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Insight to small polaron kinetics in lithium tantalate

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The formation, transport and relaxation kinetics of small polarons with strong coupling have been studied intensively in lithium niobate (LN) over the last decades. The gained knowledge helped to understand the (non-)linear optical and photoelectric properties of LN on a microscopic level. The question of the transferability of these findings to other, comparable ferroelectric crystal systems has been addressed only to a limited extent.

In this contribution, we apply the small polaron approach to lithium tantalate (LT) with the goal to highlight similarities with the model system LN, but also to uncover properties being related with the individual material properties of LT, such as the inverted sign of birefringence. For this purpose, optical and nonlinear optical experimental findings - in particular obtained by means of steady-state and dynamic spectroscopy - are determined and analyzed for LT and compared with LN. The data are used to perform numerical studies for the polaronic hopping transport, that yield characteristic relaxation times of the small polaron survival probability as well as insight into the defect-modulated migration properties. A first driving result is the variation of the polaron binding energies in comparison to LN that has a strong effect on the emergent polaron behavior in LT. In particular migration and relaxation characteristics are substantially altered between the two materials and show a dominating contribution of small polarons bound to intrinsic defects even at elevated temperatures for LT. The consequences of these findings for high-temperature applications as well as the interplay with ionic transport features for temperatures $T > 500$ K are discussed.

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