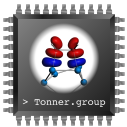
UNIVERSITÄT
LEIPZIG

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 und Mineralogie
Universität Leipzig

Introduction

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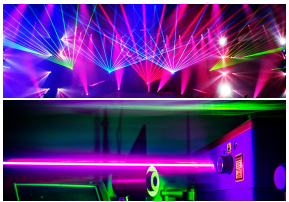

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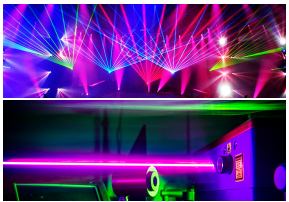

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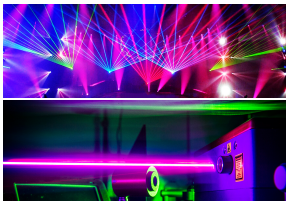

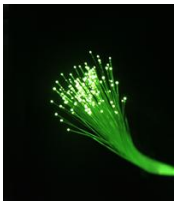

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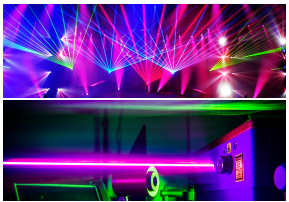

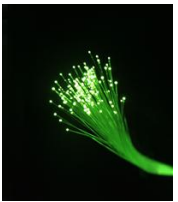

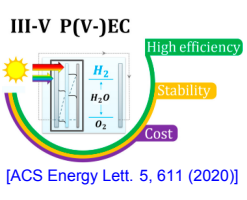

[ACS Energy Lett. 5, 611 (2020)]

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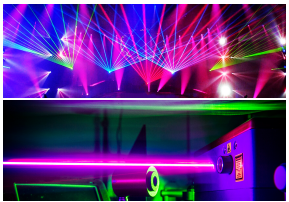
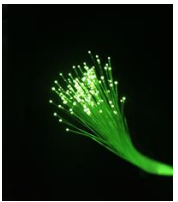
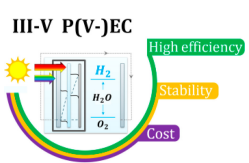
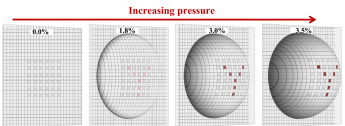






[ACS Energy Lett. 5, 611 (2020)]



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

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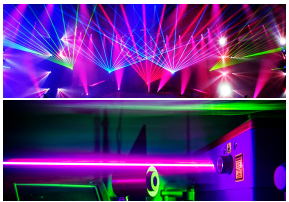

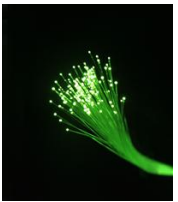

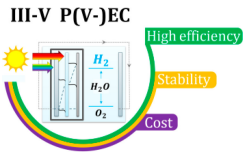

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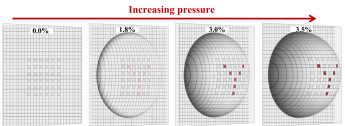

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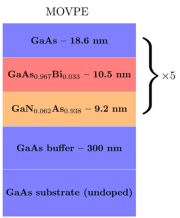

[Sci. Rep. 7, 46371 (2017)]

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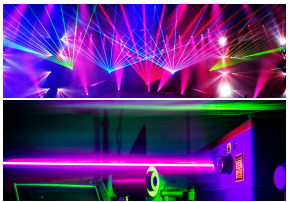

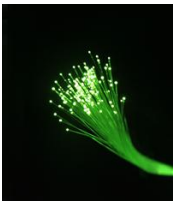

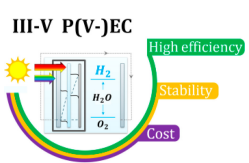

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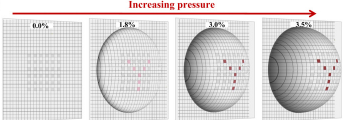

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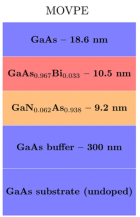

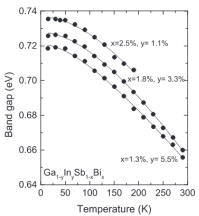

[Sci. Rep. 7, 46371 (2017)] [Semi. Sci. Tech., 073001 (2018)]

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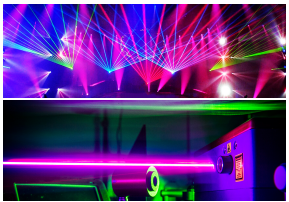

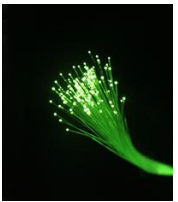

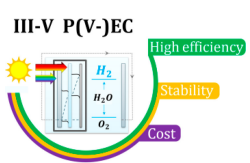

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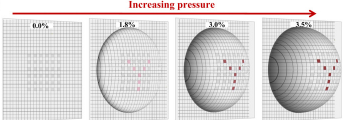

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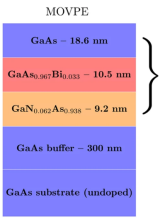

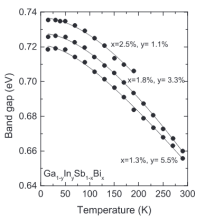

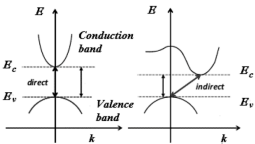

[Int. J. Sci. (2014)]

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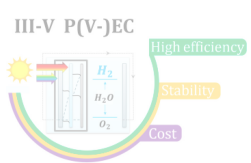

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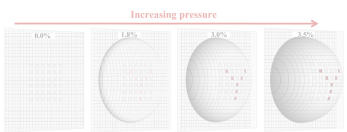

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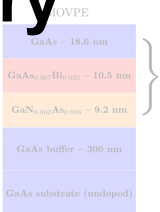

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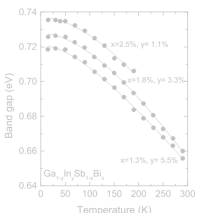

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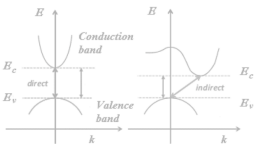

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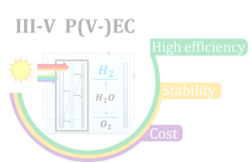

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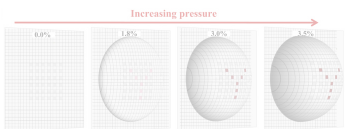

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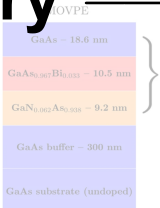

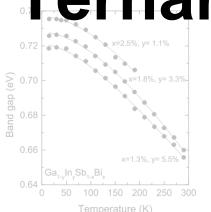

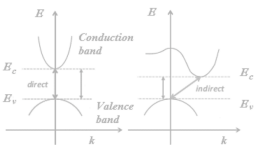

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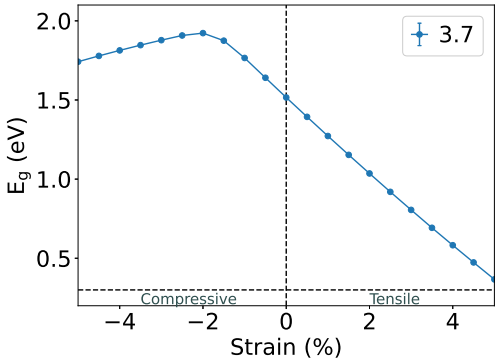
GaAsP, GaAs [100] isotropic strain [1]



[1] VASP-5.4.4, TB09, SOC, $6 \times 6 \times 6$ supercell, 10 SQS

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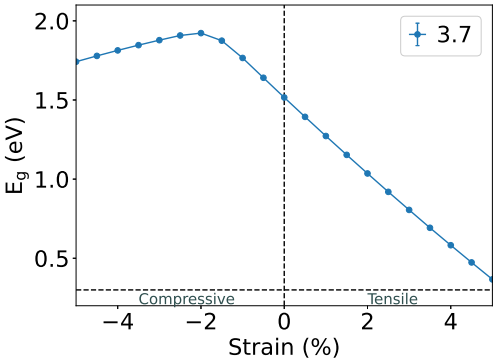
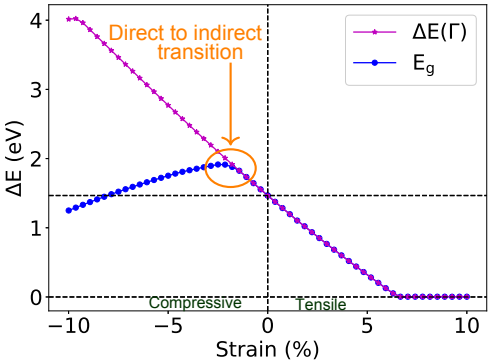
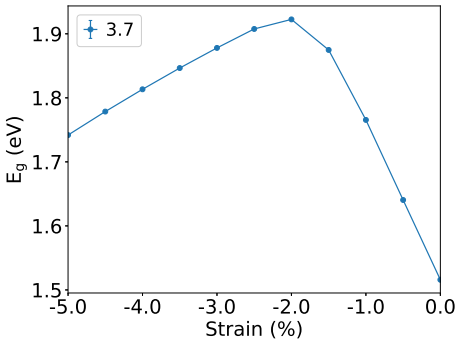




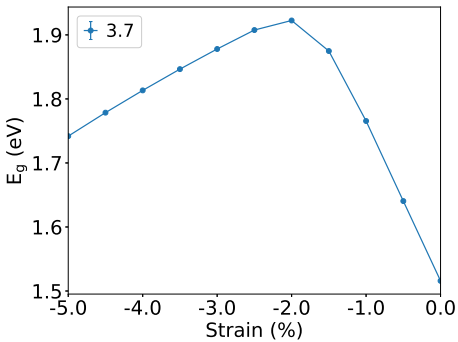
[1] VASP-5.4.4, TB09, SOC, $6 \times 6 \times 6$ supercell, 10 SQS

Ternary system: GaAsP



[Isotropic compressive strain]

Ternary system: GaAsP, Band folding[2]



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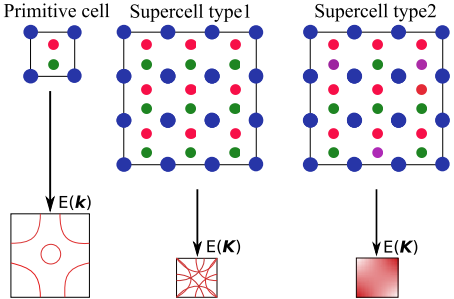
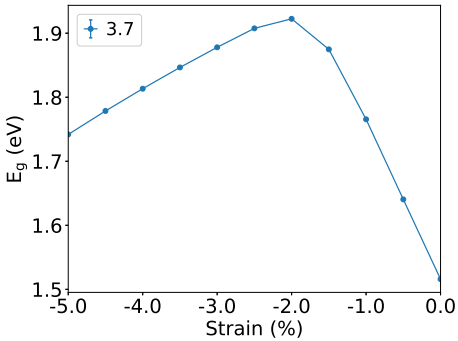
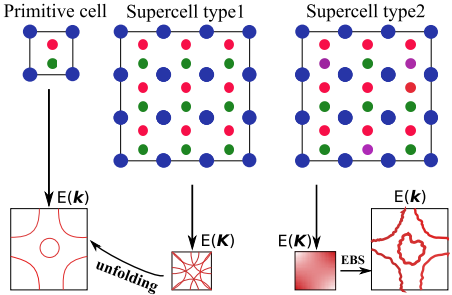


[2]S.-Y. Yang *et al.*, *Advances in Physics: X* **3**, 1414631 (2018).

Band folding: Bloch spectral density/weight[2,3,4]

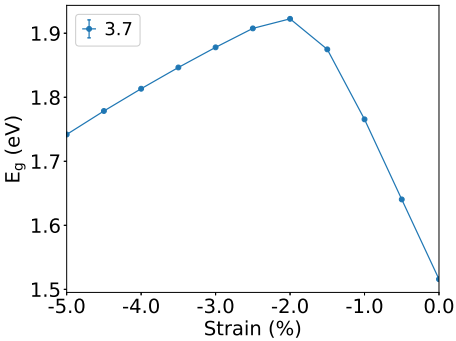


[Isotropic compressive strain]

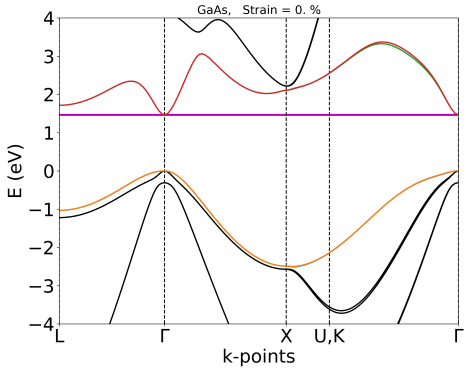


[2] L.-W. Wang *et al.*, *Phys. Rev. Lett.* **80**, 4725 (1998).
[3] V. Popescu, A. Zunger, *Phys. Rev. B* **85**, 085201 (2012).
[4] O. Rubel *et al.*, *Phys. Rev. B* **90**, 115202 (2014).

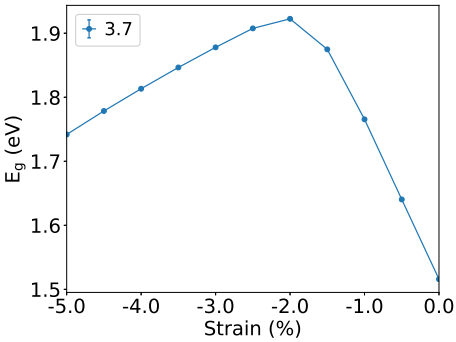
Band unfolding, Bloch weight



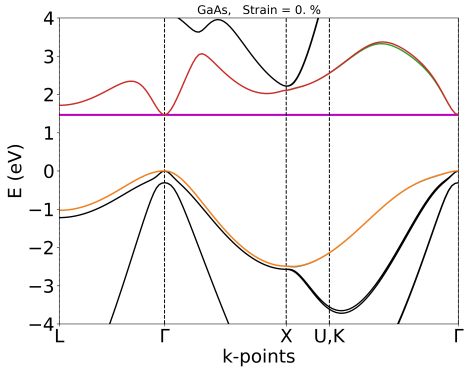
[Isotropic compressive strain]



Band unfolding, Bloch weight

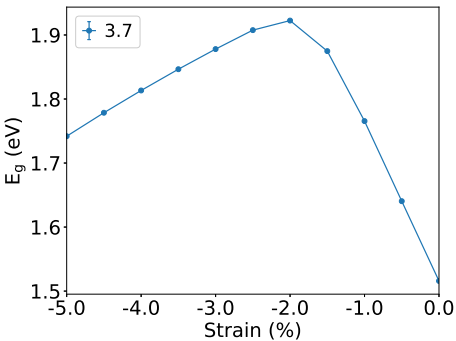


[Isotropic compressive strain]

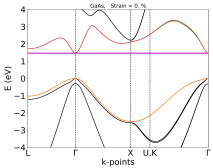


- CB: BW_Γ, BW_L, BW_X

Band unfolding, Bloch weight

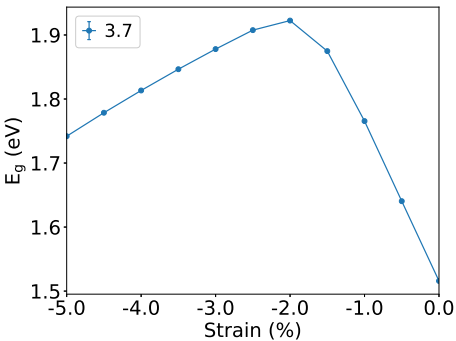


[Isotropic compressive strain]

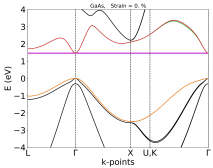


$BW_{\Gamma}:BW_{L}:BW_{X}$ = 100:0:0

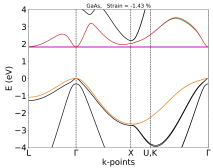
Band unfolding, Bloch weight



[Isotropic compressive strain]

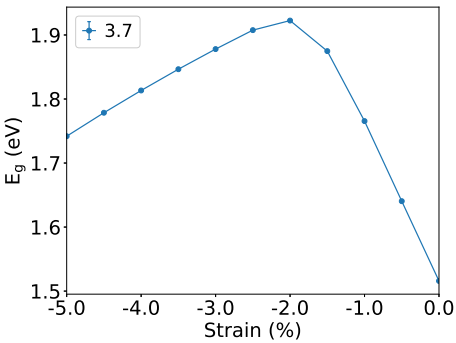


BW_Γ:BW_L:BW_X = 100:0:0

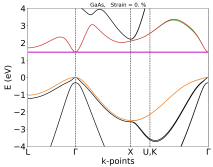


BW_Γ:BW_L:BW_X = 50:50:0

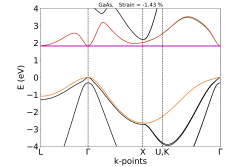
Band unfolding, Bloch weight



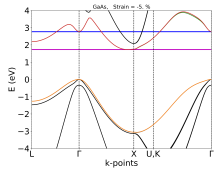
[Isotropic compressive strain]



$BW_\Gamma:BW_L:BW_X$ = 100:0:0

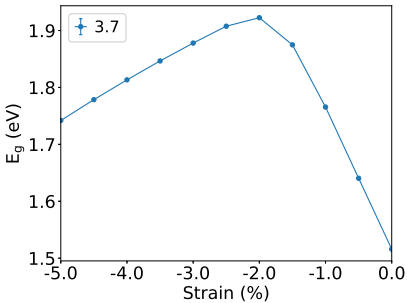


$BW_\Gamma:BW_L:BW_X$ = 50:50:0

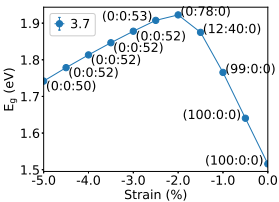


$BW_\Gamma:BW_L:BW_X$ = 0:0:100

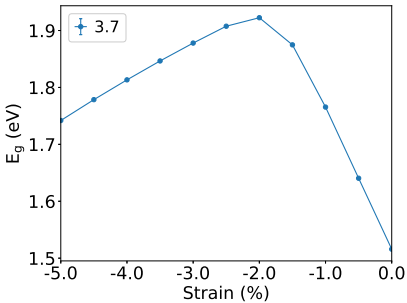
GaAsP: Direct-indirect transition



[Isotropic compressive strain]



GaAsP: Direct-indirect transition



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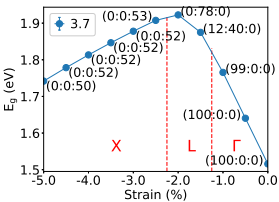
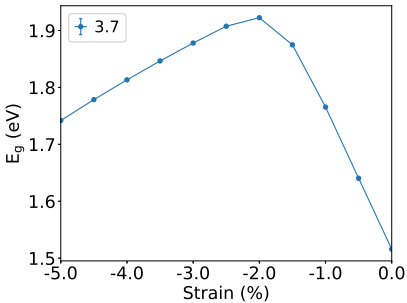
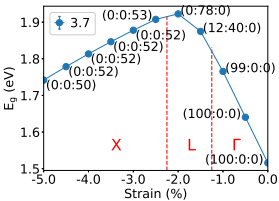
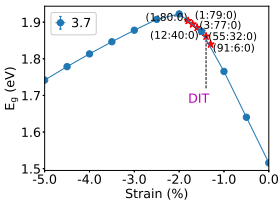


GaAsP: Direct-indirect transition

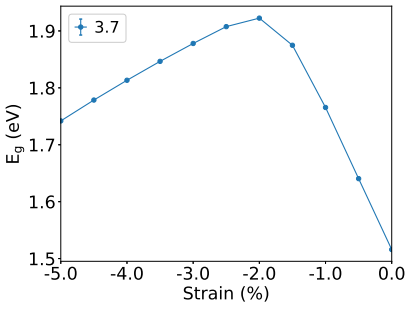


[Isotropic compressive strain]

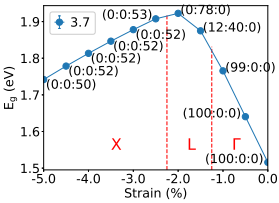


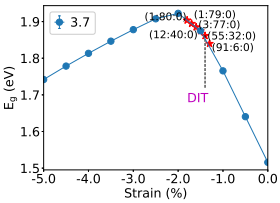


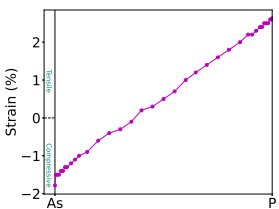
GaAsP: Direct-indirect transition



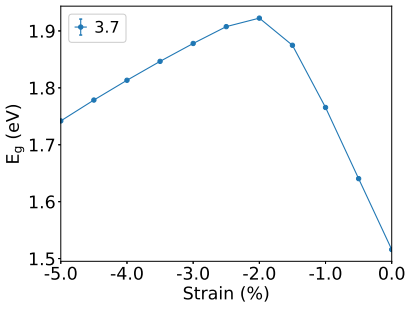
[Isotropic compressive strain]







GaAsP: Direct-indirect transition



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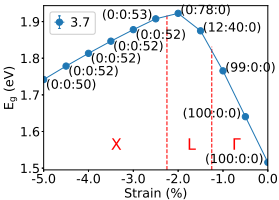
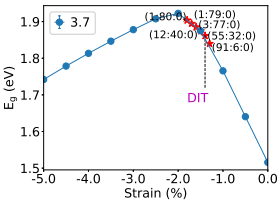
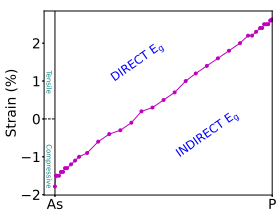
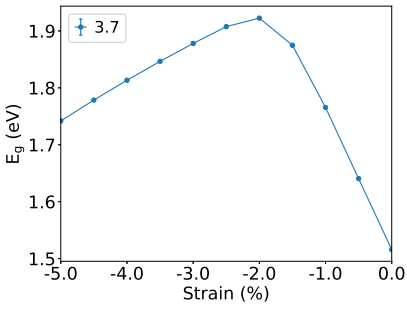






GaAsP: Direct-indirect transition



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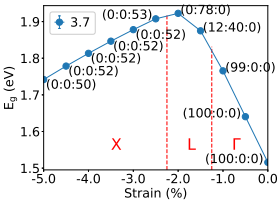
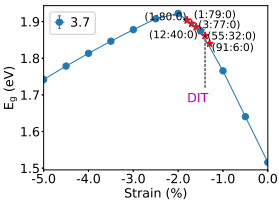
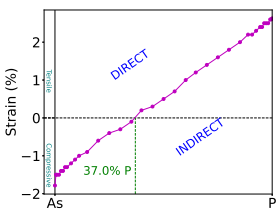
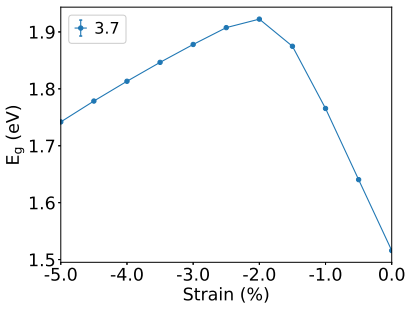


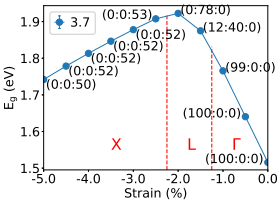


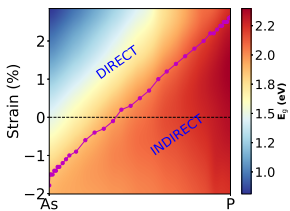


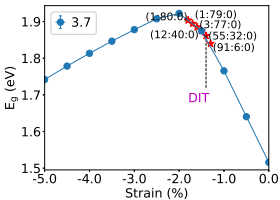
GaAsP: Direct-indirect transition



[Isotropic compressive strain]







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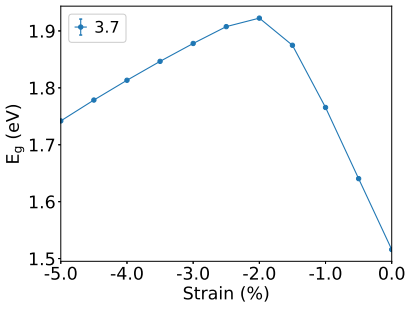

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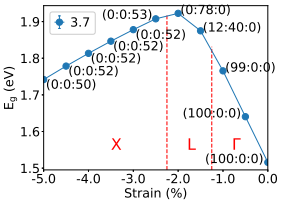
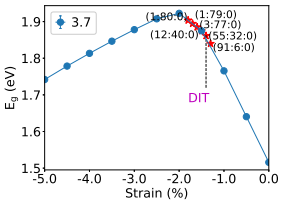
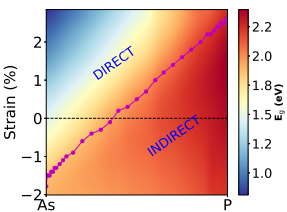
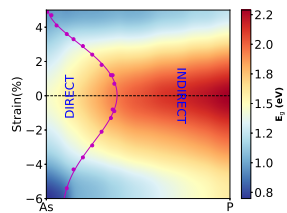
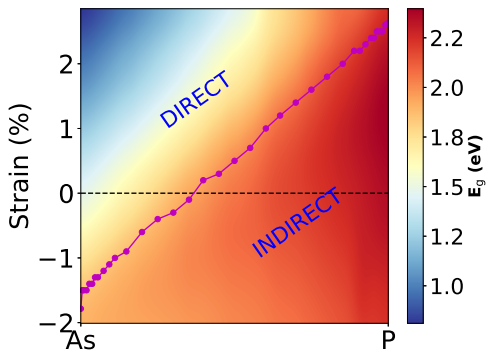


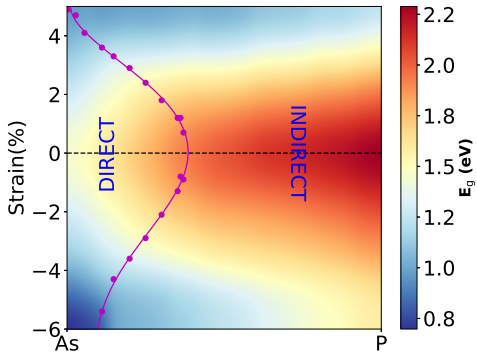






“Bandgap Phase Diagram”





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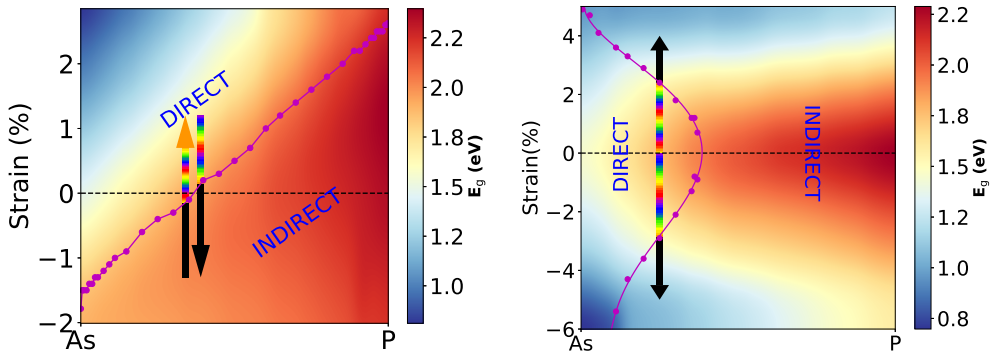

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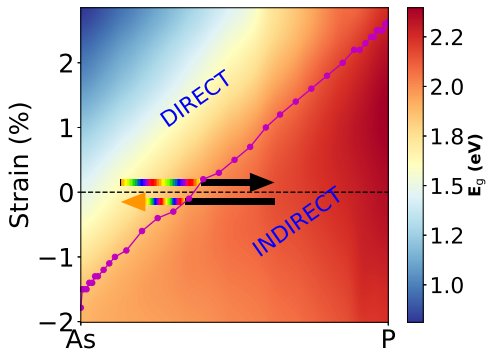
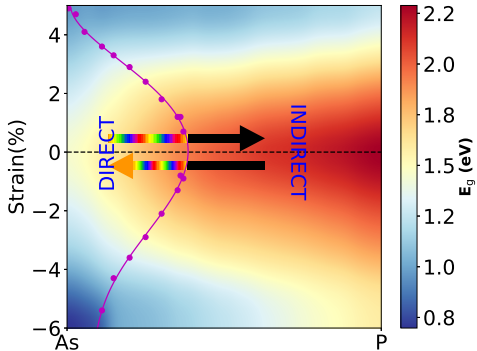
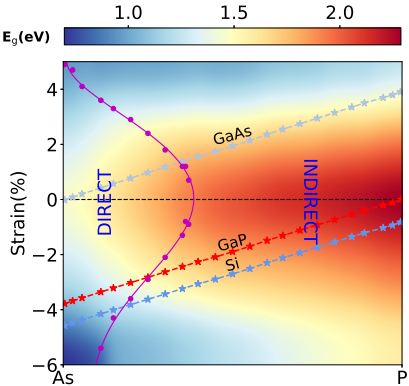




GaAsP biaxial strain: Bandgap phase diagram



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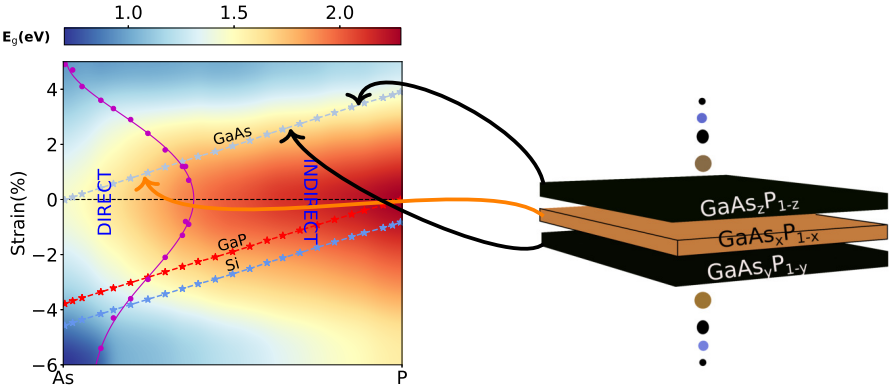

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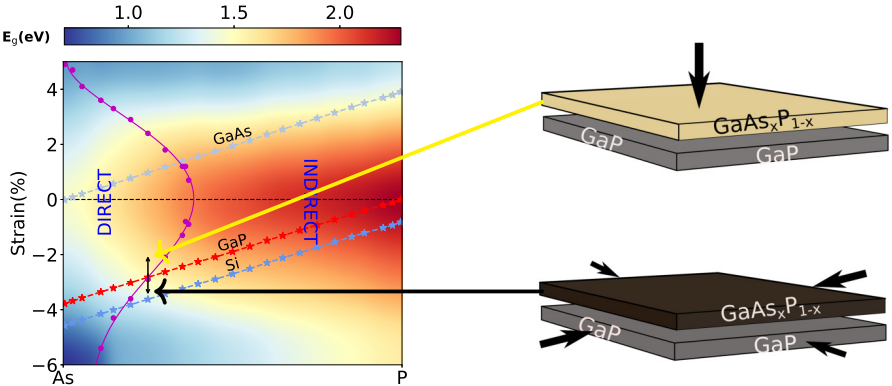
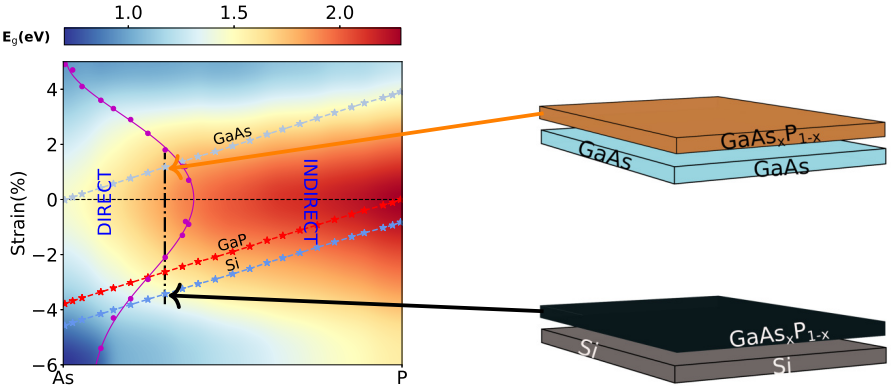
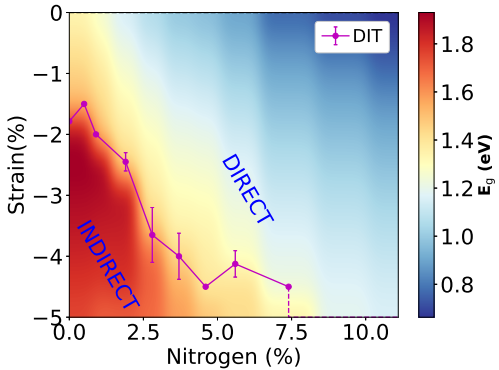


GaAsP biaxial strain: Bandgap phase diagram

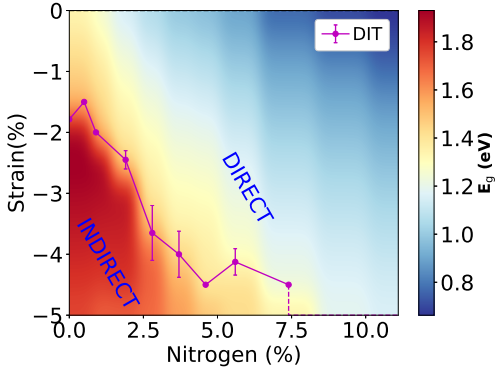


Bandgap Phase Diagram: Precision

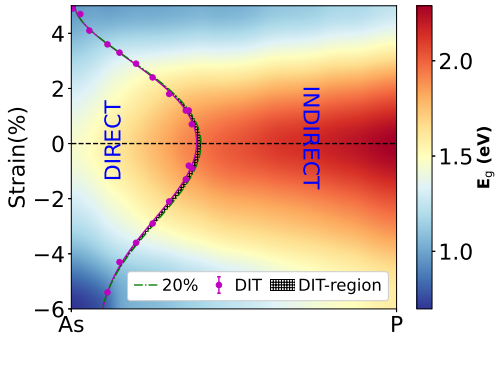


[GaAsN isotropic strain]

Bandgap Phase Diagram: Precision



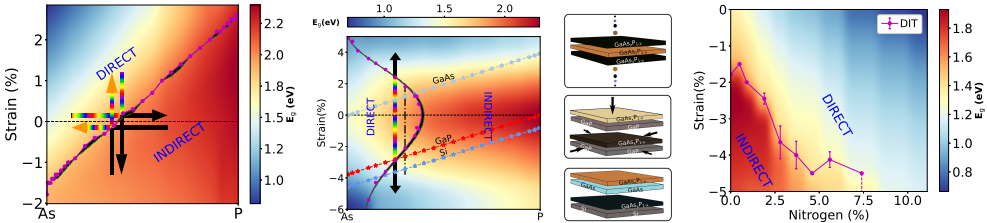
[GaAsN isotropic strain]



[GaAsP biaxial strain]

Summary

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



What next?

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- Other transitions (e.g. L-X)

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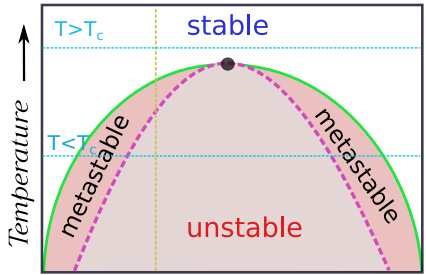
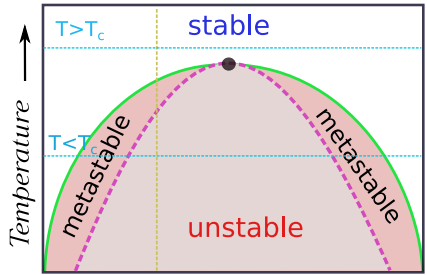
- Other transitions (e.g. L-X)
- 3rd dimension (e.g. phonon contribution)
- Higher order system
  - Machine learning
- Other material systems (e.g. II-VI, III-VI)
- Other areas (e.g. Auger recombination)

Significance



Compositional phase diagram

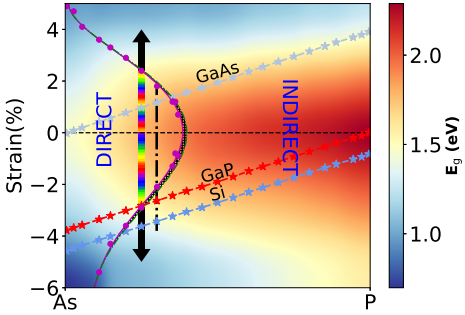
Significance



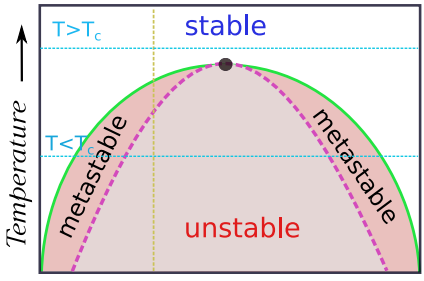
Compositional phase diagram

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

Significance



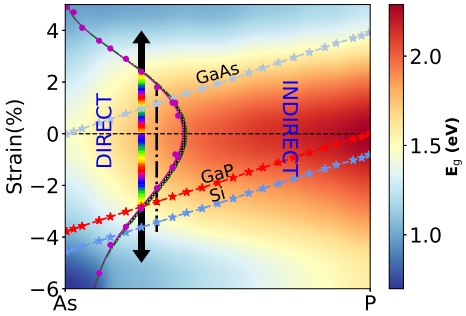
Bandgap phase diagram



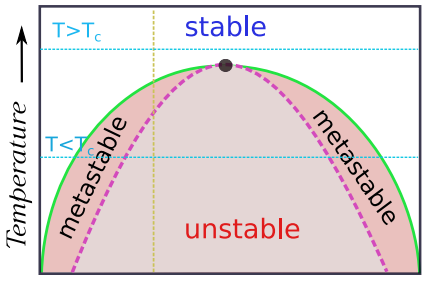
Compositional phase diagram

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

Significance

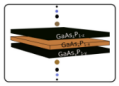


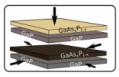
Bandgap phase diagram

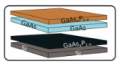


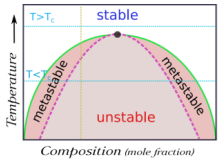
Compositional phase diagram

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

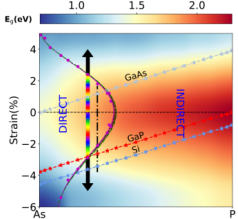








Bandgap Phase Diagram



Acknowledgements

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

Philipps Universität Marburg

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* https://bmondal94.github.io/Bandgap-Phase-Diagram/

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