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# Impact of surface passivation of III-V elements on Si (001) substrate based on absolute surface and barrier energy calculations

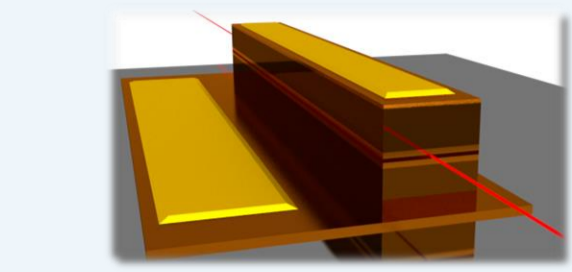
Sreejith Pallikkara Chandrasekharan<sup>1,\*</sup>, Divishth Gupta<sup>1</sup>, Laurent Pedesseau<sup>1</sup>, Charles Cornet<sup>1</sup>

(1) Univ Rennes, INSA Rennes, CNRS, Institut FOTON-UMR 6082, F-35000, Rennes, France.

## Introduction

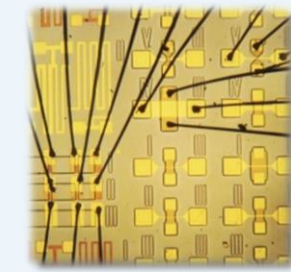
Integrating III-V compound semiconductors on (001) Si substrates is a long-standing challenge, which has driven many researches for the past 40 years. A large portfolio of passive photonic devices and their mature fabrication technology are available on the Si platform. This gives greater flexibility to design photonics integrated circuits (PICs) as compared to the pure III-V technologies and opens a number of possibilities for e.g. lasers, photovoltaic energy production, or energy storage via solar hydrogen production.

### Active photonics



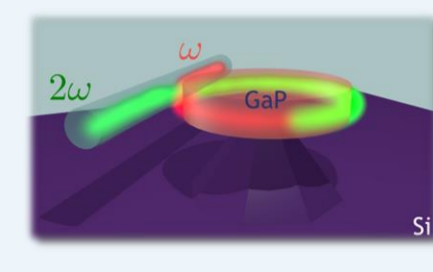
- Direct bandgaps in III-V materials for integrated lasers
- H. Liu et al., Nature Photonics 10 (5), 307 (2016) - UCL
- J. Bowers, J. Kippenberg et al. Nature 557, 81 (2018) - UCLA, EPFL, CIT, etc...

### Electronics



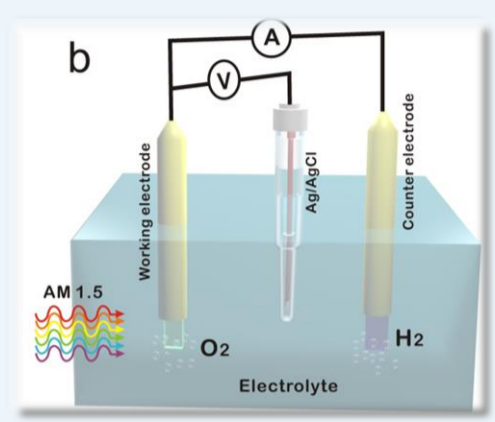
- High carriers mobilities in III-V materials for advanced CMOS concepts
- L. Ciomamaz et al., Proc. of Symposium on VLSI Technology (2015) - IBM
- C. Merckling et al. ECS Trans. 61, 107 (2014) - IMEC

### Passive photonics



- Non-linear properties of III-V materials for integrated passive devices (frequency comb generation):
- G. Roelkens et al., Opt. Express 23, 4650 (2015), Ghent Univ.-IMEC
- M. M. Fejer et al. Opt. Express 26, 26971 (2018), Stanford Univ.

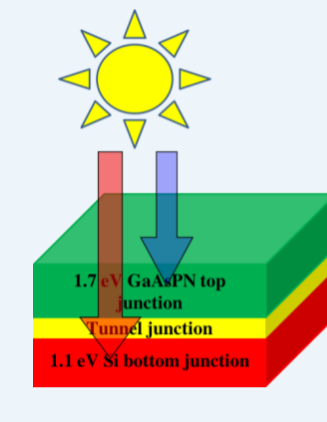
### Water splitting



- High efficiency III-V/Si photoelectrodes for solar hydrogen production
- R. Nötzel et al., Nat. Com. (2018), South China Normal Univ.
- L. Lucci et al., Adv. Funct. Mater. 28, 1801585 (2018), FOTON Inst.

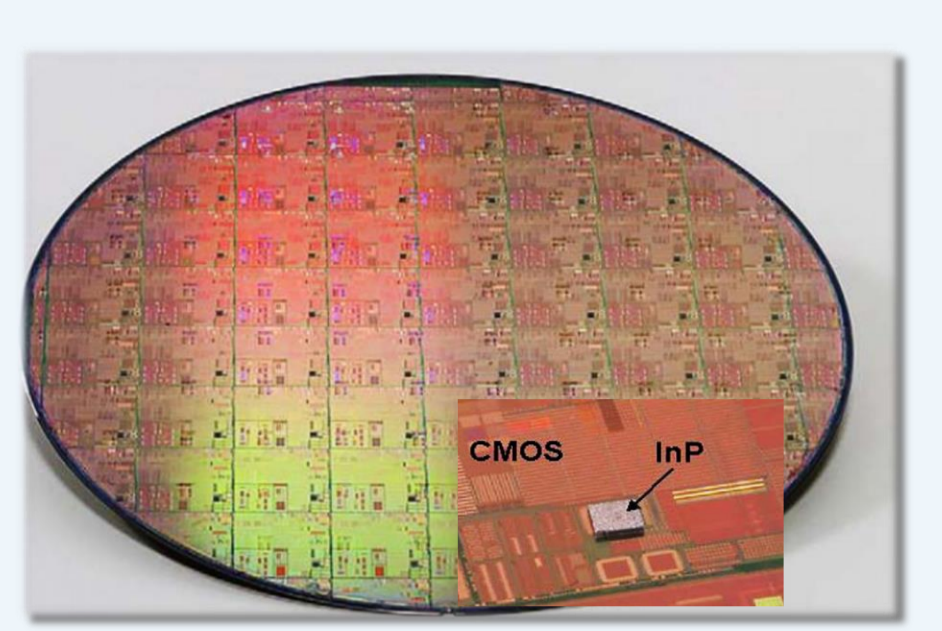
## III-V/Si co-integration

### Photovoltaics

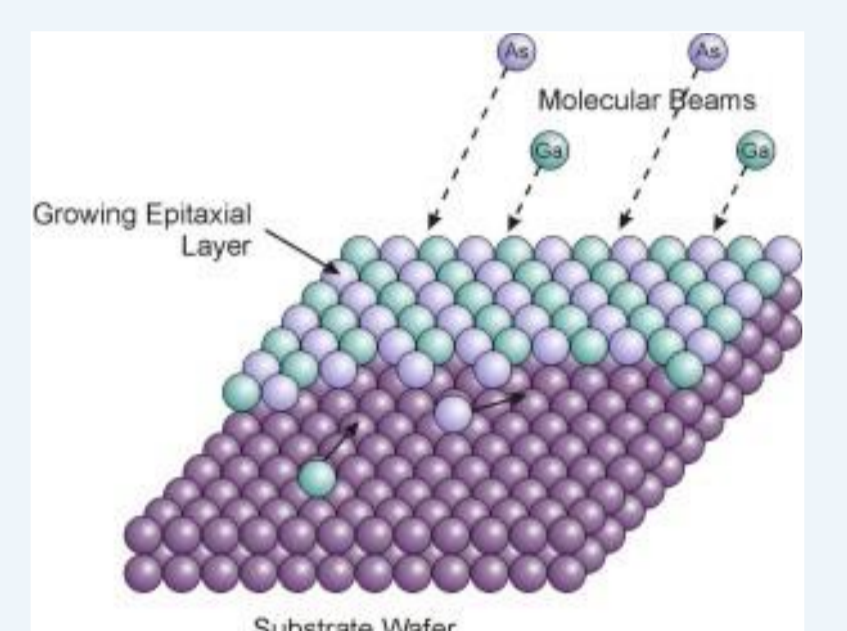


- Bandgap engineering in III-V/Si for high efficiency multijunction architectures.
- K. Volt, T. Hannappel et al., IEEE J. Photovolt. 9, 1 (2018), Marburg Univ., Ilmenau Univ.

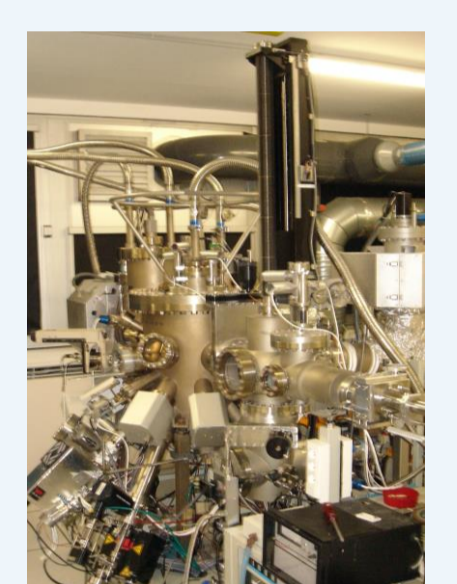
### Bonding strategies



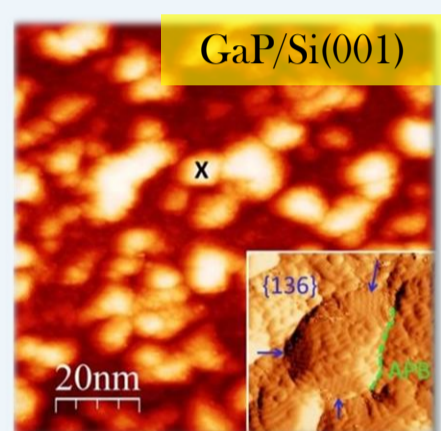
### Monolithic integration



### III-V/Si crystal growth by MBE



### Experiments

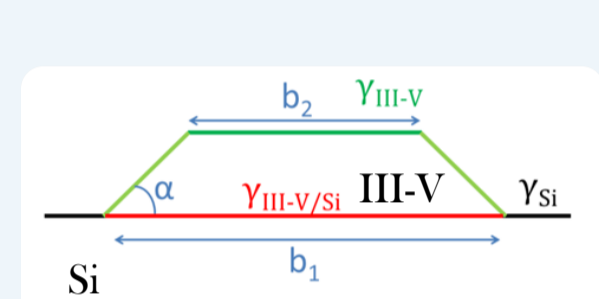


→ 3D growth  
→ Large impact on defects generation

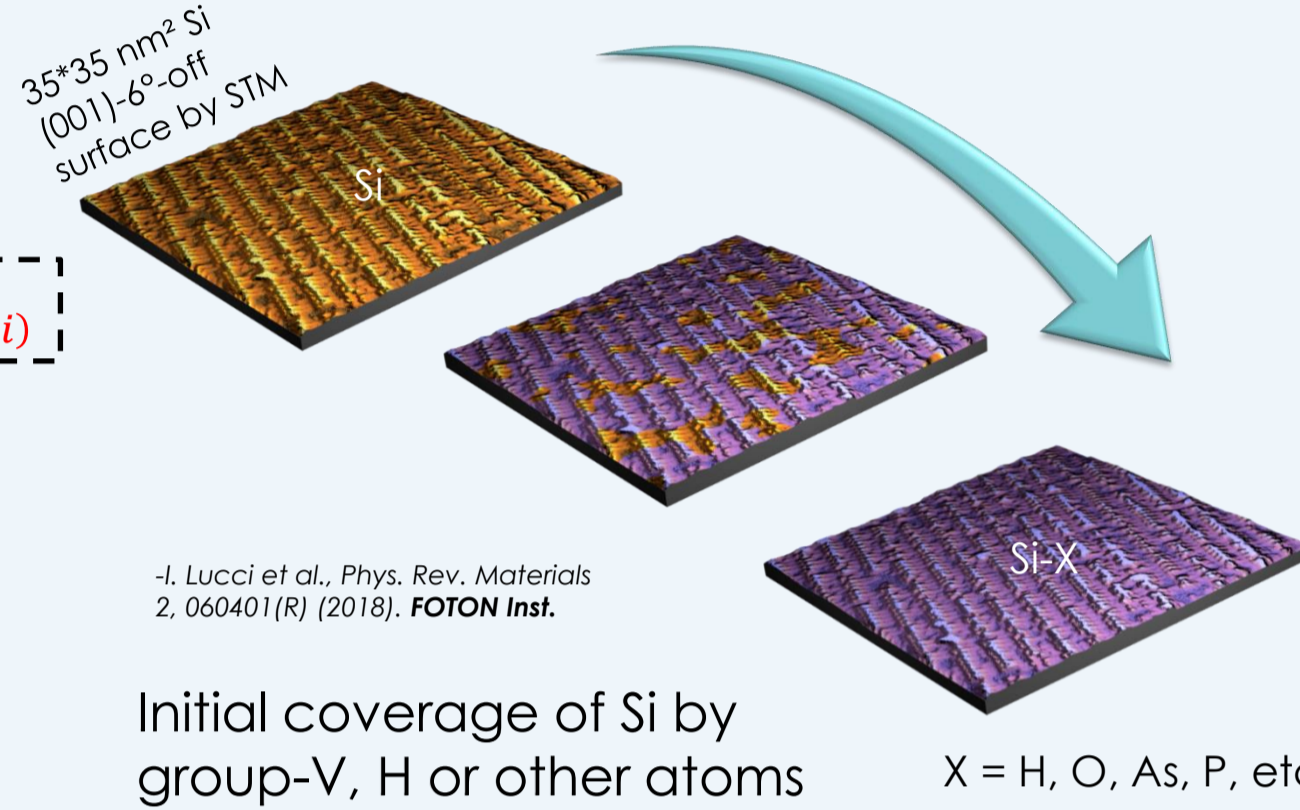
-J. Lucci et al., Phys. Rev. Materials 2, 060401 (2018), FOTON Inst.

### Wetting

$$\Omega = \gamma^S(Si) - \gamma^S(III-V) - \gamma^I(III-V/Si)$$



-Pedesseau et al., arXiv:2303.15566 (2023), FOTON Inst.



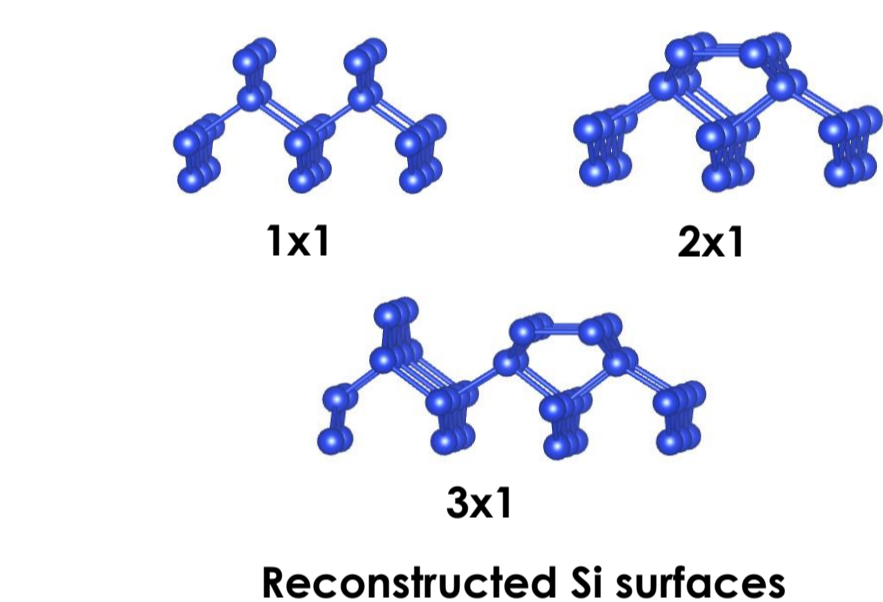
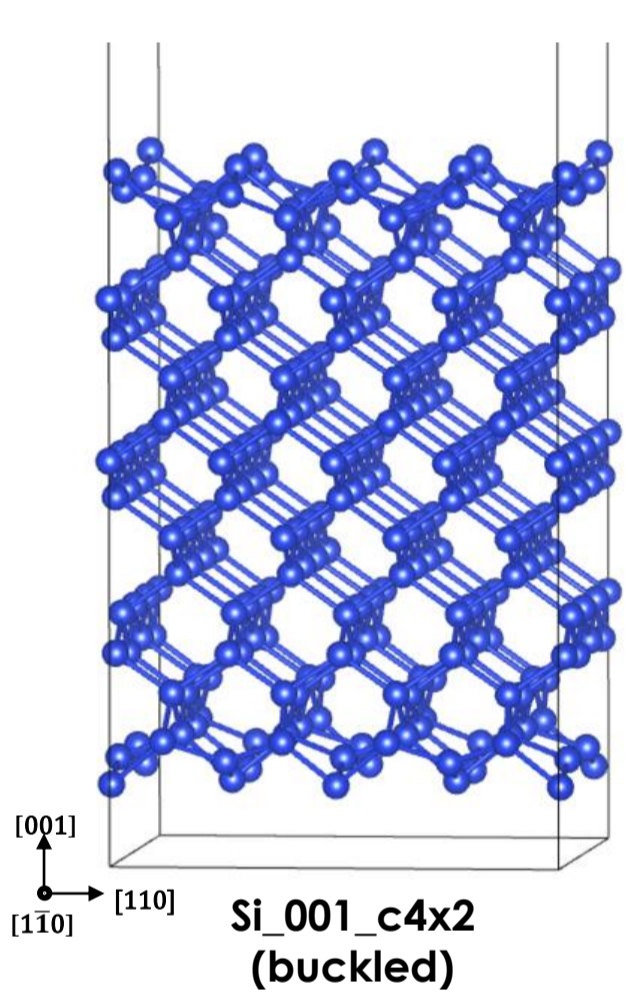
35x35 nm<sup>2</sup> Si(001)-4x8-off surface by STM

-L. Lucci et al., Phys. Rev. Materials 2, 060401 (R) (2018), FOTON Inst.

Initial coverage of Si by group-V, H or other atoms

X = H, O, As, P, etc...

## Surface



System	Surface energy calculated	Reference [1-4]
c4x2	89.37 meV/Å <sup>2</sup>	88.0-92.8 meV/Å <sup>2</sup>
1x1	146.15 meV/Å <sup>2</sup>	147.1-149.1 meV/Å <sup>2</sup>
2x1	98.68 meV/Å <sup>2</sup>	90.5-94.1 meV/Å <sup>2</sup>
3x1	119.55 meV/Å <sup>2</sup>	-

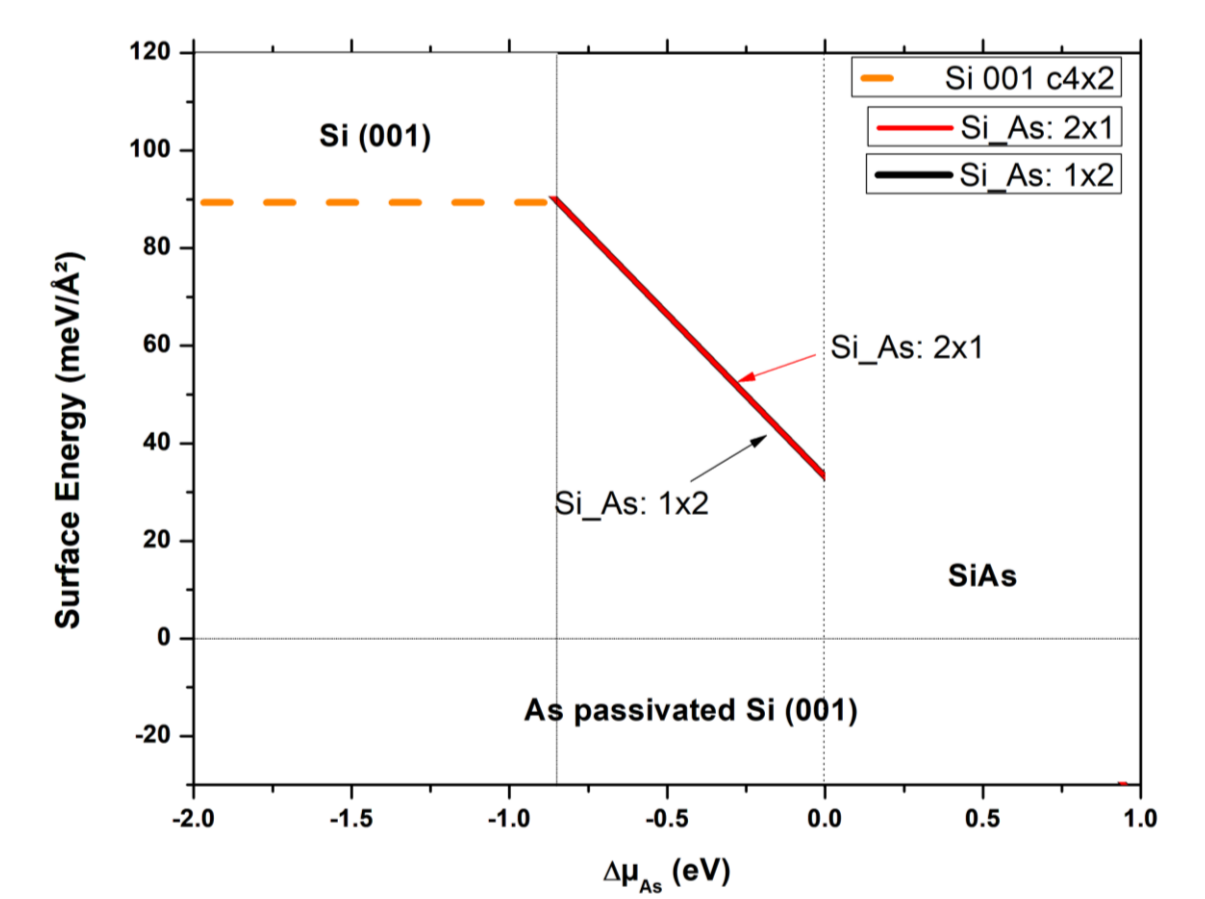
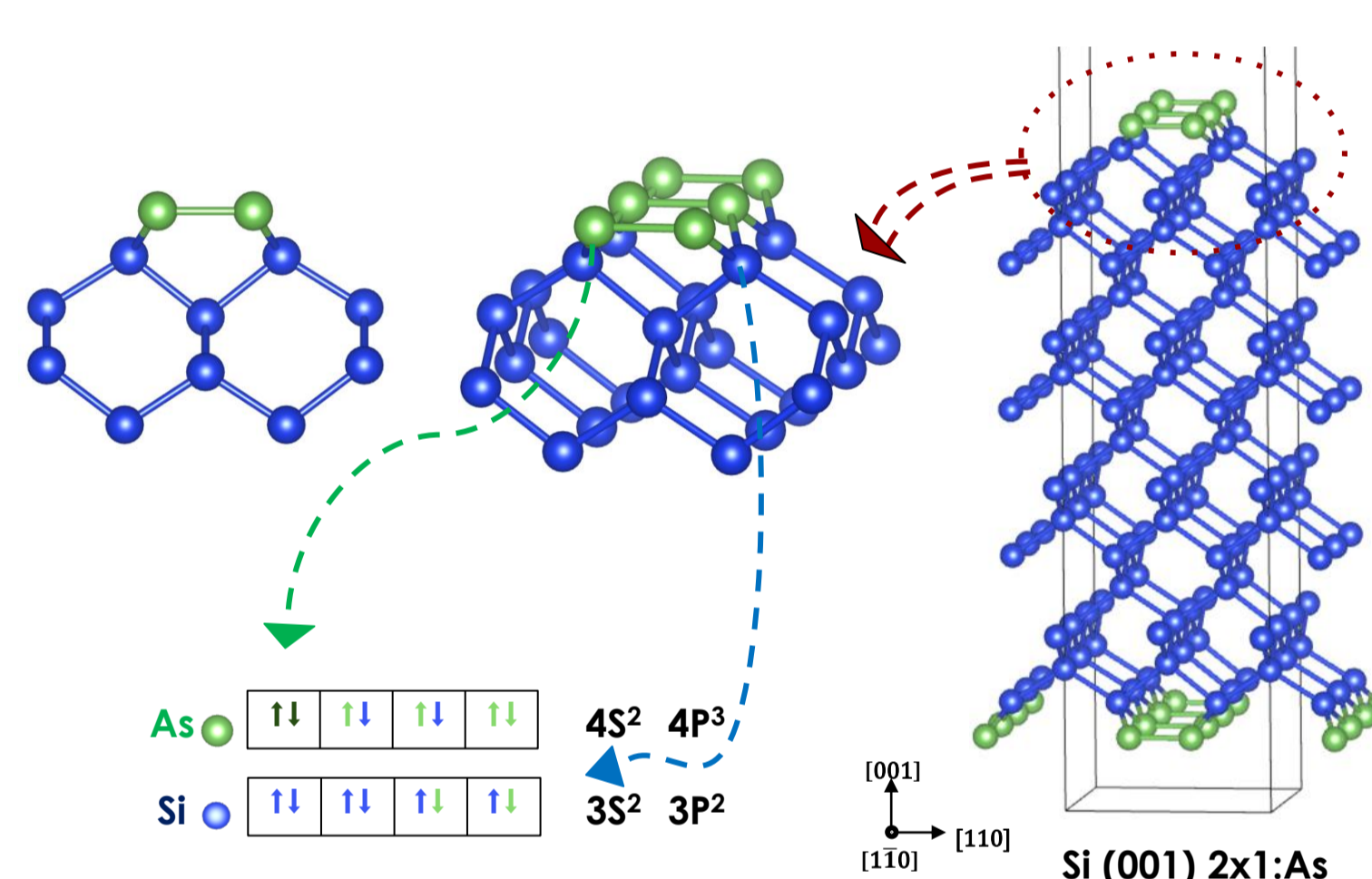
### Surface Energy

$$E_{surf} = \frac{E_{slab} - (N_{atom} * \mu_{atom})}{2A}$$

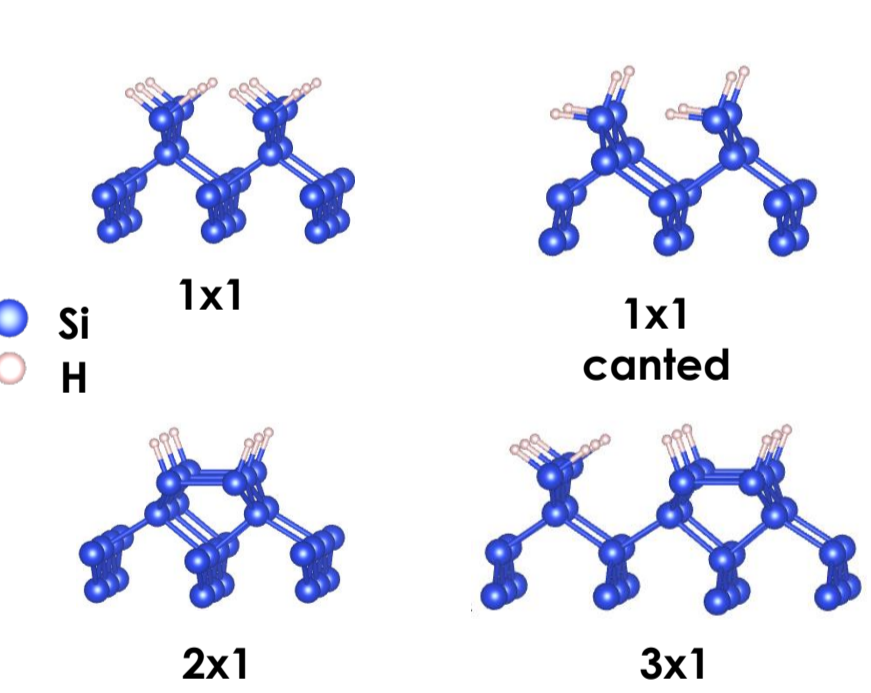
siesta

- Lu, Guang-Hong, et al. "Relative stability of Si surfaces: A first-principles study." Surface science 588, 1-3 (2005): 61-70.
- A.A. Stekolnikov, J. Furthmüller, F. Bechstedt, Phys. Rev. B 65 (2002) 115318
- A.A. Stekolnikov, J. Furthmüller, F. Bechstedt, Phys. Rev. B 67 (2003) 195332
- Lucci, Ido, et al. "Universal description of III-V/Si epitaxial growth processes." Physical Review Materials 2, 6 (2018): 060401.

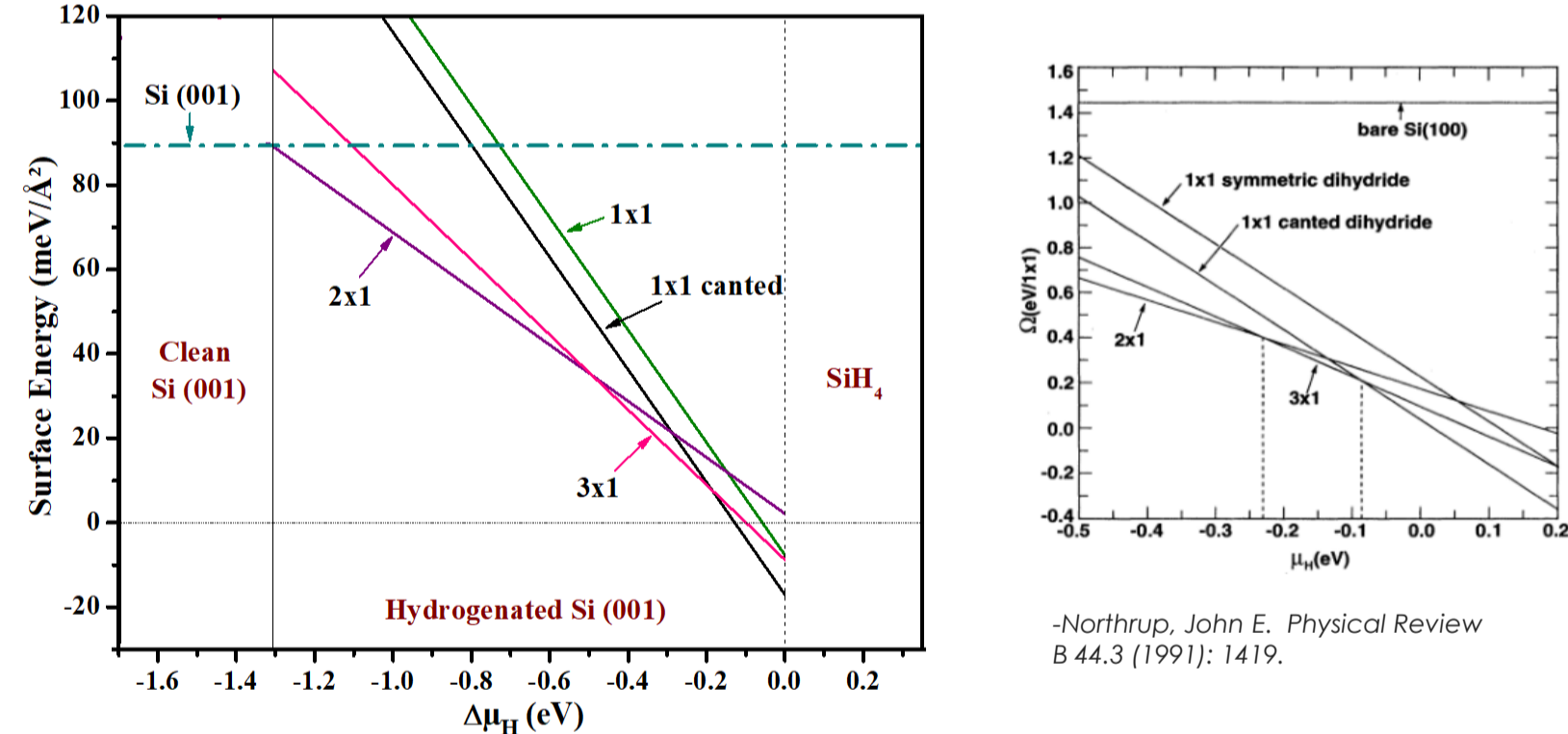
## Group V passivation on Si (001)



## H passivation on Si (001)

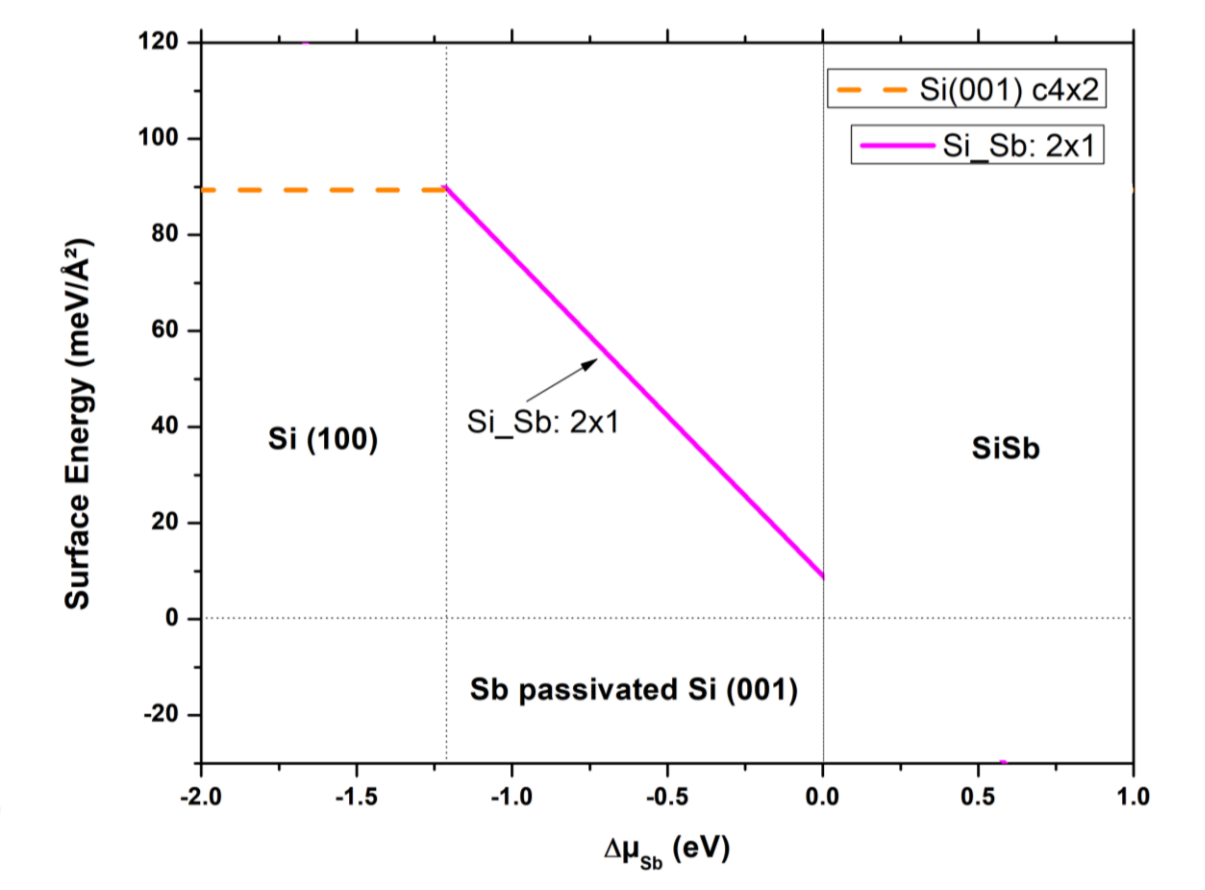
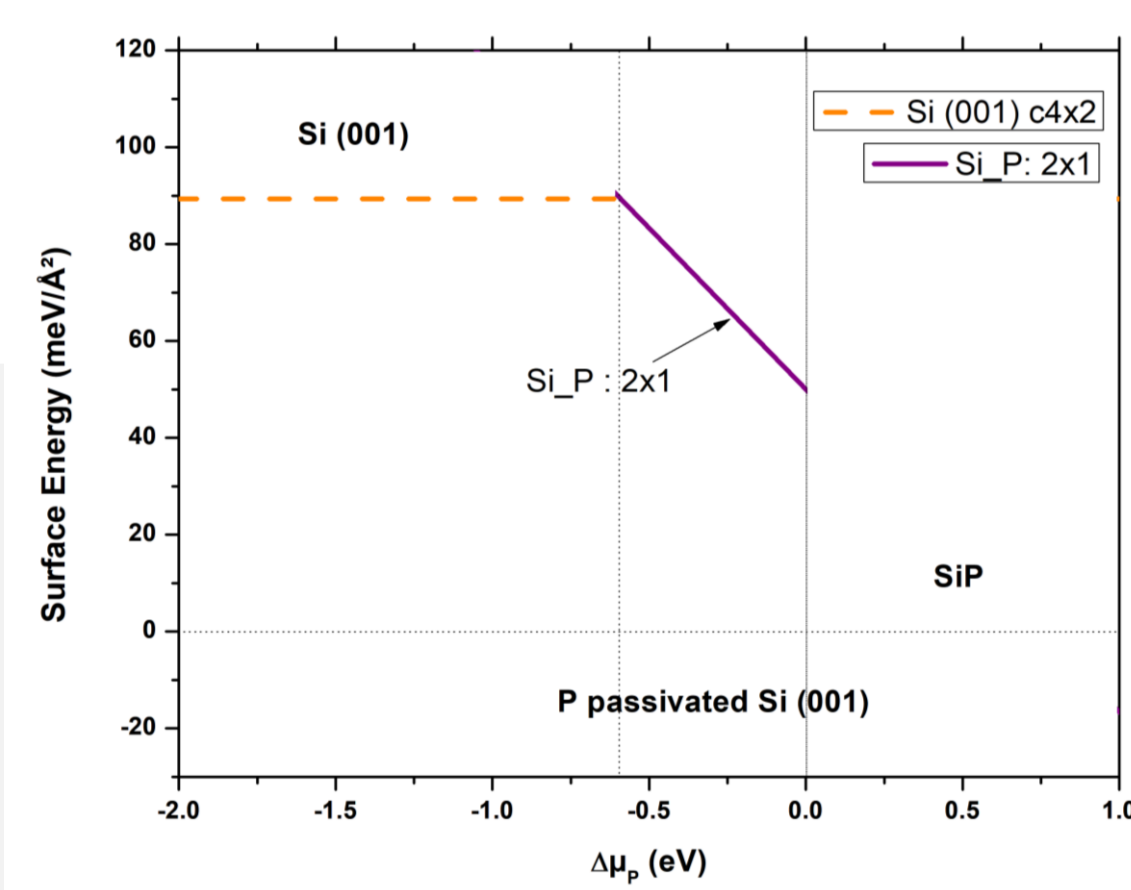


### Validation of the methodology.

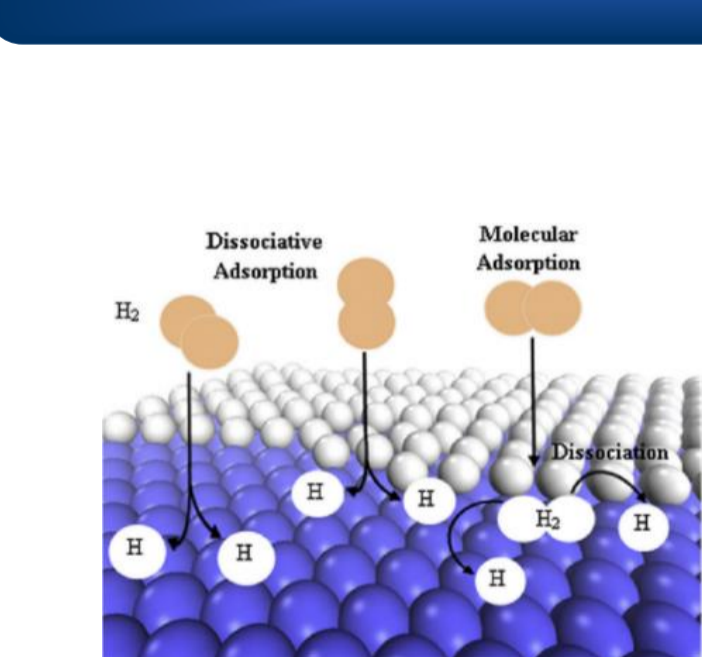


"Adapted Similar technique for other group V elements"

"First results of surface passivation diagrams of group V elements on Si (001) substrate in terms of chemical potential"



## Energy barrier

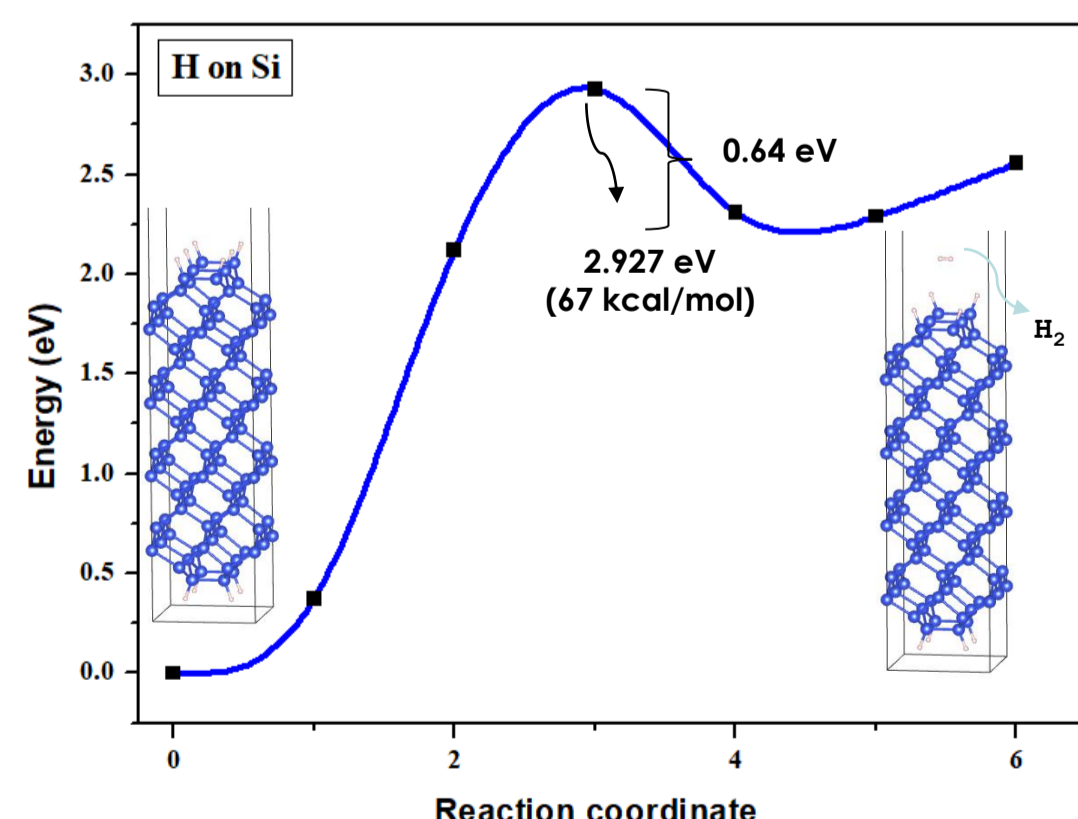


### Nudged Elastic Band Method

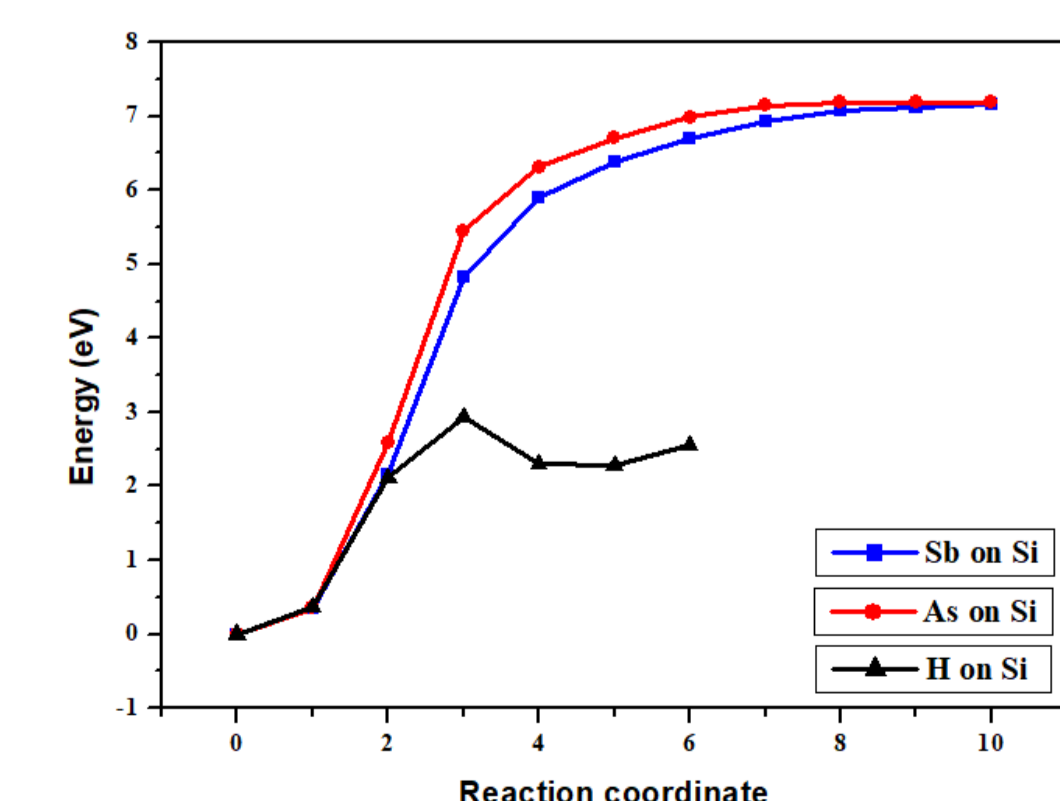
"As desorption on Si (001) behaves like molecular adsorption not dissociative adsorption for H on Si"

"The first results show that group V elements on Si (001) substrate are more stable than H"

### Validation of the methodology.



- Dür, Michael, and U. Höfer. Surface science reports 61, 12 (2006): 465-526.
- Wu, Christine J., Ilna V. Ionova, and Emily A. Carter. Surface science 295, 1-2 (1993): 64-78.



## Conclusions

- Absolute surface energies of Si (001) surfaces with mono or sub-atomic layers of H and group V elements.
- Energy barrier calculation to study the desorption of different passivating elements from the Si surface.

## Prospects

- The surface and interface energies calculations for III-V/Si.
- The influence of dislocations and antiphase boundaries.

## Acknowledgements

This research was supported by the French National Research NUAGES Project (Grant no. **ANR-21-CE24-0006**). DFT calculations were performed at FOTON Institute, and the work was granted access to the HPC resources of TGCC/CINES under the allocation **A0120911434** and **A0140911434** made by GENCI.