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DPG 2022

Strain-induced bandgap transition in III-V semiconductors

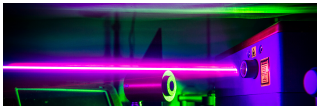
September 7, 2022

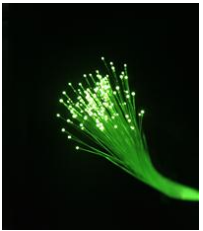
Badal Mondal and Ralf Tonner-Zech

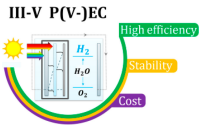
> Tonner.group

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

Introduction

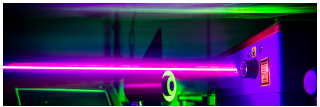


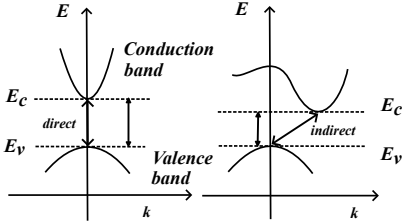




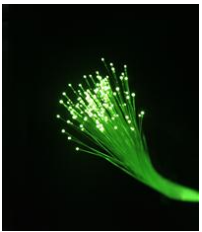
[ACS Energy Lett. 5, 611 (2020)]

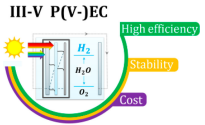
Introduction





[Int. J. Sci. (2014)]





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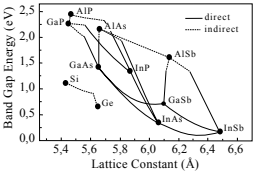
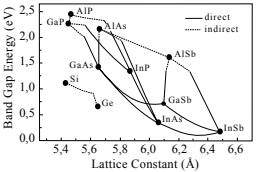
Motivation



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

– Compositional engineering

Motivation



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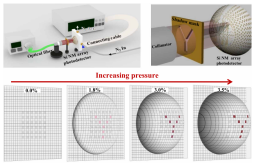
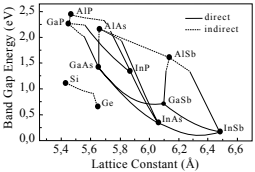


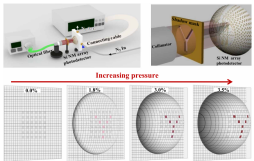
[Sci. Adv. 6, eabb0576 (2020)]

- Compositional engineering
- Strain engineering

Motivation



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



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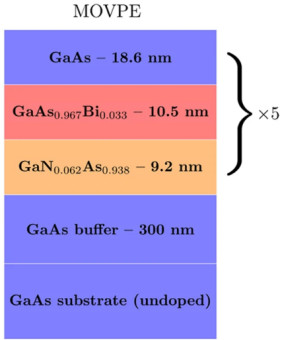
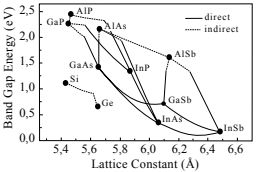


[Sci. Rep. 7, 46371 (2017)]

- Compositional engineering
- Strain engineering
- Composition + strain engineering

Motivation

composition-strain-bandgap



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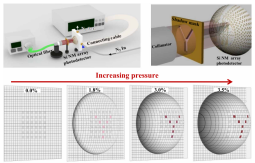

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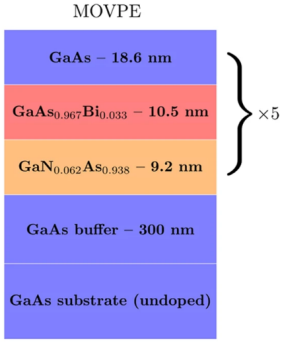

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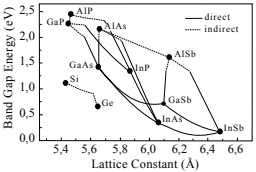

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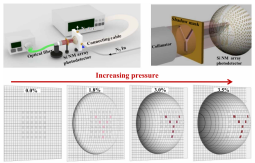

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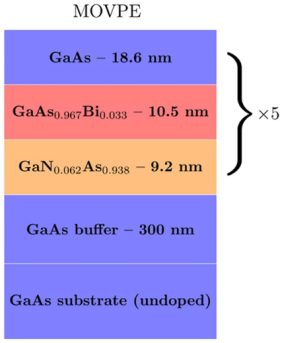

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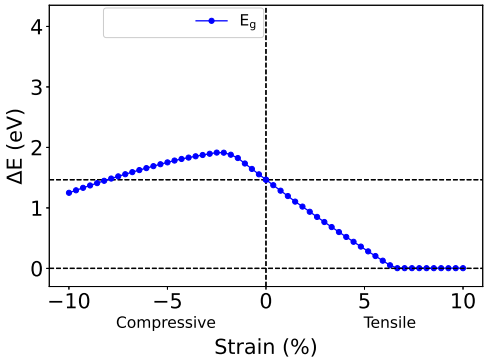
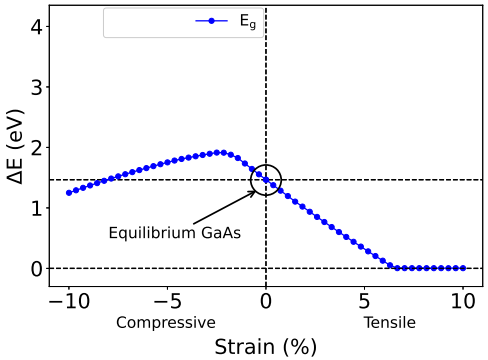
- Compositional engineering
- Strain engineering
- Composition + strain engineering
- Density functional theory

GaAs isotropic strain: strain-bandgap



* B. Mondal, R. Tonner-Zech, arXiv:2208.10596 (2022)

GaAs isotropic strain: strain-bandgap



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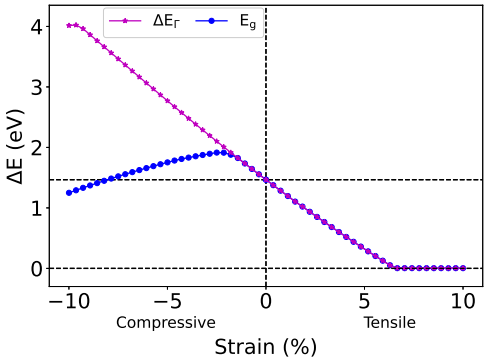

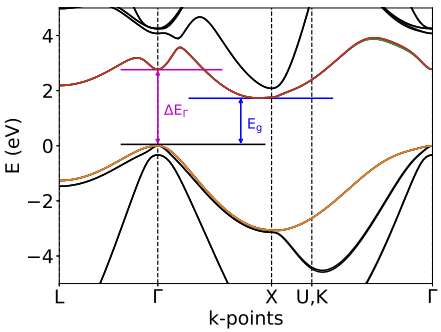

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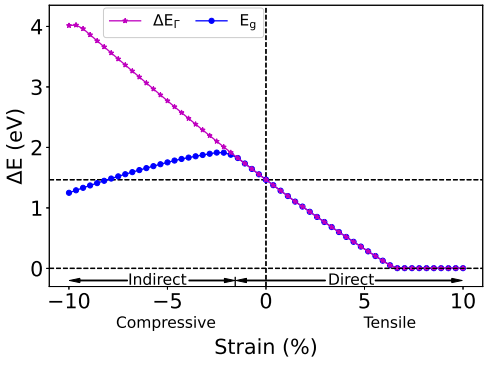

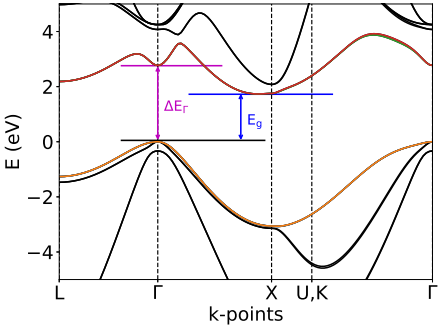

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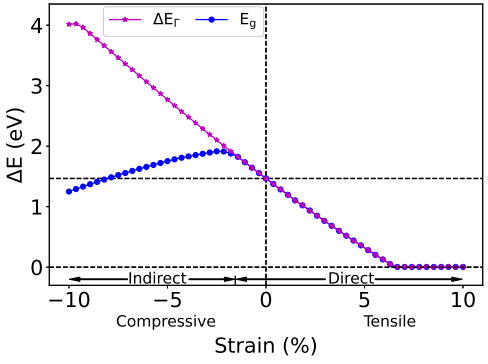

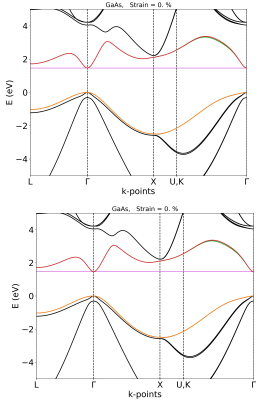

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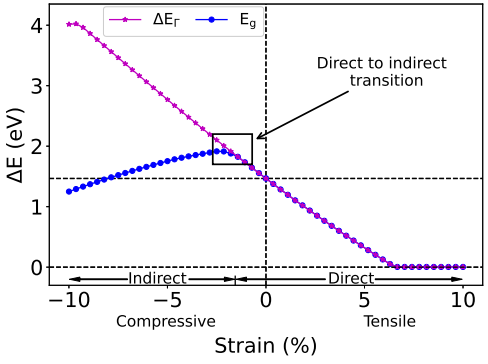

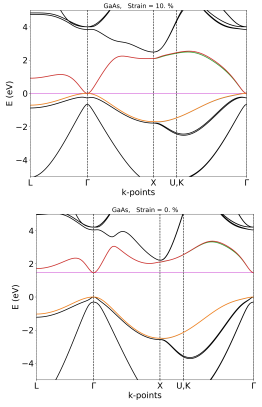

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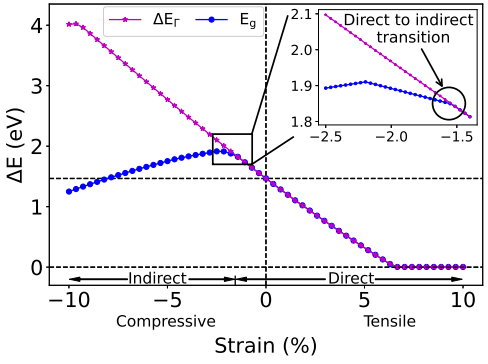

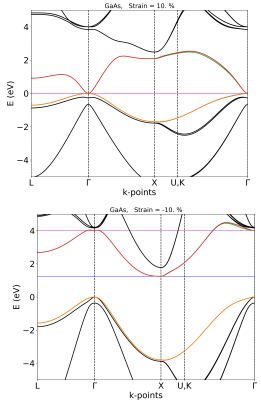

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Ga(AsP) isotropic strain: bandgap phase diagram

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

[a] S.-Y Yang *et al., Adv. Phys.: X* **3**, 1414631 (2018)
[b] V. Popescu, A. Zunger, *Phys. Rev. B* **85**, 085201 (2012)

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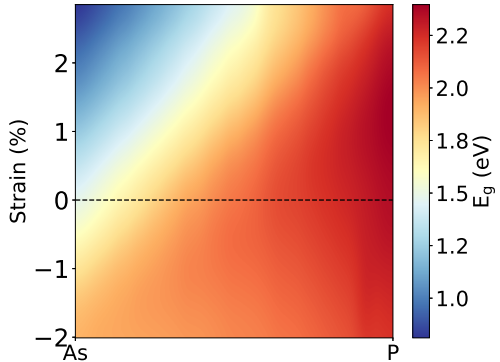

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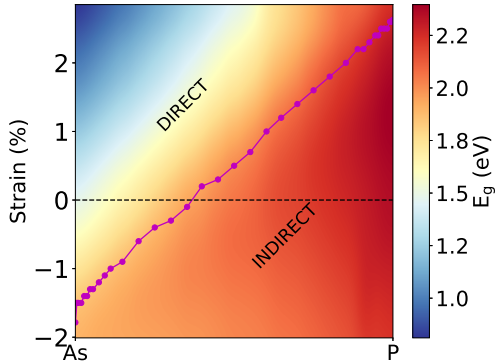

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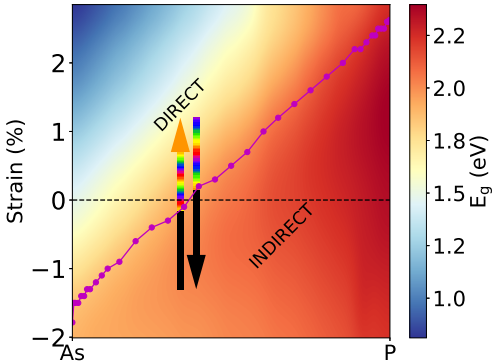

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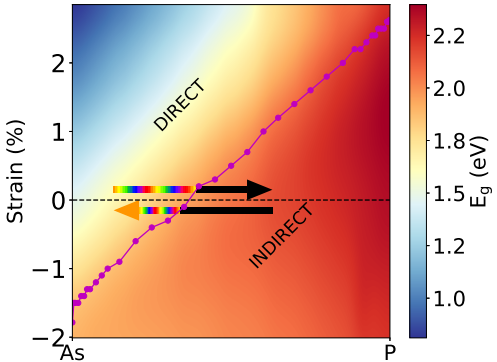

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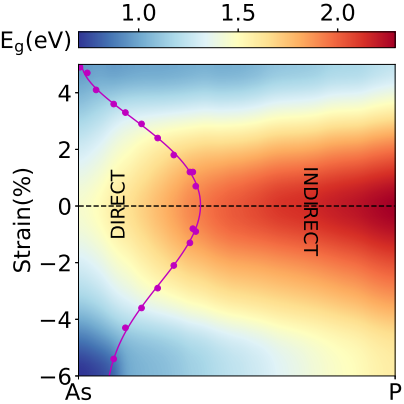
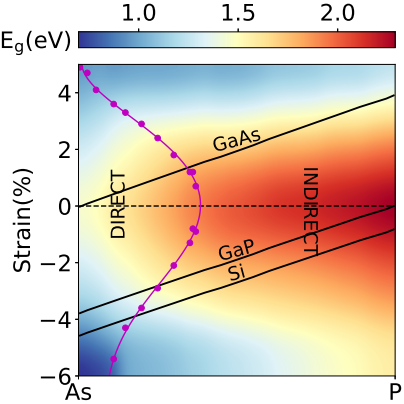
Ga(AsP) biaxial strain: bandgap phase diagram



Ga(AsP) biaxial strain: bandgap phase diagram



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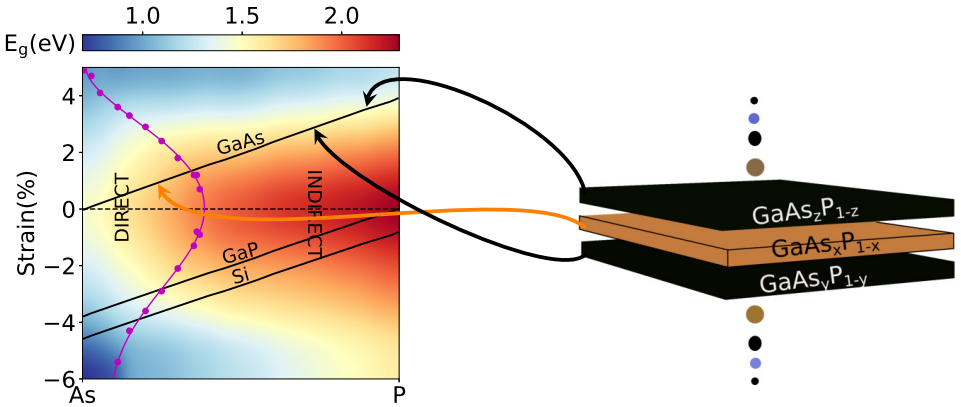

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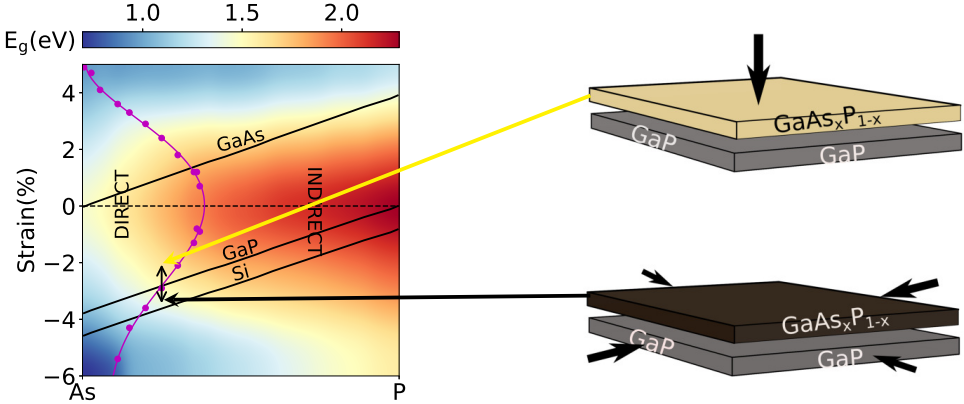

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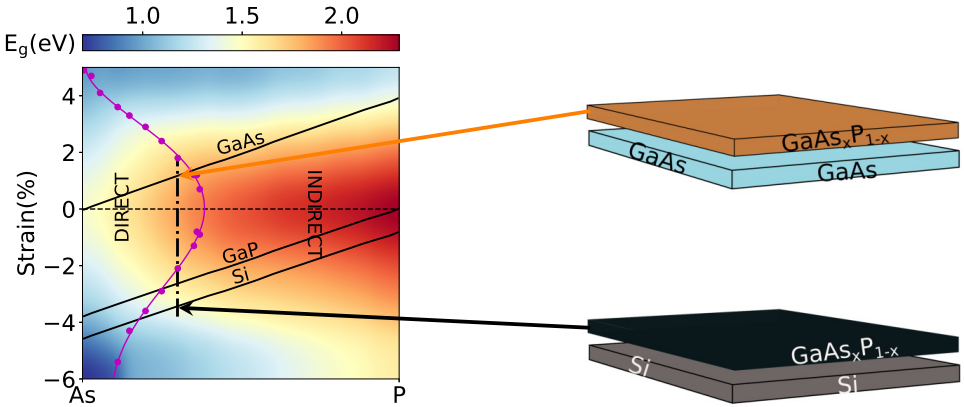
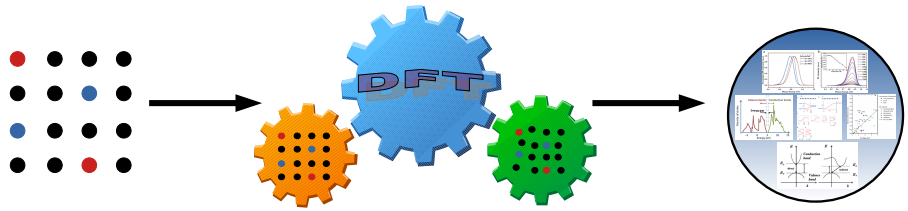
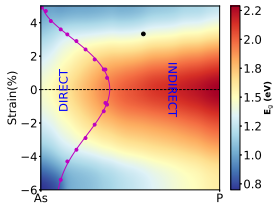
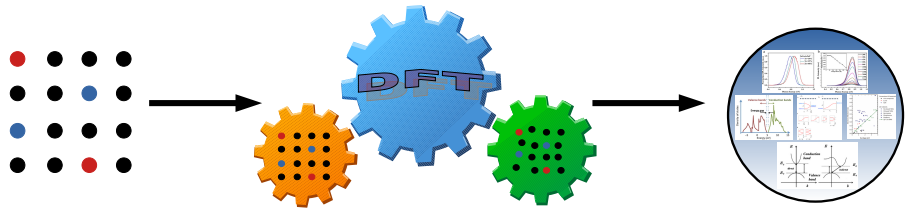


Approach

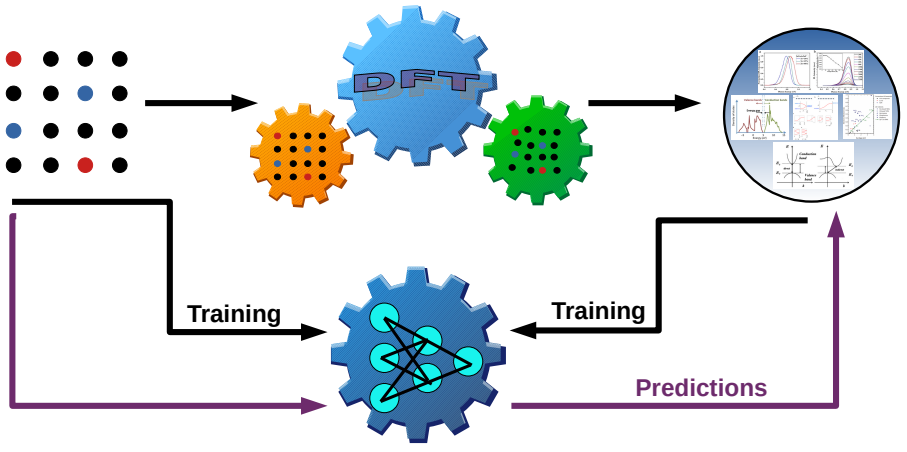

DFT


Strain(%)
4
2
0
−2
−4
−6
As
P
DIRECT
INDIRECT
2.2
2.0
1.8
1.5
1.2
1.0
0.8
E_0 (eV)

Approach

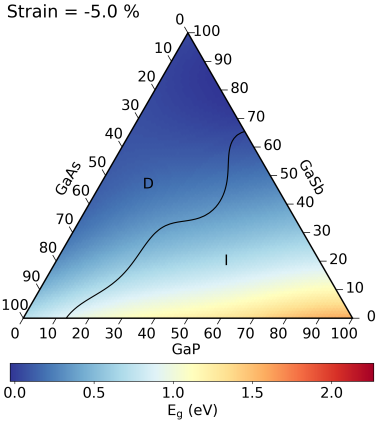

DFT
Strain(%)
DIRECT
INDIRECT
As
P
E_g (eV)
2,000
500,000
Strain=0%
A
B
C

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



[c] Z. Zhu *et al., Chin. Phys. B* **29**, 046101 (2020)
[d] Y. Huang *et al., J. Mater. Chem. C* **7**, 3238 (2019)

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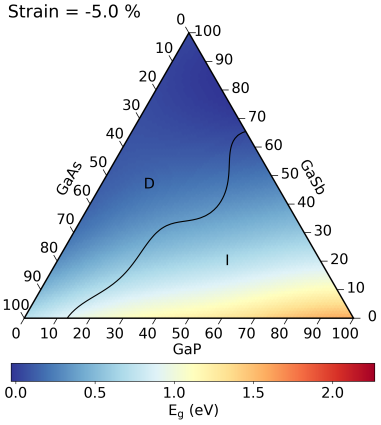

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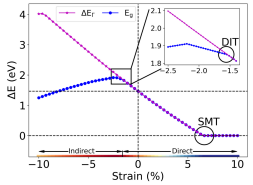
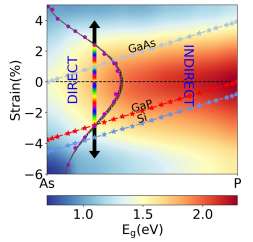
Summary

GaAs
(isotropic)



Bloch spectral weight

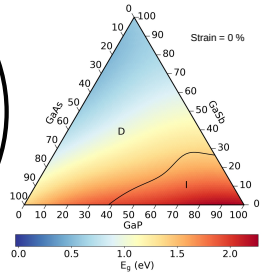


GaAsP
(biaxial)

Bandgap phase diagram

Machine learning

composition-strain-bandgap



GaAsPSb
(biaxial)

More

Systems

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

- ▾ III-V semiconductors
  - ▸ III-V binary
  - ▾ III-V ternary
    - ▾ DFT based
      - GaAsP, Computational details (uploaded on 22.09.2021), Experimental verification
      - GaAsN, Computational details (uploaded on 22.09.2021)
        - No direct-indirect transition (DIT) for GaAsN under biaxial strain within ± 5% of strain.
      - GaPSb (only biaxial), Computational details, Experimental verification
      - GaAsSb (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 (coming soon)
    - ▸ DFT + Machine learning based

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