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Photostriction in ferroelectric and multiferroic materials from first principles[1]

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The so-called Bulk Photovoltaic Effect (BPVE), occurring in materialslacking inversion symmetry, has attracted interest for the design of new solar cells. Hence, non-centrosymmetry of ferroelectrics makes themnatural candidates to the design of suchsolar cells. Itis also fundamental to their piezoelectric properties, *i.e.*the coupling of their electric polarization to strain. Therefore, ferroelectrics offer a natural route towards the realization of light-induced actuators among the class of photostrictive materials. Experimental evidences towards this goal have appeared, with intense studies of the photostriction in bismuth ferrite, in which both thesteady state response andthe transientgiant shear strain induced by femtoseconds laser pulses wereattributed to the conjunction of the BPVE and the piezoelectric effect. However, theory has not investigated the coupling of light with electromechanical properties of ferroelectrics on a microscopic scale. To tackle this problem, we employ a Δ-SCF scheme in which the occupation numbers of the Kohn-Sham orbitals are constrained. We apply this method to various prototypical ferroelectric and multiferroic materials, such as bismuth ferrite. This scheme yields a photostrictioneffect of the same order of magnitude than the ones recently observed. It also predicts a strong dependence of photostrictive response on both the reached conduction state and the crystallographic direction (along which this effect is determined). In particular, according to our results, BFO should shrink along its pseudo-cubic and polarization axes, with the pseudo-cubic angle getting closer to 90, while the directions perpendicular to the polarization, such as $[110]_{pc}$, stretches under excitation of electrons in the conduction band. Another of our main results is that photostriction is found to originate from the combination of screening of the polarization at the unit cell scale by the photoexcited carriers, and converse piezoelectric effect.

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