UNIVERSITY OF ARKANSAS

Anharmonic lattice dynamics and thermal conductivity of ZrS_2 monolayer using self-consistent phonon theory

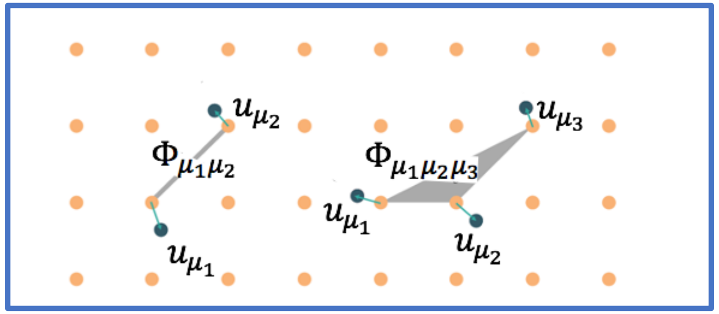
Abhiyan Pandit[1,*] and Bothina Hamad[1,2,]

[1]*Physics Department, University of Arkansas, Fayetteville, AR 72701, USA*

[2]*Physics Department, The University of Jordan, Amman-11942, Jordan*

*: apandit@uark.edu

Description: The lattice anharmonicity and temperature dependences of phonon, which play a key role to explain the lattice thermal conductivity (LTC) and thermal expansion in solids, cannot be accounted within the harmonic limit. In particular, the harmonic approximation (HA) fails in the crystals that have significant anharmonic effects and for the materials that are dynamically unstable at 0 K. The inadequate understanding of the lattice anharmonicity and its effect on the phonon dispersion and lattice thermal conductivity can be misleading in revealing the actual significance of a material, two-dimensional (2D) ZrS_2 monolayer (ML) here, in thermoelectric device applications.



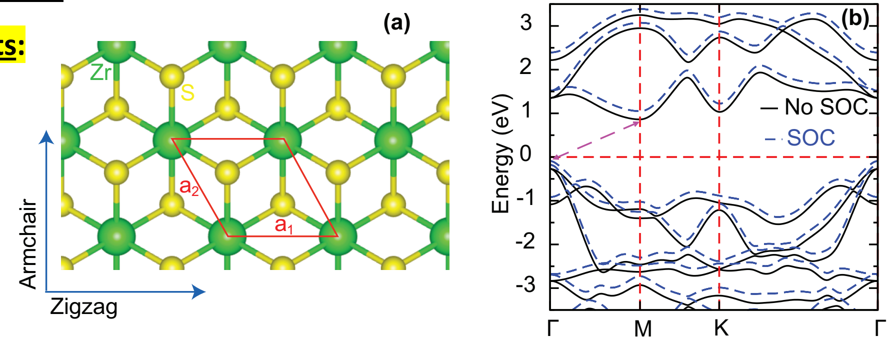
Computational Approach:

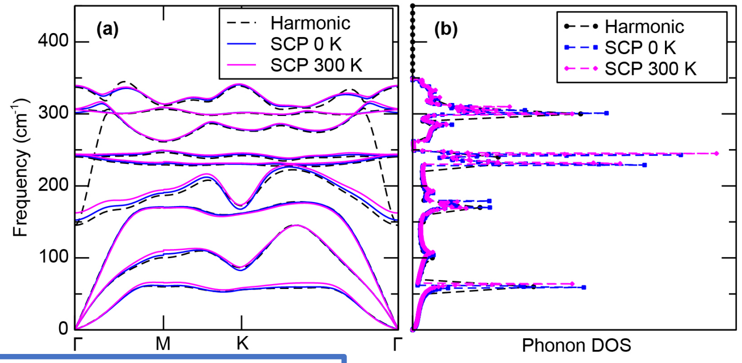
- $\Phi_{\mu_1\mu_2\mu_3 \ldots \mu_n}(l_1k_1;\ l_2k_2;\ \ldots;\ l_nk_n) = \dfrac{\partial^n U}{\partial u_{\mu_1(l_1k_1)} \ldots \partial u_{\mu_n(l_nk_n)}}\Big|_{\{u\}=0} = n^{th}$ order IFCs
- Higher order interatomic force constants (IFCs) obtained by using the compressive sensing technique, which estimates the necessary data based on the emerging machine learning program (LASSO regression followed by cross-validation technique)
- **Self-consistent phonon (SCP) theory** used to calculate the temperature-dependent lattice dynamics and LTC using the calculated interatomic force constants (IFCs) within a supercell

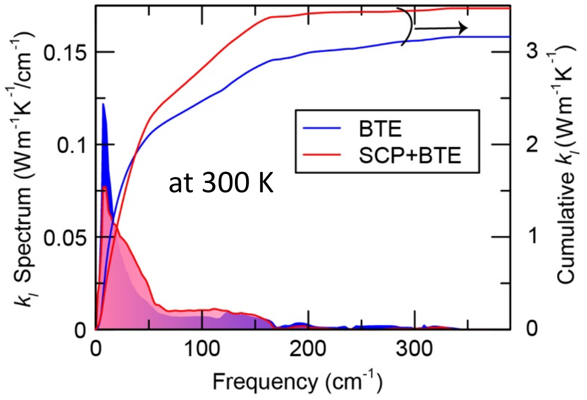
Hamiltonian $\boldsymbol{H} = \boldsymbol{\mathcal{H}_0} + (\boldsymbol{H_0} - \boldsymbol{\mathcal{H}_0} + \boldsymbol{U_3} + \boldsymbol{U_4}) = \boldsymbol{\mathcal{H}_0} + \boldsymbol{\mathcal{H}'}$;

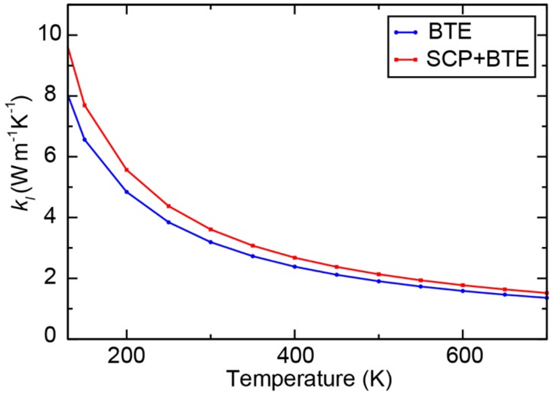
$\boldsymbol{\mathcal{H}_0} = \sum_{q,j} \hbar \boldsymbol{\Omega_{qj}} \left(\boldsymbol{a_{qj}}^{\dagger} \boldsymbol{a_{qj}} + \frac{1}{2} \right)$ = effective Hamiltonian associated with the renormalized **anharmonic phonon frequency $\boldsymbol{\Omega_q}$**

Current Results:









Future works/Challenges:

- Very few experimental works till now
- Estimate the structural phase transition temperature (T_c)
- Investigate the similar studies on the thermoelectric performance
- Study the lattice anharmonicity and its effect in other 2D materials