Ab-initio phonon and electron transport in nuclear materials

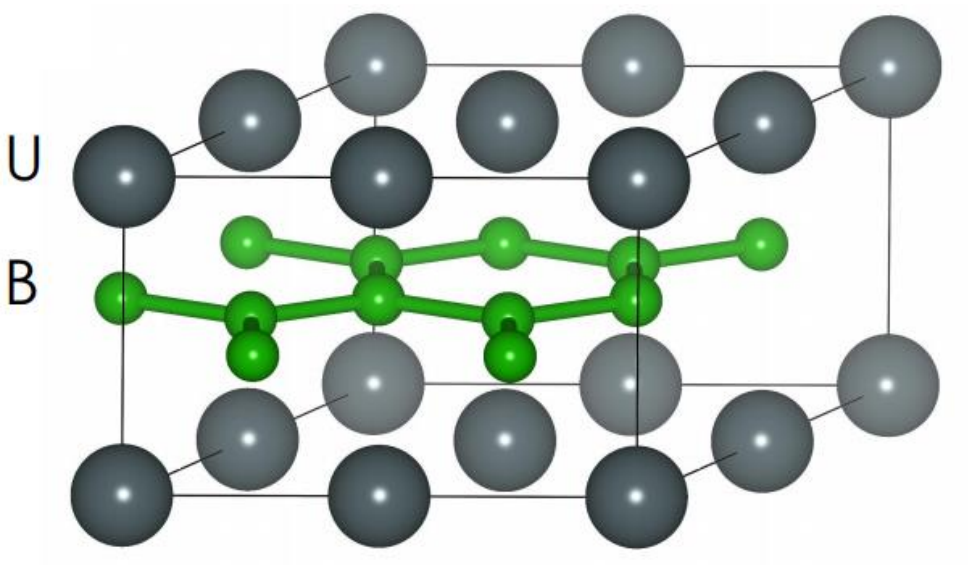
Phonons (vibrations)

[e.g. C_v, C_p, S^{vib}, K_{lat}, B(T), G(T)]

Coupling of the two!

Electrons

[e.g. σ/ρ, T_c, K_{el}, E_F (band structure)]



- Focus on UB_2 [1] (potential fuel), P6/mmm anisotropic structure
- Higher U density than UO_2

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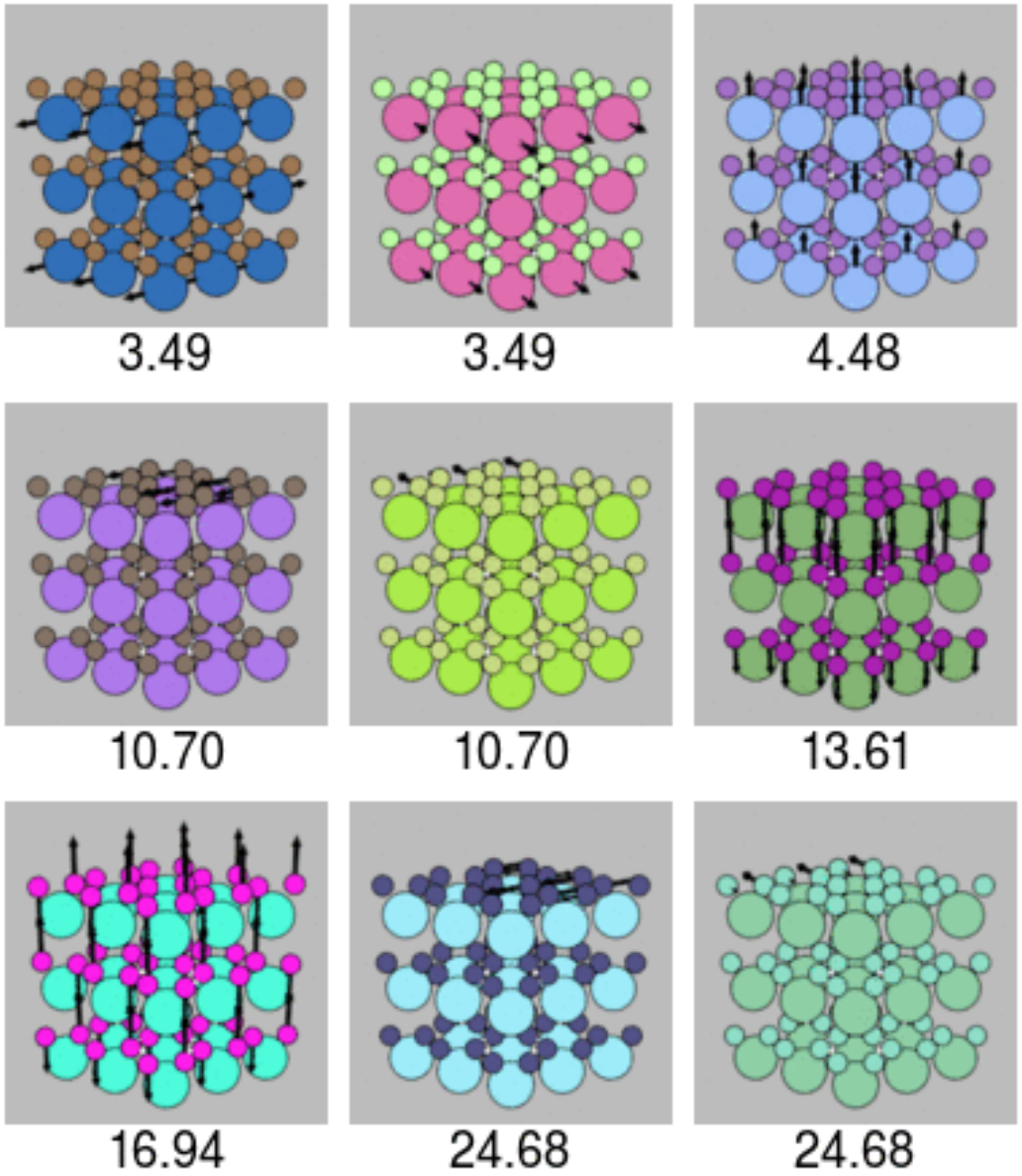
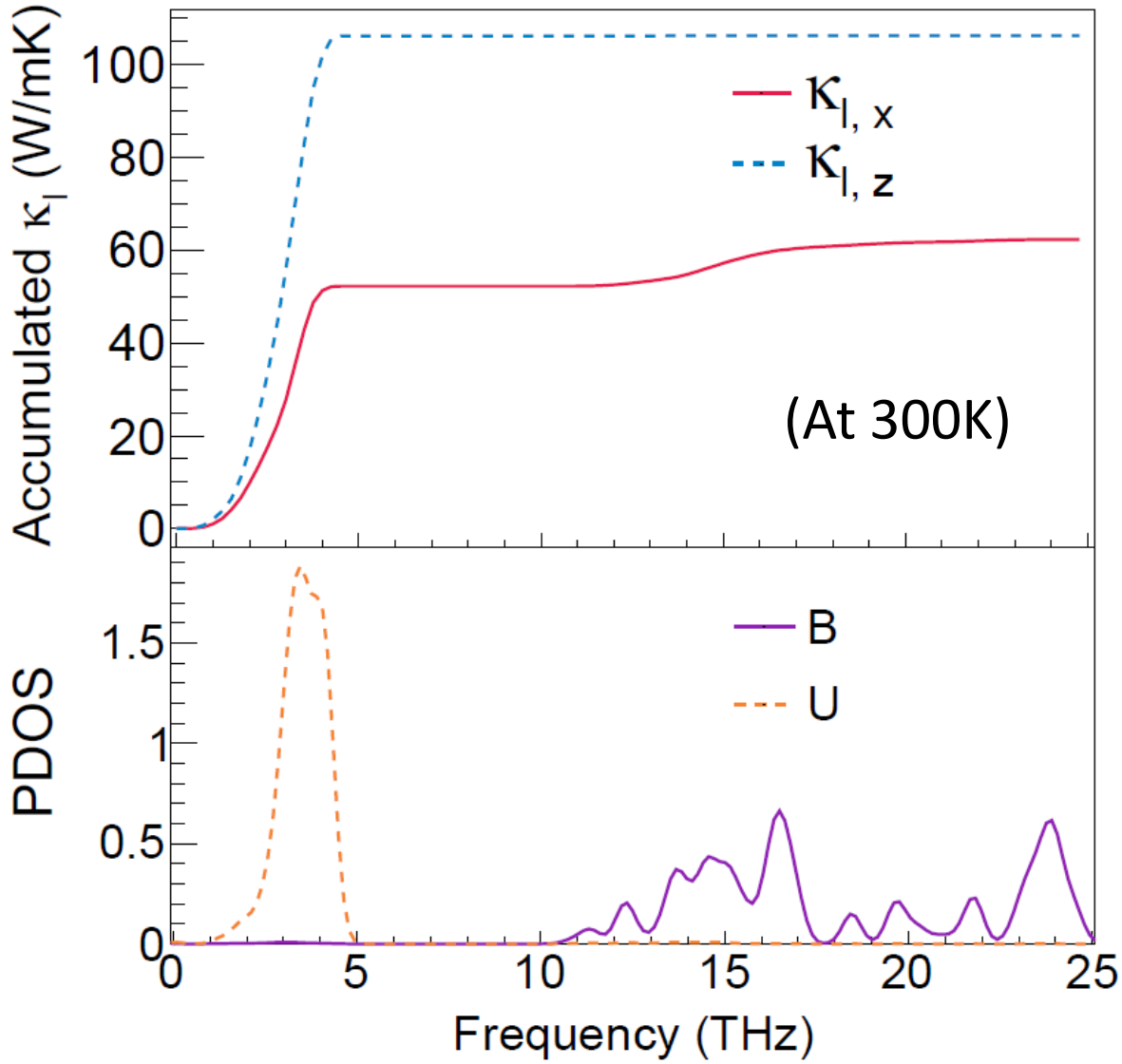
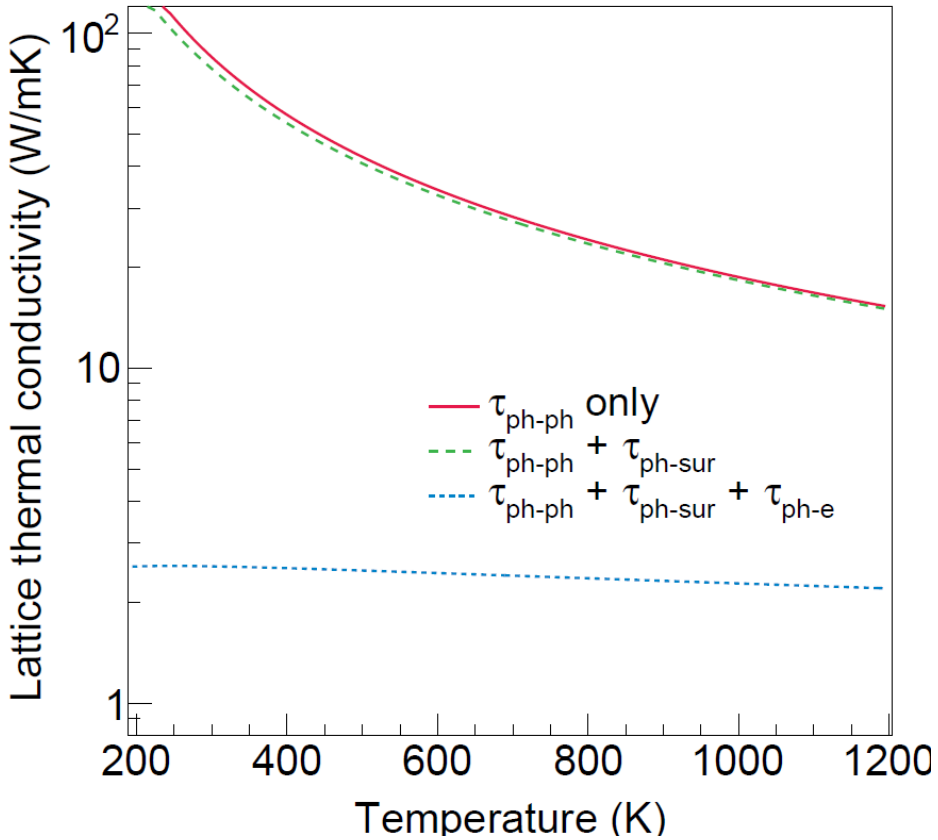
[1] J. Nucl. Mater, 528 (2020)

Phonons – breakdown of lattice thermal conductivity





Coupling phonons and electrons



$$\kappa_l = \frac{1}{3} \cdot C_v \cdot v_M^2 \cdot \tau_p$$

$$\frac{1}{\tau_p} = \frac{1}{\tau_{ph}} + \frac{1}{\tau_{def}} + \frac{1}{\tau_{sur}} + \frac{1}{\tau_{spin}} + \frac{1}{\tau_{e-}}$$

- Typically, only ph-ph scattering calculated
- ph-sur scattering estimated from typical grain size
- (Discussion of ph-isotope in paper)
- ph-e- can be calculated from coupling ab-initio phonon and electron transport calculations (electron-phonon Wannierization)

Electrons

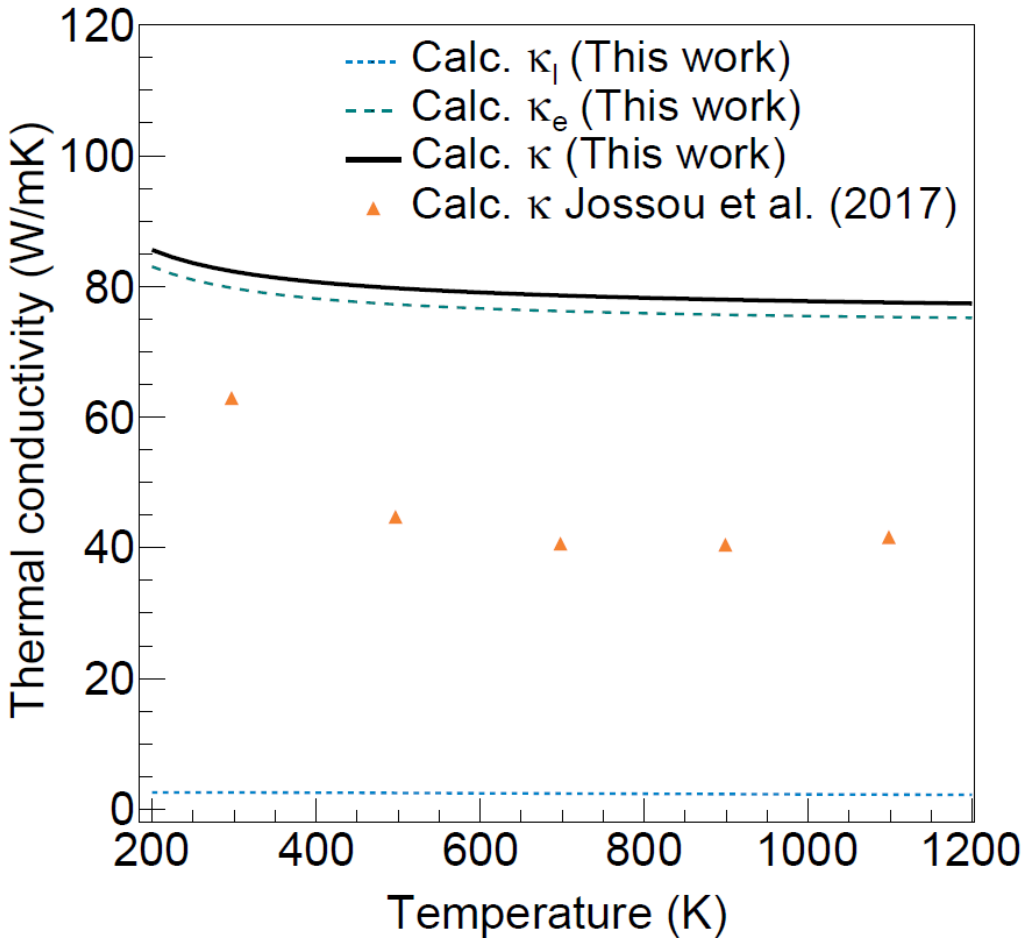
- BoltzTraP give properties as fn of σ
- Maximally localized Wannier fn:
- ρ = 9.16 μΩ cm at RT
  (expt ~10 μΩ cm [1])

$$\kappa_e^{imp} = LT/\rho$$

$$\frac{1}{\kappa_e} = \frac{1}{\kappa_e^{imp}} + \frac{1}{\kappa_e^{ph}}$$

- K^{ph}_e calc. from integrals of spectral functions, found to be negligible

Total K dominated by K_e



[1] E. Yamamoto et al, J. Phys. Soc. Jpn 67 (9) (1998)