Abstract Submitted
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First-principles calculation of the polarization-dependent force driving the E_g mode in bismuth under optical excitation.[1] EAMONN MURRAY, Tyndall National Institute, Ireland, STEPHEN FAHY, Tyndall National Institute and University College Cork, Ireland — Using first principles electronic structure methods, we calculate the induced force on the E_g (zone centre transverse optical) phonon mode in bismuth immediately after absorption of polarized light. When radiation with polarization perpendicular to the c-axis is absorbed in bismuth, the distribution of excited electrons and holes breaks the three-fold rotational symmetry and leads to a net force on the atoms in the direction perpendicular to the axis. We calculate the initial excited electronic distribution as a function of photon energy and polarization and find the resulting transverse and longitudinal forces experienced by the atoms. Using the measured, temperature-dependent rate of decay of the transverse force[2], we predict the approximate amplitude of induced atomic motion in the E_g mode as a function of temperature and optical fluence.

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[2]J.J. Li et al, Phys. Rev. Lett. 110, 047401 (2013)

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