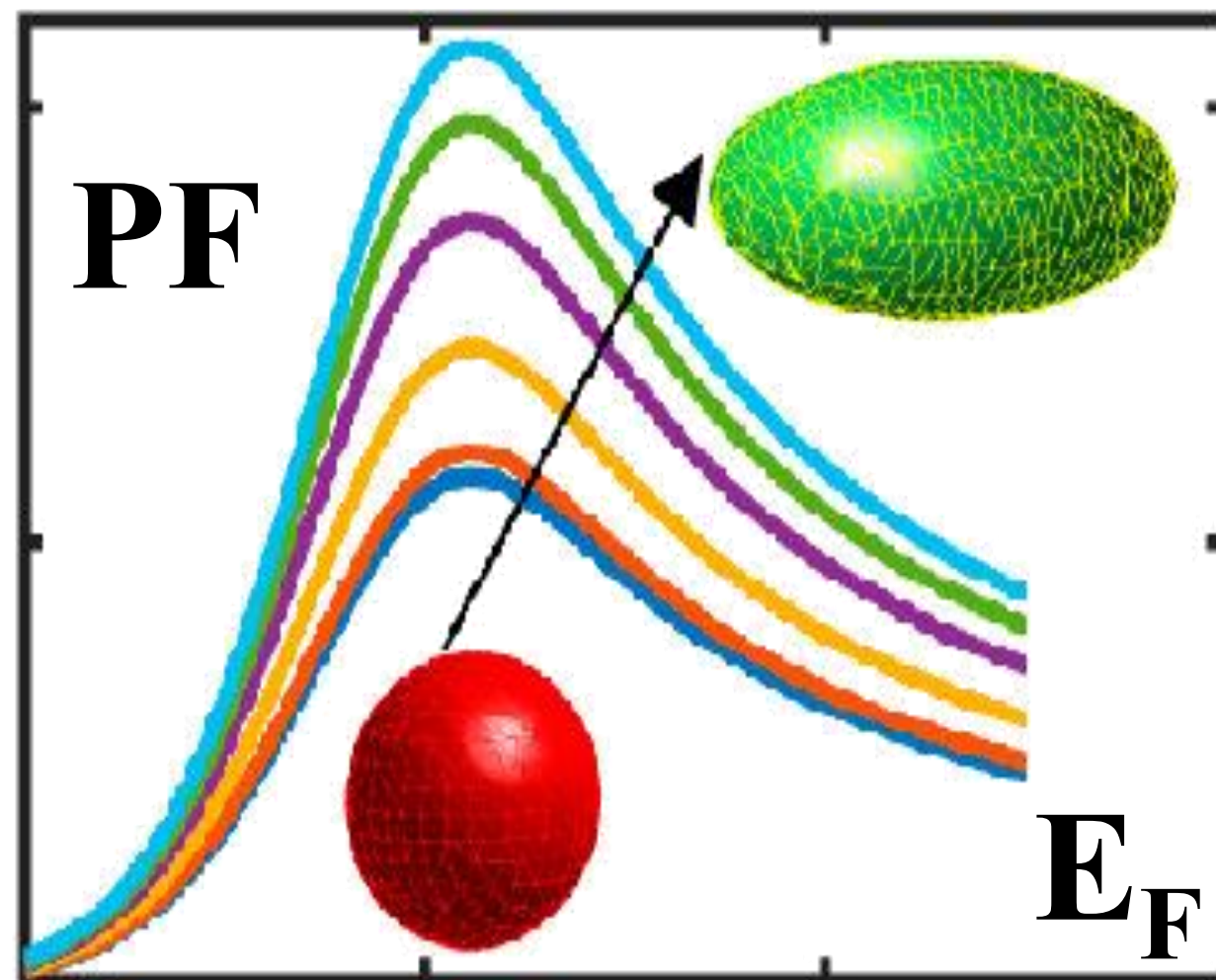


Introduction

Spherical bands:

Fe₂VAl

- “Balanced but limited”
- σ , and S are moderate.



$$m_C = 3 \left(\frac{1}{m_1} + \frac{2}{m_t} \right)^{-1}, \quad m_{DOS} = (m_1 m_t^2)^{1/3}$$

Elongated bands:

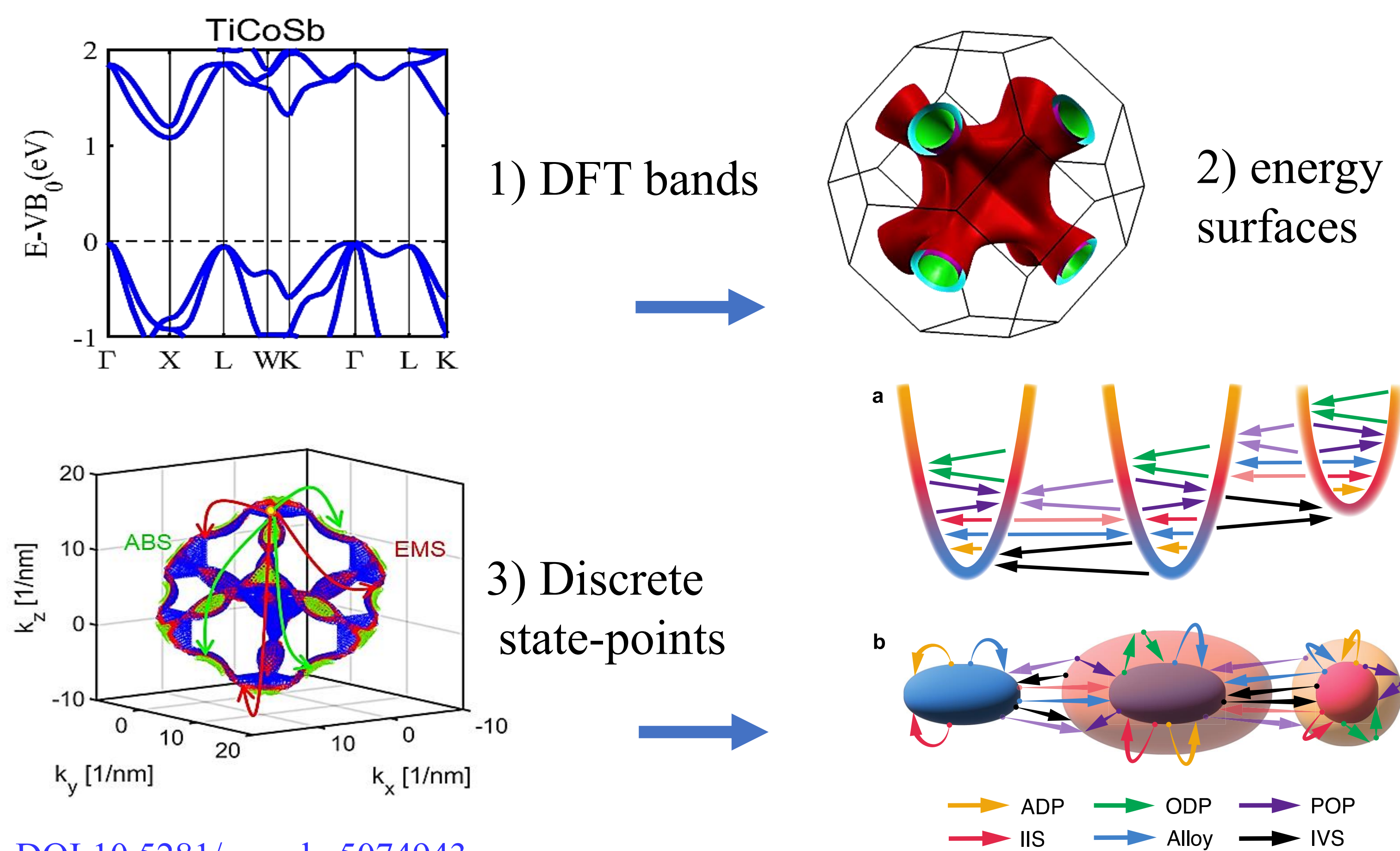
Fe₂NbAl, Fe₂TiSn

- “Best of both worlds”
- $\uparrow \sigma$ at one direction
- $\uparrow S$ at other direction

Methodology

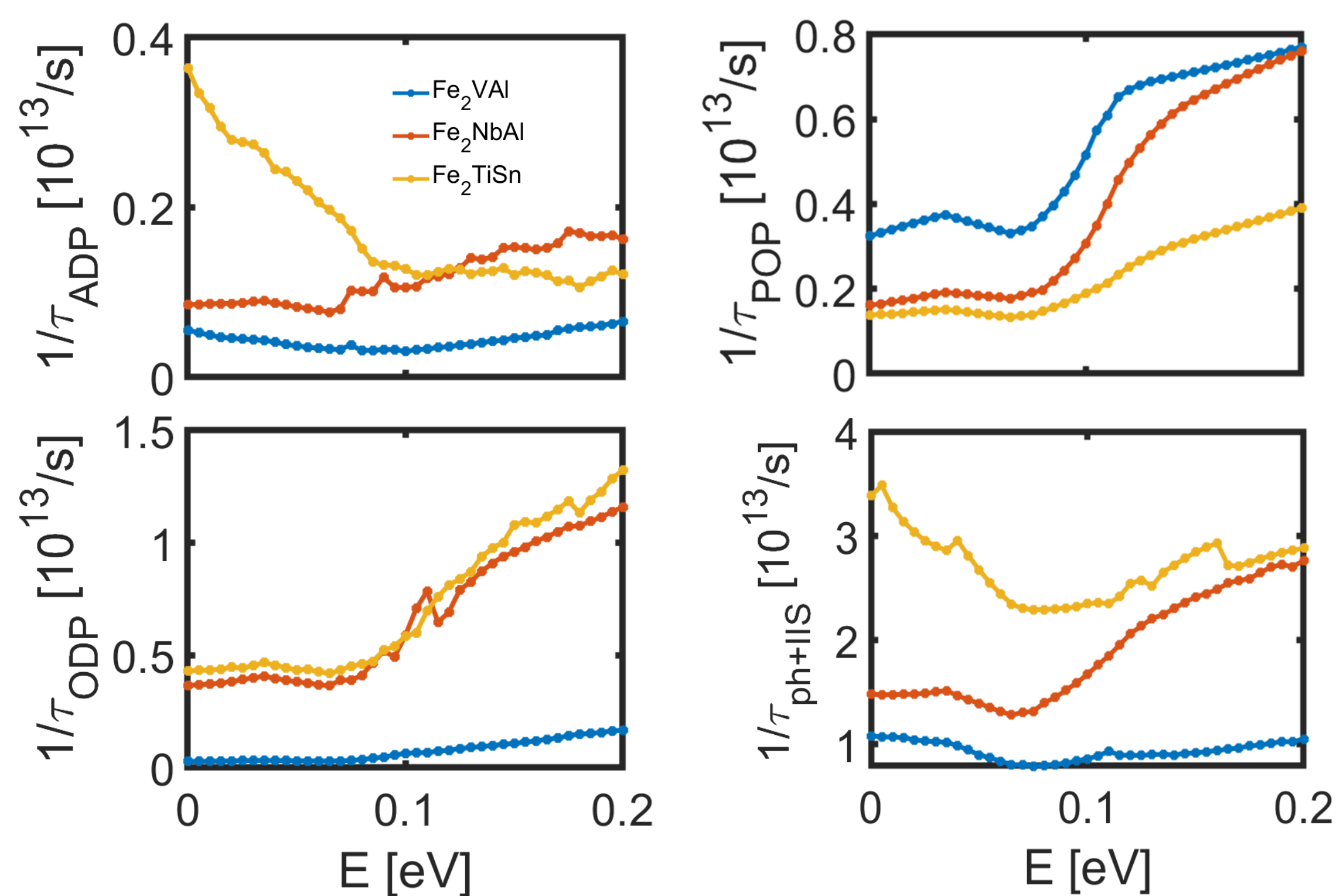
- GGA-based DFT and DFPT calculations.
- ElecTra** code for electronic transport based on Boltzmann Transport equations.

ElecTra Workflow



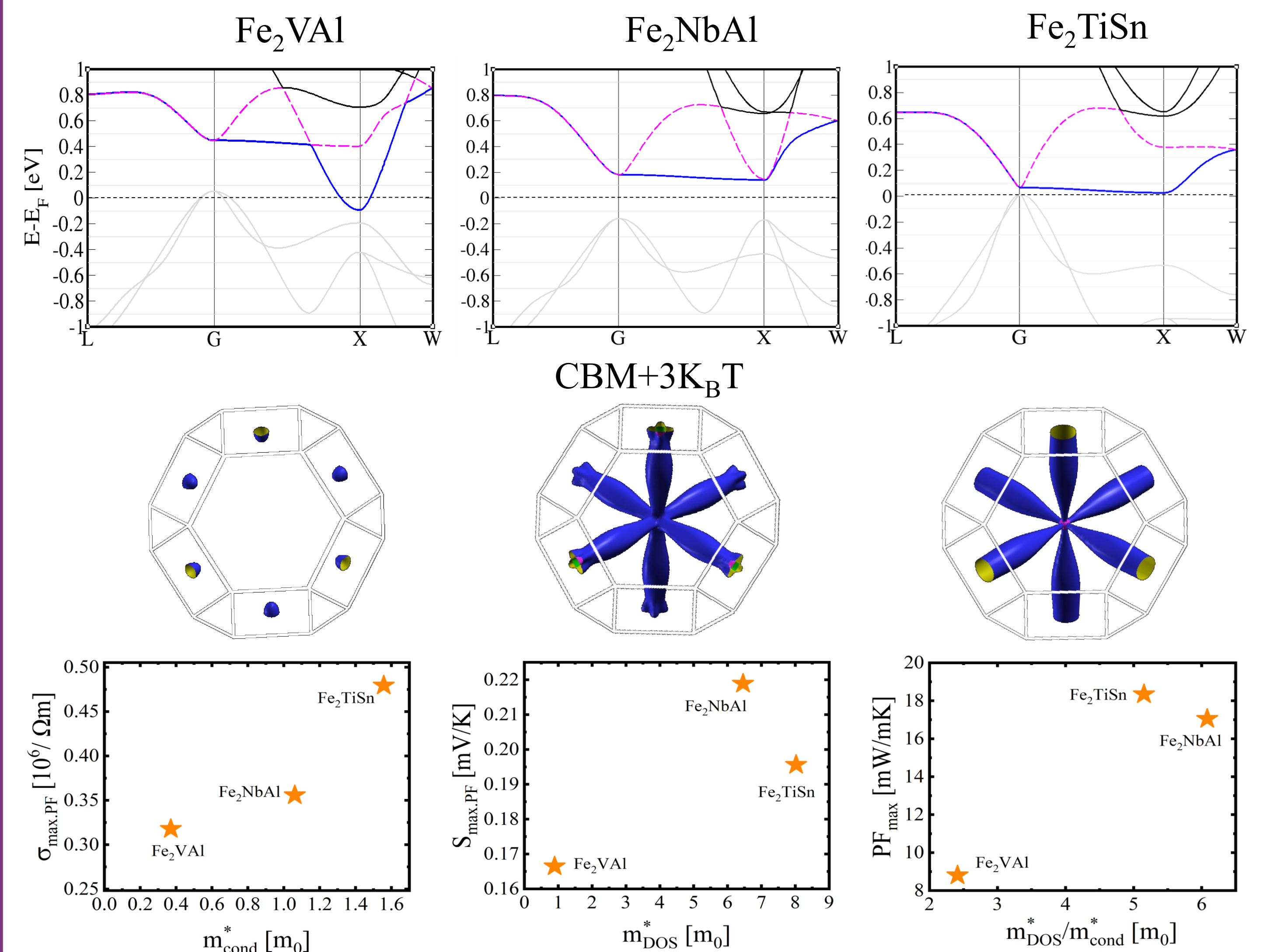
DOI:10.5281/zenodo.5074943,
<https://doi.org/10.1016/j.cpc.2023.108670>
<https://github.com/PatrizioGraziosi/ELECTRA>

Scattering rates



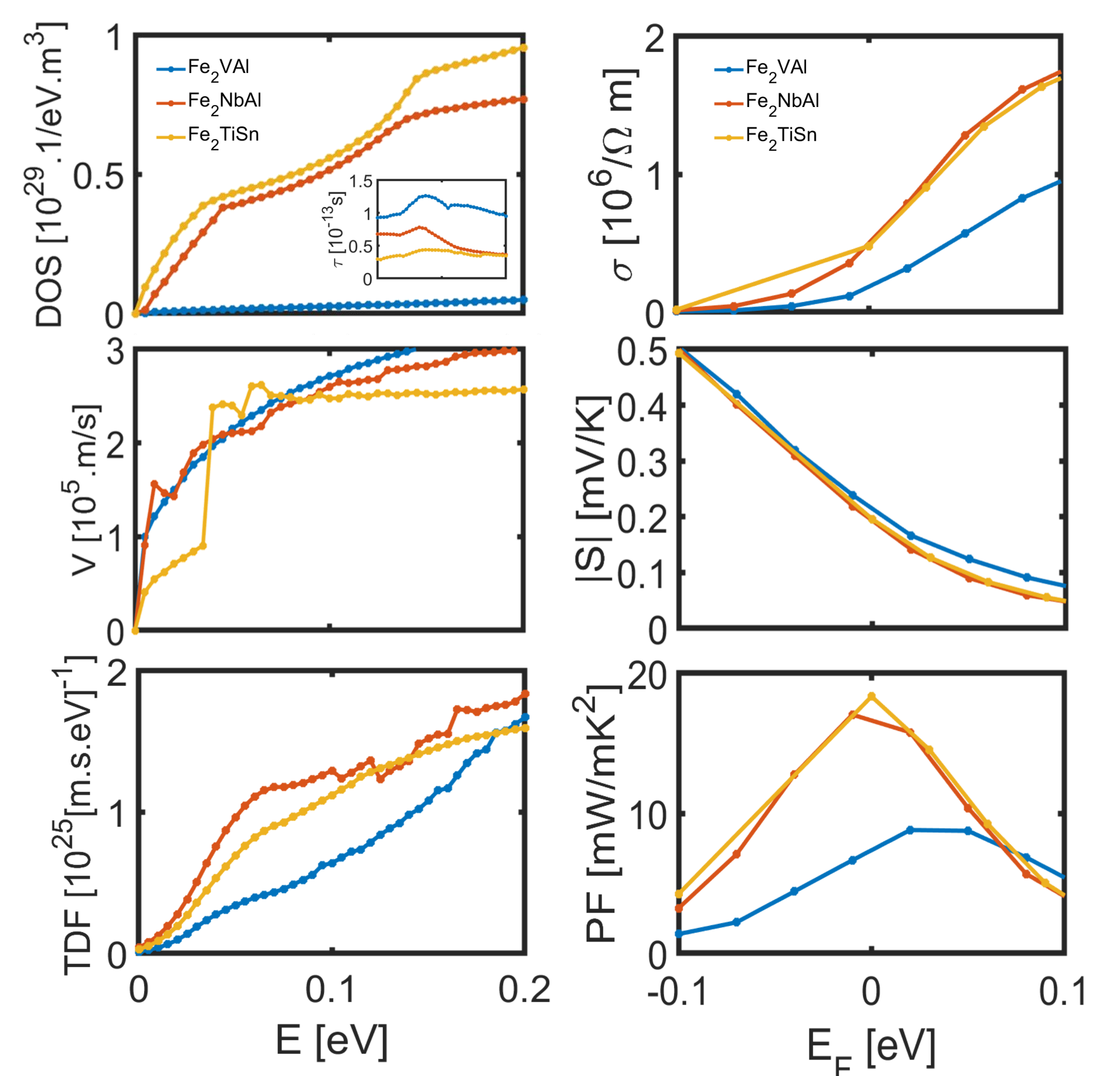
- IIS scattering dominates overall.

Electronic structures



- Anisotropic pockets raise DOS but preserve usable velocities \rightarrow large m_{DOS}/m_{cond}

Transport Coefficients



- The combination of large DOS and moderate effective conductivity mass (anisotropic pockets) results in the highest PF of Fe₂TiSn.

Conclusions

- Materials with elongated pockets have almost 2x increase in PF compared to spherical bands.
- In elongated bands anisotropy enhances both the DOS mass and the effective carrier density while keeping conductivity mass moderate, allowing larger σ and much higher PF.
- Spherical bands with low DOS and few valleys \rightarrow consistently lowest σ , S, and PF among the three.

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