Strain induced bandgap transition in III-V semiconductors

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Pictorial representation of the summary of our project on strain induced bandgap transition in III-V semiconductors.

[1] Given the extensive diverse applications in our everyday life, the III-V semiconductors family posses a great deal of attention in the scientific community. Since its discovery decades ago, people have learned a lot about its potentials, and eventually developed and mastered different techniques in the goal of fine tune their properties. One of such very successful technique in this respect is the 'strain engineering'. Sometimes, it comes as a side effect, such as in hetero-structure. So, it is worth and we did learn quite a lot about mutual correlation between strain of different flavors and different electronic properties of different III-V semiconductor materials in the hope of control them, either use them for our good or sometimes to avoid them. Despite of extensive effort in the past a complete picture in this respect of understanding of how the bandgap of III-V semiconductor materials is affected by strain is still missing. And there we came into the picture. The electronic properties that we choose as the subject of our primary interest is the so-called backbone of optical properties of semiconductors, the bandgap. In this vision, our aim is to map the variation of bandgap under strain, globally.

[2] We have established a comparatively computationally cost effective and fairly robust recipe for such analysis using computational tools, modern ab-initio density functional theory (DFT). We have shown that depending on the nature and strength of applied strain in the system the material behavior can change substantially. Namely, a direct bandgap semiconductor can transform to an indirect bandgap semiconductor and vice versa. This ultimately enables us to construct the 'bandgap phase diagram' by mapping the different direct-indirect transition points with strain and/or composition .

Binary, 1D bandgap phase diagram: [3] Let's start with the simplest, binary III-V semiconductor system. [3a] As an example, in GaAs we have shown that under isotropic compressive strain the nature of the bandgap changes from direct to indirect given by this direct to indirect transition (DIT) point. Under isotropic tensile strain the well know semiconducting GaAs become metal, given by this semiconductor to metal transition (SMT). [3b] As the valence band maxima (VBM) always remain at the Gamma point, therefore, by tracking the evolution of conduction band minima (CBM) under strain enable us to track the nature of bandgap. For example, the CBM starts at the the Gamma point at strain=0, corresponds to a direct bandgap. Then at ~1.56 % strain the CBM shifts to the L point, and the bandgap become indirect in nature; corresponds to the direct to indirect transition. After that CBM consecutively moves from L to Δm to X-point. Following the same principle, the transitions in other commonly used binary III-V semiconductors (including Si) are also analyzed.

Ternary, 2D bandgap phase diagram: [4] Following the great success in binary systems, our next goal was to extend the analyses for higher-order systems. However, in comparison to the binary systems where we could use simple primitive cells for the analysis but in multinary systems, to ensure the ideal admixing among all the components in the composition we had to go for supercell. Unfortunately, the use of this supercell resulted in the well-known 'band folding' phenomena. Due to this band folding, although it was straightforward to get the information about the magnitude of bandgap, but not the nature of bandgap. [4a] Using the idea of 'Bloch spectral density/weight' we have developed a systematic strategy for the strain-bandgap relationship in the next higher order, ternary systems; by mapping the different direct-indirect transition (DIT) points with composition **and** strain. This is such an example of bandgap phase diagram for GaAsP under biaxial strain. [4b] As the use of this bandgap phase diagram we have speculated a few possibilities within 'epitaxial growth model'.

Quaternary, quasi-2D bandgap phase diagram: Following the footstep of our previous analyses, we then extended the scope to the next higher order quaternary systems. However, given the huge compositional space, it will be an extremely daunting step to take to cover enough of the vast compositional space in quaternary systems using DFT calculations only. So, we decided to take the advantage of another uprising modern scientific tool Machine learning. The core idea is to combine our limited DFT capability with the

easily extendable ML with the hope to cover the maximum compositional space with reliable results. [5] Here is a snapshot of such a bandgap phase diagram for the quaternary compound, GaAsPSb. [5a] Using the already available DFT data for the corresponding ternary subsystems of our quaternary system of choice and some more calculations on the quaternary region we have mapped the DIT points over composition and scanned over strain. Here, we have used the Support Vector Machine (SVM) supervised machine learning model in combination with Radial Basis Function (RBF) kernel. For the prediction of bandgap nature, we used the classification version of the SVM model, known as Support Vector Classification (SVC) model with an accuracy of 95.4%. [5b] And the regression version of SVM, the Support Vector Regression (SVR) model for the prediction of the bandgap with an accuracy (r2 score) of 99%.

[6] [6a] In conclusion, the best analogy we came up with in this this respect is, 'bandgap phase diagram' is like a navigation map. Similar to a navigation map bandgap phase diagram can help one to chose or determine 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. [6b] However, one should realize that bandgap phase diagram alone is not enough for this purpose. Alongside electronic properties, the realization of efficient and stable optoelectronics requires smooth transportation of electrons through the system. The presence of any kind of dislocation, heterogeneity in the material composition, or roughness in the heterostructure interfaces can tremendously hinder the electronic mobility and hence, the performance and long-term stability of the devices. 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. Although, we had compositional phase diagram in the picture for quite a long time, but this other one was missing. And now we are giving you the missing piece. We no longer have to rely on our experience or trial and error method but now we have a scientifically consistent systematic way to make our choice superior.

[7] As the extension of this project, among others, few of the most important propositions that we are currently working on are

1. Extension of our bandgap phase transition analysis to the next higher order systems. Given the limitations in visualization we can go up to at least 5 components systems.
2. What about other material systems, for e.g. II-VI or III-VI systems?
3. We have just seen only one of the transition, the direct-indirect transition. But in the similar fashion one can analyze other transitions in indirect region itself such as L-X and so on, given the needs.
4. One can also extend this idea to other contexts. For e.g. using this idea of Bloch weight we aim to map the correlation between bandgap and split-off energy in the direct bandgap regions, which can be used for e.g. in Auger recombination type analyses.
5.

In short, we have have accomplished so far 3 projects in this regard, 1D bandgap phase diagram in Binary systems, 2D bandgap phase diagram in Ternary systems, and quasi-2D bandgap phase diagram in Quaternary systems. With quite confidence, I can say that going from binary to ternary was really an important and a great step forward; a great achievement in terms of developing a completely new idea for cracking a deep scientific problem. With the 4^{th} corner of this square as the future outlook, let me finish with our long term goal. [8] In long term our goal is to make this rectangle to a circle.

[9] We have also designed a fairly detail map of this whole topic and you can find it here. That includes our results, details of the calculation procedure, latest updates in this regard etc. and so on. Feel free to contact us if you have any further questions, any new ideas from your side. The details you will find there.

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And finally, thank you all for your attention, and being here till the end.