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Laurent Pedesseau, Lipin Chen, Ida Lucci, Divishth Gutpa, Charles Cornet. Determination of absolute “surface/interface” energies in heterogeneous materials and hetero-interfaces: A theoretical approach. European Materials Research Society - Fall Meeting 2022 (E-MRS 2022 Fall Meeting), Sep 2022, Warsaw, Poland. hal-03788415

HAL Id: hal-03788415

<https://hal.science/hal-03788415>

Submitted on 27 Sep 2022

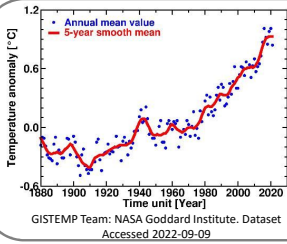
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Determination of absolute "surface/interface" energies in heterogeneous materials and hetero-interfaces: A theoretical approach

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Introduction

The climate change and its impacts are nowadays well established and cannot be ignored [1]. The international community agrees to have a fast energy transition, which translates in developing more efficient photovoltaic cells, light emitting and photocatalytic devices. To deal with this irreversible problem, new or advanced semiconductors have to be found for the next generation of optoelectronic applications such as Laser, Light Emitting Devices (LED), Photodetection, Photocatalysis.

[1] Obama, B. The Irreversible Momentum of Clean Energy. *Science* 2017, 355 (6321), 126.

Abstract

The determination of absolute surface and interface energies of materials is one challenging issue in today's epitaxial developments, as it fundamentally governs the nucleation and physical properties of heterogeneously integrated materials and devices for photonics, electronics or energy harvesting applications.[1] Especially, determining the hetero-interface absolute energies remain tricky, because of the difference of chemistry between the two materials considered. In this work, we use Density Functional Theory, with a fictitious hydrogen atoms charge compensation strategy, to determine the surface and interface absolute energies in the III-V/Si heterogeneous materials association case [1,2]. This method is expected to be applicable for all other heterogeneous materials association. We finally show how, in the specific case of III-V/Si heterogeneous epitaxy, it allows understanding structural properties of samples, and consider their use for applications in photonics, solar cells, or solar hydrogen production through water splitting [3,4].

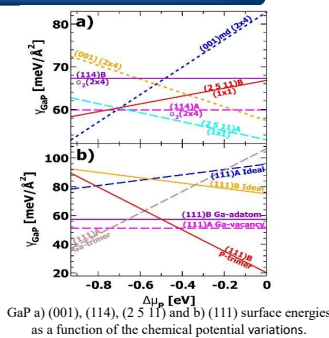
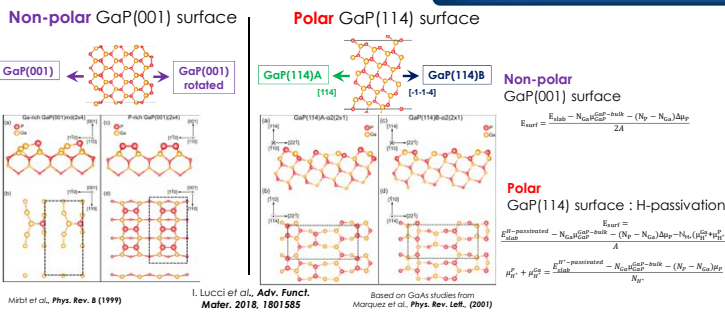
[1] I. Lucci *et al.*, *Physical Review Materials* 2 (6), 060401, 2018

[2] I. Lucci *et al.*, *Advanced Functional Materials*, 28(30):1801585, 2018.

[3] M. Alqahtani *et al.*, *Sustainable Energy & Fuels* 3, 2019.

[4] L. Chen *et al.*, *Advanced Science*, 9, 2101661, 2022

Surface



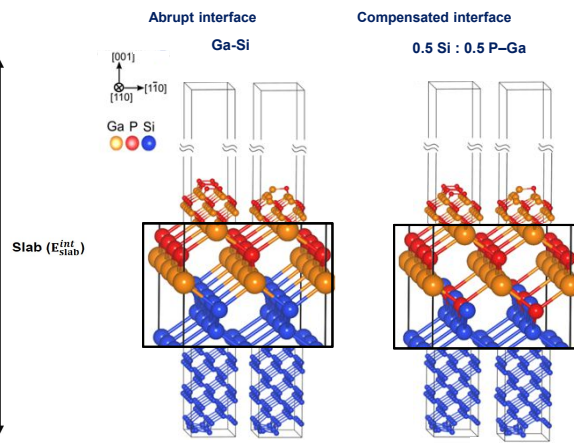
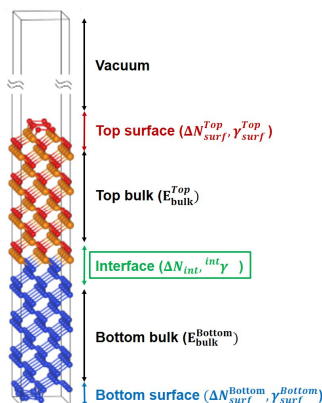
Stable GaP and Si surface energies computed by DFT

Surface	Energy (meV/A ²)	
	P-rich	Ga-rich
Si(001) c(2x4)		92.8
GaP(001) c(2x4)	57.4	72.4
GaP(001) md (2x4)	82.8	52.9
GaP(114)B c2(2x1)	67.3	67.3
GaP(114)A c2(2x1)	59.9	59.9
GaP(2 5 1)B (1x1) Ga-dimer	66.8	58.3
GaP(2 5 1)A (1x1) P-dimer	52.9	62.7
GaP(111)A Ideal	95.7	78.4
GaP(111)B Ideal	75.1	92.3
GaP(111)A Ga-vacancy	51.2	51.2
GaP(111)B Ga-adatom	57.3	57.3
GaP(111)A Ga-trimer	106.4	37.3
GaP(111)B P-trimer	20.2	89.3

How can we determine the non-polar and polar surface energy?

Interface

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



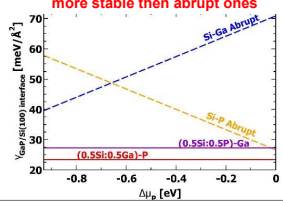
The stoichiometry of the interface for a slab

$$\Delta N_{int} = \Delta N_{slab} - \Delta N_{top\ surface} - \Delta N_{bottom\ surface}$$

Here, the stoichiometry of the silicon surface at the bottom is equal to 0, $\Delta N_{bottom} = 0$

Slab configuration	ΔN_{slab}	$\Delta N_{top\ surface}$	ΔN_{int}	$\frac{\Delta N_{int}}{A} = S_{int}$
Si-Ga ₂ Si (100)				
GaP (001) 2x4	-2	2	-4	-1
Si-P ₂ Si (100)				
YGaP (001) 2x4	6	2	4	1
1.5Si-0.5P-Ga ₂ Si (100)	2	2	0	0
YGaP (001) 2x4	2	2	0	0

GaP/Si(001) compensated interfaces are more stable than abrupt ones



Acknowledgements

This research was supported by the French National Research Agency PIANIST Project (Grant no. ANR-21-CE09-0020), and NUAGES Project (Grant no. ANR-21-CE24-0006).

DFT calculations were performed at Institut FOTON, and the work was granted access to the HPC resources of TGCC/CINES under the allocation 2021-A0100911434 and 2022-A0120911434 made by GENCI.