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# (G*) Atomic insights into the lattice dynamics driving the relaxation of charged defects

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Electron-driven lattice rearrangements commonly exist in phenomena such as electron/hole transfer, defect ionization, photoexcitation, and polaron formation. These phenomena are manifested in a variety of important technologies employing energy harvesting and conversion materials. Hence, lattice equilibration processes at the atomic scale need to be more deeply understood in order to tailor the physical properties of such materials. In this work [1], we adopt the $F^+$-center in NaCl as a model system and study its femtosecond-resolved lattice dynamics driven by charge localization changes. Our results reveal that the excess energy is imparted amongst the highest optical phonon modes with no clear localization preference. The overall phonon decay trends are found to be largely exponential in the temporal domain and the corresponding phonon lifetimes are shown to be temperature dependent. The lifetimes of the local kinetic energy (decaying near the defect in real space) have a different timescale and display less variation at non-cryogenic temperatures. Moreover, a phenomenological first-order analytical model based on Langevin dynamics is provided to interpret the exponential decay trend of the phonon modes in the temporal domain and a first-order quantum rate mode is applied to interpret the temperature dependency of the phonon lifetime. In addition, this work also provides technical contributions in terms of showing the limitations caused by supercell size effects and the challenge posed by the extensive statistical sampling needed to reach convergent trends in lattice dissipation calculations. The calculation procedure and analysis methods in this work are transferable to study such formation dynamics in defects from first-principles. In general, the findings demonstrate how the charged-center dynamics may play a crucial role in the performance of many energy materials.

[1] Yuan, S., Kantorovich, L., Shluger, A. L. & Bevan, K. H. Atomistic insight into the formation dynamics of charged point defects: A classical molecular dynamics study of $F^+$-centers in NaCl. Phys. Rev. Mater. 6, 15404 (2022).

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