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International Union of Materials Research Societies–
International Conference on Electronic Materials
04 to 08 July 2016, Suntec Singapore

Symposium N; Materials by Theoretical/Computational Design
Session; Alloys and Nano Materials
15:15, 6 Jul 2016 (W)
Room 323

Oxygen Adsorption Behavior on InAs surfaces by Ab-Initio Calculations

In Won Yeu[1,2], Cheol Seong Hwang[2], and Jung-Hae Choi[1]

[1]Center for electronic Materials Research, Korea Institute of Science and Technology (KIST)

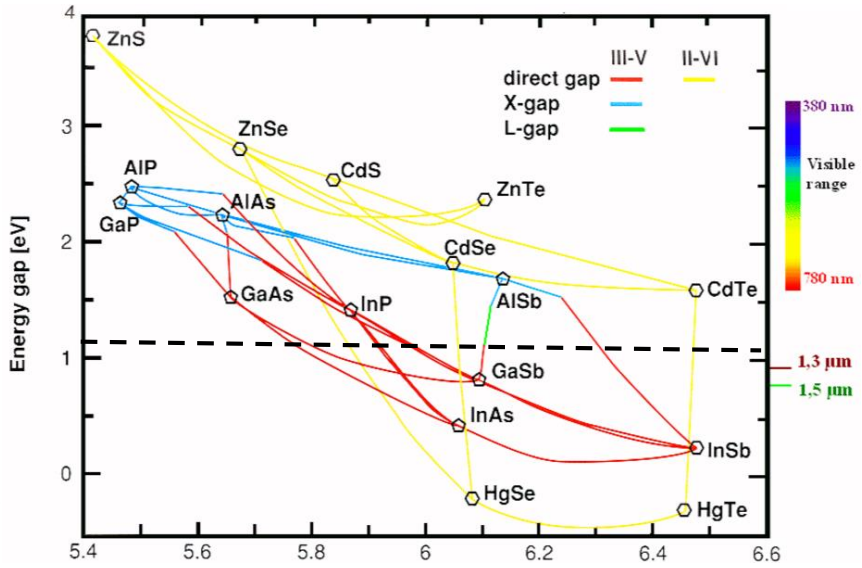
[2]Department of Materials Science and Engineering, Seoul National University

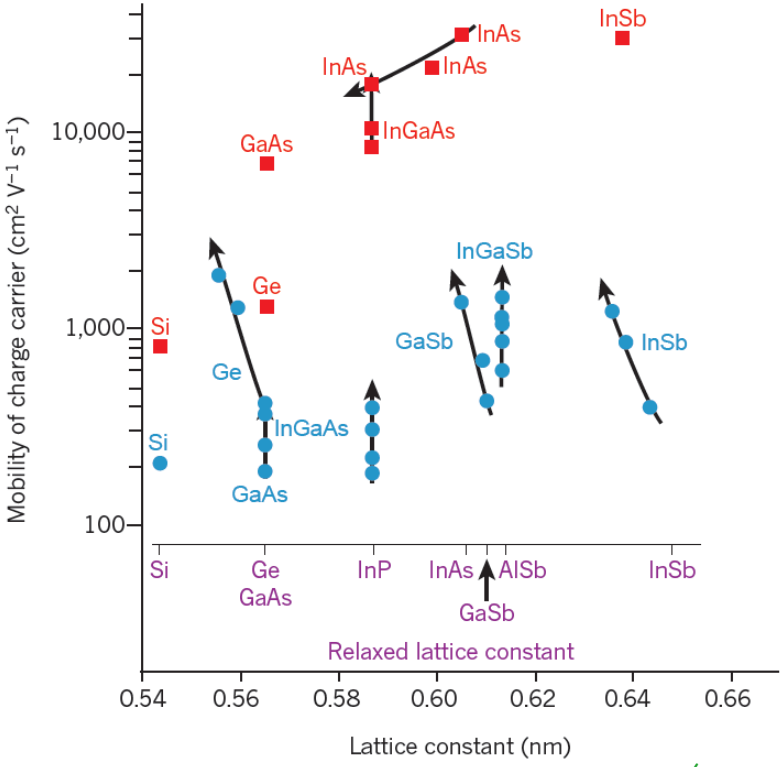
Seoul, Korea

III–V compound semiconductors

High Electron & Hole mobilities

- High speed of charge (electron/hole)
  > 10 times w.r.t Si
- Smaller band gap
  Low voltage operation [3-5 CMOS] (1/10)
- Direct band gap
  Electron + photon [Si-Photonics]
  → low power to send a signal (< 1/10)





Nature, 479, 317 (2011).

Material	Si	Ge	GaAs	InGaAs	InAs
Mobility (electrons) in $cm^2 V^{-1} s^{-1}$	1350	3600	8000	11 200	30 000
Mobility (holes) in $cm^2 V^{-1} s^{-1}$	480	1800	300	300	450

Appl. Phys. Lett. 96, 122105 (2010).

Interface between III–V and oxide

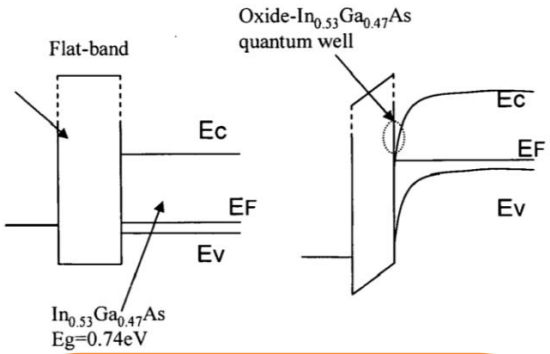
gate

gate oxide

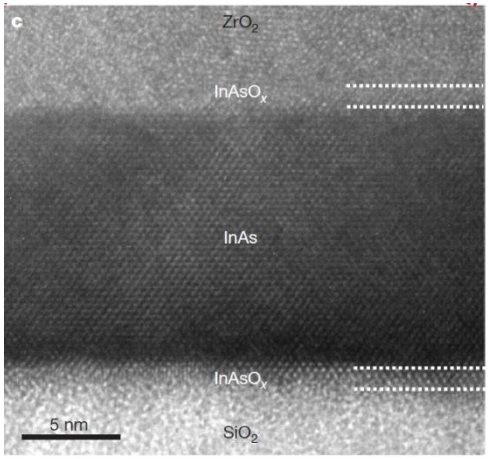
channel

Al_2O_3
Eg= 9eV

Fermi level pinning

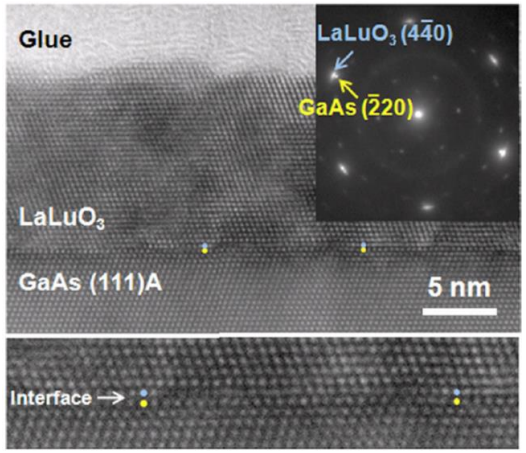


Surface treatment



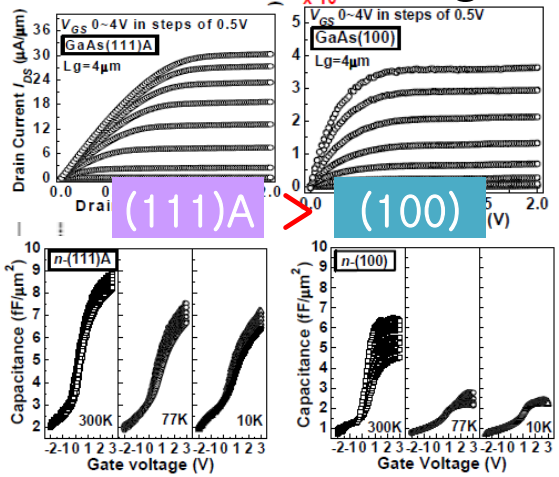
Nature 468, 286 (2010).

Crystalline oxide



Appl. Phys. Lett. 97, 162910 (2010).

Orientation change

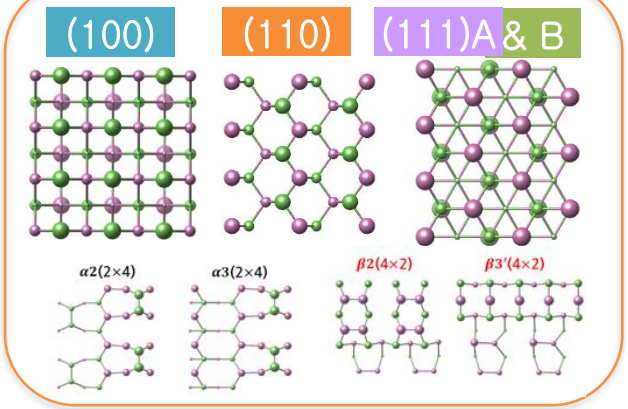


IEDM, 865. (2009).

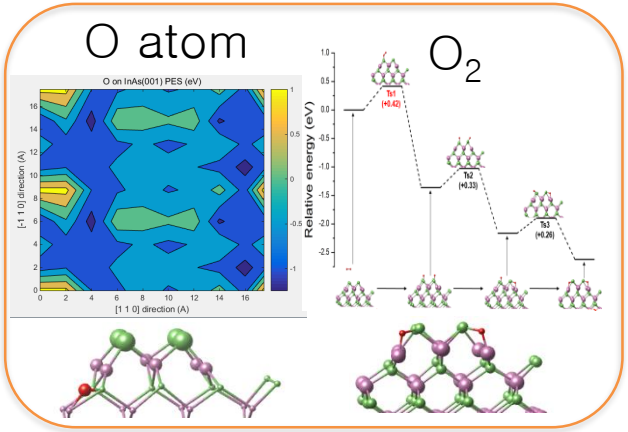
Effects of surface reconstruction & initial oxidation of InAs

Contents

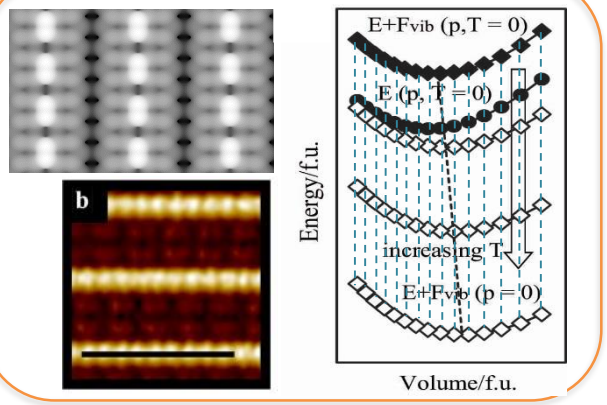
Surface



Oxygen adsorption



Non-0K surface



Xc-functional ; PBE

cutoff energy =500 eV

Spin-polarization

Nudged Elastic Band

Xc-functional ; LDA

cutoff energy =300 eV

DFPT;

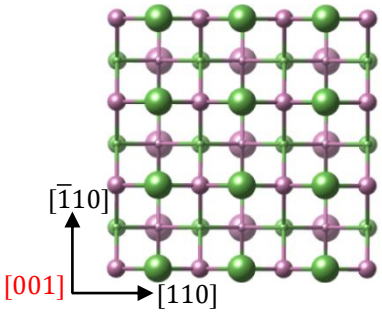
"PHONOPY"

All calculations are performed using VASP.

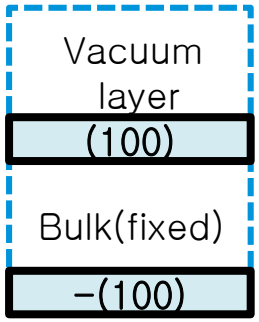
Surface

Calculation of surface energy

(100) = (-100)



i .

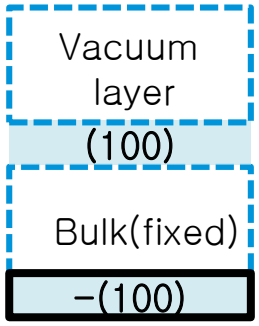


H-covered layer (fixed)

H-covered layer (fixed)

$\gamma_{(100)-H}=(E_{tot} - \mu_{Ga}N_{Ga} - \mu_{As}N_{As})/2A$

ii .

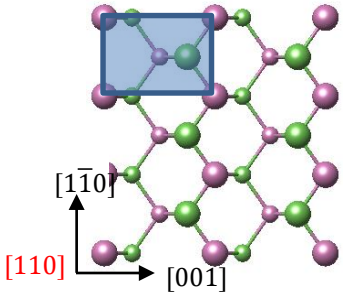


Relaxed/reconstructed surface(movable)

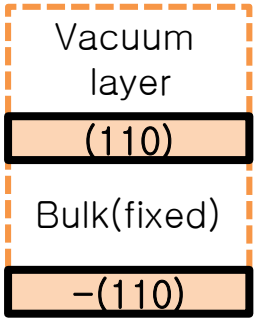
H-covered surface (fixed)

$\gamma_{(100)}=(E_{tot}-\mu_{Ga}N_{Ga}-\mu_{As}N_{As})/A-\gamma_{(100)-H}$

(110) = (-1-10)

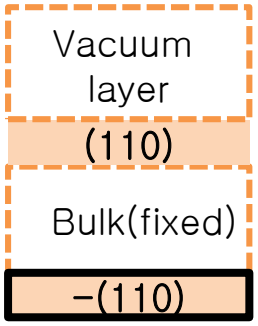


i .



$\gamma_{(110)-H}=(E_{tot} - \mu_{Ga}N_{Ga} - \mu_{As}N_{As})/2A$

ii .

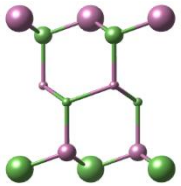


$\gamma_{(110)}=(E_{tot}-\mu_{Ga}N_{Ga}-\mu_{As}N_{As})/A-\gamma_{(110)-H}$

Calculation of surface energy of {111}

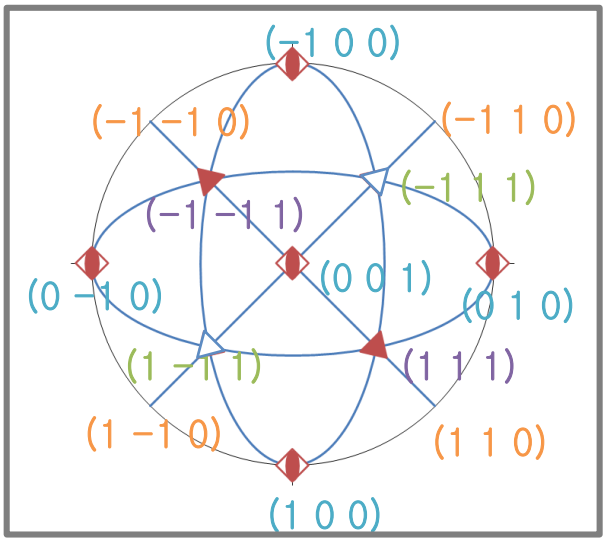
(111)A
; In-terminated

<111>A

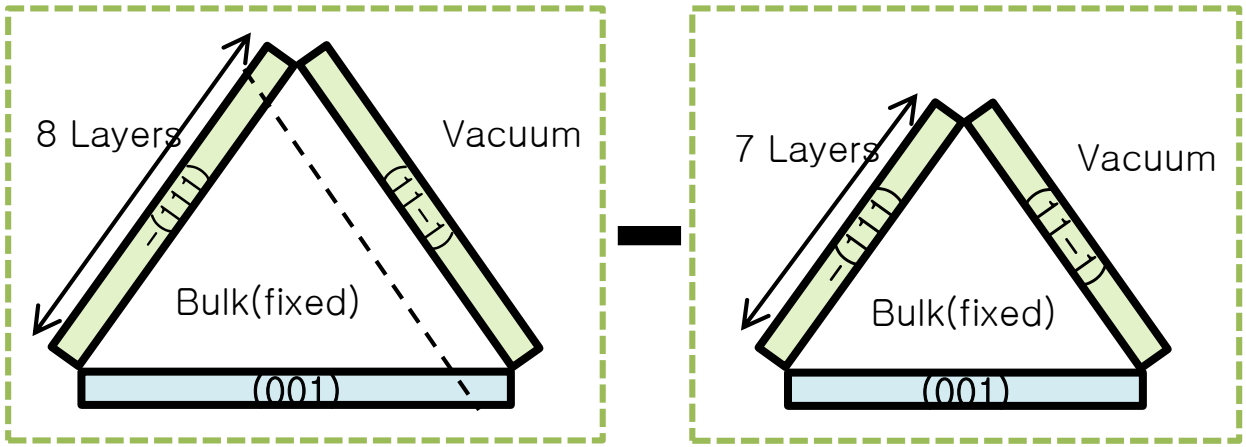


<111>B

(111)B
; As-terminated

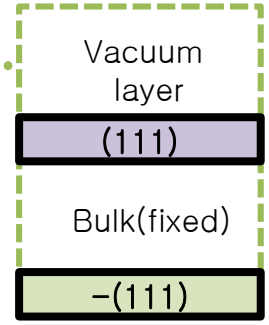


i.



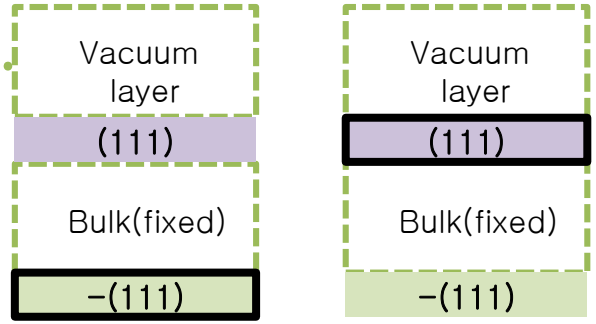
$\delta E = E_{tot}(n=8;\ 36AB) - E_{tot}(n=7;\ 28AB) - 8\mu_{AB}$
$= 2\gamma_{(-1-1-1)-H} + \gamma_{(-1\ 0\ 0)-H}$ Phys. Rev. Lett. 92 086102 (2004).

ii.



$\gamma_{(111)-H} = (E_{tot} - \mu_{Ga}N_{Ga} - \mu_{As}N_{As})/A - \gamma_{(-1-1-1)-H}$

iii.

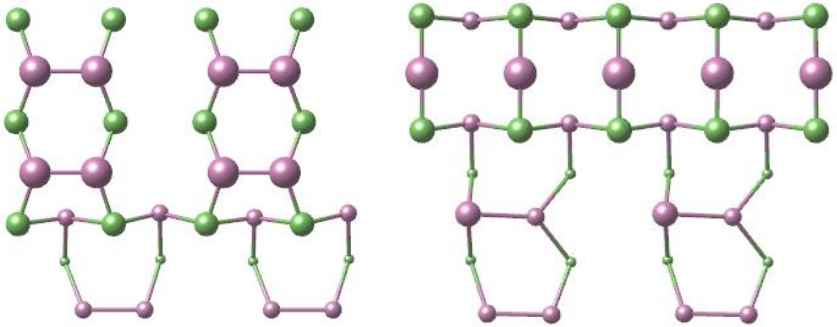


$\gamma_{(111)} = (E_{tot} - \mu_{Ga}N_{Ga} - \mu_{As}N_{As})/A - \gamma_{(-1-1-1)-H}$
$\gamma_{(-1-1-1)} = (E_{tot} - \mu_{Ga}N_{Ga} - \mu_{As}N_{As})/A - \gamma_{(111)-H}$

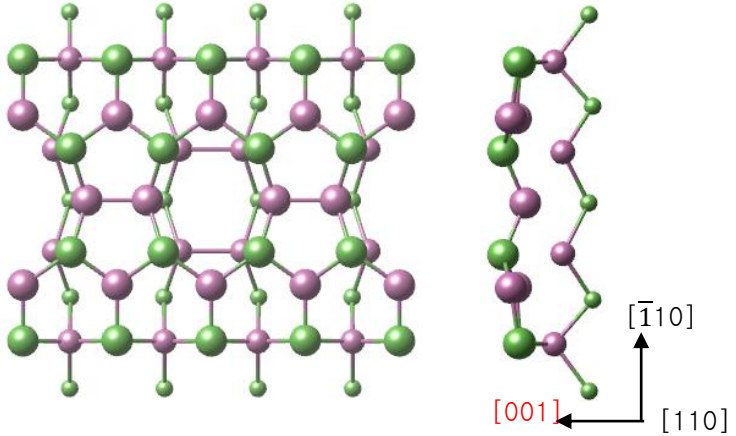
Surface reconstruction of InAs(100)

In-dimer along [110]

$\beta 2(4\times2)$ $\beta 3'(4\times2)$

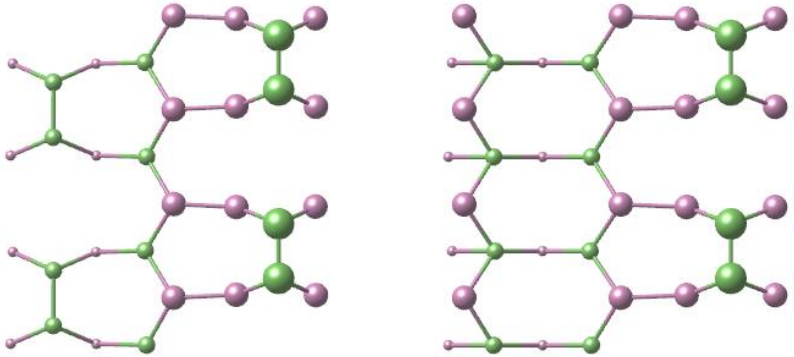


$\xi(4\times2)$

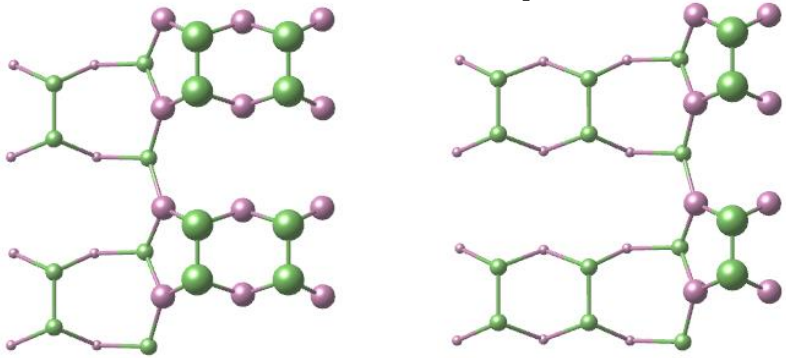


As-dimer along [-110]

$\alpha 2(2\times4)$ $\alpha 3(2\times4)$



$\beta 2(2\times4)$ $\beta 3(2\times4)$

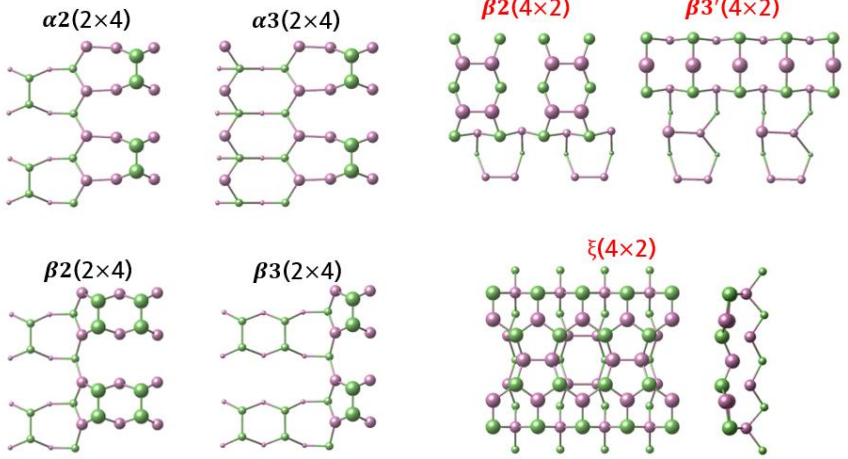


In As

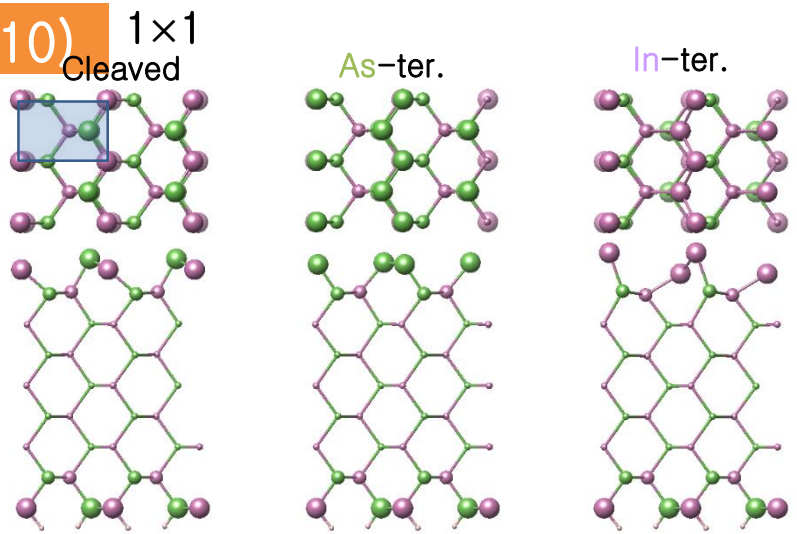
Surface reconstruction of InAs

In
As

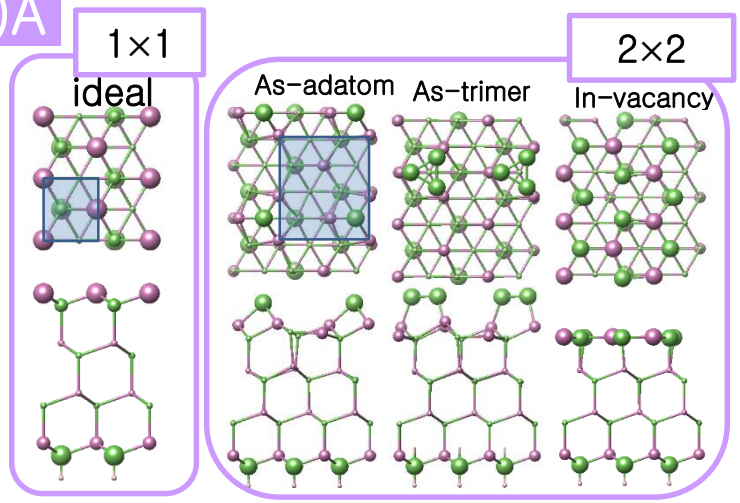
(100)



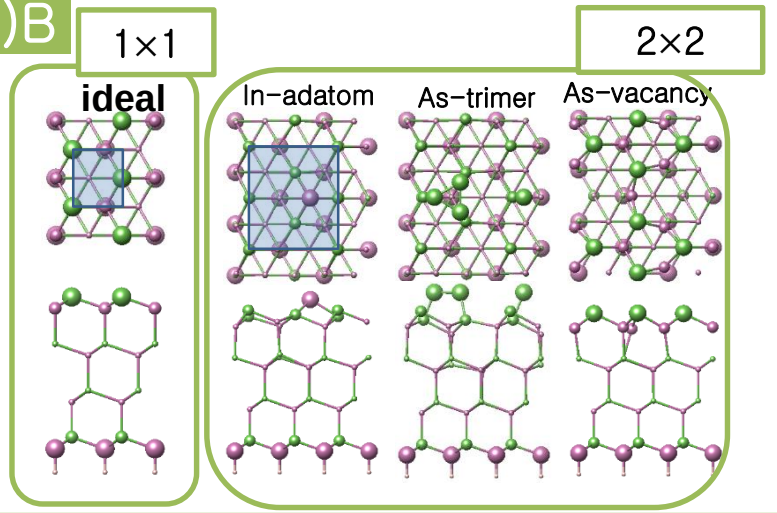
(110)



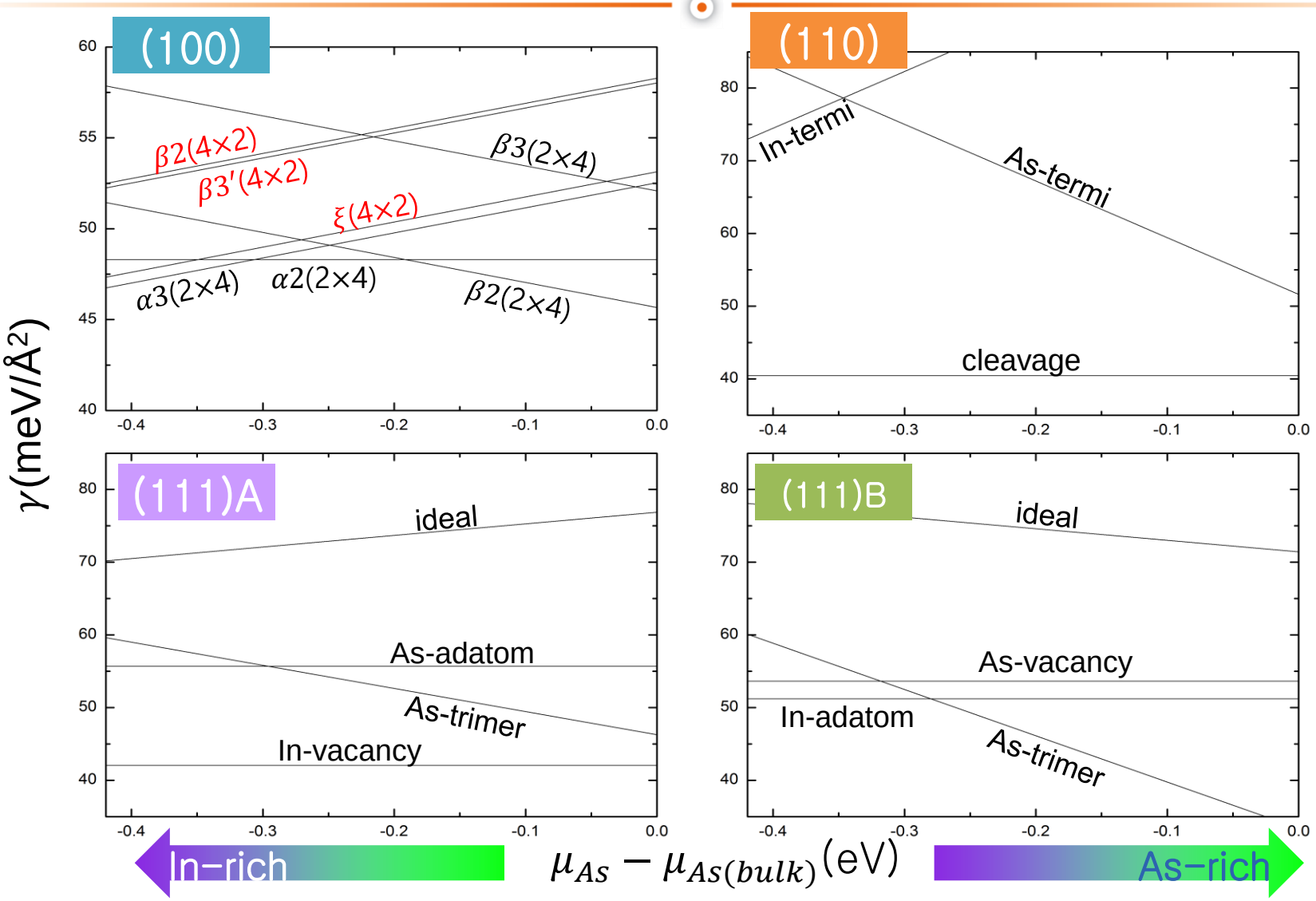
(111)A



(111)B

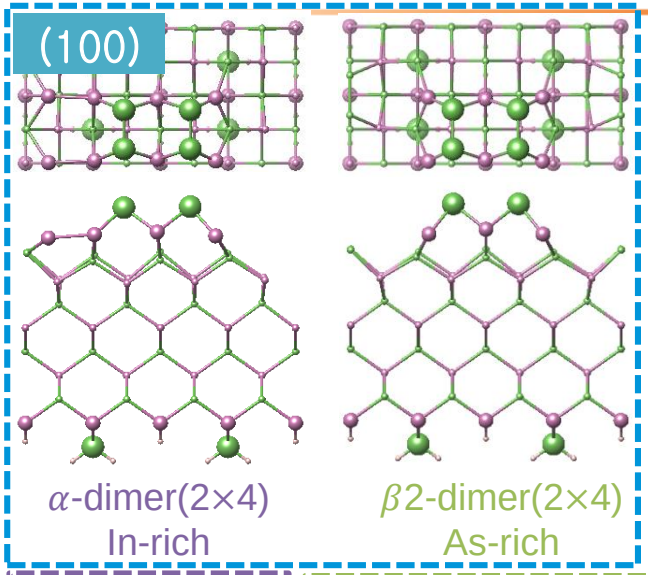


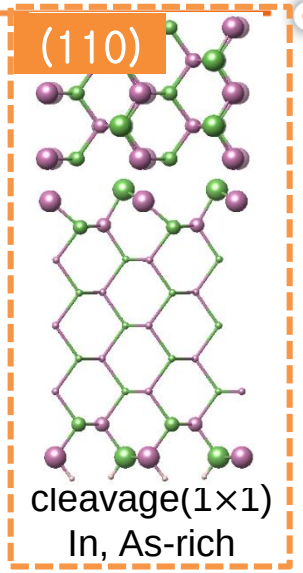
Surface energy

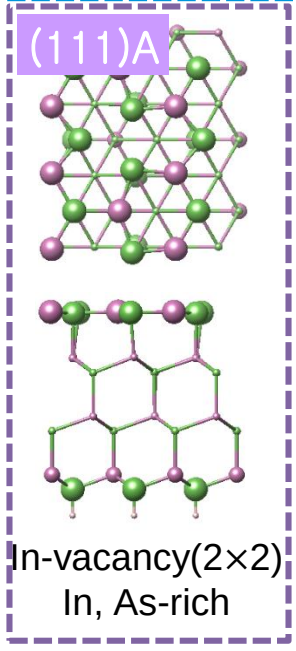


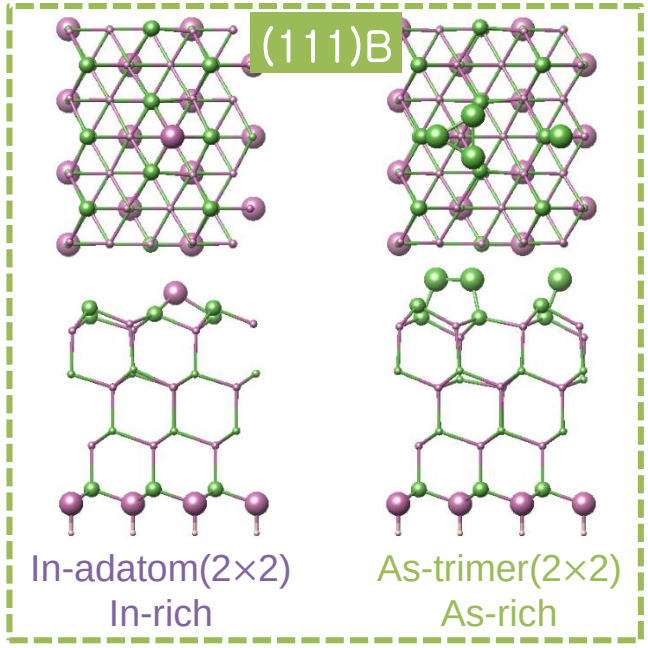
The surface energies of InAs is ~10 meV/Å² (0.16 J/m²) lower than those of GaAs.

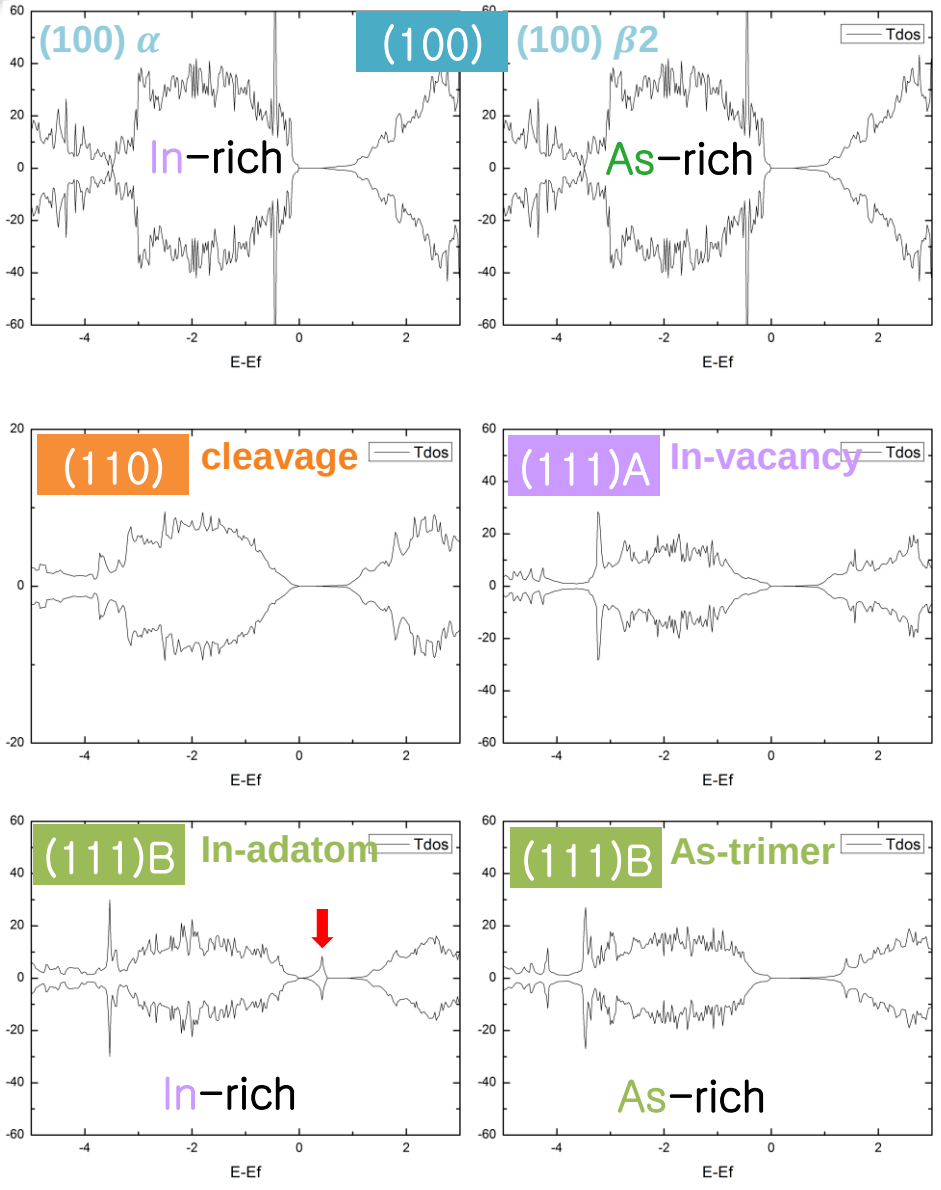
Stable surface & density of states





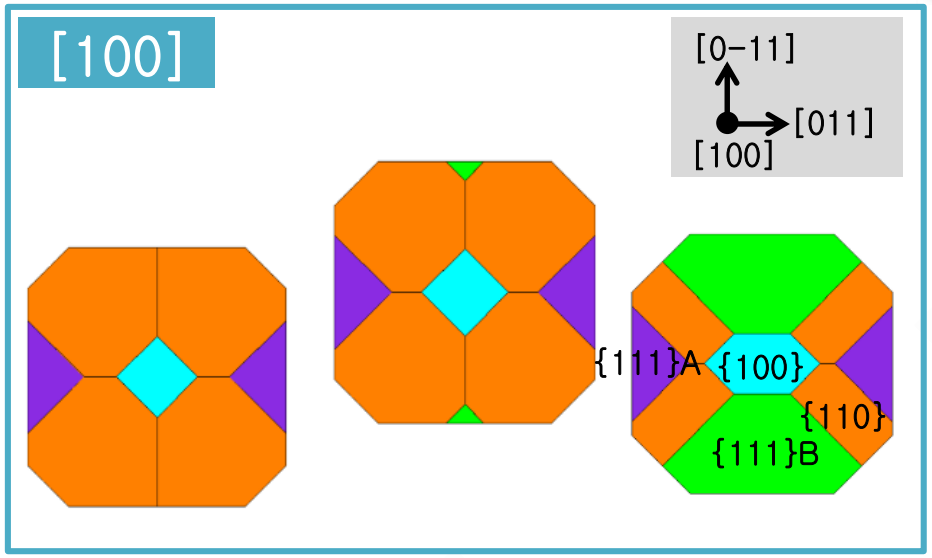


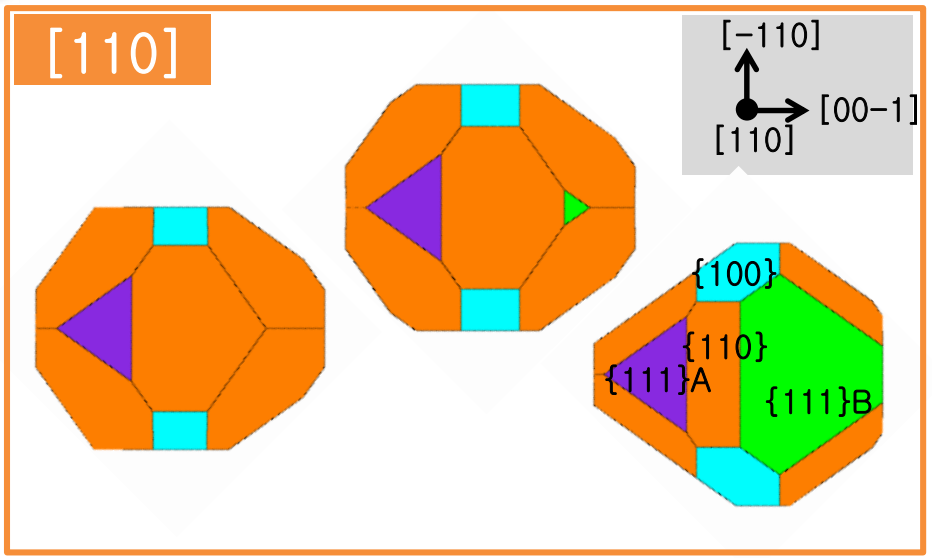


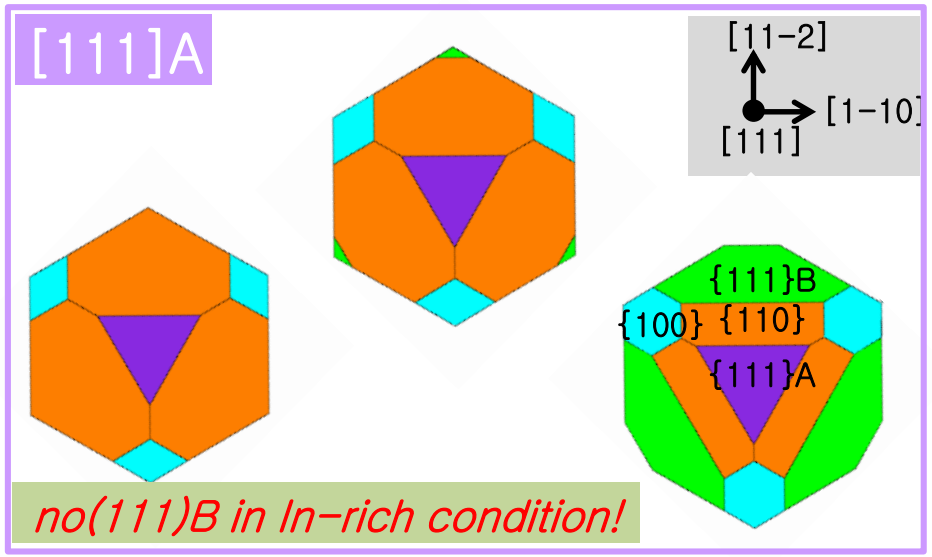


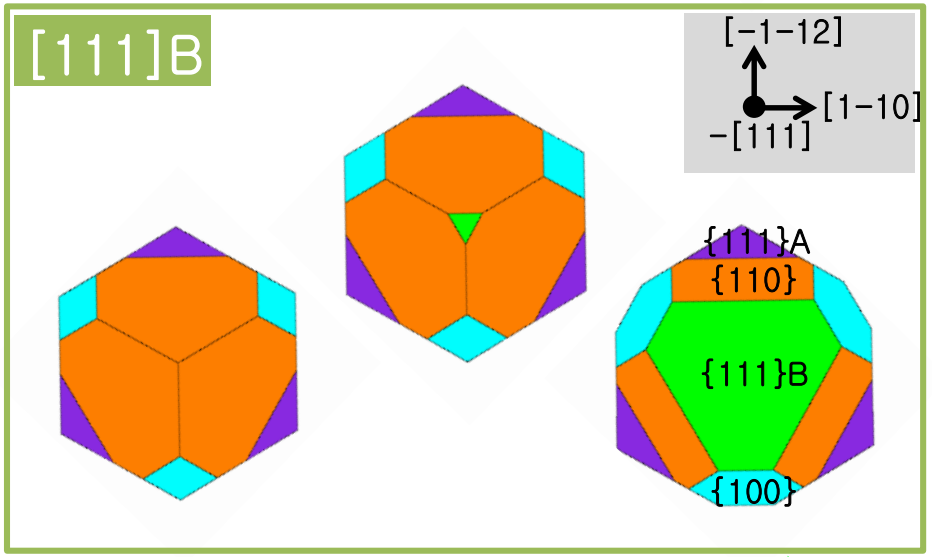
The bare surface structures do not have the gap states except (111)B.

Equilibrium shape of InAs









In-rich As-rich

In-rich As-rich

Equilibrium shape of InAs

[100]

[0-11]

[011]

[110]

[-110]

[00-1]

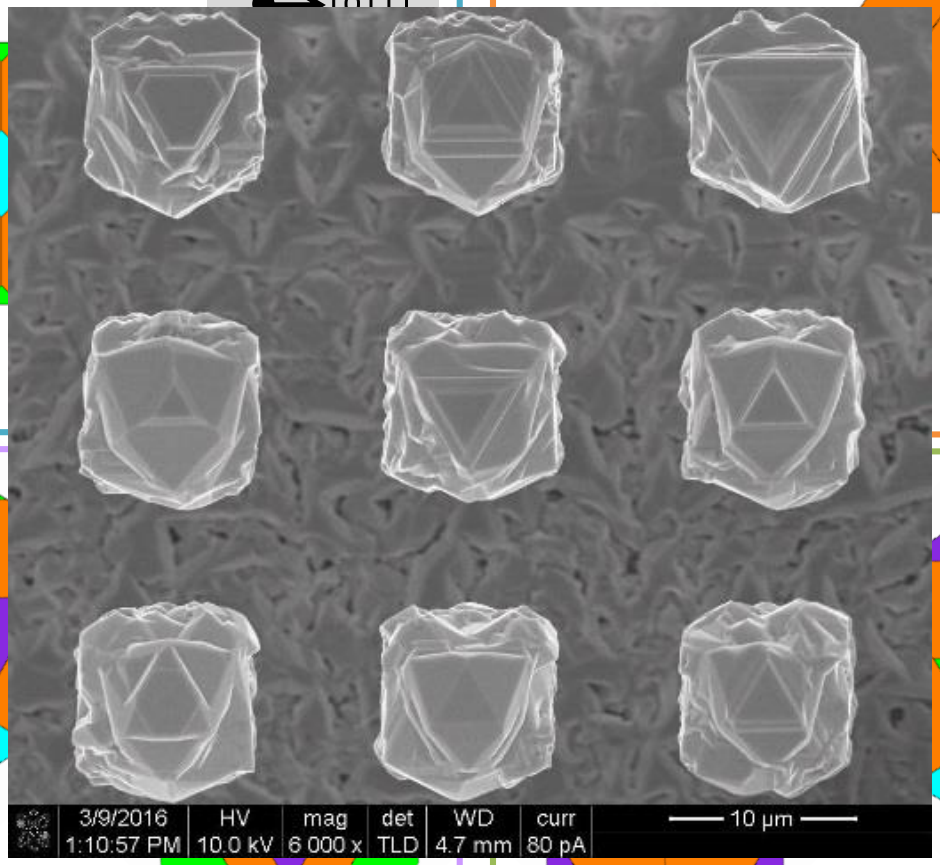
[110]

{100}

{110}

{111}A

{111}B



[111]A

no(111)B in In-rich condition!

[-1-12]

[1-10]

-[111]

{111}A

{110}

{111}B

{100}

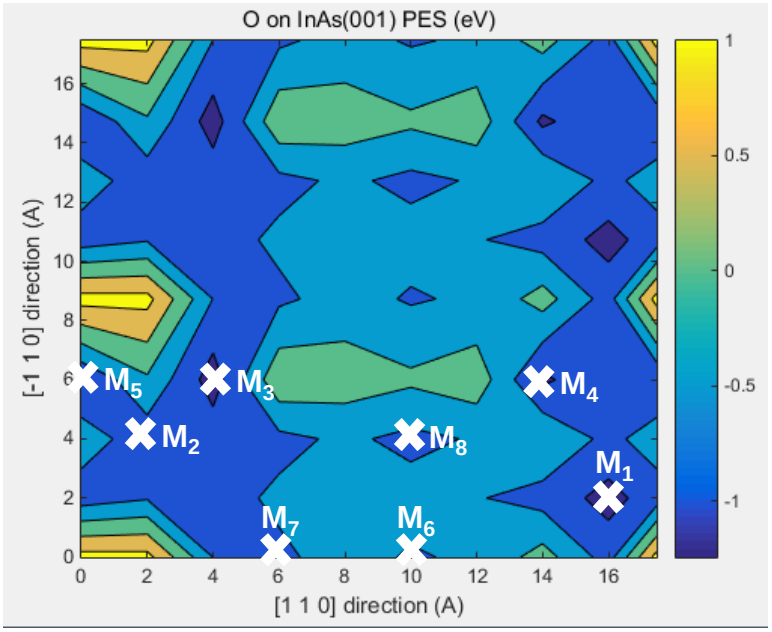
In-rich As-rich

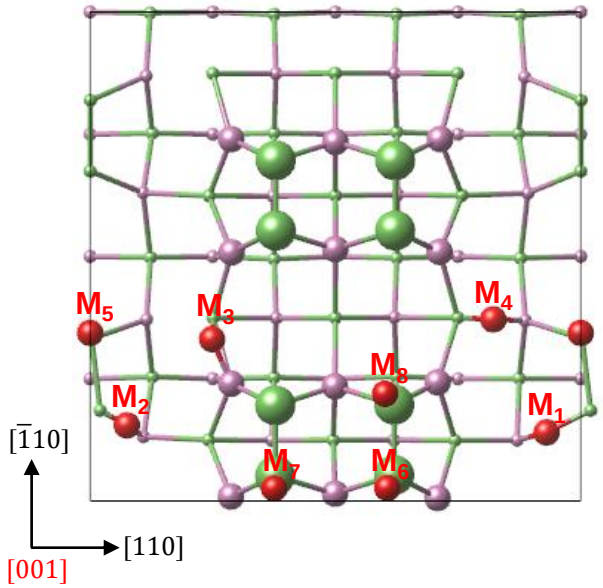
In-rich As-rich

Adsorption of O atom

Potential Energy Surface of O atom on (100)

As−rich $\beta2(2\times4)$





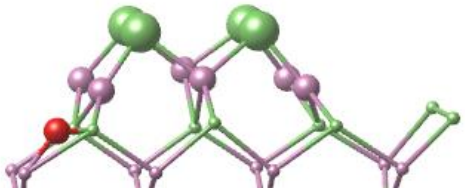
In

As

O

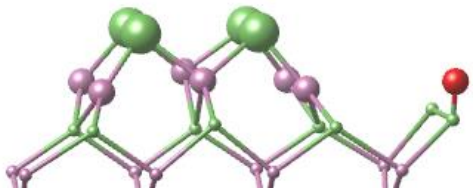
Adsorption energy & Stability

Site	M_1	M_2	M_3	M_4	M_5	M_6	M_7	M_8
E_{ads} (eV/O)	−1.41	−1.41	−1.38	−1.26	−0.97	−0.75	−0.74	−0.73



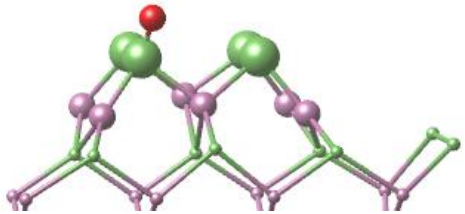
As-O-In bridge
(M_1~M_4)

>



2nd layer As=O
(M_5)

>



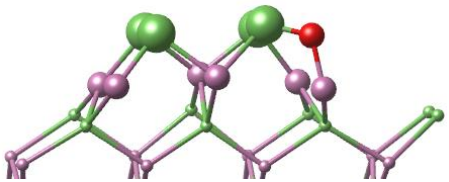
1st layer As=O
(M_6~M_9)

Adsorption energies of O atom

As−rich condition

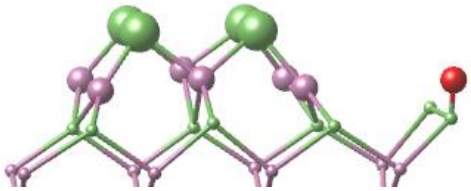
(100)

E_{sur} (meV/Å^2) = 44 ~ 50



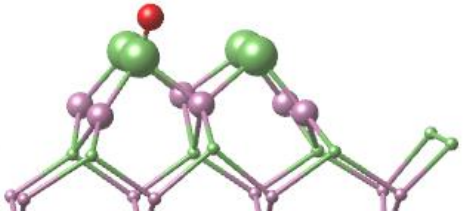
As-O-In bridge
(E_{ads} = -1.36 eV/O)

>



2nd layer As=O
(E_{ads} = -0.98 eV/O)

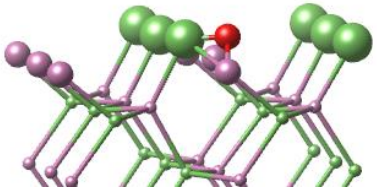
>



1st layer As=O
(E_{ads} = -0.75 eV/O)

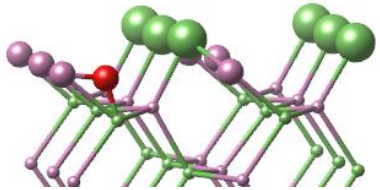
(110)

E_{sur} (meV/Å^2) = 40 ~ 40



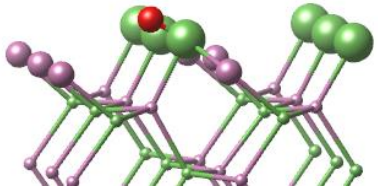
1st layer As-O-In
(E_{ads} = -1.31 eV/O)

>



2nd layer As-O-In
(E_{ads} = -1.12 eV/O)

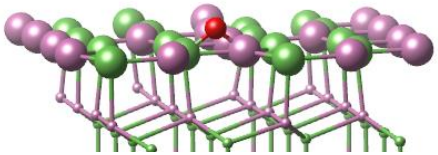
>



As=O
(E_{ads} = -0.64 eV/O)

(111)A

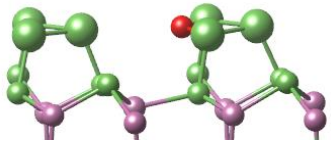
E_{sur} (meV/Å^2) = 42 ~ 42



1st layer As-O-In
(E_{ads} = -1.28 eV/O)

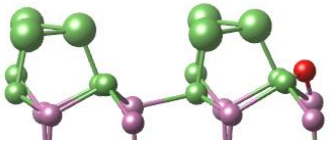
(111)B

E_{sur} (meV/Å^2) = 33 ~ 60



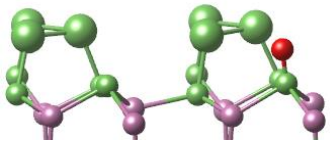
As-O-As
(E_{ads} = -1.37 eV/O)

>



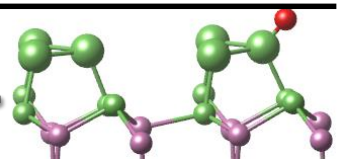
As-O-In
(E_{ads} = -1.09 eV/O)

>



2nd layer As=O
(E_{ads} = -0.61 eV/O)

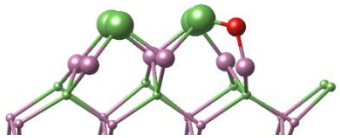
>



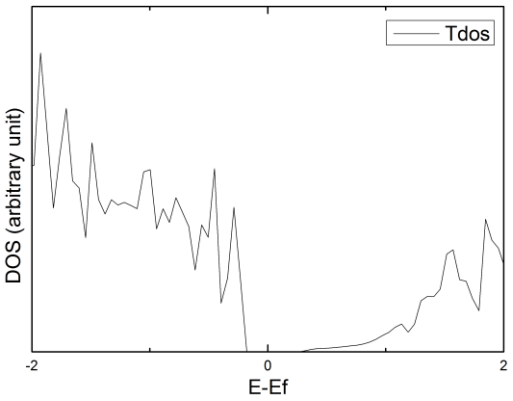
1st layer As=O
(E_{ads} = -0.51 eV/O)

Stable site for O adsorption & DOS

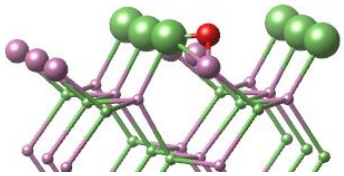
(100) As–O–In



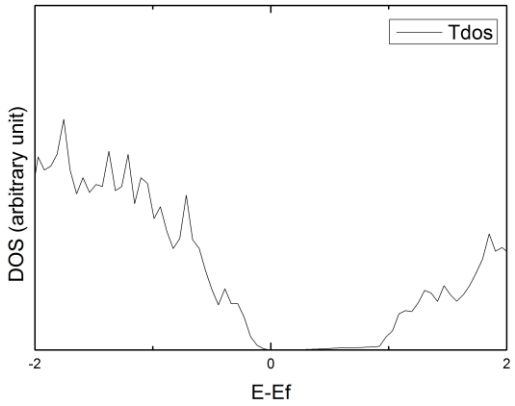
E_{ads} = −1.36 eV



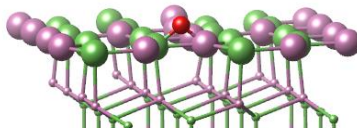
(110) As–O–In



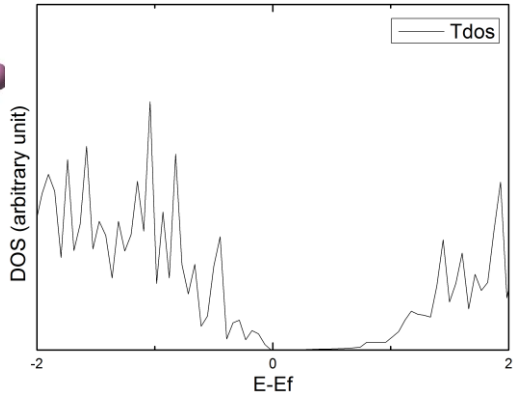
E_{ads} = −1.31 eV



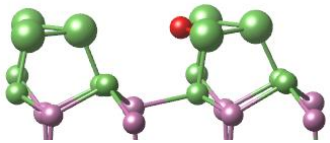
(111)A As–O–In



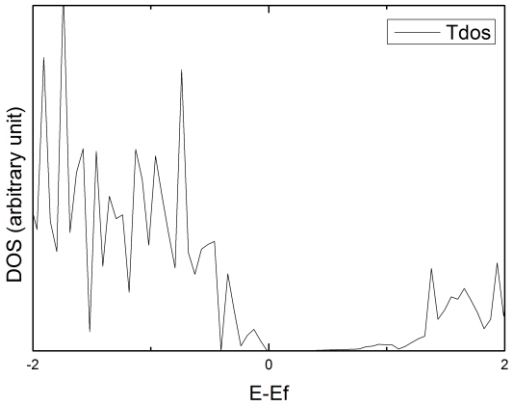
E_{ads} = −1.28 eV



(111)B As–O–As



E_{ads} = −1.37 eV



Adsorption of atomic O does not produce the gap states.

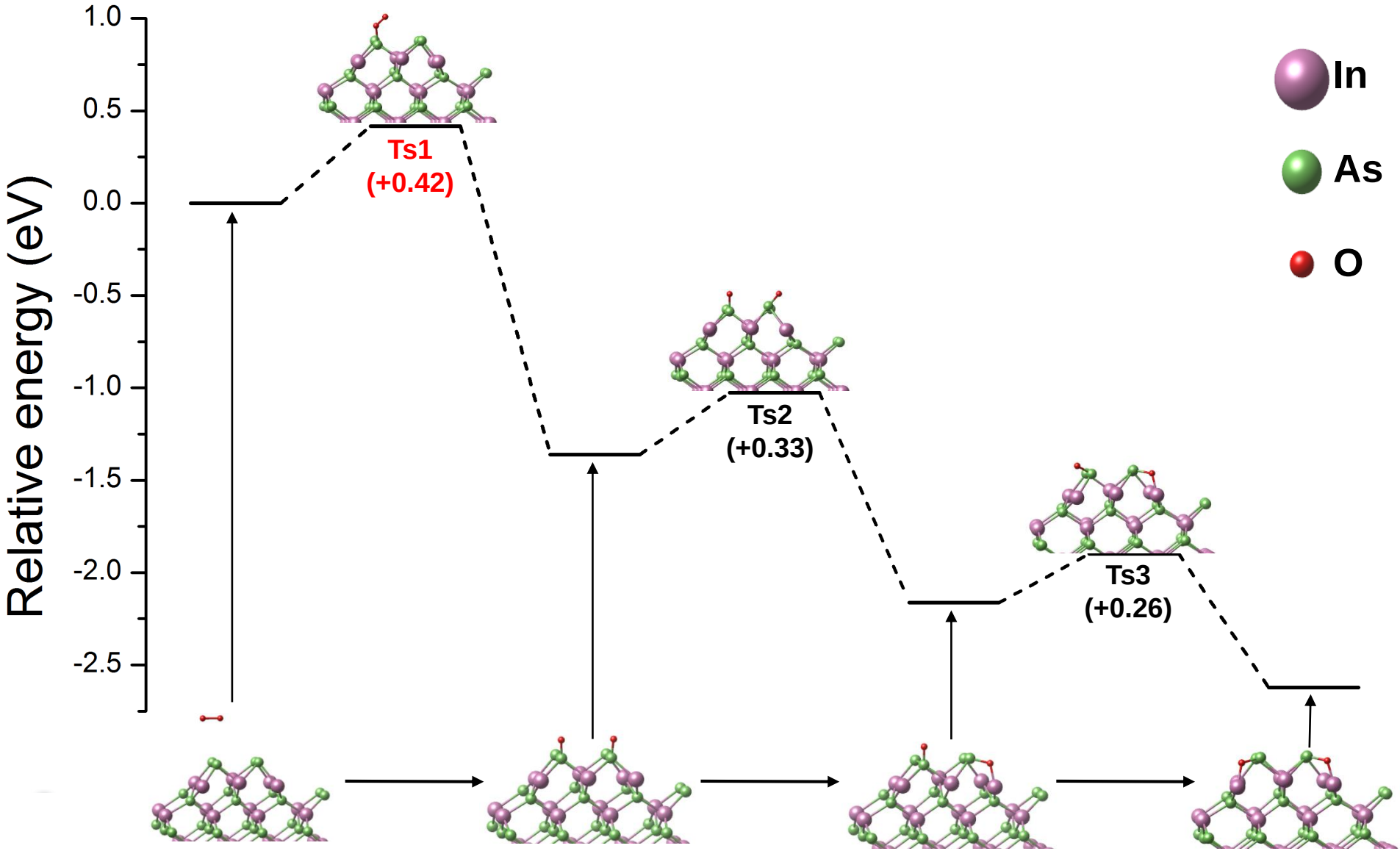
In

As

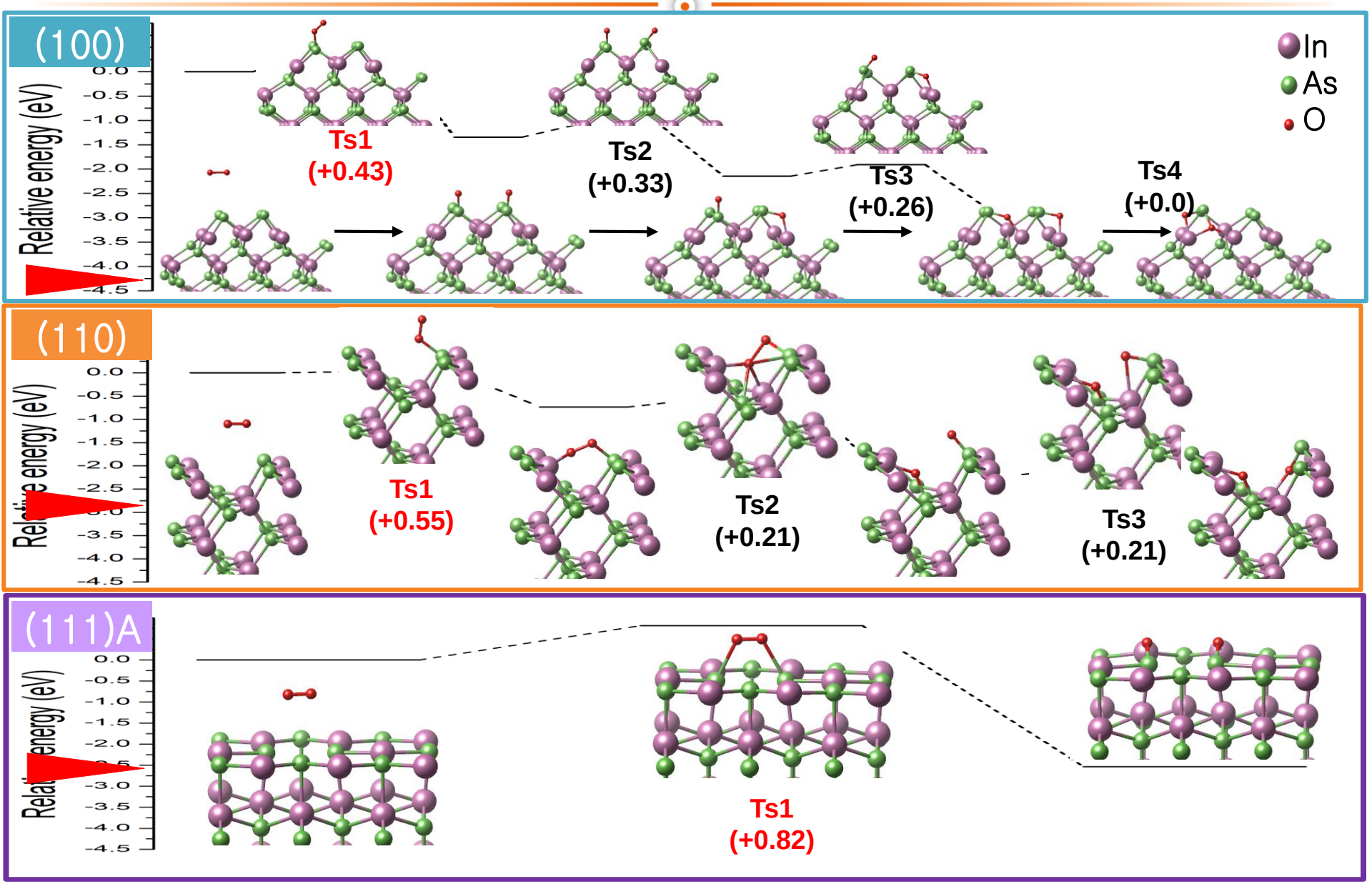
Adsorption of O_2 molecule

Dissociation of O_2 molecule on (100)

As−rich $\beta2(2\times4)$



Dissociation of O_2 on InAs surface

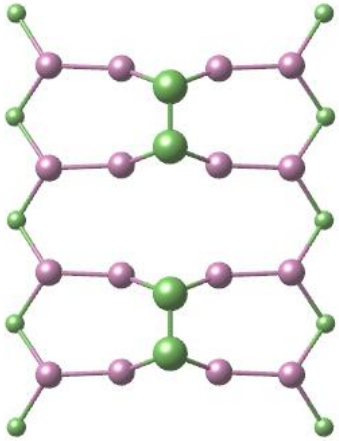


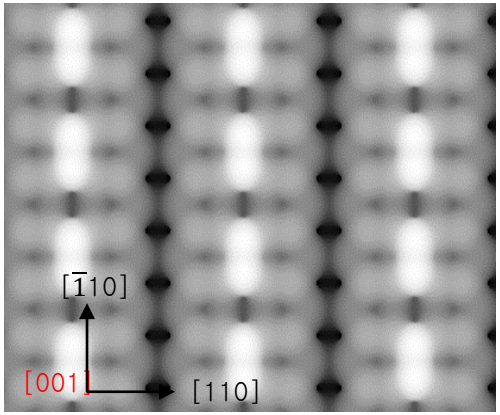
Non-0K (100) surface

STM of In-rich InAs(100)

Simulated STM at 0K
$\alpha 3(2\times4)$; As-dimer along [-110]

Experimental STM at 300 K
(4×2) ; In-dimer along [110]





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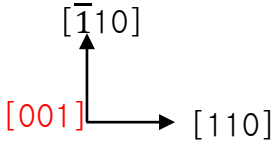
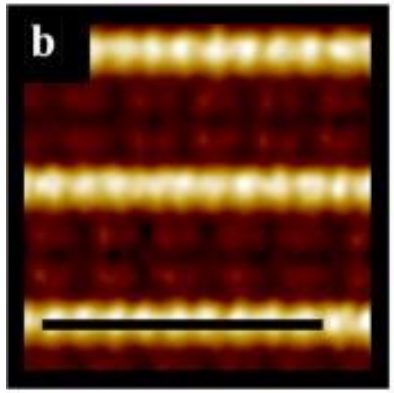
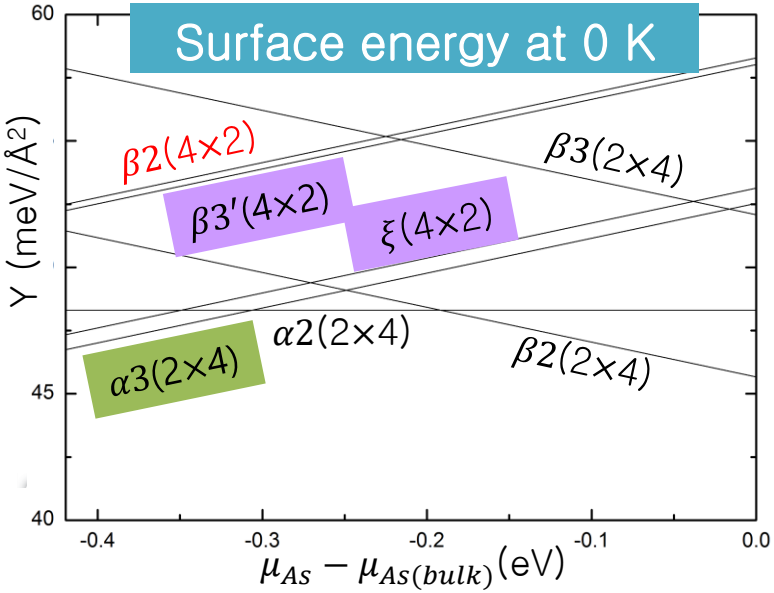




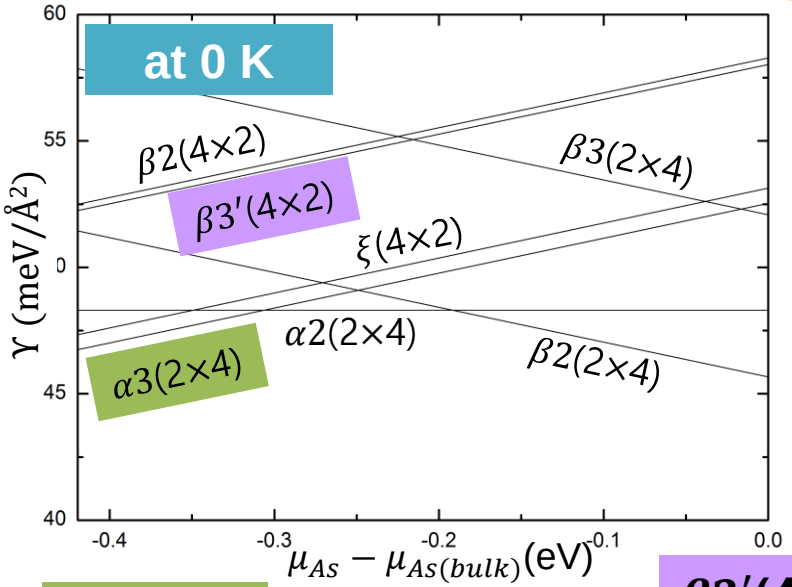
Surf. Sci. 603, 3321 (2009).



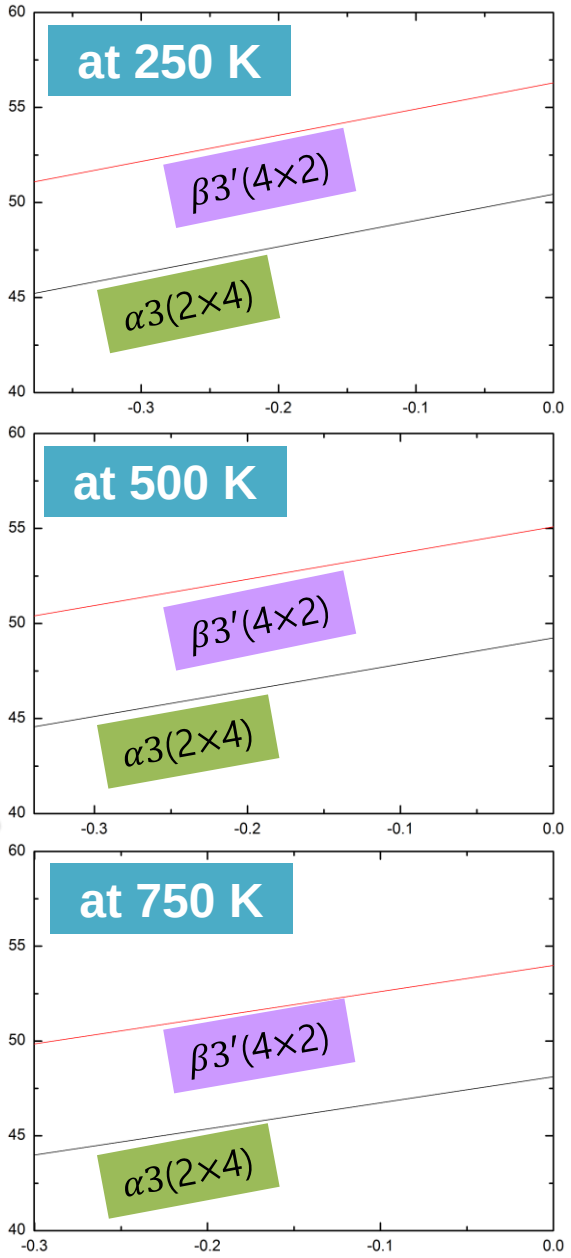
???

at 0 K: $\alpha 3(2\times4) < \xi(4\times2) < \beta 3'(4\times2)$
at non-0 K: $\beta 3'(4\times2)$ or $\xi(4\times2) < \alpha 3(2\times4)$

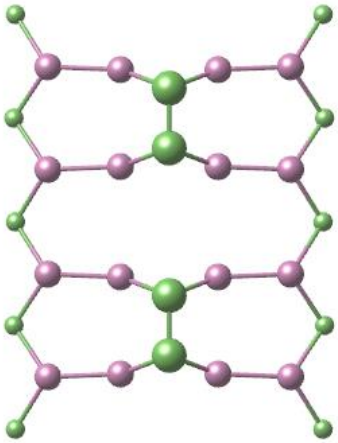
Surface energy of InAs(100) (T > 0 K); S_{vib}



+vibrational entropy

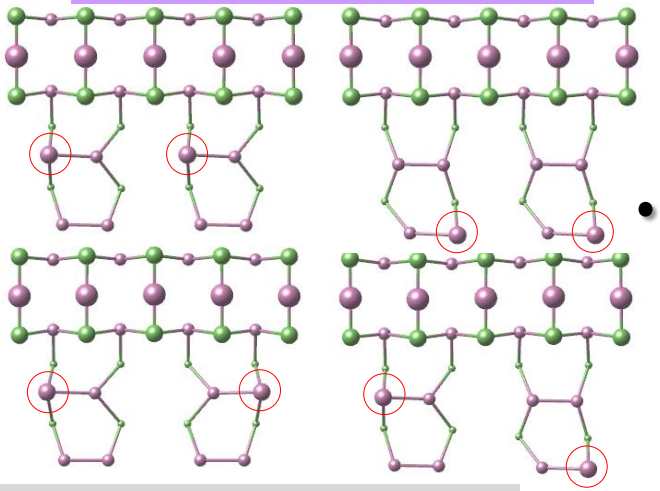


α3(2×4)



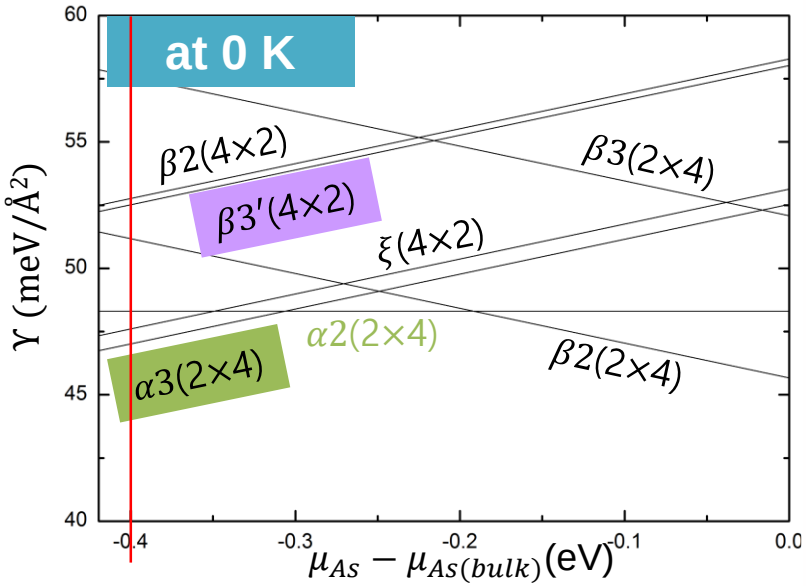
+5.5 meV/Å²

β3′(4×2) or β3′(4×4)



T ↑ → *Surface energy* ↓
but no reversal of stability

Surface energy of InAs(100) (T > 0 K); S_{conf}



+configurational entropy

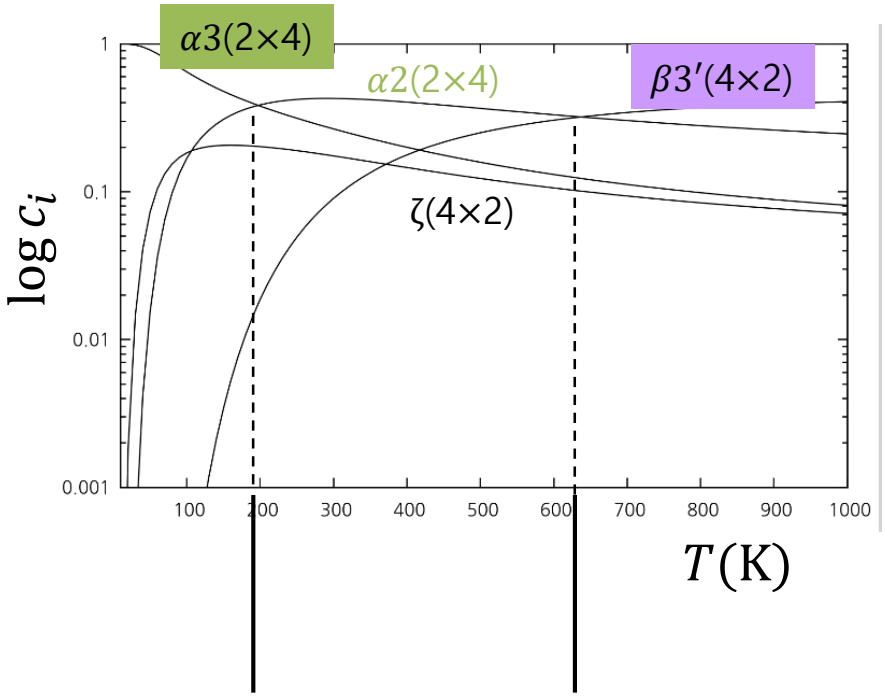
$$Z = \sum_i Z_i = \sum_i g_i \exp(-\frac{\Delta\gamma_i A}{k_B T})$$

$$c_i = \frac{Z_i}{Z} \; where \; i \in S(\alpha2, \alpha3, \beta2, \beta3, \beta3', \zeta)$$

Phys. Rev. Lett. 93, 146102 (2004).

$In-rich\ condition$

$\Delta\mu_{As} = -0.40$ eV

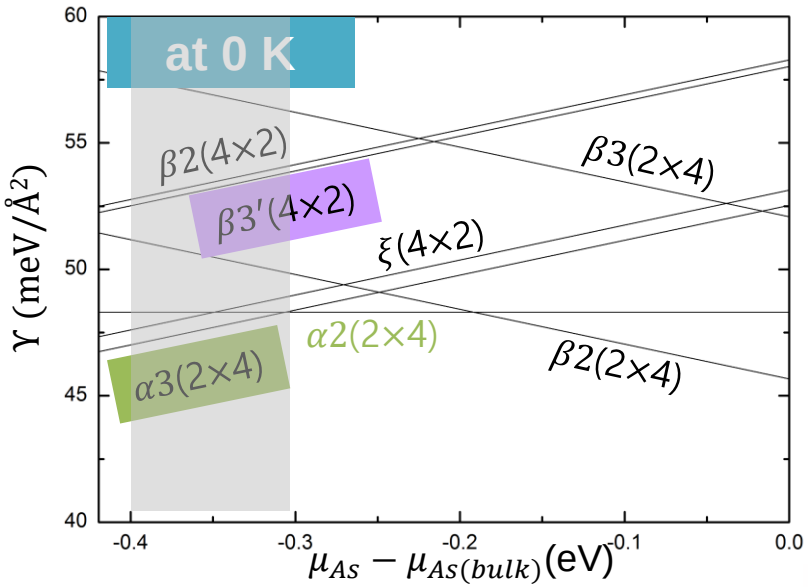


$\alpha3(2\times4)$ 195 K $\alpha2(2\times4)$ 635 K $\beta3'(4\times2)$

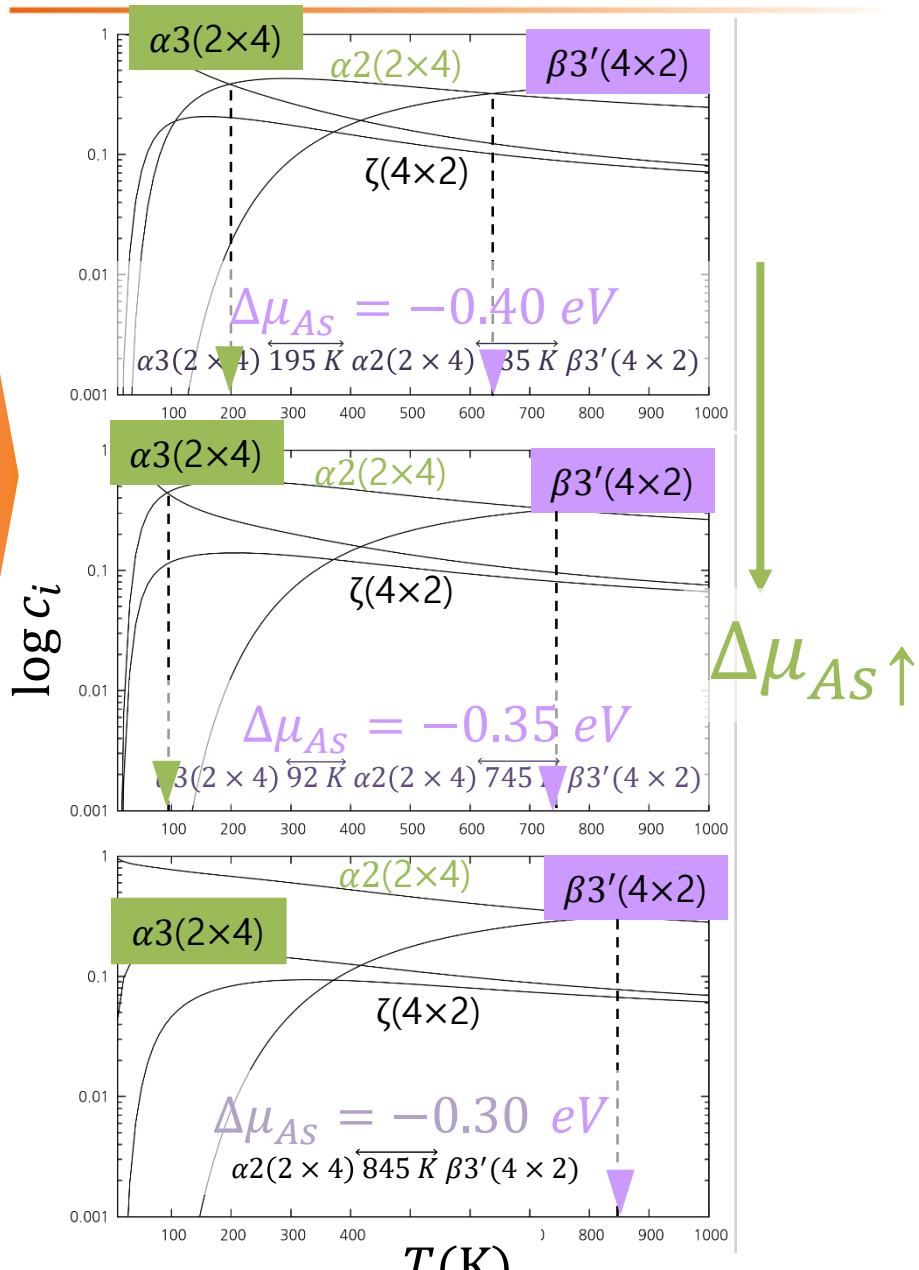
723 K annealing → (4×2)

Surf. Sci. 604 1859 (2010).

Surface energy of InAs(100) (T > 0 K); S_{conf}



+configurational entropy



$$Z = \sum_i Z_i = \sum_i g_i \exp(-\frac{\Delta\gamma_i A}{k_B T})$$

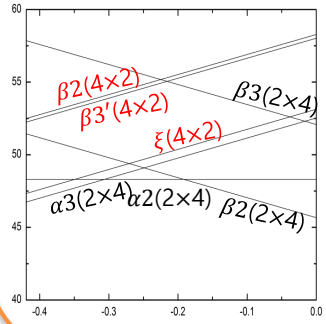
$$c_i = \frac{Z_i}{Z} \text{ where } i \in S(\alpha 2, \alpha 3, \beta 2, \beta 3, \beta 3', \zeta)$$

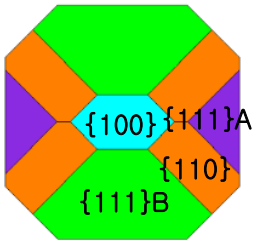
Phys. Rev. Lett. 93, 146102 (2004).

Summary

Surface

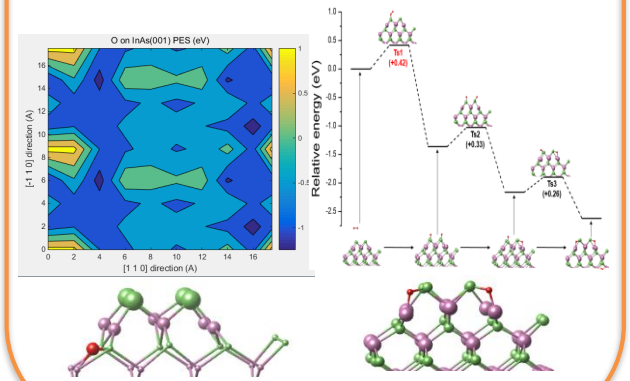
- Surface energy
  $\gamma_{InAs} < \gamma_{GaAs}$
- Surface reconstruction
- Equilibrium shape





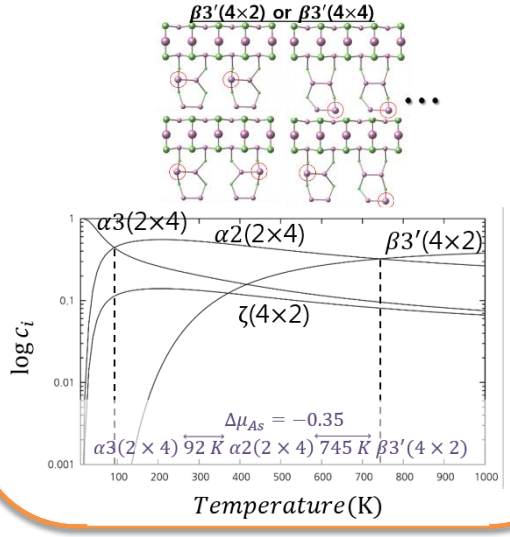
Oxygen adsorption

- Adsorption of O atom
- Adsorption of O_2
- Dissociation of O_2



Non-0K surface

- In-rich surface
- +vibration
- +configuration



→ will be expanded to (In,Ga)As

→ strain & interface will be considered.

Thank you !