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Sreejith Pallikkara Chandrasekharan, Divishth Gutpa, C. Cornet, Laurent Pedesseau. Impact of initial surface passivation on wetting properties analysis during III-V/Si epitaxy. E-MRS 2024 Spring meeting, May 2024, Strasbourg, France. hal-04597986

HAL Id: hal-04597986

<https://hal.science/hal-04597986v1>

Submitted on 3 Jun 2024

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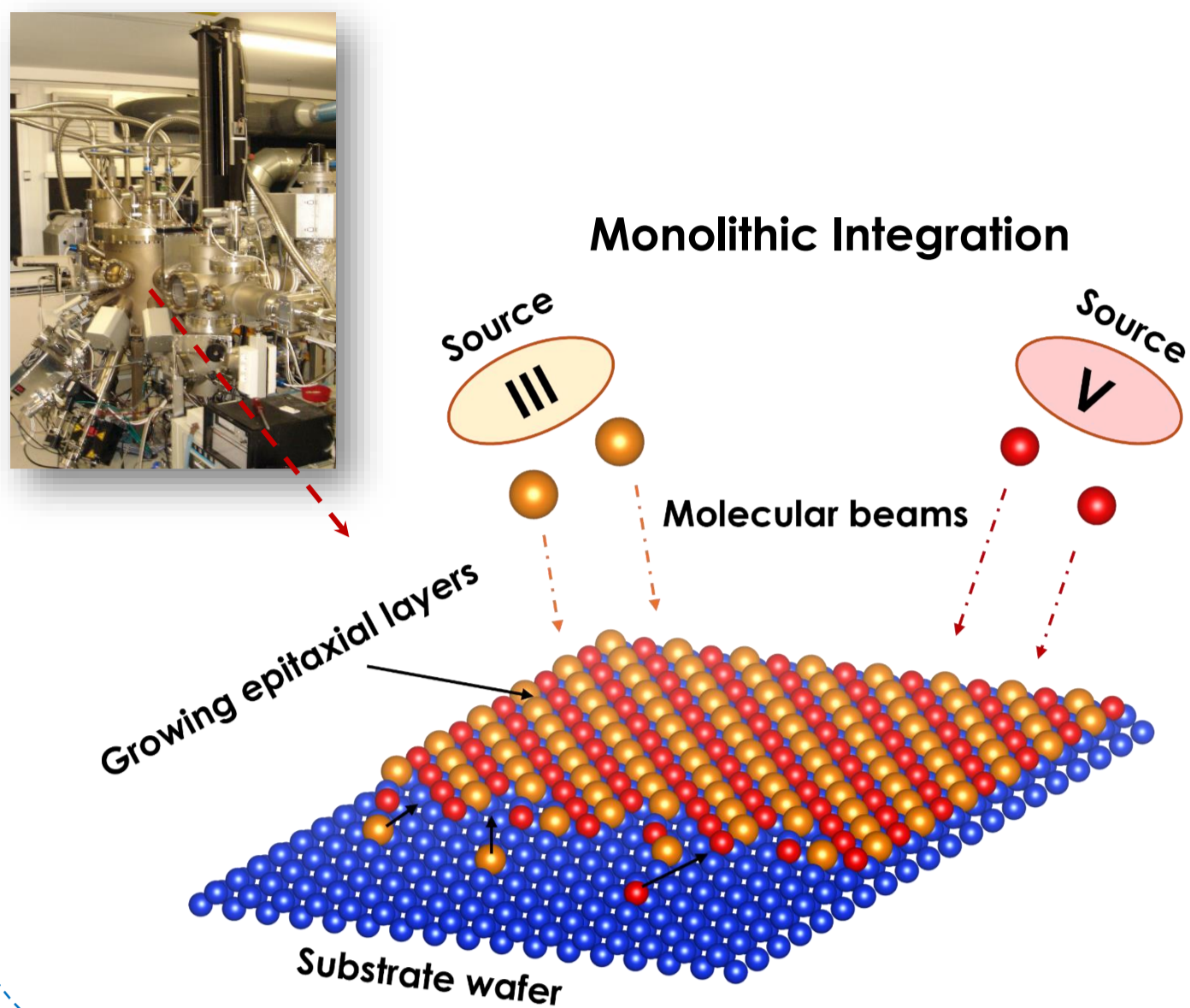
Impact of initial surface passivation on wetting properties analysis during III-V/Si epitaxy

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

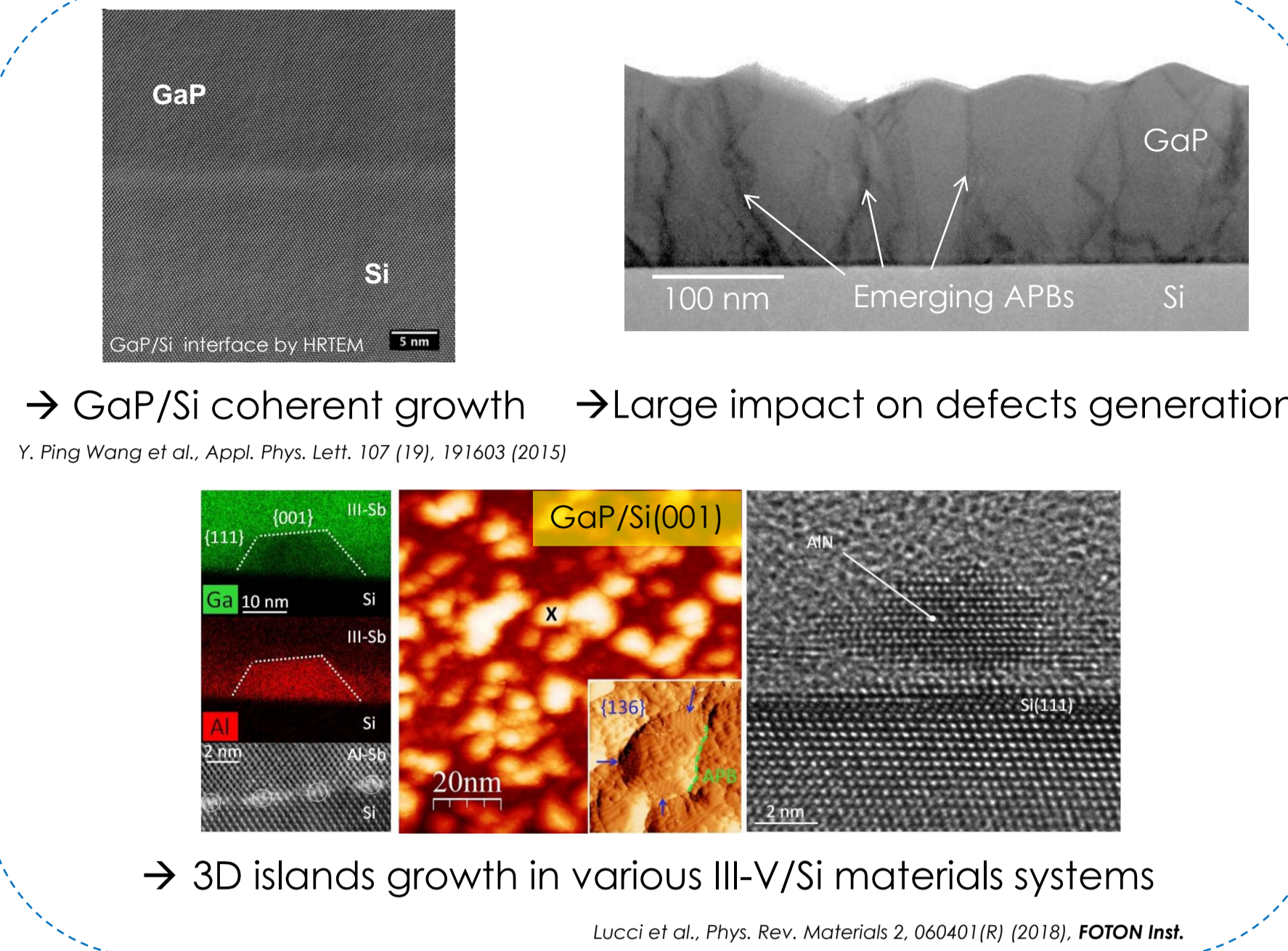
(1) Univ Rennes, INSA Rennes, CNRS, Institut FOTON-UMR 6082, F-35000, Rennes, France.

Introduction

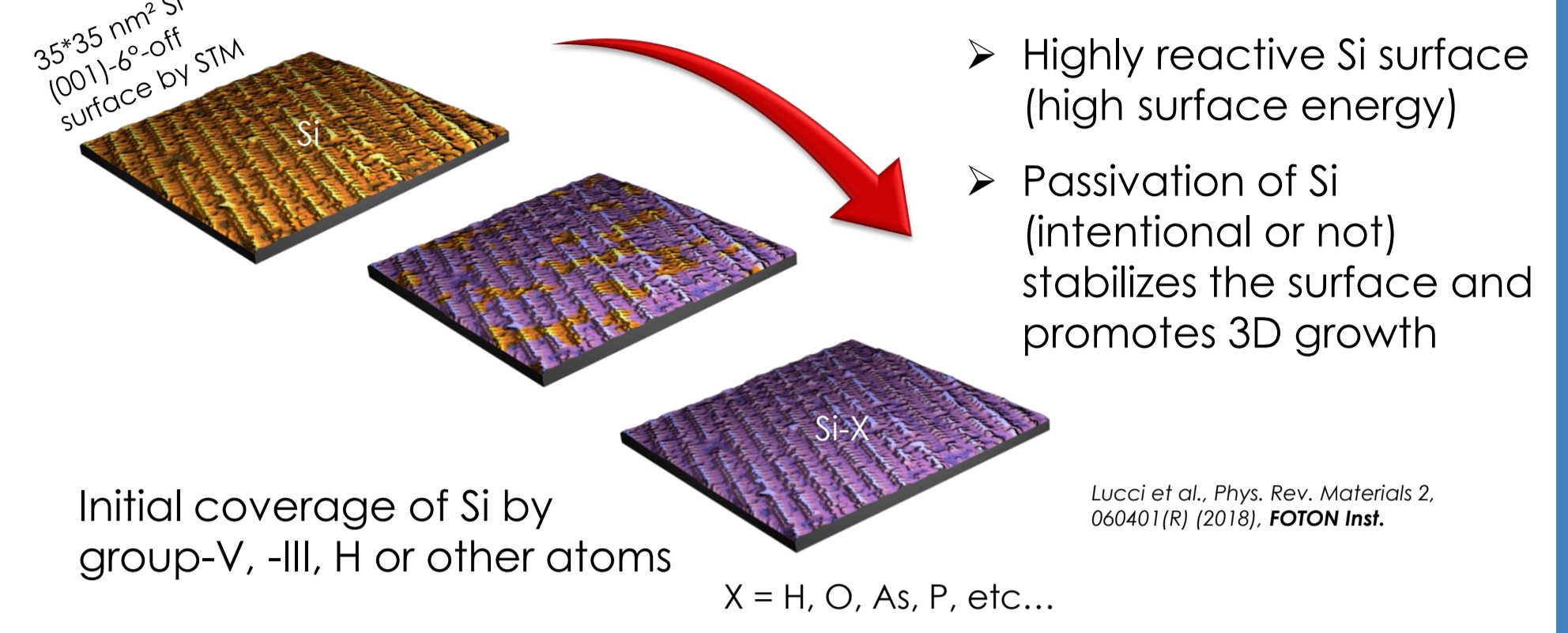
Molecular beam epitaxy



Experimental observations



Objectives



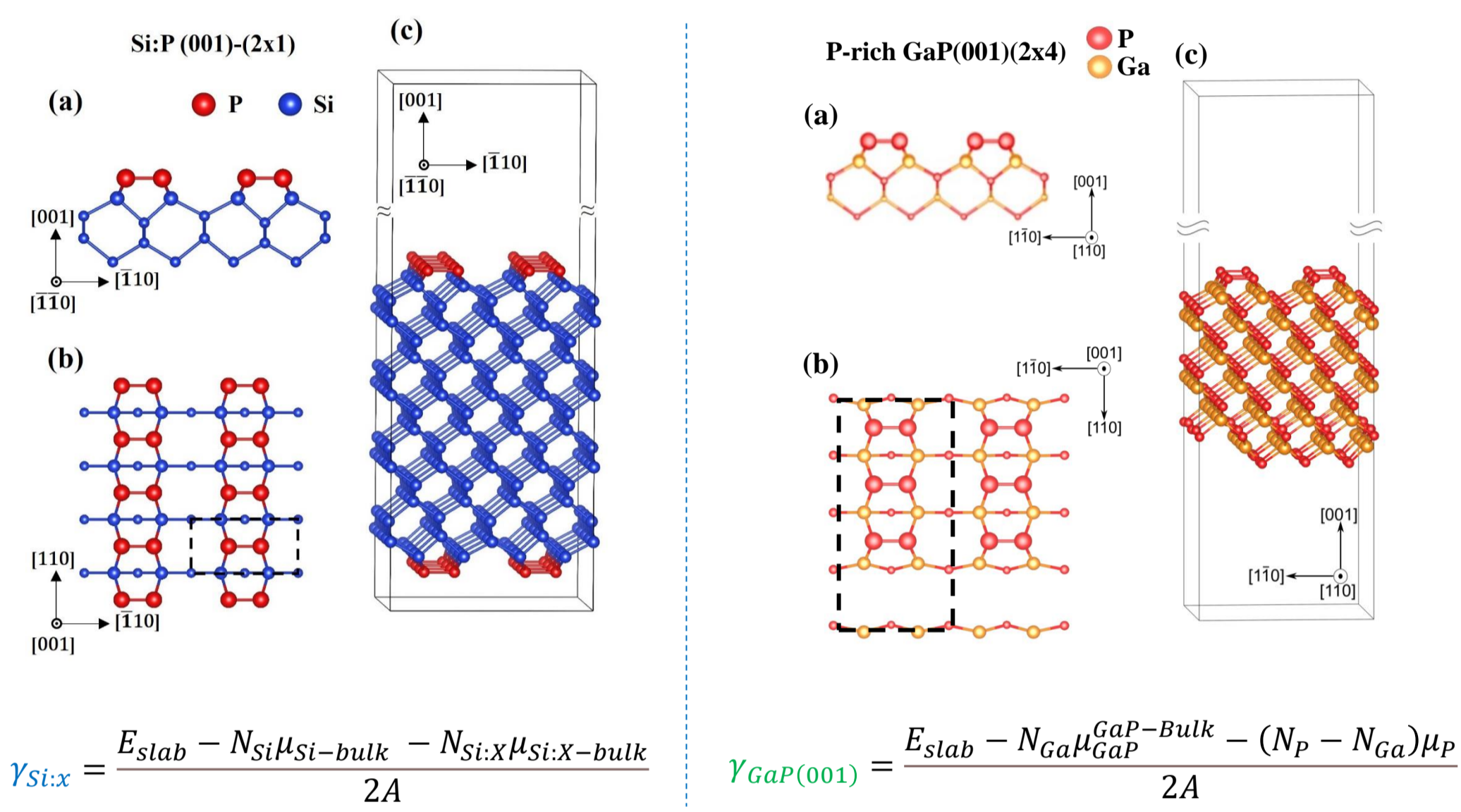
Initial coverage of Si by group-V, -III, H or other atoms

Spreading parameter (solid wetting theory)...

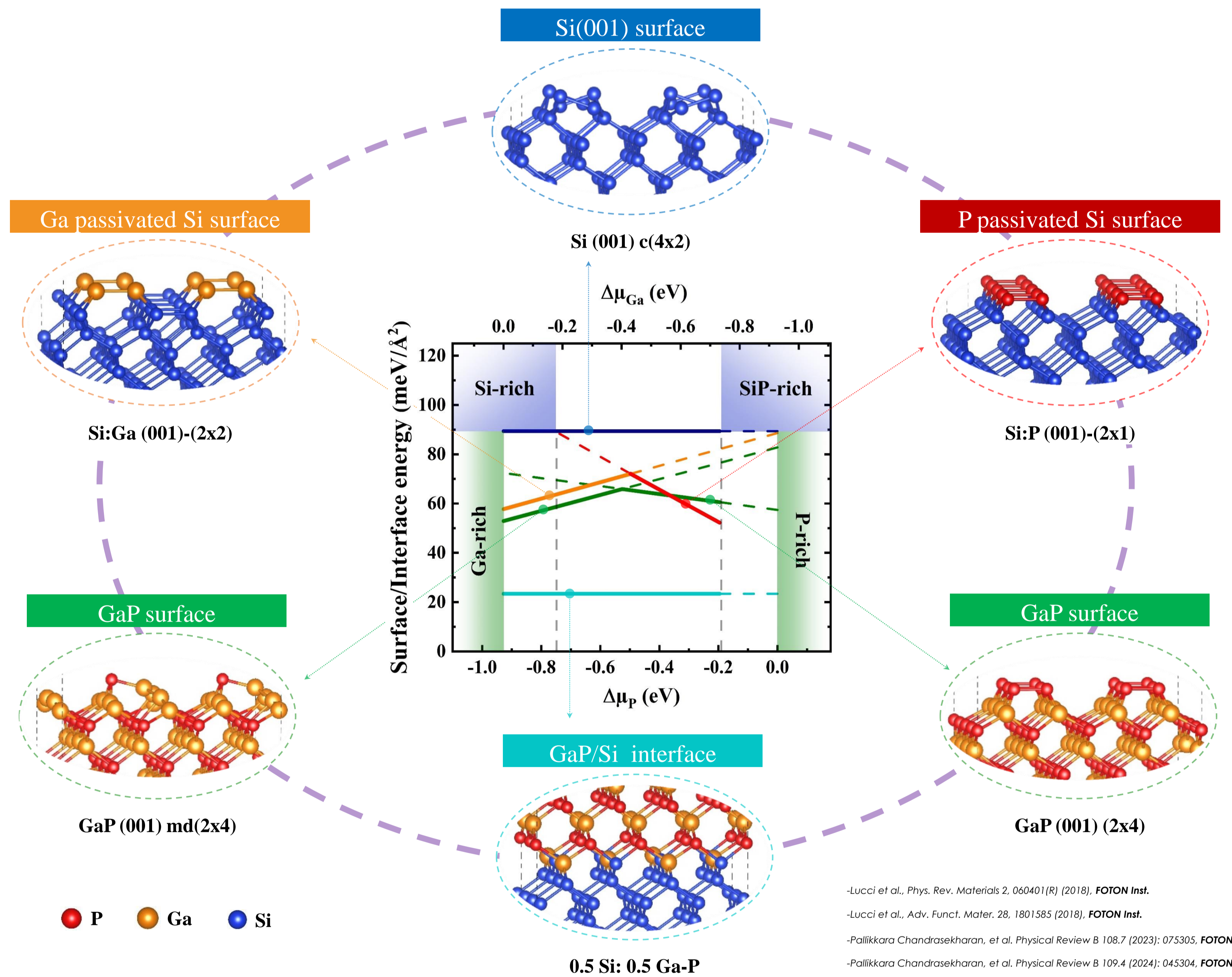
$$\Omega = \gamma_{(Si-x)}^S - \gamma_{(III-V)}^S - \gamma_{(III-V/Si)}^I$$

$\Omega > 0$, complete wetting
 $\Omega < 0$, partial wetting

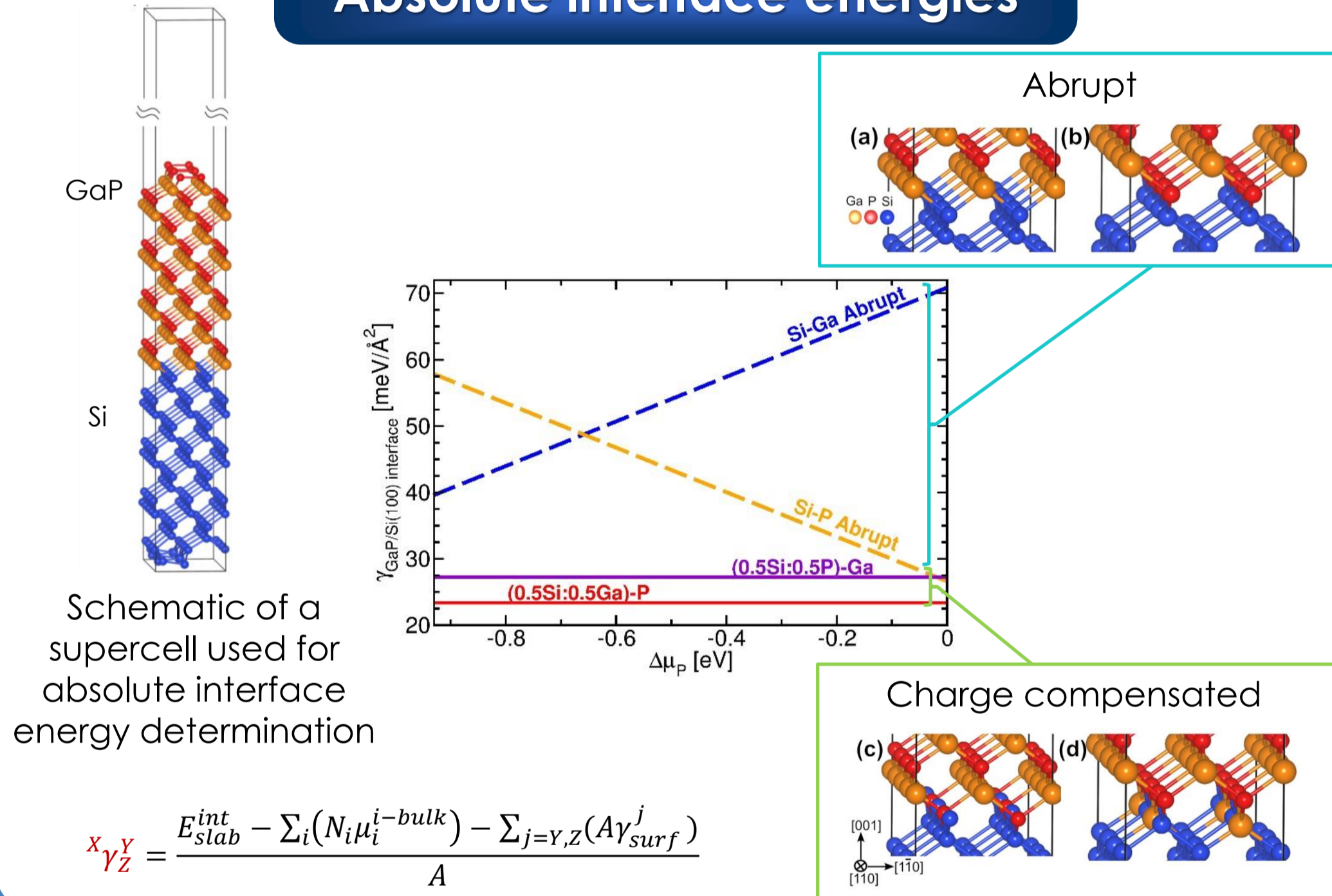
Absolute surface energies



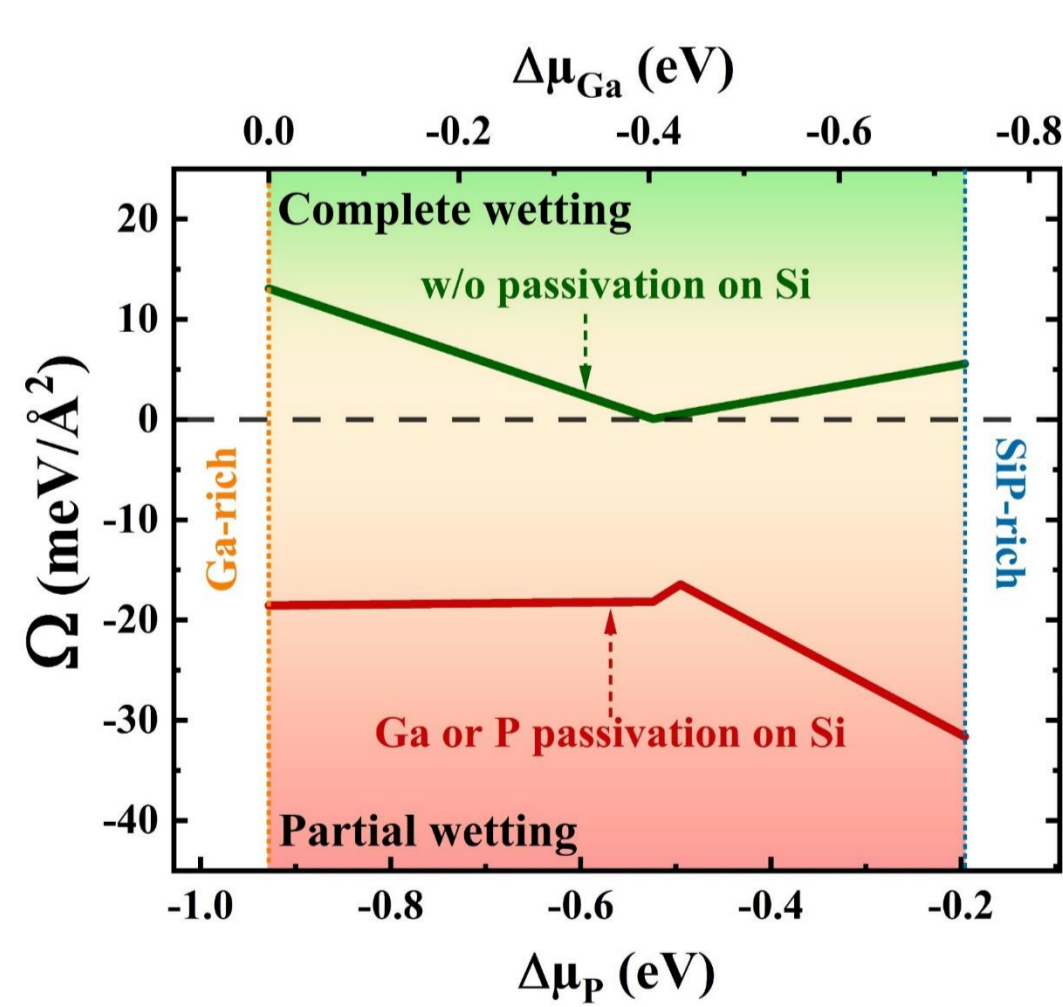
Surface and interface energies vs chemical potentials for GaP/Si



Absolute interface energies



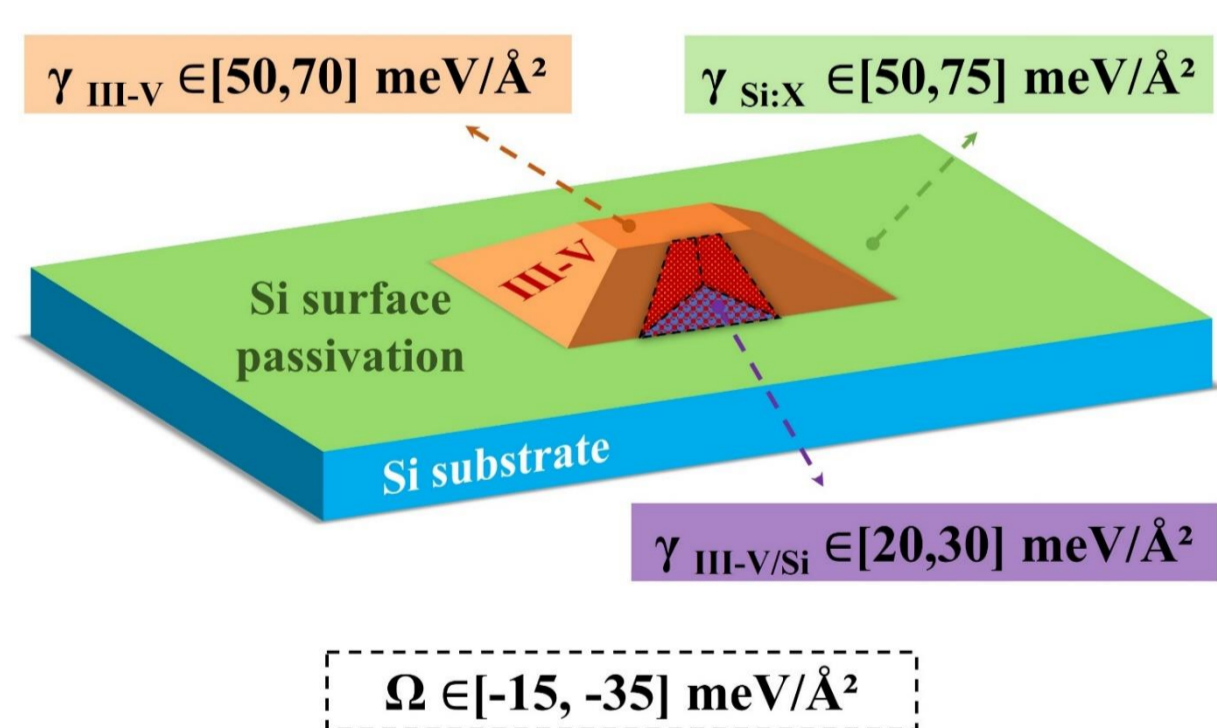
Wetting properties



Young-Dupré spreading parameter Ω

- Passivation promotes partial wetting conditions.

*Pallikkara Chandrasekharan, et al. Physical Review B 109.4 (2024): 045304, FOTON Inst.

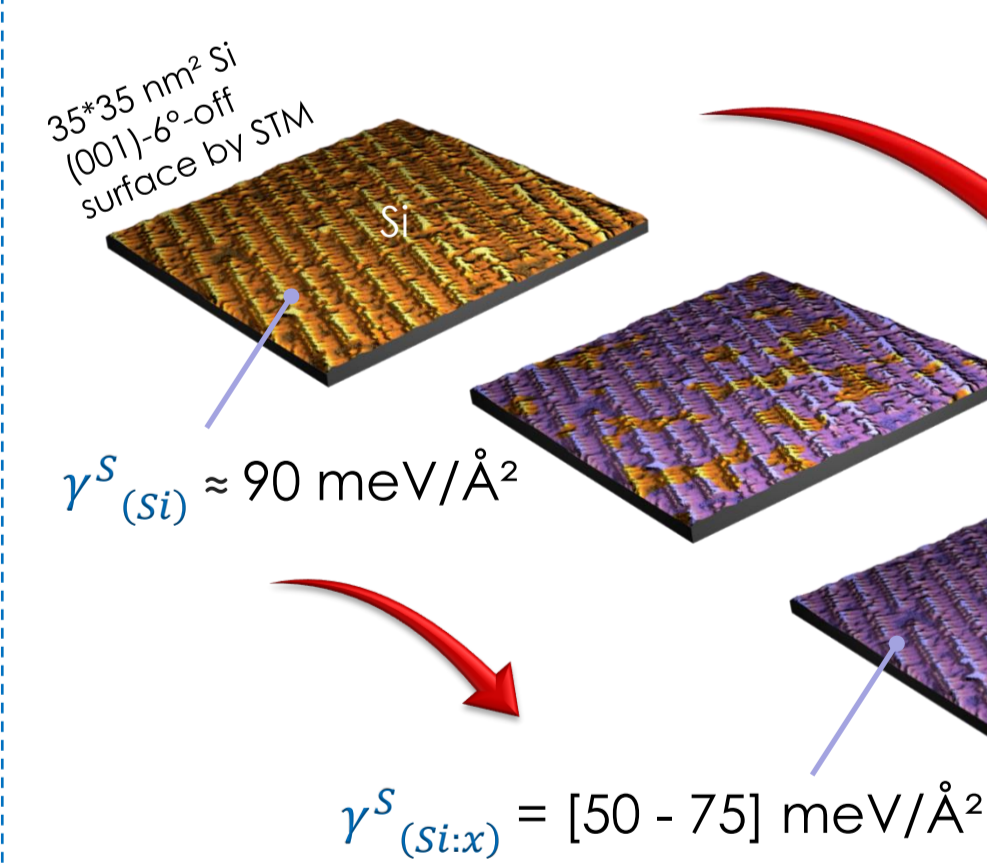


"Illustration summarizing the energies involved in the 3D island formation of GaP on the Si substrate with a range of possible energy values"

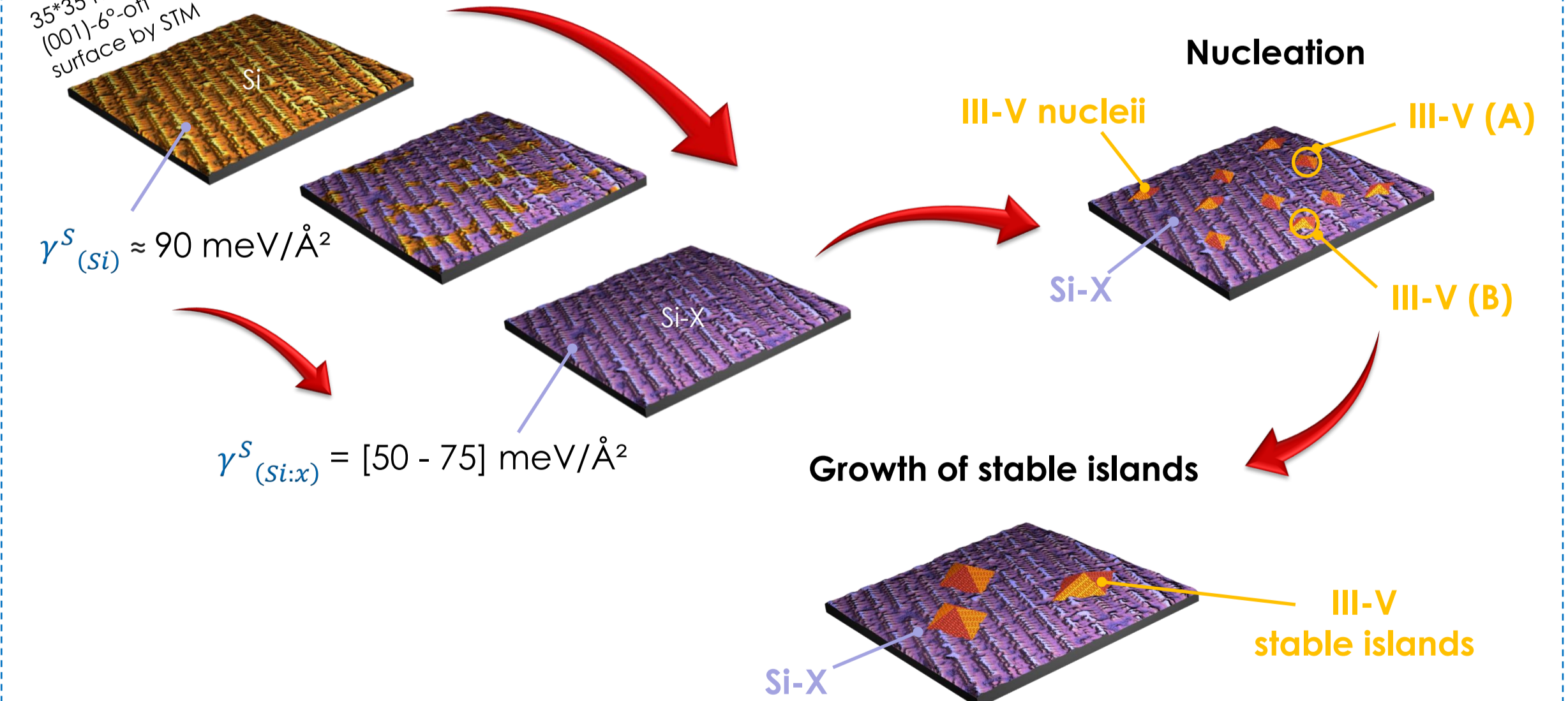
- Stable surface and interface energies support the growth of 3D islands.

*Pallikkara Chandrasekharan, et al. Physical Review B 109.4 (2024): 045304, FOTON Inst.

Initial surface passivation



Proposed III-V/Si growth steps



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

Conclusions

- Inevitable passivation of Si prior to GaP/Si heteroepitaxy leads to a large decrease of the substrate surface energy.
- This decrease leads to a significant reduction in the spreading parameter.
- Destabilizing a passivated Si surface by at least 15 meV/Å² or stabilizing the III-V (001) surface makes a complete wetting situation possible.
- Si passivation is a driving force for the formation of 3D stable islands, which leads to the emergence of structural defects due to their coalescence.

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**, **A0140911434**, and **A0160911434** made by GENCI.