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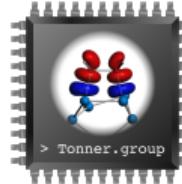
Epi-seminar 2022

Strain effect on III-V semiconductor bandgap

January 10, 2022

Badal Mondal

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



Introduction



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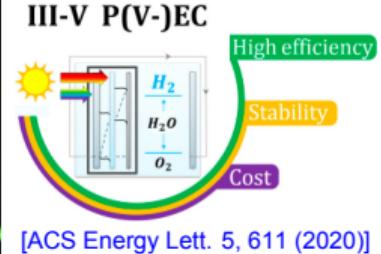
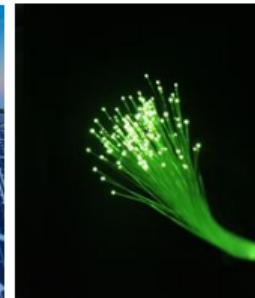
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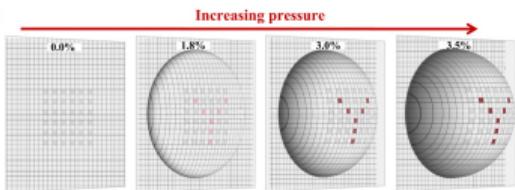
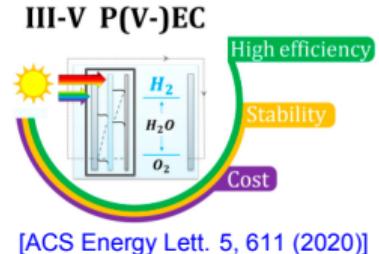
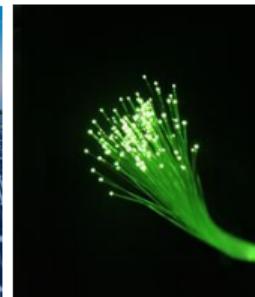
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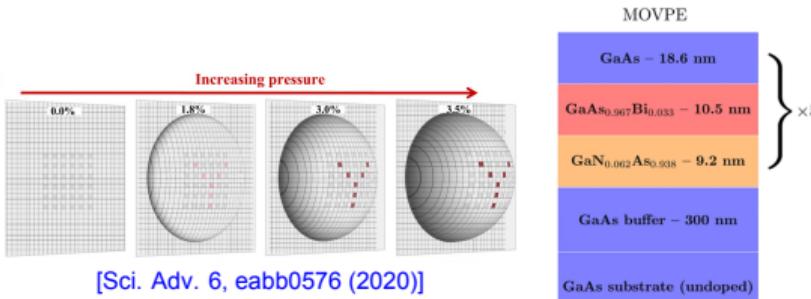
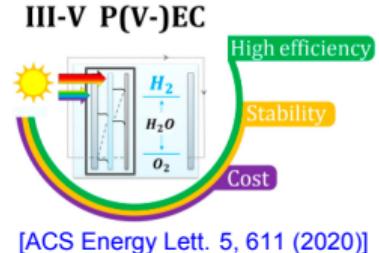
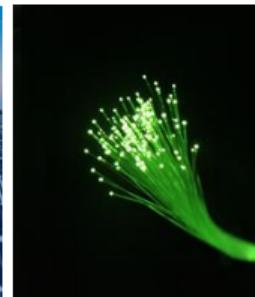


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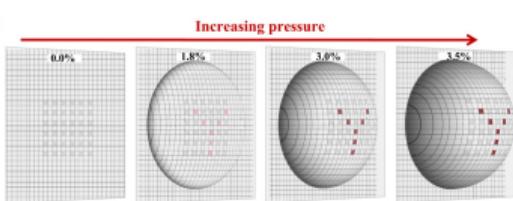
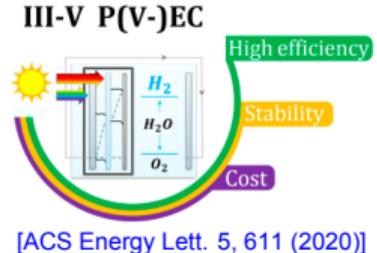
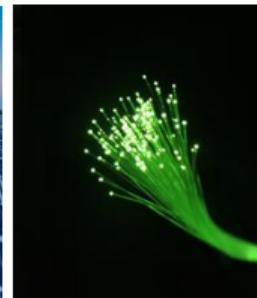


[Sci. Adv. 6, eabb0576 (2020)]

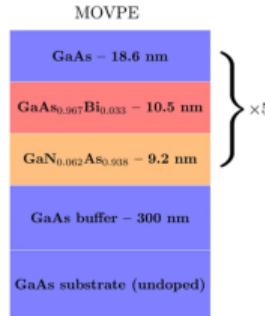
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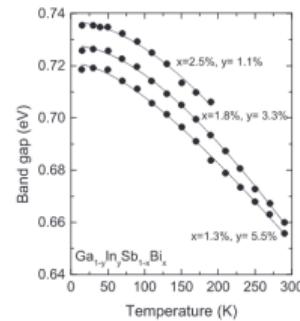
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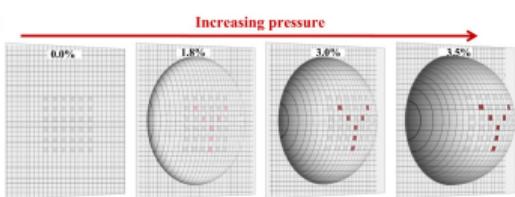
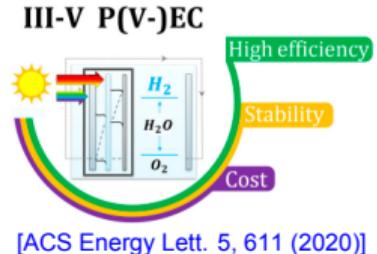
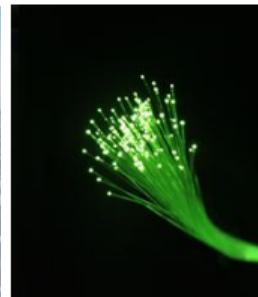
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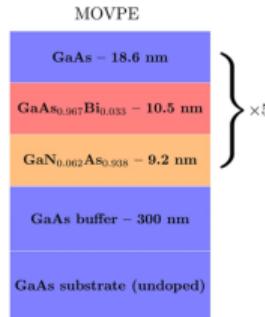
[Sci. Rep. 6, 46371 (2017)] [Semi. Sci. Tech., 073001 (2018)]



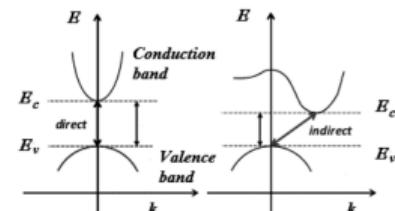
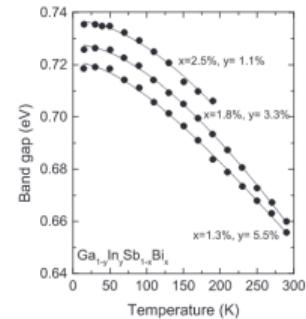
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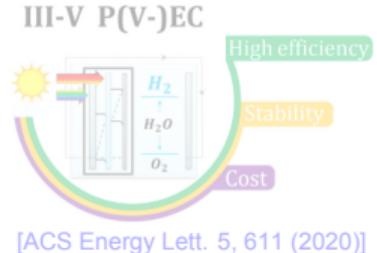


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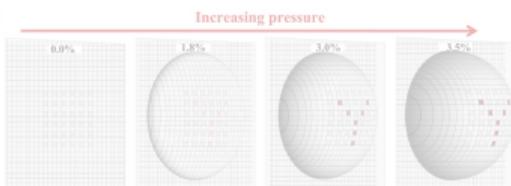


[Int. J. Sci. (2014)]

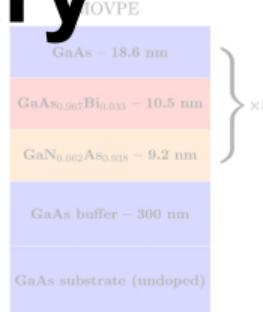
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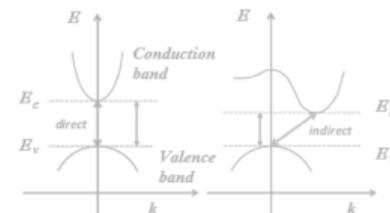
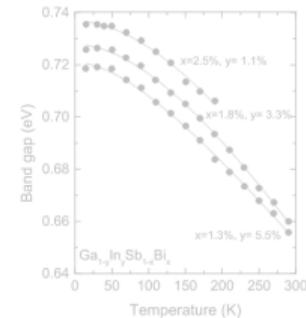
Binary



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

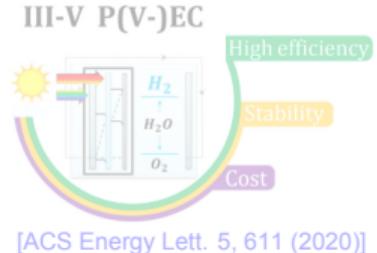


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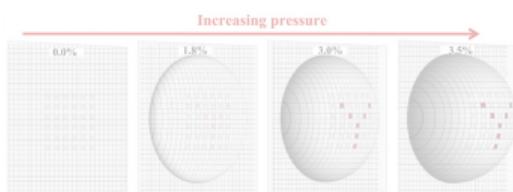


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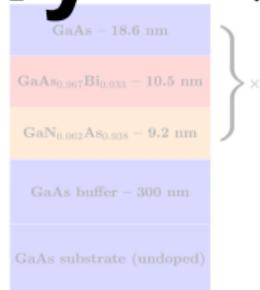
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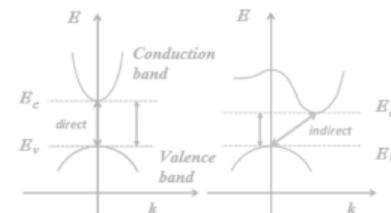
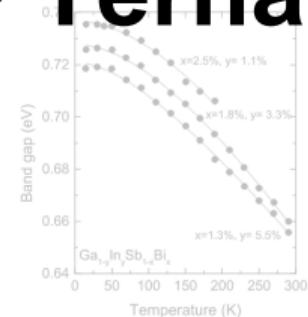
Binary → Ternary



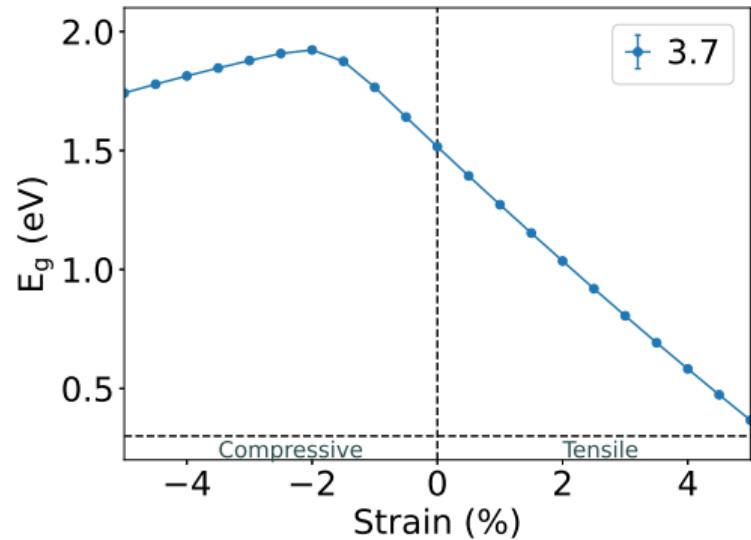
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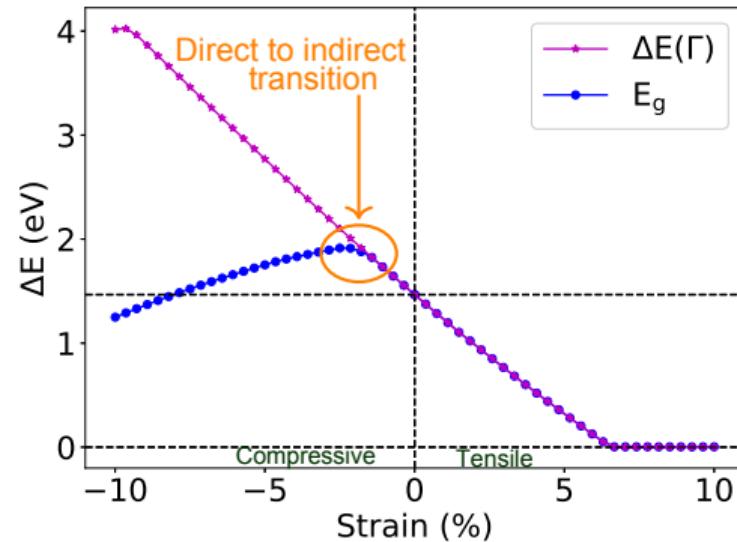
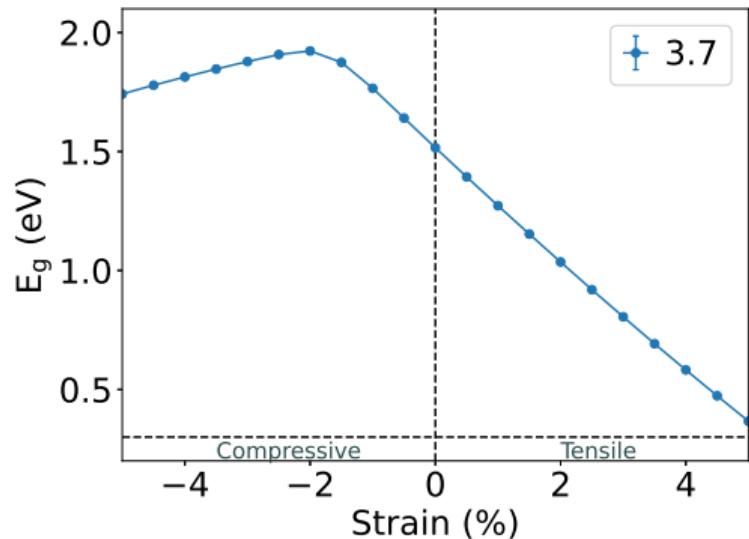
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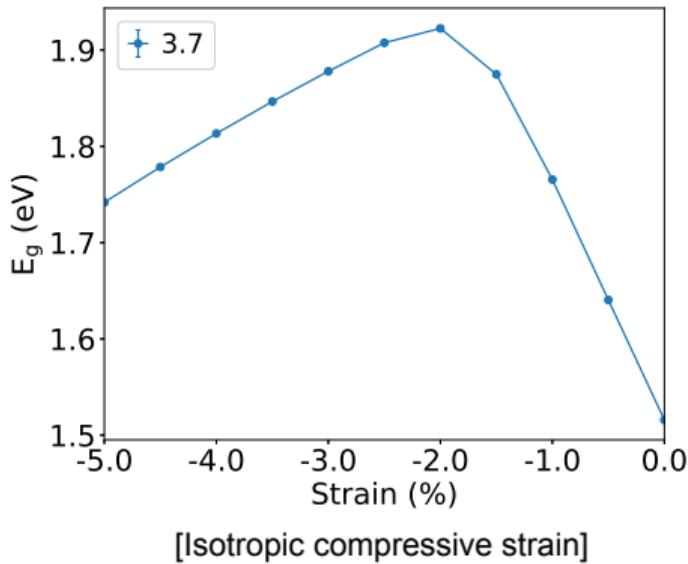
GaAsP, GaAs [100] isotropic strain ¹



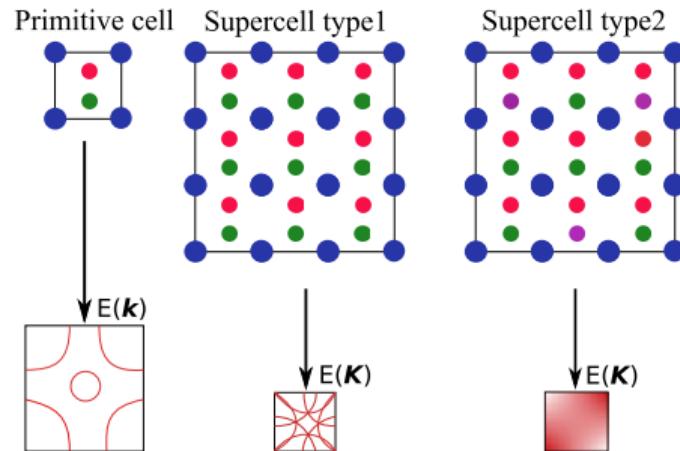
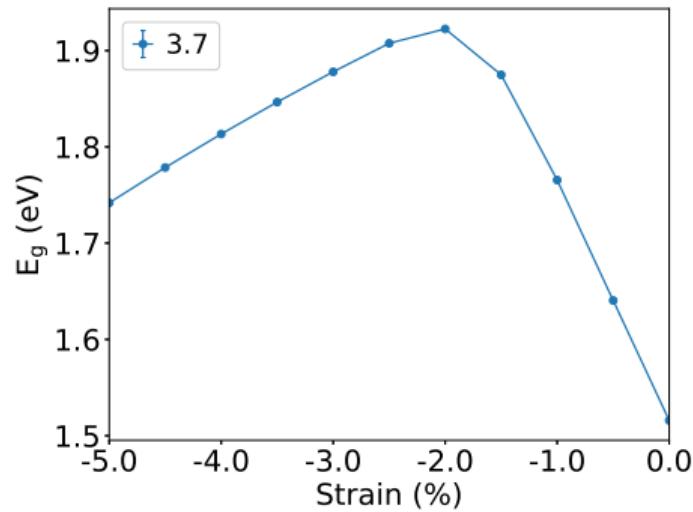
GaAsP, GaAs [100] isotropic strain ¹



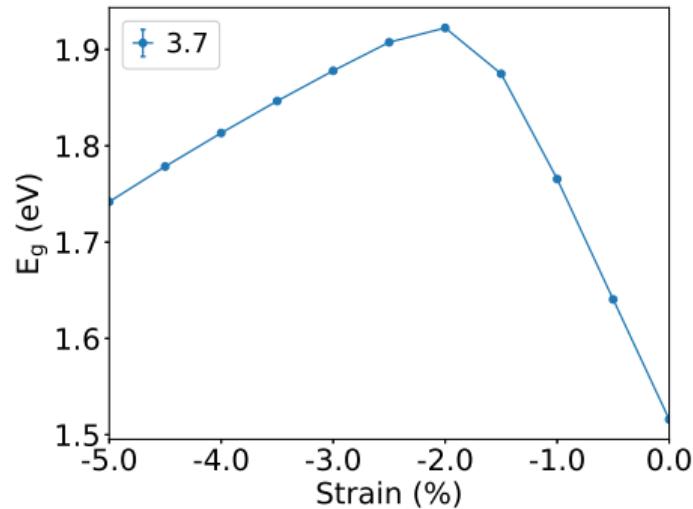
Ternary system: GaAsP



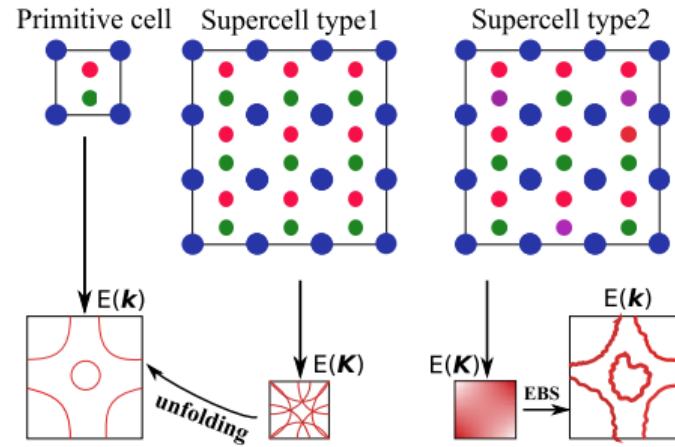
Ternary system: GaAsP, Band folding²



Band folding: Bloch spectral density/weight^{2,3,4}



[Isotropic compressive strain]

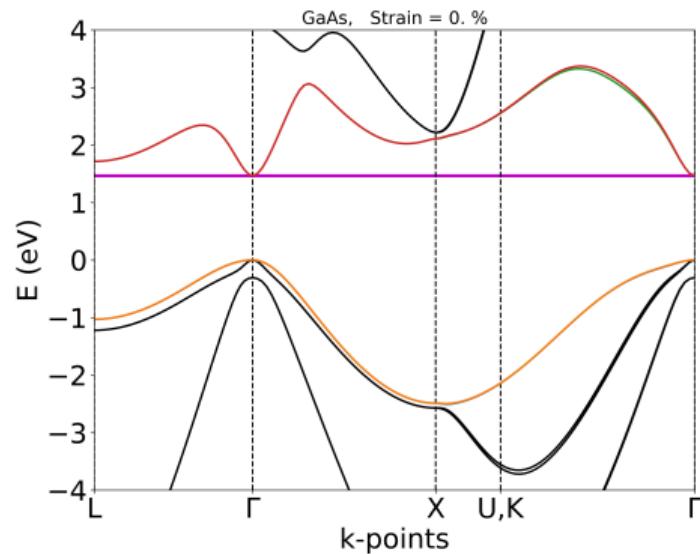
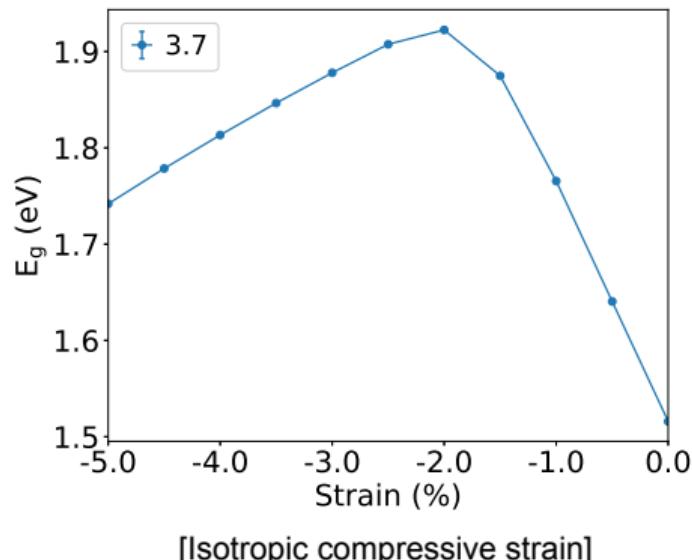


²L.-W. Wang *et al.*, *Phys. Rev. Lett.* **80**, 4725 (1998).

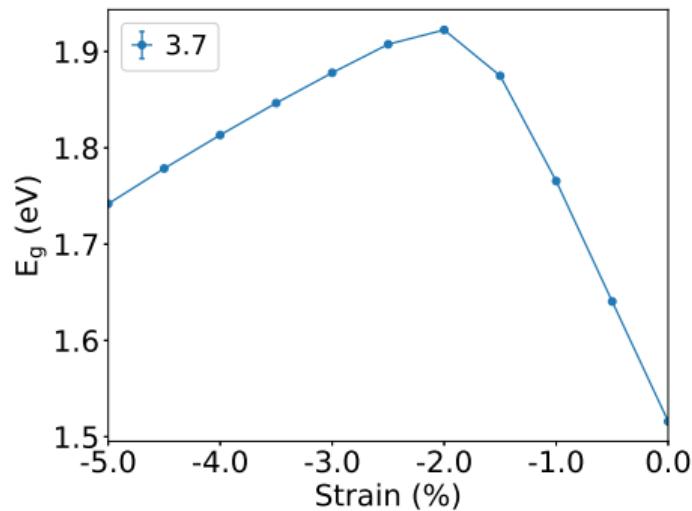
³V. Popescu, A. Zunger, *Phys. Rev. B* **85**, 085201 (2012).

⁴O. Rubel *et al.*, *Phys. Rev. B* **90**, 115202 (2014).

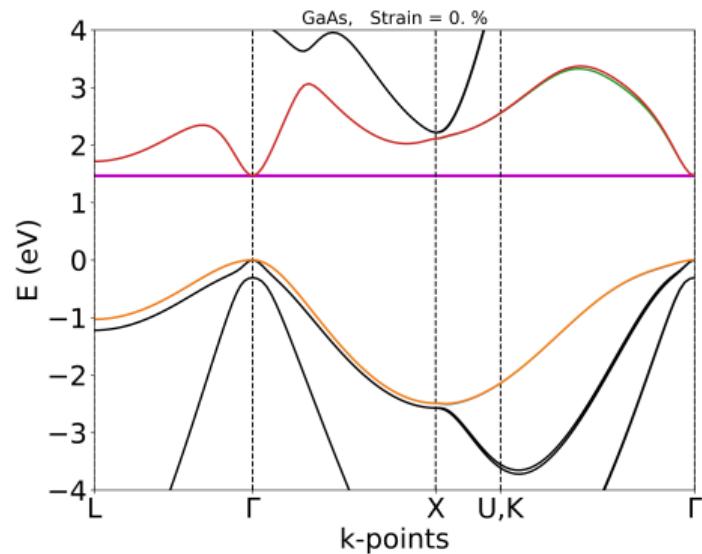
Band unfolding, Bloch weight



Band unfolding, Bloch weight

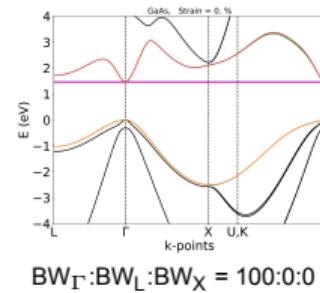
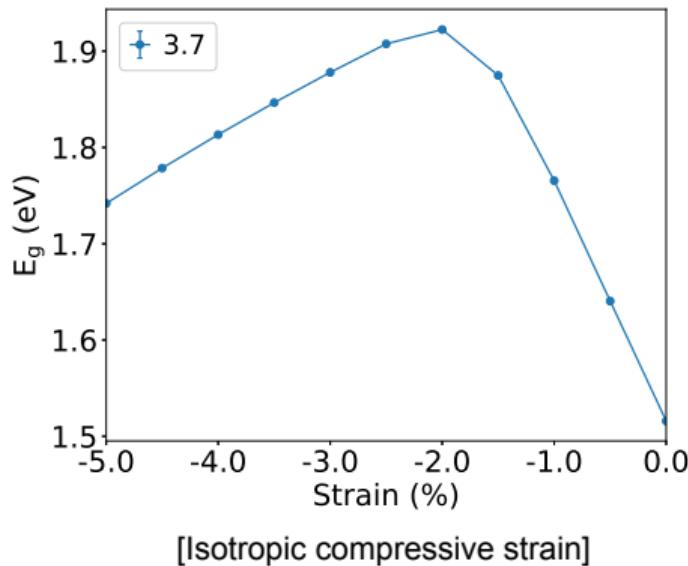


[Isotropic compressive strain]

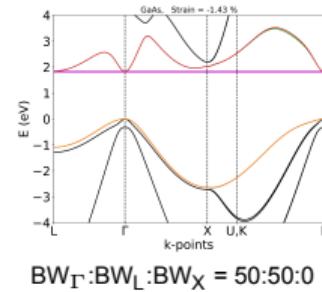
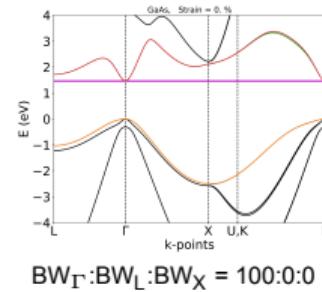
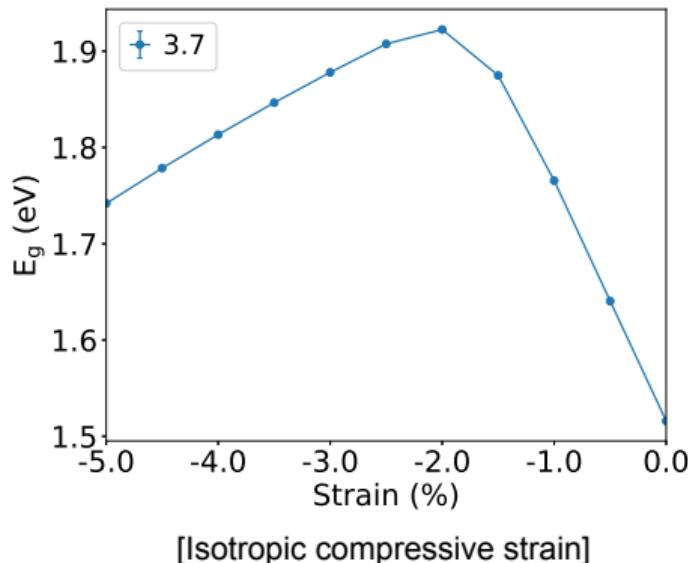


► CB: BW_{Γ} , BW_L , BW_X

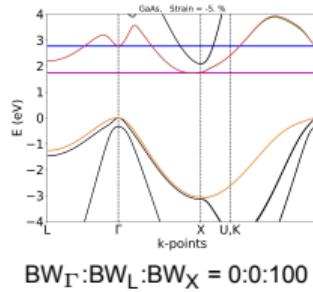
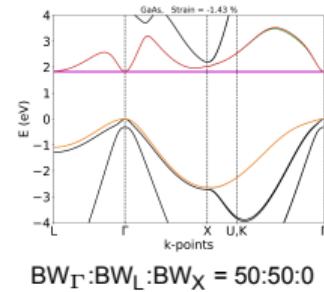
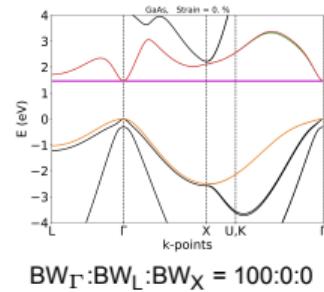
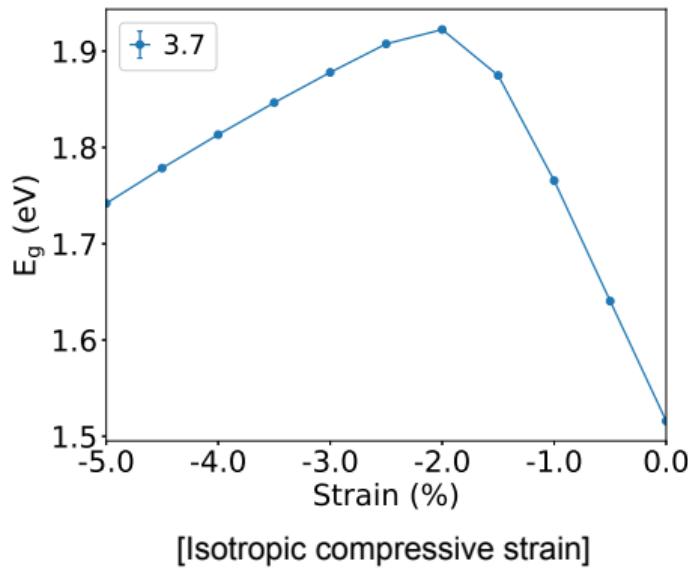
Band unfolding, Bloch weight



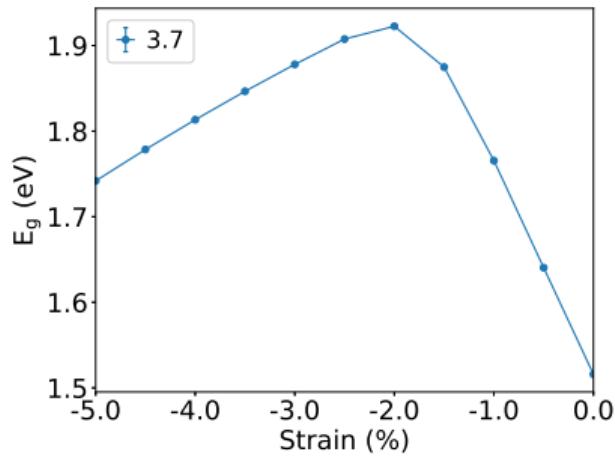
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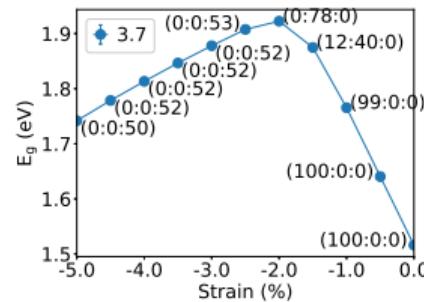
Band unfolding, Bloch weight



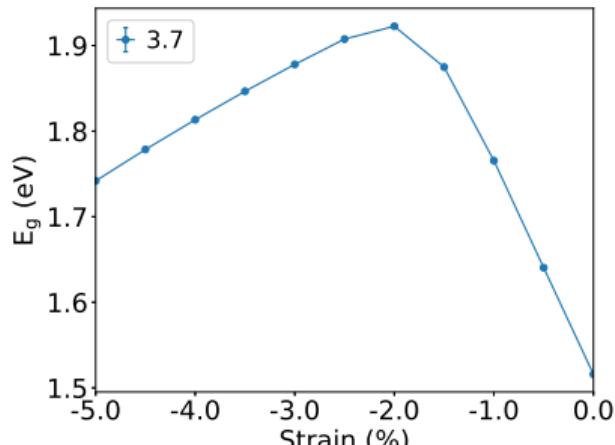
GaAsP: Direct-indirect transition



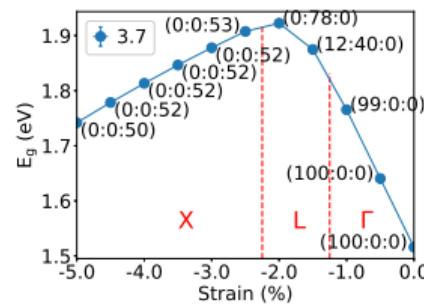
[Isotropic compressive strain]



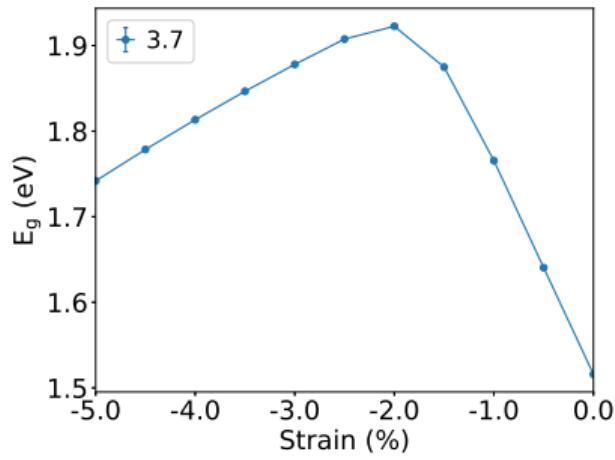
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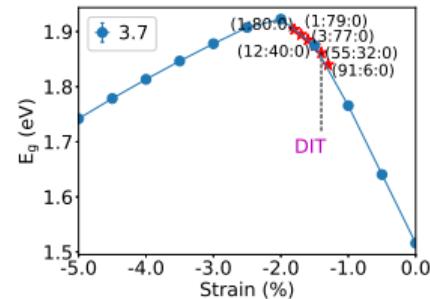
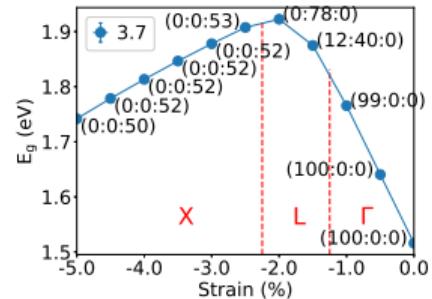
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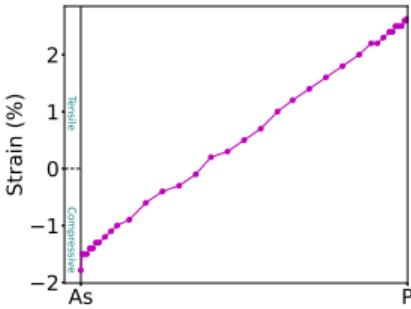
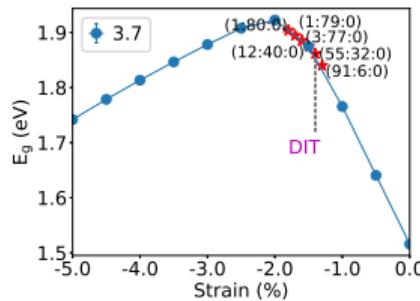
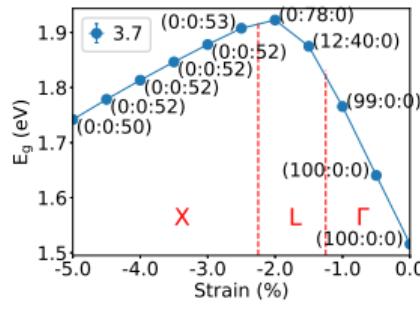
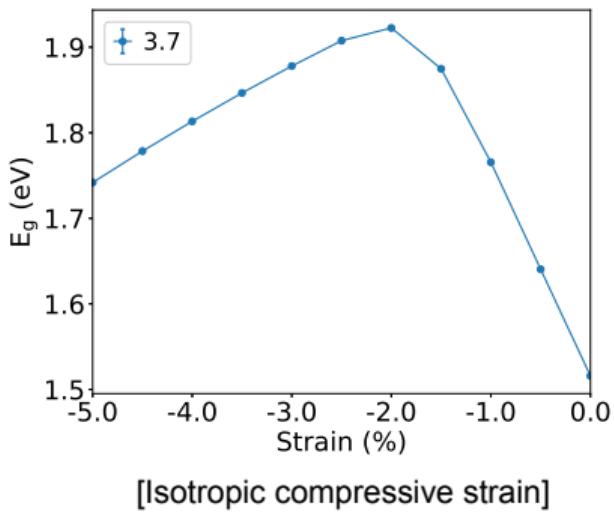
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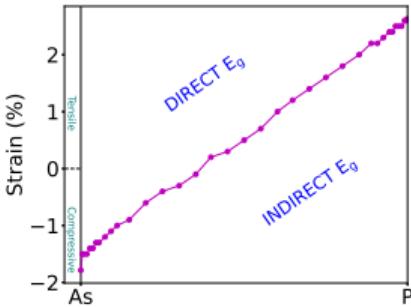
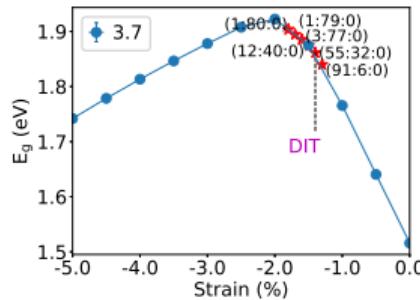
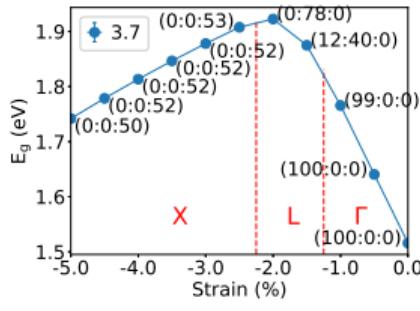
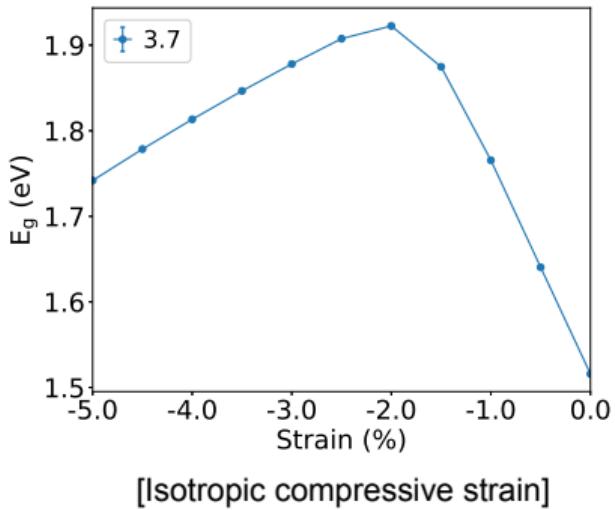
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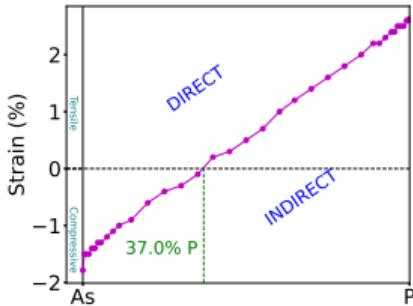
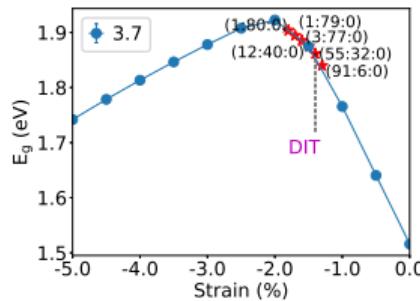
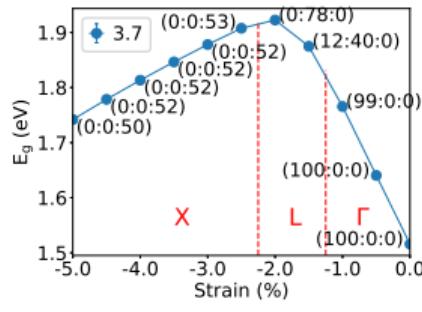
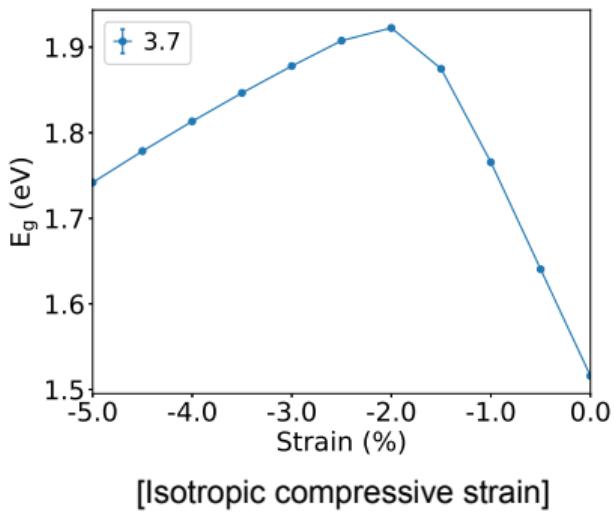
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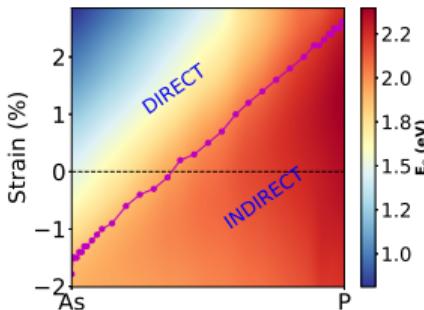
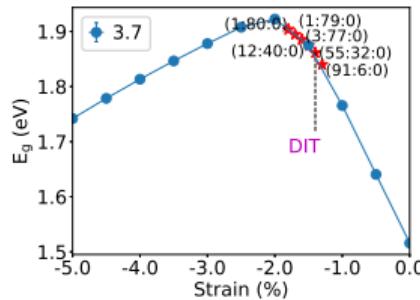
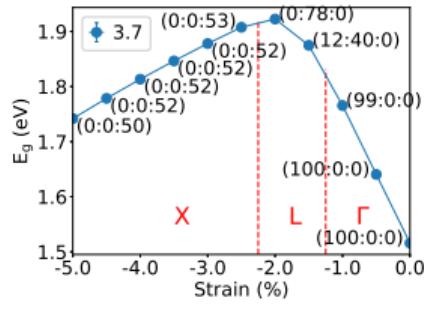
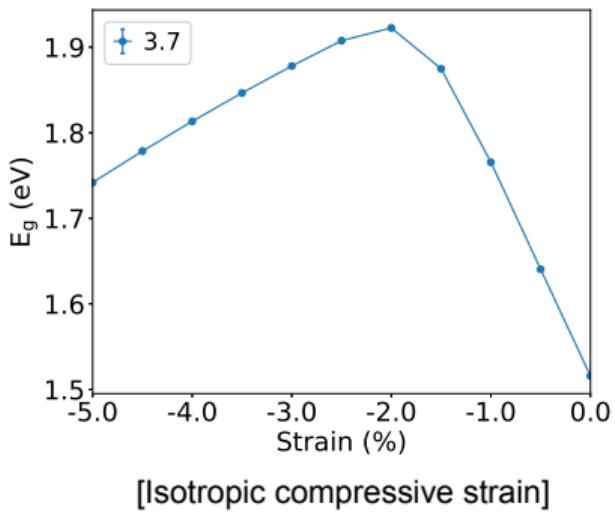
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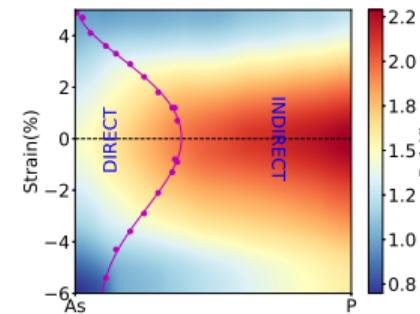
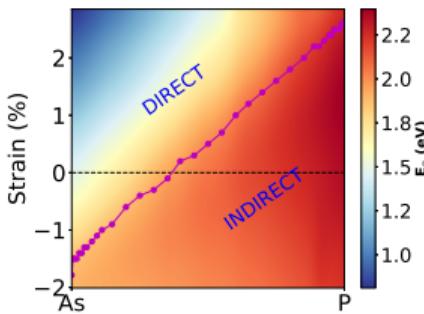
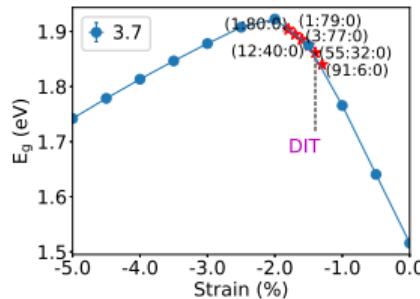
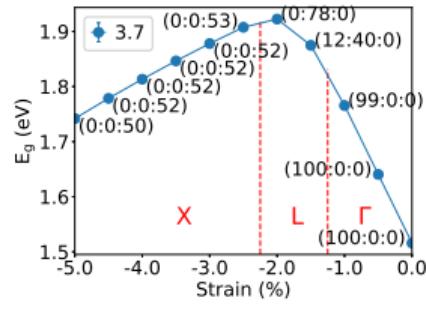
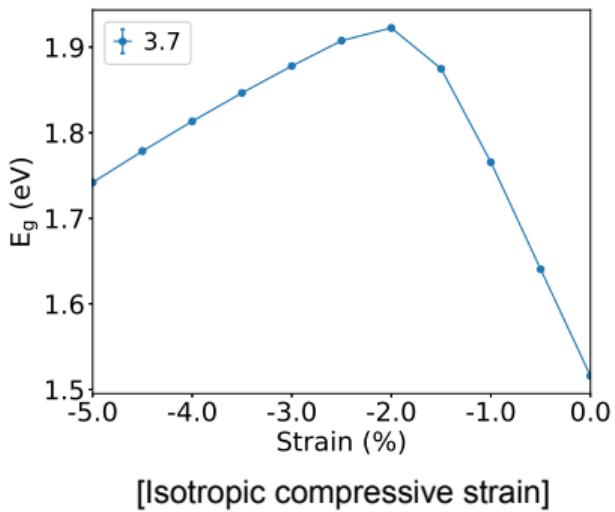
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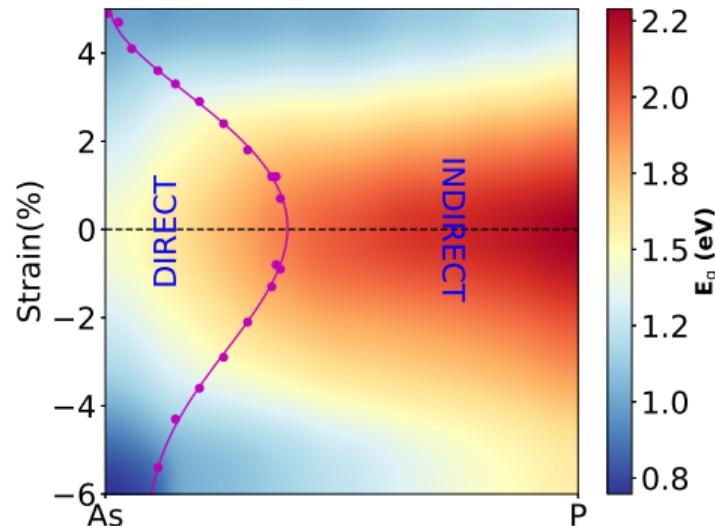
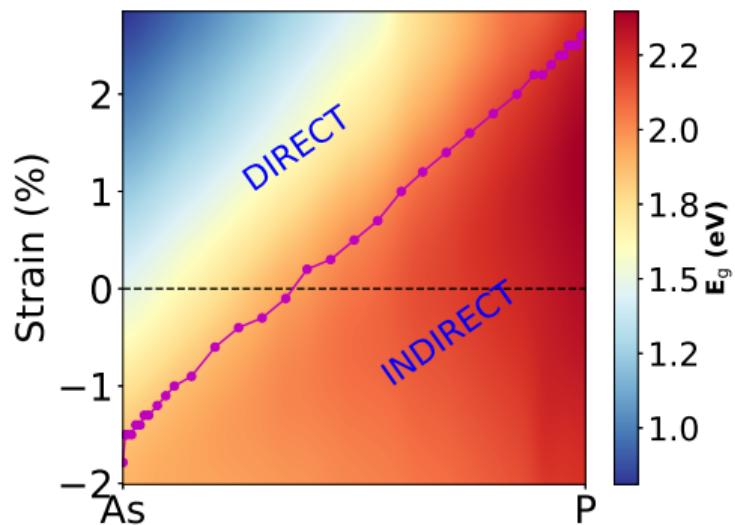
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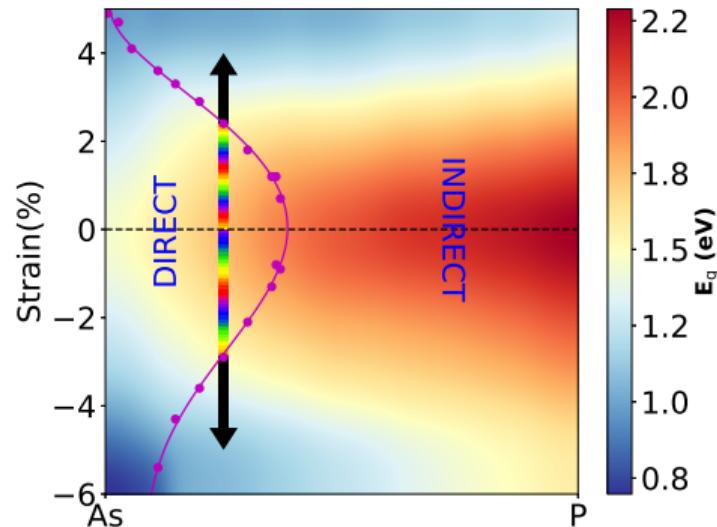
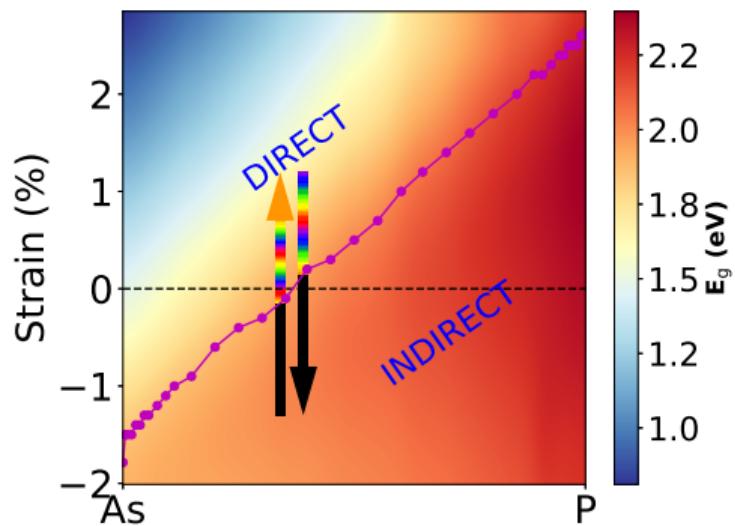
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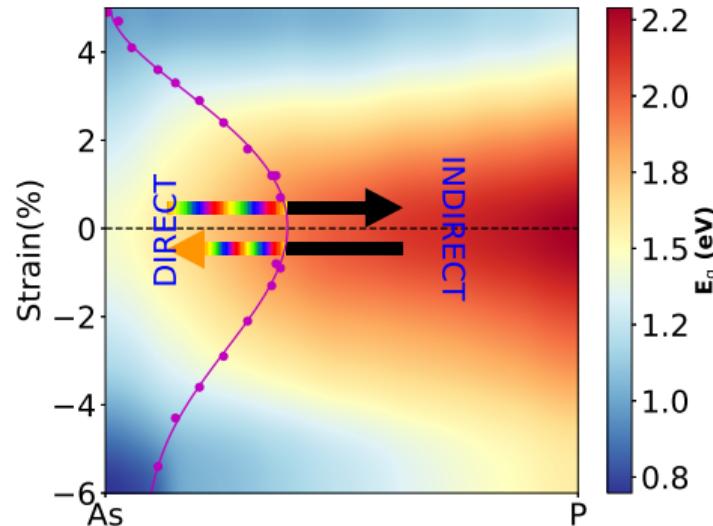
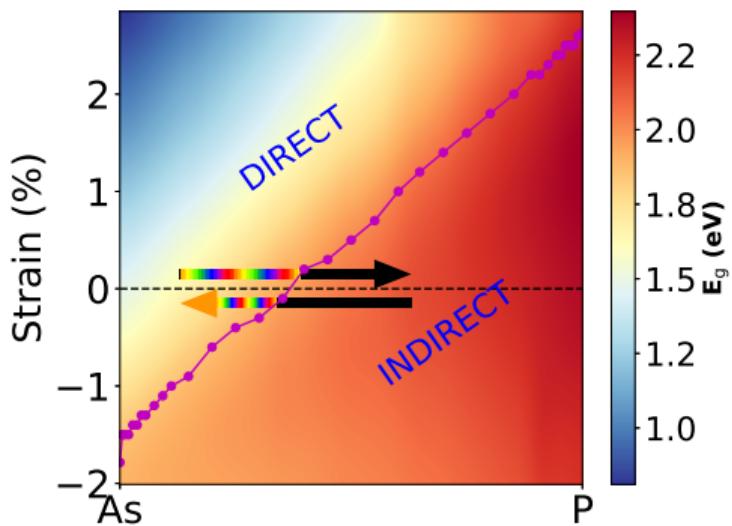
“Bandgap Phase Diagram”



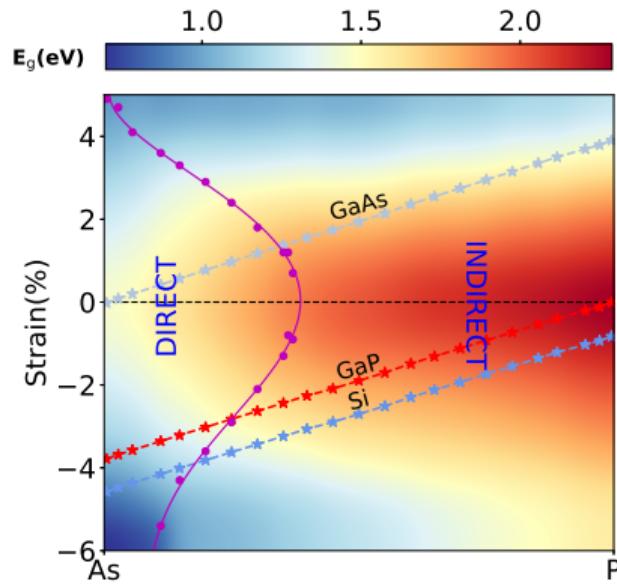
“Bandgap Phase Diagram”



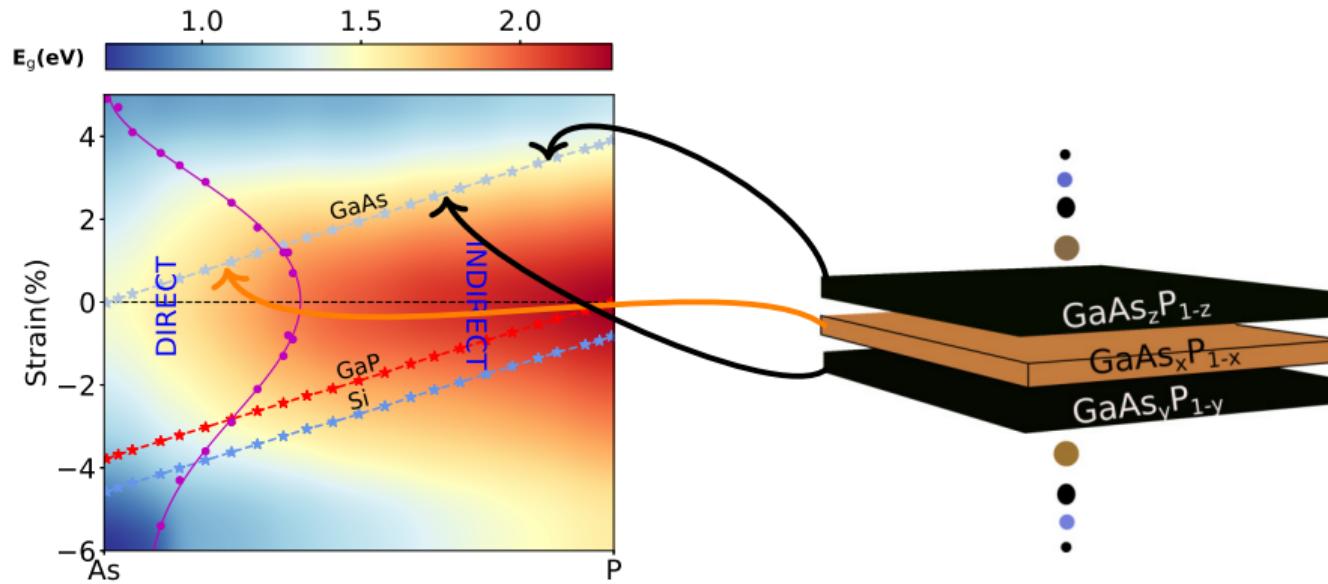
“Bandgap Phase Diagram”



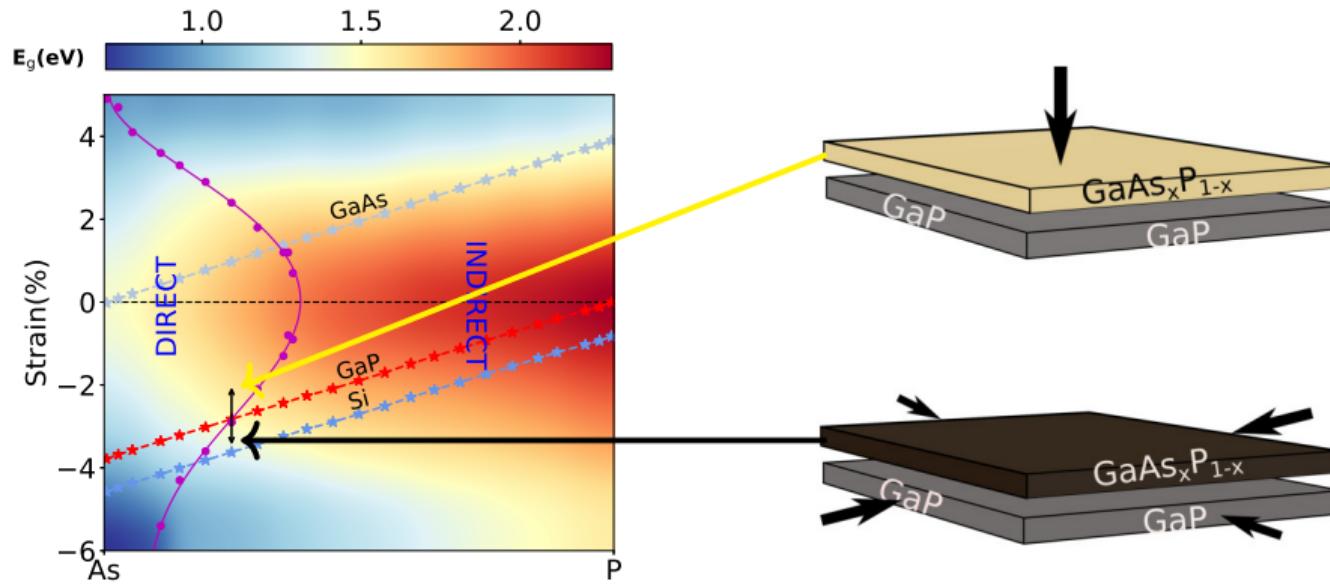
GaAsP biaxial strain: Bandgap phase diagram



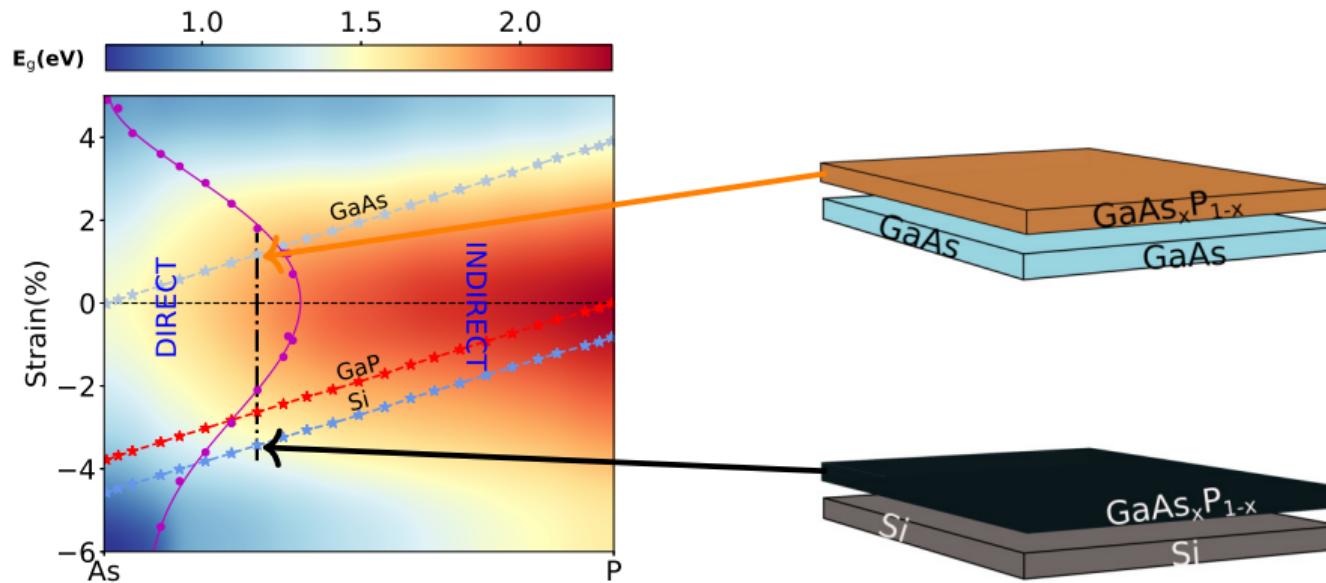
GaAsP biaxial strain: Bandgap phase diagram



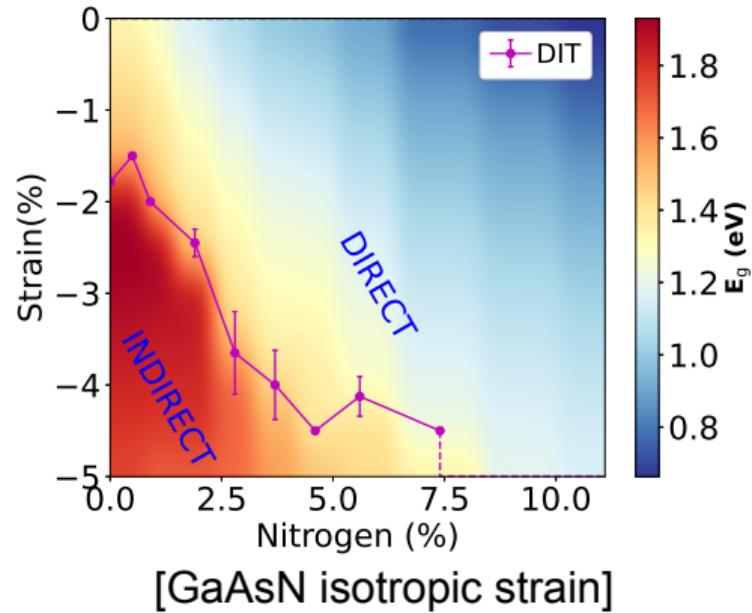
GaAsP biaxial strain: Bandgap phase diagram



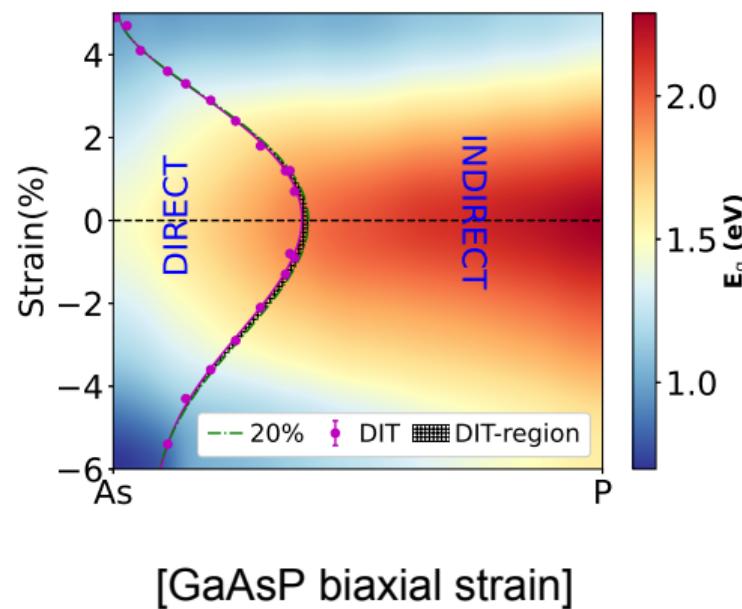
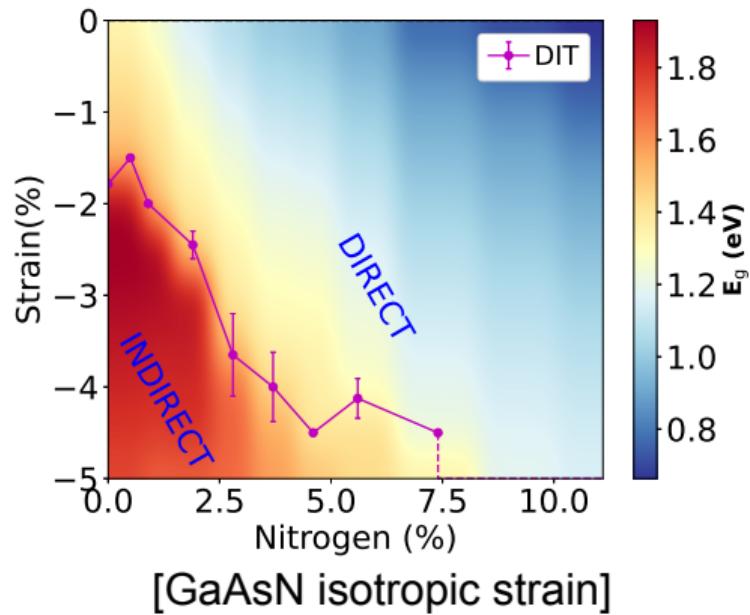
GaAsP biaxial strain: Bandgap phase diagram



Bandgap Phase Diagram: Precision

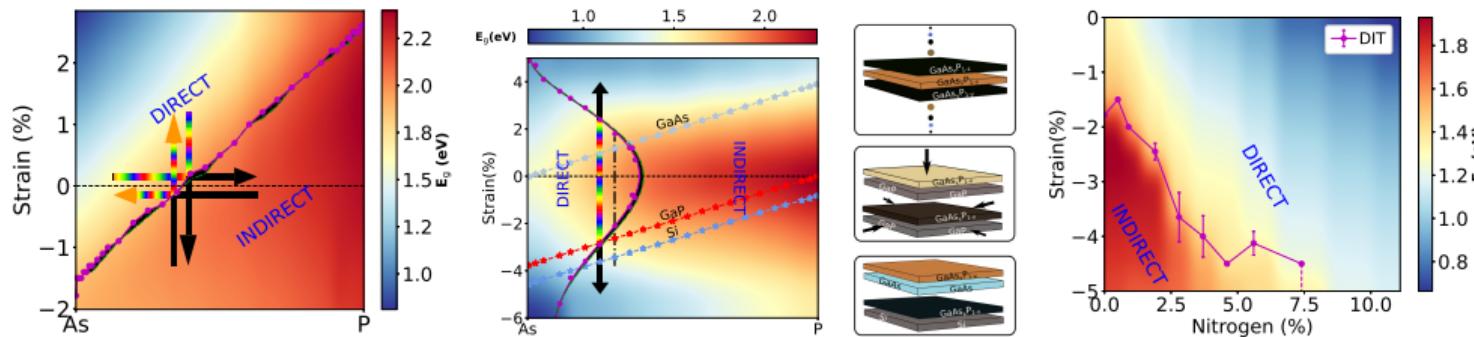


Bandgap Phase Diagram: Precision



Summary

- ▶ Direct-indirect transition: ternary system
 - ▶ Bloch spectral density
 - ▶ Bandgap phase diagram [\[https://bmondal94.github.io/Bandgap-Phase-Diagram/\]](https://bmondal94.github.io/Bandgap-Phase-Diagram/)



What next?

What next?

- ▶ Other transitions (e.g. L-X)

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 - ▶ Machine learning

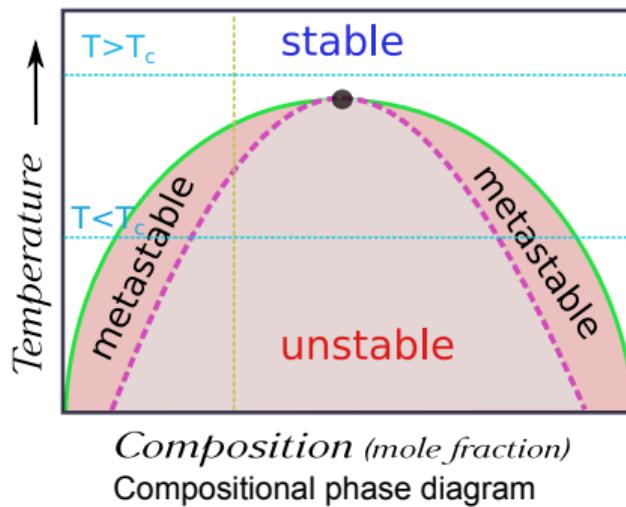
What next?

- ▶ Other transitions (e.g. L-X)
- ▶ 3rd dimension (e.g. phonon contribution)
- ▶ Higher order system
 - ▶ Machine learning
- ▶ Other material systems (e.g. II-VI, III-VI)

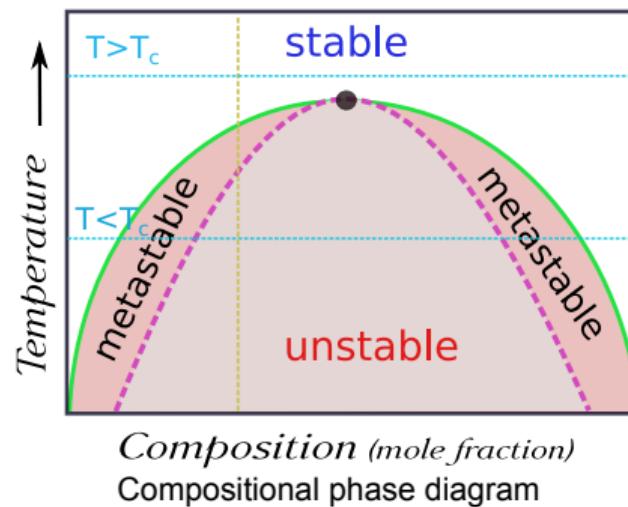
What next?

- ▶ Other transitions (e.g. L-X)
- ▶ 3rd dimension (e.g. phonon contribution)
- ▶ Higher order system
 - ▶ Machine learning
- ▶ Other material systems (e.g. II-VI, III-VI)
- ▶ Other areas (e.g. Auger recombination)

Significance

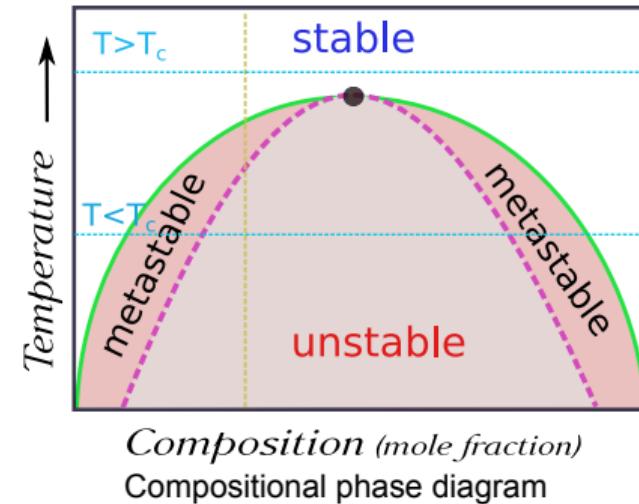
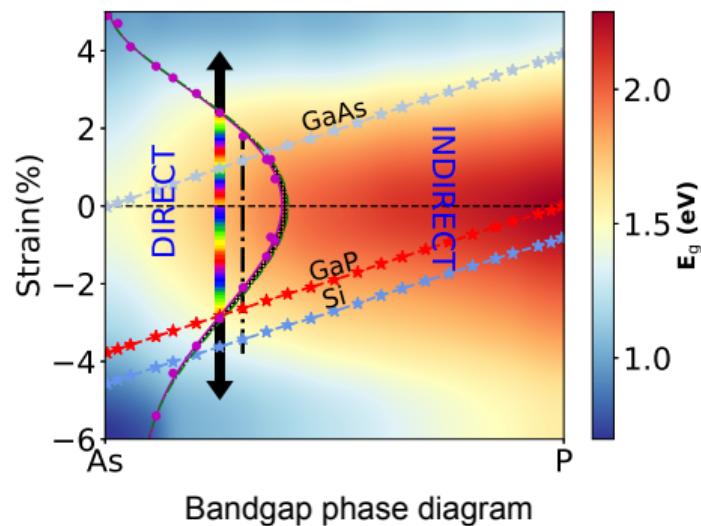


Significance



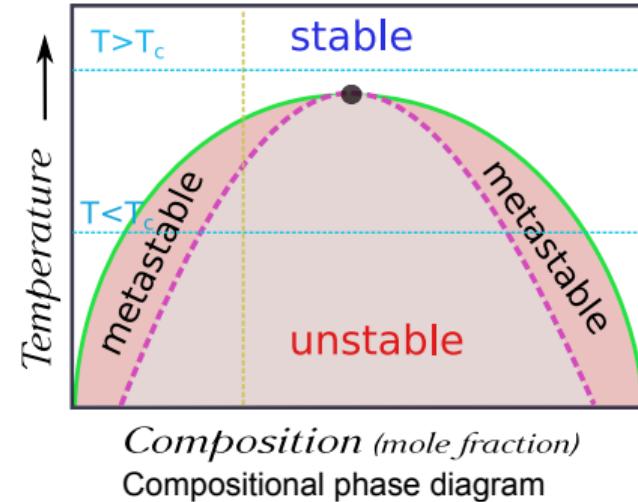
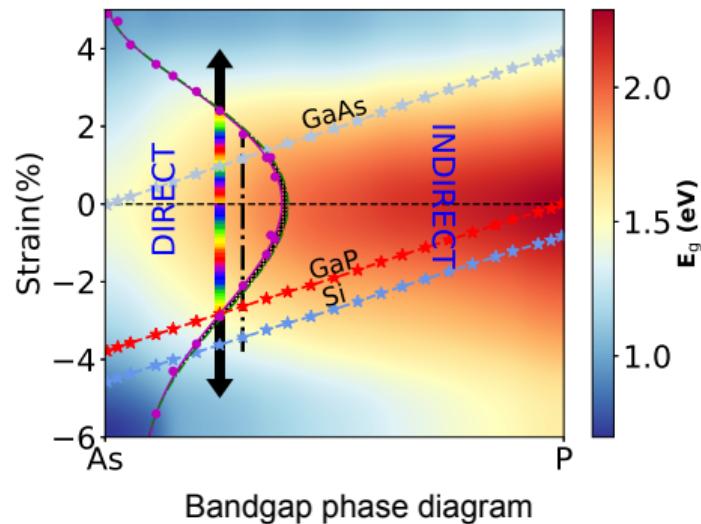
- Compositional phase diagram: **Can you grow?**

Significance

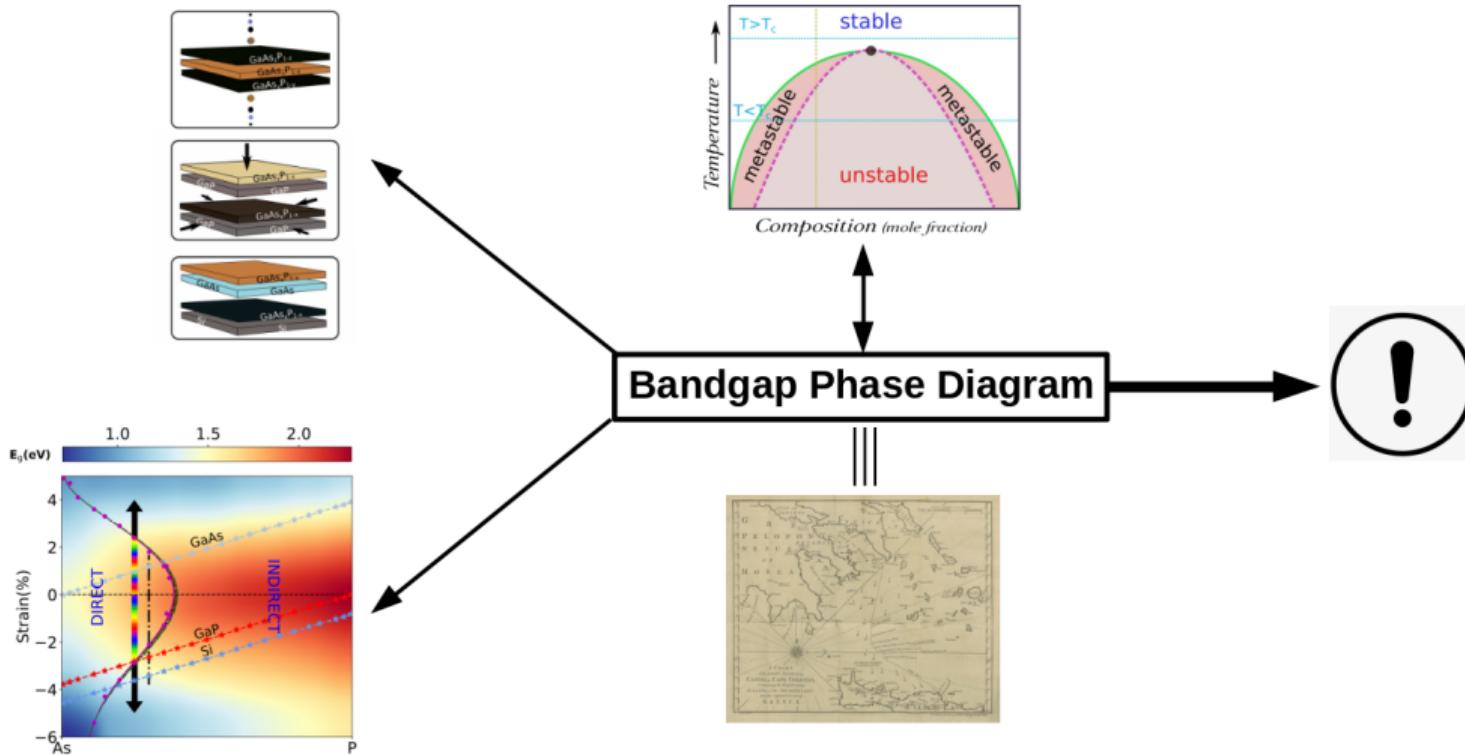


- Compositional phase diagram: **Can you grow?**

Significance



- ▶ Bandgap phase diagram: **What do you want to grow?**
- ▶ Compositional phase diagram: **Can you grow?**



Acknowledgements

- ▶ Prof. Dr. Ralf Tonner-Zech
- ▶ All of my group members

Philipps



Universität
Marburg



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Functionalization
of Semiconductors

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Universität
Marburg



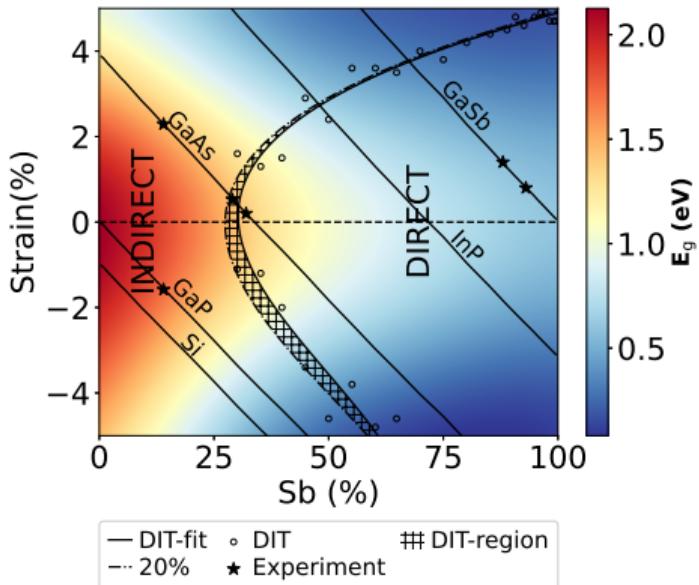
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Thank you

GaPSb 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

Binary systems

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

System	Si	GaSb	GaAs	GaP	InSb	InAs	InP
T 1 (%) [¶]	~ 15 [@]	2.85	6.67	~ 13 [@]	0.34	2.10	8.20
T 2 (%) [□]	10.31 (t)	1.00 (c)	1.56 (c)	2.63 (t)	5.18 (c)	7.41 (c)	4.40 (c)
T 3 (%) ^{**}	×	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.

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^{**} DIT or IDT transition under bi-axial strain

Bloch spectral weight

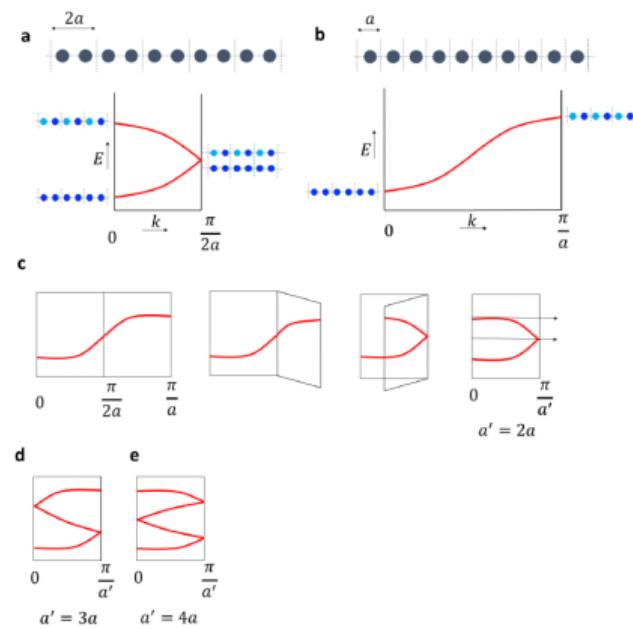
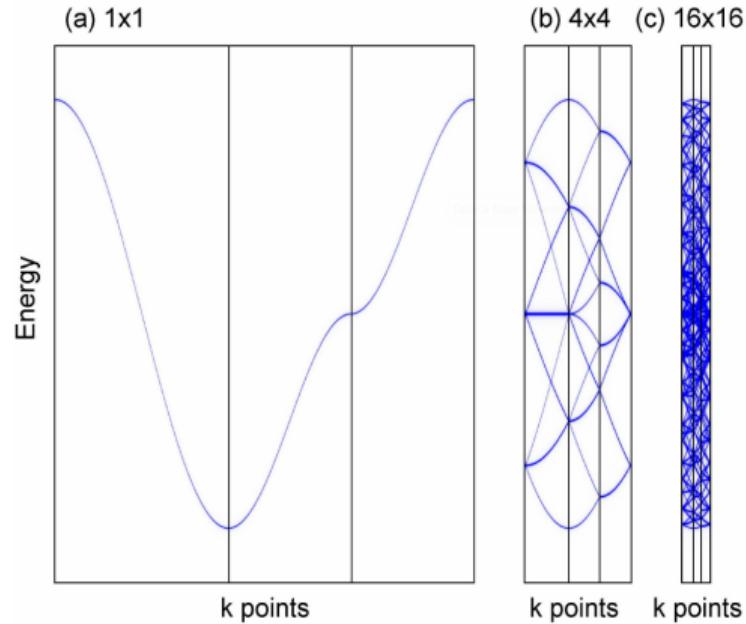
$$|\vec{K}m\rangle = \sum_{i=1}^{N_{\vec{K}}} \underbrace{w(\vec{k}_i, n; \vec{K}, m)}_{\text{contribution of } |\vec{k}_i n\rangle \text{ to SC eigenstate } |\vec{K}m\rangle} |\vec{k}_i n\rangle \Rightarrow \sum_{i=1}^{N_{\vec{K}}} \sum_n w(\vec{k}_i, n; \vec{K}, m) |\vec{k}_i n\rangle$$

- ▶ $w(\vec{k}_i, n; \vec{K}, m) = |\langle \vec{K}m | \vec{k}_i n \rangle|^2$
- ▶ Spectral weight: fold2Bloch^{††}

$$P_{\vec{K}m}(\vec{k}_i) = \sum_n |\langle \vec{K}m | \vec{k}_i n \rangle|^2 = \sum_{\vec{g}} |C_{\vec{K}m}(\vec{g} + \vec{k}_i - \vec{K})|^2$$

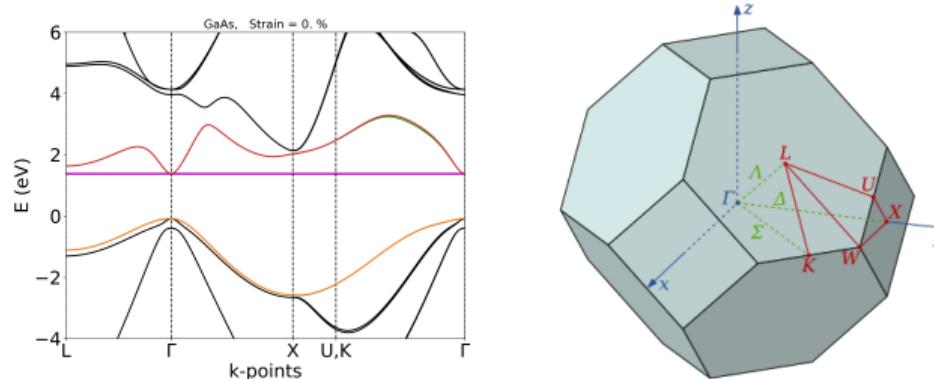
$$\Psi_{\vec{K}m}(\vec{r}) = |\vec{K}m\rangle = \sum_{\vec{G}} C_{\vec{K}m}(\vec{G}) e^{i(\vec{K} + \vec{G}) \cdot \vec{r}}$$

Band folding pattern*,†

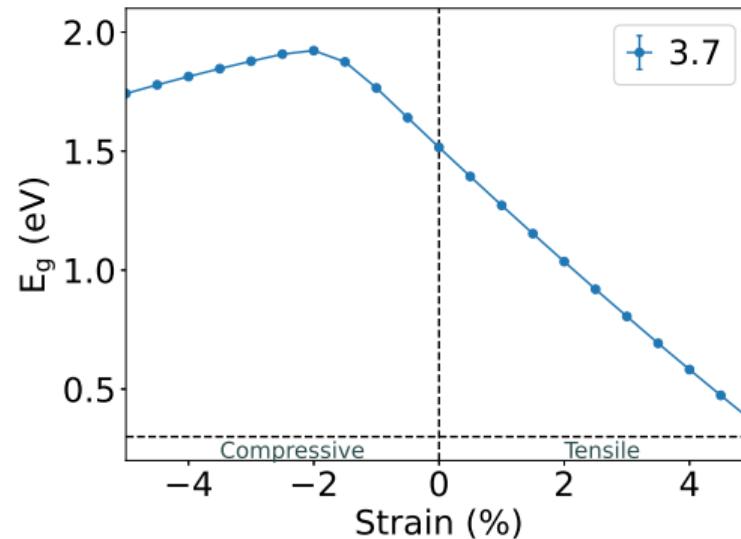
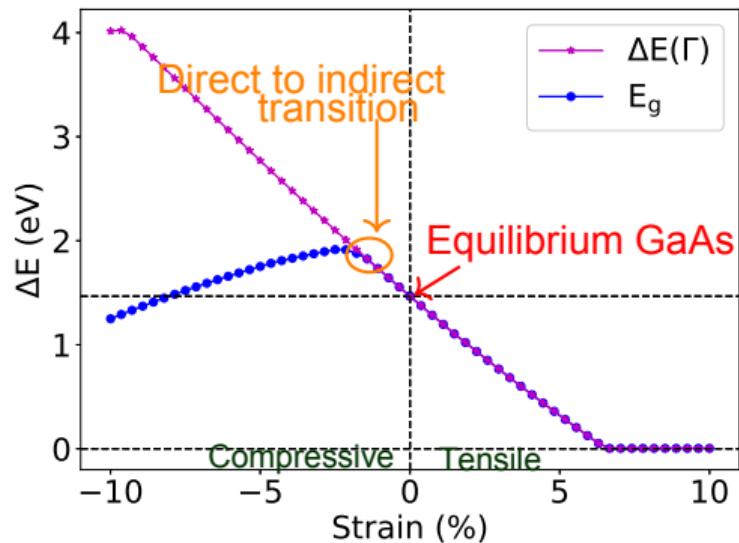


BW → CB

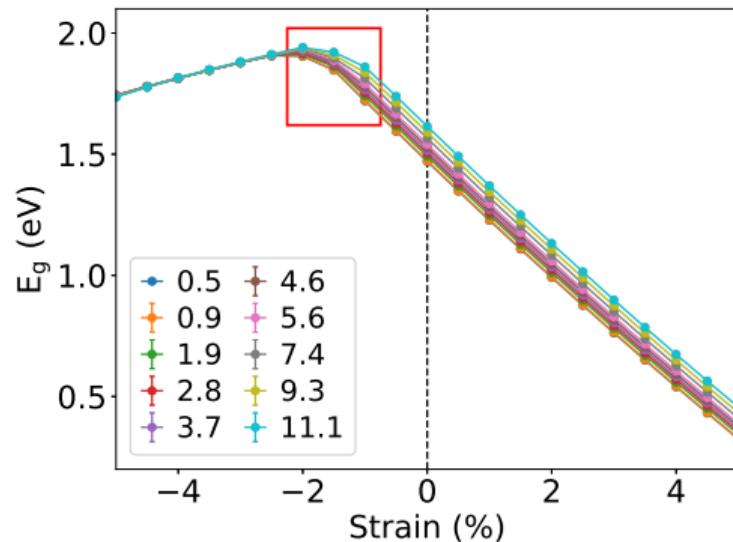
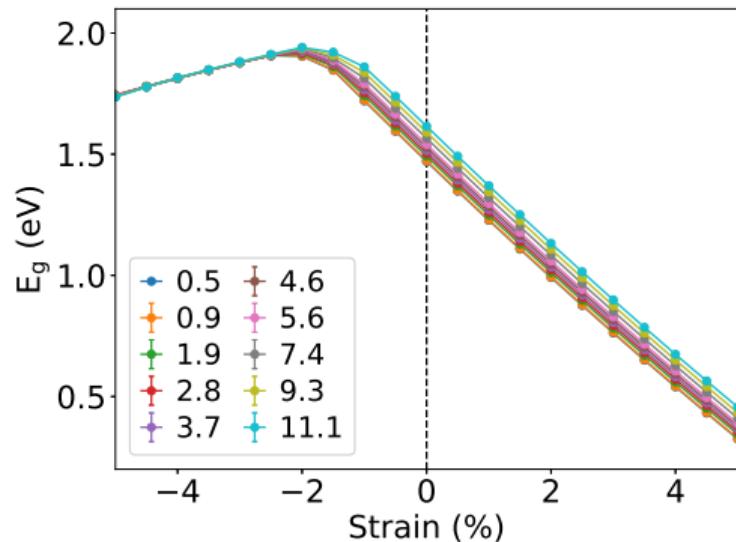
- ▶ Γ^f point: [0.0000 0.0000 0.0000]
 - ▶ Γ : [0.0 0.0 0.0]
 - ▶ L: [0.0 0.0 0.5], [0.0 0.5 0.0], [0.5 0.0 0.0], [0.5 0.5 0.5]
 - ▶ X: [0.0 0.5 0.5], [0.5 0.0 0.5], [0.5 0.5 0.0]



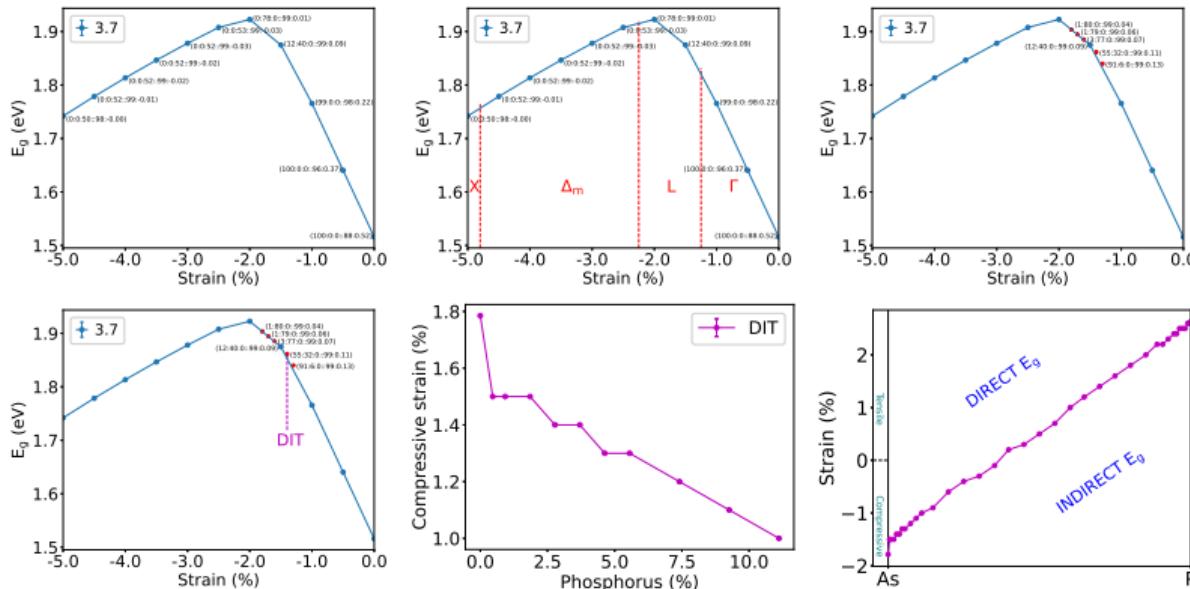
Revisit: GaAs, GaAsP [100] isotropic strain



GaAsP isotropic strain: Bandgap variation



GaAsP isotropic strain: BW=(Γ:L:X::Δ_m:ΔE=(Δ_m^f - Γ^f))



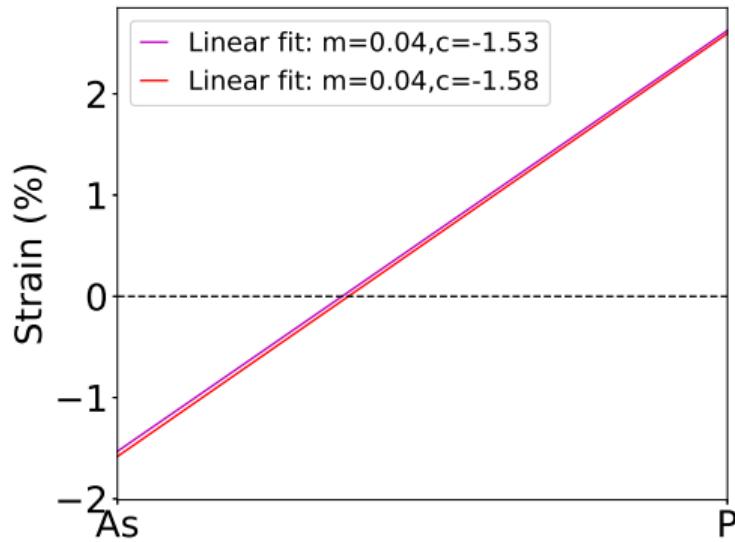
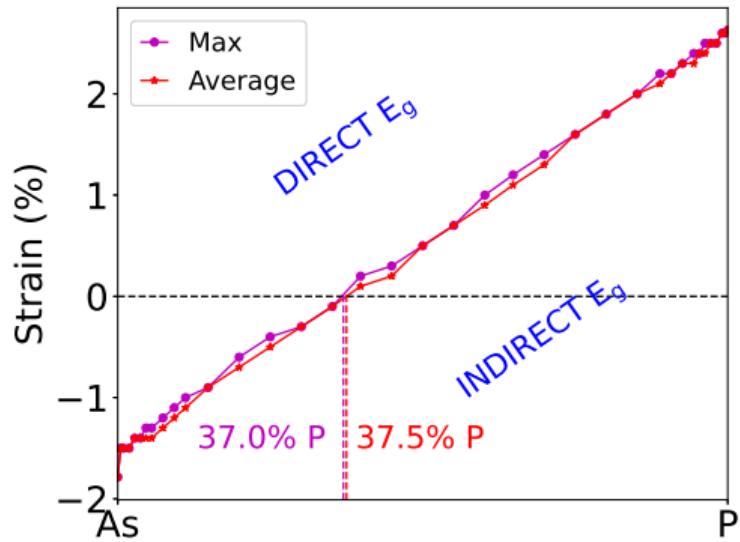
Ternary DIT Assumptions/ Errors/ Limitations

- ▶ 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)

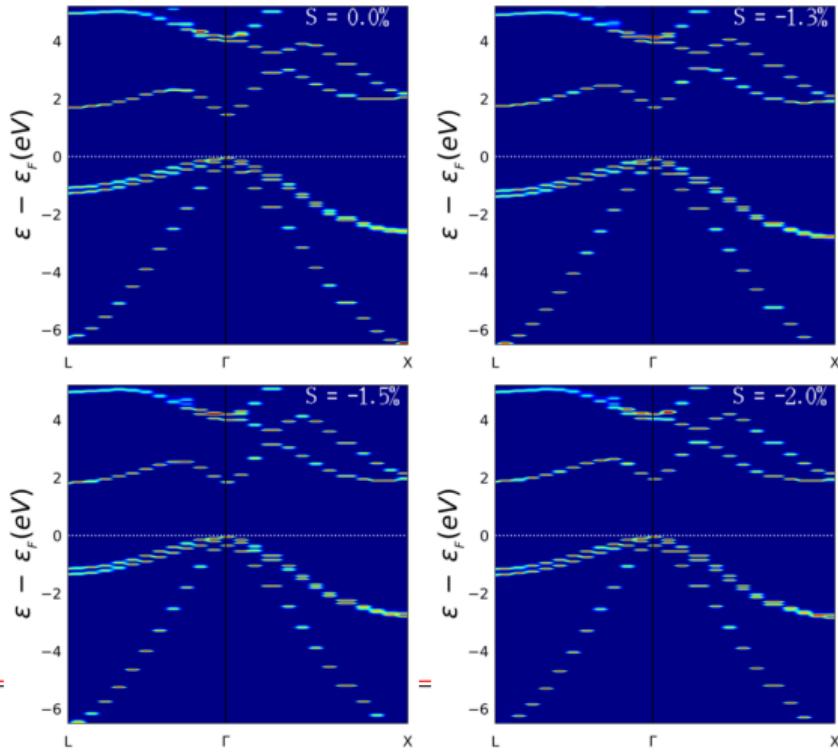
Computational details

- ▶ VASP 5.4.4
- ▶ $6 \times 6 \times 6$ supercell
- ▶ PBE (optimization), DFT-D3, TB09 (band gap)
- ▶ 450 eV (for optimization), 350 eV ENCUT (for band gap)
- ▶ Convergency criteria (optimization): 10^{-6} eV (electronic energy); 10^{-2} eVÅ⁻¹ (force)
- ▶ Convergency criteria (bandgap): 10^{-4} eV (electronic energy); 10^{-2} eVÅ⁻¹ (force)
- ▶ Spin-orbit coupling during bandgap calculation
- ▶ 10 sqs for each composition and strain point

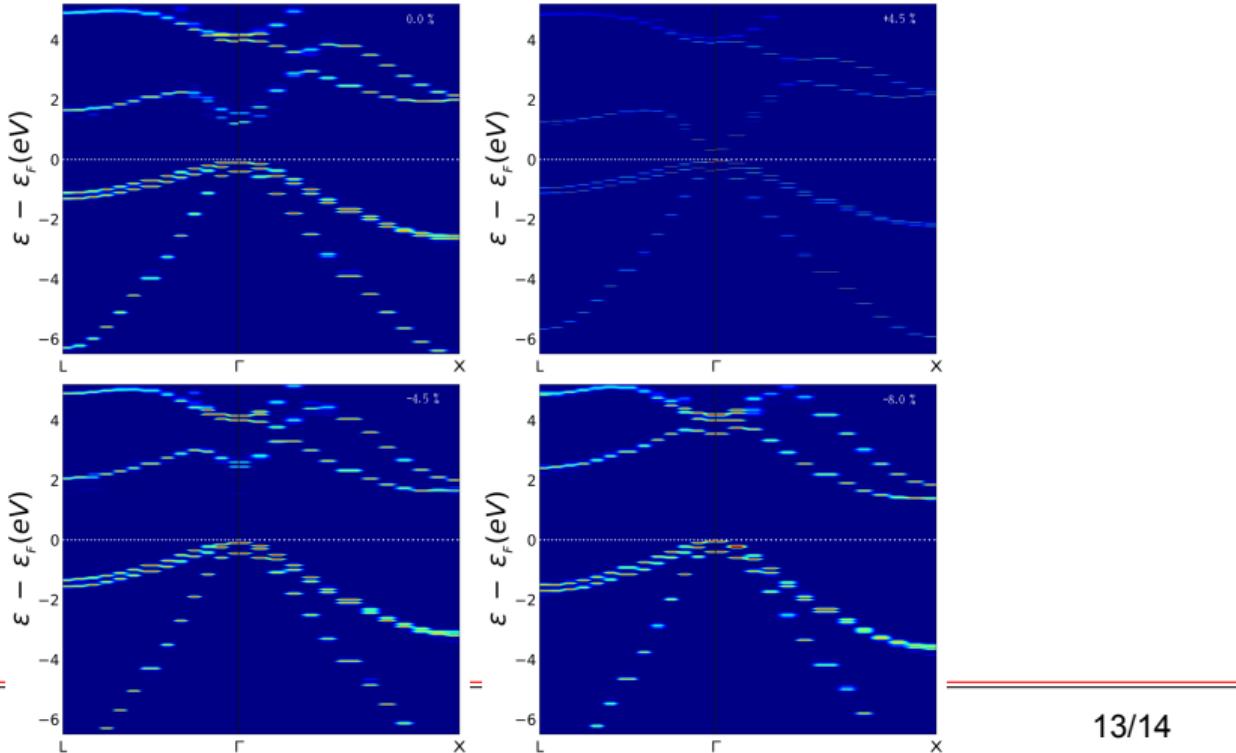
Average vs maximum BW



GaAsP bandstructure



GaAsN: 0.5% N bandstructure



GaAsN: 11.1% N, S0, S-5 bandstructure

