The origin of out-of-equilibrium ferroelectricity in $SrTiO_3$ under resonant ultrafast THz pumping

Lorenzo Monacelli, *Department of Physics, Sapienza University of Rome, Italy*

Advancements in laser technology have unlocked the potential to observe the real-time dynamics of nuclei on the femtosecond scale. Strontium titanate ($SrTiO_3$) presents a unique case as a quantum paraelectric material characterized by its near-ferroelectric transition at low temperatures, which is inhibited by quantum nuclear fluctuations. In this study, we simulate from first principles the time-resolved quantum nuclear dynamics of $SrTiO_3$ under pulsed THz radiation targeting the mode responsible for ferroelectricity. Our novel approach, entirely based on first principles simulations[1], accurately replicates the spectral features identified in time-resolved X-ray signals (like energy upconversion[2]) without any fitted parameter but also reveals the complex energy redistribution processes among all modes following phonon-phonon scattering. We also show how it is possible to stabilize a dynamical ferroelectric phase[3,4] thanks to the transient strain induced by the nonlinear dynamics of nuclei.

[1] L Monacelli and F Mauri, Phys. Rev. B 103, 104305 (2021)
[2] M Kozina et al, Nat Phys, 15, 387 (2019)
[3] T F Nova et al, Science, 364, 1075 (2019)
[4] X Li et al, Science, 364, 1079 (2019)