

Abstract Submitted
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Calculation of phonon dispersion relations and softening in photo-excited bismuth EAMONN MURRAY, Tyndall National Institute, Ireland, STEPHEN FAHY, Tyndall National Institute, Ireland — The phonon dispersion relations for equilibrium and photo-excited bismuth are calculated using density functional theory, combined with constrained density functional theory. The dependence of phonon frequency on photo-excited electron-hole plasma density is found for modes throughout the Brillouin Zone. The results are in excellent agreement with available neutron scattering data for the equilibrium occupation of electronic bands. We find the effect of phonon softening by the electron-hole plasma to be larger in the optical modes than in the acoustic modes.

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