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Coherent phonon generation in time-dependent density functional theory¹

GEORGE BERTSCH, University of Washington

We apply the time-dependent density functional theory (TDDFT) to the generation of coherent optical phonons in Si and Sb crystals. The computations are carried out by real-time evolution of the orbital wave functions on a coordinate-space mesh. The theory reproduces the main phenomena observed experimentally: dependence on polarization, strong growth at the direct band gap, and the change in phase from below to above the band gap. Comparing with more phenomenological models, we find that the TDDFT supports the impulsively stimulated Raman mechanism at low frequencies and the qualitative aspects of the displacive mechanism at higher frequencies. We also compare with the more detailed model of displacive excitation by Stevens, Kuhl, and Merlin.

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