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Lattice dynamics and electron-phonon coupling calculations using nondiagonal supercells[1] JONATHAN LLOYD-WILLIAMS, University of Cambridge, BARTOMEU MONSERRAT, Rutgers University — Quantities derived from electron-phonon coupling matrix elements require a fine sampling of the vibrational Brillouin zone. Converged results are typically not obtainable using the direct method, in which a perturbation is frozen into the system and the total energy derivatives are calculated using a finite difference approach, because the size of simulation cell needed is prohibitively large. We show that it is possible to determine the response of a periodic system to a perturbation characterized by a wave vector with reduced fractional coordinates $(m_1/n_1, m_2/n_2, m_3/n_3)$ using a supercell containing a number of primitive cells equal to the least common multiple of n_1, n_2, and n_3. This is accomplished by utilizing supercell matrices containing nonzero off-diagonal elements. We present the results of electron-phonon coupling calculations using the direct method to sample the vibrational Brillouin zone with grids of unprecedented size for a range of systems, including the canonical example of diamond. We also demonstrate that the use of nondiagonal supercells reduces by over an order of magnitude the computational cost of obtaining converged vibrational densities of states and phonon dispersion curves.

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