



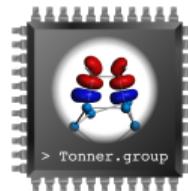
UNIVERSITÄT
LEIPZIG

ICMOVPE XX, 2022

Strain-induced bandgap transition in III-V semiconductors

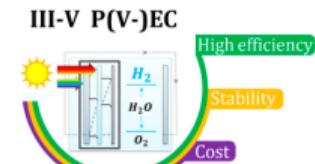
July 14, 2022

Badal Mondal and Ralf Tonner-Zech



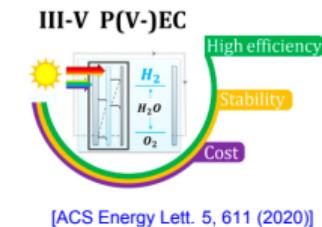
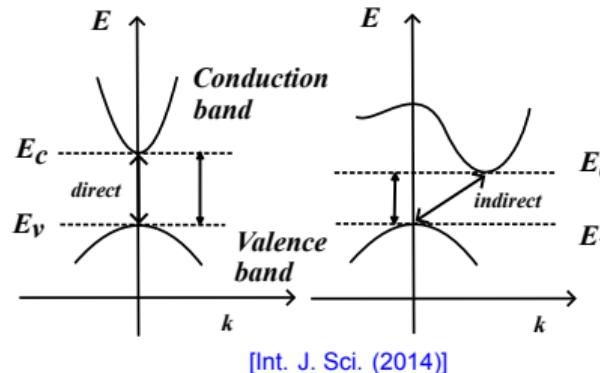
Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie
Fakultät für Chemie und Mineralogie
Universität Leipzig

Introduction

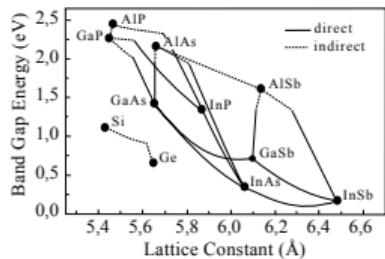


[ACS Energy Lett. 5, 611 (2020)]

Introduction



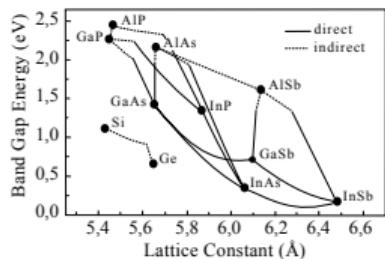
Motivation



[Appl. Phys. A 69, 119 (1999)]

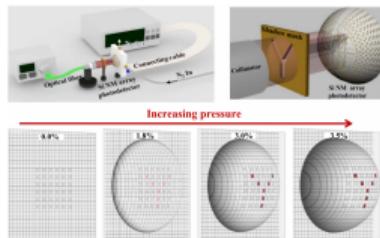
— Compositional engineering

Motivation



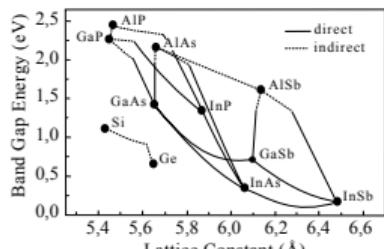
[Appl. Phys. A 69, 119 (1999)]

- Compositional engineering
- Strain engineering

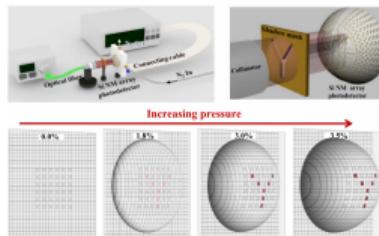


[Sci. Adv. 6, eabb0576 (2020)]

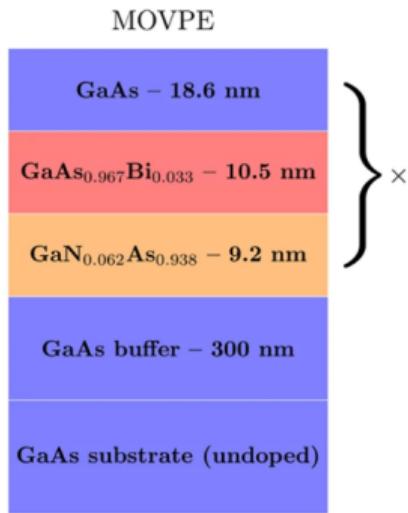
Motivation



[Appl. Phys. A 69, 119 (1999)]



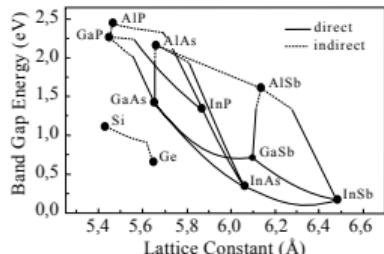
[Sci. Adv. 6, eabb0576 (2020)]



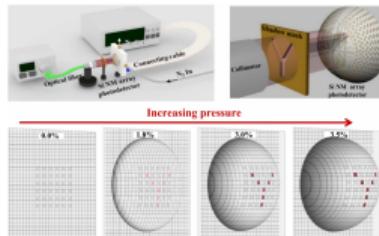
[Sci. Rep. 7, 46371 (2017)]

- Compositional engineering
- Strain engineering
- Composition + strain engineering

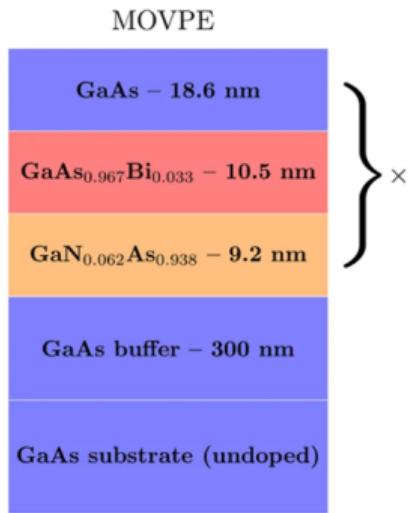
Motivation



[Appl. Phys. A 69, 119 (1999)]



[Sci. Adv. 6, eabb0576 (2020)]

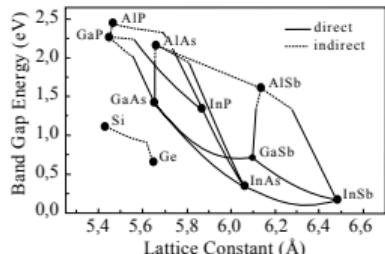


[Sci. Rep. 7, 46371 (2017)]

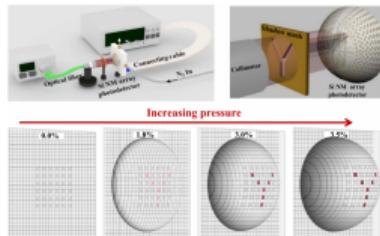
composition-strain-bandgap

- Compositional engineering
- Strain engineering
- Composition + strain engineering

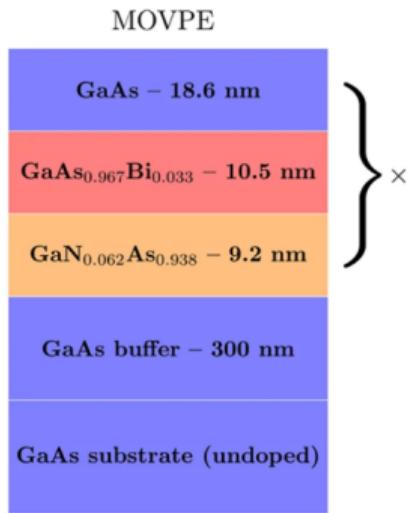
Motivation



[Appl. Phys. A 69, 119 (1999)]



[Sci. Adv. 6, eabb0576 (2020)]

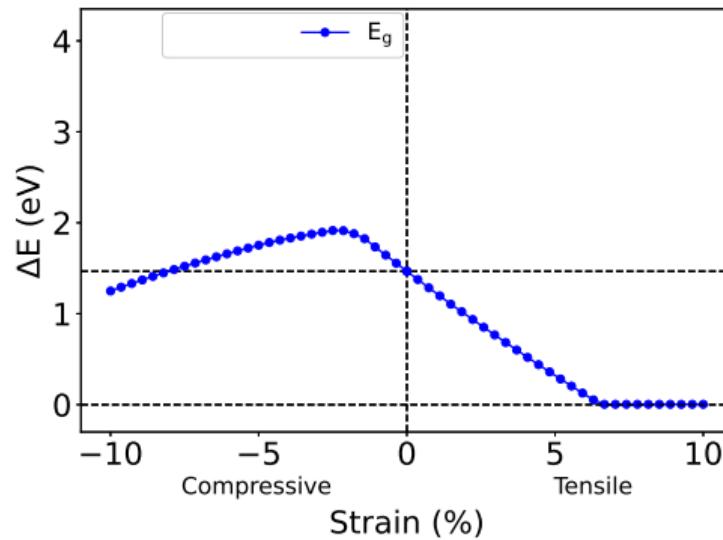


[Sci. Rep. 7, 46371 (2017)]

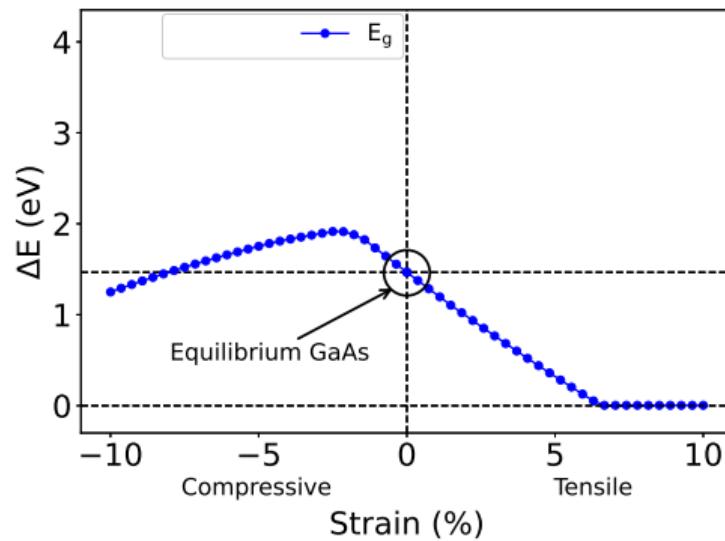
composition-strain-bandgap

- Compositional engineering
- Strain engineering
- Composition + strain engineering
- Density functional theory

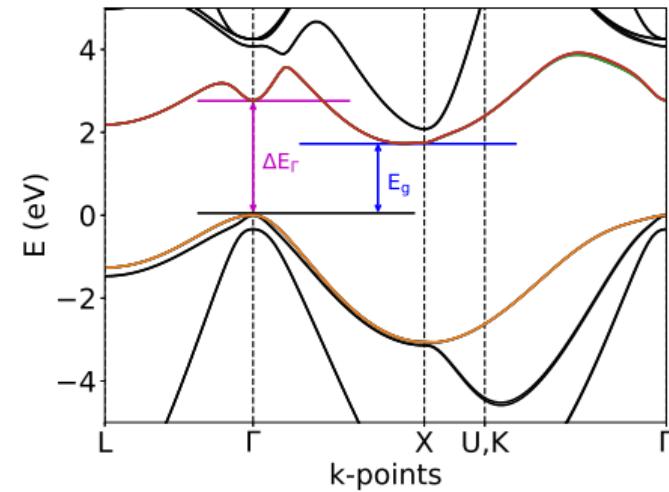
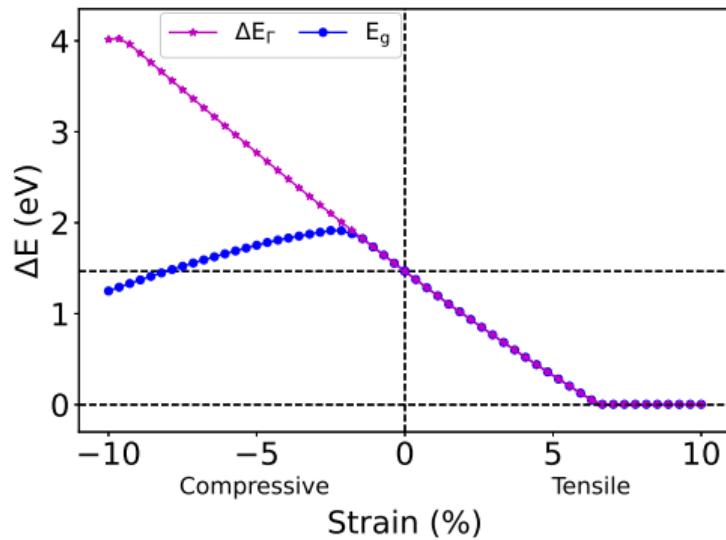
GaAs isotropic strain: strain-bandgap



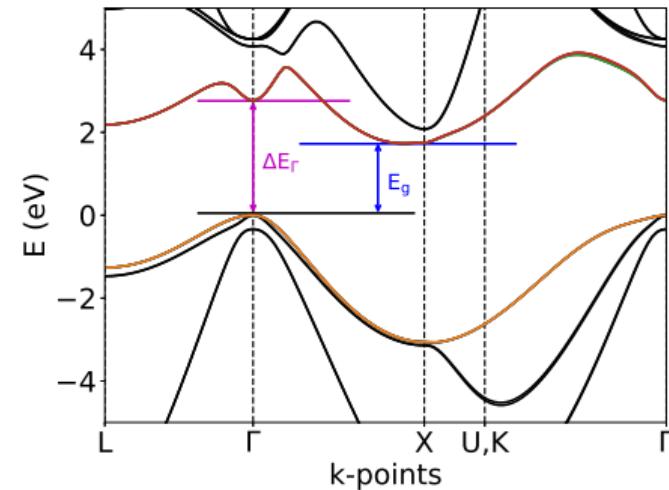
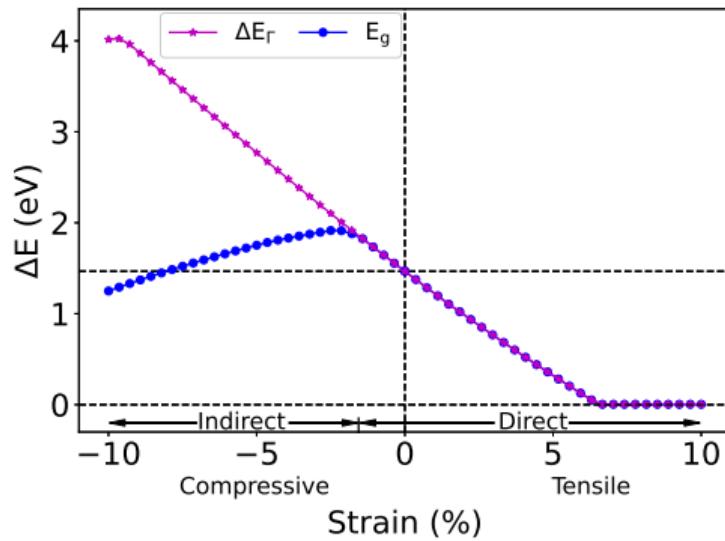
GaAs isotropic strain: strain-bandgap



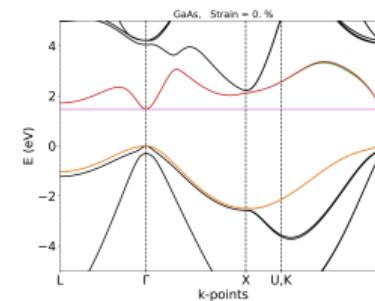
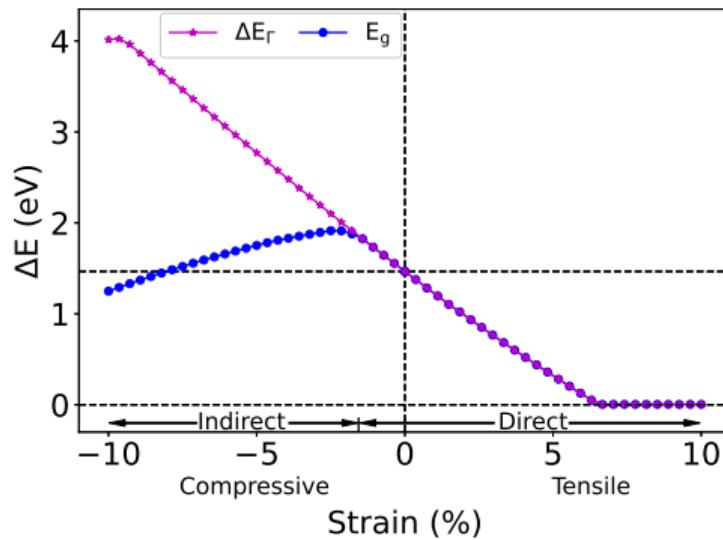
GaAs isotropic strain: strain-bandgap



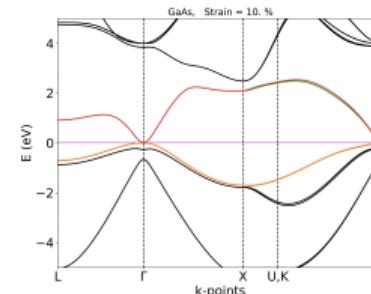
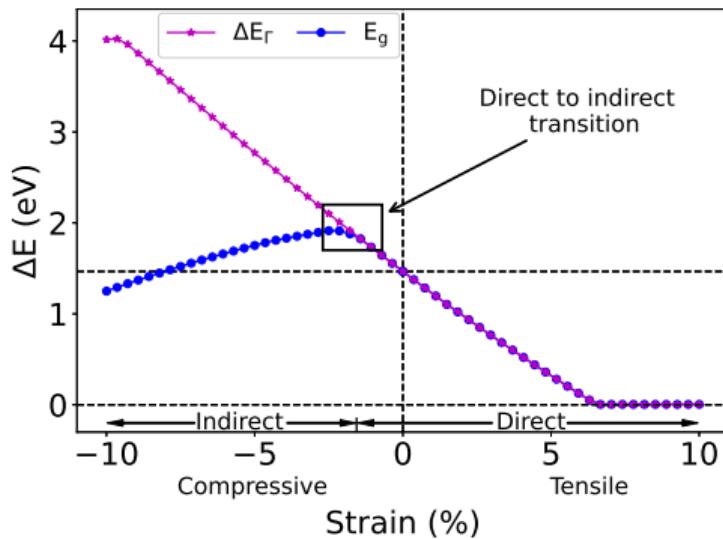
GaAs isotropic strain: strain-bandgap



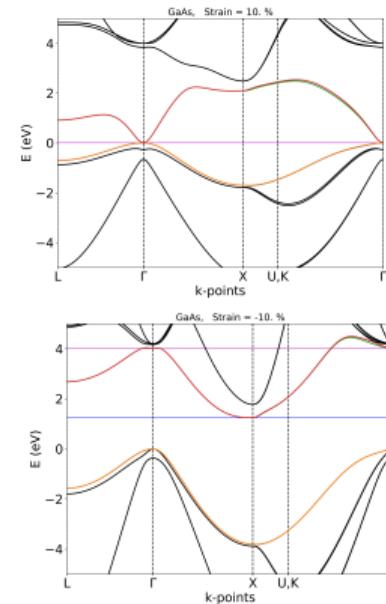
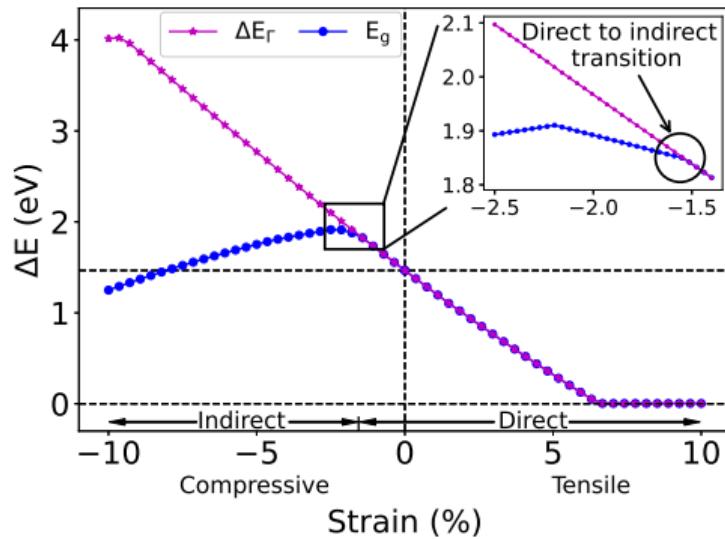
GaAs isotropic strain: strain-bandgap



GaAs isotropic strain: strain-bandgap



GaAs isotropic strain: strain-bandgap

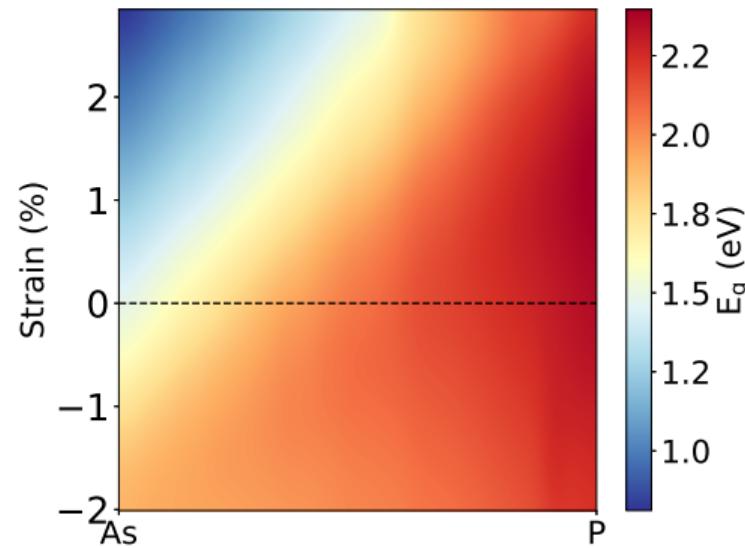


Ga(AsP) isotropic strain: bandgap phase diagram

- Composition-strain-bandgap
- Challenge
 - Supercell: band folding^a
 - Bandgap nature?
- Effective band structure^b
 - Bloch spectral weight
 - Band unfolding

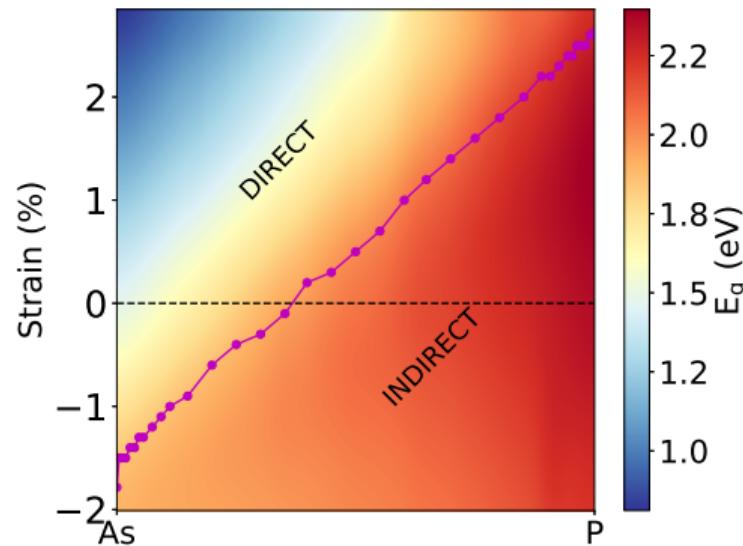
Ga(AsP) isotropic strain: bandgap phase diagram

- Composition-strain-bandgap
- Challenge
 - Supercell: band folding^a
 - Bandgap nature?
- Effective band structure^b
 - Bloch spectral weight
 - Band unfolding



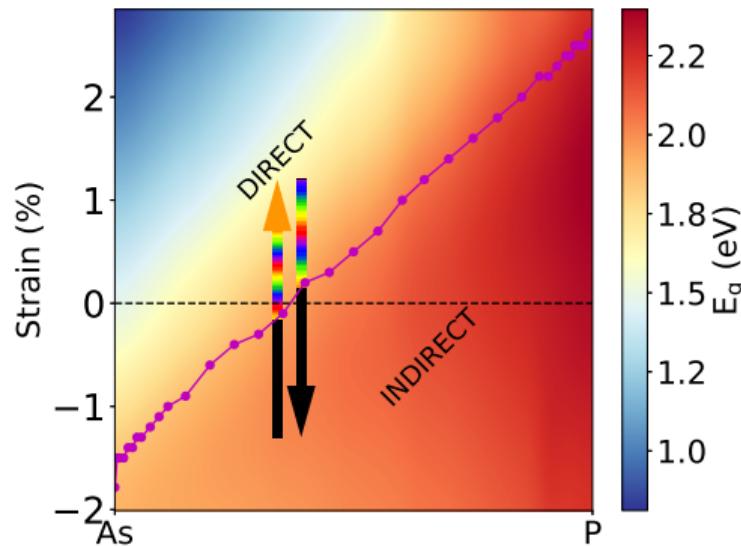
Ga(AsP) isotropic strain: bandgap phase diagram

- Composition-strain-bandgap
- Challenge
 - Supercell: band folding^a
 - Bandgap nature?
- Effective band structure^b
 - Bloch spectral weight
 - Band unfolding



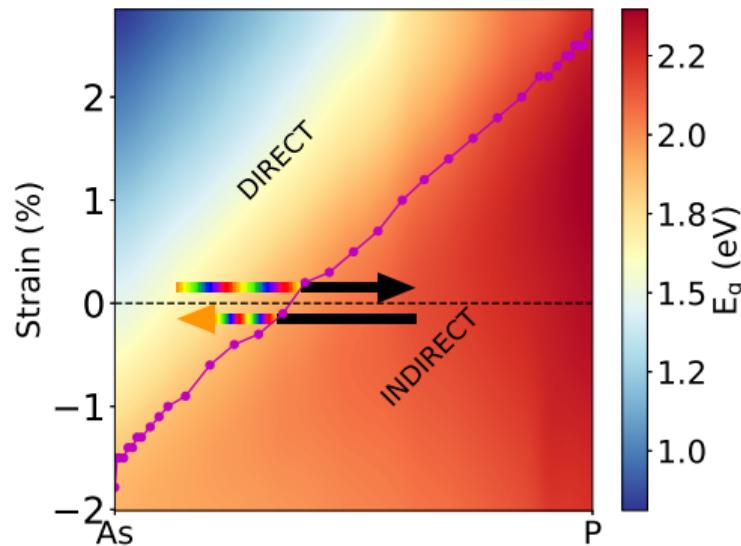
Ga(AsP) isotropic strain: bandgap phase diagram

- Composition-strain-bandgap
- Challenge
 - Supercell: band folding^a
 - Bandgap nature?
- Effective band structure^b
 - Bloch spectral weight
 - Band unfolding

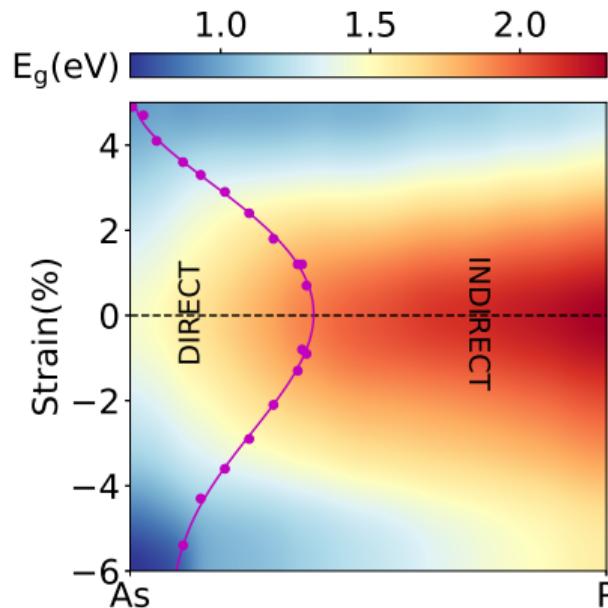


Ga(AsP) isotropic strain: bandgap phase diagram

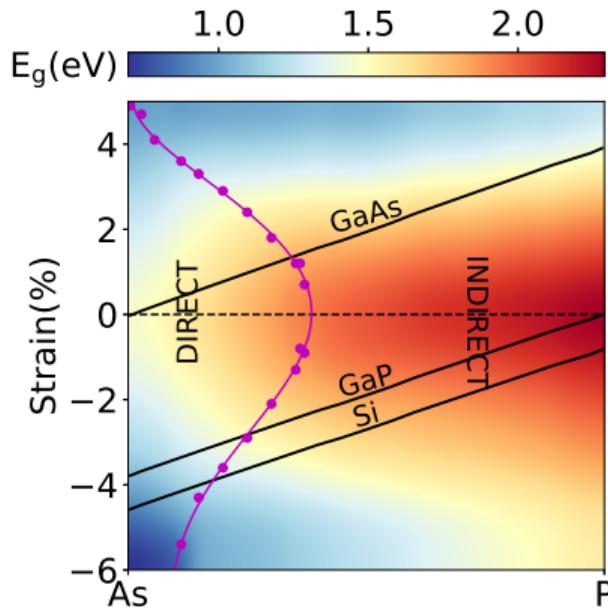
- Composition-strain-bandgap
- Challenge
 - Supercell: band folding^a
 - Bandgap nature?
- Effective band structure^b
 - Bloch spectral weight
 - Band unfolding



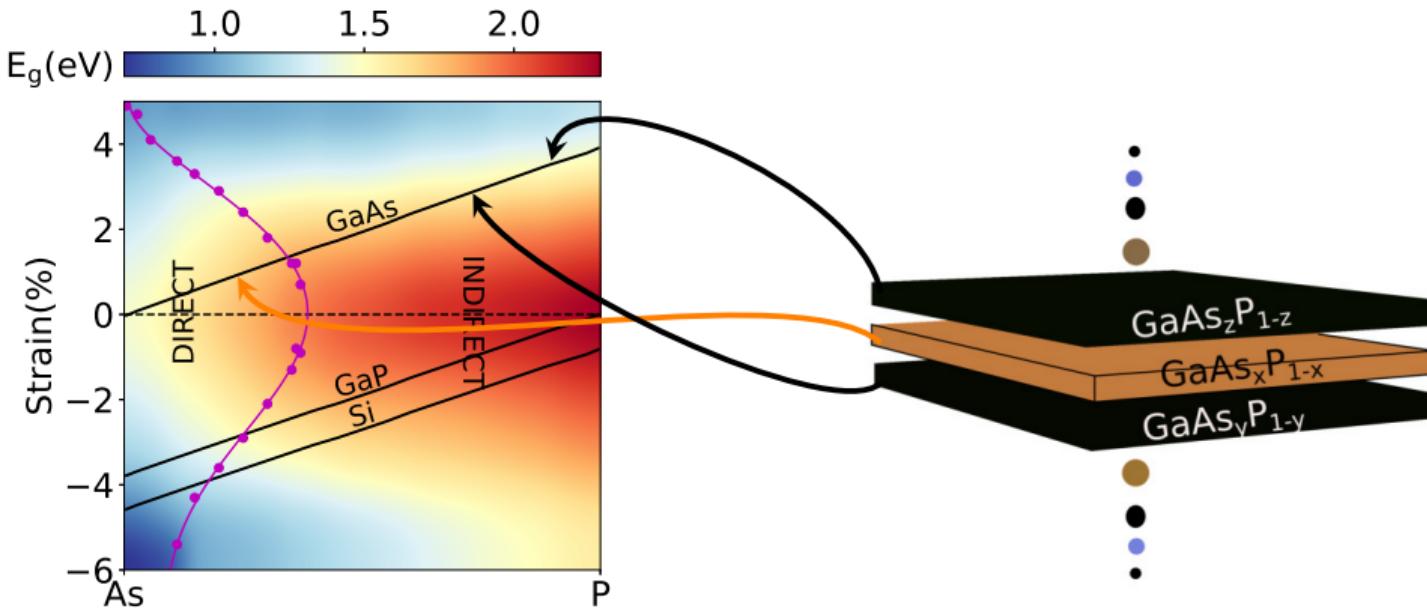
Ga(AsP) biaxial strain: bandgap phase diagram



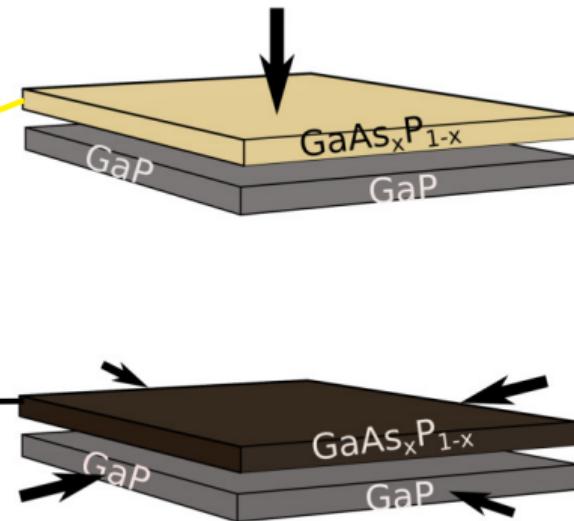
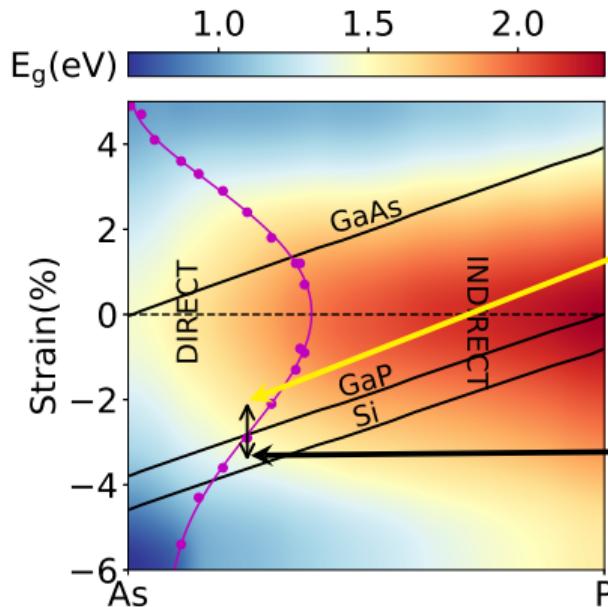
Ga(AsP) biaxial strain: bandgap phase diagram



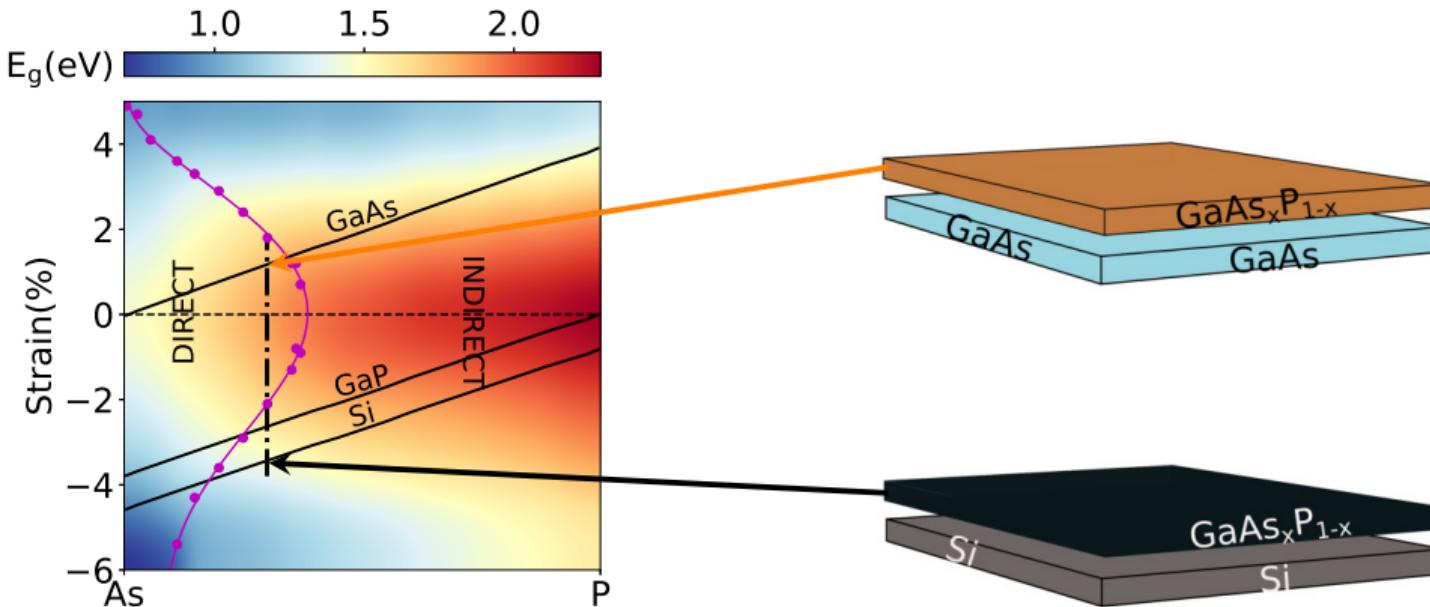
Ga(AsP) biaxial strain: bandgap phase diagram



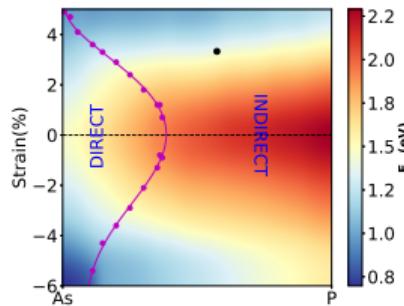
Ga(AsP) biaxial strain: bandgap phase diagram



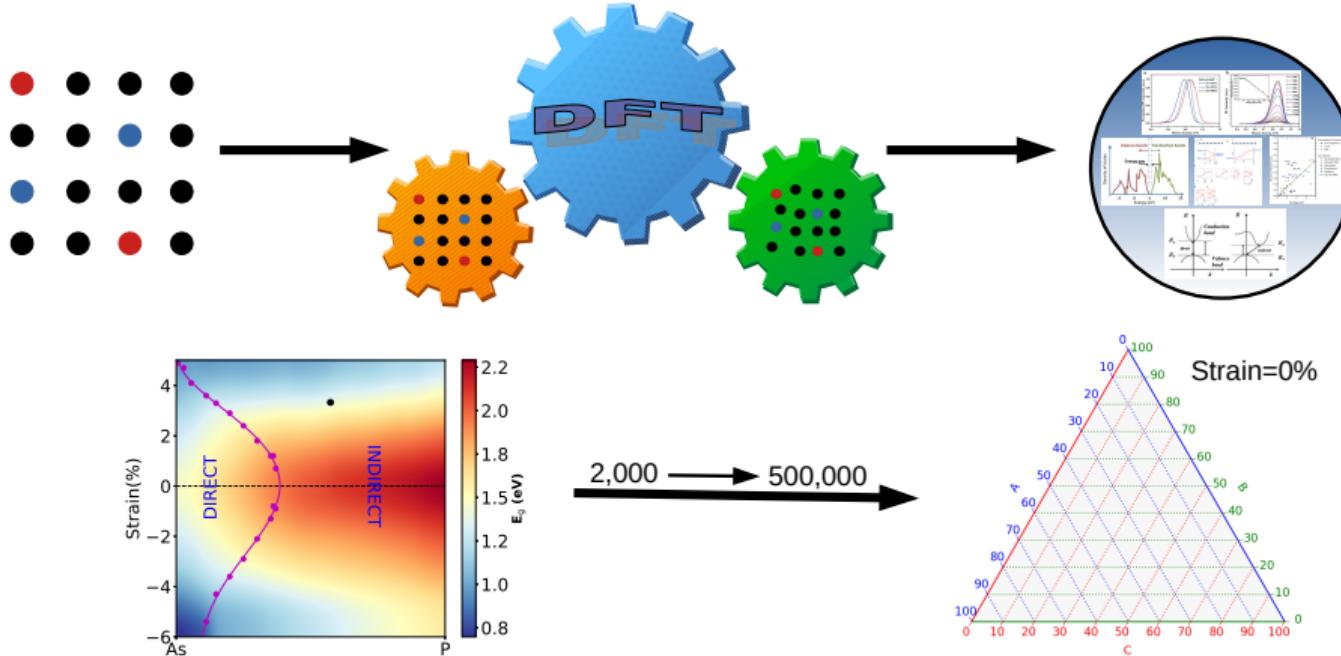
Ga(AsP) biaxial strain: bandgap phase diagram



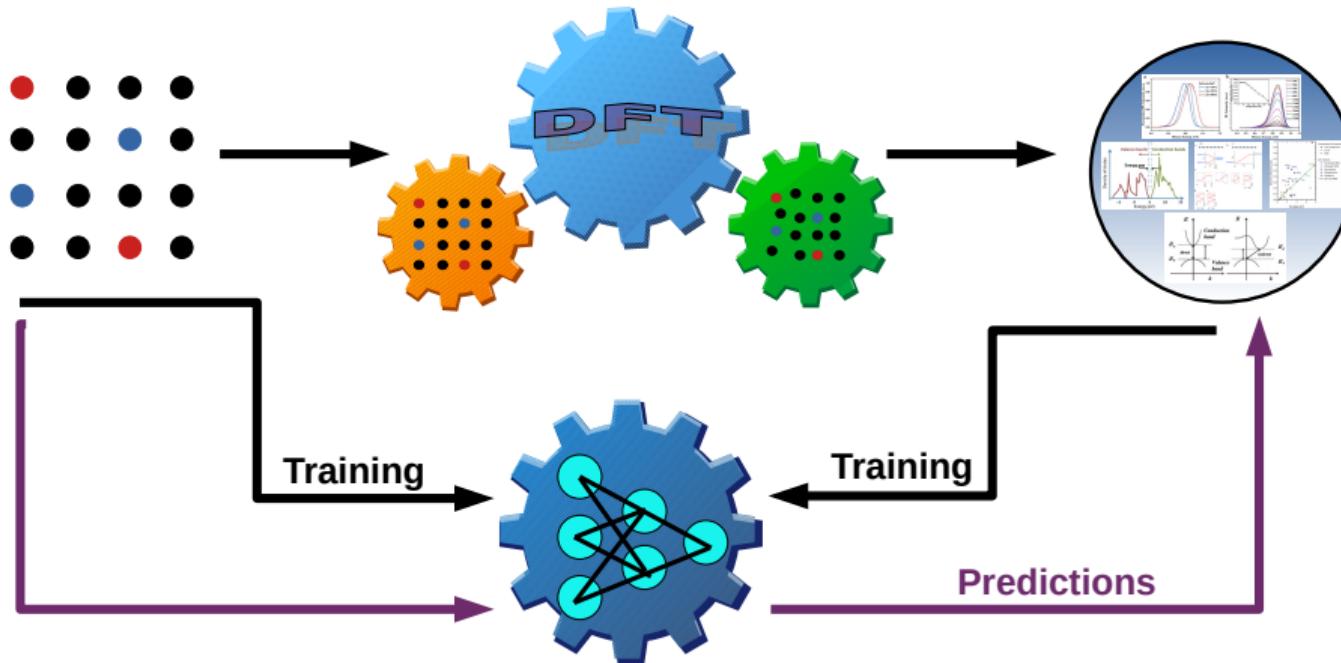
Approach



Approach

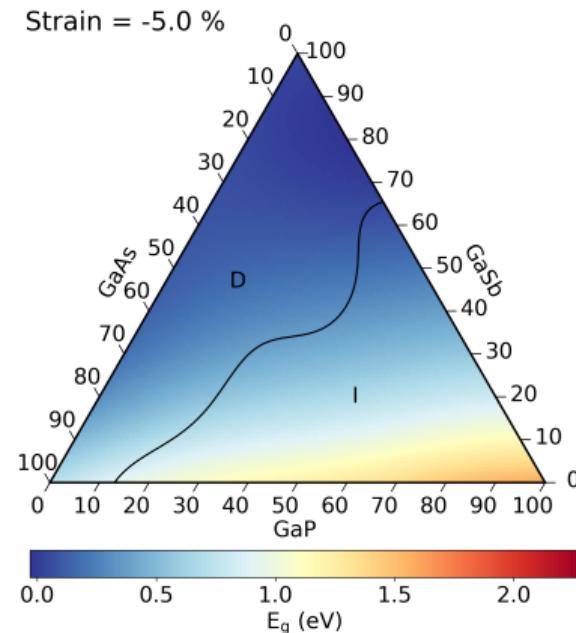


Approach



Ga(AsPSb) biaxial strain: bandgap phase diagram

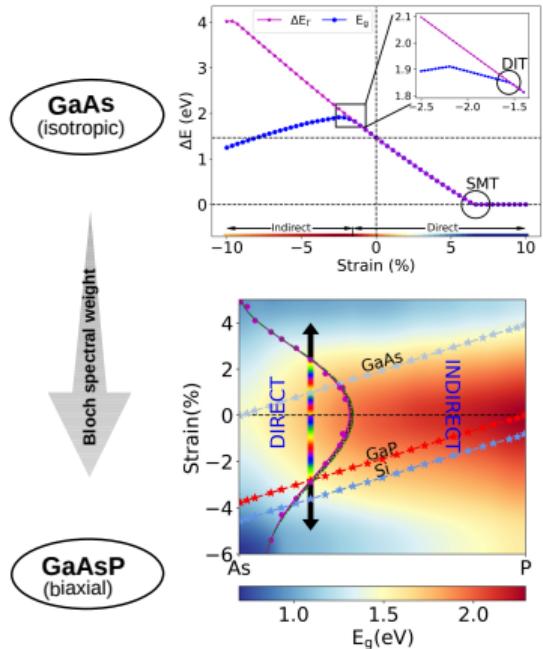
- Machine learning model^{c, d}
 - Support Vector Machine(rbf)
 - Radial Basis Function kernel
 - Training set: 4000 data points
 - Accuracy
 - Bandgap: R2 score = 0.99
 - Bandgap nature: accuracy = 0.95



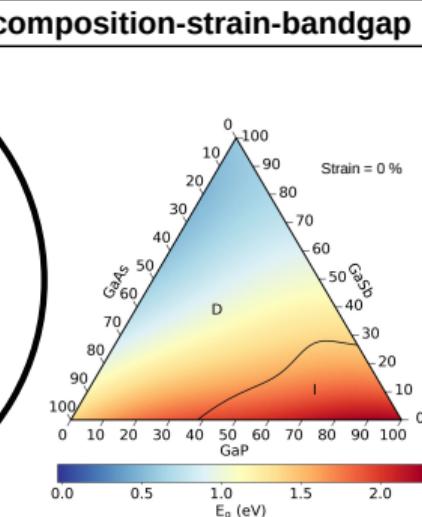
Ga(AsPSb) biaxial strain: bandgap phase diagram

- Machine learning model^{c, d}
 - Support Vector Machine(rbf)
 - Radial Basis Function kernel
 - Training set: 4000 data points
 - Accuracy
 - Bandgap: R2 score = 0.99
 - Bandgap nature: accuracy = 0.95

Summary



Bandgap phase diagram



GaAsPSb
(biaxial)

More

Systems

▼ III-V semiconductors

► III-V binary

▼ III-V ternary

▼ DFT based

- [GaAsP Computational details](#) (uploaded on 22.09.2021)
- [GaAsN Computational details](#) (uploaded on 22.09.2021)
 - No direct-indirect transition (DIT) for GaAsN under biaxial strain within $\pm 5\%$ of strain.
- [GaPSb](#) (only biaxial) [Computational details](#)
- [GaPSb](#) (only biaxial) [Computational details](#)
- GaPBi (only biaxial) (* available only on personal contact), [Computational details](#)
- GaAsBi (only biaxial) (* available only on personal contact), [Computational details](#)
- [Important notes](#)

▼ III-V quaternary (comming soon)

► DFT + Machine learning based

<https://bmondal94.github.io/Bandgap-Phase-Diagram/>

Acknowledgements

- Prof. Dr. Ralf Tonner-Zech
- Prof. Dr. Kerstin Volz
- Late Prof. Dr. Bruno Eckhardt
- HRZ Marburg, GOETHE-CSC Frankfurt, ZIH Dresden, HLR Stuttgart
- GRK 1782: Functionalization of Semiconductors



GRK 1782
Functionalization
of Semiconductors

Philipps



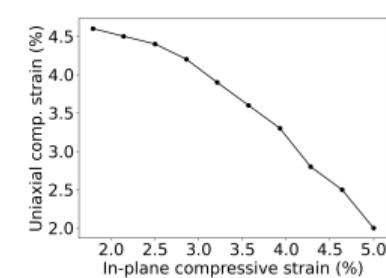
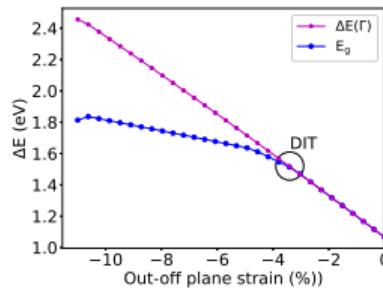
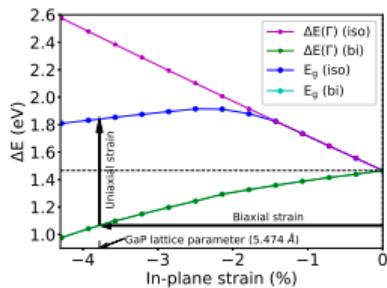
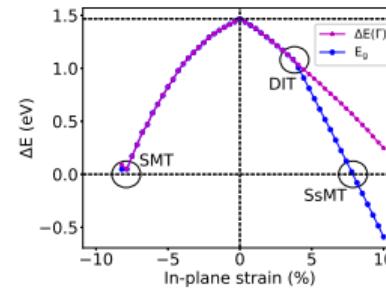
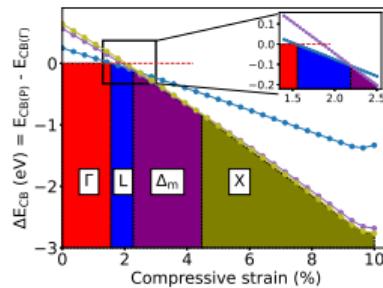
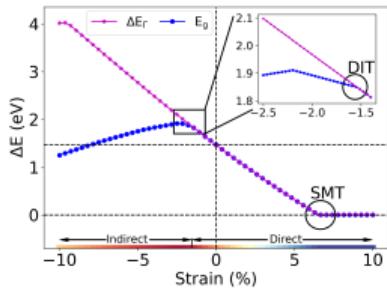
Universität
Marburg



UNIVERSITÄT
LEIPZIG



GaAs system summary



Binary systems

System	Transition	Transition path (iso)	Transition path (bi)
Si	IDT	$\Delta_m \rightarrow L \rightarrow \Gamma$ (t)	$\Delta_m \rightarrow K \rightarrow L$ (c)
GaP	IDT	$\Delta_m \rightarrow L \rightarrow \Gamma$ (t)	$\Delta_m \rightarrow L$ (c)
GaAs	DIT	$\Gamma \rightarrow L \rightarrow \Delta_m \rightarrow X$ (c)	$\Gamma \rightarrow \Delta_m$ (t)
GaSb	DIT	$\Gamma \rightarrow L \rightarrow \Delta_m$ (c)	$\Gamma \rightarrow \Delta_m$ (t)
InP	DIT	$\Gamma \rightarrow X$ (c)	$\Gamma \rightarrow \Delta_m$ (t)
InAs	DIT	$\Gamma \rightarrow X$ (c)	×
InSb	DIT	$\Gamma \rightarrow L \rightarrow \Delta_m$ (c)	×

System	Si	GaSb	GaAs	GaP	InSb	InAs	InP
T1 (%) * [@]	~ 15	2.85	6.67	~ 13	0.34	2.10	8.20
T2 (%) †	10.31 (t)	1.00 (c)	1.56 (c)	2.63 (t)	5.18 (c)	7.41 (c)	4.40 (c)
T3 (%) ‡	×	3.71 (t)	3.52 (t)	×	×	×	7.66 (t)

't' and 'c' in brackets indicate to tensile and compressive strain, respectively.

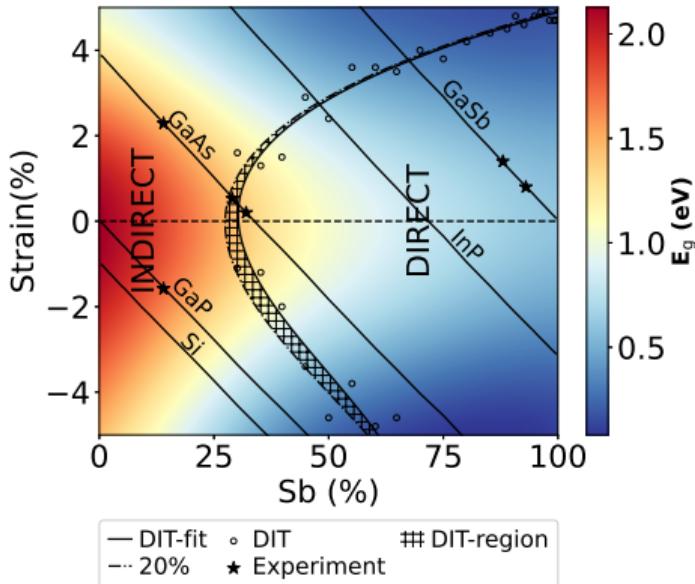
@ Linear extrapolation

* Semiconductor to metal transition under isotropic tensile strain

† Direct to indirect (DIT) or indirect to direct (IDT) transition under isotropic strain.

‡ DIT or IDT transition under bi-axial strain

Ga(PSb) bandgap phase diagram

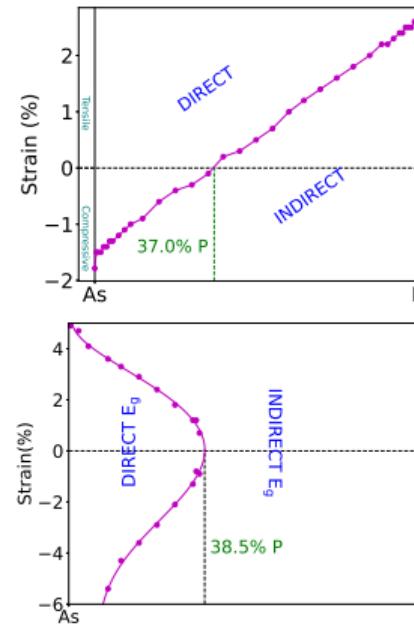
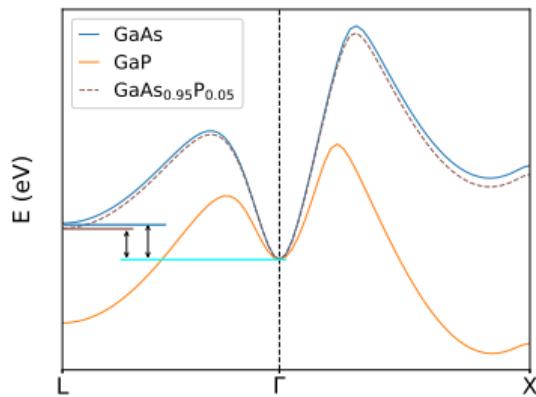


substrate	Sb (%)	E_g (eV)	exp. E_g (eV)*
GaAs	14	1.63	1.61
	14	1.60	1.61
	29	1.44	1.39
	32	1.38	1.31
	33	1.36	1.40
GaSb	93	0.61	0.73

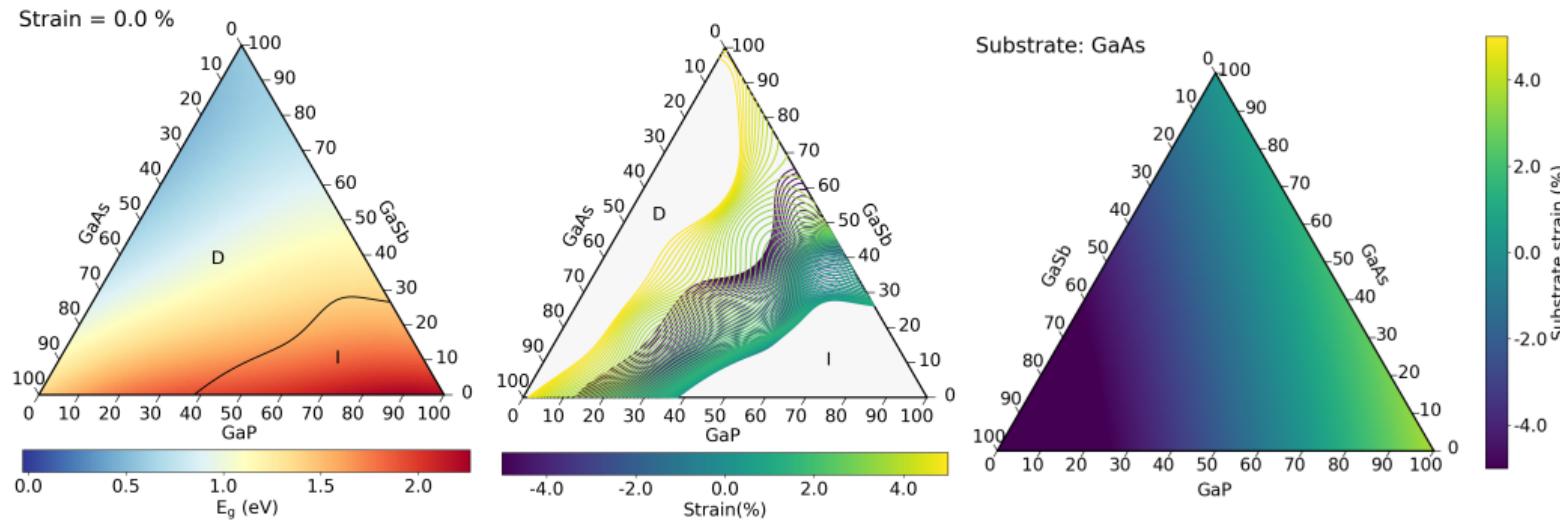
Ternary DIT Assumptions/ Errors/ Limitations

- Statistical error: Finite resolution (in strain and conc.), SQS
- Inherent error: Effective Bloch weight.
- Uncertainty in exact DIT: $BW_G = BW_L$
 - $BW_G: BW_L = 40:60$ vs $60:40$
 - Cutoff criteria for minimum BW %
- k-point error: DIT at other k-point
- BW's directional dependency in L and X point (biaxial strain)
- Energetically closely spaced bands: Average, Near flat bands
- Extremely sparse BWs in bands
- Not generizable to higher(lower) bands other than CB(VB)

Binary approximation: Ga(AsP) isotropic strain



Quaternary



DFT computational details [§]

- VASP 5.4.4
- $6 \times 6 \times 6$ supercell
- Geometry optimization: PBE + DFT-D3; Bandgap: TB09
- 450 eV (for optimization), 350 eV ENCUT (for band gap)
- Convergency criteria (optimization): 10^{-7} eV (electronic energy); 10^{-2} eVÅ⁻¹ (force)
- Convergency criteria (bandgap): 10^{-6} eV (electronic energy); 10^{-2} eVÅ⁻¹ (force)
- Spin-orbit coupling during bandgap calculation
- 10 sqs for each composition and strain point