Contribution submission to the conference SKM 2023

Predicting bandgap in strain-engineered multinary III-V semiconductors — •Badal Mondal and Ralf Tonner-Zech — Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, 04103 Leipzig, Germany

The tuning of the type and size of bandgaps of III-V semiconductors is a major goal for optoelectronic applications. Varying the relative composition of several III- or V-components in compound semiconductors is one of the major approaches here. Alternatively, straining the system can be used to modify the bandgaps. By combining these two approaches, bandgaps can be tuned over a wide range of values, and direct or indirect semiconductors can be designed. However, an optimal choice of composition and strain to a target bandgap requires complete material-specific composition, strain, and bandgap knowledge. Exploring the vast chemical space of all possible combinations of III- and V-elements with variation in composition and strain is experimentally not feasible. We thus developed a density-functional-theory-based predictive computational approach for such an exhaustive exploration. This enabled us to construct the 'bandgap phase diagram' [1] by mapping the bandgap in terms of its magnitude and nature over the whole composition-strain space. Further, we have developed efficient machine-learning models to accelerate such mapping. We will show the application to binary [2], ternary and quaternary material combinations and the possible impact on device design.

[1] https://bmondal94.github.io/Bandgap-Phase-Diagram , 2022
[2] https://arxiv.org/abs/2208.10596

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