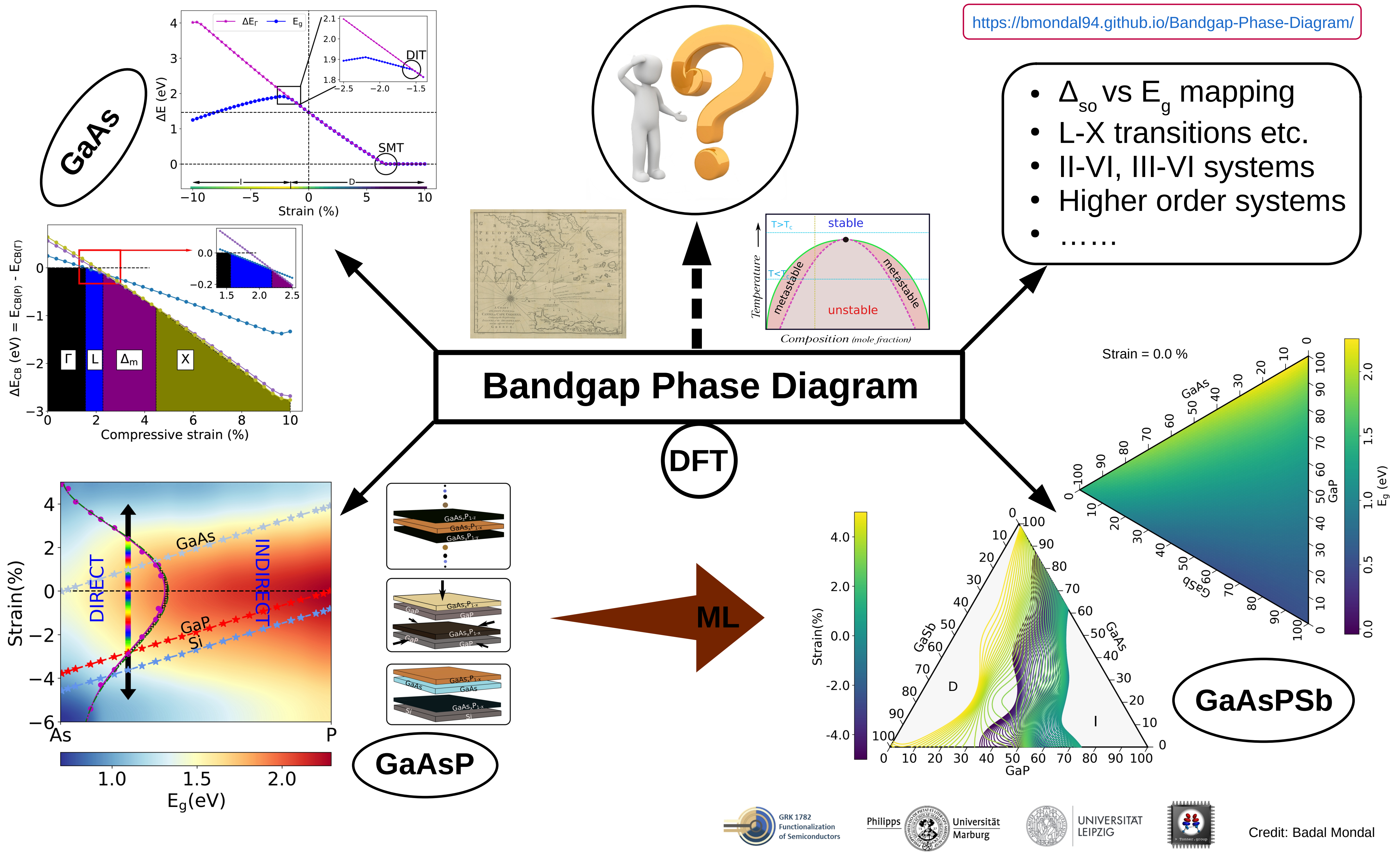
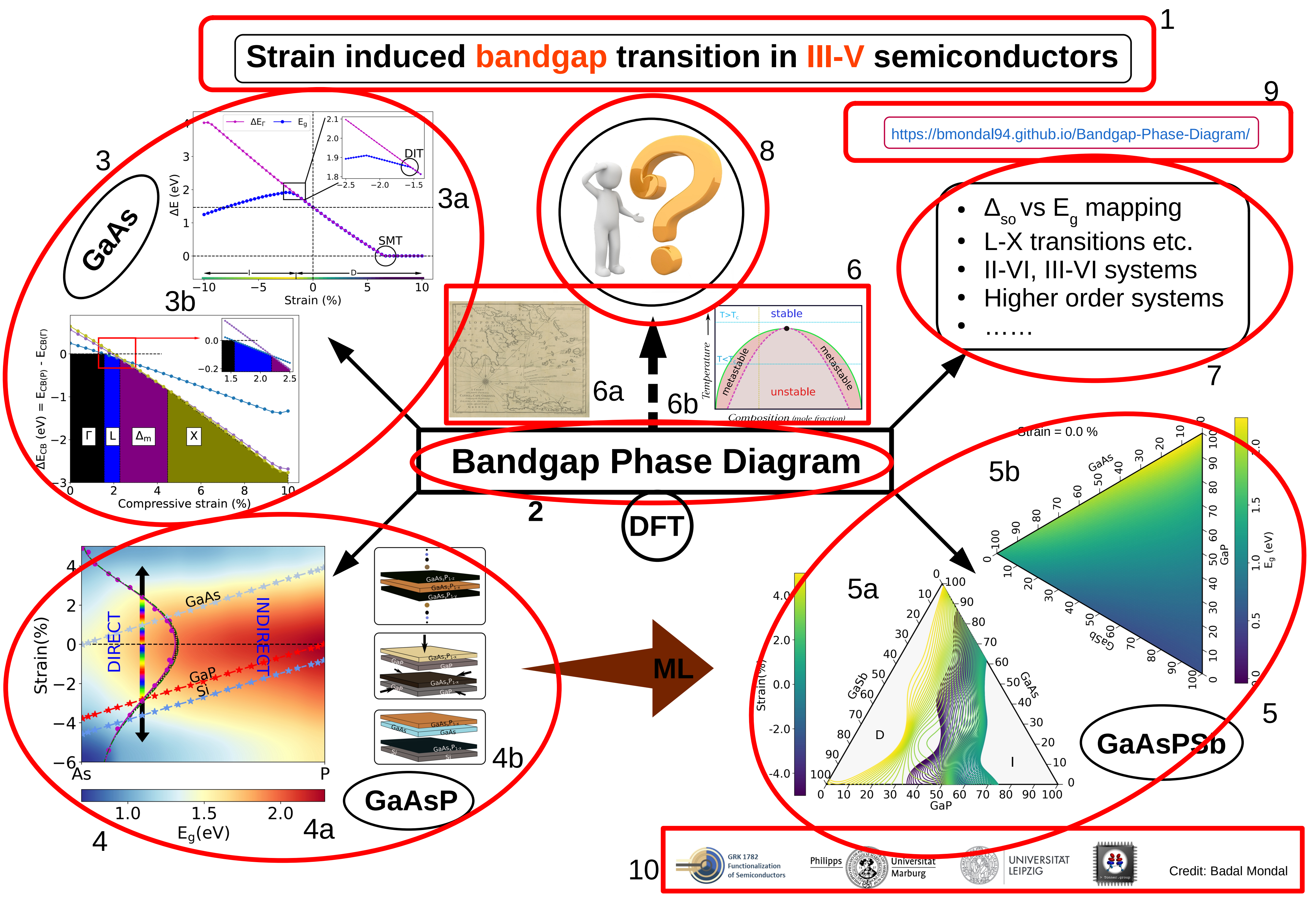
Strain induced bandgap transition in III-V semiconductors





1
Strain induced bandgap transition in III-V semiconductors
9
https://bmondal94.github.io/Bandgap-Phase-Diagram/
3
GaAs
3a
ΔE (eV)
Strain (%)
ΔEΓ
Eg
DIT
SMT
3b
ΔE_CB (eV) = E_CB(P) - E_CB(Γ)
Compressive strain (%)
Γ
L
Δm
X
8
6
6a
6b
stable
metastable
unstable
Temperature
Composition (mole fraction)
7
Δso vs Eg mapping
L-X transitions etc.
II-VI, III-VI systems
Higher order systems
……
Bandgap Phase Diagram
2
DFT
4
4a
Strain(%)
DIRECT
INDIRECT
GaAs
GaP
Si
As
P
Eg(eV)
4b
GaAsP
ML
5
5a
5b
Strain = 0.0 %
GaSb
GaAs
GaP
Strain(%)
D
I
Eg (eV)
GaAsPSb
10
GRK 1782 Functionalization of Semiconductors
Philipps Universität Marburg
UNIVERSITÄT LEIPZIG
Credit: Badal Mondal

1. Title of the project
2. Topic of the project
3. Binary system: GaAs under isotropic strain
   a) Variation of energy difference between conduction band minima (CBM) and valence band maxima (VBM) at the Γ-point, ΔE_{Γ} and bandgap (E_g) under strain application. The positive and negative strain correspond to the tensile and compressive strain respectively. The deviation of the E_g curve from the ΔE_{Γ} curve corresponds to the direct to indirect transition (DIT) in the nature of bandgap, ~1.56 % of isotropic compressive strain. At ~6.67% of isotropic tensile strain the bandgap of GaAs becomes zero, corresponds to the semiconductor to metal transition (SMT). The color scale is the bandgap magnitude. 'D' and 'I' symbolize the 'Direct' and 'Indirect' bandgap nature regions, respectively.
   b) Change in the position of CBM under isotropic compressive strain in GaAs. ΔE_{CB} measures the energy difference between conduction band energy at the Γ and other important k-points (L, X, and Δ_m). The VBM always remain at the Γ-point. Therefore, the evolution of CBM under strain determines the nature of nature of bandgap. From the figure clearly the CBM starts at the Γ-point at strain=0%, corresponds to a direct bandgap. Then at ~1.56 % strain the CBM shifts to the L point, corresponds to the DIT. After that CBM consecutively moves from L to Δ_m to X-point. Δ_m=[0.0000,0.4231,0.4231] in reciprocal space.
4. Ternary system: GaAsP under biaxial strain (for further details please refer to the below Epi-seminar presentation)
   a) The mapping of bandgap magnitude (E_g), the color scale, and the DIT points, magenta dots, with strain and composition. The DIT points are fitted with 5^{th} order polynomial. The GaAs, GaP and Si lines are the substrate strain lines under epitaxial growth model.
   b) Few speculations of the use of bandgap phase diagram.
5. Quaternary system: GaAsPSb under biaxial strain
   a) The mapping of DIT lines in composition and scan over strain within ±5% of strain. The 'D' and 'I' symbolize the 'Direct' and 'Indirect' bandgap nature regions, respectively.
   b) The mapping of bandgap magnitudes in composition at strain=0%, equilibrium configurations.
6. Significance of bandgap phase diagram
   a) The analogy of bandgap phase diagram. This is like a map. Similar to a navigation map bandgap phase diagram can help one to chose the best option in configuration (composition and strain) given an application (such as a device) in mind; and vice versa, given a configuration what can be done with it.
   b) The schematic of binary compositional phase diagram. Alongside electronic properties, the realization of efficient and stable optoelectronics requires smooth transportation of electrons through the system. Therefore, 'only' in combination with the compositional (thermodynamic) phase diagram, bandgap phase diagram can significantly improve the future development in terms of strategic choice of certain application-oriented most suited material systems or vice versa.
7. The future outlooks.
8. Long term goal of the project: Make the rectangle to a circle.
9. The website for reference. The updates regarding bandgap phase diagram will be published here.
10. Acknowledgments