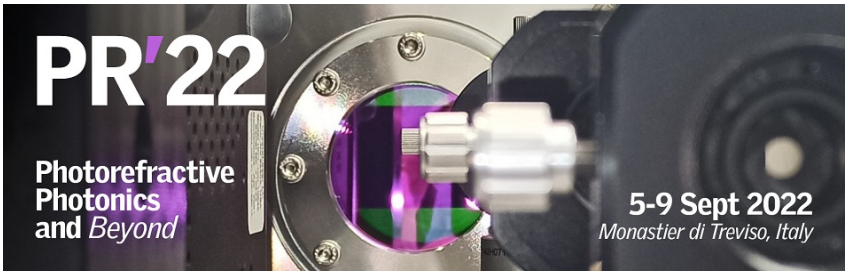

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Optical response of strained LiNbO3 crystals from first principles

Thursday, 8 September 2022 16:40 (1h 30m)

As X-ray measurements have shown, domain walls in $LiNbO_3$ exhibit the structure of compressed bulk material [1]. Hence, knowledge of the optical response of $LiNbO_3$ as a function of compression can help to characterize the domain walls of $LiNbO_3$ and yields information about their optical signatures.

In our work, we model linear and non-linear optical properties of $LiNbO_3$ in dependence on uniaxial compressive strain in x-, y- and z-direction from first principles using time-dependent density functional theory (TDDFT) [2]. This includes the calculation of the energy dependent second (SHG) and third harmonic generation (THG). We find changes for all components of the second- and third-order polarizability tensor χ^2 and χ^3. In particular, for $|\chi^2_{zzz}|$ we obtain a linear increase with applied compression in z-direction. Due to the threefold rotational symmetry, $LiNbO_3$ has four independent χ^2 elements [3]. However, compression in x- and y-direction reduces the symmetry, lifting the degeneracy of identical χ^2 components. Additionally, from the calculated dielectric tensor the refractive index and birefringence as a function of compression is obtained. Knowledge of both these properties under compression is particularly important for the application of Ti waveguides.

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