Abstract Submitted
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Zone Unfolding and Approximate Bandstructure Calculations in Tight-Binding[1] TIMOTHY BOYKIN, University of Alabama-Huntsville, NEERAV KHARCHE, Purdue University, MATHIEU LUISIER, ETH Zurich, GERHARD KLIMECK, Purdue University — Tight-binding electronic structure calculations for periodic systems are often carried out in non-primitive unit cells, or for imperfect (e.g. random-alloy) nanostructures, such as nanowires. In the first case bands exist but they are difficult to identify due to the choice of unit cell for the calculation, while in the second case bands only exist in an approximate sense. The Brillouin zone unfolding technique applied to tight-binding calculations provides a powerful tool for extracting the true primitive-cell bands from non-primitive cells. Also, it is the starting point for approximate nanowire band calculations. We discuss zone unfolding in tight-binding and its application to both perfect and imperfect systems.

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