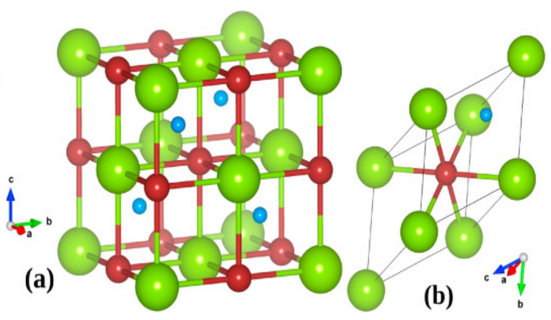
Carrier scattering considerations and thermoelectric power factors of half-Heuslers

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Introduction

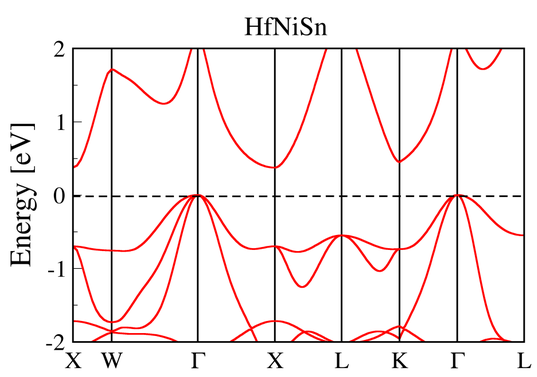
- Investigation of electronic and thermoelectric (TE) properties of half Heuslers (HH)
- Different scattering mechanisms
  - Non-polar ADP, ODP,
  - Fröhlich interaction (POP),
  - Ionized Impurtiy scattering (IIS)
- Effect of elastic and inelastic scattering on Seebeck
- Role of multi-bands on the TE properties.



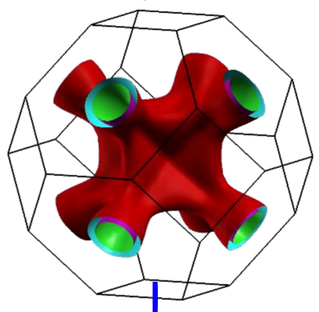
Method

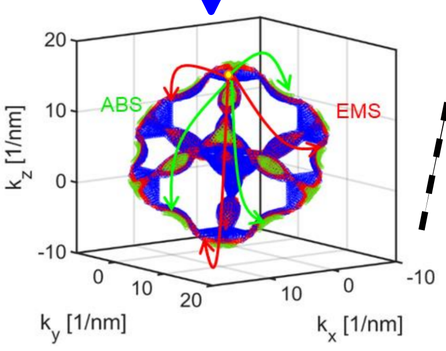
- Density functional theory based calcuations: Quantum Espresso with GGA exchange-correlation
- Boltzmann transport
  ElecTra code for electronic transport

DFT bands

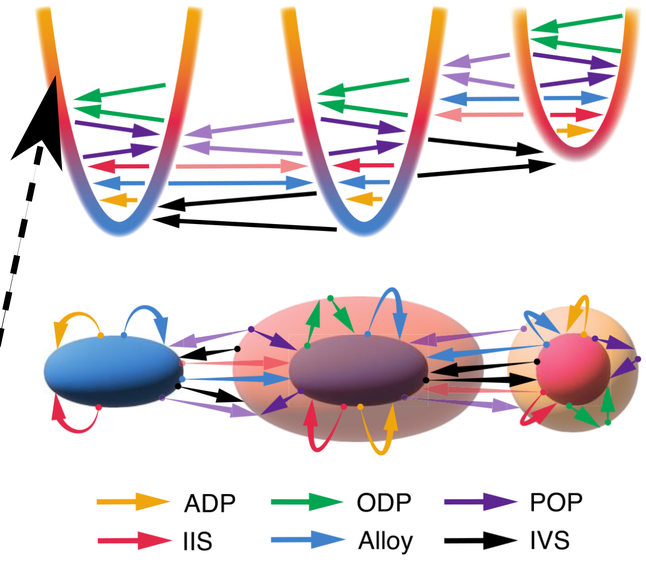


Energy surfaces





Discrete state-points



Careful consideration of scattering process

$$\frac{1}{\tau^{(i)}_{x,k,n,E}} = \frac{1}{(2\pi)^3}\sum_{k'}|S^{(i)}_{k,k'}|\left(1-\frac{v_{x,k'}}{v_{x,k,n,E}}\right)$$

$$|S^{ADP}_{k,k'}| = 2\frac{\pi}{\hbar}D^2_{ADP}\frac{k_BT}{\rho v_s^2}g_{k'}$$

$$|S^{ODP}_{k,k'}| = \frac{\pi D^2_{ODP}}{\rho\omega}\left(N_{\omega BE}+\frac{1}{2}\mp\frac{1}{2}\right)g_{k'}$$

$$|S^{POP}_{k,k'}| = \frac{\pi e^2\omega}{|k-k'|^2\epsilon}\left(\frac{1}{k_\infty}-\frac{1}{k_0}\right)\left(N_{\omega BE}+\frac{1}{2}\mp\frac{1}{2}\right)g_{k'}$$

$$|S^{IVS}_{k,k'}| = \frac{\pi D^2_{IVS}}{\rho\omega}\left(N_{\omega}+\frac{1}{2}\mp\frac{1}{2}\right)g_{k'}$$

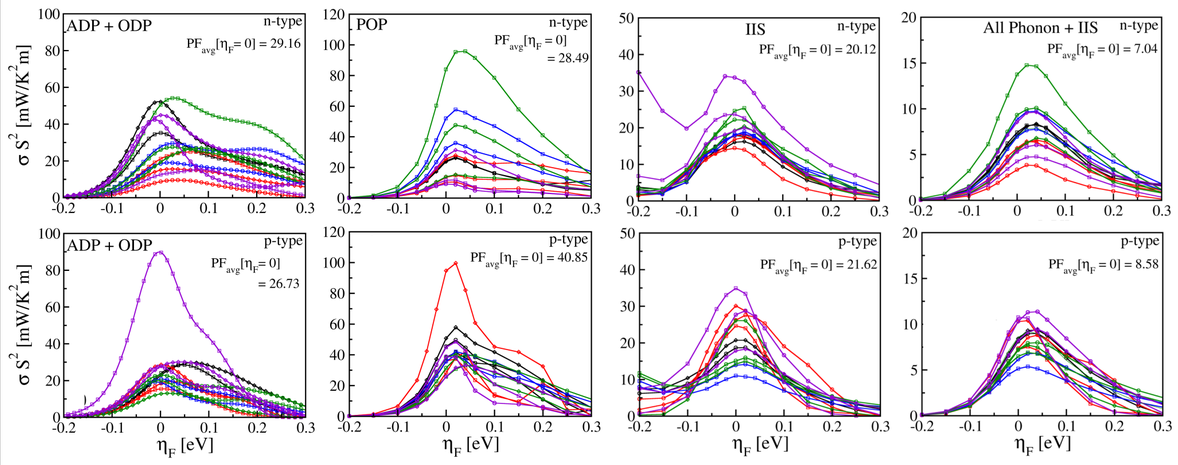
$$|S^{IIS}_{k,k'}| = \frac{2\pi}{\hbar}\frac{Z^2e^4}{k_s^2\epsilon_0^2}\frac{N_{imp}}{\left(|k-k'|^2+\frac{1}{L_D^2}\right)^2}g_{k'}$$

Screening for POP $\left(\frac{(|k-k'|)^2}{|k-k'|^2+\frac{1}{L_D^2}^2}\right)^2$

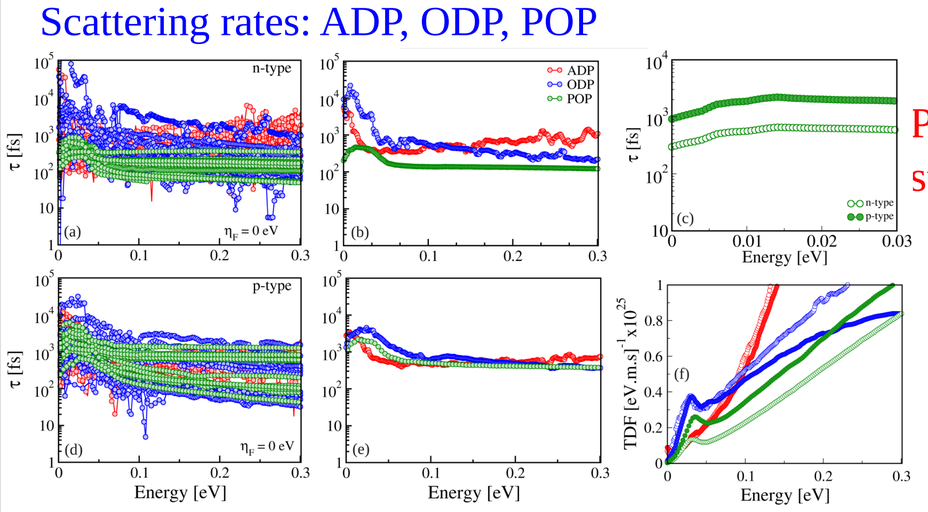
DOI:10.5281/zenodo.5074943
https://github.com/PatrizioGraziosi/ELECTRA

Transport Properties

PF vs scattering mechanisms:

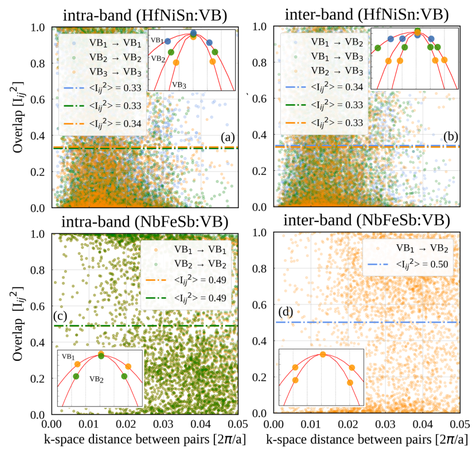


Scattering rates: ADP, ODP, POP

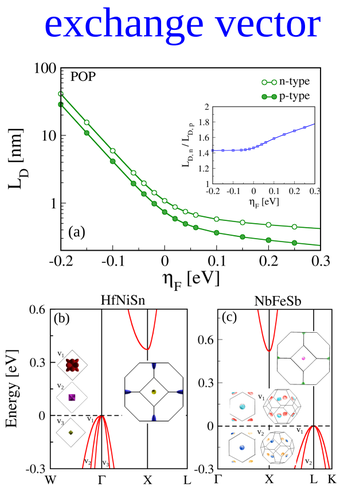


POP: stronger for CB

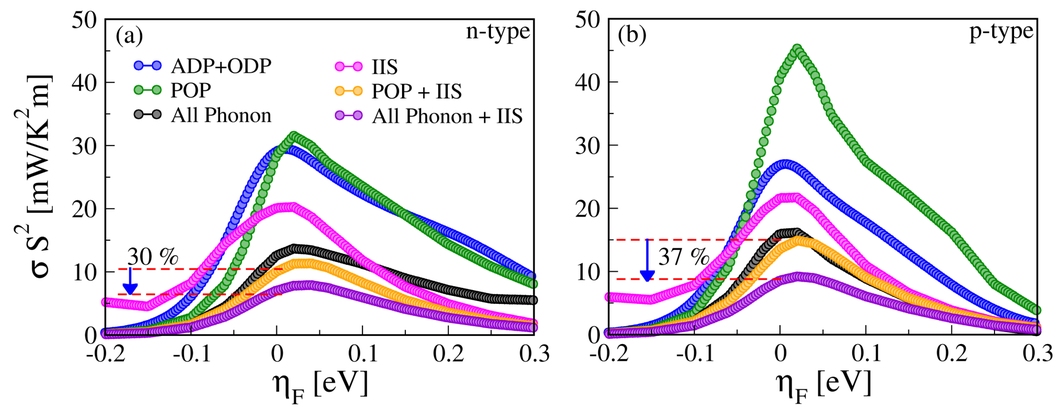
Role of Overlap Interaction



Screening length and exchange vector



Average PF with different scattering



Conclusions

- TE properties of 13 HH alloys investigated.
  Detailed comparison of different scattering mechanisms
- POP stronger than non-polar ADP, ODP
- Seebeck coefficient decreases due to inelastic scattering, with an even greater reduction in VB
- IIS is stronger compared to all other mechanisms
- POP and IIS combined determine 67% of PF in n-type and 82% in p-type HH alloys

References:
1. Patrizio Graziosi, Zhen Li, N. Neophytou Comput. Phys Commun. 287, 108670 (2023).
2. Zhen Li, Patrizio Graziosi, N. Neophytou npj Compu. Mat.. 10 (1), 8 (2024)
3. Zhen Li, Patrizio Graziosi, N. N Phys. Rev. B. 104(19), 195201 (2021).
4. R. Dutt, B. Sahni, Y. Zhao, Y. Go, S.E.A. Akhtar, A. Kumar, S. Kukreti, Z. Li, P. Graziosi J. Mater. Chem. A 14 (17), 10332 (2026).

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