Strain-induced bandgap transition in III-V semiconductors

Badal Mondal[1,2] and Ralf Tonner-Zech[2]

[1]Fachbereich Physik, Philipps-Universität Marburg, 35032 Marburg, Germany
[2]Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, 04103 Leipzig, Germany

III-V semiconductor compounds attract a great amount of attention both in science and technology due to their diverse applications in areas such as optoelectronics. One of the most important fundamental properties determining the optical properties of semiconductor materials is the bandgap. Varying the relative composition is one of the major approaches to tailor the bandgap in compound semiconductors. Strain can be used further to systematically fine-tune the bandgaps. In combination, they can be used to customize the bandgaps over a wide range of values and induce the transition in the nature of bandgaps.

Previously, the density functional theory (DFT) with the TB09 exchange-correlation functional [1] had been successfully demonstrated to predict the electronic properties of unstrained III-V compound semiconductors [1, 2]. Here, we have shown that this approach can also be successfully used for strained materials over a wide range of structural strains. Using this computational method, we have established a methodology for the analysis of the mutual correlation of composition, strain, and the bandgap of material. Using the idea of Bloch spectral weight [3, 4], we have developed a systematic strategy for the predictive mapping of composition-strain-bandgap relationship in multinary III-V semiconductor compounds. We have shown that straining the system not only changes the bandgap in terms of its magnitude but can also modify the nature of bandgap itself. Depending on the nature and strength of applied strain in the system, a direct bandgap semiconductor can transform into an indirect bandgap semiconductor and vice versa. This has ultimately enabled us to construct the 'bandgap phase diagram' [5] by mapping the different direct-indirect transition points with composition and strain. By combining the advanced tools of machine learning with DFT, we have further developed an efficient approach for such mapping in multinary systems. We have demonstrated the huge impact and effectiveness of this new predictive mapping in choosing the best-suited material system targeting certain applications, or vice versa.

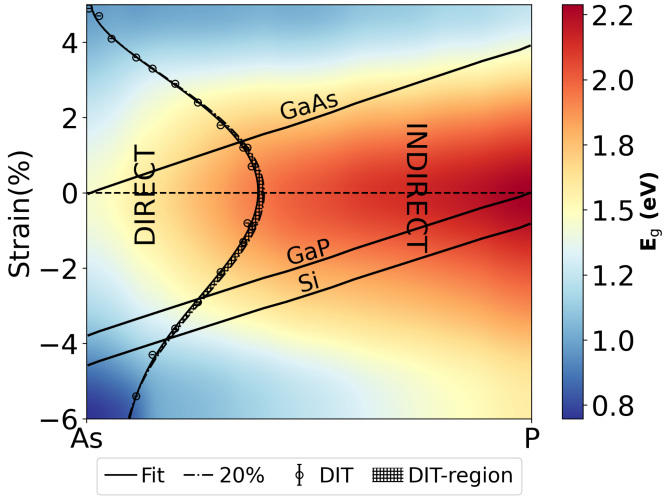

Figure: GaAsP bandgap phase diagram under bi-axial strain. 'DIRECT' and 'INDIRECT' indicate the region of compositions having bandgap direct and indirect in nature, respectively. The colorbar shows the bandgap magnitude (E_g). The direct-indirect transition (DIT) points are shown in black circles. The DIT points are fitted with a polynomial of order 5. The DIT-region is the uncertainty in the determination of bandgap nature. The 20% line corresponds to the cutoff of 20% Bloch weight is considered as the minimum criteria in defining a state. The GaAs, GaP, and Si lines correspond to the substrate strain line under the 'epitaxial growth' model.

References:

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