



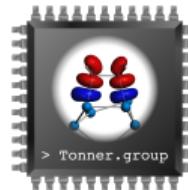
UNIVERSITÄT
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ICMOVPE XX, 2022

Strain-induced bandgap transition in III-V semiconductors

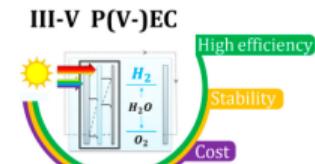
July 14, 2022

Badal Mondal and Ralf Tonner-Zech



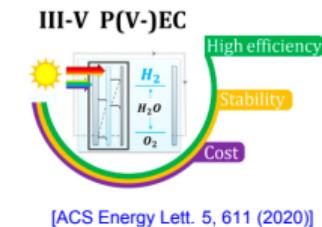
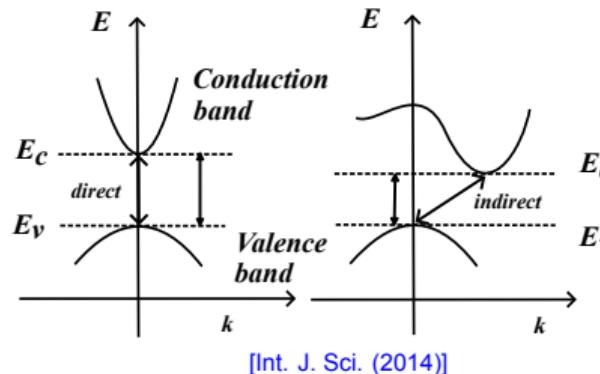
Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie
Fakultät für Chemie und Mineralogie
Universität Leipzig

Introduction

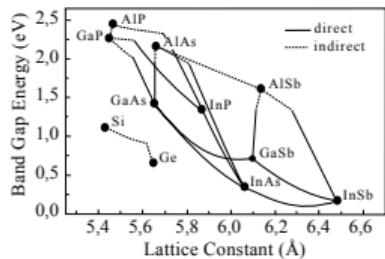


[ACS Energy Lett. 5, 611 (2020)]

Introduction



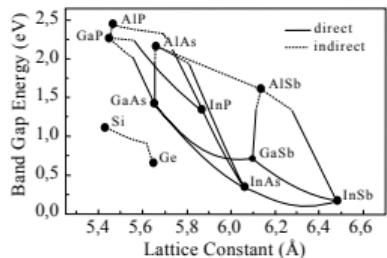
Motivation



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

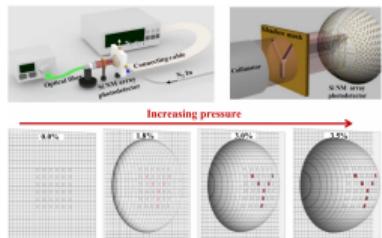
— Compositional engineering

Motivation



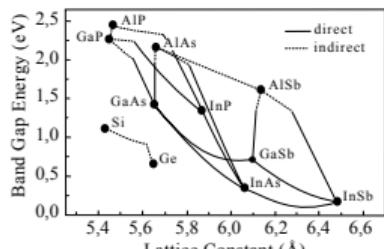
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- Compositional engineering
- Strain engineering

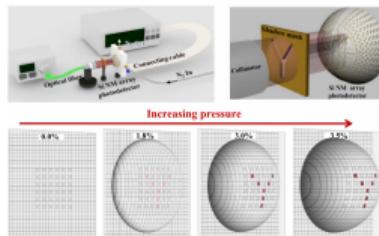


[Sci. Adv. 6, eabb0576 (2020)]

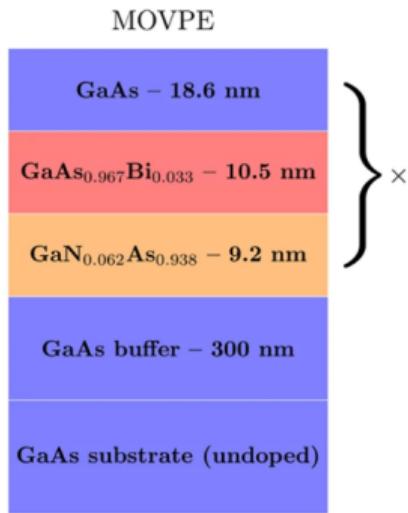
Motivation



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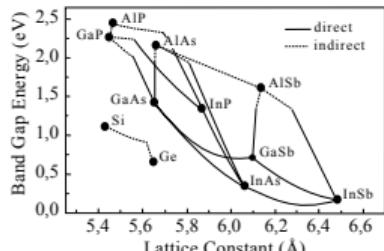
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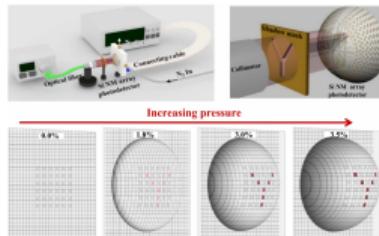
[Sci. Rep. 7, 46371 (2017)]

- Compositional engineering
- Strain engineering
- Composition + strain engineering

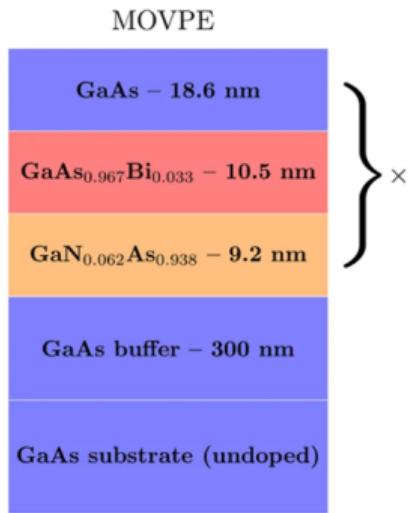
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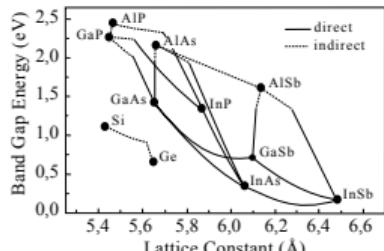


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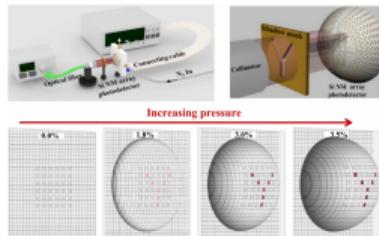
composition-strain-bandgap

- Compositional engineering
- Strain engineering
- Composition + strain engineering

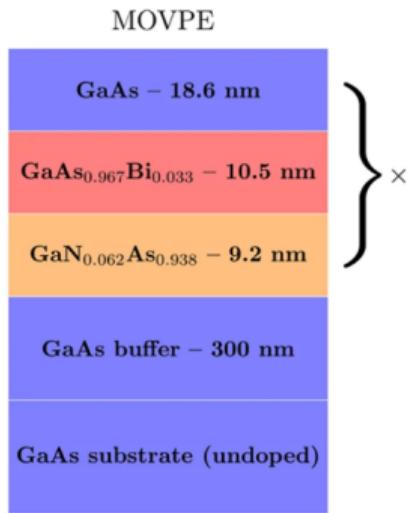
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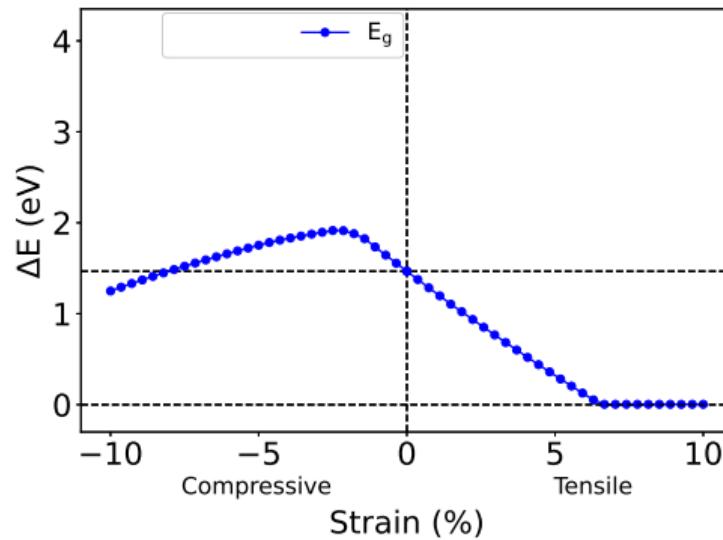


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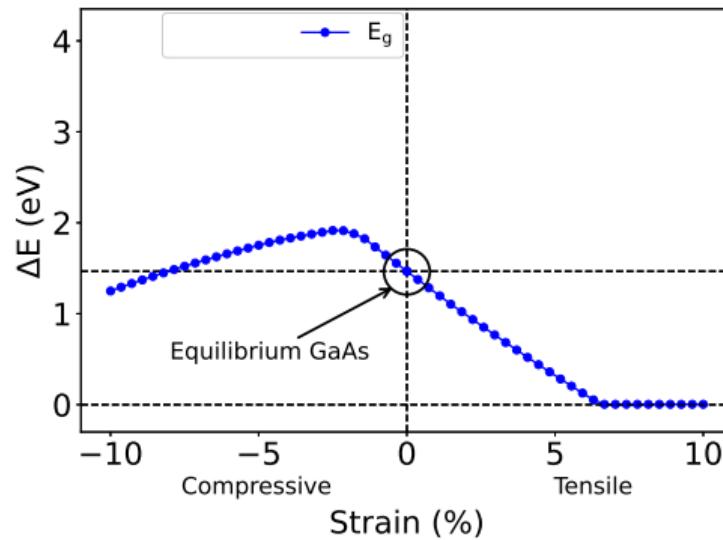
composition-strain-bandgap

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

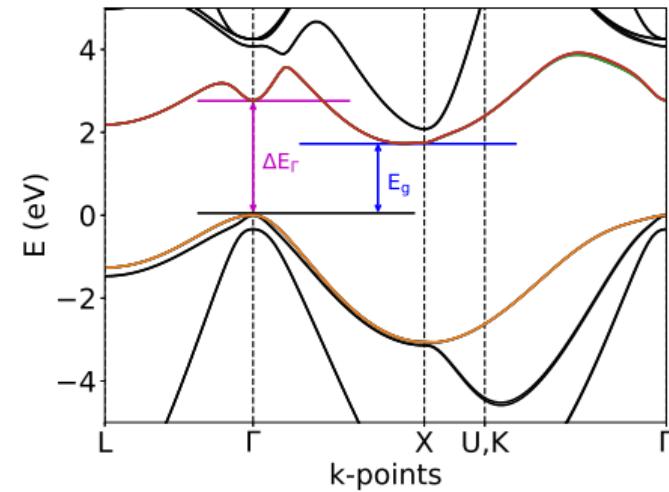
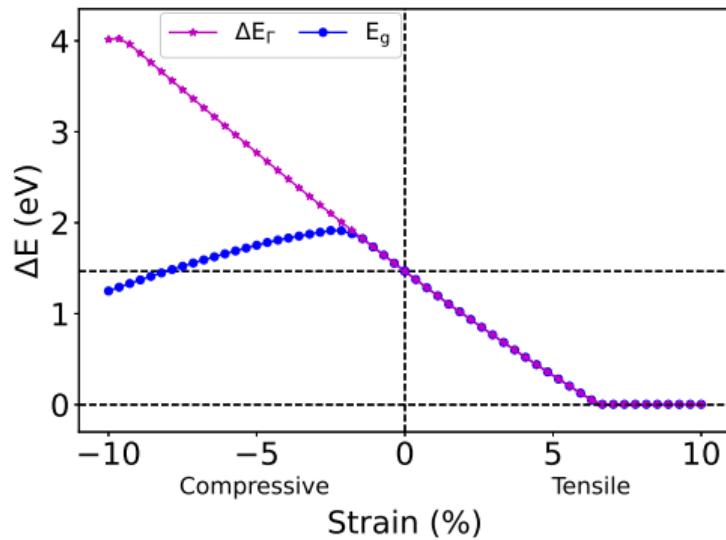
GaAs isotropic strain: strain-bandgap



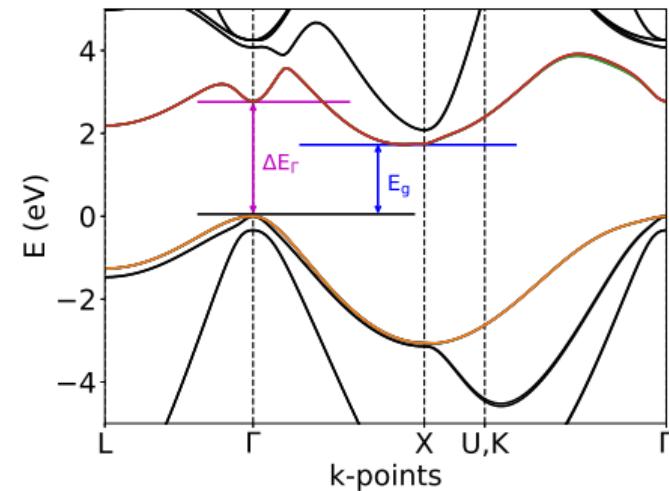
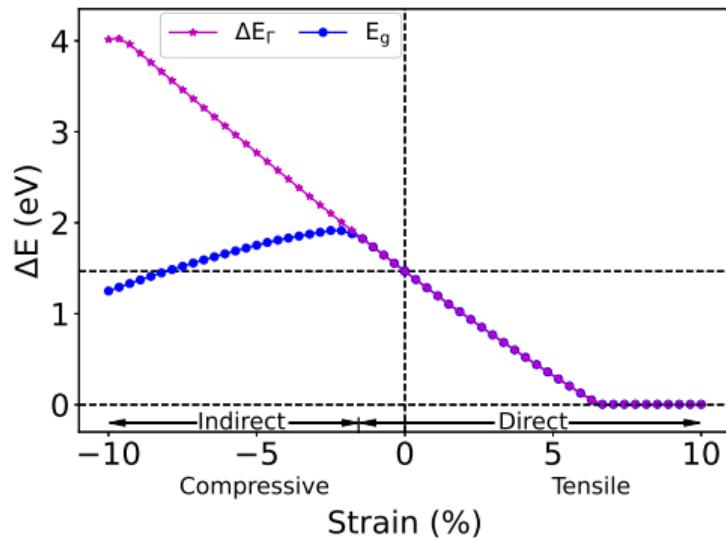
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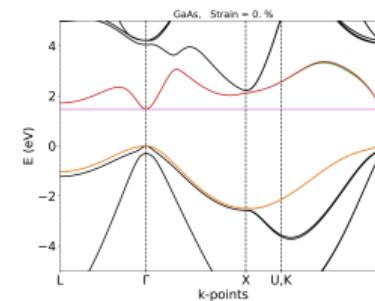
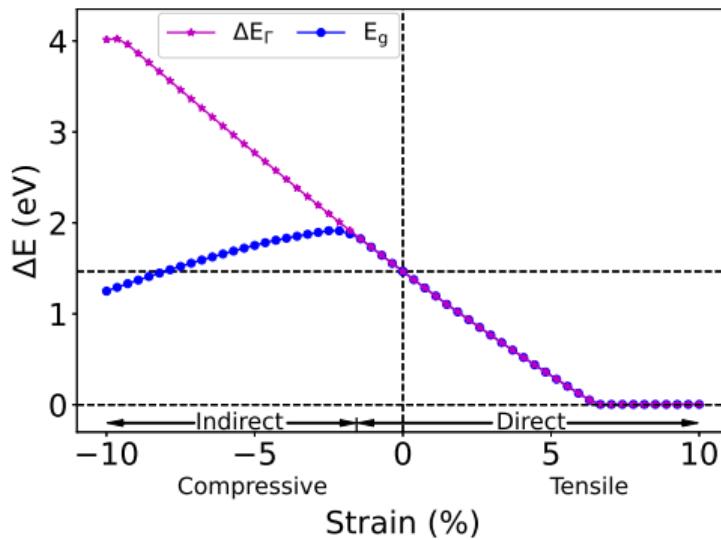
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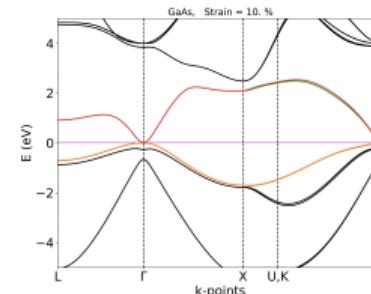
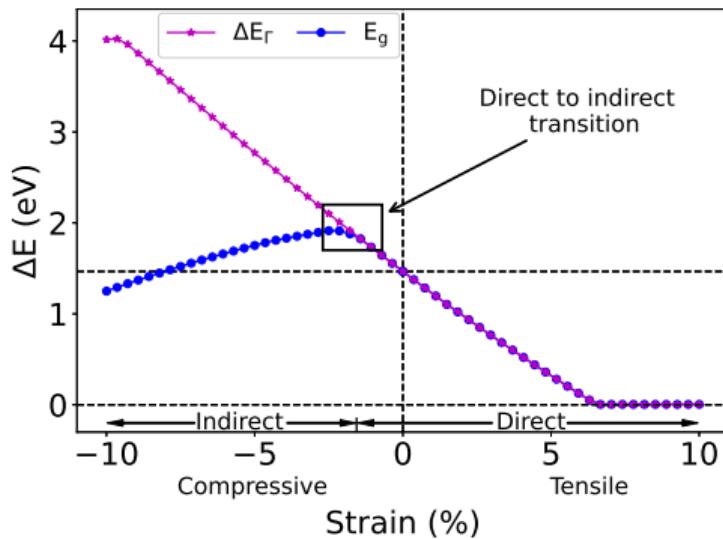
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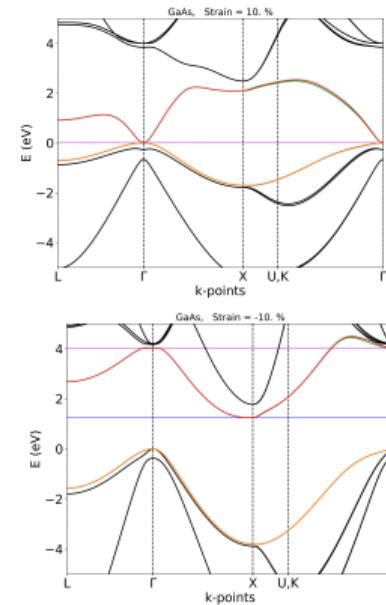
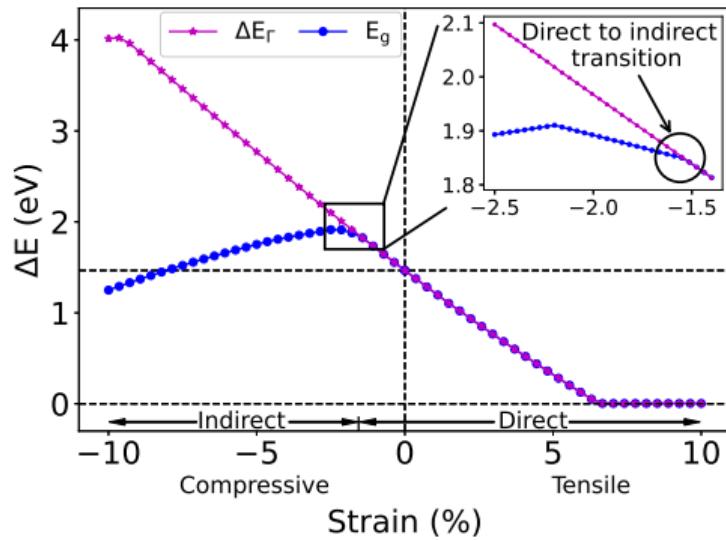
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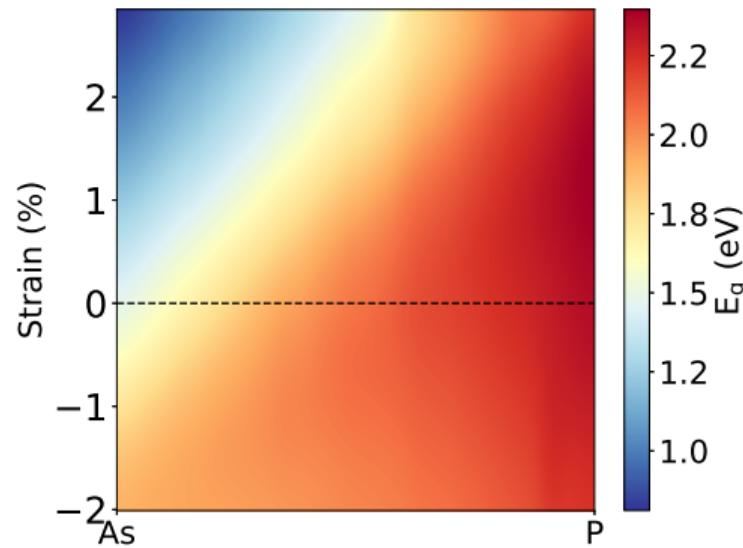


Ga(AsP) isotropic strain: bandgap phase diagram

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

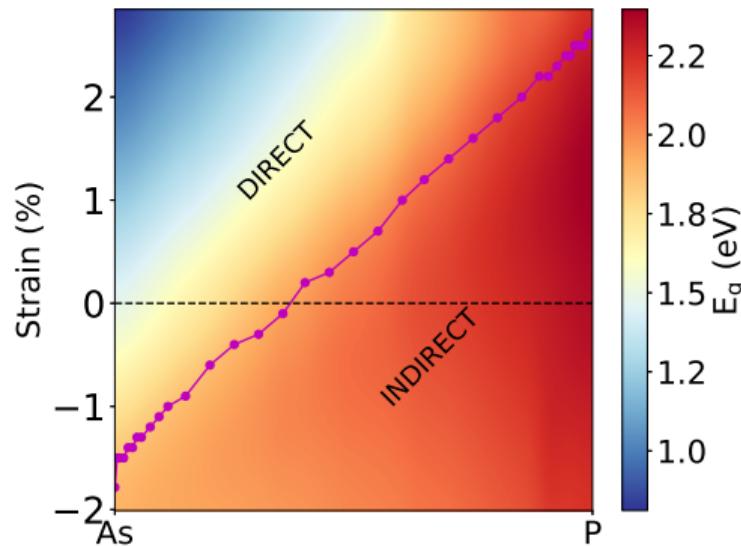
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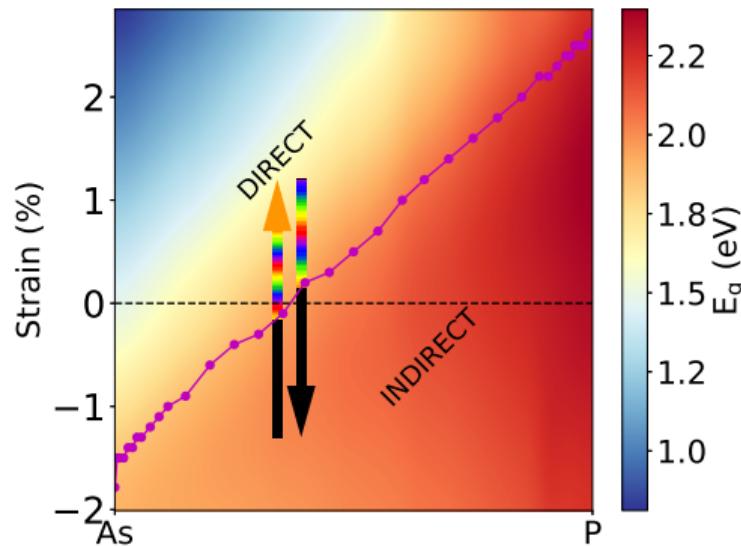
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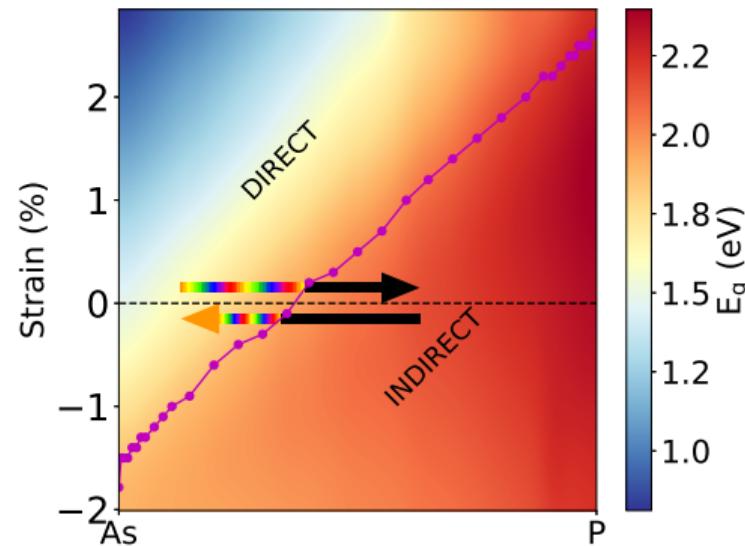
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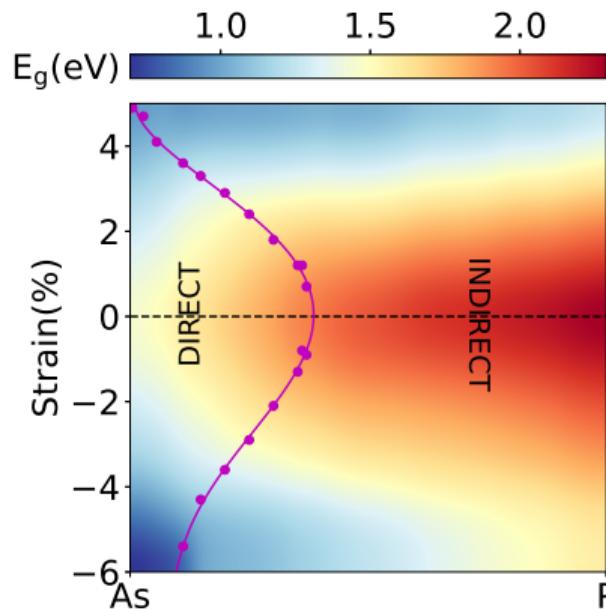


Ga(AsP) isotropic strain: bandgap phase diagram

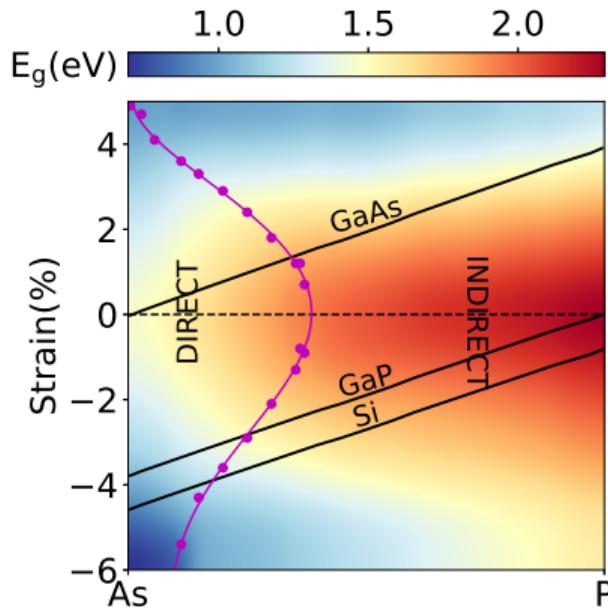
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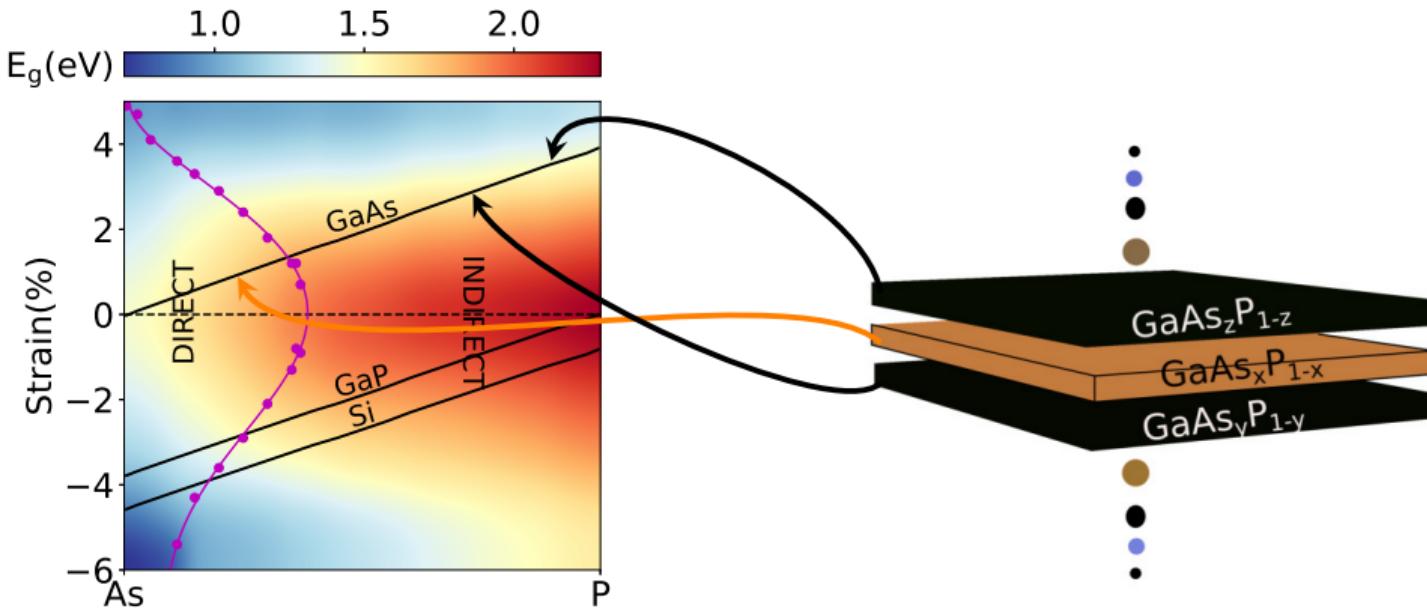
Ga(AsP) biaxial strain: bandgap phase diagram



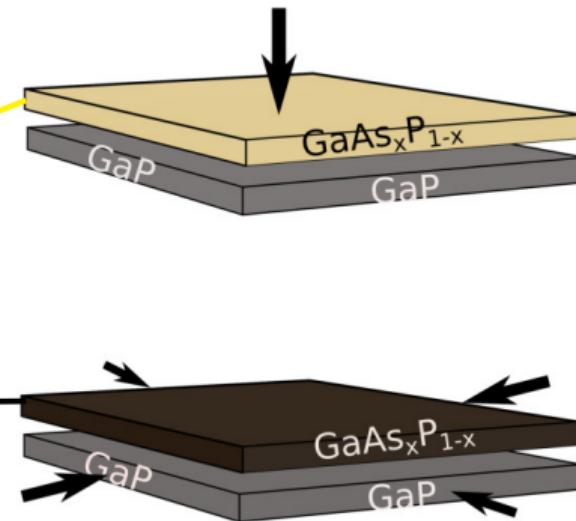
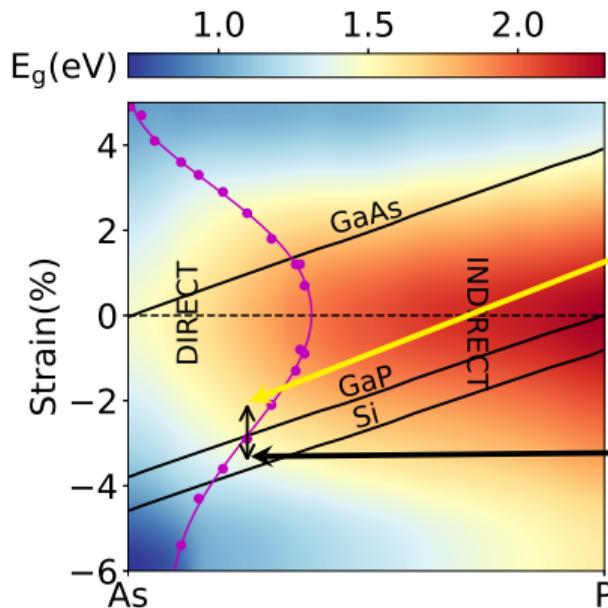
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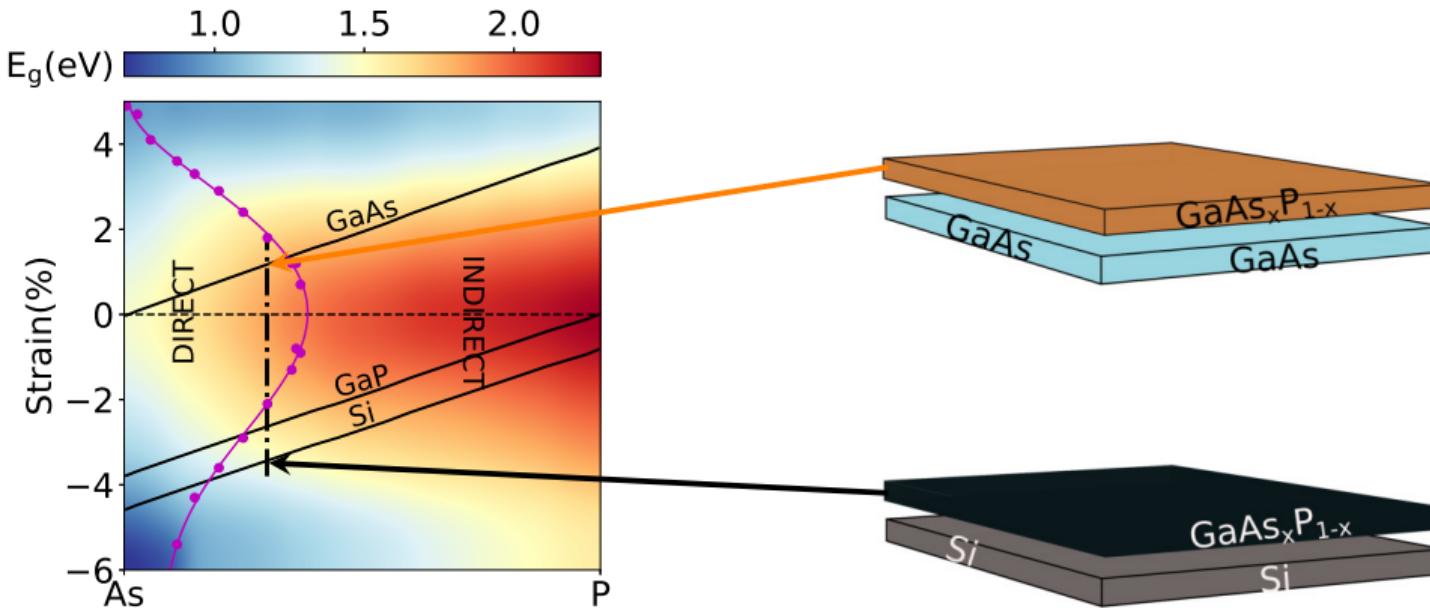
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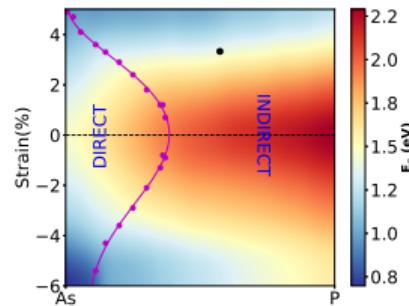
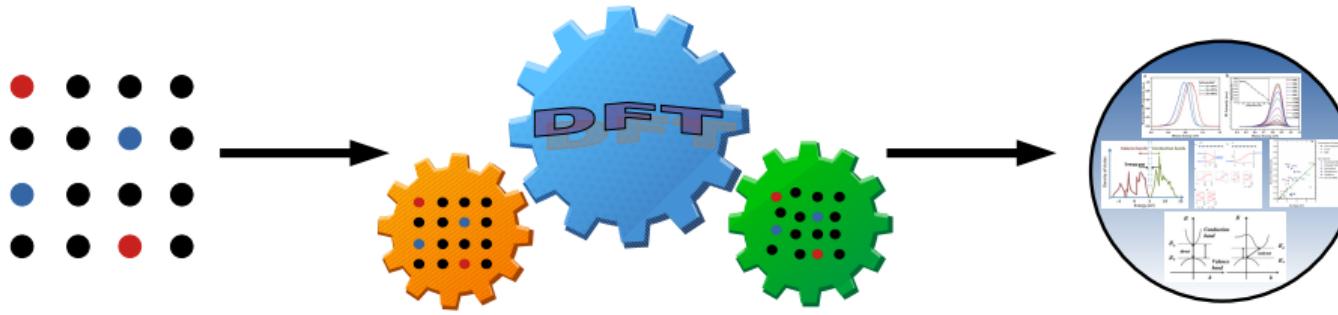
Ga(AsP) biaxial strain: bandgap phase diagram



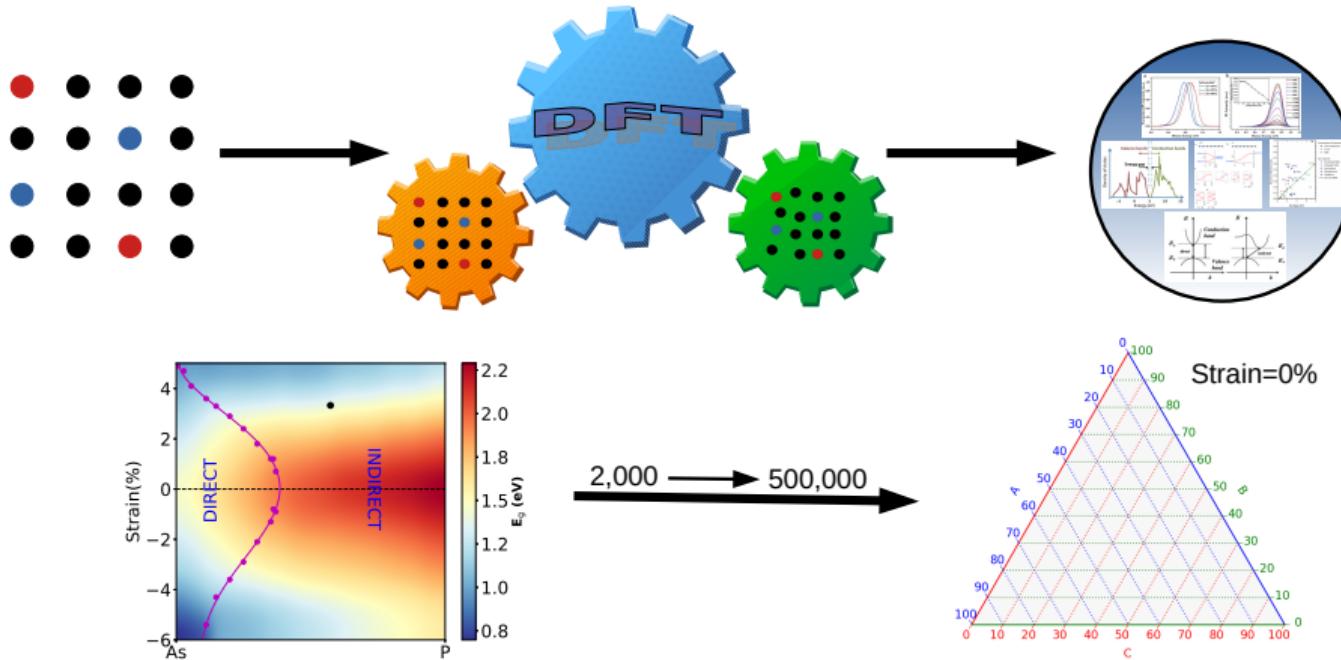
Ga(AsP) biaxial strain: bandgap phase diagram



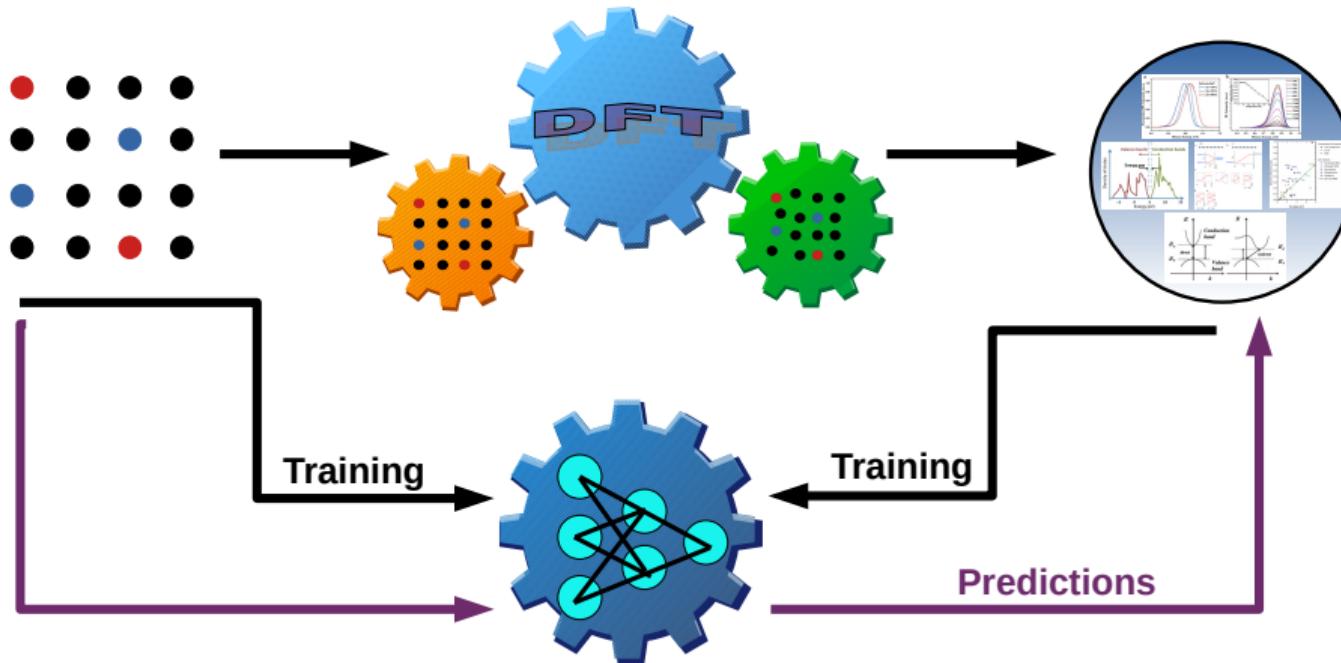
Approach



Approach

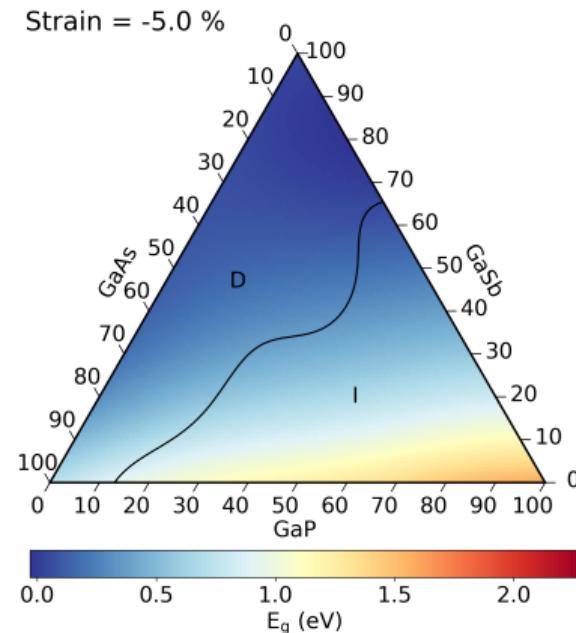


Approach



Ga(AsPSb) biaxial strain: bandgap phase diagram

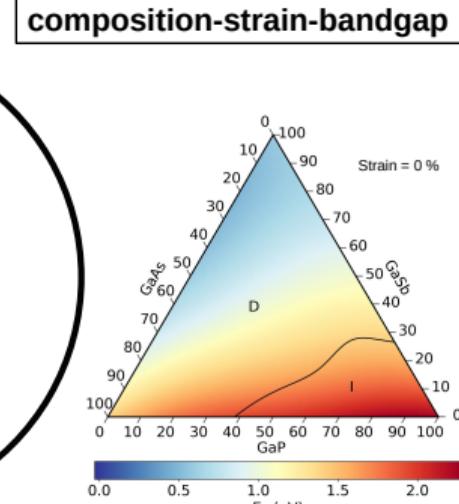
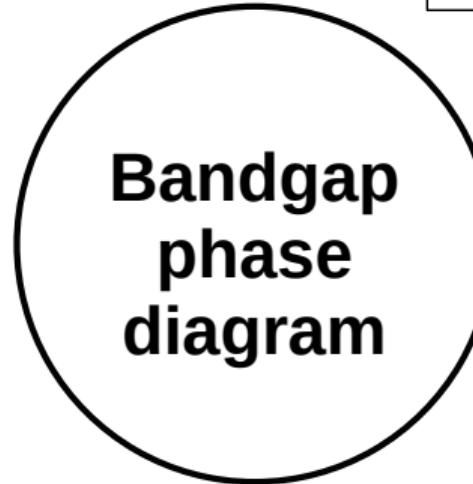
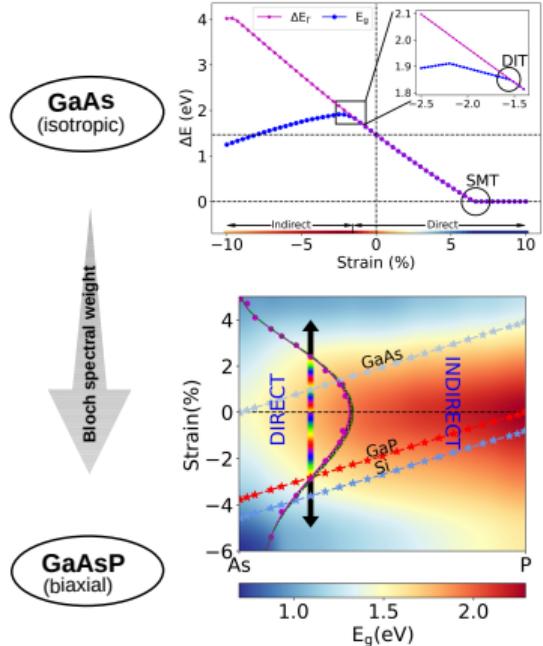
- Machine learning model^{c, d}
 - Support Vector Machine(rbf)
 - Radial Basis Function kernel
 - Training set: 4000 data points
 - Accuracy
 - Bandgap: R2 score = 0.99
 - Bandgap nature: accuracy = 0.95



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



GaAsPb
(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](#)

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

▼ III-V quaternary (comming 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



GRK 1782
Functionalization
of Semiconductors



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