Supplementary Information for "Light-driven dynamical tuning of the thermal conductivity in ferroelectrics"

Claudio Cazorla and Carlos Escorihuela-Sayalero

Departament de Física, Universitat Politècnica de Catalunya, Campus Nord B4-B5, Barcelona 08034, Spain

Sebastian Bichelmaier and Jesús Carrete

Institute of Materials Chemistry, TU Wien, A-1060 Vienna, Austria

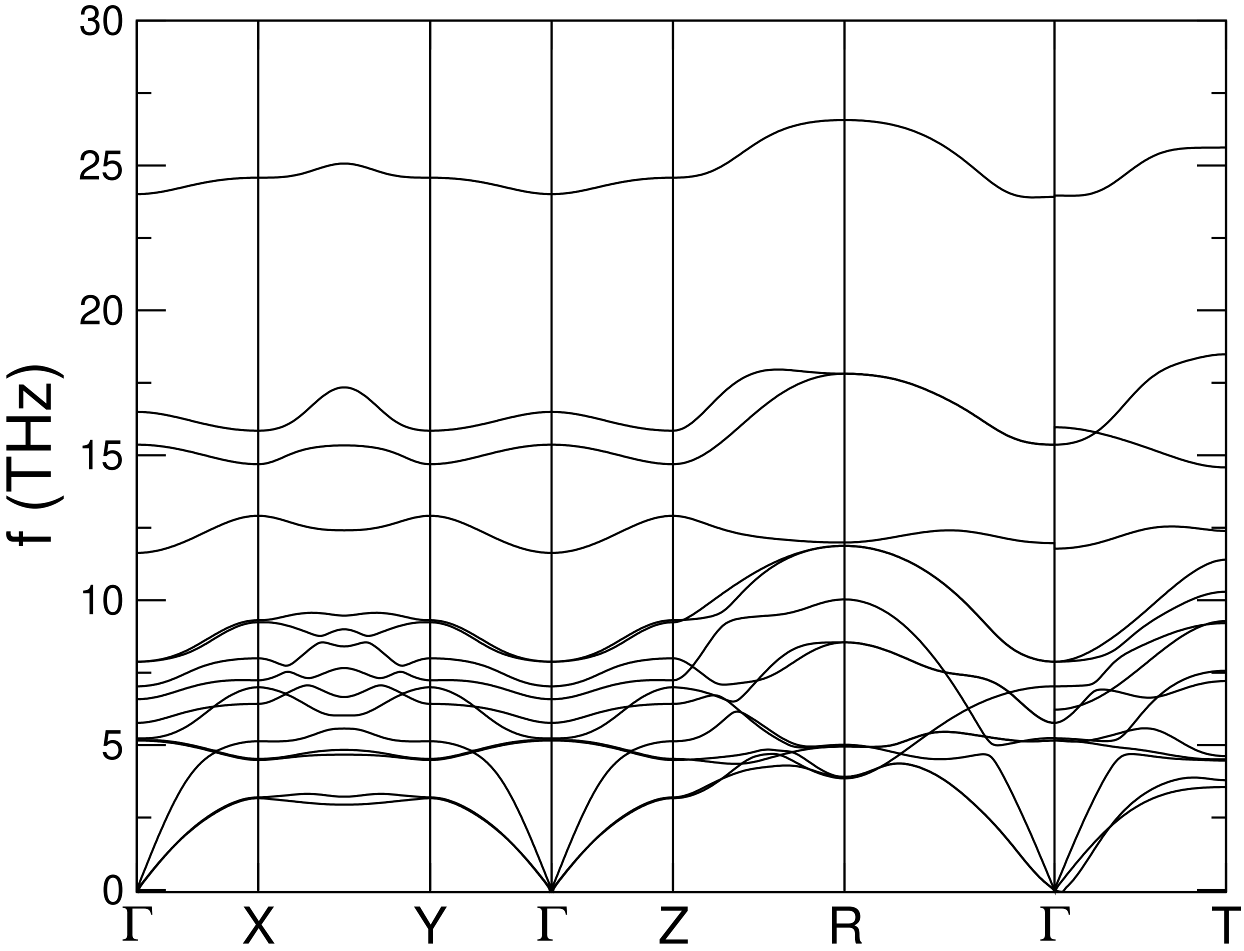
Jorge Íñiguez

Materials Research and Technology Department, Luxembourg Institute of Science and Technology (LIST), Avenue des Hauts-Fourneaux 5, L-4362 Esch/Alzette, Luxembourg and Department of Physics and Materials Science, University of Luxembourg, 41 Rue du Brill, L-4422 Belvaux, Luxembourg

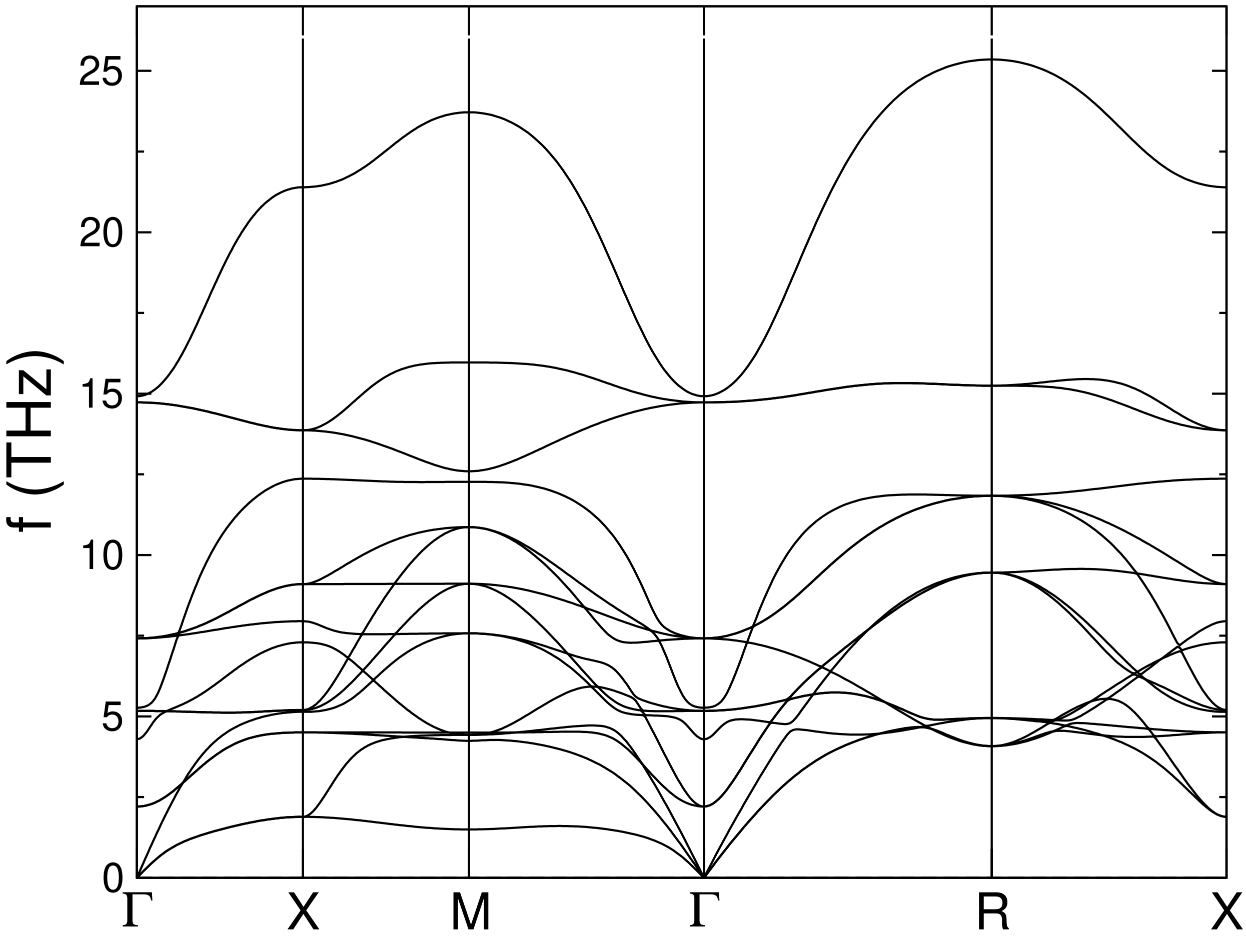
Riccardo Rurali

Institut de Ciència de Materials de Barcelona, ICMAB–CSIC, Campus UAB, 08193 Bellaterra, Spain[*]

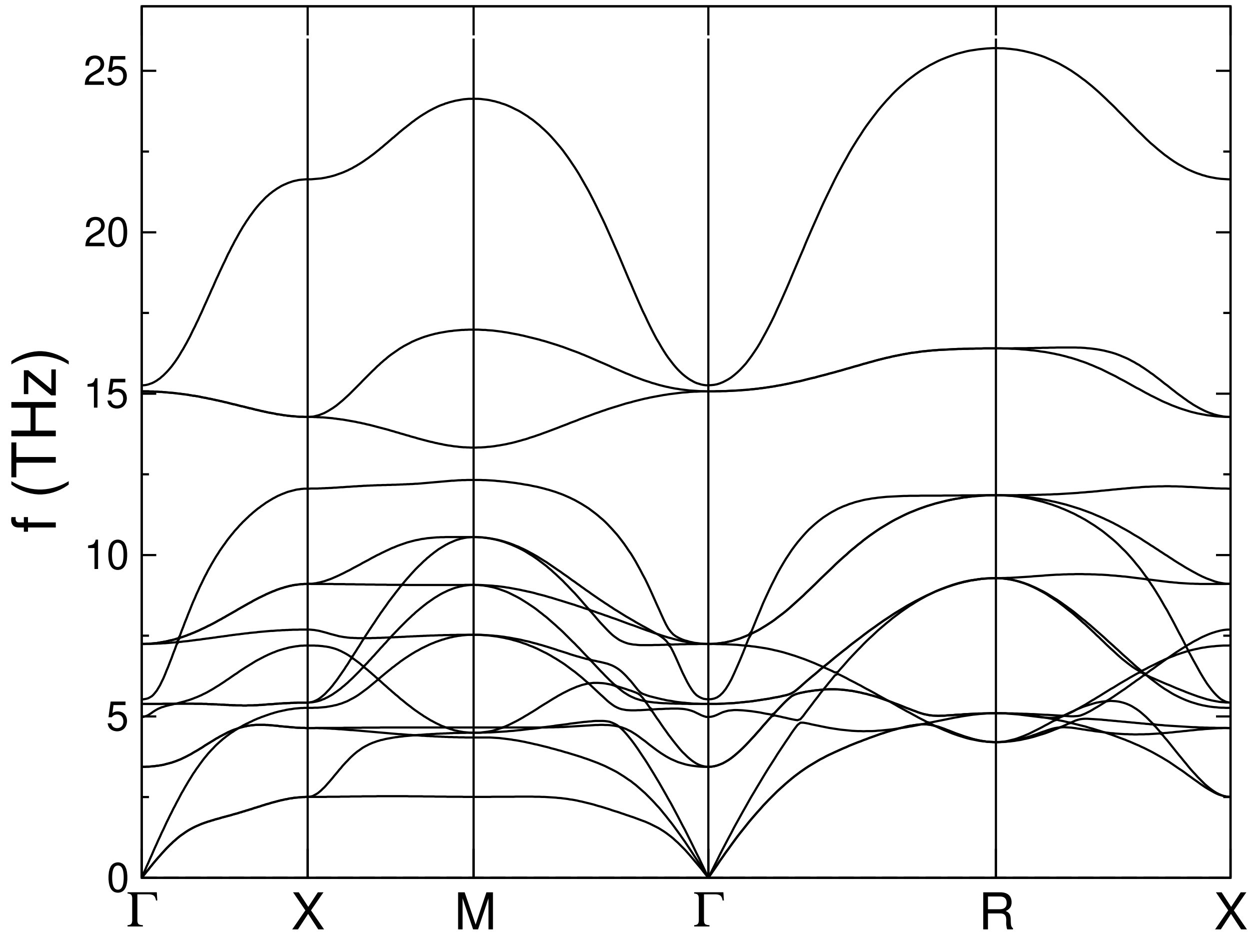
[*]Electronic address: rrurali@icmab.es



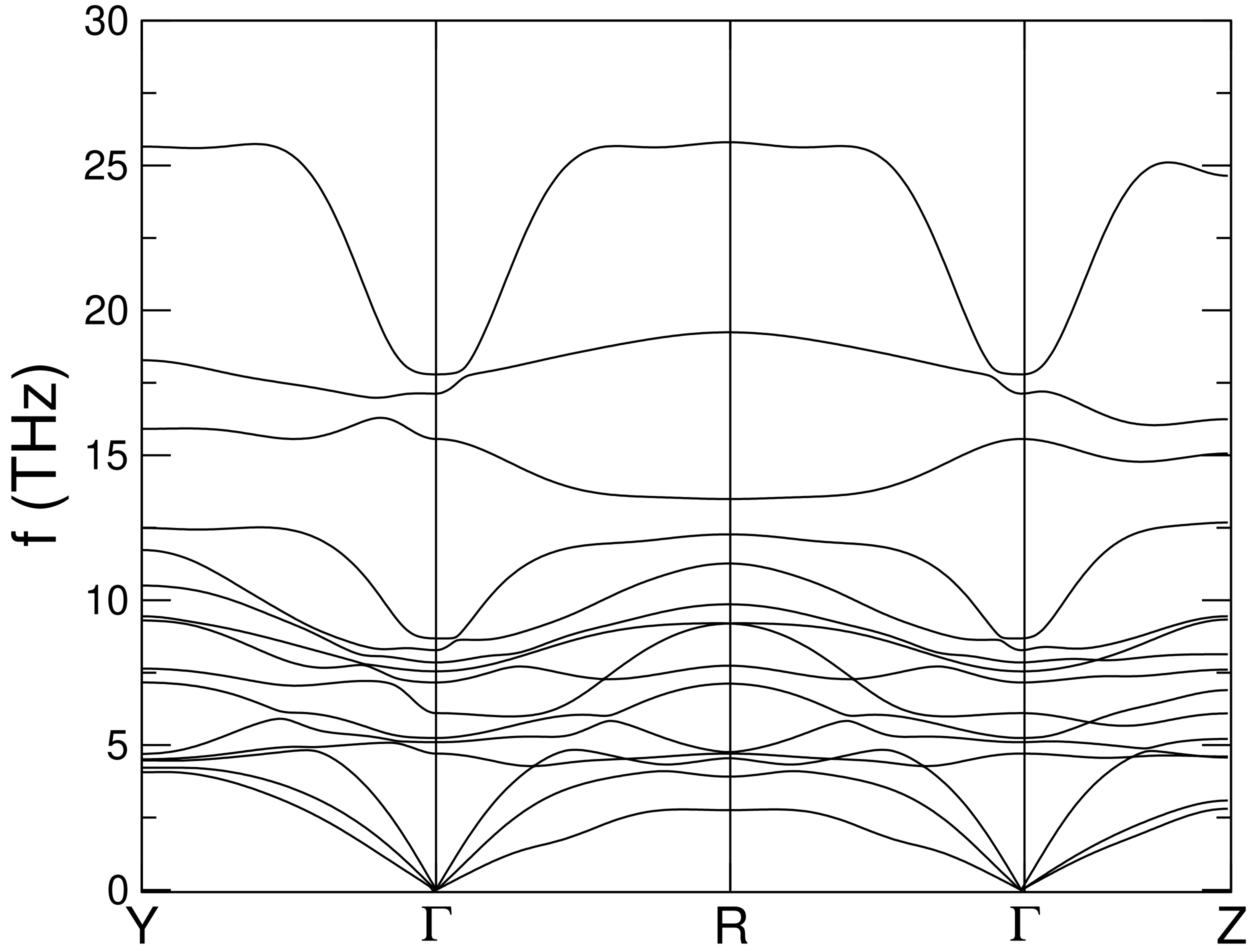
Supplementary Figure 1: Phonon dispersion of KNO in the $R3m$ phase ($\Gamma = 0.0, 0.0, 0.0$; $X = 0.5, 0.0, 0.0$; $Y = 0.0, 0.5, 0.0$; $Z = 0.0, 0.0, 0.5$; $R = 0.5, 0.5, 0.5$; $T = 0.0, 0.5, 0.5$).



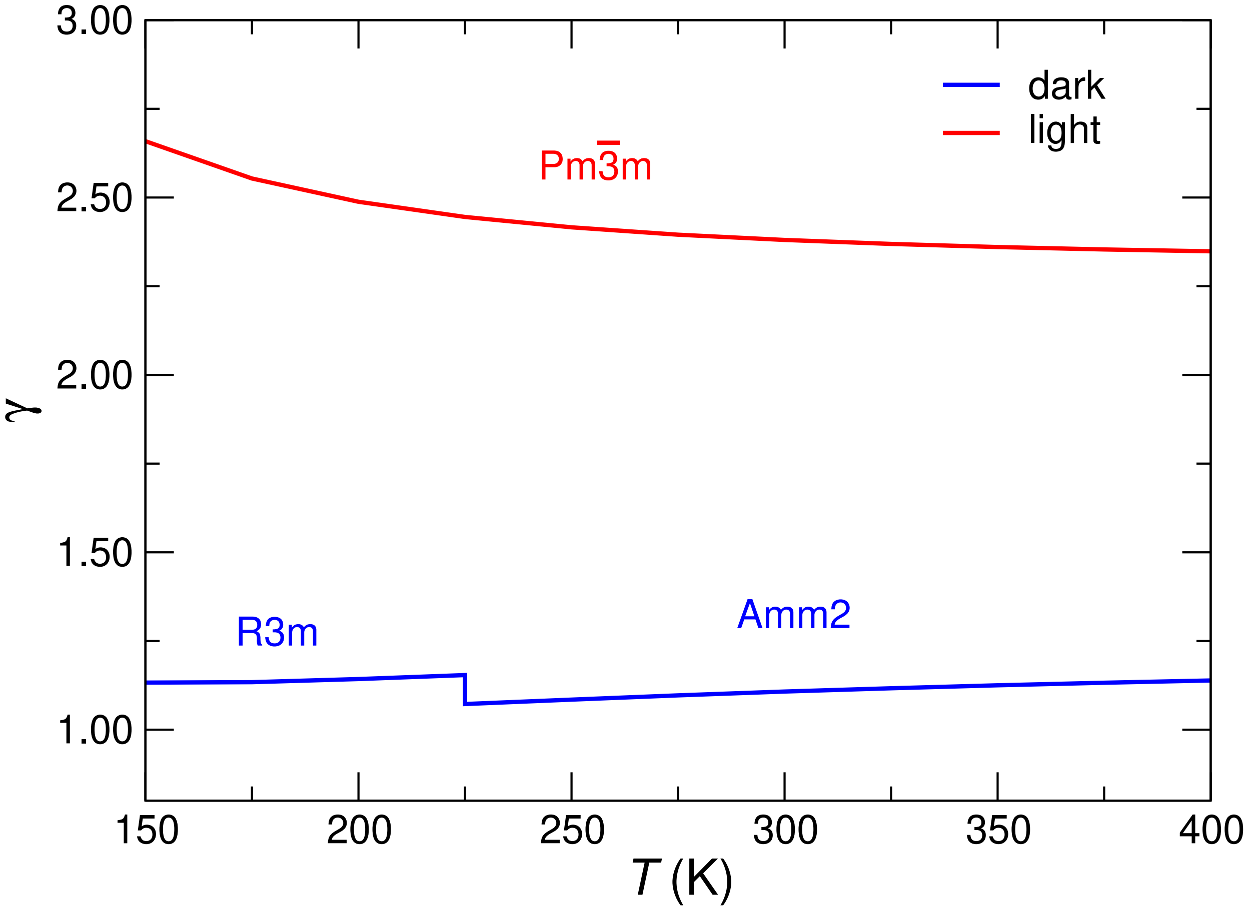
Supplementary Figure 2: Phonon dispersion of KNO in the $Pm\bar{3}m$ phase stabilized by photoexcitation; carrier denisty in the conduction band is $n = 2.69 \cdot 10^{21}\text{cm}^{-3}$. ($\Gamma = 0.0, 0.0, 0.0$; $X = 0.0, 0.5, 0.0$; $M = 0.5, 0.5, 0.0$; $R = 0.5, 0.5, 0.5$).



Supplementary Figure 3: Phonon dispersion at $T = 300$ K of KNO in the $Pm\bar{3}m$ phase stabilized by photoexcitation; carrier denisty in the conduction band is $n = 2.69 \cdot 10^{21}\text{cm}^{-3}$. Phonons were renormalized with a normal-mode-decomposition technique [1]. ($\Gamma = 0.0, 0.0, 0.0$; $X = 0.0, 0.5, 0.0$; $M = 0.5, 0.5, 0.0$; $R = 0.5, 0.5, 0.5$).



Supplementary Figure 4: Phonon dispersion at $T = 300$ K of KNO in the $Amm2$ phase. Phonons were renormalized with a normal-mode-decomposition technique [1]. Similar results were also obtained from the QSCAILD [2, 3] method. ($Y = -0.5, 0.5, 0.0$; $\Gamma = 0.0, 0.0, 0.0$; $R = 0.0, 0.5, 0.5$; $Z = 0.0, 0.0, 0.5$).



Supplementary Figure 5: Grüneisen parameter, γ, computed beyond the quasiharmonic approximation, by a linear combination of the third-order force constants.

	Phonon population	Irradiation conditions	Figure in main text
$R3m$	f_{BE}	dark	3
$Amm2$	renorm$^{300\ \mathrm{K}}$	dark	3
$Pm\bar{3}m$	f_{BE}	light	3, 7a
$Pm\bar{3}m$	renorm$^{300\ \mathrm{K}}$	dark	3, 7b
$Pm\bar{3}m$	renorm$^{800\ \mathrm{K}}$	dark	7c

Supplementary Table 1. Summary of how $\boldsymbol{\kappa}$, as displayed in Figure 3 and 7, has been computed in the different cases. The first column indicates how phonon population at a given temperature was accounted for: f_{BE} indicates that phonons were computed in the standard way by finite displacements at zero Kelvin and that phonon states were then populated following Bose-Einstein statistics; renorm$^{300\ K}$ indicates that an explicit finite temperature calculations of phonons at 300 K was also carried out (see Methods); similarly for renorm$^{800\ K}$. The second column indicates the irradiation state, dark vs. light, of each phase. We recall here that photoexcitation was achieved by tuning the smearing of the electron distribution function (see Methods). The third column inidicates in which Figure(s) os the main text the corresponding $\boldsymbol{\kappa}(T)$ is shown.

[1] A. Carreras, A. Togo, and I. Tanaka, Comput. Phys. Commun. **221**, 221 (2017).

[2] A. van Roekeghem, J. Carrete, and N. Mingo, Comput. Phys. Commun. **263**, 107945 (2021).

[3] S. Bichelmaier, J. Carrete, M. Nelhiebel, and G. K. H. Madsen, Phys. Status Solidi Rapid Res. Lett. **16**, 2100642 (2022).