Band-transport and thermoelectricity.

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Overview

- Band transport
  - electric and magnetic fields and thermal gradients
  - Semi-classic theory
  - Program: Transport
- Thermoelectrics
  - The figure of merrit
  - Phonon Glass - Electron crystal
  - Skutterudites
  - Clathrates
  - Phonon DOS
- Outlook

Transport

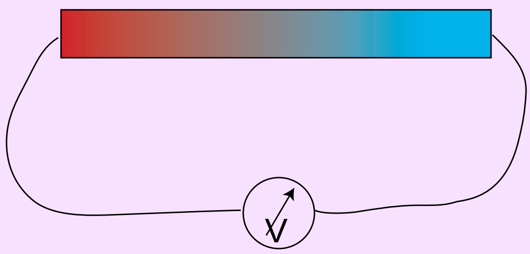
Transport equation

$$j_i = \sigma_{ij} E_j + \sigma_{ijk} E_j B_k + \sigma_{ijkl} E_j B_k B_l + \nu_{ij} \nabla_j T + \cdots$$

- j current density
- σ conductivity tensors
- E electric field
- B magnetic field

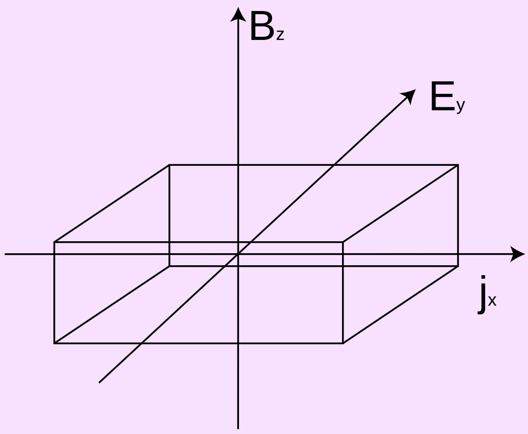
Seebeck coefficient

$$S_{ij} = E_i (\nabla_j T)^{-1} = \sigma^{-1}_{i\alpha} \nu_{j\alpha}$$



Hall coefficient

$$R_{ijk} = j_i^{-1} E_j B_k^{-1} = \sigma^{-1}_{j\alpha} \sigma^{-1}_{i\beta} \sigma_{\alpha\beta k}$$

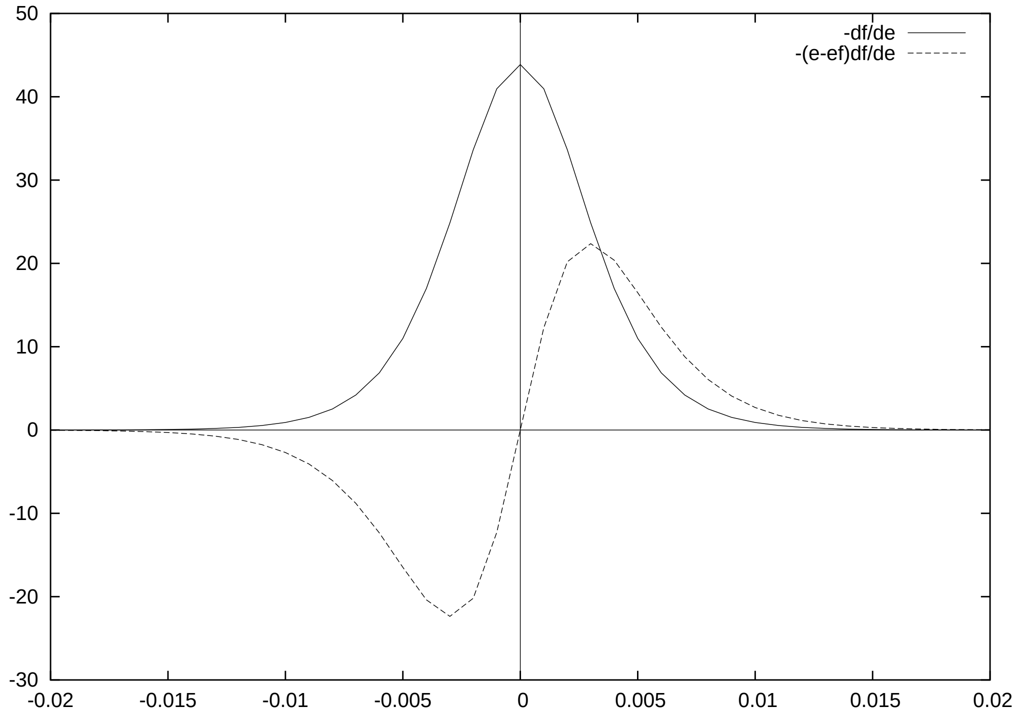


Semi-classic approximation

$$\sigma_{\alpha\beta} = \frac{e^2\tau}{\Omega}\sum_{\mathbf{k}} v_\alpha(\mathbf{k})v_\beta(\mathbf{k})\left(-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right) \qquad (1)$$

$$\nu_{\alpha\beta} = \frac{e^2\tau}{\Omega T}\sum_{\mathbf{k}} v_\alpha(\mathbf{k})v_\beta(\mathbf{k})(\varepsilon_{\mathbf{k}}-\mu)\left(-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right) \qquad (2)$$

$$\sigma_{\alpha\beta\gamma} = \frac{e^3\tau^2}{\hbar\Omega}\sum_{\mathbf{k}} v_\alpha(\mathbf{k})[\mathbf{v}(\mathbf{k})\times\boldsymbol{\nabla}_{\mathbf{k}}]_\gamma v_\beta(\mathbf{k})\left(-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right) \qquad (3)$$



J. M. Ziman, *Electrons and Phonons* (Oxford Classics Series, Clarendon Press, Oxford, 2001).

Program: Transport

Smoothed Fourier expansion of band energies.

$$\varepsilon(\mathbf{k}) = \sum \varepsilon_m S_m(\mathbf{k}) \quad , \quad S_m(\mathbf{k}) = 1/n \sum_{\Lambda} e^{ik\Lambda R_m}$$

$$\begin{array}{ccc} FFT(\varepsilon_m) & FFT(\varepsilon_m k_{mi}) & FFT(\varepsilon_m k_{mi} k_{mj}) \\ \downarrow & \downarrow & \downarrow \\ N(\varepsilon) & N(\varepsilon)\sigma_{ij} & N(\varepsilon)\sigma_{ijk} \end{array}$$

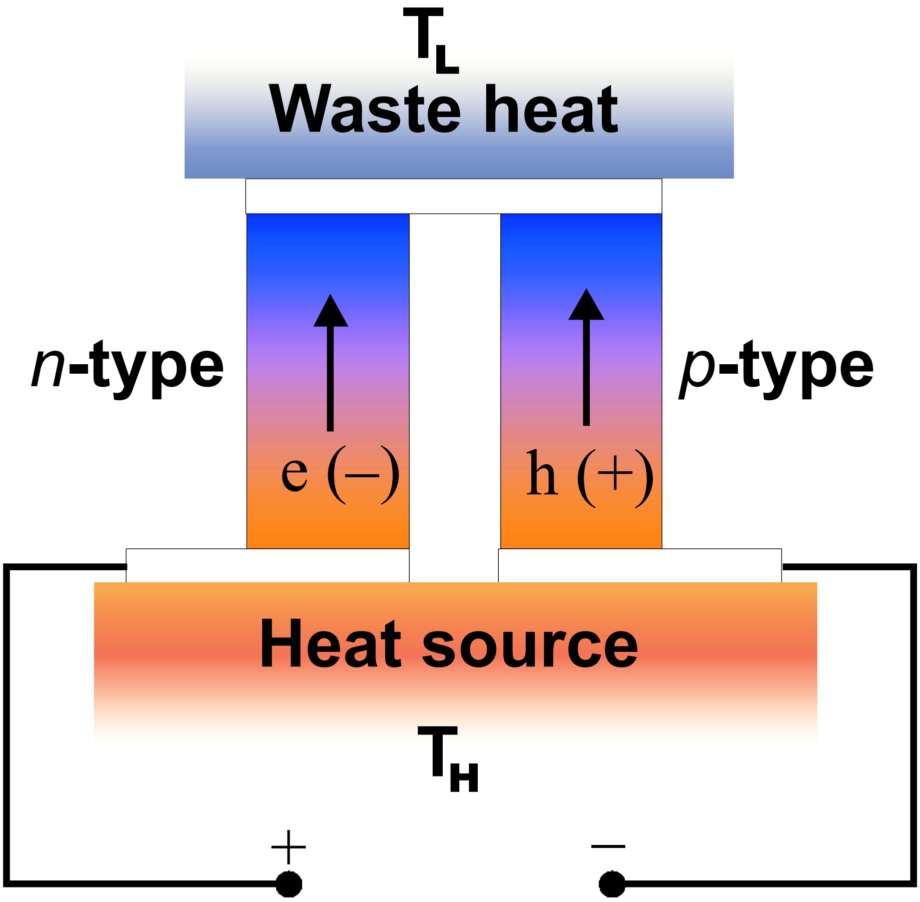
$$\sigma_{ij} = \int N(\varepsilon)\sigma_{ij}(\varepsilon) d\varepsilon$$

$$S_{ij} = \sigma^{-1}_{i\alpha} \int N(\varepsilon)\sigma_{j\alpha}(\varepsilon)(\varepsilon - \mu) d\varepsilon$$

$$R_{ijk} = \sigma^{-1}_{j\alpha}\sigma^{-1}_{i\beta} \int N(\varepsilon)\sigma_{\alpha\beta k}(\varepsilon) d\varepsilon$$

W. E. Pickett, H. Krakauer, and P. B. Allen, Phys. Rev. B **38**, 2721 (1988).

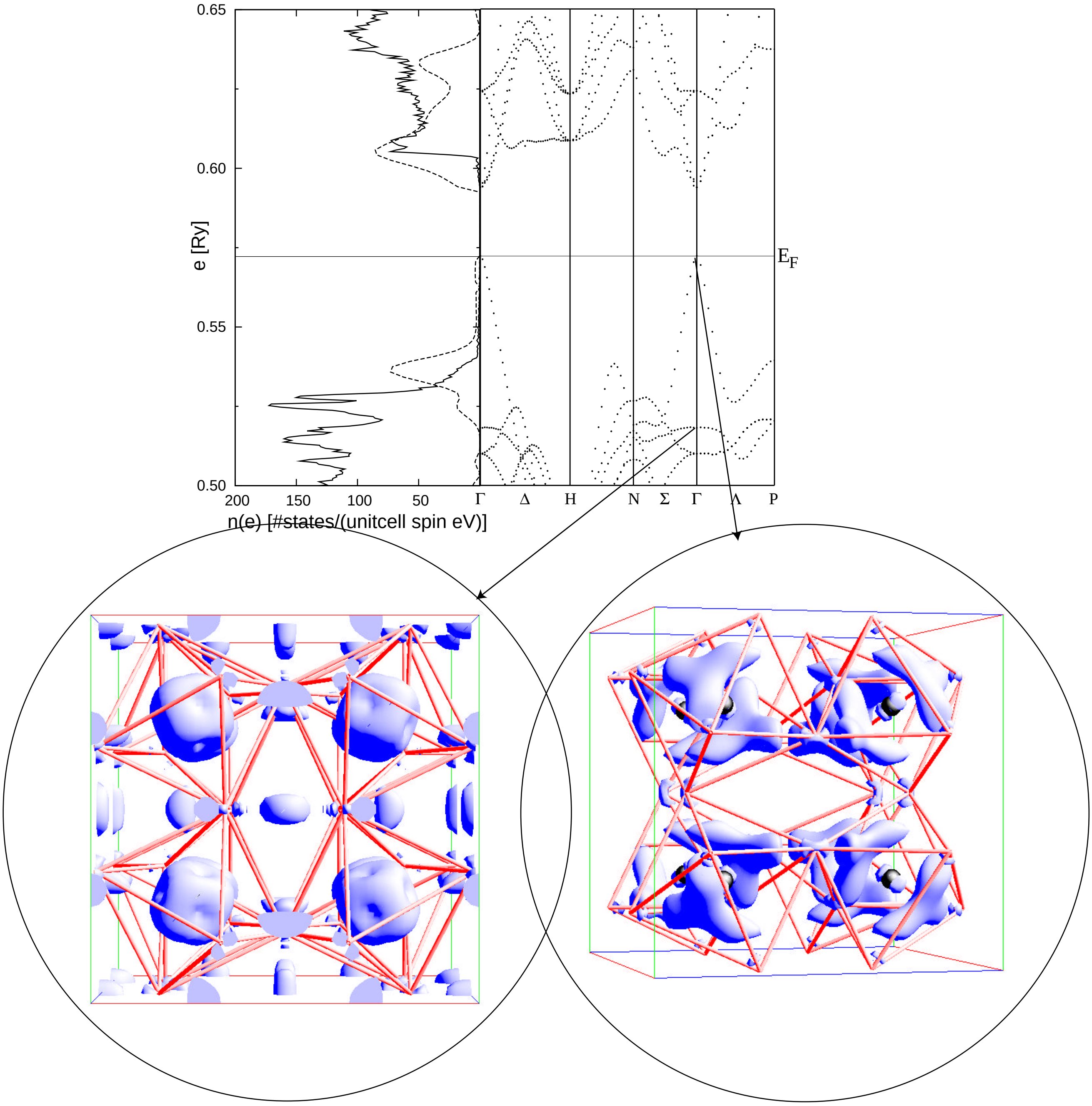
Figure of merrit



$$ZT = (\sigma T/\kappa)S^2$$

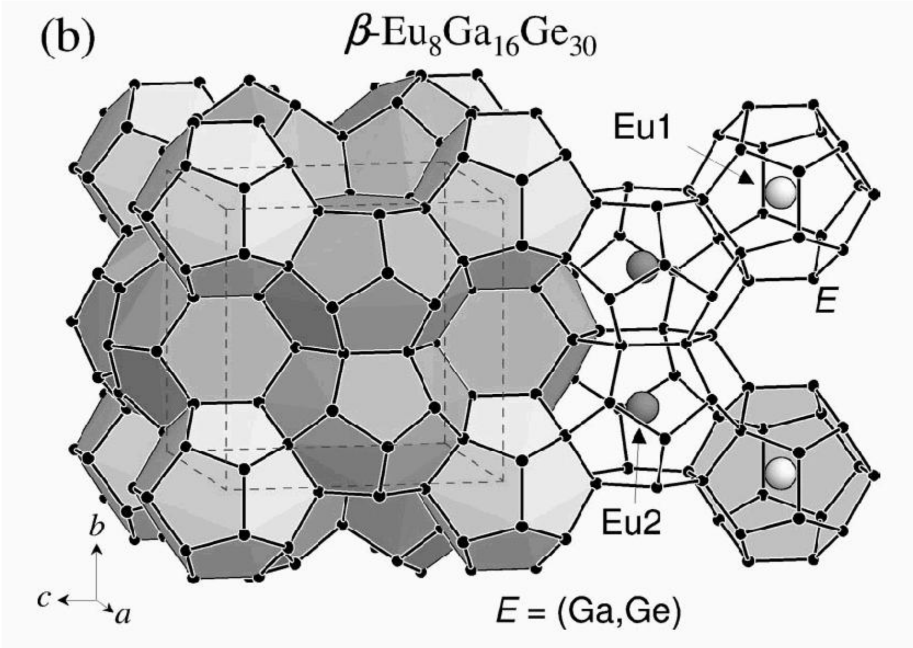
- Electrical conductivity, σ
- Thermal conductivity (electronic and lattice), κ
- Seebeck coefficient, S

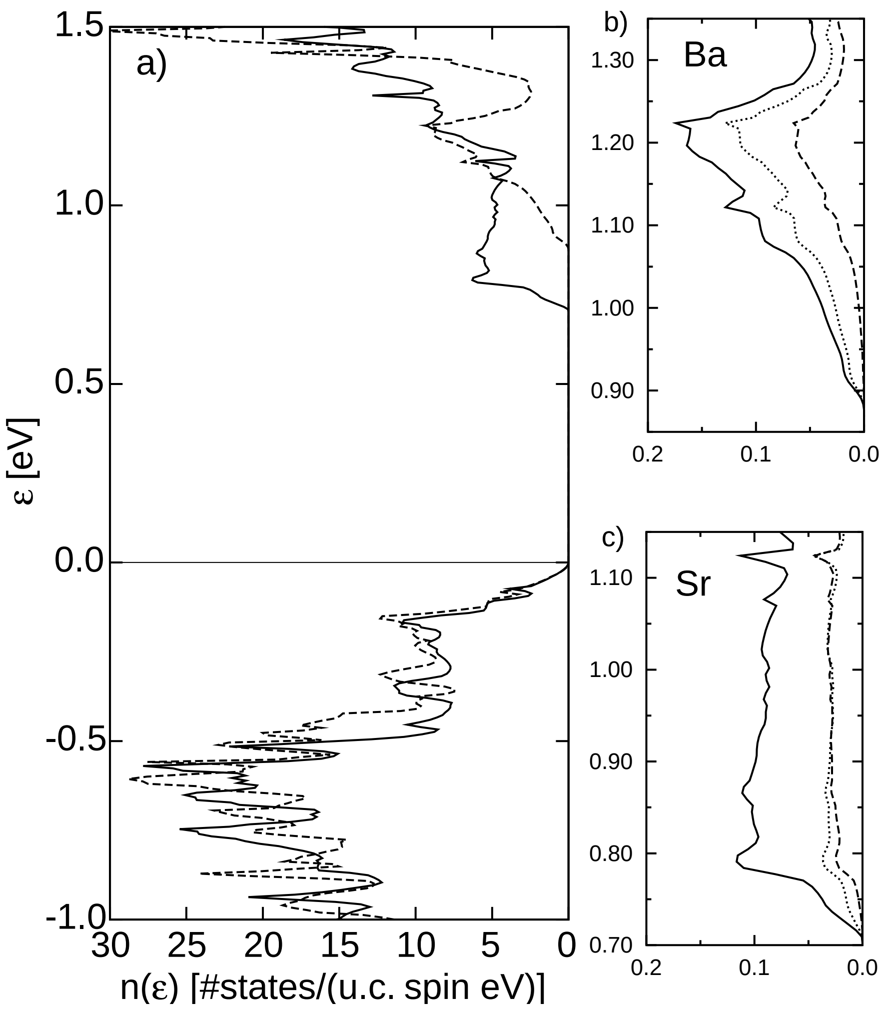
CoSb3



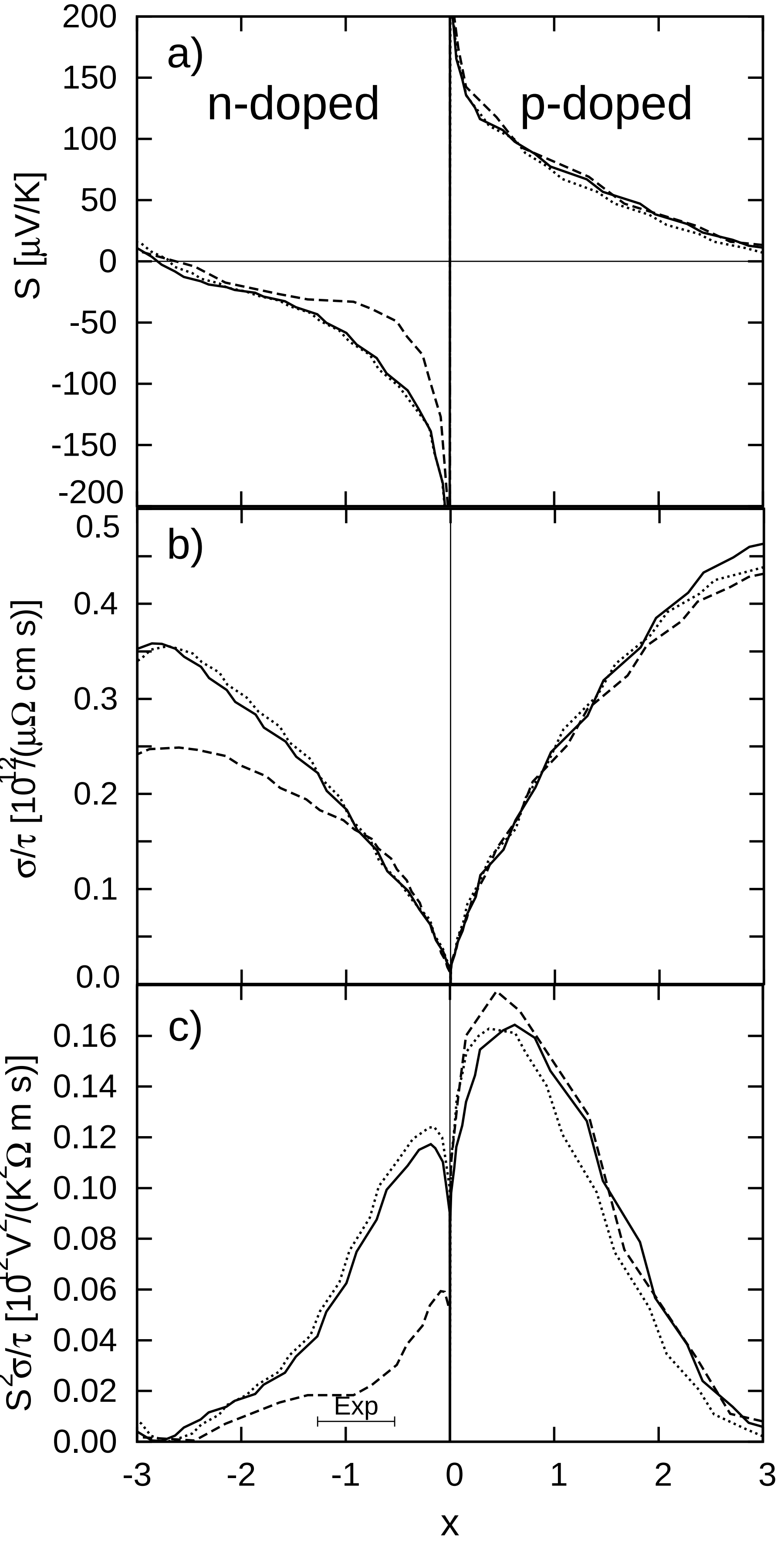
D. J. Singh and I. I. Mazin, Phys. Rev. B **56**, 1650 (1997).

Zintl clathrates. $(II)_8(III)_{16+x}(IV)_{30-x}$

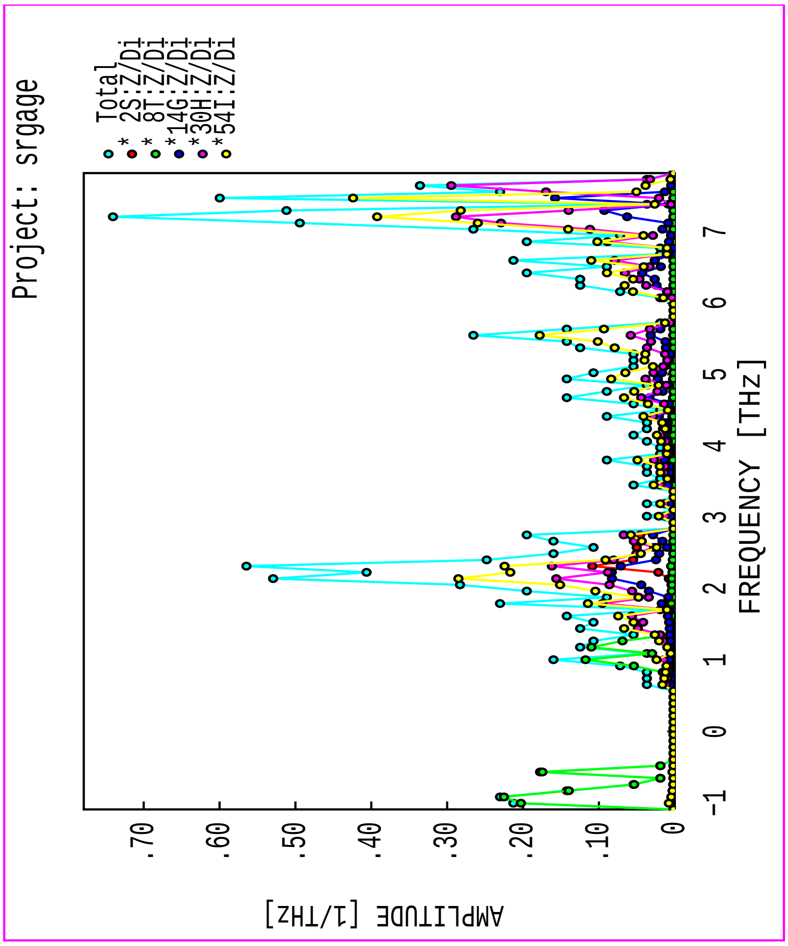


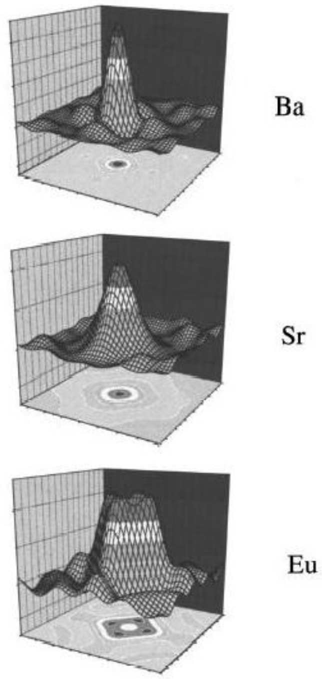


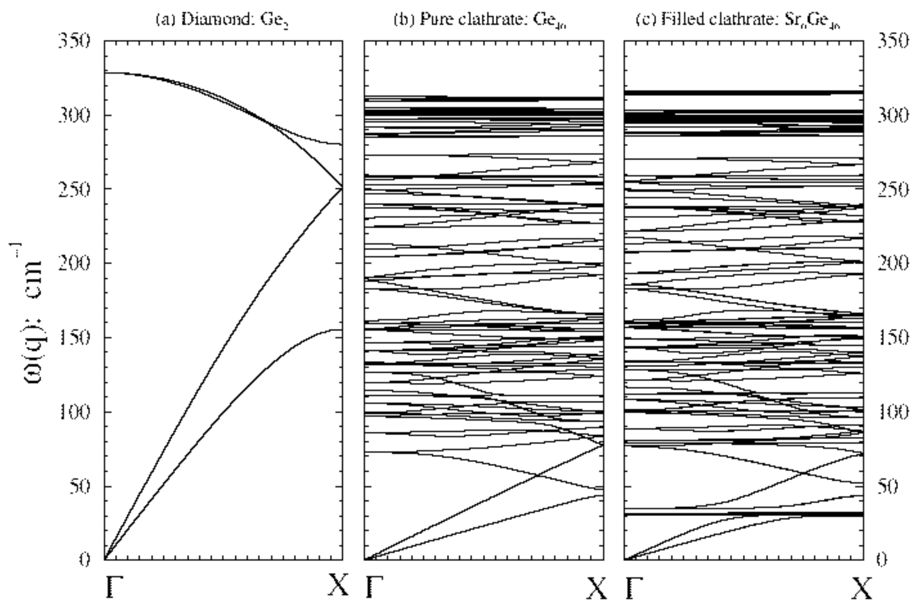
Type-I transport



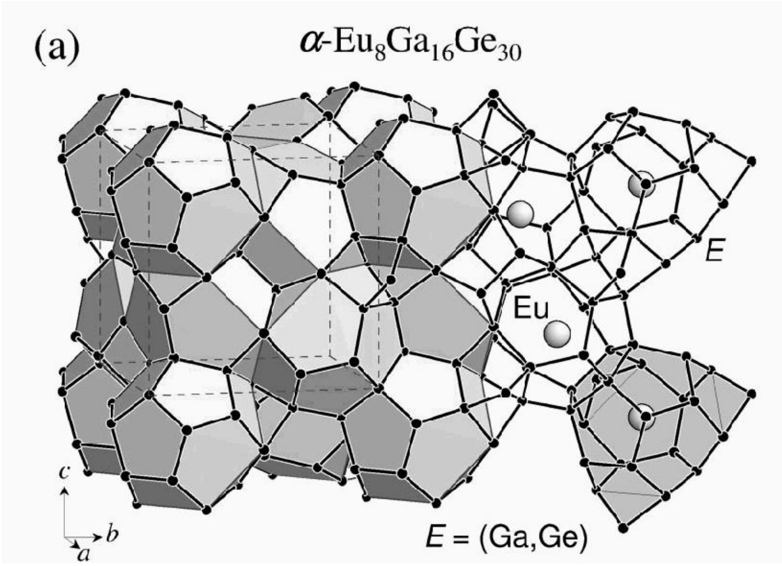
Type-I phonon DOS



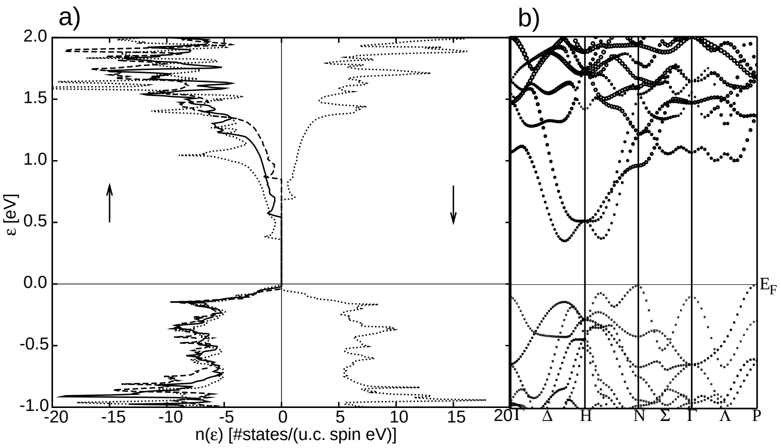




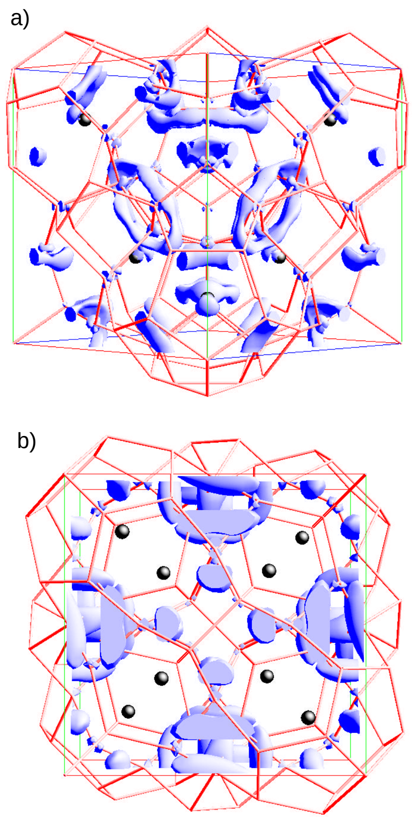
Type-VIII



(a)
α-Eu8Ga16Ge30
E
Eu
E = (Ga,Ge)
c
b
a

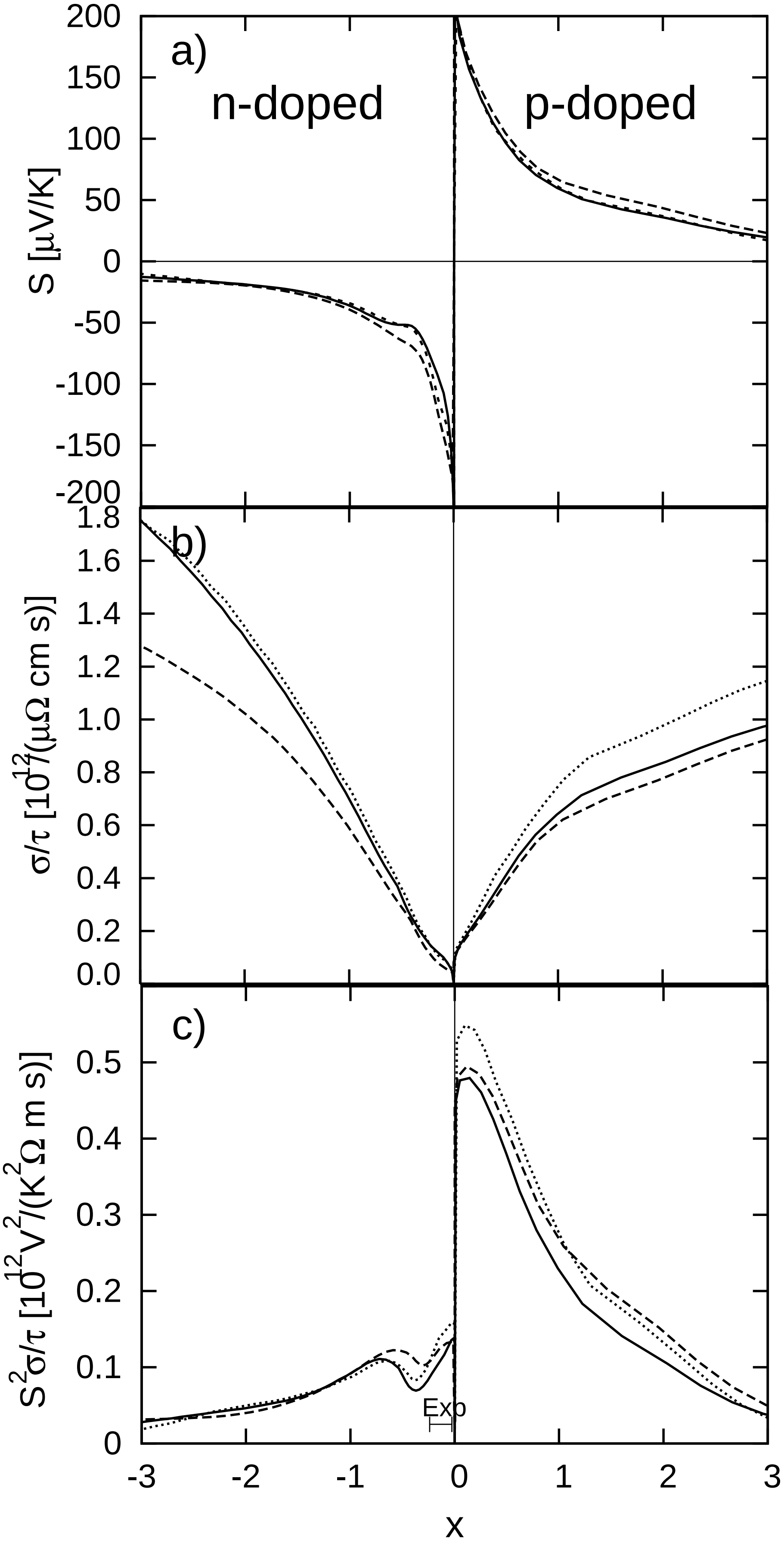


a)
b)
ε [eV]
n(ε) [#states/(u.c. spin eV)]
E_F
Γ
Δ
H
N
Σ
Γ
Λ
P

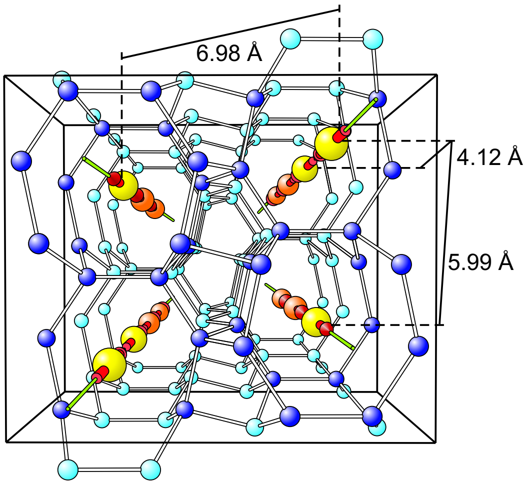


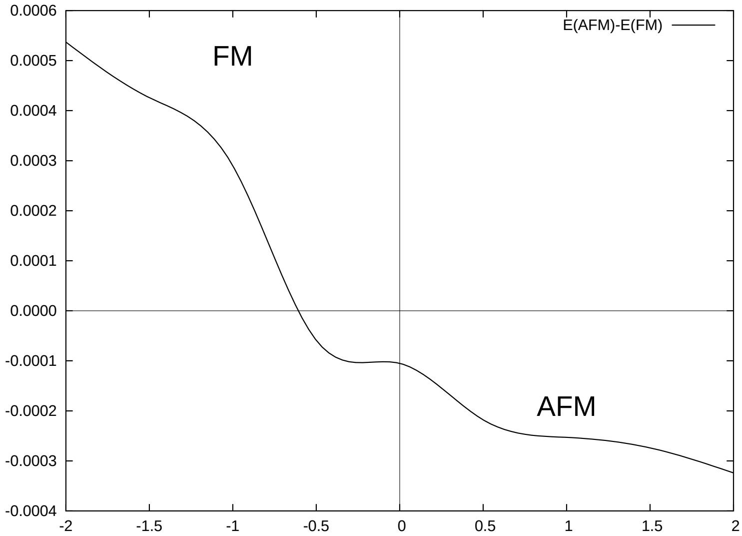
a)
b)

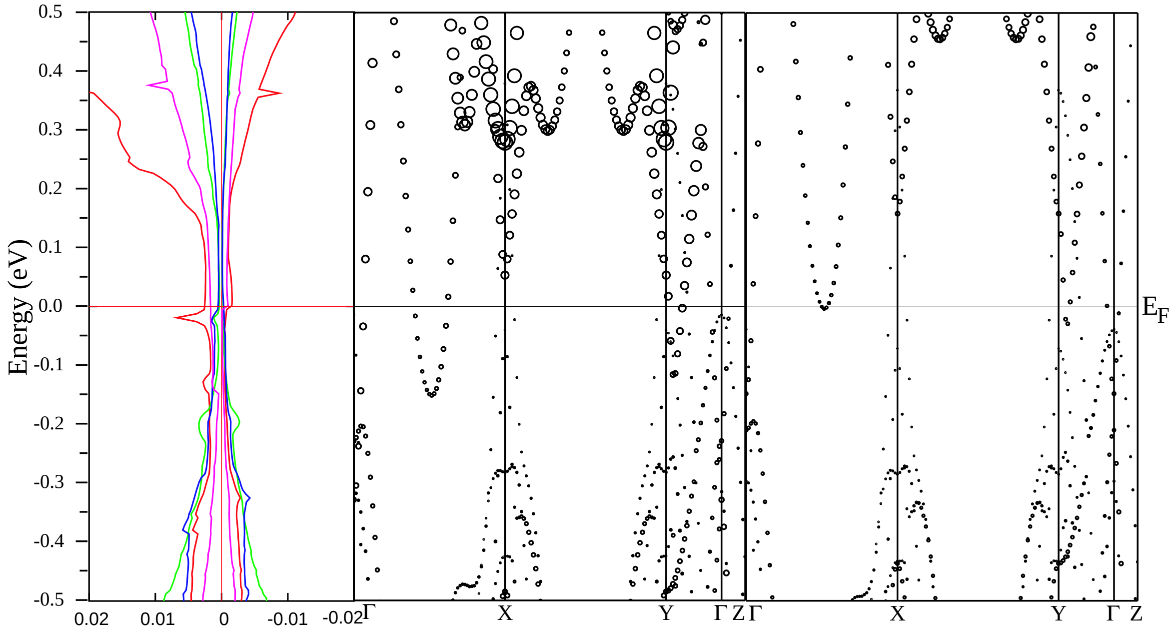
Type-VIII transport

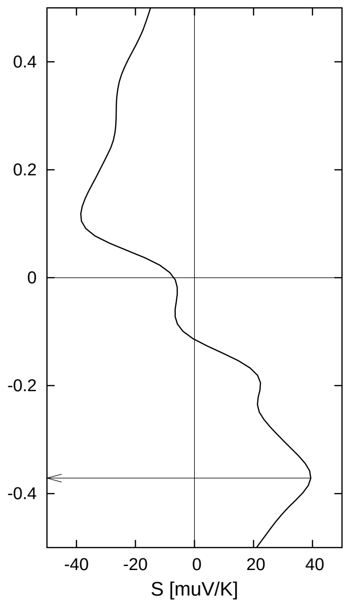


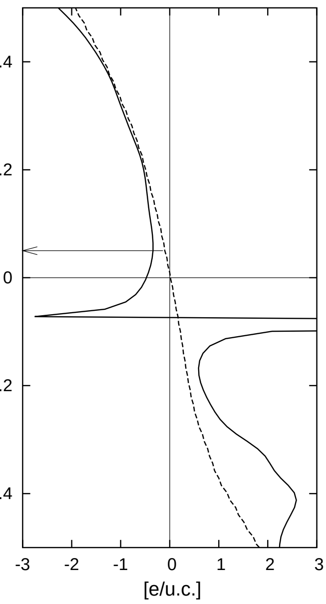
Type-IV AFM clathrate











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