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Absolute surface and interface energy analysis of III-V/Si and its consequences on wetting characteristics

S. Pallikkara Chandrasekharan^{1,*}, I. Lucci¹, D. Gupta¹, C. Cornet¹, L. Pedesseau¹

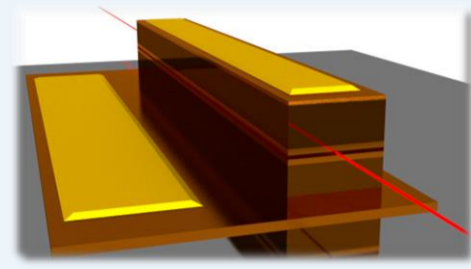
(1) Univ Rennes, INSA Rennes, CNRS, Institut FOTON-UMR 6082, F-35000, Rennes, France.

Introduction

The epitaxial growth of heterogeneous materials with different physical properties is of greatest interest in materials science, as they enable huge promise, especially in integrated photonics, electronics and energy harvesting applications. Such heterogeneous material associations strongly depend on the hybrid interface atomic configurations. Thus, a quantitative determination of interface energies impacts the description of the wetting properties of the system.

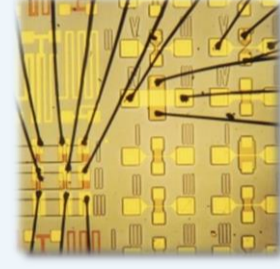
III-V/Si integration

Active photonics



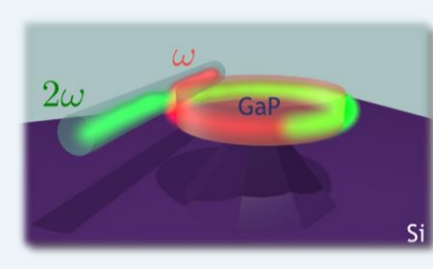
- Direct bandgaps in III-V materials for integrated lasers
- H. Liu et al., *Nature Photonics* 10 (5), 307 (2016), **UCL**
- J. Bowers, J. Kippenberg et al. *Nature* 557, 81 (2018), **UCLA, EPFL, CIT, etc...**
- M. R. Calvo et al., *Optica* 7, 263 (2020), **IES- Uni. of Montpellier**

Electronics



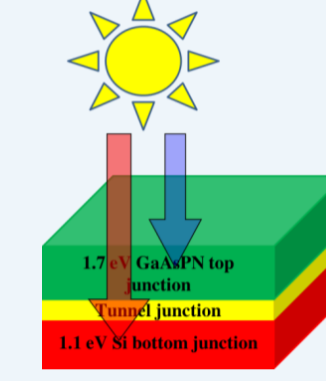
- High carriers mobilities in III-V materials for advanced CMOS concepts
- L. Ciomaz et al., *Proc. of Symposium on VLSI Technology* (2015), **IBM**
- C. Merckling et al. *ECS Trans.* 61, 107 (2014), **IMEC**

Passive photonics



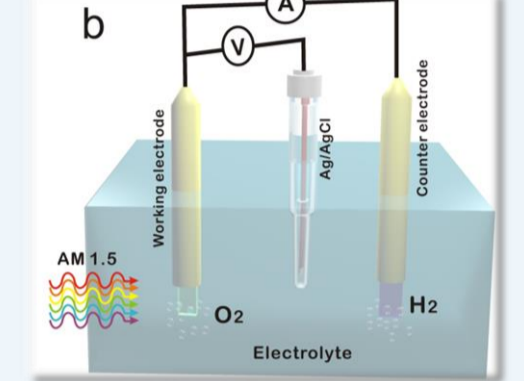
- Non-linear properties of III-V materials for integrated passive devices (frequency comb generation)
- G. Roelkens et al., *Opt. Express* 23, 4650 (2015), **Ghent Uni.- IMEC**
- M. M. Fejer et al. *Opt. Express* 26, 26971 (2018), **Stanford Uni.**

Photovoltaics



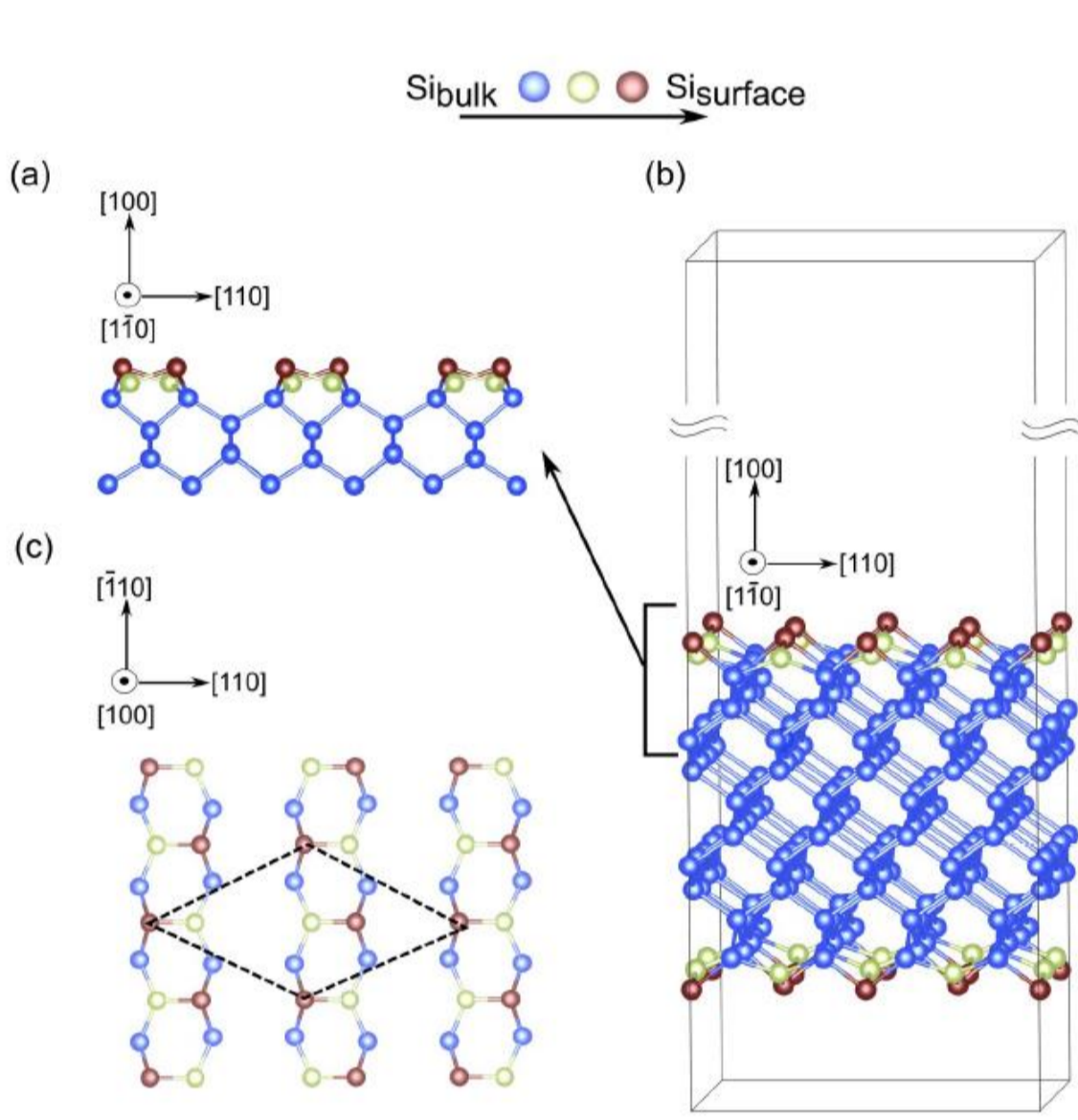
- Bandgap engineering in III-V/Si for high efficiency multijunction architectures
- K. Vola, T. Harnappel et al., *IEEE J. Photovolt.* 99, 1 (2018), **Marburg Uni., Ilmenau Uni.**

Water splitting



- High efficiency III-V/Si photo-electrodes for solar hydrogen production
- R. Nötzel et al., *Nat. Com.* (2018), **South China Normal Uni.**
- L. Chen et al., *Adv. Sci.* 9, 2101661 (2022); M. Pilyev et al., *Sol. Energy Mater. Sol. Cells* 251, 112138 (2023), **FOTON Inst.**

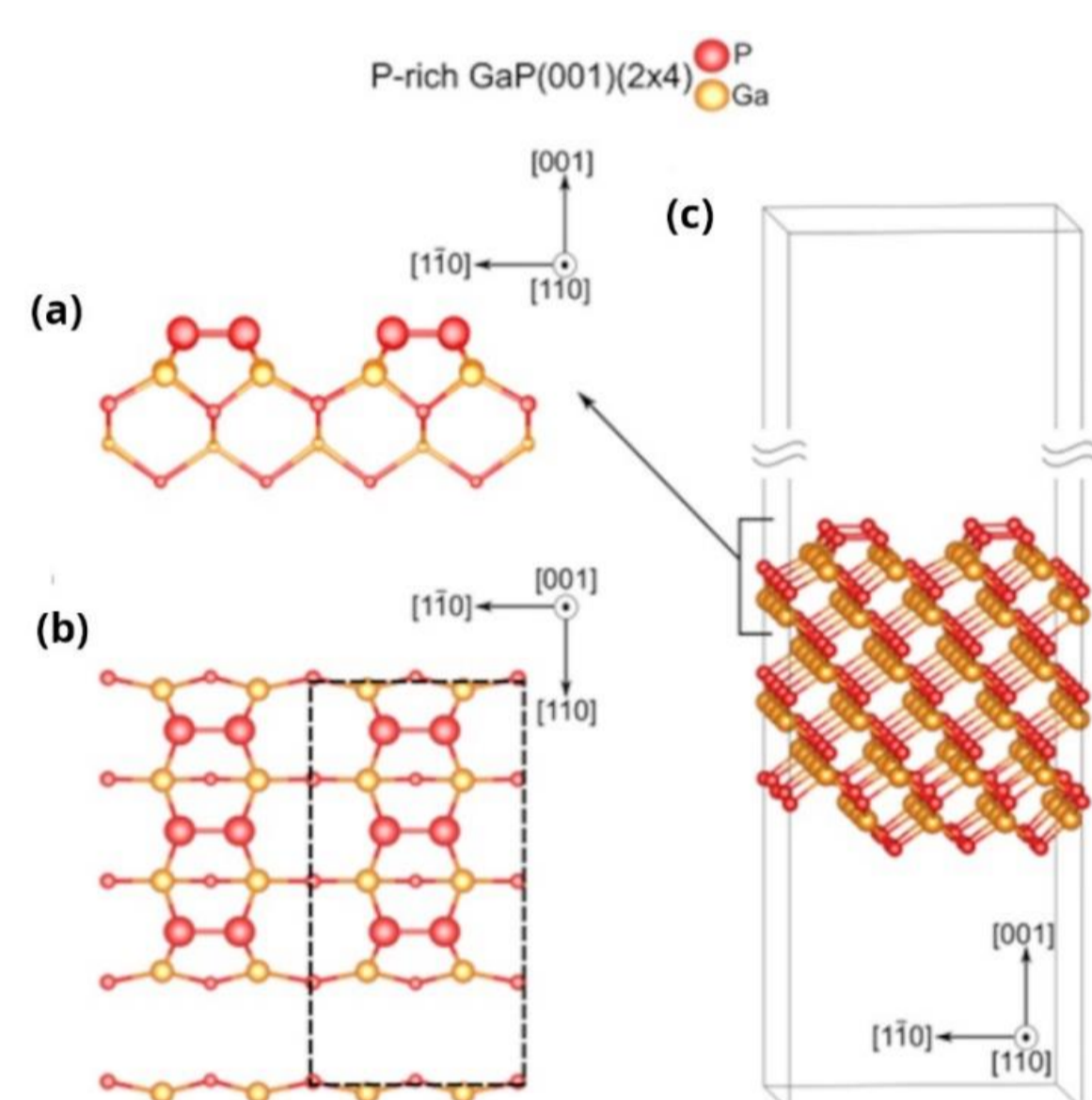
Absolute surface energies



Si(001) surface

$$\gamma_{Si} = \frac{E_{slab} - N_{Si}\mu_{Si}^{bulk}}{2A}$$

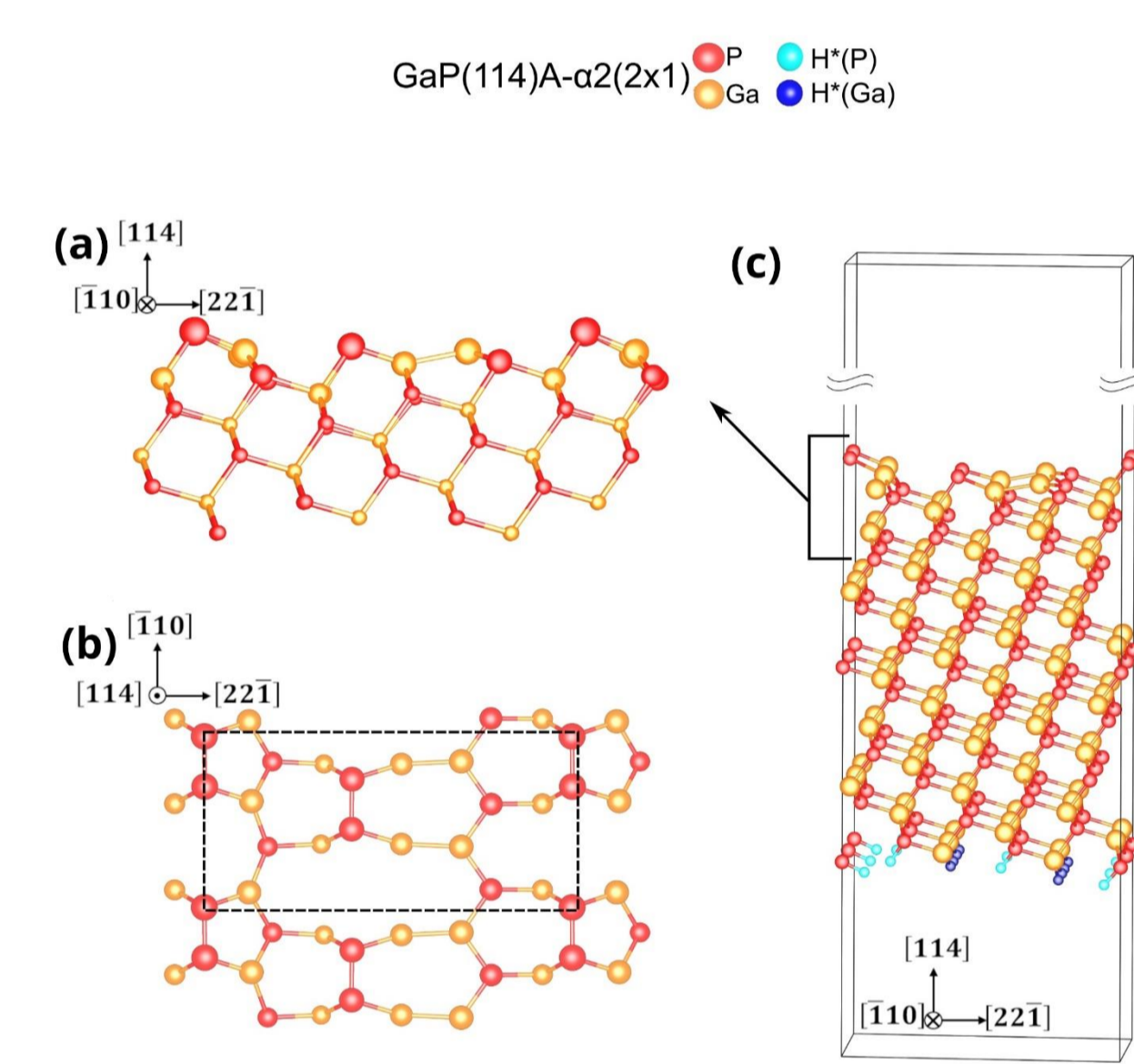
-Pallikkara Chandrasekharan, et al. *Physical Review B* 108,7 (2023); 075305, **FOTON Inst.**



Non-polar GaP surface

$$\gamma_{GaP(001)} = \frac{E_{slab} - N_{Ga}\mu_{Ga}^{bulk} - (N_P - N_{Ga})\mu_P}{2A}$$

-Pallikkara Chandrasekharan, et al. *Physical Review B* 108,7 (2023); 075305, **FOTON Inst.**



The polar surface investigated is on top and the bottom surface is H*-passivated

$$\gamma_{polar} = \frac{E_{slab} - N_{Ga}\mu_{Ga}^{bulk} - (N_P - N_{Ga})\mu_P - N_{H^*}\mu_{H^*}}{A}$$

$$\gamma_{polar} = \frac{E_{slab} - N_{Ga}\mu_{Ga}^{bulk} - (N_P - N_{Ga})\mu_P - N_{H^*}\mu_{H^*}}{A}$$

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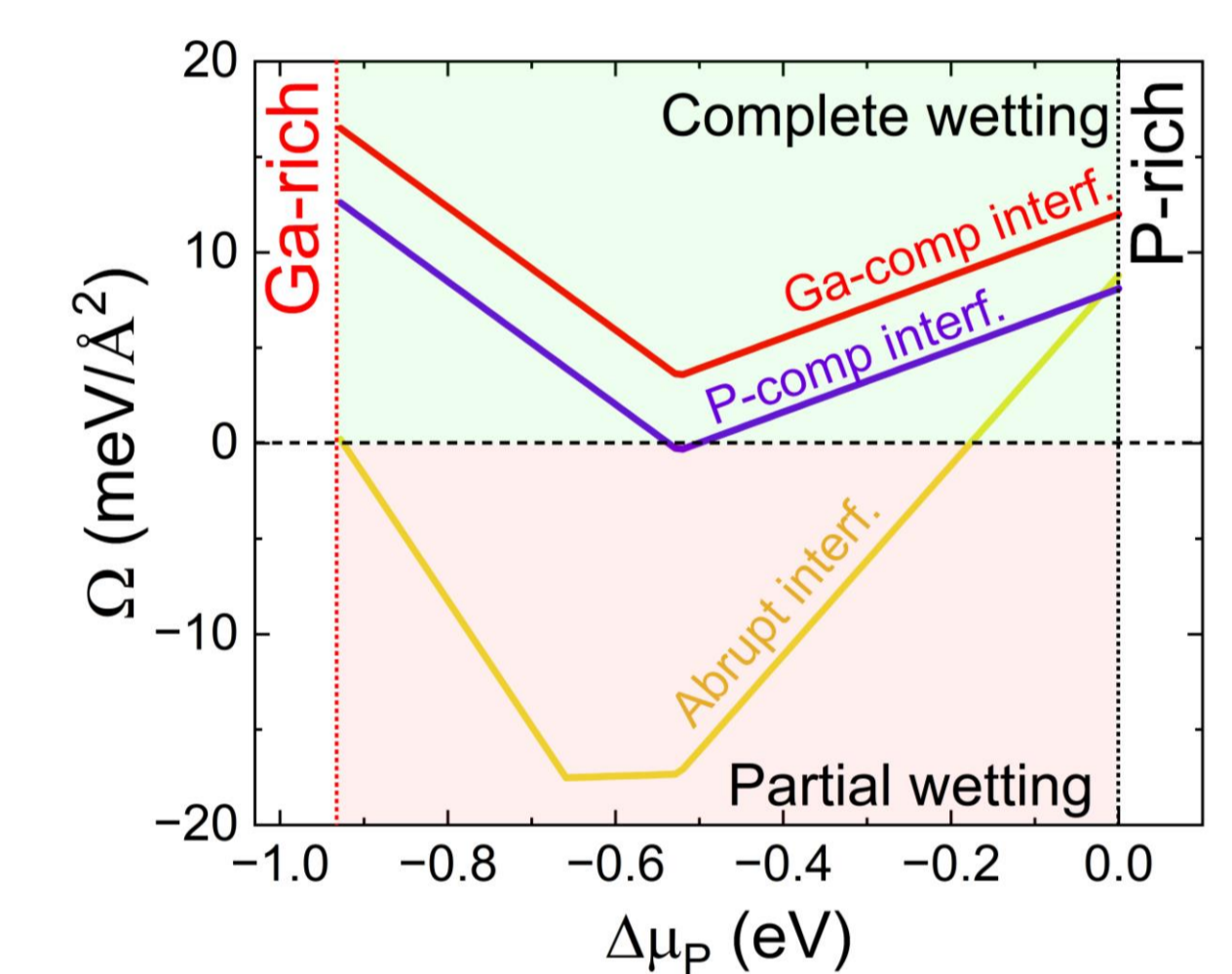
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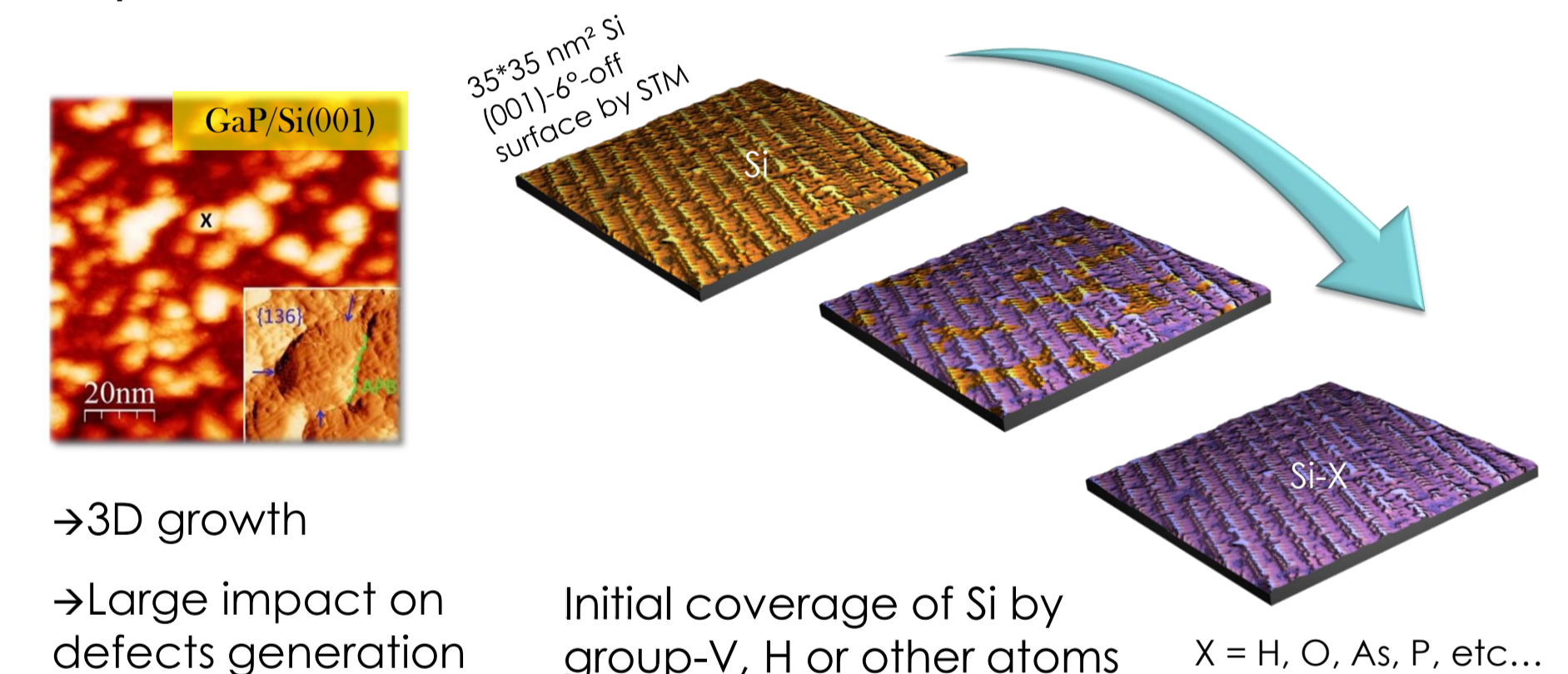
Wetting

$$\Omega = \gamma_{Si}^S - \gamma_{III-V}^S - \gamma_{III-V/Si}^I$$



Young-Dupré spreading parameter Ω calculated for the different interface atomic configurations.

Experiments



→3D growth

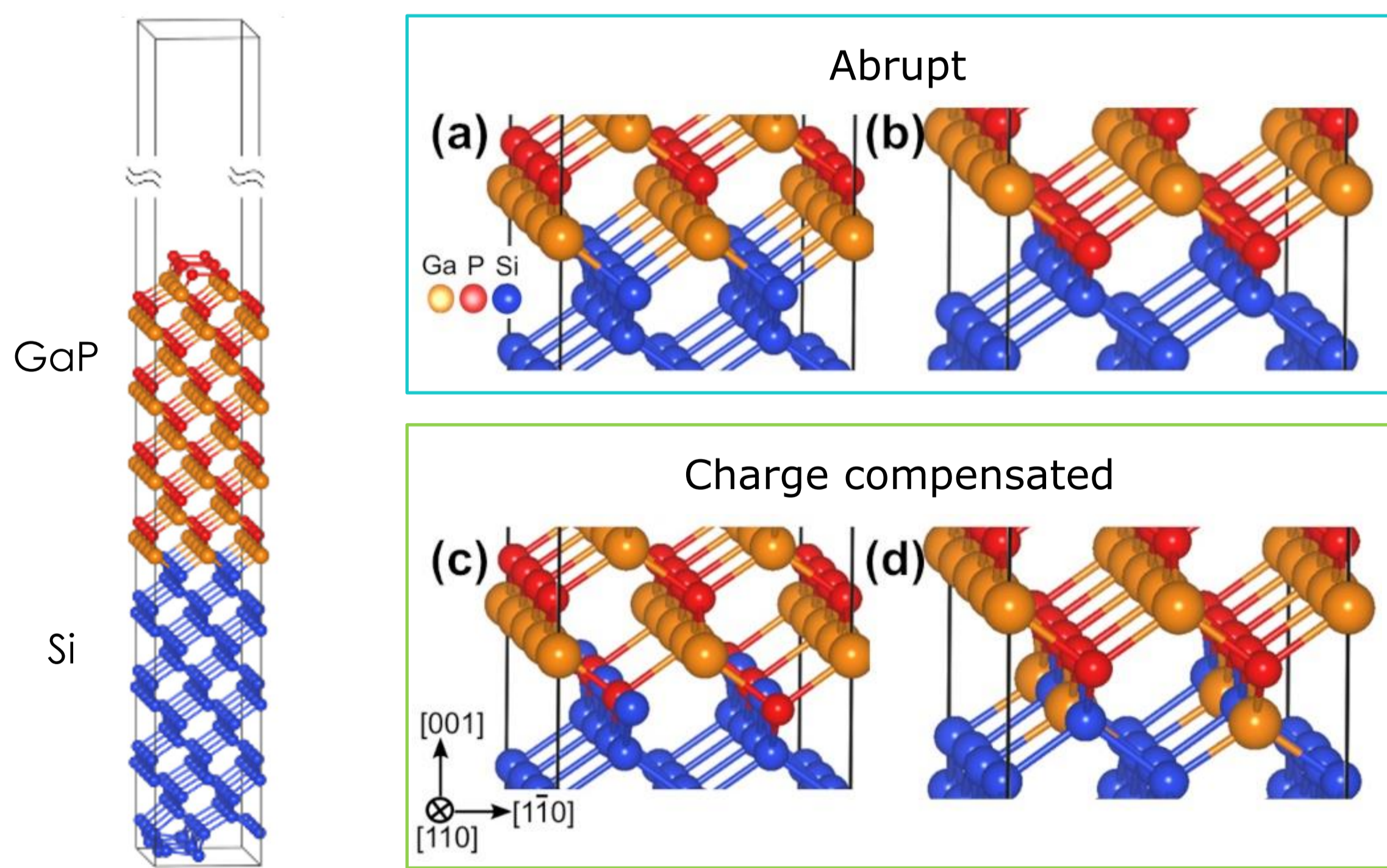
→Large impact on defects generation

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

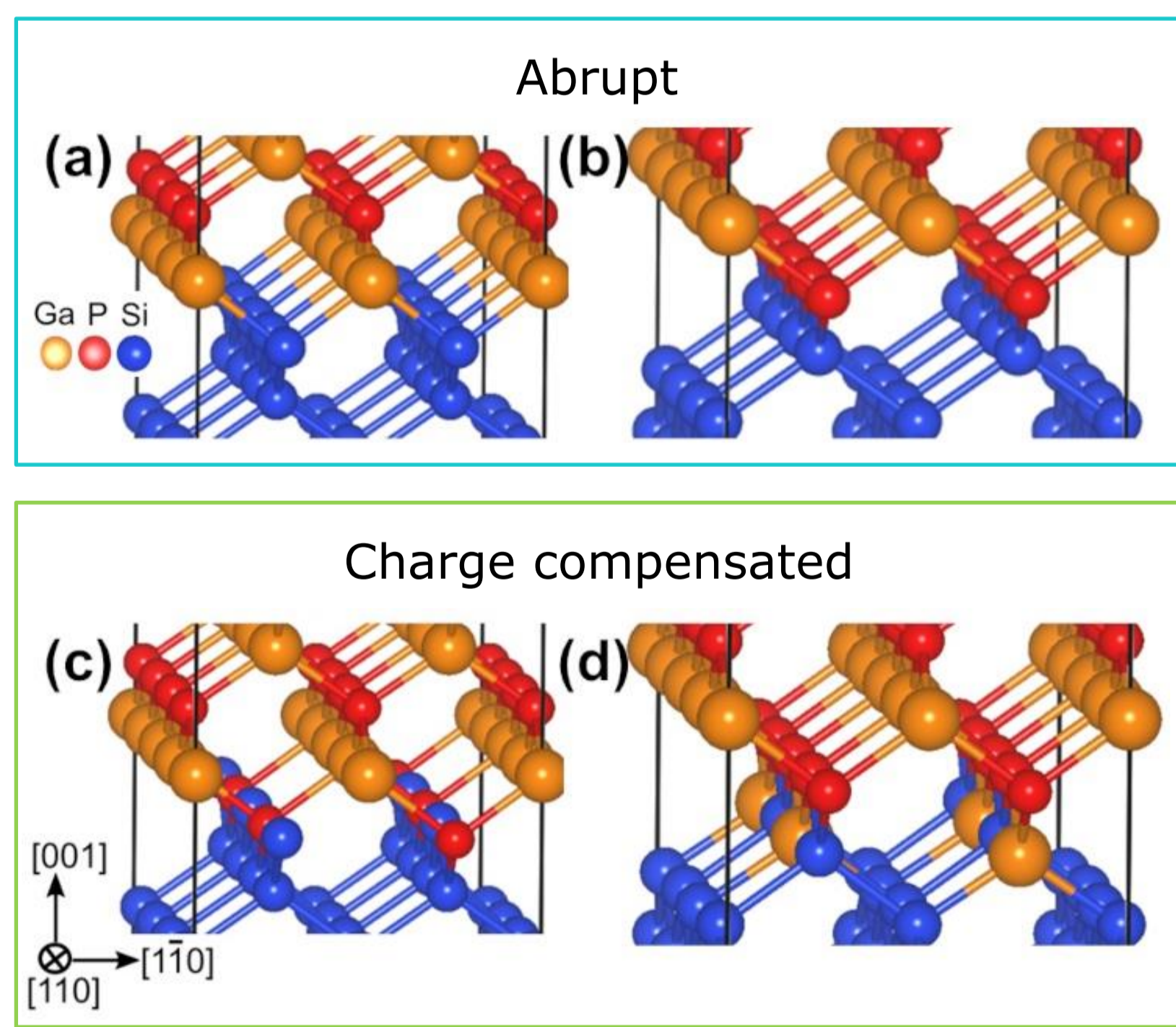
X = H, O, As, P, etc...

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

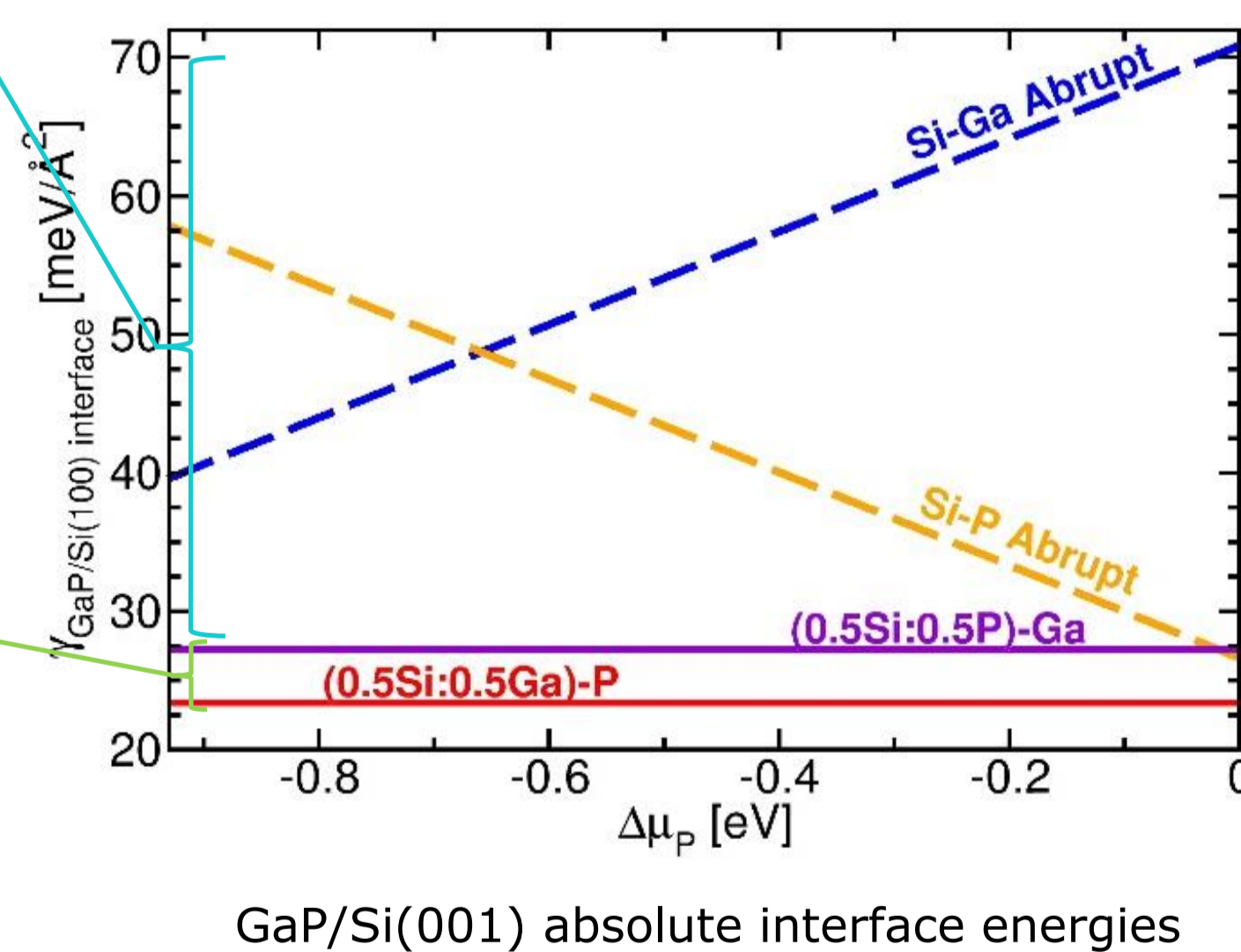
Absolute Interface energies



Schematic of a supercell used for absolute interface energy determination



$$\gamma_{YZ}^I = \frac{E_{slab}^{int} - \sum_i (N_i \mu_i^{bulk}) - \sum_{j=Y,Z} (A \gamma_{surf}^j)}{A}$$



GaP/Si(001) absolute interface energies

The large stabilization of the III-V/Si interface through charge compensation promotes the complete wetting conditions in the system.

-Pallikkara Chandrasekharan, et al. *Physical Review B* 108,7 (2023); 075305, **FOTON Inst.**

Conclusions

- Large stability of charge compensated III-V/Si interfaces as compared to abrupt ones.
- The stable compensated III-V/Si interfaces promote complete wetting conditions.
- This can be easily counterbalanced by the substrate initial passivation, which favors partial wetting conditions.

Acknowledgements

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