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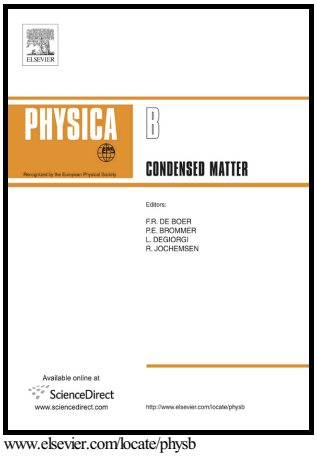

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Unfolding and effective bandstructure calculations as discrete real- and reciprocal-space operations

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ABSTRACT
In recent years, alloy electronic structure calculations based on supercell Brillouin zone unfolding have become popular. There are a number of formulations of the method which on the surface might appear different. Here we show that a discrete real-space description, based on discrete Fourier transforms, is fully general. Furthermore, such an approach can more easily show the effects of alloy scattering. We present such a method for treating the random alloy problem. This treatment features straightforward mathematics and a transparent physical interpretation of the calculated effective (i.e., approximate) energy bands.

Keywords: unfolding; supercell; alloy

1. Introduction

Approximate concepts in physics are often the most difficult to articulate and quantify, but quantification is essential for it establishes the range of validity of the approximation. The alloy concept is one which is particularly easy to explain in qualitative terms but which can be problematic to quantify. Semiconductor alloys are of particular technological interest, being found in lasers and transistors incorporated into nearly all consumer and industrial electronic