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Reduced Bloch mode expansion for fast band structure calculations MAHMOUD HUSSEIN, University of Colorado at Boulder — In this paper, we present reduced Bloch mode expansion for fast band structure calculations in lattice dynamics. The expansion employs a natural basis composed of a selected reduced set of Bloch eigenfunctions. The reduced basis is selected within the irreducible Brillouin zone at high symmetry points determined by the medium's crystal structure and group theory. At each of the reciprocal lattice selection points, a number of Bloch eigenfunctions are selected up to the frequency/energy range of interest for the band structure calculations. Being in line with the well known concept of modal analysis, the proposed approach maintains accuracy while reducing the computation time by up to two orders of magnitudes or more depending on the size and extent of the calculations. Results are presented for Si-Ge quantum dot superlattice band structures.

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