Reconstruction structure of InAs surfaces and their effects on electronic structure

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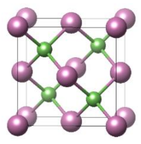
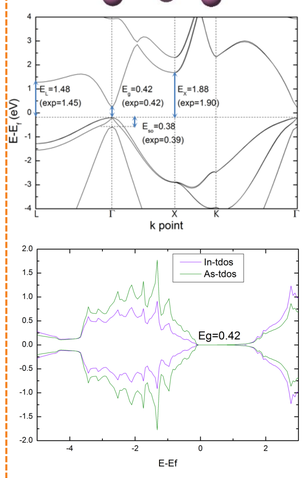
Computational Materials Design

INTRODUCTION

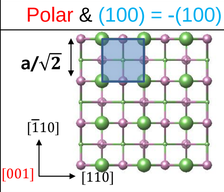
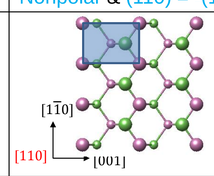
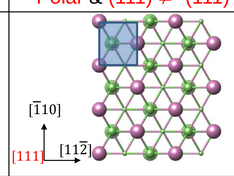
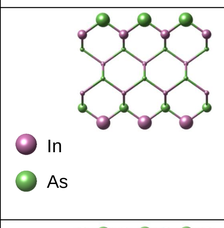
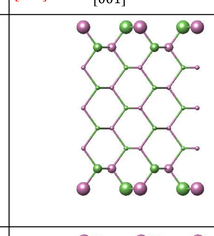
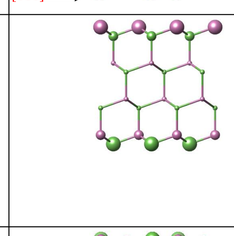
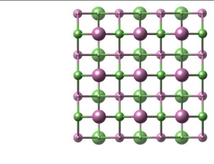
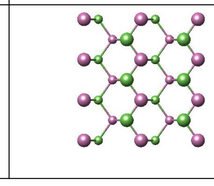
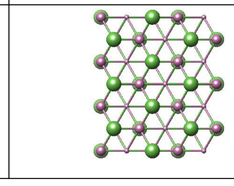
A. InAs Bulk





exposed to vacuum

B. InAs surface

	(100) Surface	(110) Surface	(111) Surface
	Polar & (100) = -(100)	Nonpolar & (110) = -(110)	Polar & (111) ≠ -(111)
Top			
Side			
bottom			

In
As

Any Change? ?

COPMUTATIONAL DETAILS

A. Computational details

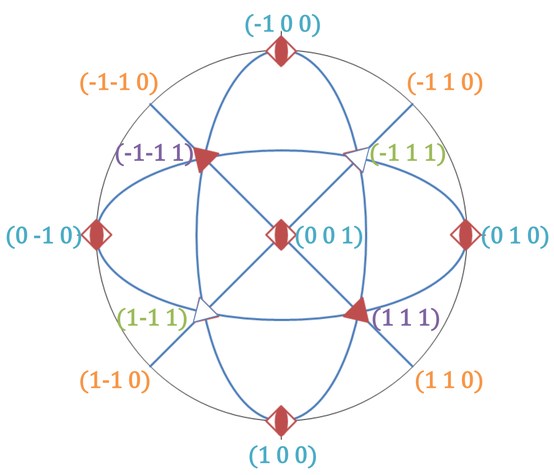
- Code : VASP (Vienna *ab-initio* Simulation Package)
- xc-functional : LDA-CA
- Cutoff energy : 300 eV
- k-points : converged for various slab structures
- Valence treatment : Ga=$3d^{10}4s^24p^1$, As=$4s^24p^3$, In=$4d^{10}5s^25p^1$
- Vacuum thickness : 10 Å
- The top 5 layers of the total 9 layers were allowed to move.
- The bottom layer was saturated with hydrogen and fixed.

B. Equilibrium condition

- $\mu_{In} + \mu_{As} = \mu_{InAs} = \mu_{In(bulk)} + \mu_{As(bulk)} - \Delta H_f$
- $0 < -\mu_{In} + \mu_{In(bulk)} = \mu_{As} - \mu_{As(bulk)} + \Delta H_f$
- $-\Delta H_f < \mu_{As} - \mu_{As(bulk)} < 0$
- $\gamma_{surface}A = E_{tot} - \mu_{In}N_{Ga} - \mu_{In}N_{As} = E_{tot} - \mu_{InAs}N_{In} - \mu_{As}(N_{As} - N_{In})$

METHODOLOGY

A. Polar InAs {111}



In-terminated surface = (111)A
: (111), (-1-1 1), (1 -1-1), (-1 1-1)

As-terminated surface = (111)B
: (-1-1-1), (1 1-1), (-1 1 1), (1-1 1)

B. Calculation procedure for surface energy

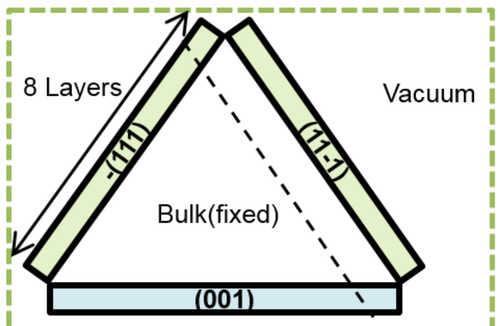
i. Vacuum layer / **(100)** / H-covered layer (fixed) / Bulk(fixed) / **-(100)** / H-covered layer (fixed)

$\gamma_{(100),(110)\text{-}H} = (E_{tot} - \mu_{Ga}N_{Ga} - \mu_{As}N_{As})/2A$

ii. Vacuum layer / **(100)** / Relaxed surface / Bulk(fixed) / **-(100)** / H-covered layer (fixed)

$\gamma_{(100),(110)} = (E_{tot} - \mu_{Ga}N_{Ga} - \mu_{As}N_{As})/A - \gamma_{(100),(110)\text{-}H}$

i. Vacuum layer / **(110)** / Bulk(fixed) / **-(110)**



$\delta E = E_{tot}(n=8;\ 36AB) - E_{tot}(n=7;\ 28AB) - 8\mu_{AB} = 2\gamma_{(-1-1-1)\text{-}H} + \gamma_{(-1\,0\,0)\text{-}H}$

ii. Vacuum layer / **(111)** / Bulk(fixed) / **-(111)**

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

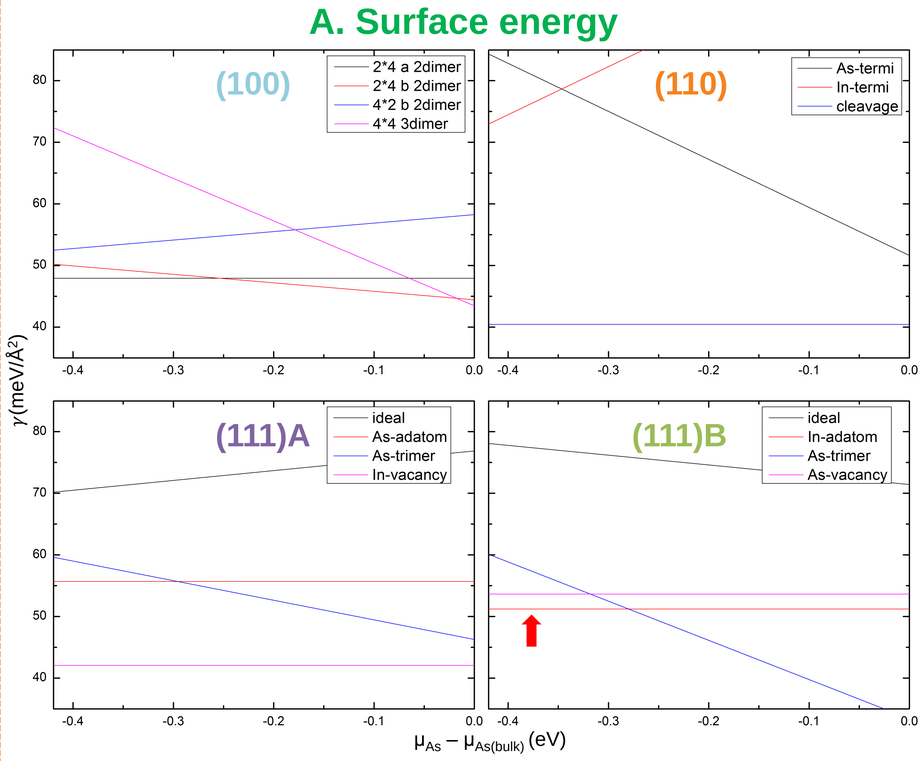
iii. Vacuum layer / **(111)** / Bulk(fixed) / **-(111)** ; Vacuum layer / **(111)** / **-(111)**

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

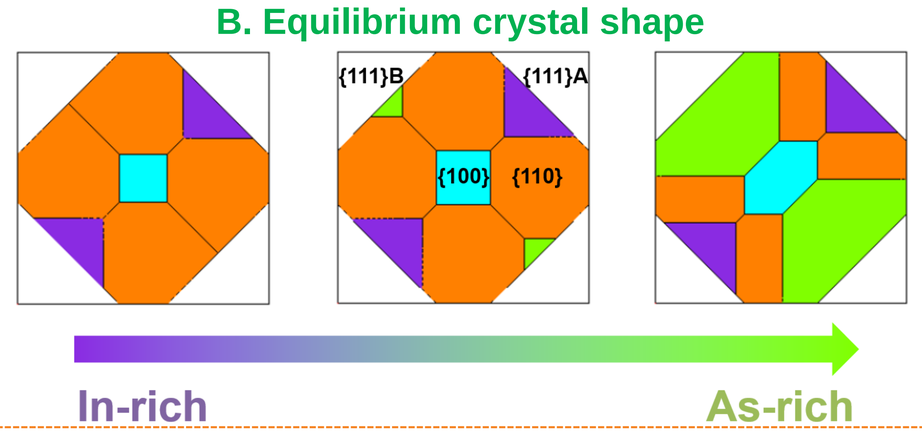
Summary
Top=Bottom → Slab geometry
Top≠Bottom → Prism geometry to separate two different surfaces

Results & discussions

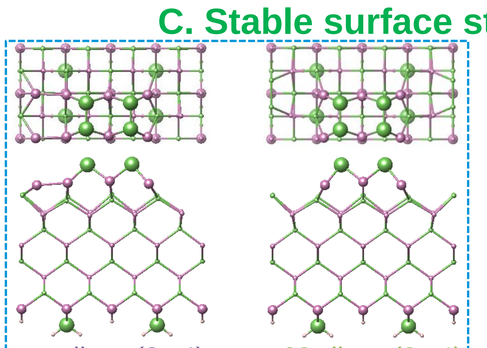
A. Surface energy



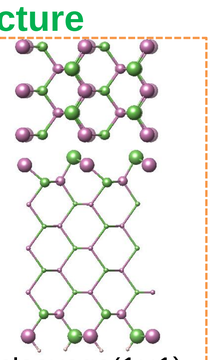
B. Equilibrium crystal shape



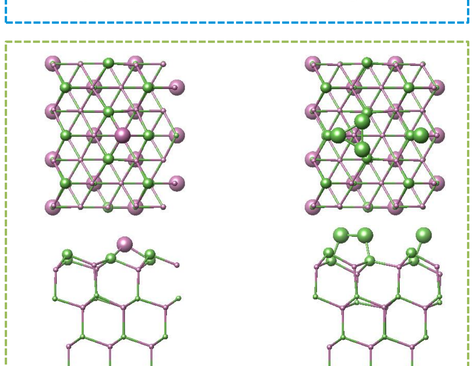
C. Stable surface structure



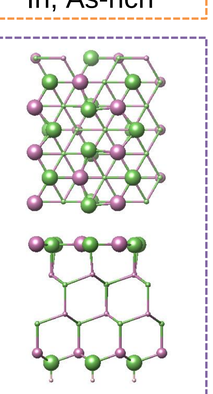
α-dimer(2×4) In-rich
β2-dimer(2×4) As-rich



cleavage(1×1) In, As-rich

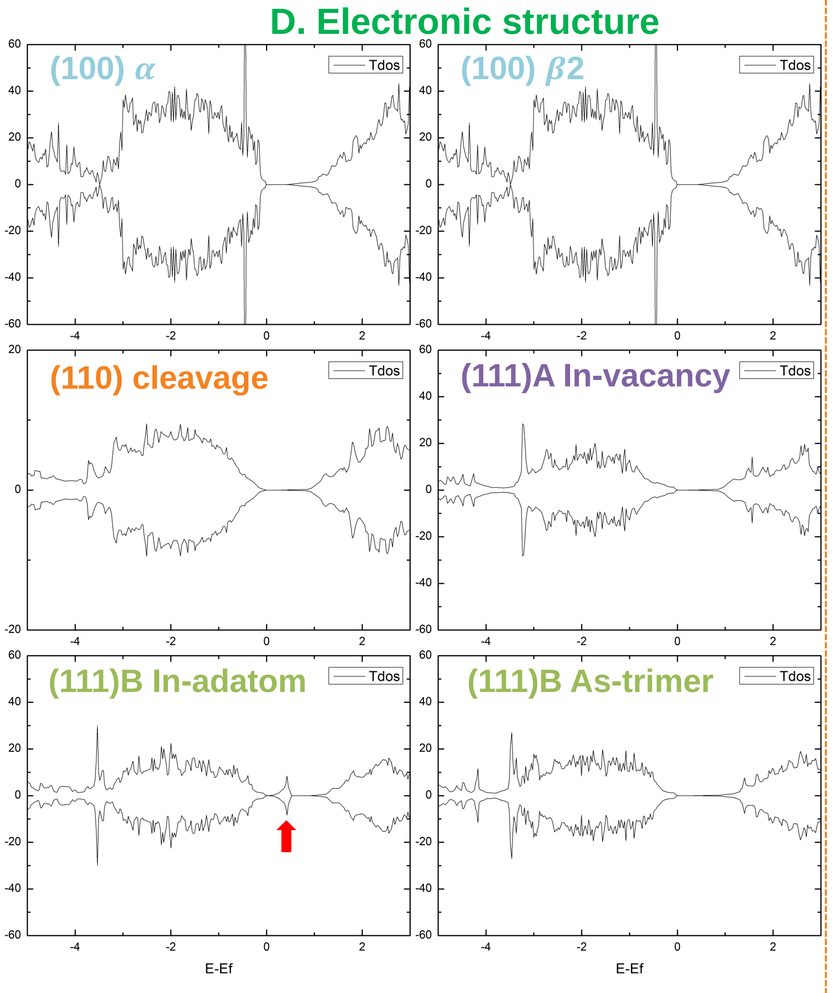


In-adatom(2×2) In-rich
As-trimer(2×2) As-rich



In-vacancy(2×2) In, As-rich

D. Electronic structure



Summary
A. The most stable orientation? (110) at In-rich → (111)B at As-rich
B. All surface orientations exist? (111)B does not exist at In-rich → (111)B dominates at As-rich
C. How to lower surface energy? Atom addition and reconstruction of the polar surfaces
D. States in the band gap? Only for (111)B In-adatom at In-rich condition, but it does not exist at the equilibrium condition

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