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Temperature Waves In Layered Correlated Materials And Temperonic Crystals

Marco Gandolfi

Giacomo Mazza,
Massimo Capone,
Francesco Banfi,
Claudio Giannetti

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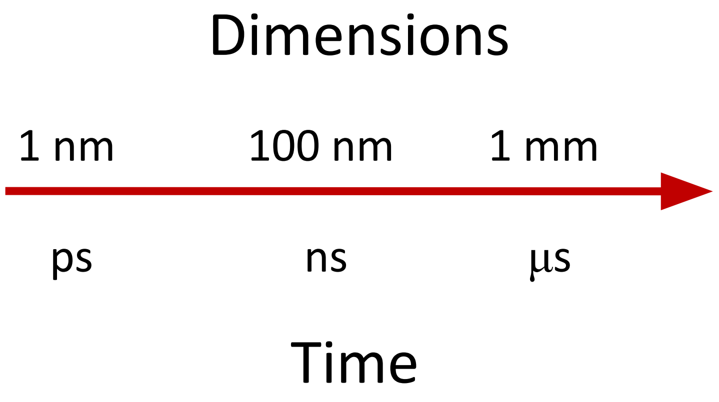
Beyond Fourier Paris 2022

9th September 2022

Introduction

Nano-scale heat transport



Beyond Fourier’s Law … a dispersion relation perspective

Temperature waves: graphite and correlated materials

Temperonic Crystal

Beyond Fourier's Law

$$\boldsymbol{q}(\boldsymbol{x},t) = -k_T \nabla T(\boldsymbol{x},t)$$

→ no causality

Dual-Phase-Lag-Model

$$\boldsymbol{q}(\boldsymbol{x},t+\tau_q) = -k_T \nabla T(\boldsymbol{x},t+\tau_T)$$

↓ + conservation of energy

$$\left(\frac{\tau_q}{\alpha}\right)\frac{\partial^2 T}{\partial t^2} - \frac{\partial^2 T}{\partial x^2} + \frac{1}{\alpha}\frac{\partial T}{\partial t} - \tau_T \frac{\partial^3 T}{\partial x^2 \partial t} = 0$$

$$\boldsymbol{q}(\boldsymbol{x},t) = -k_T \nabla T(\boldsymbol{x},t) \quad \Rightarrow \quad \text{no causality}$$

Dual-Phase-Lag-Model

$$\boldsymbol{q}(\boldsymbol{x},t+\tau_q) = -k_T \nabla T(\boldsymbol{x},t+\tau_T)$$

+ conservation of energy

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Waves | Diffusion damping | Damping

$$\left(\frac{\tau_q}{\alpha}\right)\frac{\partial^2 T}{\partial t^2} - \frac{\partial^2 T}{\partial x^2} + \frac{1}{\alpha}\frac{\partial T}{\partial t} - \tau_T \frac{\partial^3 T}{\partial x^2 \partial t} = 0$$

∇T Cause → $\boldsymbol{q}$ effect

$$\boldsymbol{q}(\boldsymbol{x},t) = -k_T \nabla T(\boldsymbol{x},t)$$ → no causality

Dual-Phase-Lag-Model

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$$\left(\frac{\tau_q}{\alpha}\right)\frac{\partial^2 T}{\partial t^2} - \frac{\partial^2 T}{\partial x^2} + \frac{1}{\alpha}\frac{\partial T}{\partial t} - \tau_T \frac{\partial^3 T}{\partial x^2 \partial t} = 0$$ → ∇T Cause → $\boldsymbol{q}$ effect → Temperature «wave»

International Journal of Heat and Mass Transfer
Volume 143, November 2019, 118553

Accessing temperature waves: A dispersion relation perspective

Marco Gandolfi [a, b], Giulio Benetti [c, b], Christ Glorieux [a], Claudio Giannetti [b], Francesco Banfi [d]

$$\boldsymbol{q}(\boldsymbol{x},t) = -k_T \nabla T(\boldsymbol{x},t)$$ → no causality

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Frequency ω

Wave vector k

Dispersion relation:

$$(1 + i\omega\tau_T)k^2 = \left(\frac{\tau_q}{\alpha}\right)\left(1 - \frac{i}{\omega\tau_q}\right)\omega^2$$

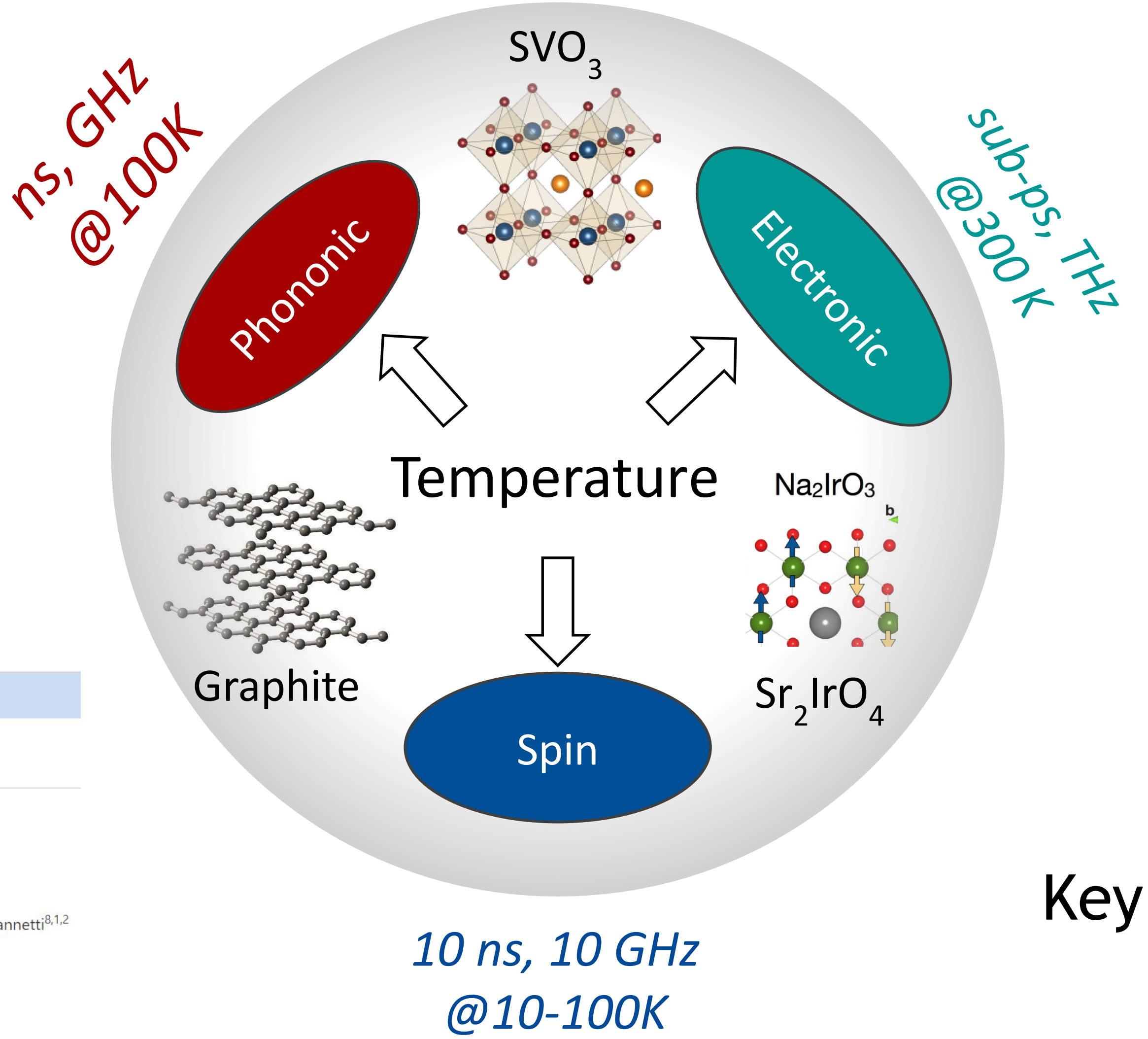
Q-factor

$$\left(\frac{\tau_q}{\alpha}\right)\frac{\partial^2 T}{\partial t^2} - \frac{\partial^2 T}{\partial x^2} + \frac{1}{\alpha}\frac{\partial T}{\partial t} - \tau_T \frac{\partial^3 T}{\partial x^2 \partial t} = 0$$

→ ∇T Cause → $\boldsymbol{q}$ effect → Temperature «wave»

Dispersion relation perspective

Generality



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Emergent ultrafast phenomena in correlated oxides and heterostructures

M Gandolfi[1,2,3], G L Celardo[1,2,4], F Borgonovi[1,2,4], G Ferrini[1,2], A Avella[5,6,7], F Banfi[1,2] and C Giannetti[8,1,2]

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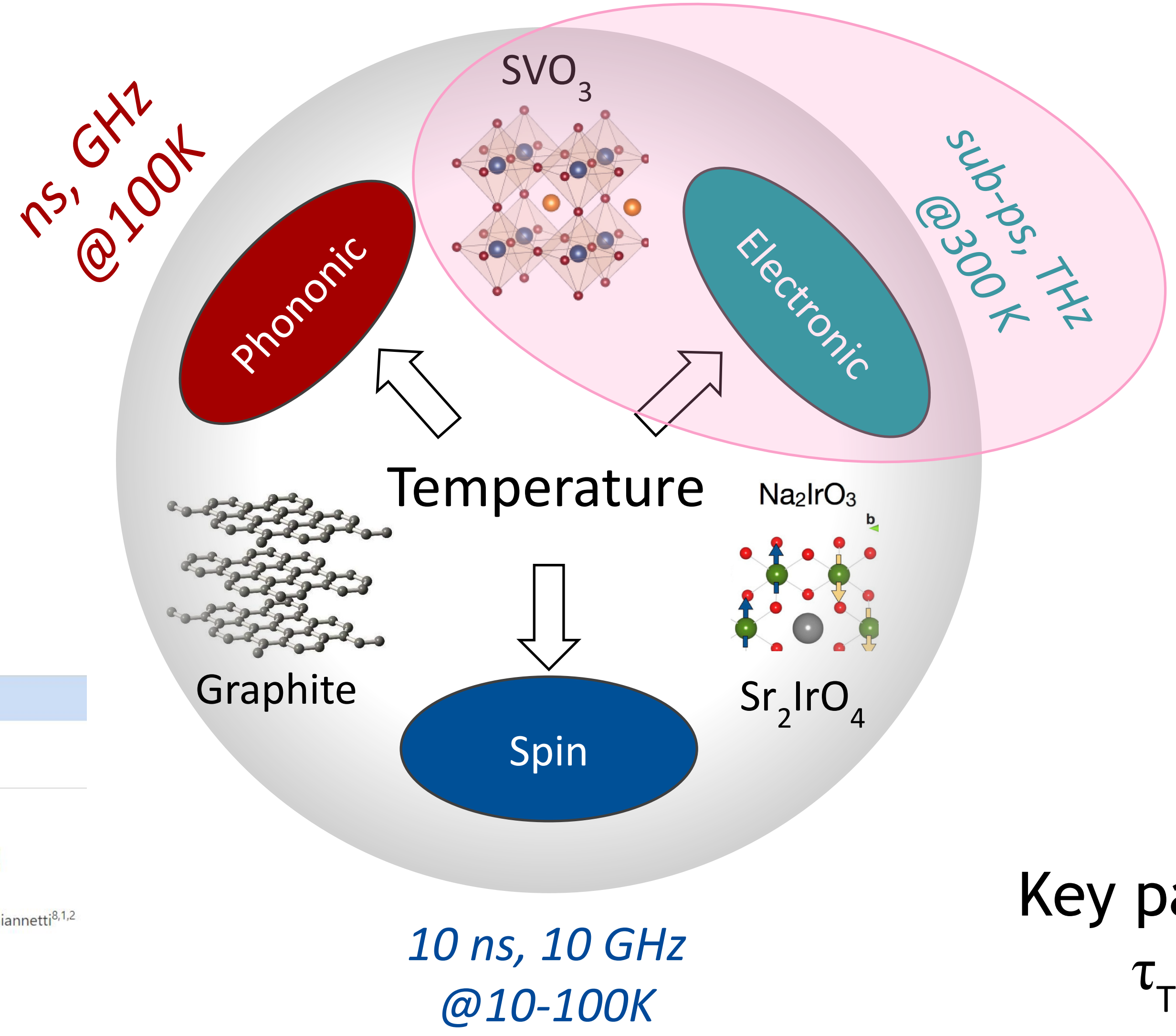
Physica Scripta, Volume 92, Number 3

Focus issue on Ultrafast Bandgap Photonics

Citation M Gandolfi *et al* 2017 *Phys. Scr.* **92** 034004

Key parameters:
τ_T and τ_Q

Generality



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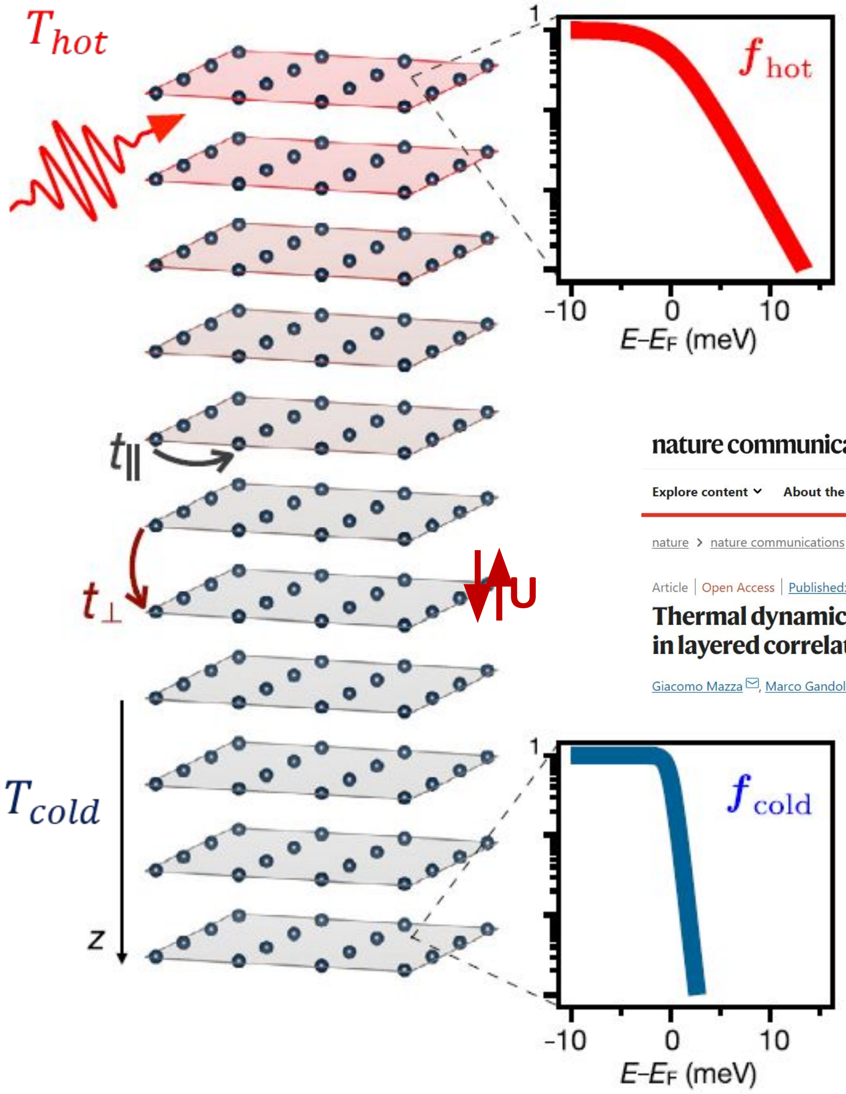


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Hubbard Model

$$H = \sum_{n=1}^{L} h_n + \sum_{n=1}^{L-1} \tau_{n,n+1}$$

$$h_n = \sum_{<i,j>\sigma} t_{\|} c^{\dagger}_{in\sigma} c_{jn\sigma} + U \sum_{i} n_{in\uparrow} n_{in\downarrow}$$

$$\tau_{n,n+1} = \sum_{\sigma} t_{\perp} c^{\dagger}_{in\sigma} c_{in+1\sigma} + h.c.$$

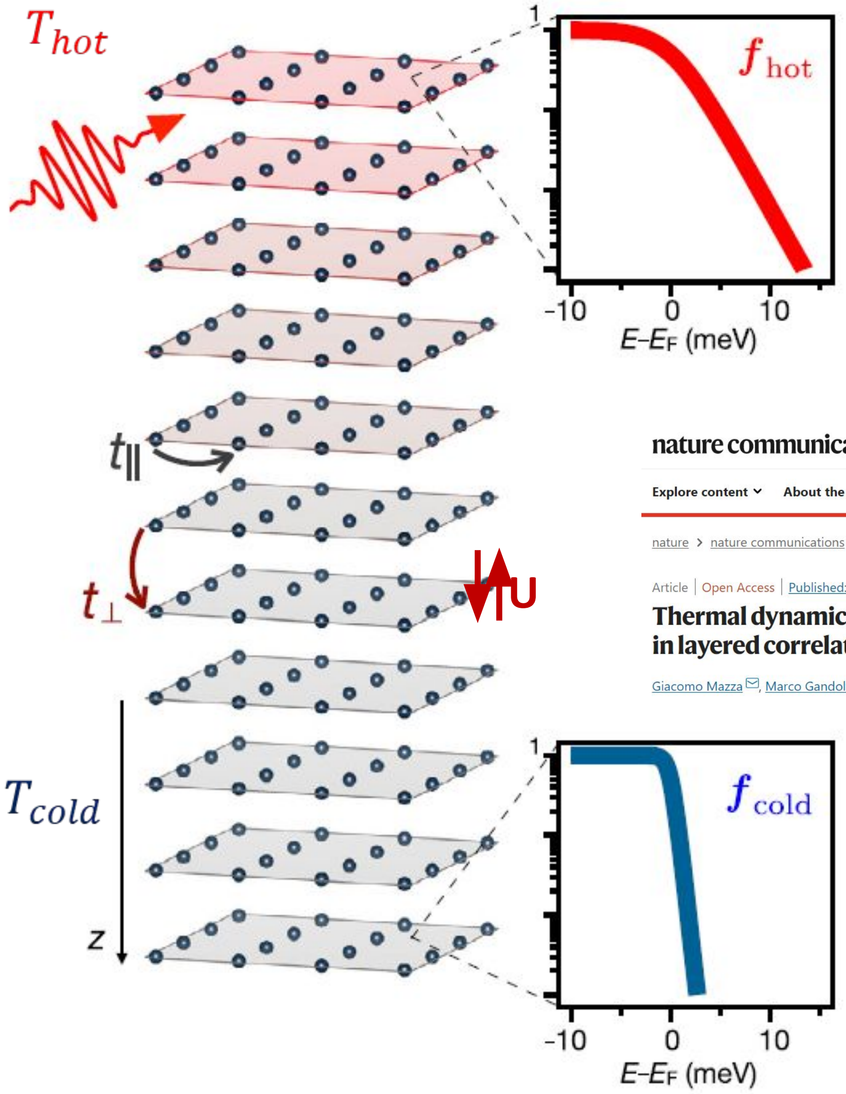
$t_{\|}$ interlayer hopping

$t_{\perp}$ intra-layer hopping

U Coulomb interaction

G. Mazza et al., *Nat. Comm.* (2021)

Layered Correlated Materials



$$N_n^{neq}(\varepsilon,t) = f_{hot}\rho_{hot} + f_{cold}(1-\rho_{hot})$$

$$f_{hot} = \frac{1}{\exp\left(\frac{\varepsilon}{k_B T_{hot}}\right)+1} \qquad f_{cold} = \frac{1}{\exp\left(\frac{\varepsilon}{k_B T_{cold}(n,t)}\right)+1}$$

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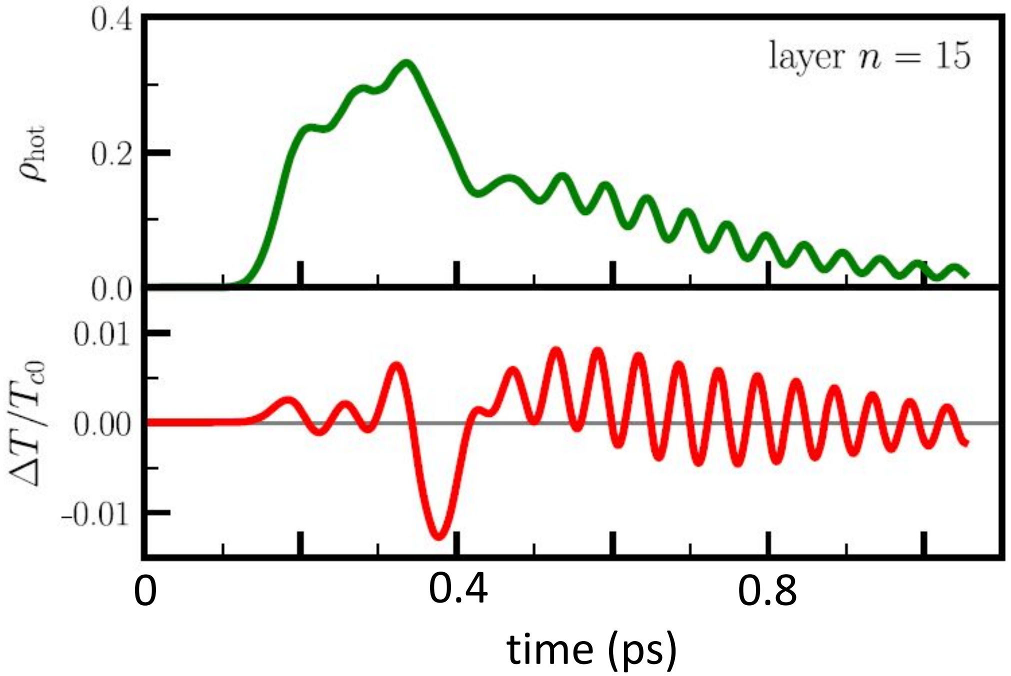
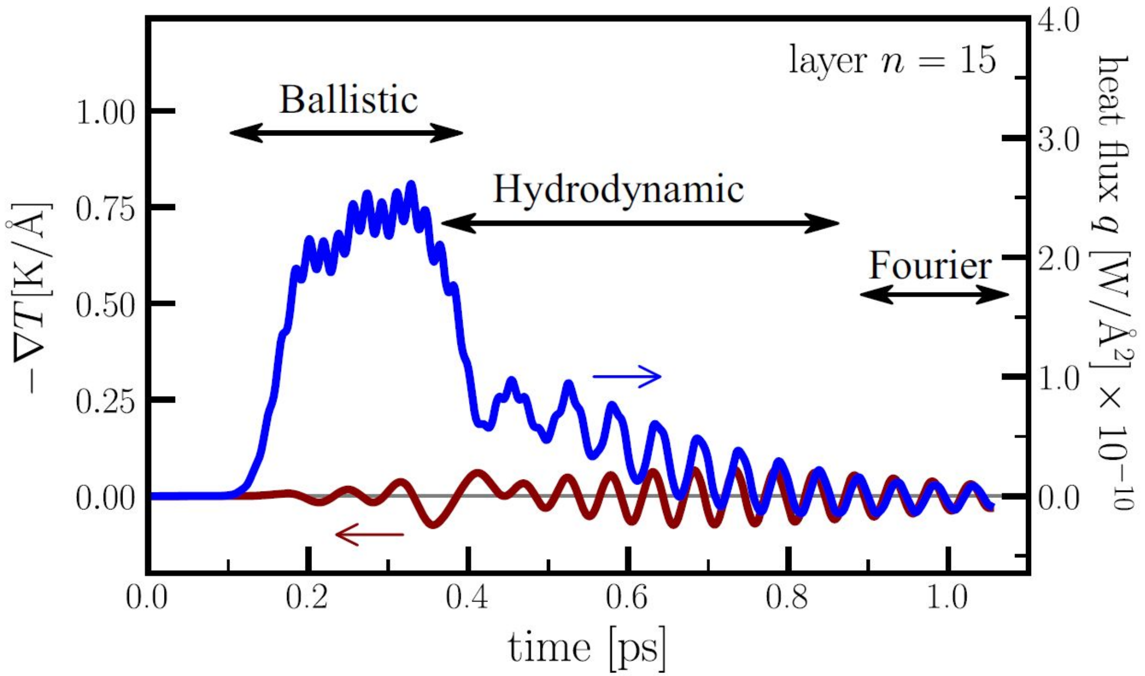


Energy density $E_n(t)$ → Heat flux $\frac{\partial q_n}{\partial z} + \frac{\partial E_n}{\partial t} = 0$

Heat diffusion regimes



- Ballistic: large heat flux, no temperature dynamics
- Hydrodynamic: positive heat flux, temperature oscillations
- Fourier: $q \propto -\nabla T$

For $SrVO_3$

$\tau_T \sim 5$ fs (scattering time from optics)

$\tau_q \sim 500$ fs (from neq. dynamics)

$k = 10 - 20 \text{ W m}^{-1} \text{ K}^{-1}$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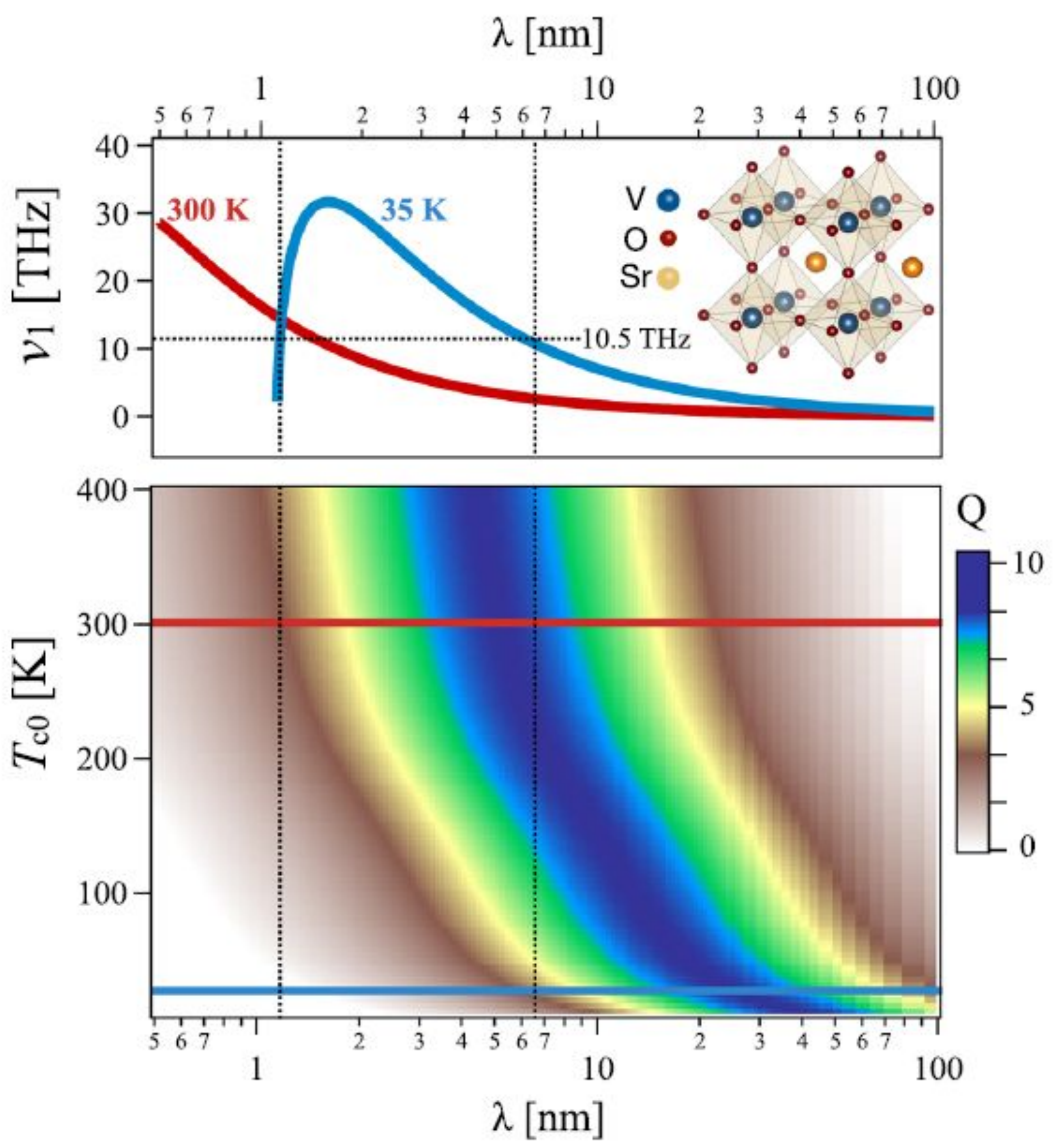


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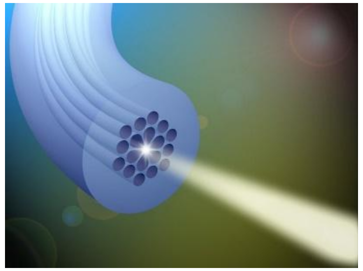
Marco Gandolfi, Claudio Giannetti, and Francesco Banfi

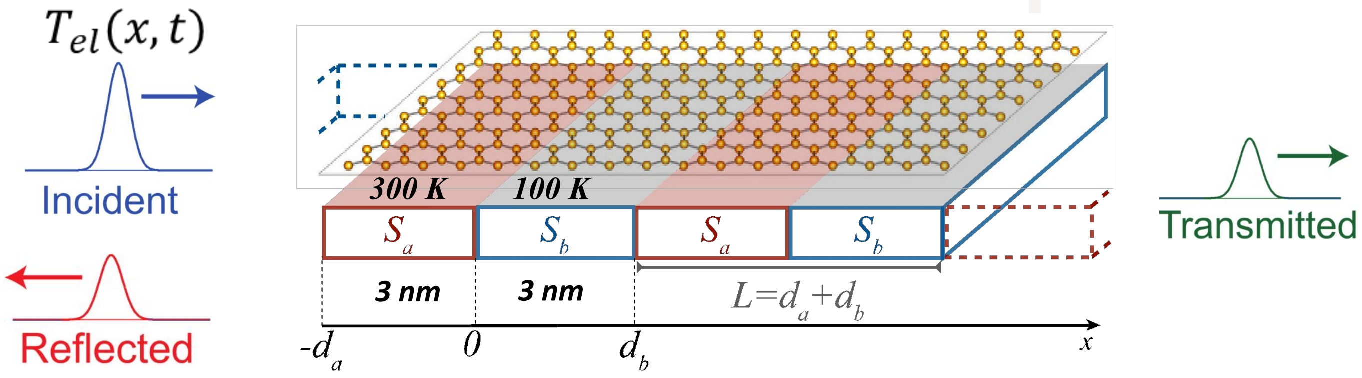
Phys. Rev. Lett. **125**, 265901 – Published 31 December 2020

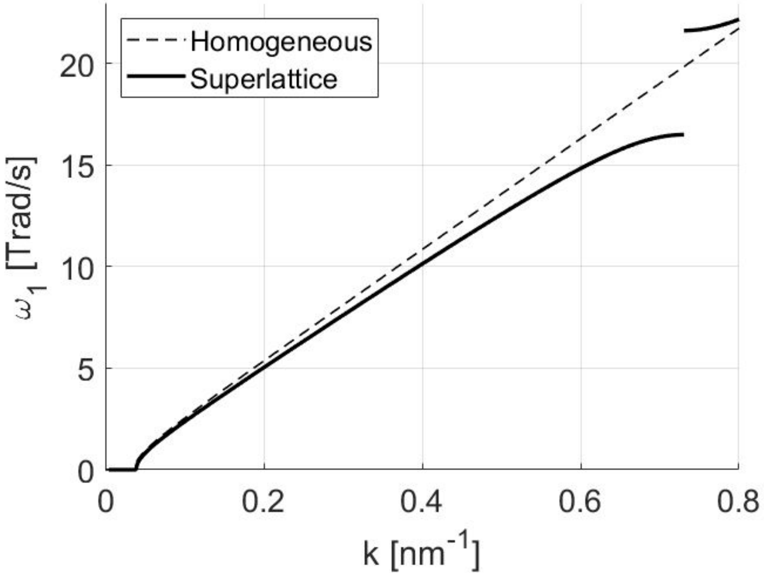
A Superlattice for Temperature Waves in Correlated Materials

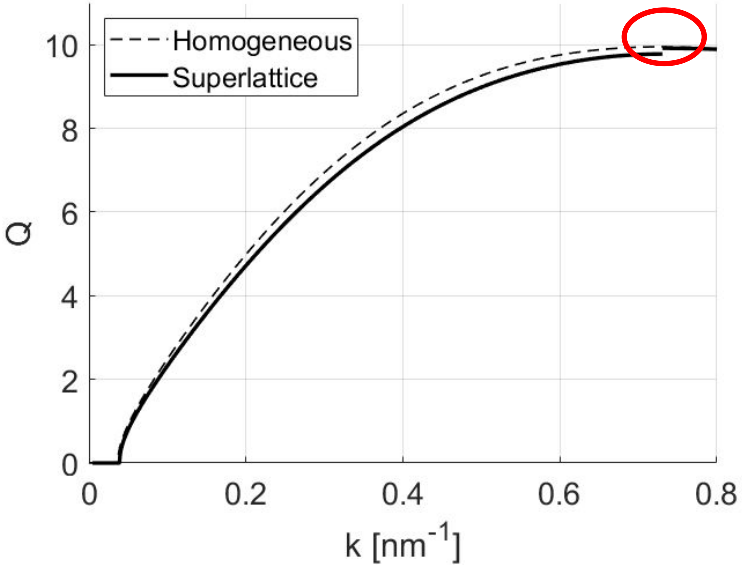
Phononic Crystal

Photonic Crystal







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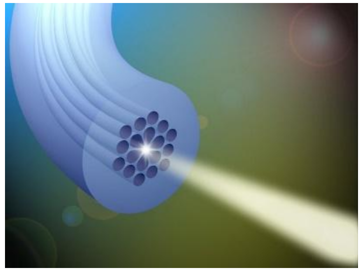
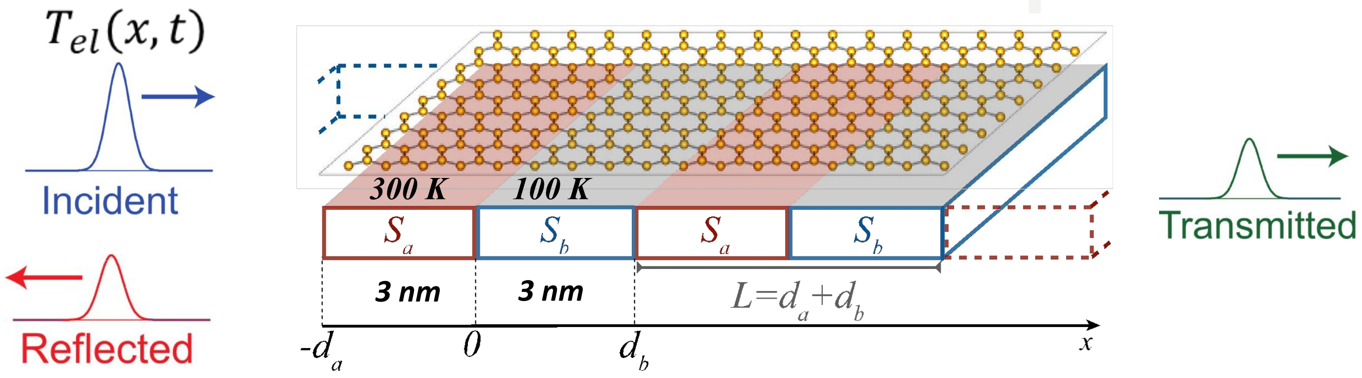
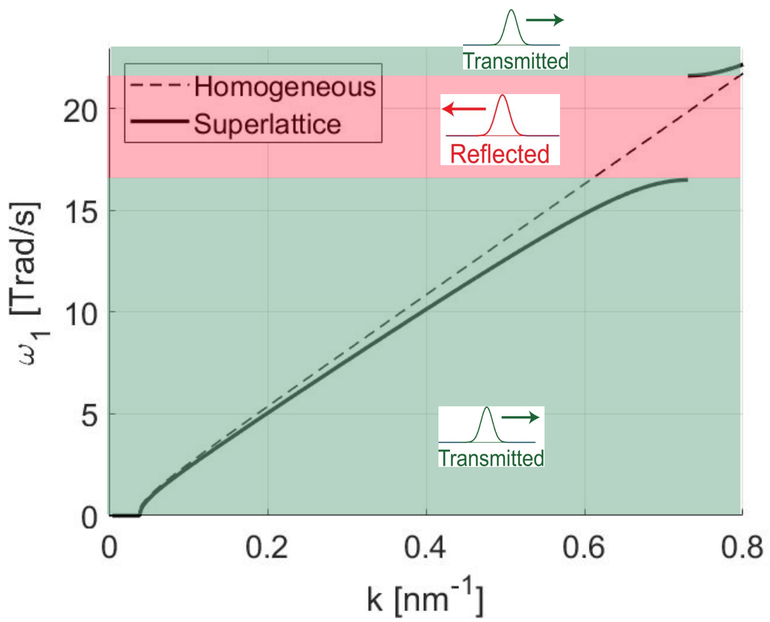
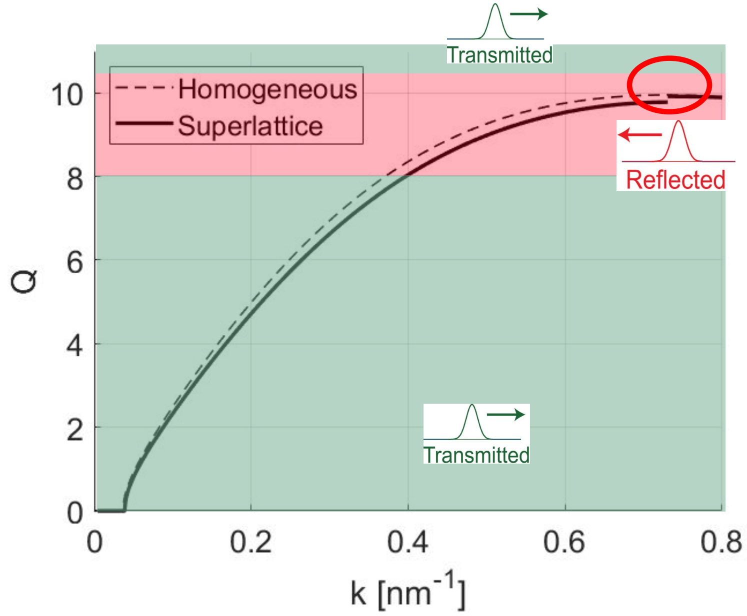
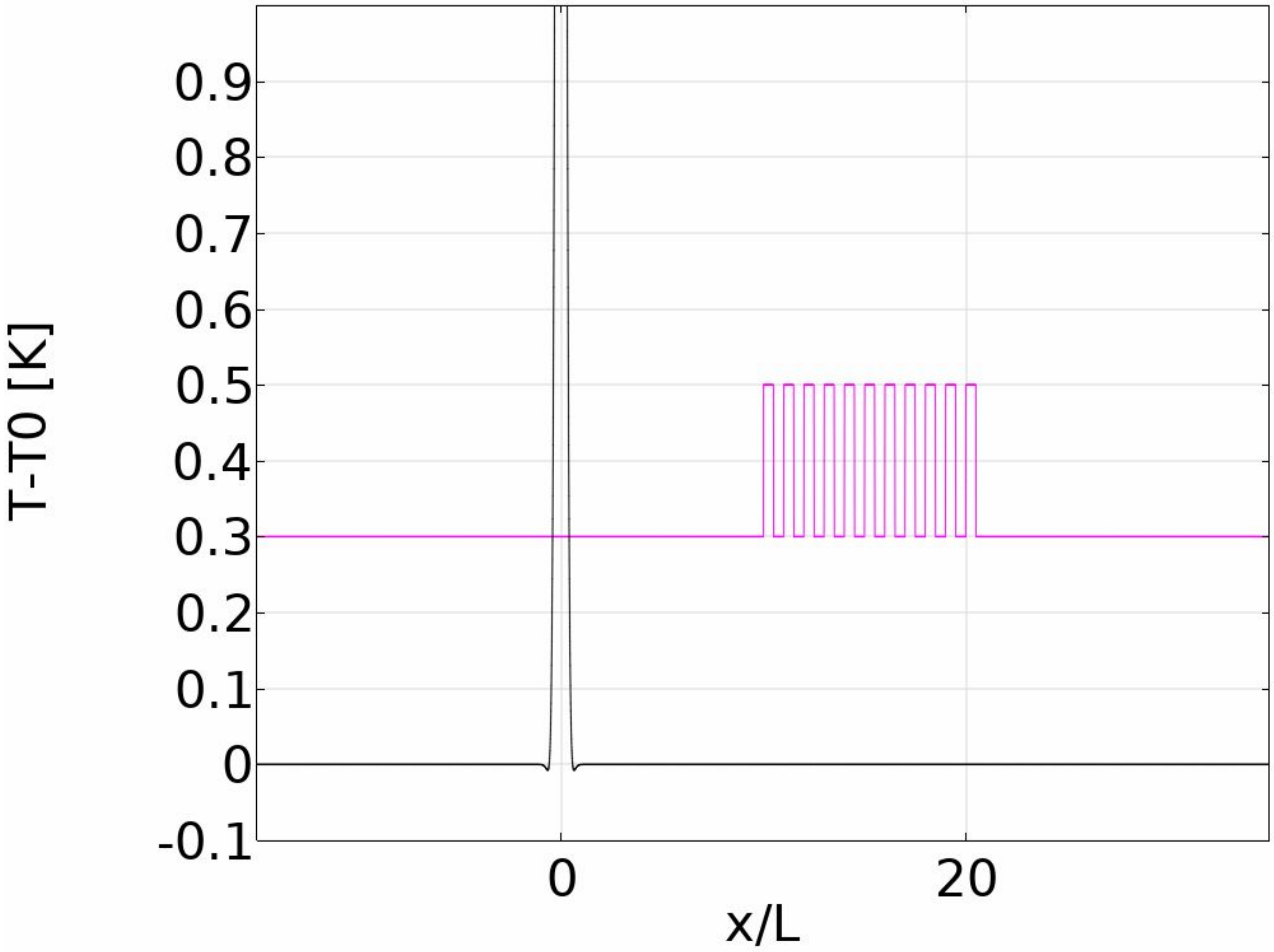








Spatio-temporal evolution of temperature



Temperonic crystal:

extendible to graphene…

Conclusions

Beyond Fourier's Law … a dispersion relation perspective

Temperonic Materials

Temperonic Crystal

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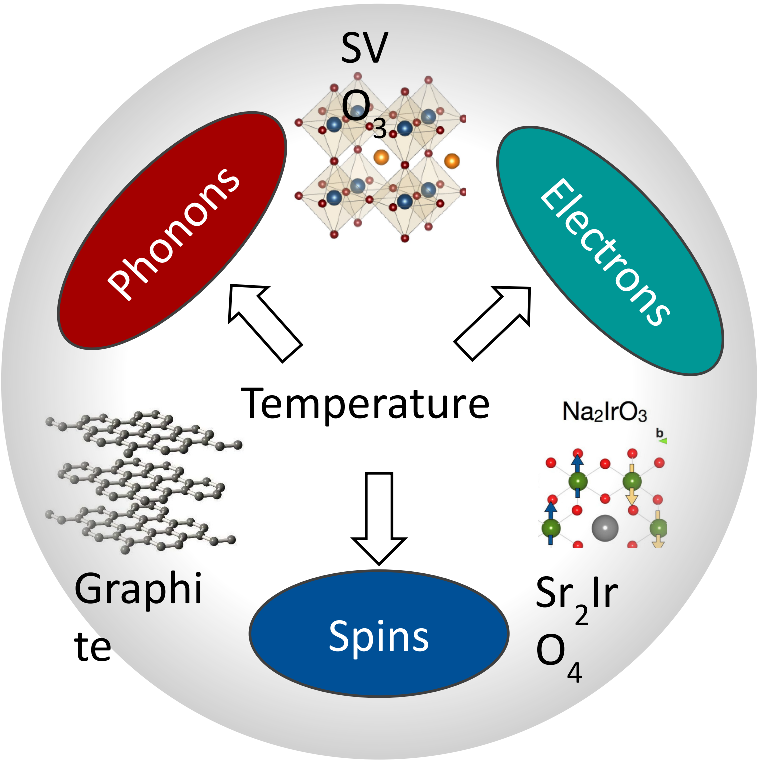

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