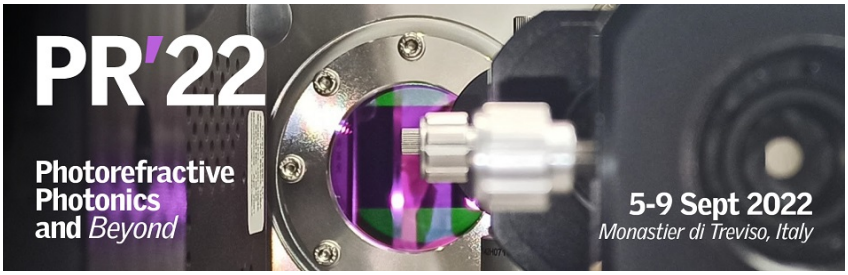

Contribution ID: **58** Type: **Poster**

Composition dependent optical properties of LiNb_xTa_(1-x)O3 solid solutions

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

Lithium niobate (LN) and lithium tantalate (LT) are ferroelectric crystals with a wide range of applications, extending from piezoelectric sensors to integrated photonics. Their structural similarities enable the combination of these materials to $LiNb_xTa_{1-x}O_3$ (LNT) alloys. As the optical absorption edge depends on the stoichiometry, it can be used to determine the crystal composition non destructively.
\\
Here, we use special quasi-random structures to simulate LNT crystals with different compositions. These structures mimic an ideal random alloy, even when periodic boundary conditions are employed. Furthermore, we use the Li-vacancy model as well as the Nb-antisite model [1] to simulate congruent LN crystals, as they are commonly used in experiments.
\\
We calculate the first order dielectric tensor of these materials by combining density-functional theory with the indepent particle approximation. A clear correlation between the absorption edge and the Li-concentration of LN can be seen, as it has been described in [2]. Modifications of the electronic band structure, can be attributed to the absence of Li-2s states near the fundamental band gap.
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[1]: Yanlu Li, W. G. Schmidt, and S. Sanna, Defect complexes in congruent
LiNbO3 and their optical signature. Phys. Rev. B 91, 174106 (2015).\\
\url{ https://link.aps.org/doi/10.1103/PhysRevB.91.174106}

[2]: Földvári, I., Polgár, K. & Mecseki, A. Nonstoichiometry as a source of "intrinsic impurities"in LiNbO3 crystals. Acta Physica Hungarica 55, 321–327 (1984). \url{https://doi.org/10.1007/BF03155945}

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Session Classification: Poster session - in presence

Track Classification: Nonlinear light-matter interaction and applications