

The Inverse Band Structure Approach: Given the desired electronic property, find the atomic configuration

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ABSTRACT

Modern crystal-growth techniques, such as molecular beam epitaxy or metal-organic chemical-vapour deposition, are capable of producing prescribed crystal structures, sometimes even in defiance of equilibrium, bulk thermodynamics. These techniques open up the possibility of exploring different atomic arrangements in search of a configuration that possesses given electronic and optical properties. Unfortunately, the number of possible combinations is so vast, and the electronic properties are so sensitive to the details of the crystal structure, that simple trial-and-error methods (such as those used in combinatorial synthesis) are unlikely to be successful. Here we describe a theoretical method that addresses the problem of finding the atomic configuration of a complex, multi-component system having a target electronic-structure property. As an example, we predict that the configuration of an $\text{Al}_{0.25}\text{Ga}_{0.75}\text{As}$ alloy having the largest optical bandgap is a $(\text{GaAs})_2(\text{AlAs})_1(\text{GaAs})_4(\text{AlAs})_1$ superlattice oriented in the $[201]$ direction.

Keywords: inverse band structure, atomic configuration.

1 INTRODUCTION

The idea is as follows: Conventional electronic-structure theory of solids, clusters and molecules proceeds by first specifying the spatial coordinates of all atomic species involved, and then calculating the ensuing energy levels and wavefunctions:

$$\text{Atomic Configuration} \rightarrow \text{Electronic Structure} \quad (1)$$

We are interested in the counterpart to this direct approach: the "inverse approach" of finding the atomic configuration that produces a prescribed electronic structure:

$$\text{Electronic Structure} \rightarrow \text{Atomic Configuration} \quad (2)$$

In the context of optical properties, such a method would provide answers to questions like "For a given superlattice orientation, what is the layer sequence that has the maximum bandgap (or a pre-assigned bandgap, say 2 eV)?" In the context of transport properties, one could ask: "What is the crystal structure whose band structure maximizes Auger carrier multiplication? Similar 'inverse problems' can be addressed in the context of vibrational and photonic properties, as well as for molecules and low-dimensional systems.

We describe here a solution to the 'inverse band-structure problem' based on a direct exploration of the space of atomic configurations in search of the configuration possessing given electronic properties.

This method can be compared with a direct "Linear Expansion in Geometric Objects" approach in which the LDA-calculated band gap is expanded in "geometric objects" (GO) such as atom-pairs, triangles, etc. Once the contribution of each GO to the band gap is known, one can search many possible configurations for the one that has a desired gap. This method produces similar results as the Inverse Band Structure.

2 CONCLUSION

These two approaches -- "Inverse Band Structure" (IBS) and "Linear Expansion in Geometric Objects" (LEGO) form a new basis for rational material design.