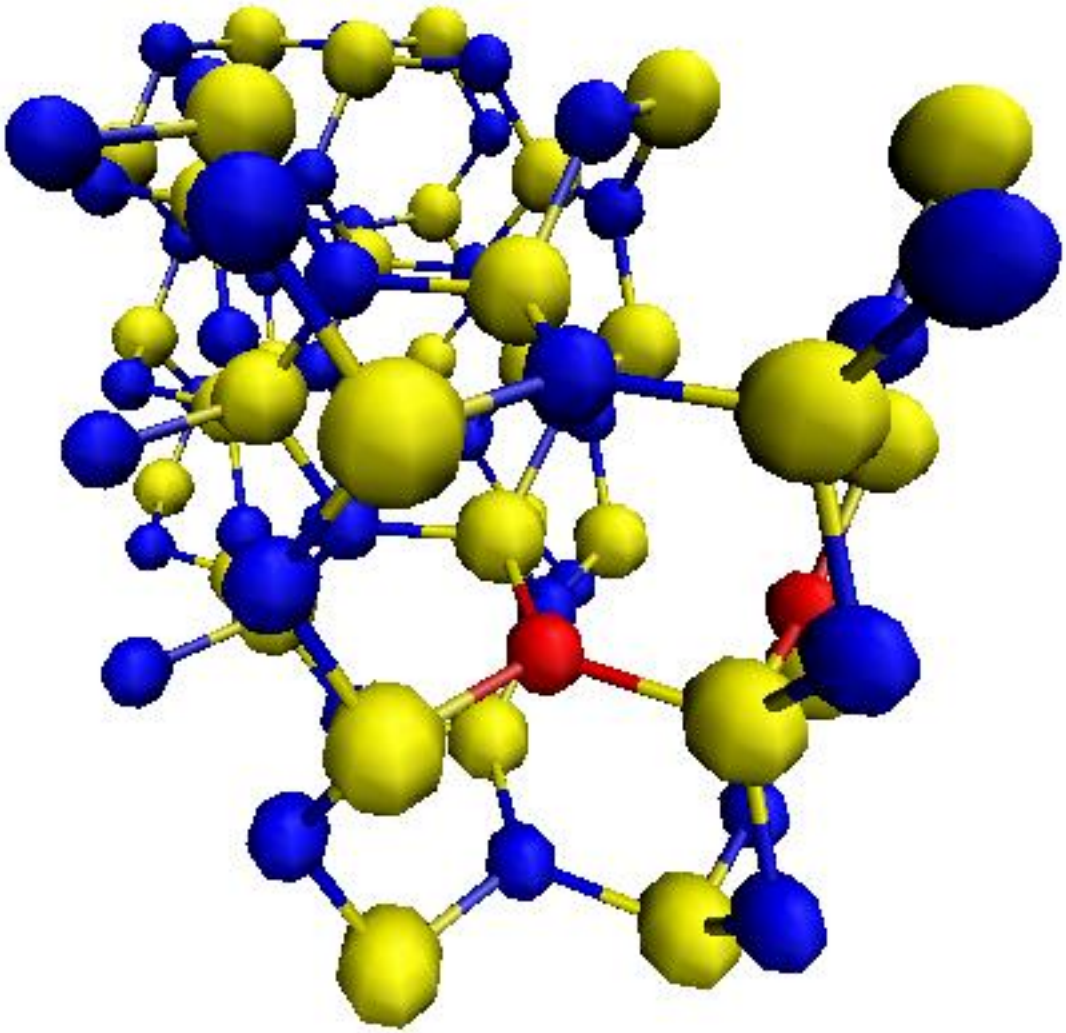
Structural change by program operation



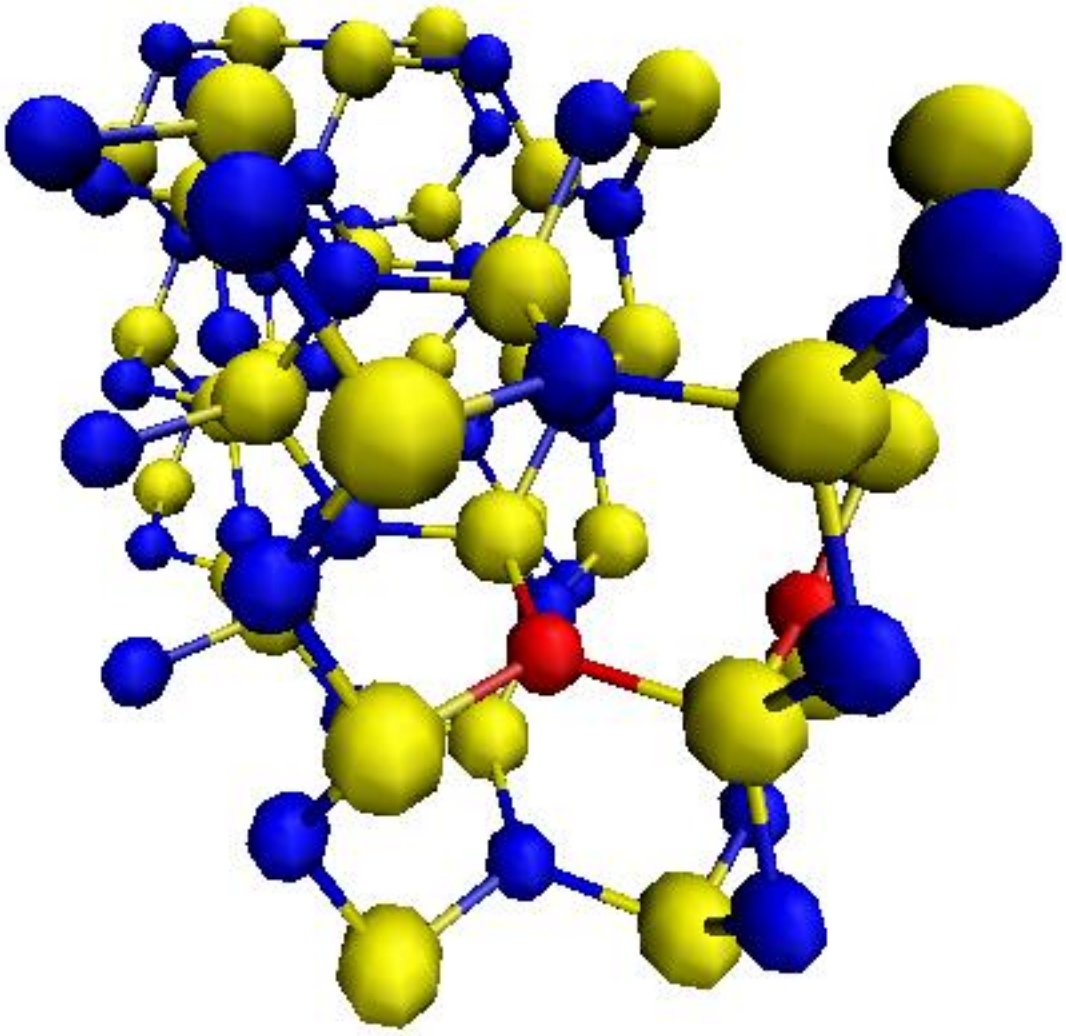




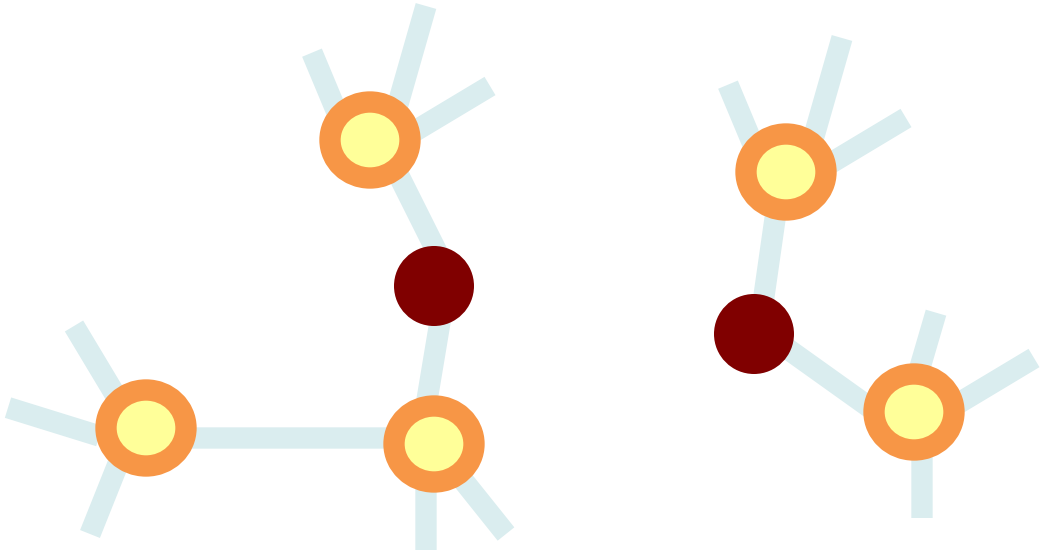




After program operation



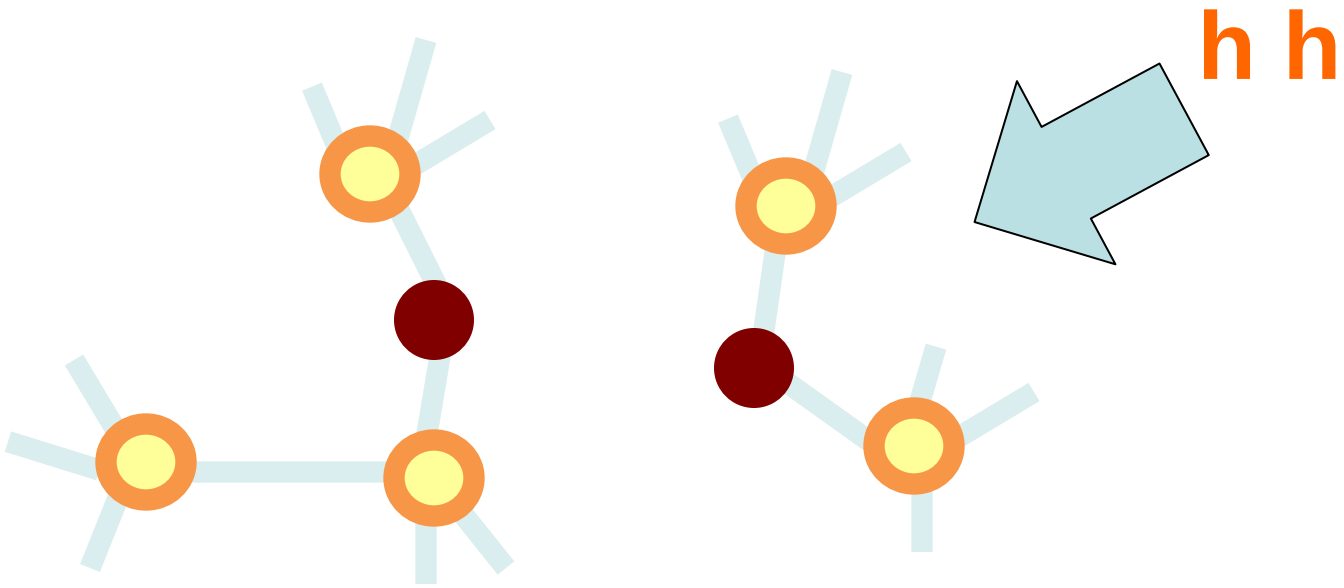
Initial structure



Step 0

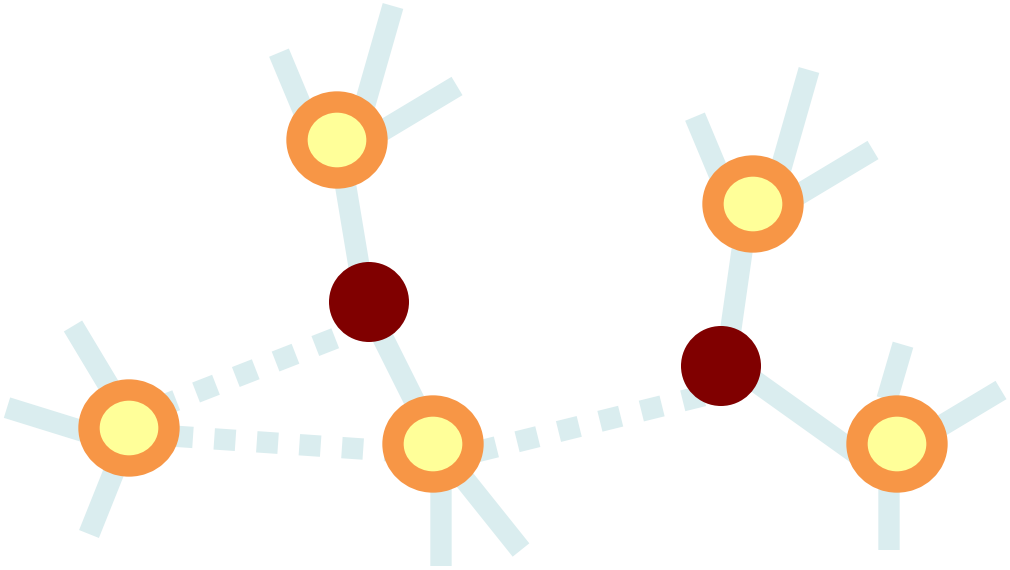
:Si **:O**

Program operation

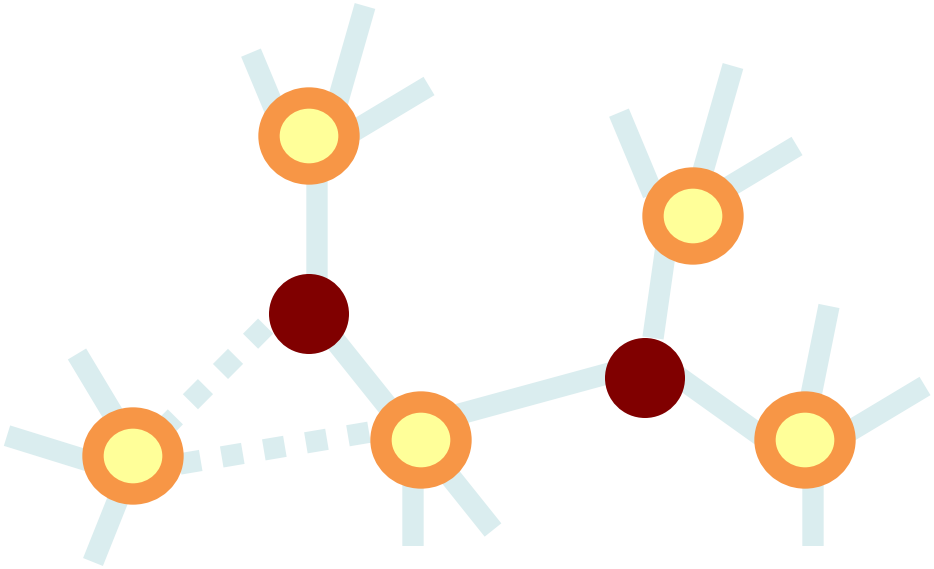


Step 0

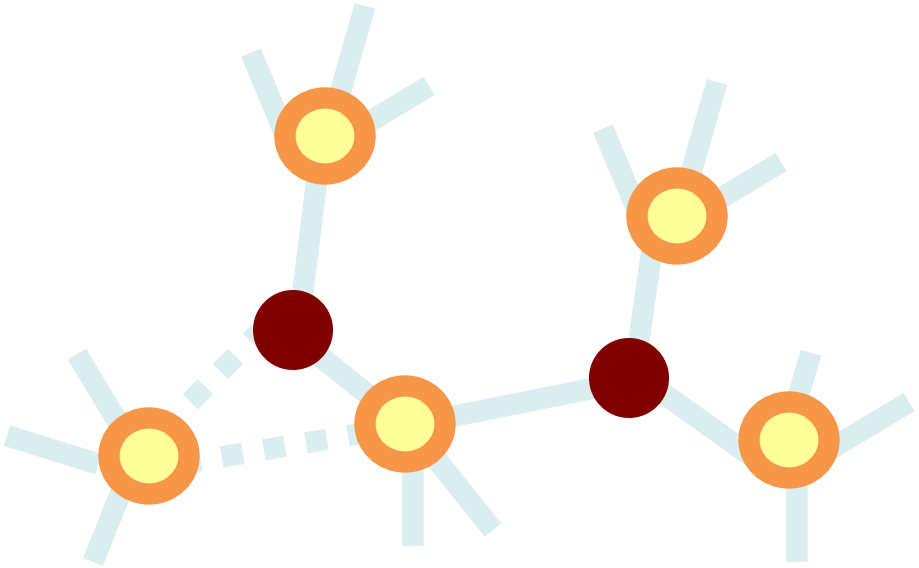
:Si :O



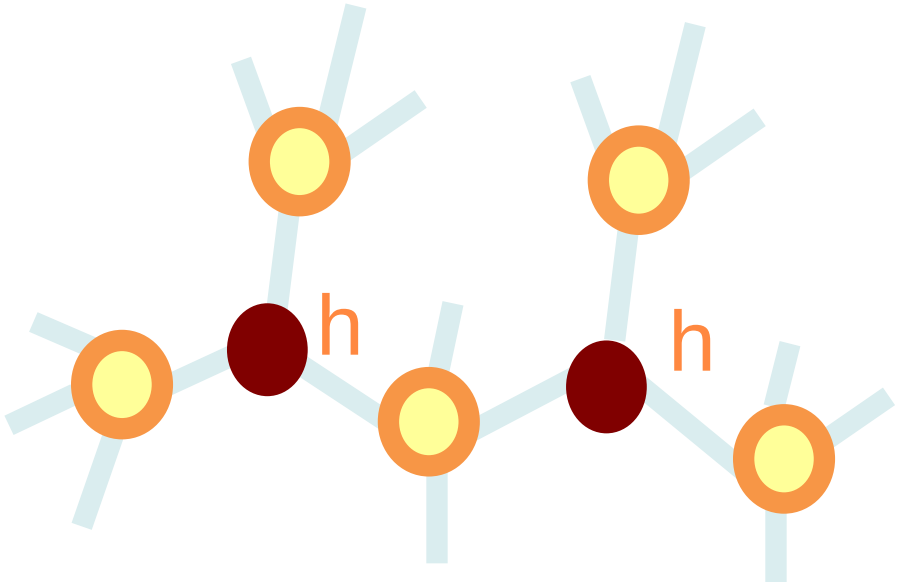
Step 1



Step 2

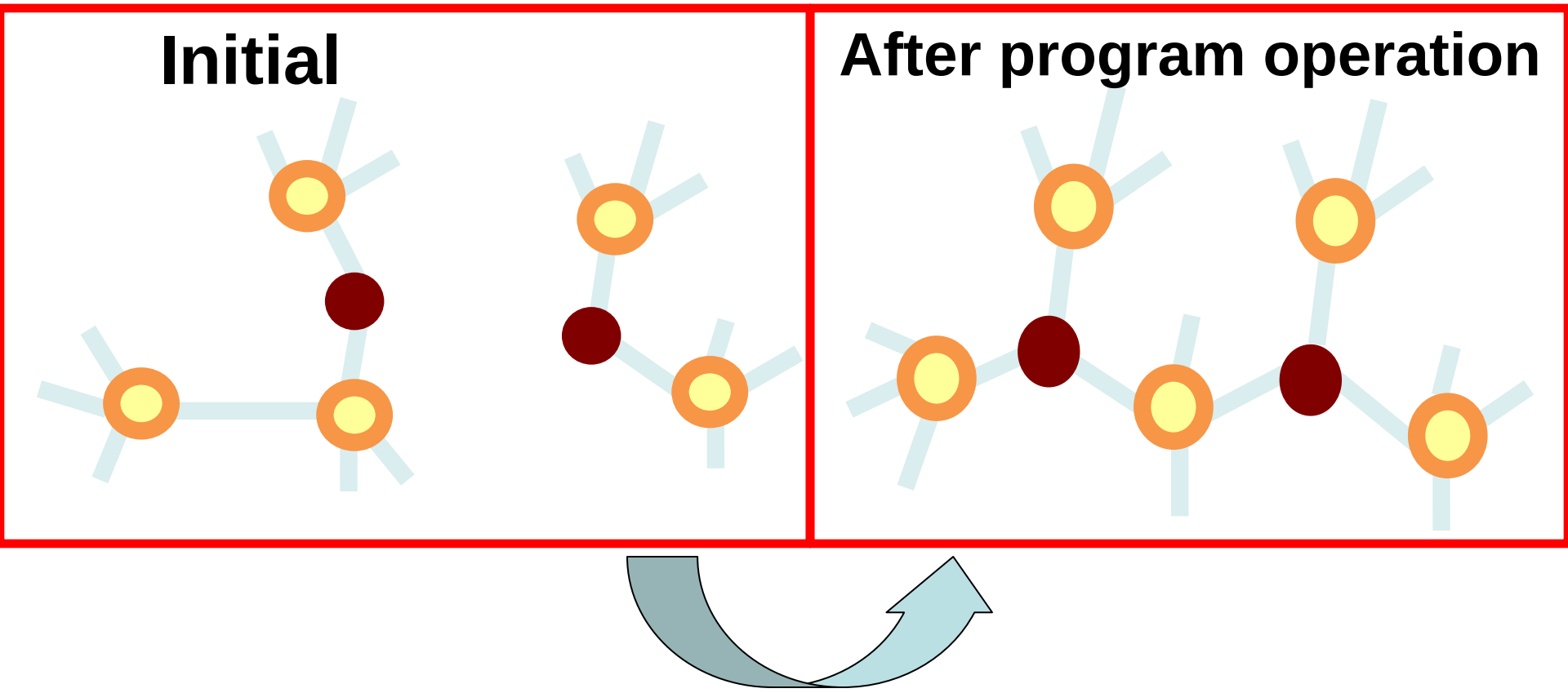


Step 3



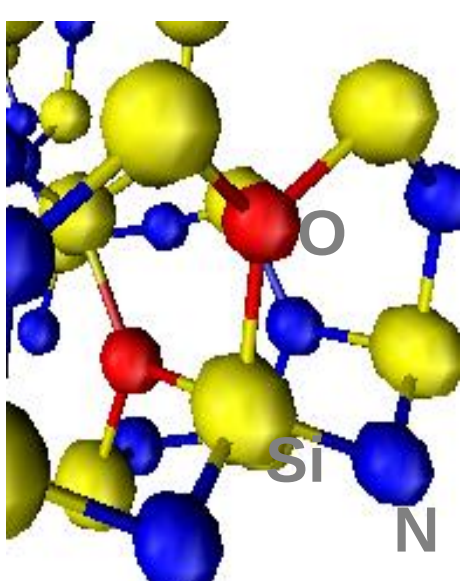
Step 4

Schematic view of structural change by program operation



Drastic structural change

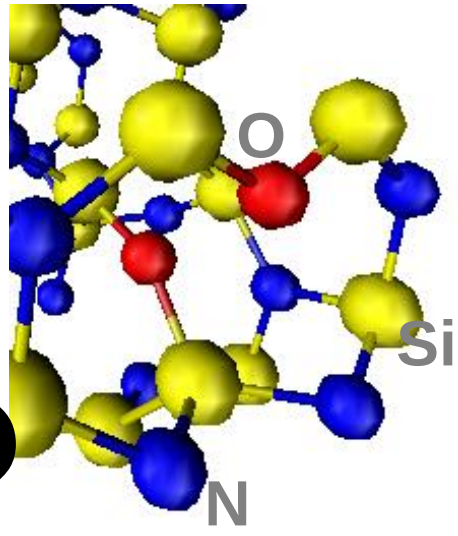
Is the structure recovered after erase operation?

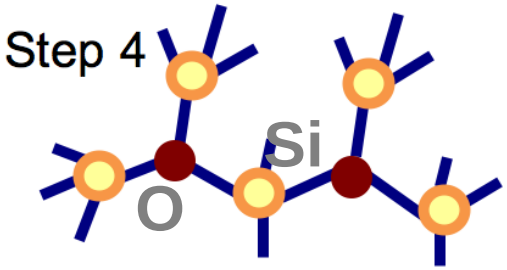


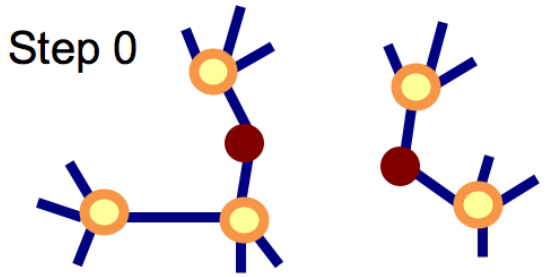
Hole

Erase

?



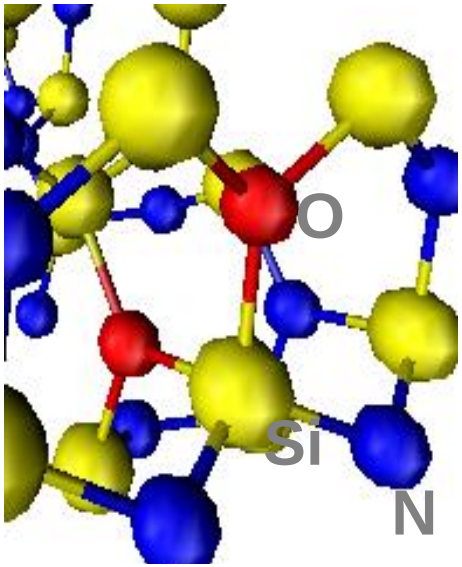




Initial

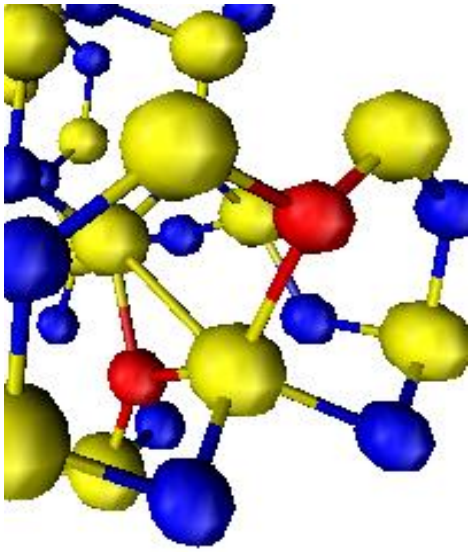
After erase operation

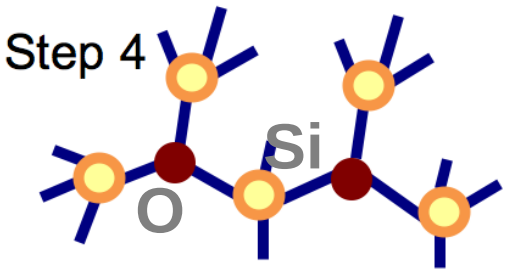
Erase operation (carrier removal)

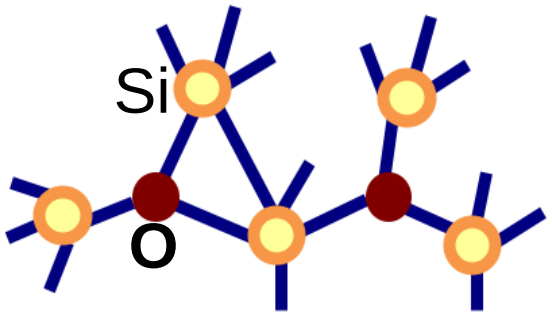


Hole

Erase



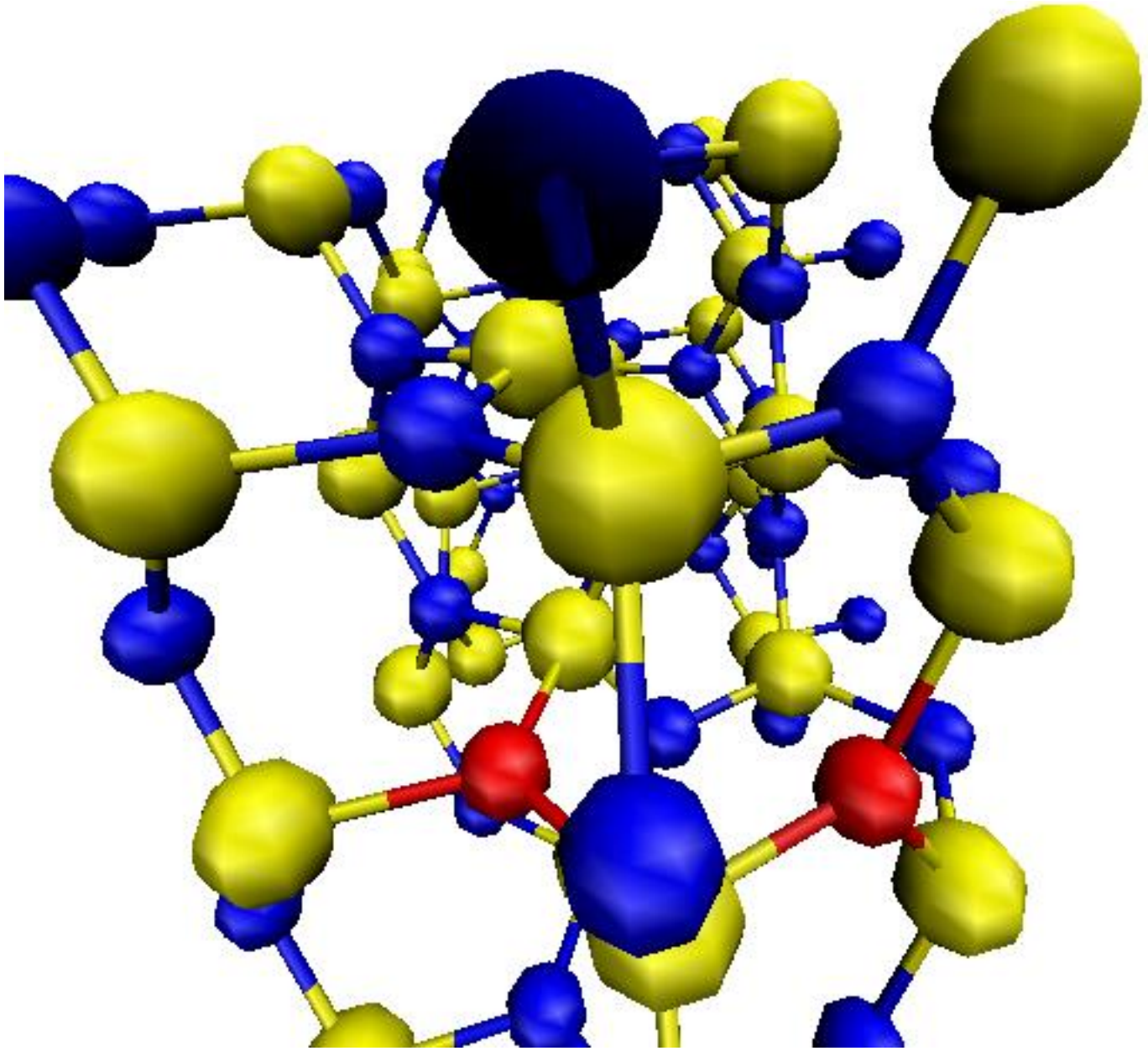


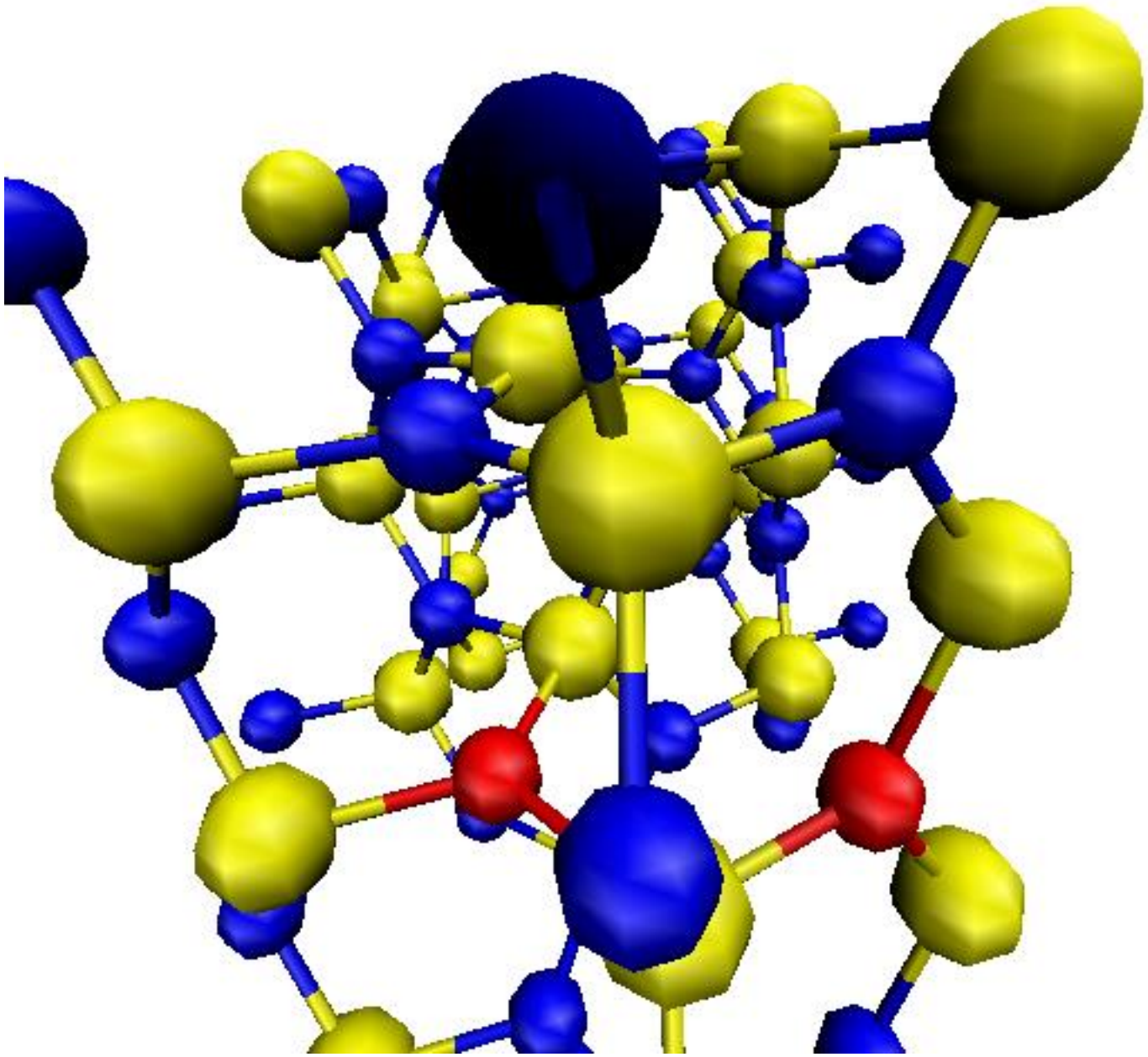


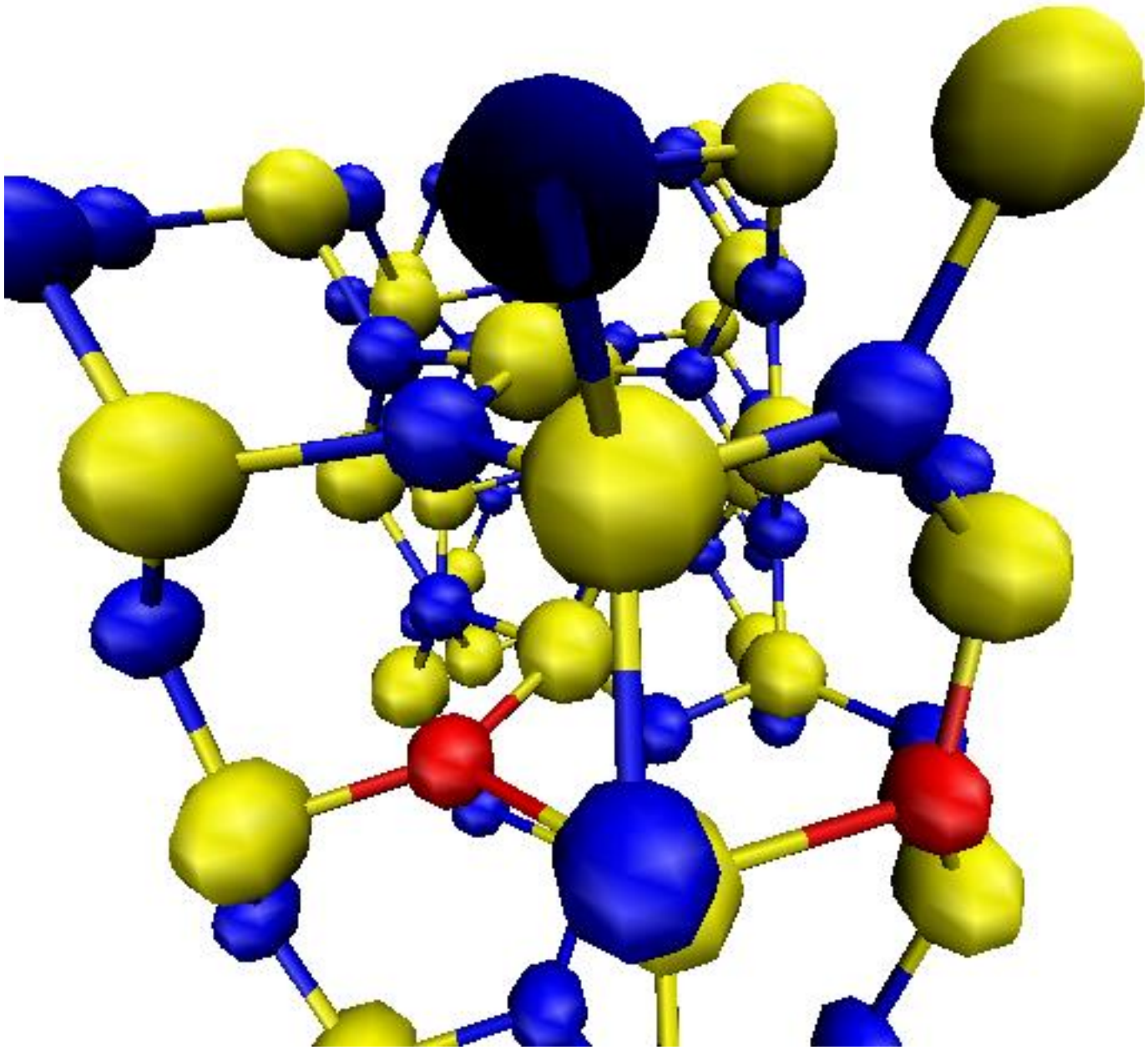
Before erase **After erase**

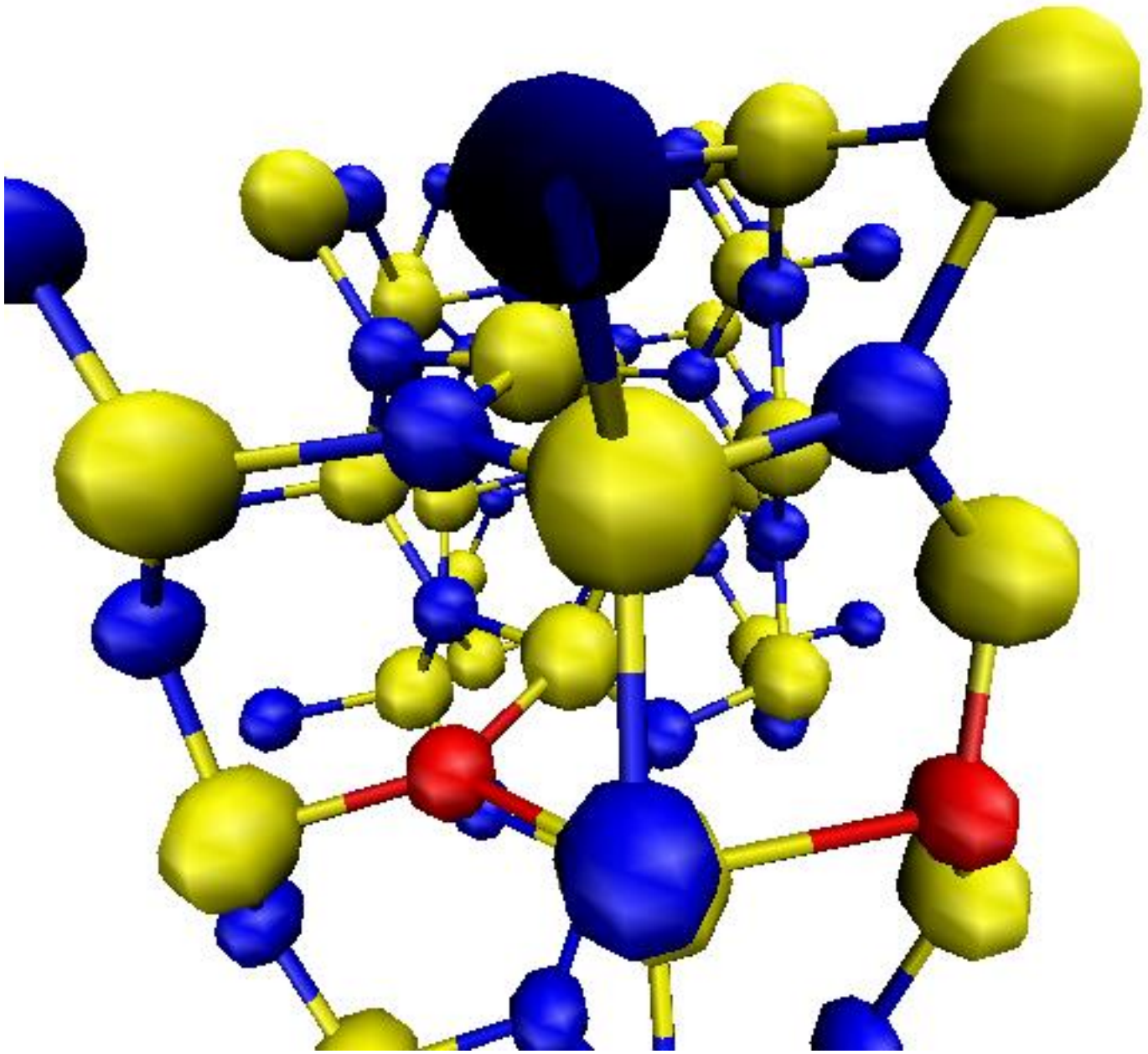
Very little structural change.

Structural change by erase operation

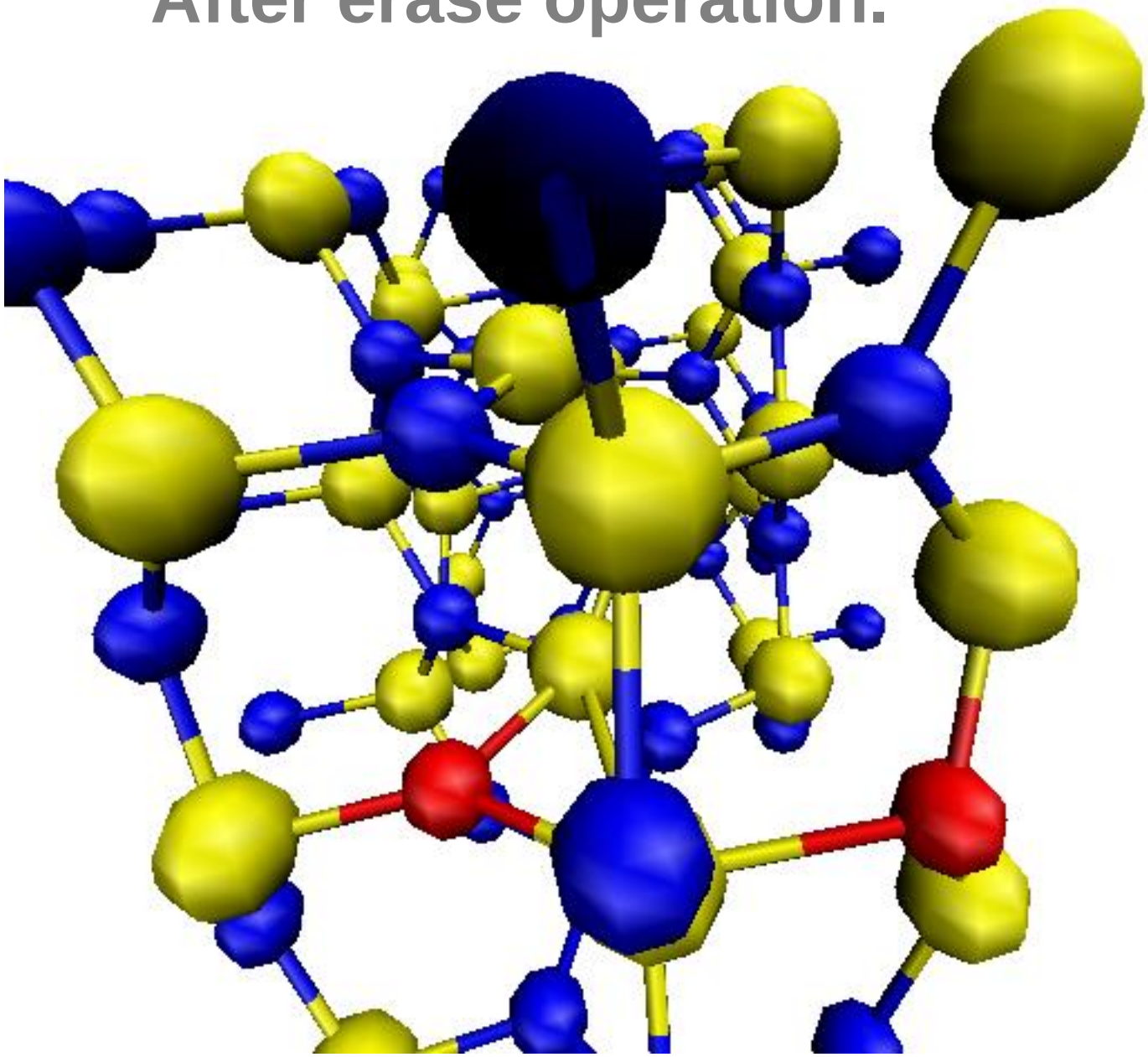




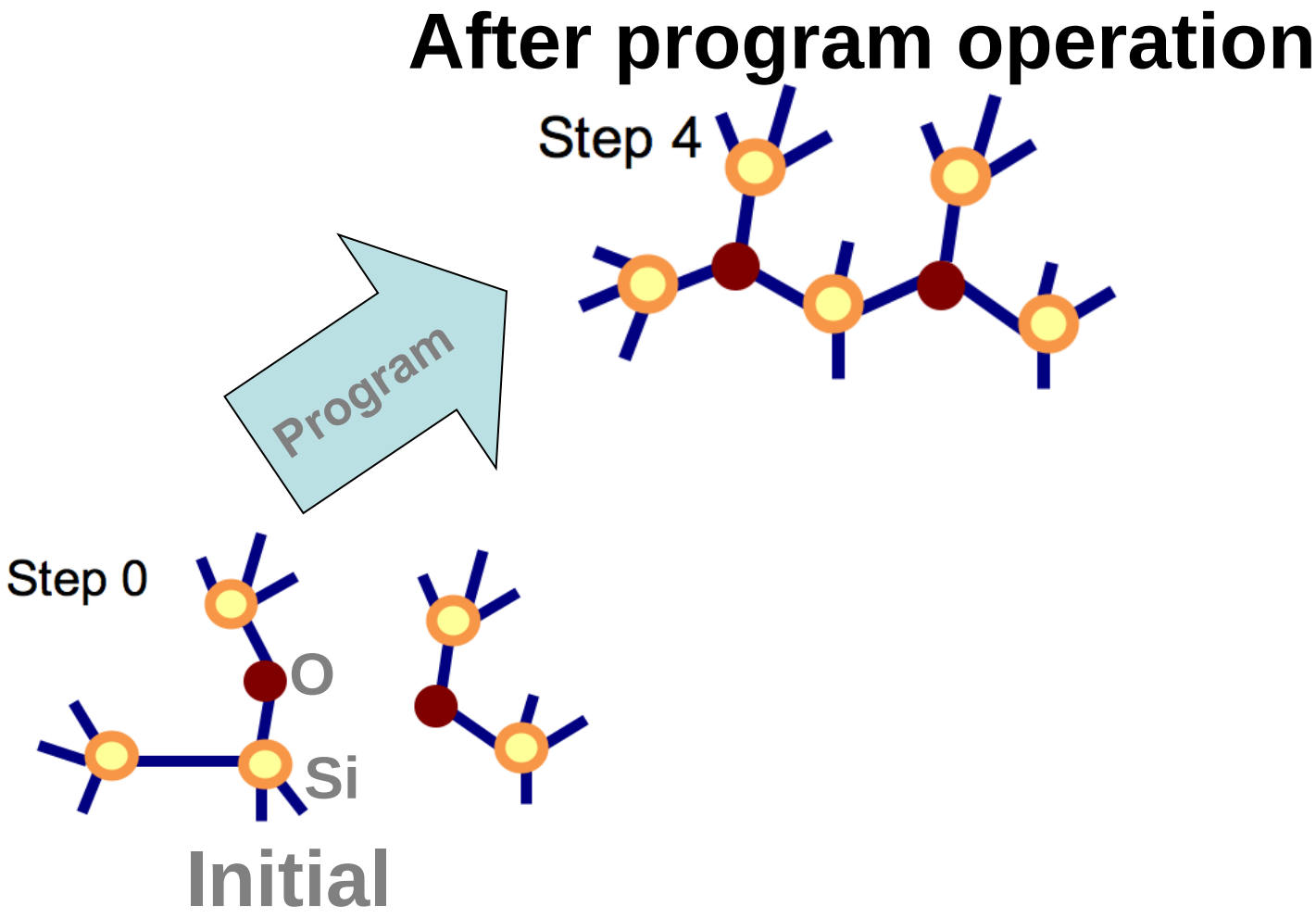




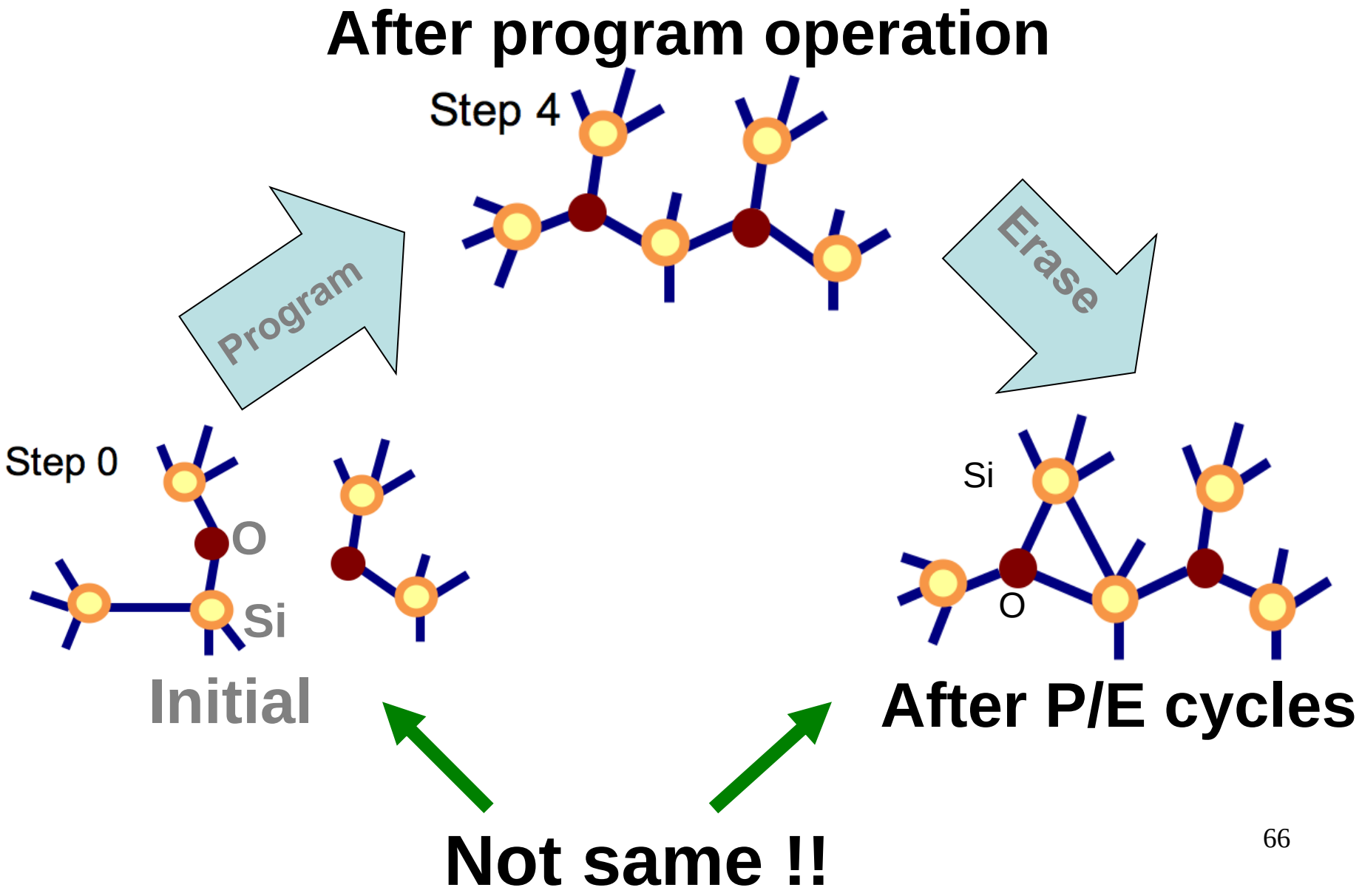
After erase operation.



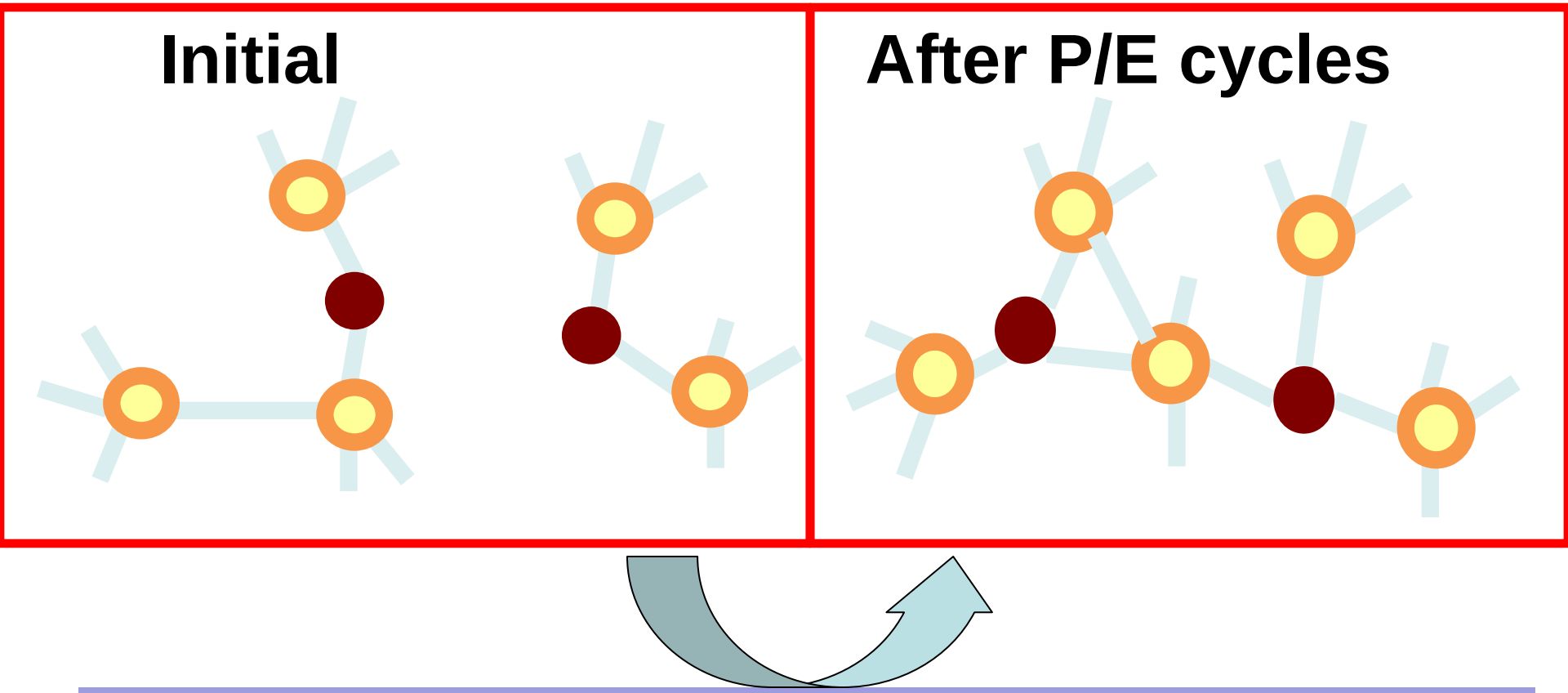
Structural change during program



Structural change during program/erase cycles

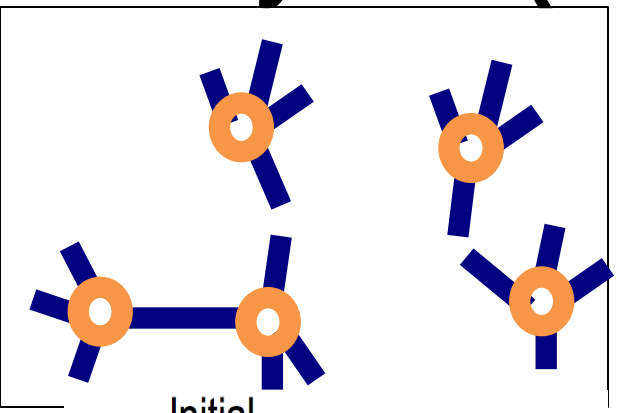


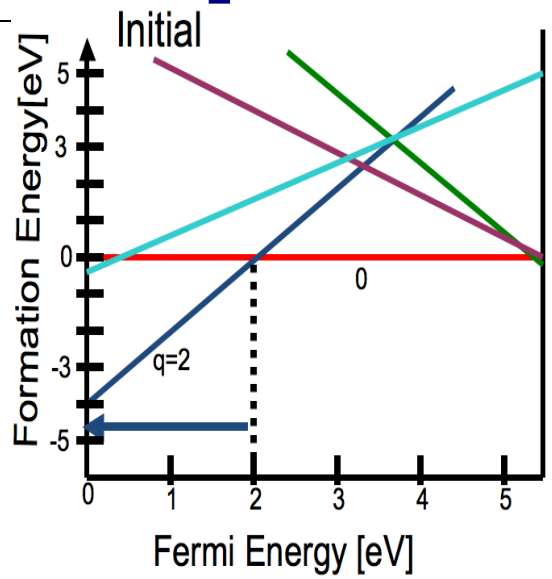
Summary of structural change during P/E cycles.



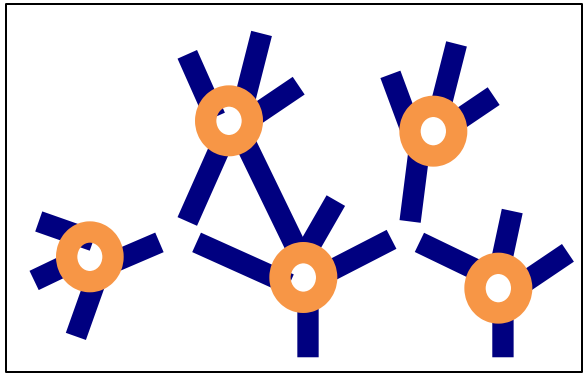
Drastic irreversible structural change
During P/E cycles.

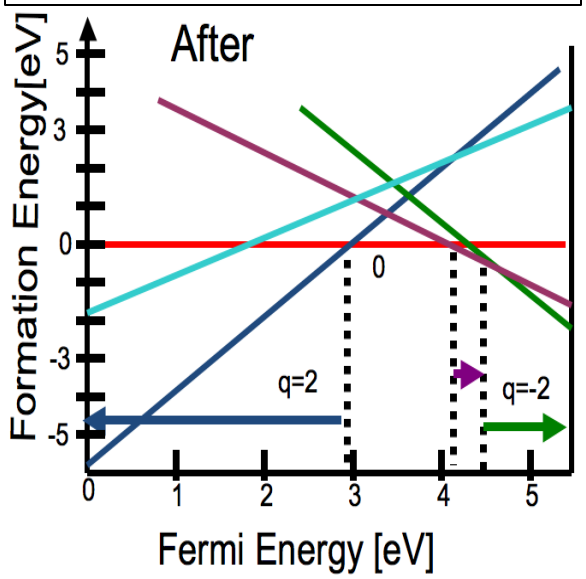
Irreversible structural change leads to degradation of memory functions during P/E cycles (Vt shift et. al.).





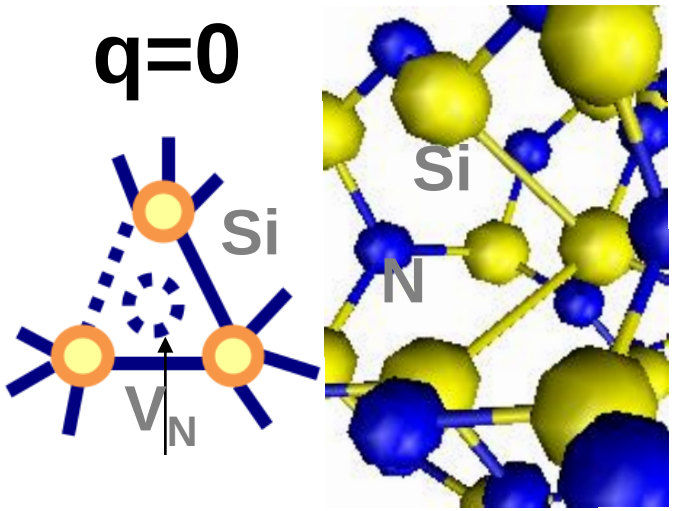
P/E cycles

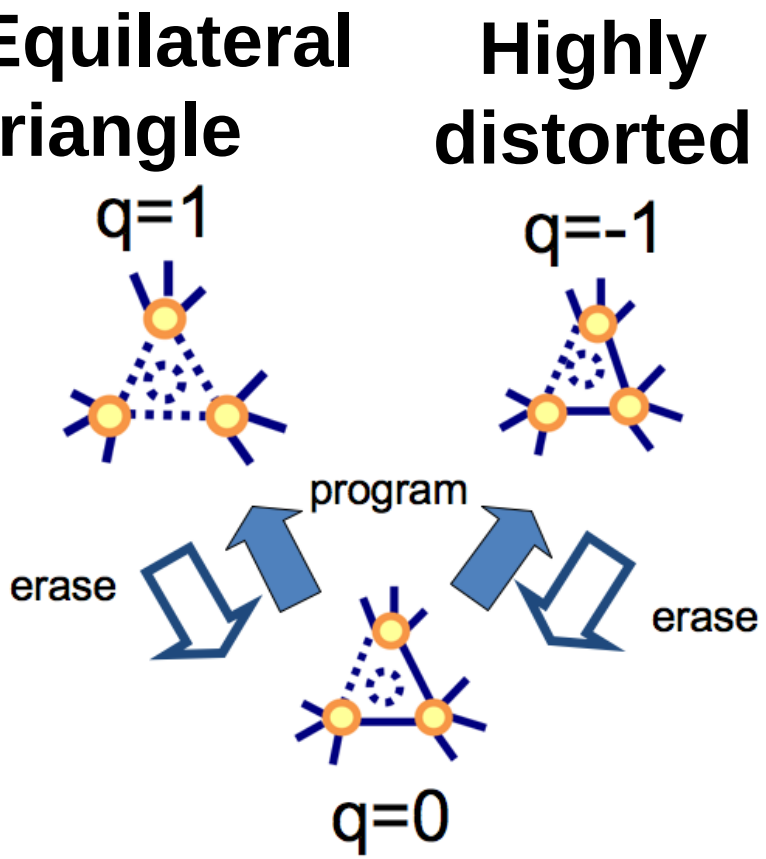




Memory characteristic changes drastically

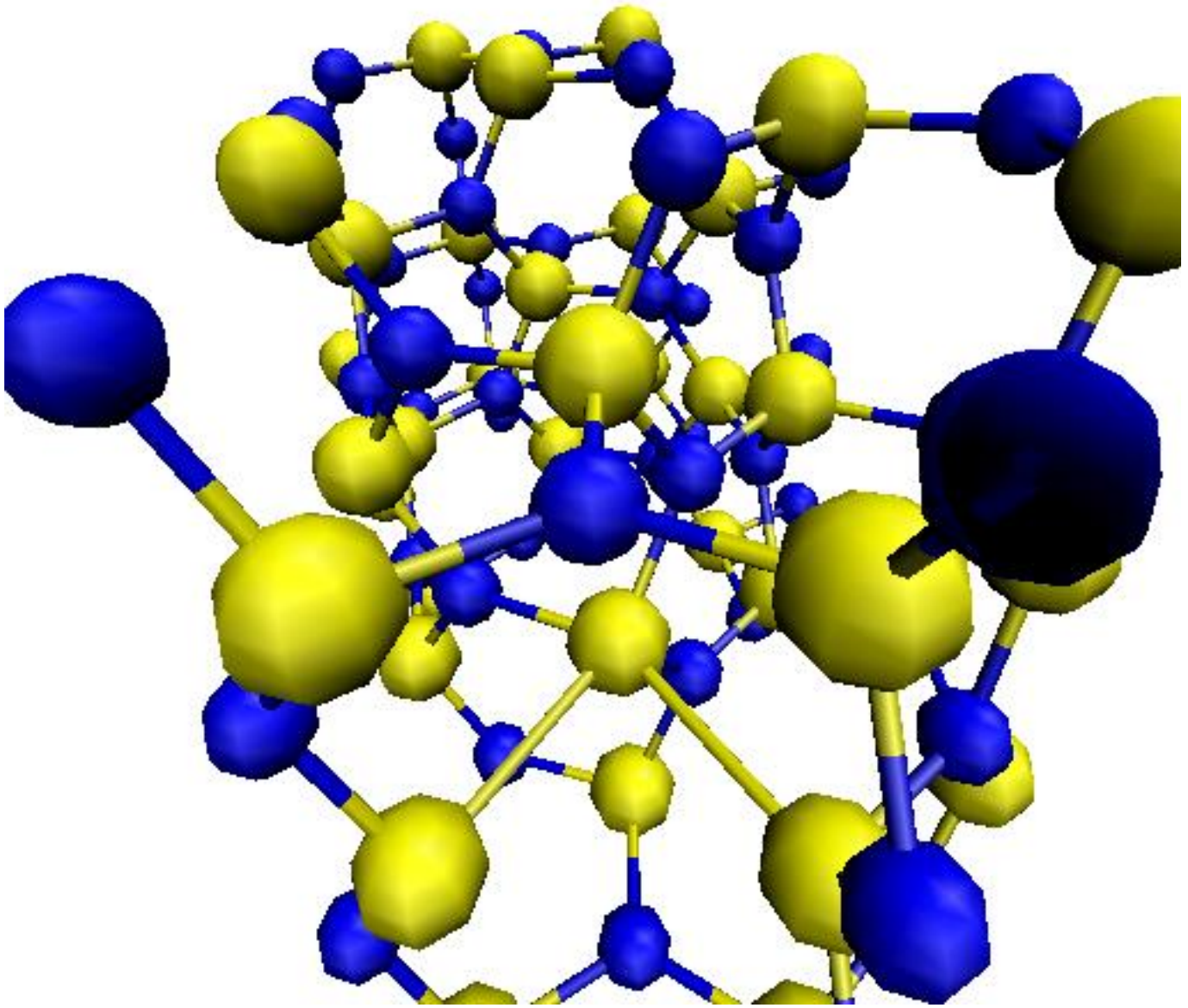
3.2 N vacancy



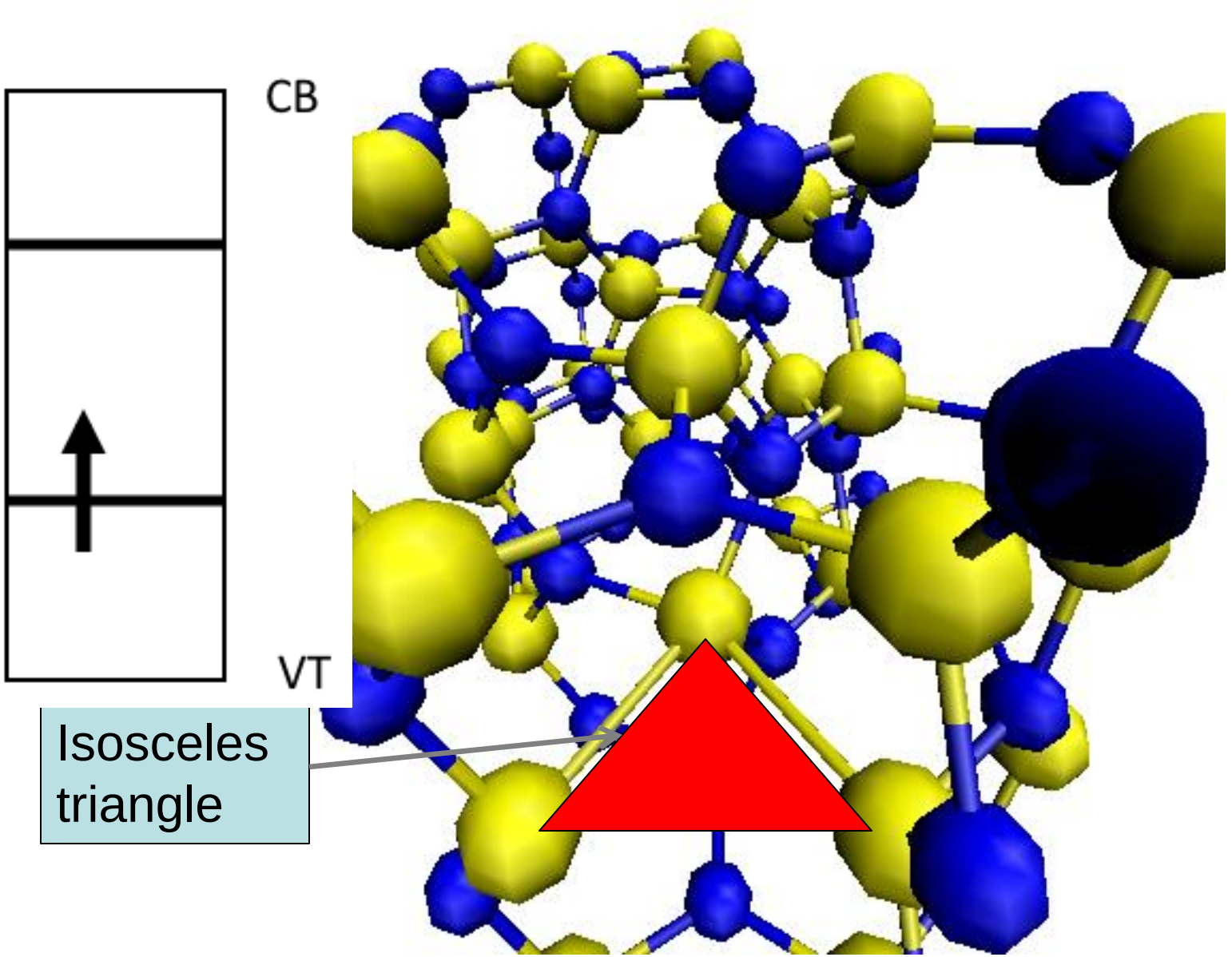


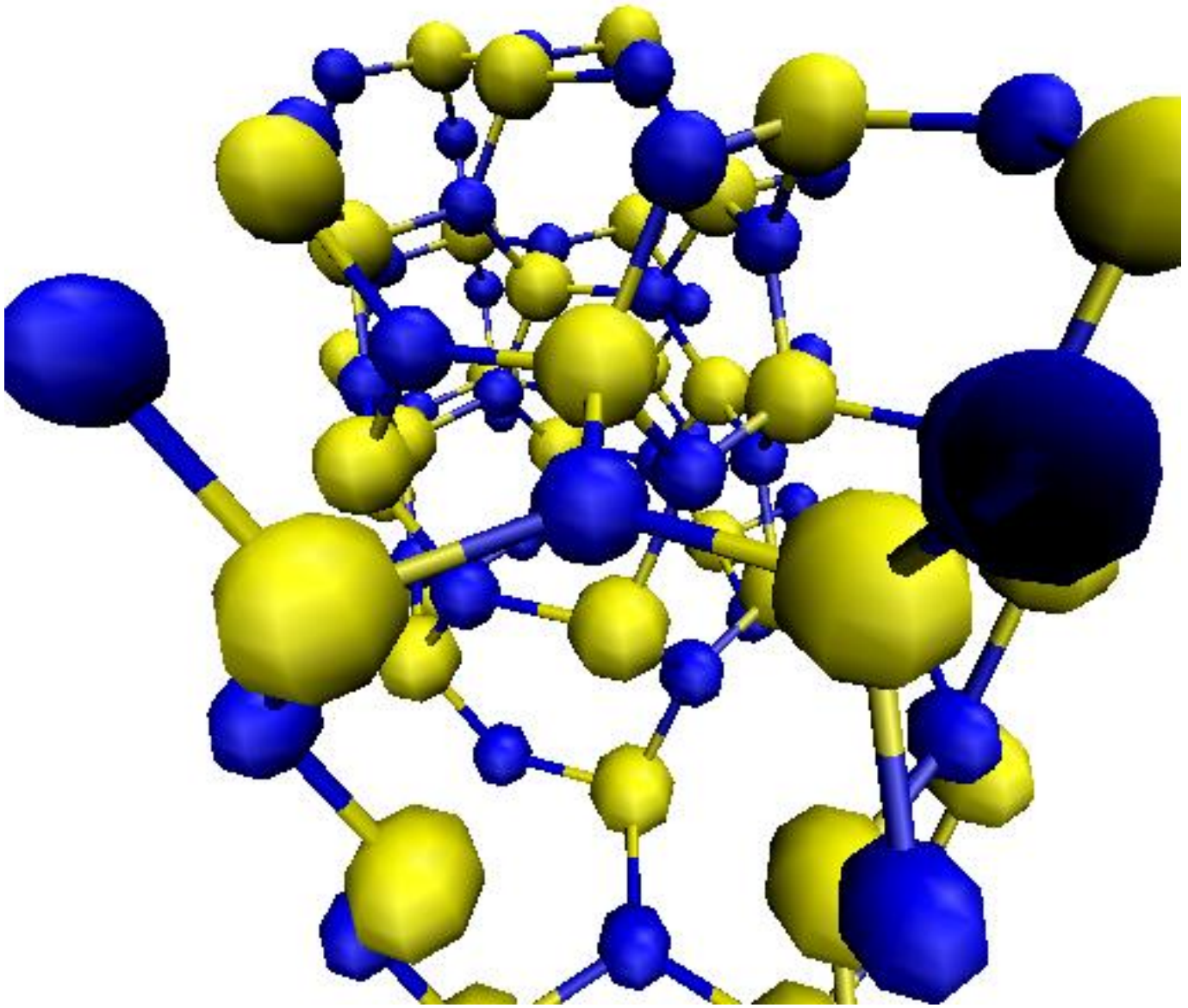
The atomistic structural change during P/E cycles is reversible.

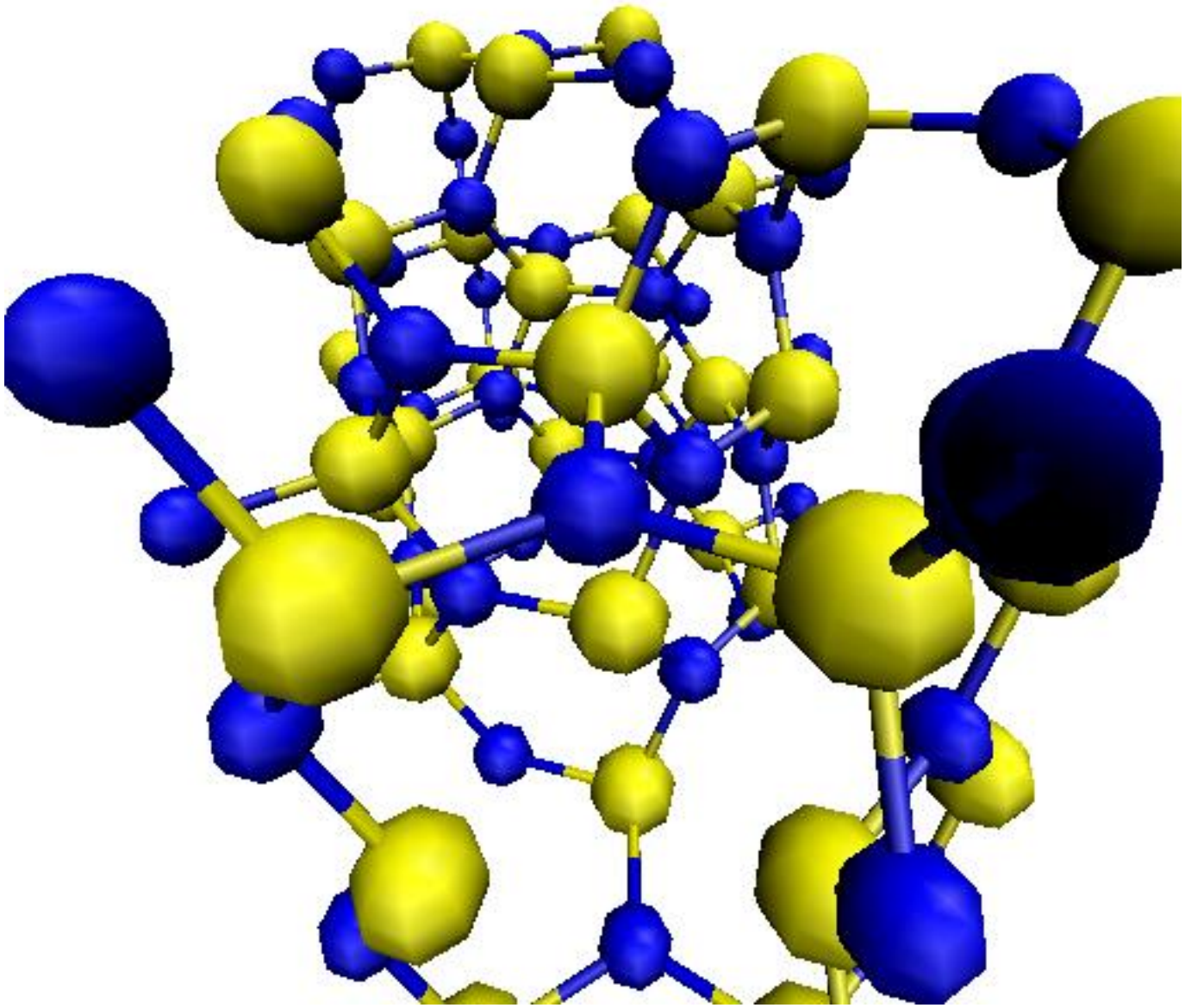
Jahn-Teller Effect



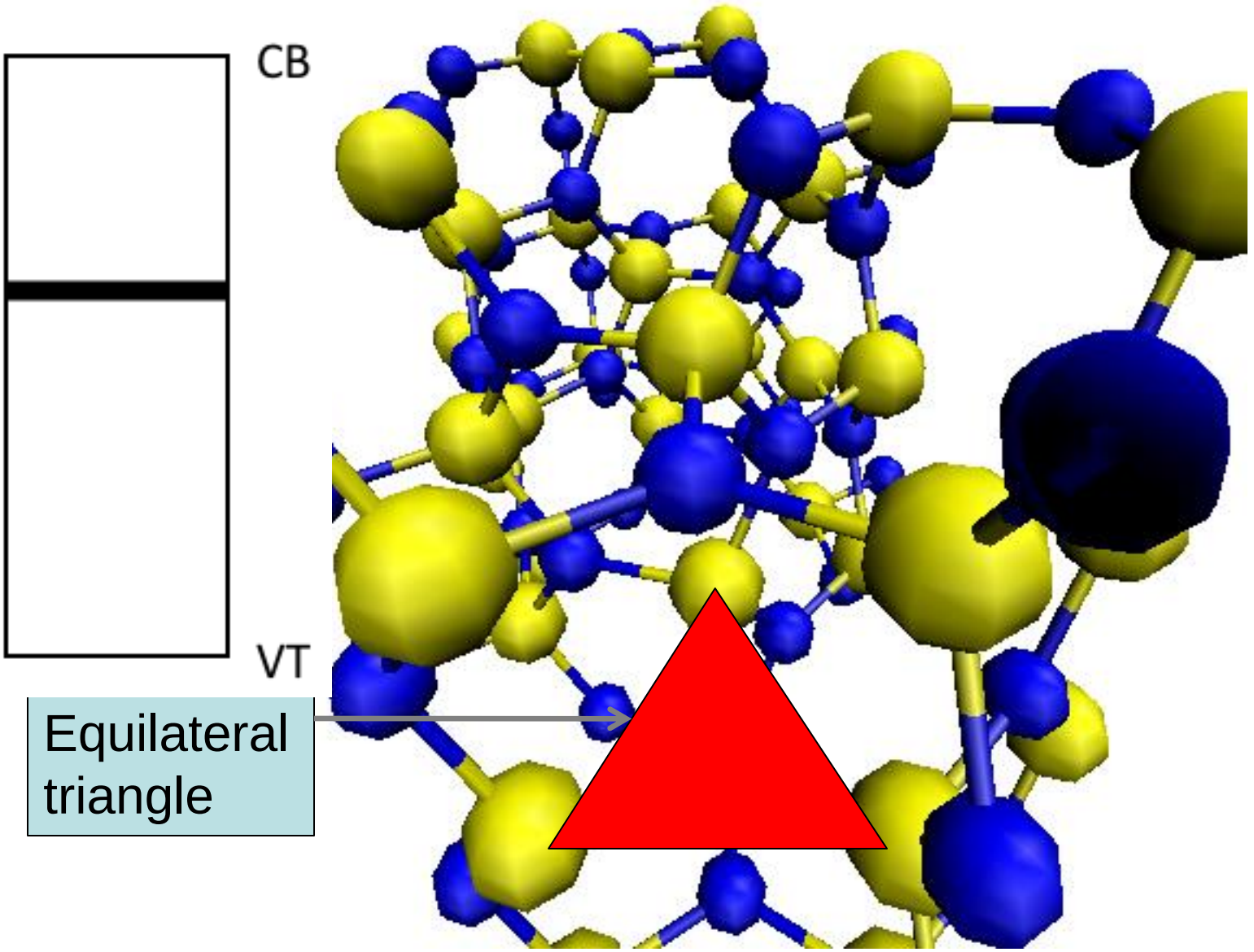
Initial



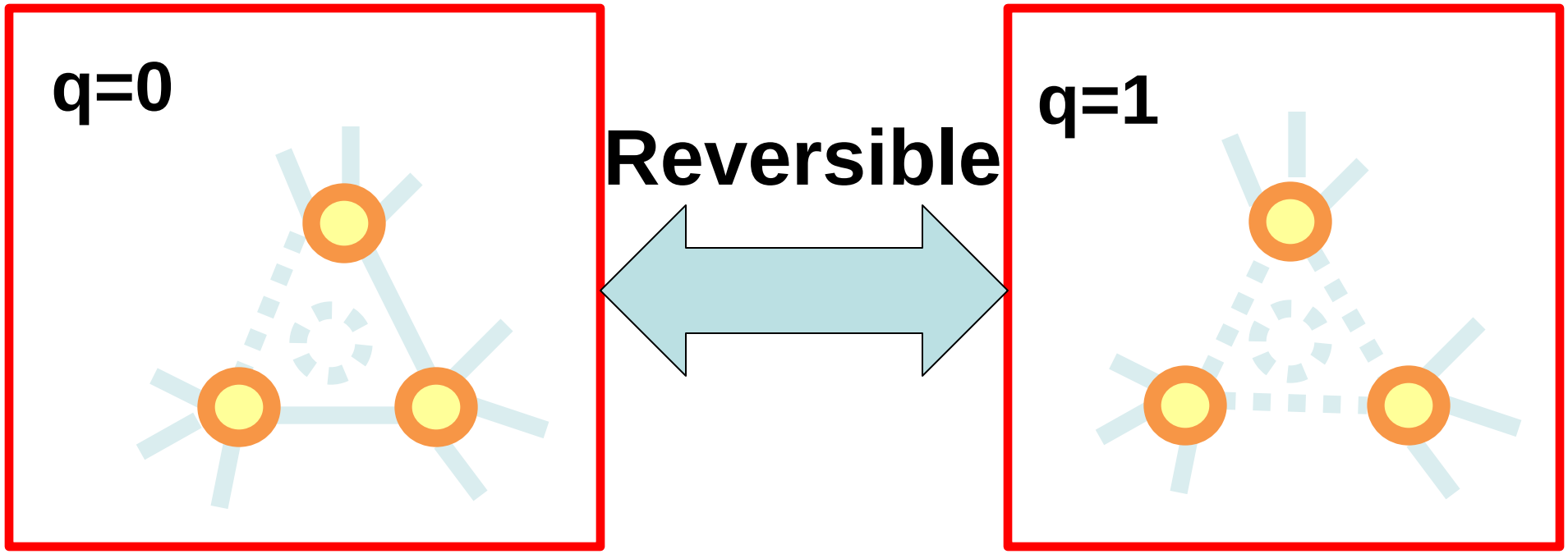




After hole injection

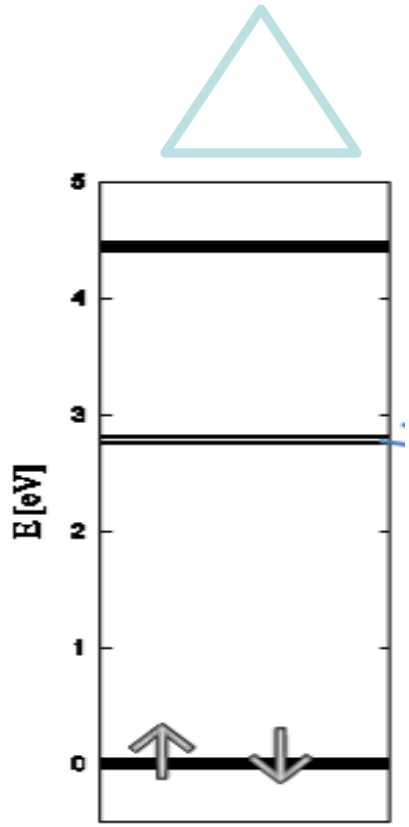


Structural change during P/E cycles



Without rearrangement of the covalent bond networks

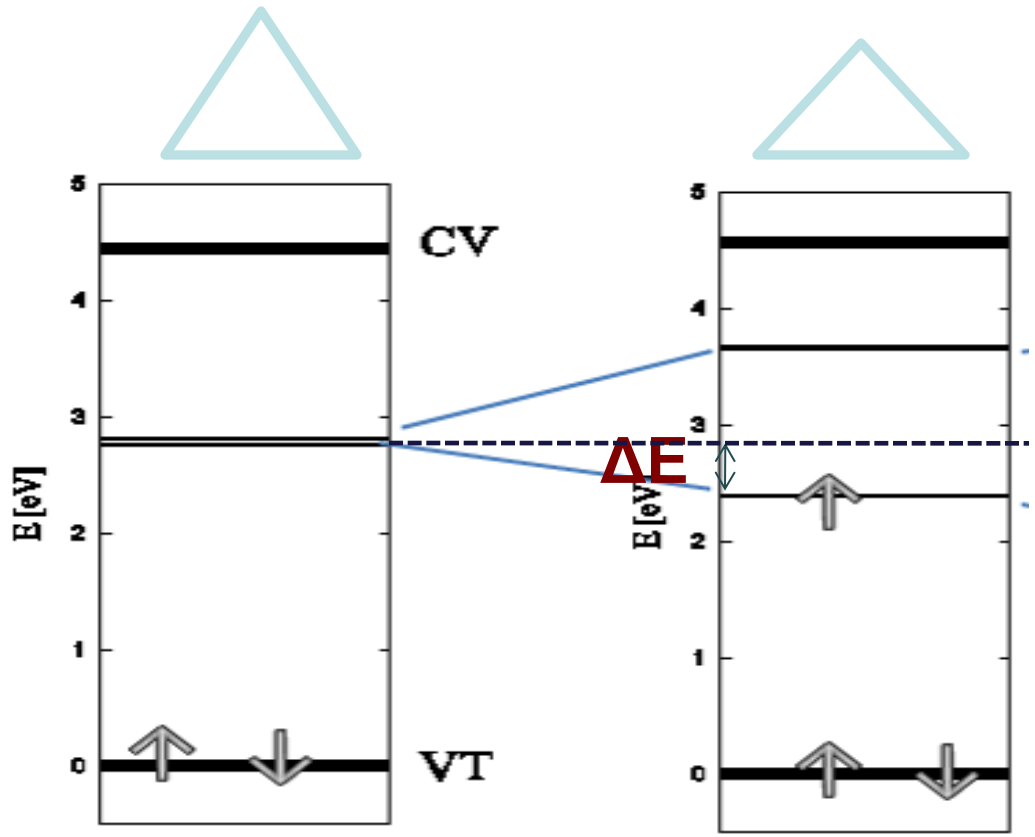
Jahn-Teller Effect



Positive charged state

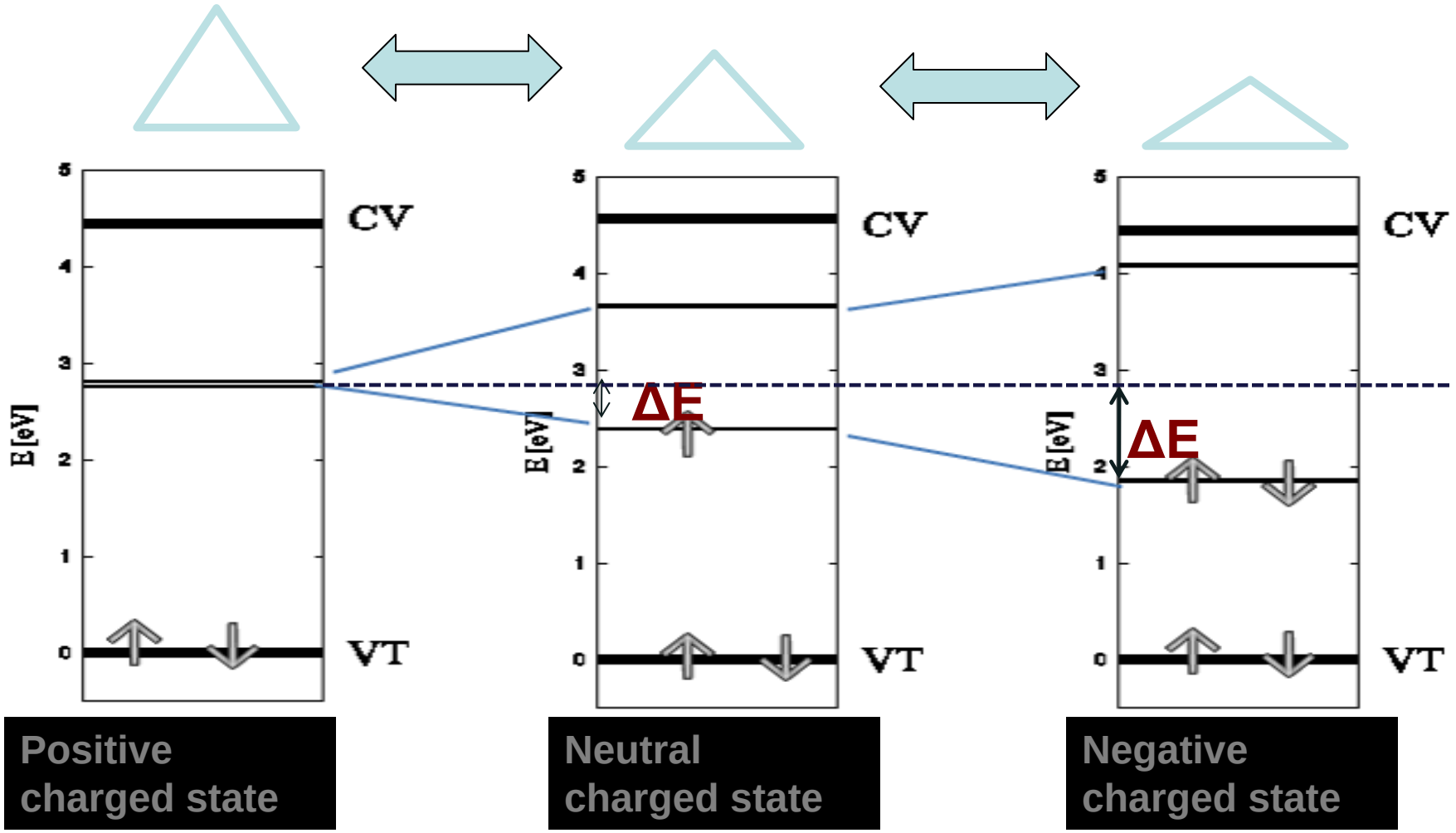
Spontaneous symmetry breaking structural change stabilize the electron energy by splitting degenerate levels.

Jahn-Teller Effect



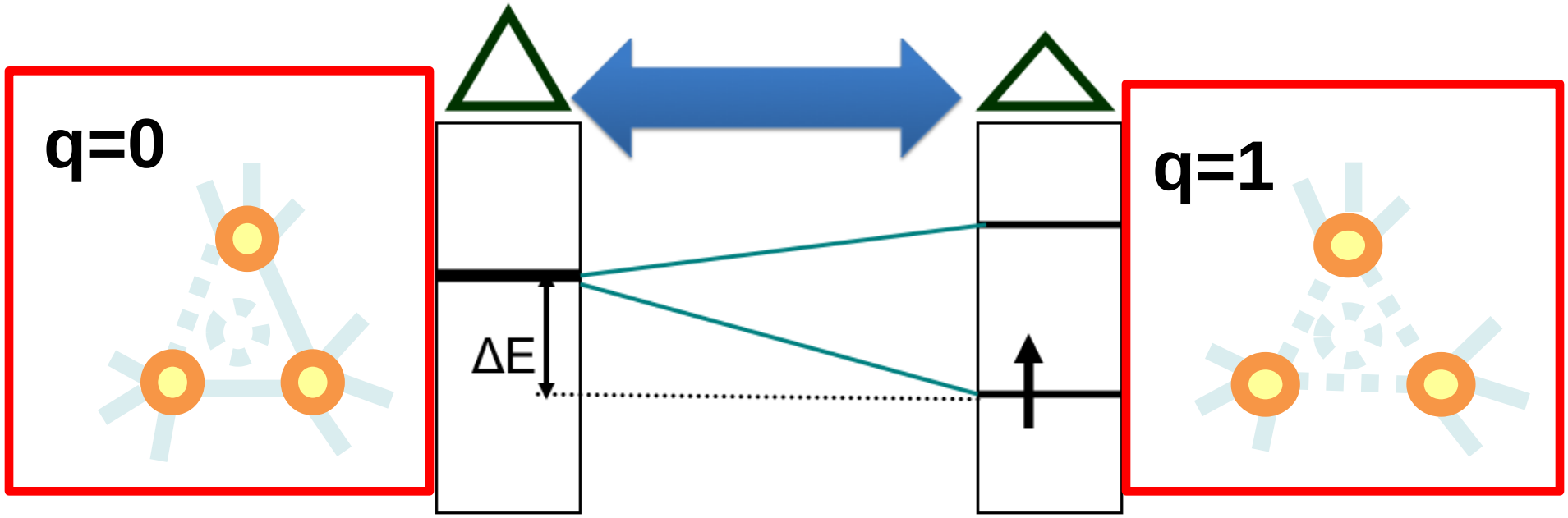
Spontaneous symmetry breaking structural change stabilize the electron energy by splitting degenerate levels.

Jahn-Teller Effect



Spontaneous symmetry breaking structural change stabilize the electron energy by splitting degenerate levels.

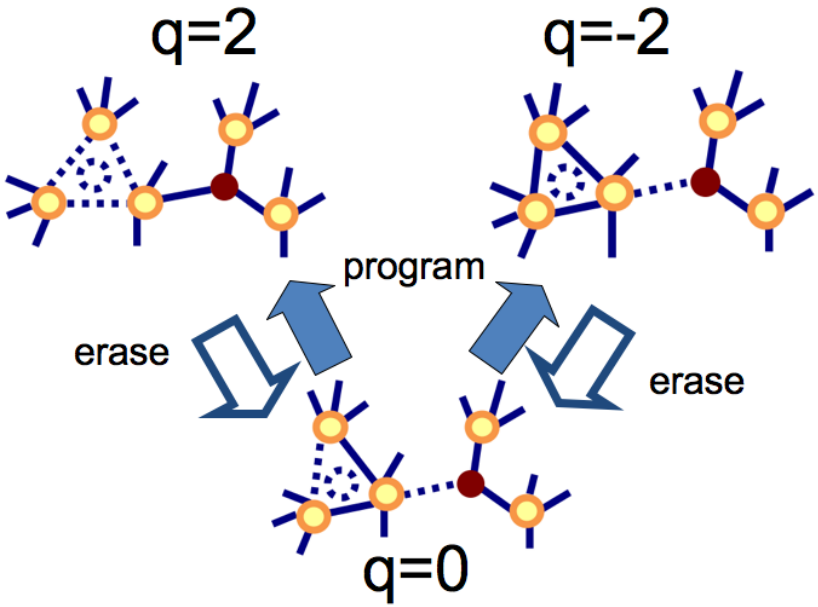
Defects with Jhan-Teller effect has reversible structural change during P/E cycles



High P/E cycle endurance

N vacancy is ideal charge trap for MONOS memory (Jahn-Teller governs structural change)

3.3 N vacancy with O atom



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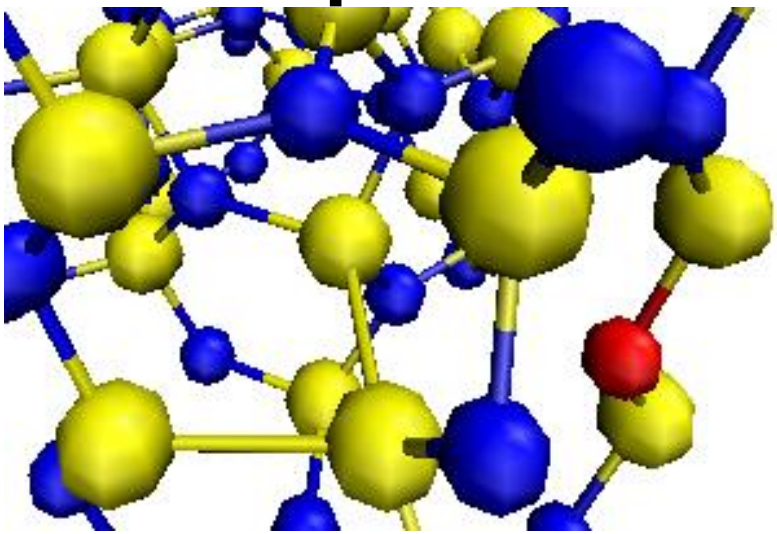


The atomistic structural change during P/E cycles is reversible.

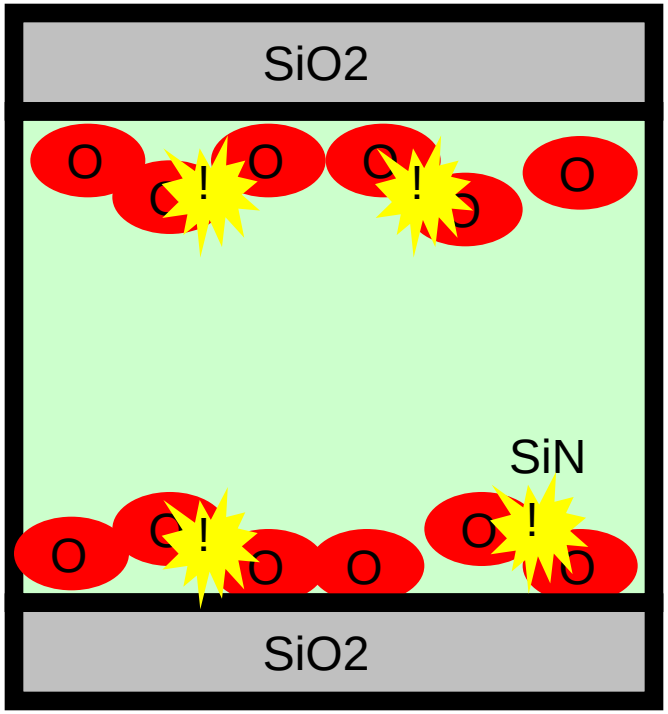
Summary of calculation result

- Excess O leads to memory degradation

- Jahn-Teller type defects suffers no degradation due to its spontaneous symmetry breaking property

  (It can be a common guiding principle for all types of charge trap memories)

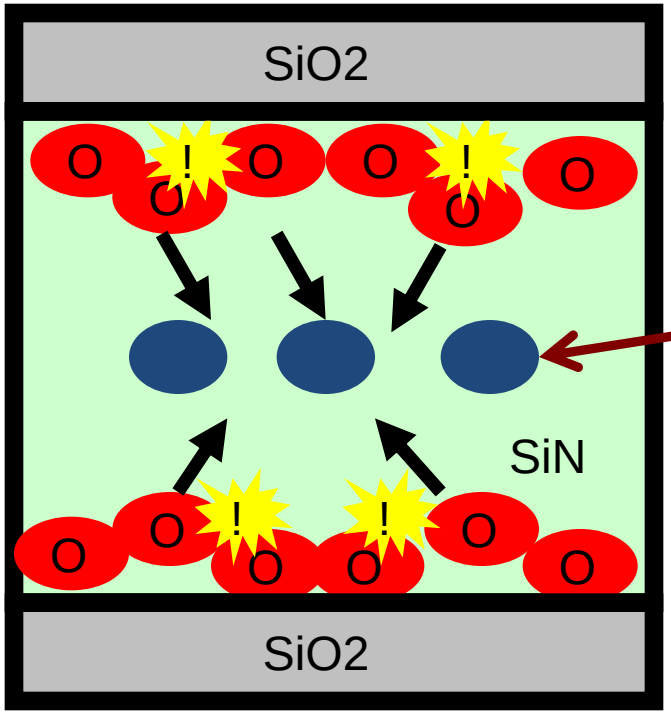
3.4 Recipe for High Quality MONOS Memories



Excess O atoms form defects with irreversible structural change.

Reducing the excess O atoms should be effective for high P/E cycle endurance.

Recipe for High Quality MONOS Memories

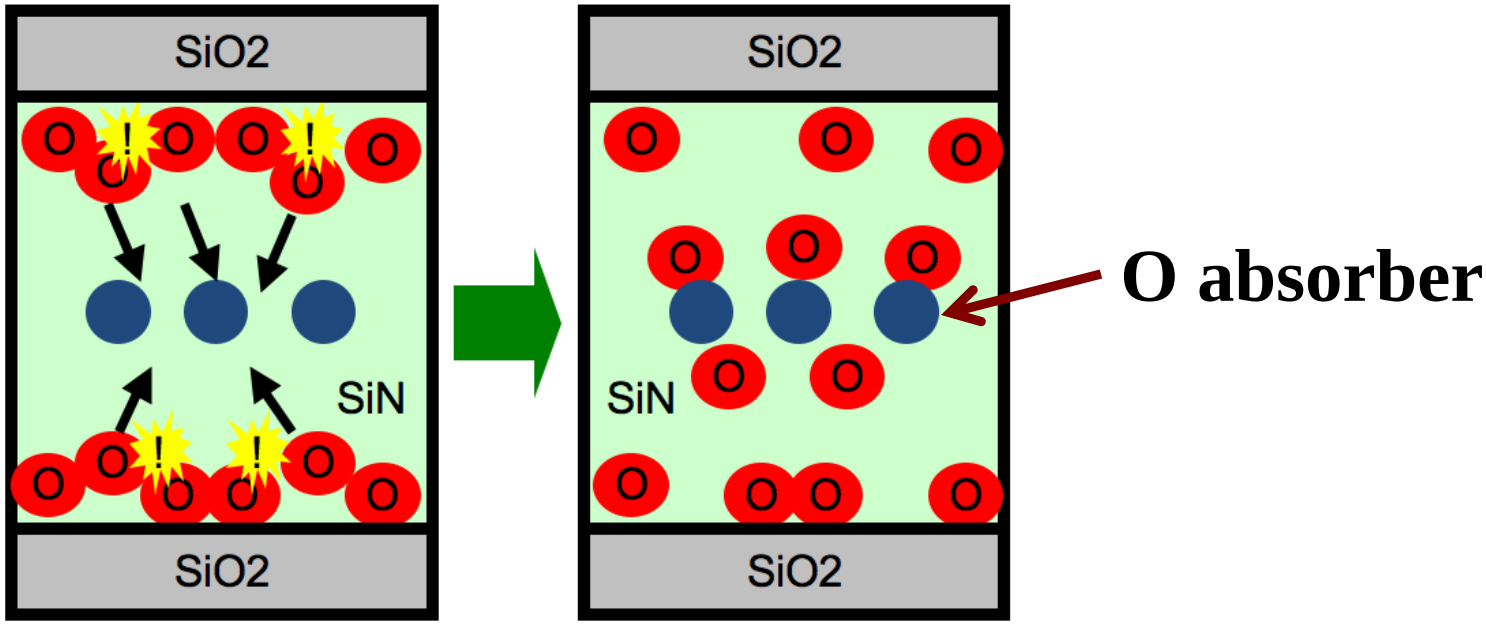


O absorber

Excess O atoms form defects with irreversible structural change.

Reducing the excess O atoms should be effective for high P/E cycle endurance.

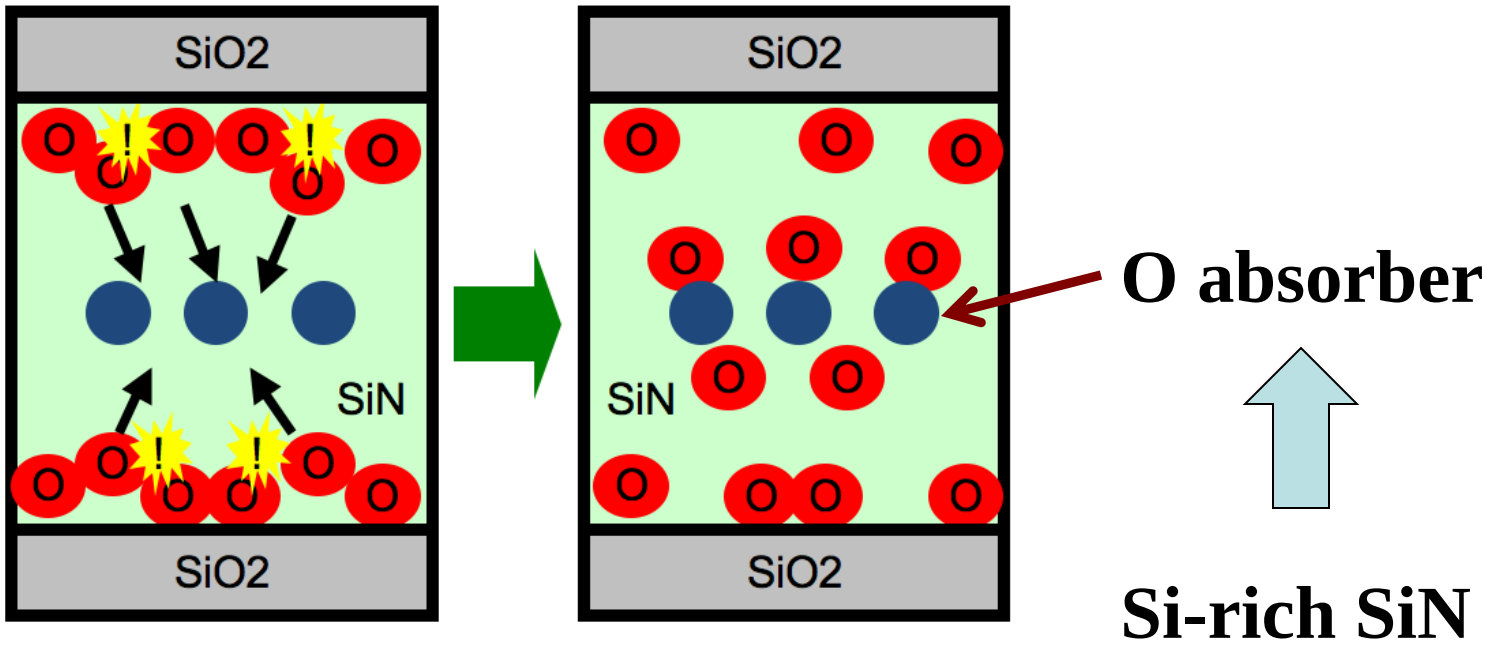
Recipe for High Quality MONOS Memories



Absorbing excess O atoms from SiN/SiO_2 interfaces and efficiently reduce the irreversible defects.

High P/E cycle endurance

Recipe for High Quality MONOS Memories

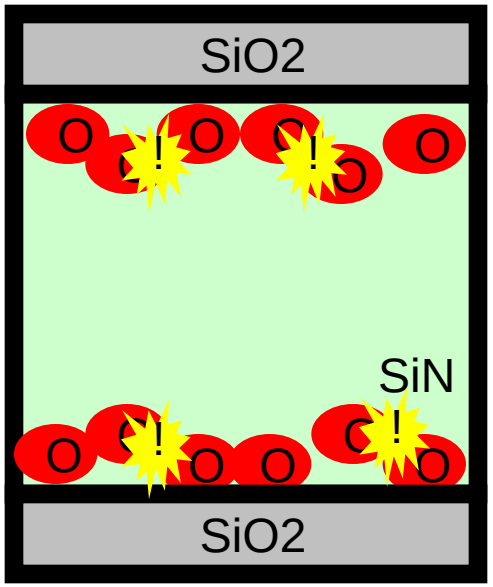


T. Mine et al., Extend. Abst. 2006 IWDTF, p.19 (2006)

Absorbing excess O atoms from SiN/SiO_2 interfaces and efficiently reduce the irreversible defects.

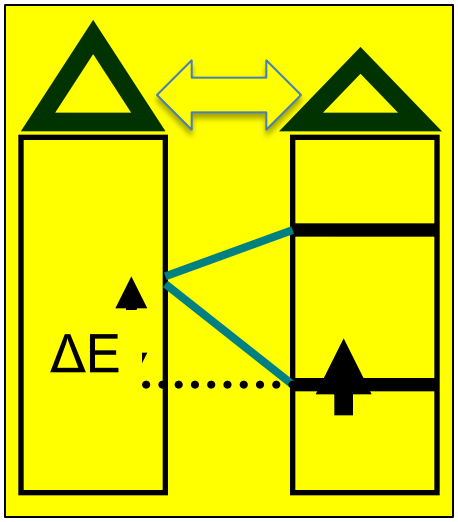
High P/E cycle endurance

Conclusion



- We have clarify the detailed atomistic behavior of defects of MONOS memory by the *ab initio* calculation.
- The excess O atoms cause an irreversible structural change in the SiN layer.

→The suppression of excess O atoms is effective to improve the MONOS characteristic.



- Defects with Jahn-Teller effect are the most suitable for charge-trap memories.

This first principles knowledge
becomes key knowledge for developing automobile memories by using MONOS structures!
→ Mass production is realized by Renesass Electronics!!

Now many automobiles such as Prius uses MONOS memories!!

First principles calculations really contributed to industry!!
(Market size is huge, since it contributed to the whole car industry!!)

High-k Gate Dielectrics and so on

Mass production of modern LSI is realized by Intel (2008), Panasonic (2010) and IBM (2011) based on the knowledge of nano-interface physics of HfO_2 which we obtained by first principles calculations in 2004.(High-k dielectrics)

Moreover, we have performed design of new types of memories (Resistive random access memory and Phase change memory) as well as a collaborative research with astrophysics

Summary

- We have performed large scale first principles calculations
- We really succeeded the first principles based mass production of modern devices.

  High-k Metal gate: Modern LSIs

  MONOS Memories: Memory devices for automobiles (Toyota, GM, Nissan)

Collaboration

- International

  Stanford University, Prof. Y. Nishi

  CNRS(France), Prof. M. Boero

  POSTECH(Korea), Prof. Hwaung

Budget(FY2008-FY2013)

- KAKENHI: Si nano electronics (2008-2010)
- JST-CREST: Ohmori (2009-2013)
- NEDO: Si nanowire (2008-2012)
- NEDO: Collaboration with LEAP (2012-2014)
- JST-CREST: Oshiyama (2008-2010)