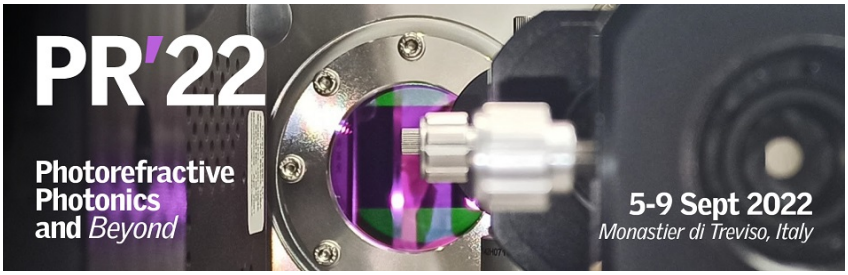

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Optical response of LiNb_{x}Ta_{1-x}O3 solid solutions calculated from first principles.

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In the last decade, our knowledge of the linear and nonlinear optical response of LiNbO3 crystals has substantially improved [1]. Precise optical measurements on samples of well known composition allowed to distinguish, e.g., polaronic signatures, while refined ab initio models allowed to disentangle the various effects contributing to the measured spectra and to assign spectral signatures to determined structural features. In this contribution, we review the actual knowledge of the linear and nonlinear optical response of LiNbO3 crystals from a theoretical point of view. The optical properties calculated with different approaches of different precision [2], ranging from the independent particle approximation to the GW-approach are shown and compared to experimental data. The role of intrinsic and extrinsic defects and temperature is discussed in detail [1,3]. Additionally, we discuss a few possibilities to tailor the materials optical response (e.g., the second harmonic generation) by structural strain or by tuning the crystal composition for specific applications. In this respect, LiNb_{x}Ta_{1-x}O3 solid solutions offer a further knob to realize crystals with optimized optical properties. The talk is concluded with an overview of actual research fields of theoretical materials science concerning the linear and nonlinear optical response of LiNbO3 and related materials.

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