제 23회 한국반도체학술대회
세션: [WK2-E] Ⅲ-Ⅴ Device

Oxidation study on the (100), (110) and (111) surfaces of InAs by ab-initio calculations

2016. 02. 24

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Computational Materials Design

Contents

Intro.

- **Motivation –** why oxidation of different surfaces of InAs?
- **Purpose & Methods**

Results

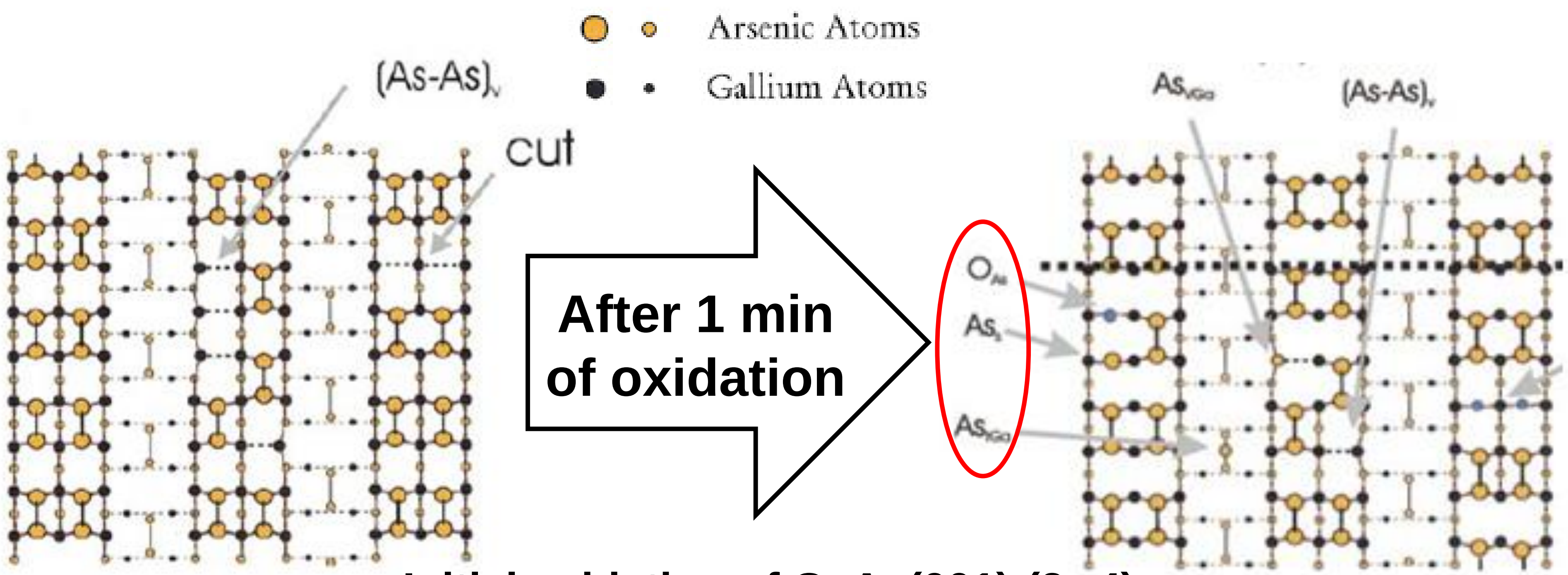
- **Surface energy –** to find stable surface structures.
- **Adsorption of O atom –** to find stable sites.
- **Adsorption of O_2 molecule –** to find barrier for antisite defects.

Summary

- **Summary –** comparison with GaAs surfaces.

Why oxidation?-Difficulty of avoiding oxidation

Exposure of Ⅲ-Ⅴ surfaces to oxygen results in 'Fermi-level pinning'

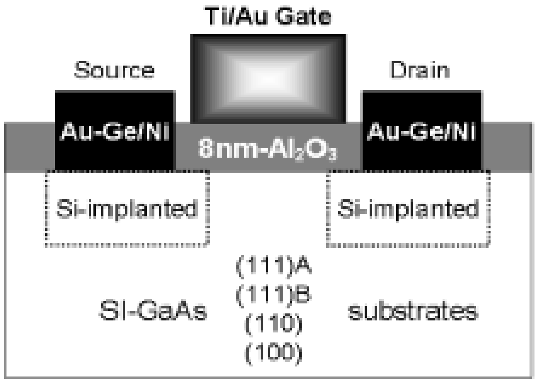


Initial oxidation of GaAs(001)-(2×4)

→ **Oxygen displaces a single As atom (O_{As}) in the top layer.**
→ **The displaced As atoms form As_{Ga} antisites,**
which is believed to cause Fermi-level pinning.

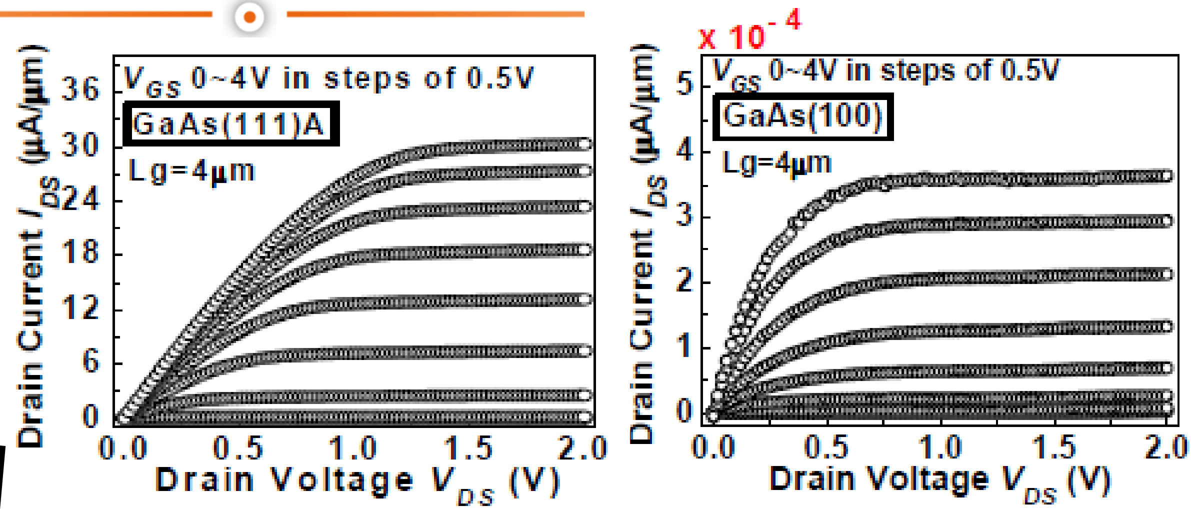
Yi, S. I., Kruse, P., Hale, M., & Kummel, A. C. (2001). The Journal of Chemical Physics, 114(7), 3215-3223.

Why various surfaces?-Impact of surface orientations



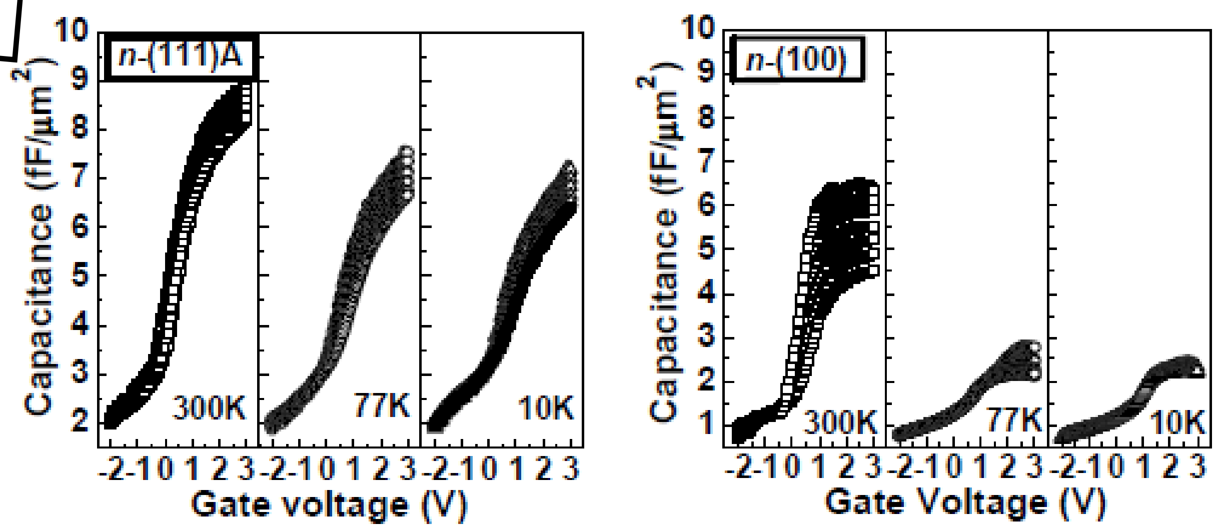
GaAs NMOSFET

I-V



→ **Maximum I_d is $30\ \mu A/\mu m$ for (111)A and $3.5 \times 10^{-4}\ \mu A/\mu m$ for (100)**

C-V



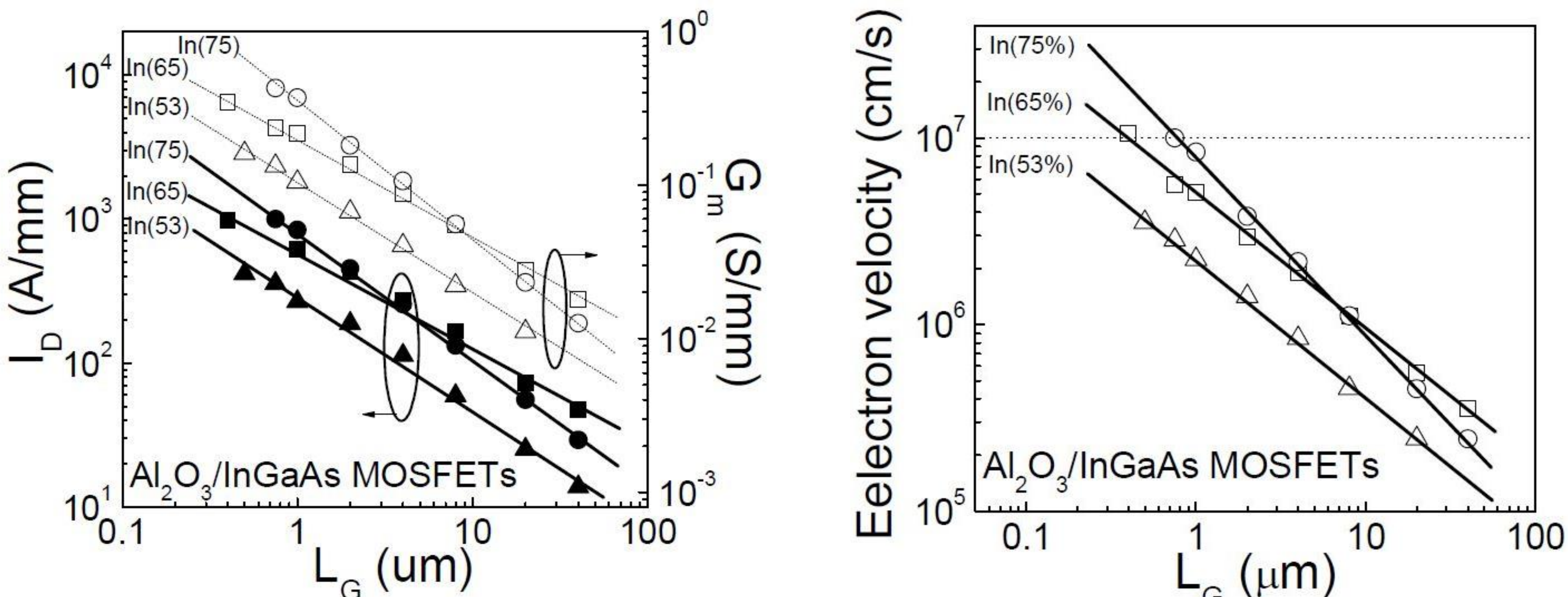
Xu M, Xu K, Contreras R, Milojevic M, Shen T, Koybasi O, et al., editors. IEEE int. Electron Devices Meeting. 865-868 (IEEE, 2009).

Why InAs?-Better intrinsic properties of $In_xGa_{1-x}As$

The device characteristics improve significantly as increasing In content

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

T. P. Ma, Appl. Phys. Lett. 96, 122105 (2010).



P.D. Ye, Y. Xuan, Y.Q. Wu, and M. Xu, ECS trans. 19, 605 (2009).

Purpose & methods of this investigation

By studying the initial oxidation of InAs on the atomic scale, Explanation of the effect of the surface orientation on the device performance

VASP: Vienna Ab-initio Simulation Package

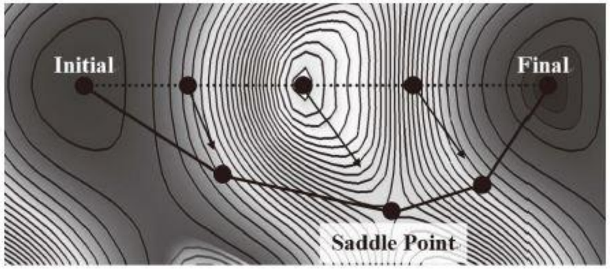
DFT

$$\hat{H}\Psi = E\Psi$$

- Structure optimization
- Electronic properties

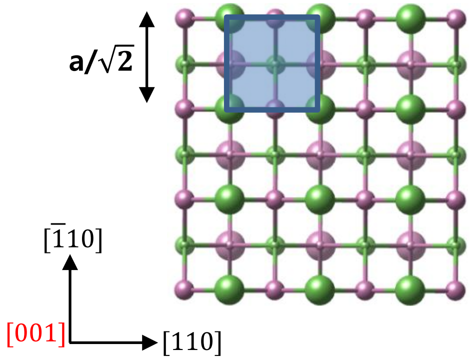
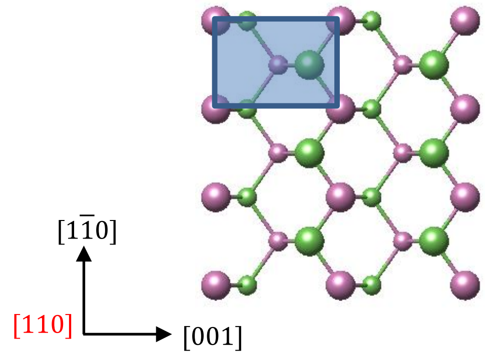
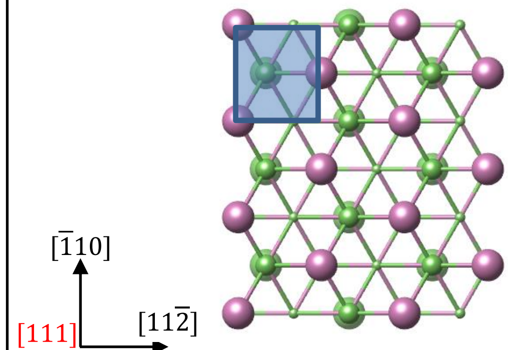
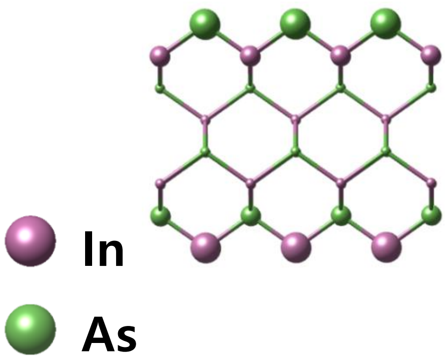
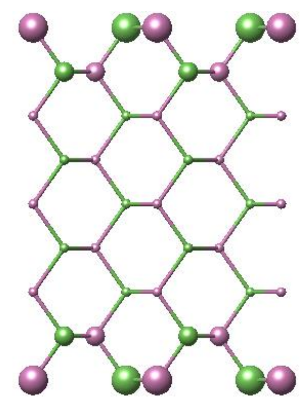
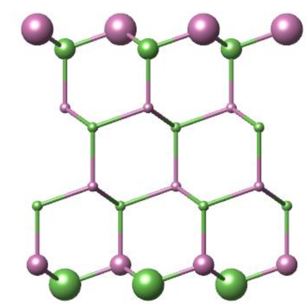
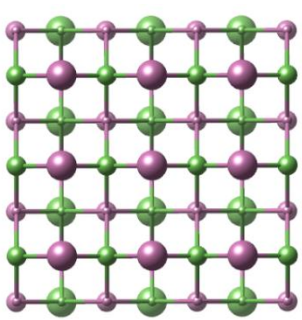
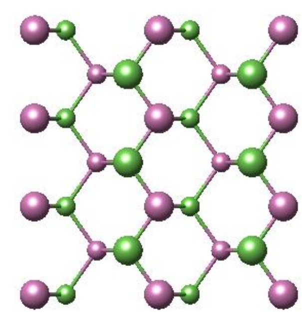
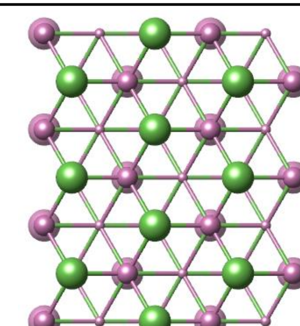
- PBE potential
- ENCUT 500 eV

NEB



- Minimum Energy Path between initial and final state

InAs unit surface

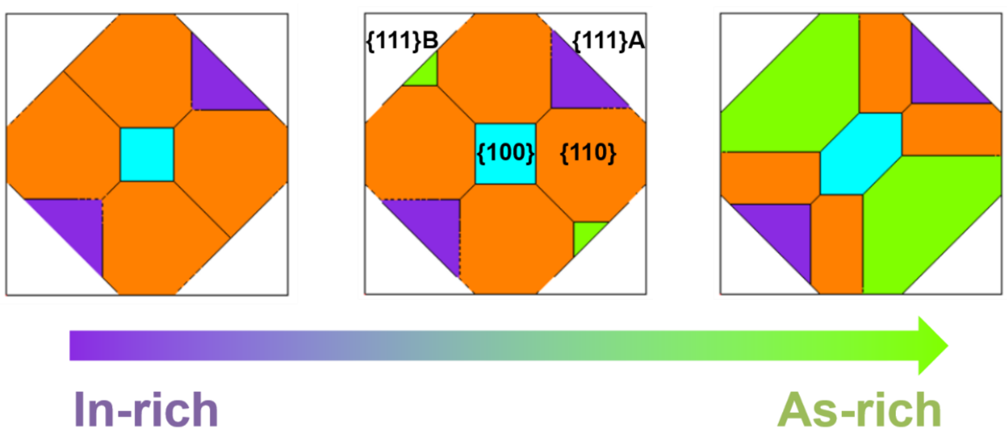
	(100) Surface	(110) Surface	(111) Surface
area	$a^2/2$ per one atom (100) = -(100)	$a^2/\sqrt{2}$ per two atom (110) = -(110)	$\sqrt{3}a^2/4$ per one atom (111) ≠ -(111)
Top			
Side			
bottom			

Surface energy: GaAs vs InAs

Ⅲ-rich condition			V-rich condition	
GaAs [1]	InAs [this study]	Orientation	GaAs [1]	InAs [this study]
65	48	(100)	45	43
52	40	(110)	45	40
54	42	(111)A	51	42
69	51	(111)B	43	33

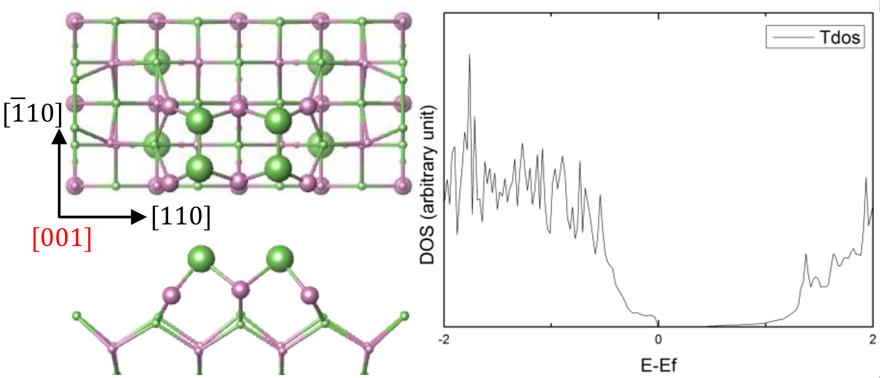
[1] N. Moll, A. Kley, E. Pehlke, M. Scheffler, Phys. Rev. B 54, 8844 (1996).

(meV/Å²)

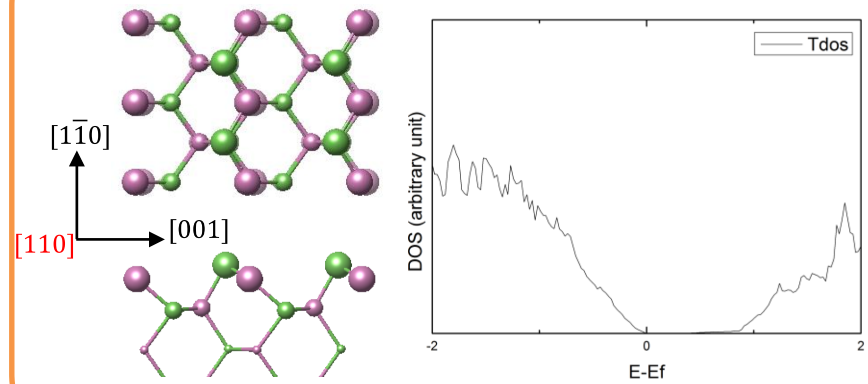


InAs: Stable surface structure and the DOS

(100) β2



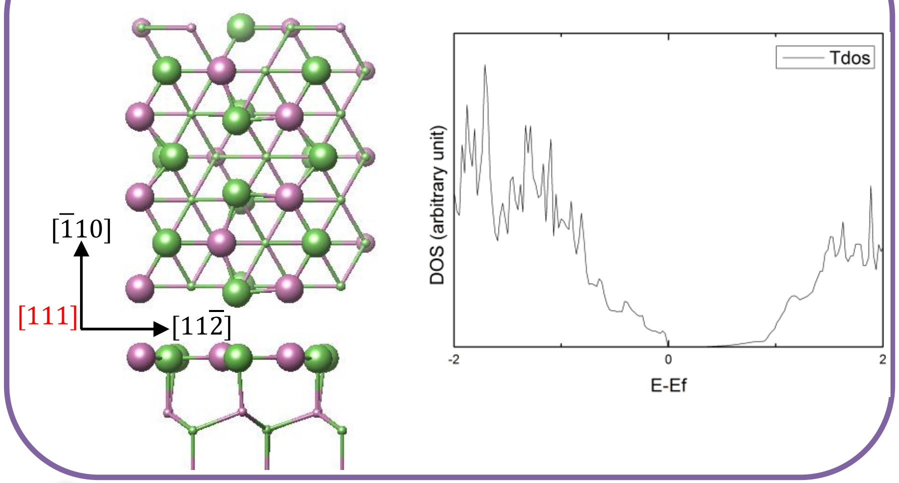
(110) cleavage



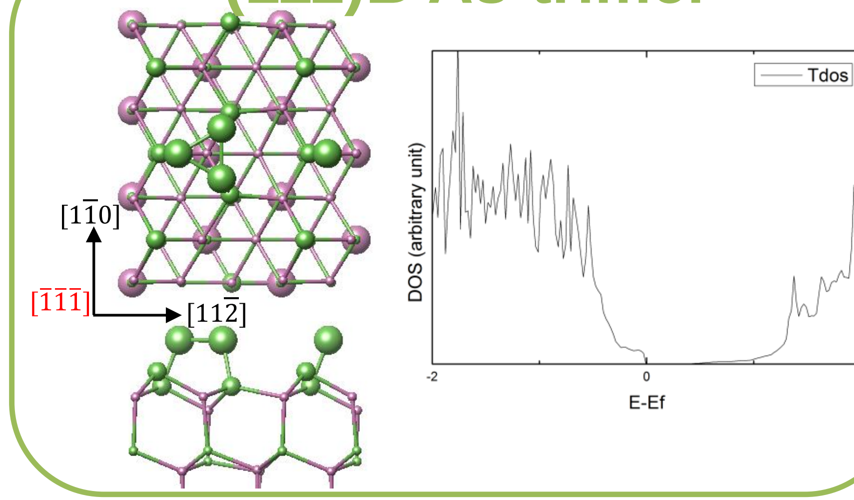
In

As

(111)A In-vacancy



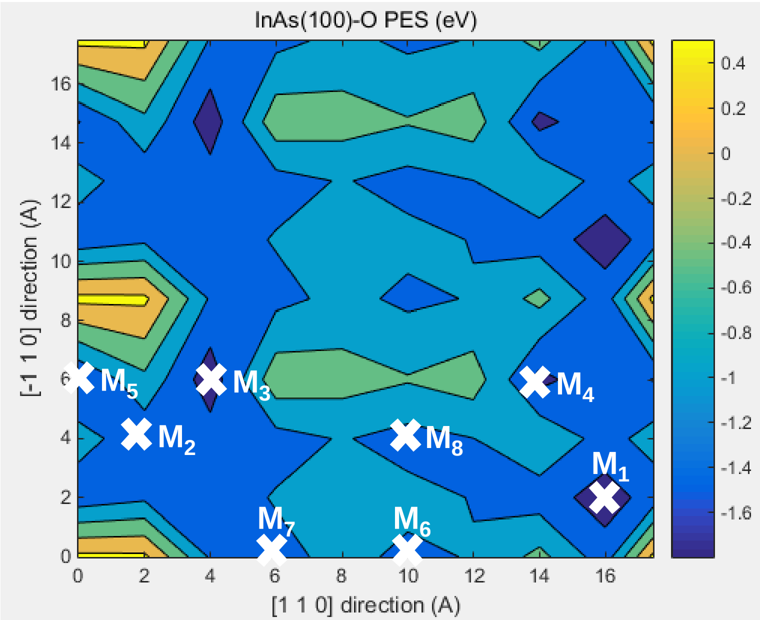
(111)B As-trimer

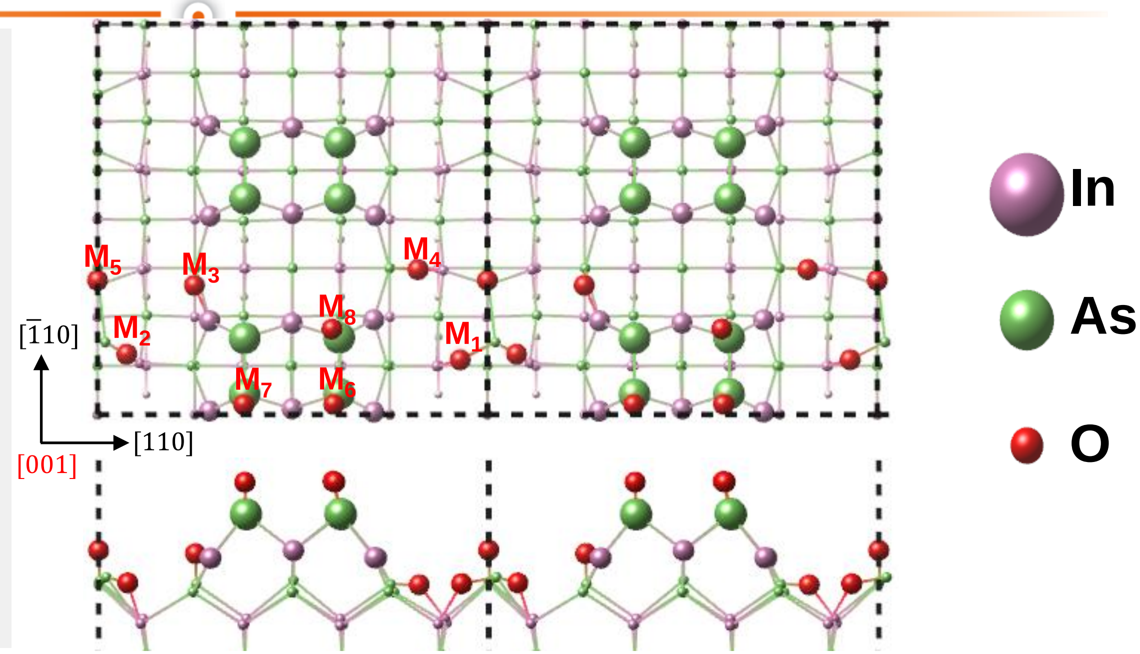


The bare surface structures have no states in the gap.

Computational Materials Design

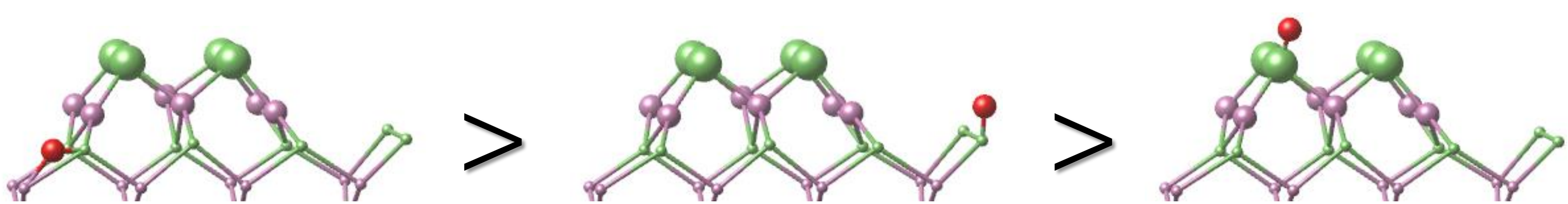
Potential Energy Surface of O atom on (100)





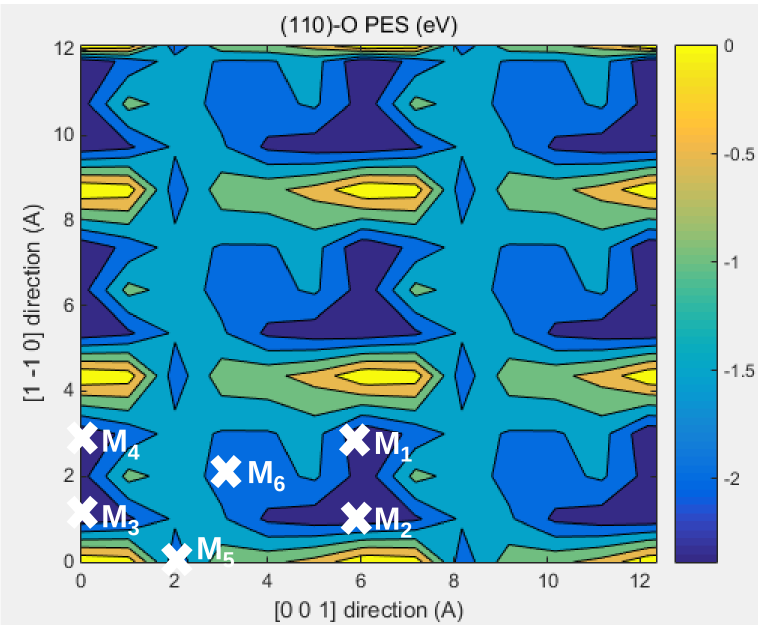
Adsorption energy & Stability

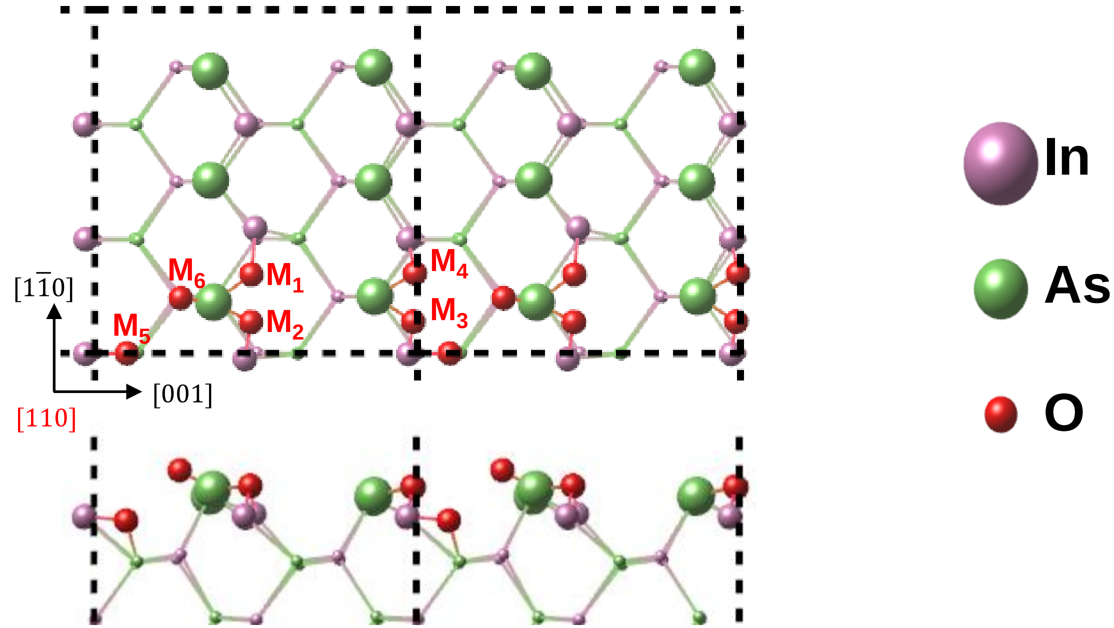
Site	M_1	M_2	M_3	M_4	M_5	M_6	M_7	M_8
E_{ads} (eV/O)	-1.96	-1.96	-1.93	-1.81	-1.52	-1.30	-1.29	-1.28



As-O-In bridge (M_1~M_4) > 2nd layer As=O (M_5) > 1st layer As=O (M_6~M_9)

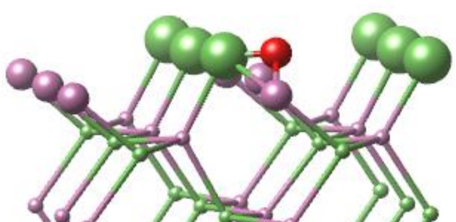
Potential Energy Surface of O atom on (110)





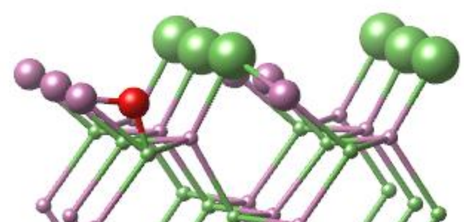
Adsorption energy & Stability

Site	M$_1$	M$_2$	M$_3$	M$_4$	M$_5$	M$_6$
E_{ads} (eV/O)	-2.38	-2.38	-2.38	-2.38	-2.19	-1.71



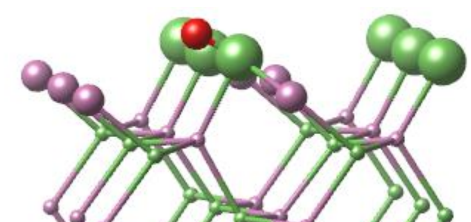
1st layer As-O-In
(M$_1$~M$_4$)

>



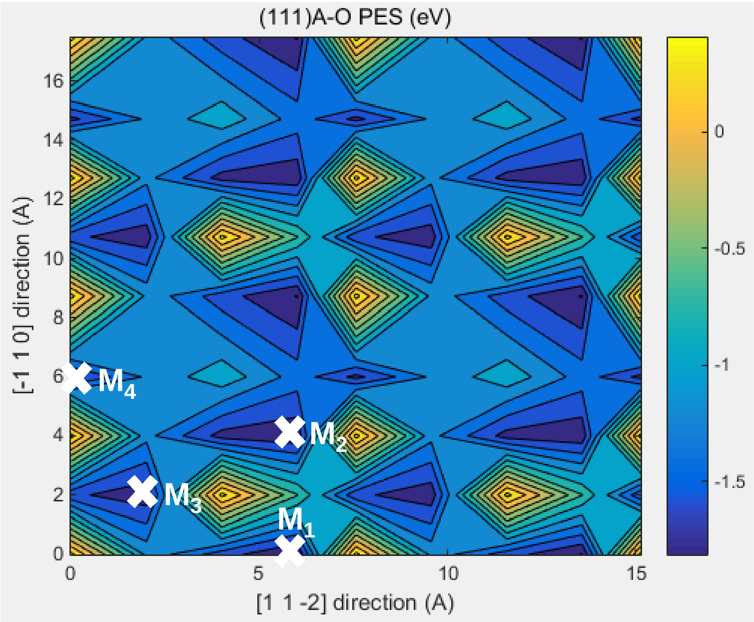
2nd layer As-O-In
(M$_5$)

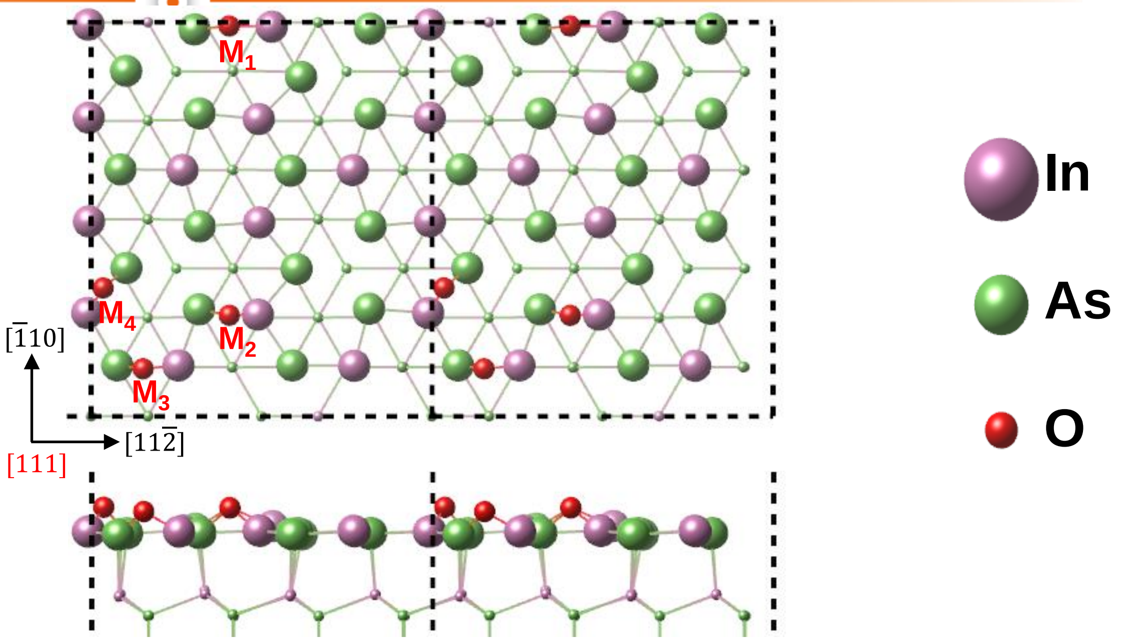
>



As=O
(M$_6$)

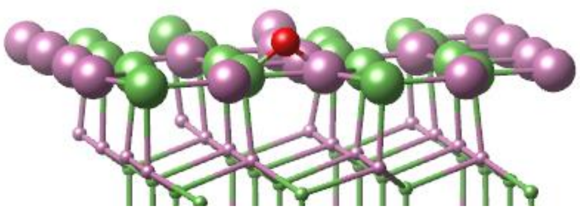
Potential Energy Surface of O atom on (111)A





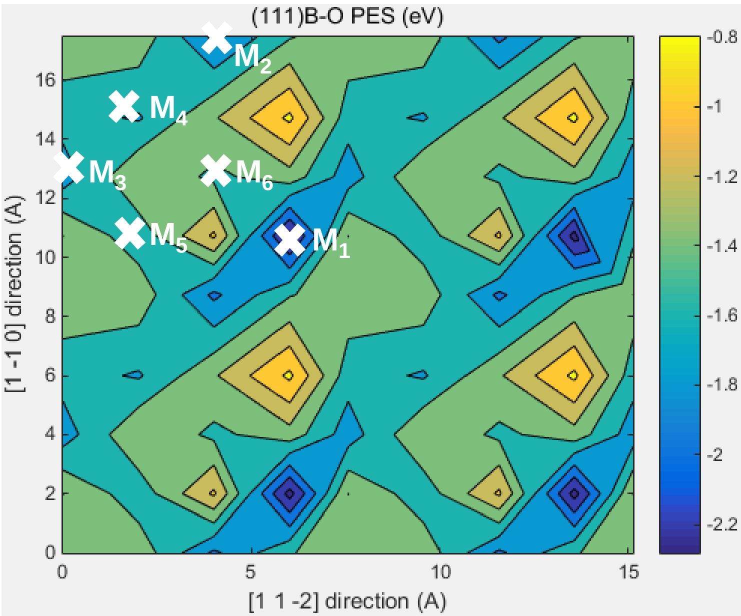
Adsorption energy & Stability

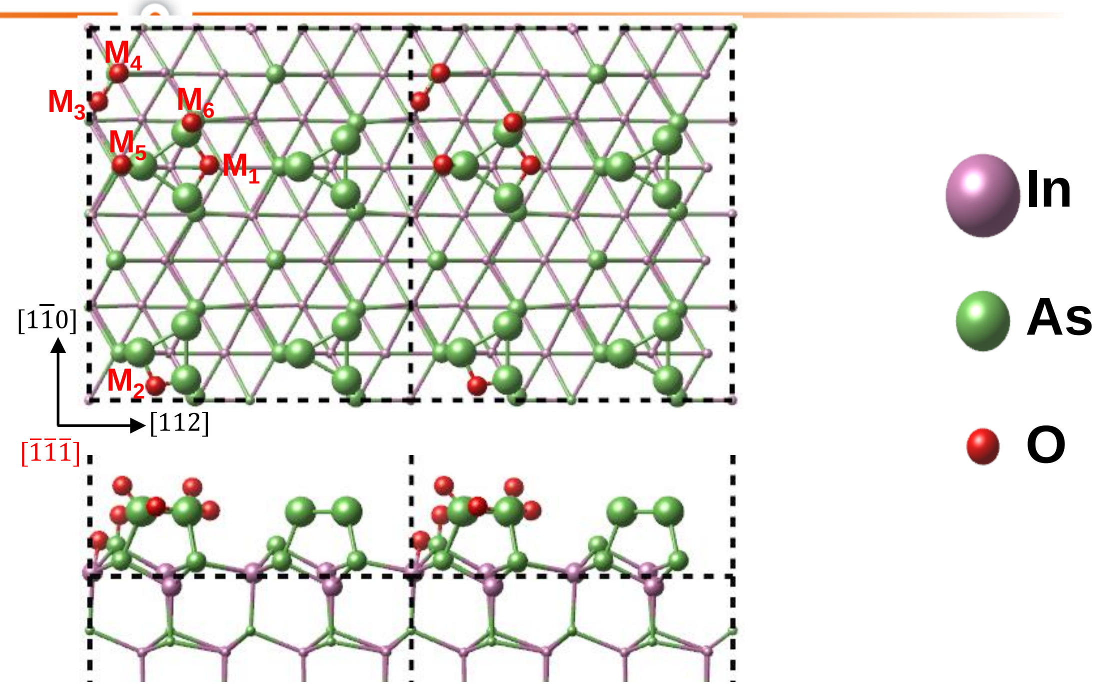
Site	M_1	M_2	M_3	M_4
E_{ads} (eV/O)	-1.85	-1.85	-1.85	-1.80



1st layer As-O-In
(M_1~M_4)

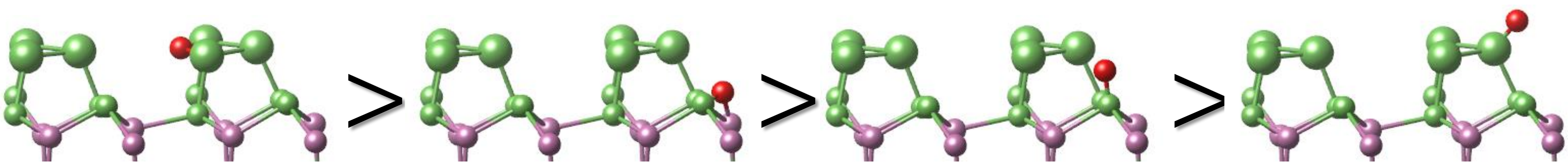
Potential Energy Surface of O atom on (111)B





Adsorption energy & Stability

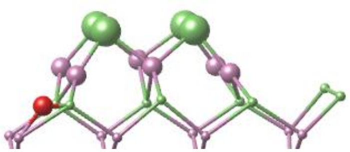
Site	M_1	M_2	M_3	M_4	M_5	M_6
E_{ads} (eV/O)	-2.51	-2.46	-2.22	-1.74	-1.64	-1.64



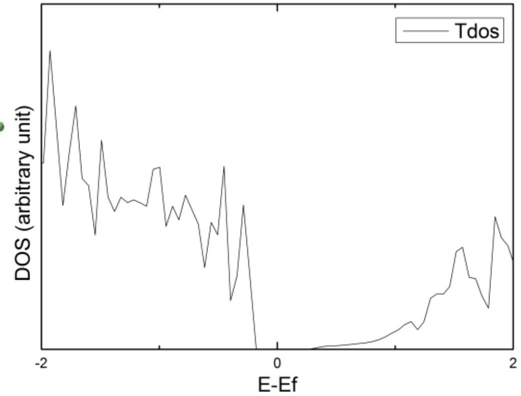
As-O-As (M_1~M_2) > As-O-In (M_3) > 2nd layer As=O (M_4) > 1st layer As=O (M_5~M_6)

The most stable O adsorption site and DOS

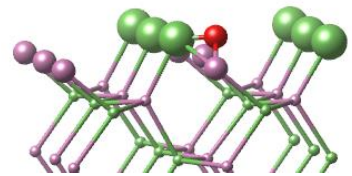
As-O-In on (100)



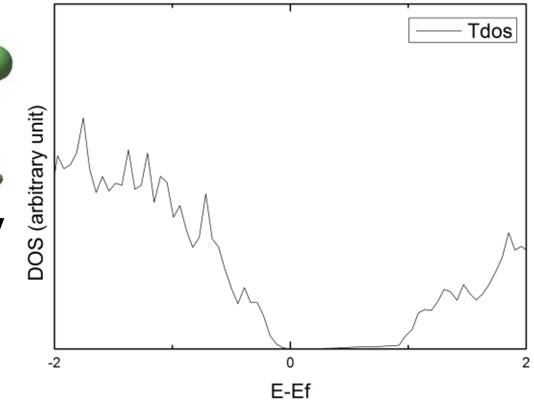
E_{ads} = -1.96 eV

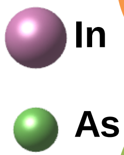


As-O-In on (110)

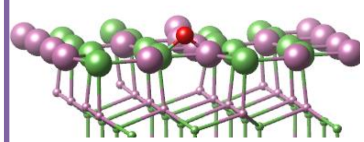


E_{ads} = -2.38 eV

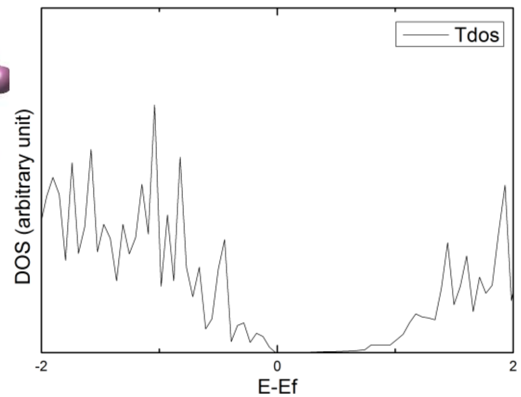




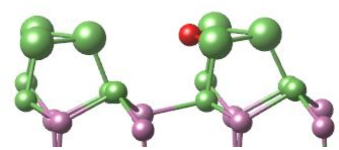
As-O-In on (111)A



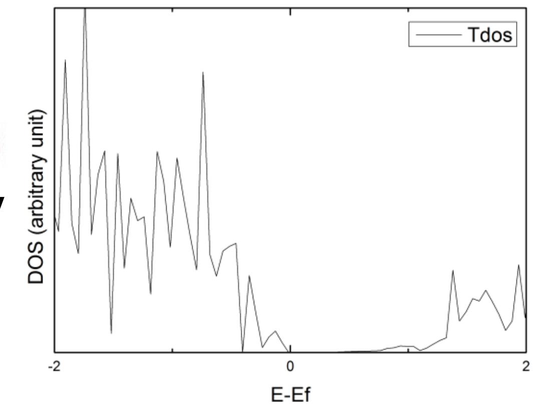
E_{ads} = -1.85 eV



As-O-As on (111)B

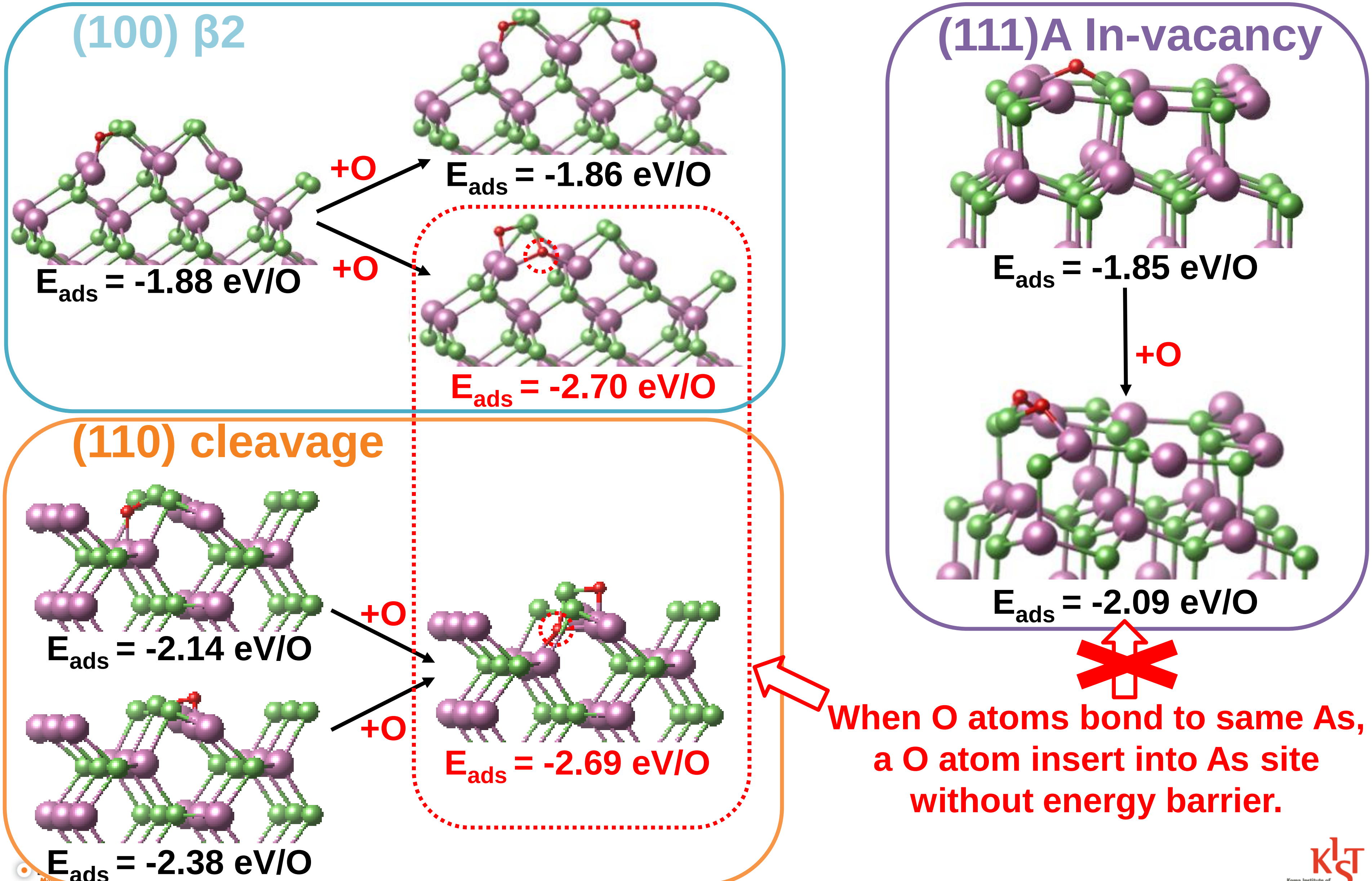


E_{ads} = -2.51 eV

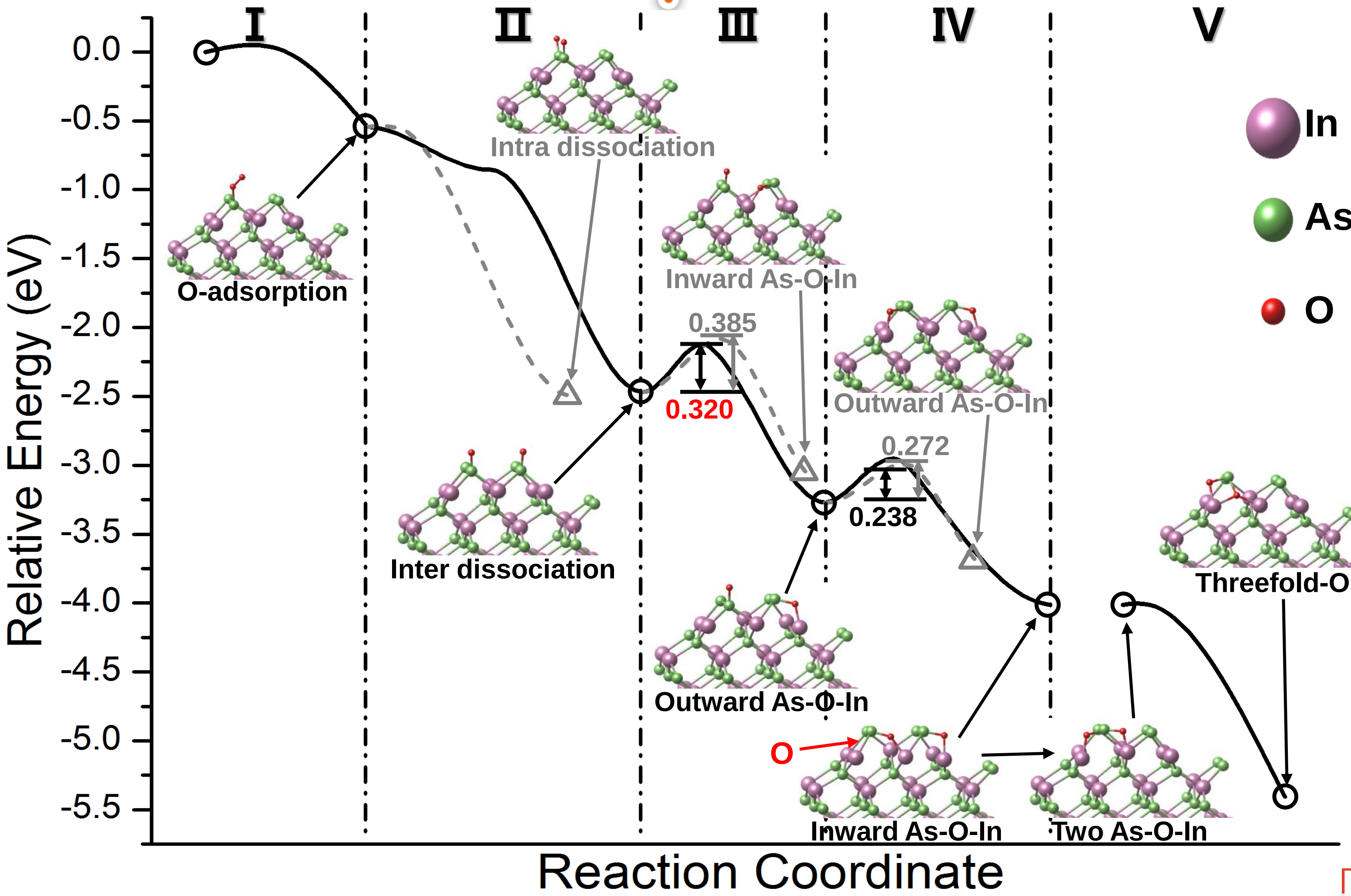


Atomic O adsorbed surfaces have no states in the gap.

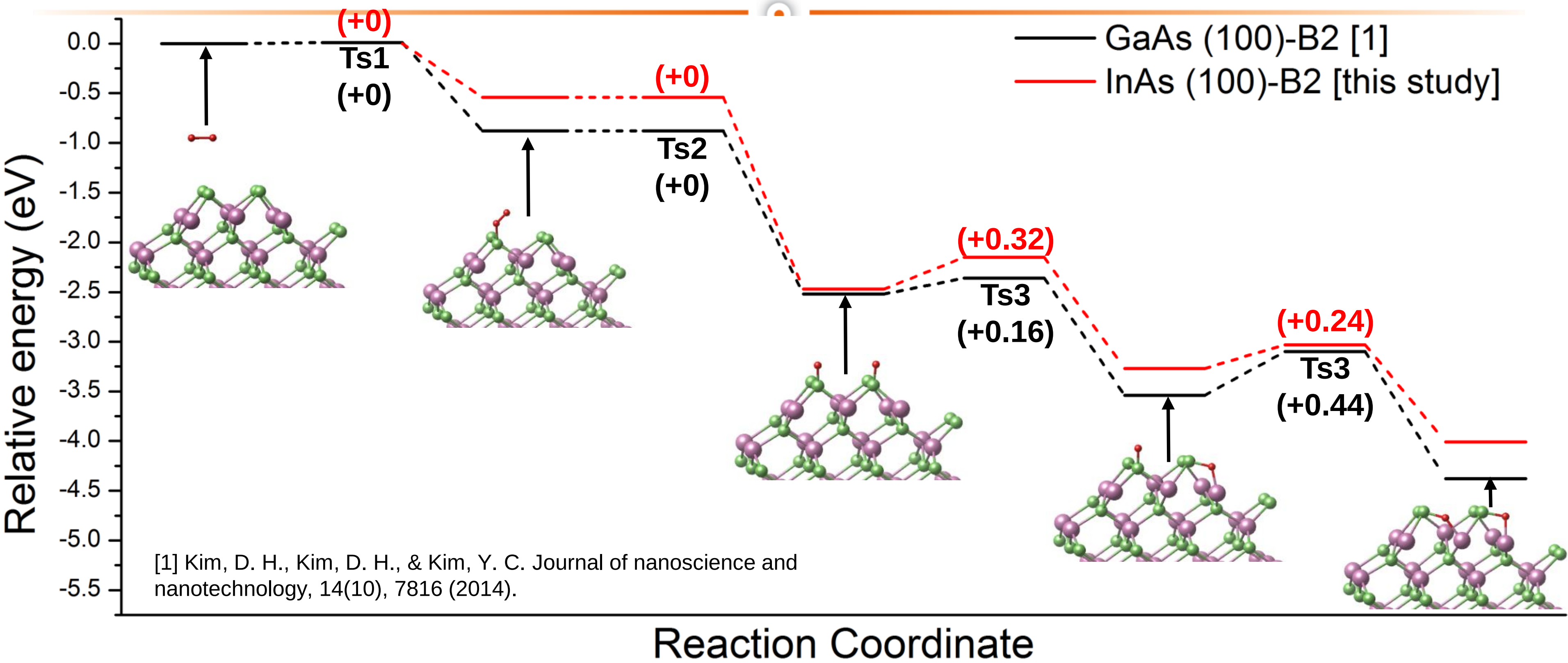
The mechanism of O_{As} antisite



Behavior of O_2 molecule on InAs(100)



Summary: comparison with GaAs surfaces



Orientation	Possibility to generate O_{As} by O_2	E_a (eV) for O_{as}
(100)	O	0.32 (c.f. 0.44 for GaAs)
(110)	O	Not yet
(111)A	X	-