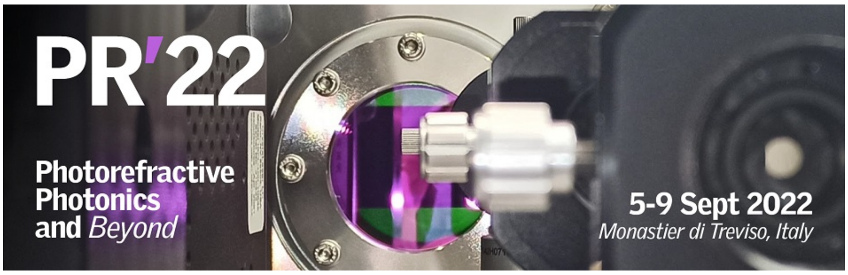

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Small polaron hopping in Fe:LiNbO3 from microscopic modelling to macroscopic observables

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Lithium niobate is nowadays one of the most used ferroelectrics oxides in the realization of optical modulators, waveguides and optical sensor due to its large acousto-optical, electro-optical and nonlinear optical coefficients. Further tailoring of these applications requires a deeper scientific insight to the relation between the microscopic structure and the macroscopic observables.
In this framework, it is already accepted that the photophysical charge transport properties can be understood to a large extend in terms of small polaron hopping. Carriers are photo-generated from deep donor centers in the first step and subsequently emitted with a preferential direction in the conduction band. Here, they lose energy by interaction with the lattice and condensate into a new state, self-localizing in the structure via distortion of the local ionic environment, i.e. a polaron is formed. According on which site the charge is localized at, different types of polarons can be distinguished. Each of them can later move by thermal assisted hopping among different sites, until a deep trap is encountered.
Despite this advanced level of understanding, there is still a lack of knowledge on the relation between the macroscopic observables such as polaron mobility and lifetime with the basic polaron hopping processes. In this contribution we try to fill this gap by combining experimental results with numerical analysis based on Monte Carlo methods.

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