A DMFT insight into the Earth's core: many-electron effects in iron under extreme conditions

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Workshop « Dynamical Mean-Field Theory and Beyond: Recent Developments»

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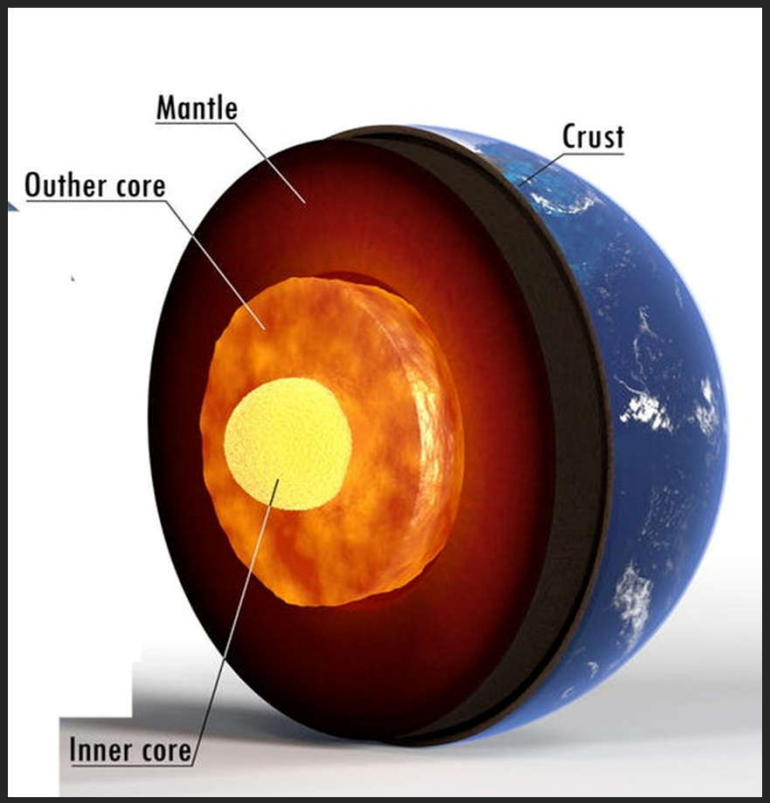
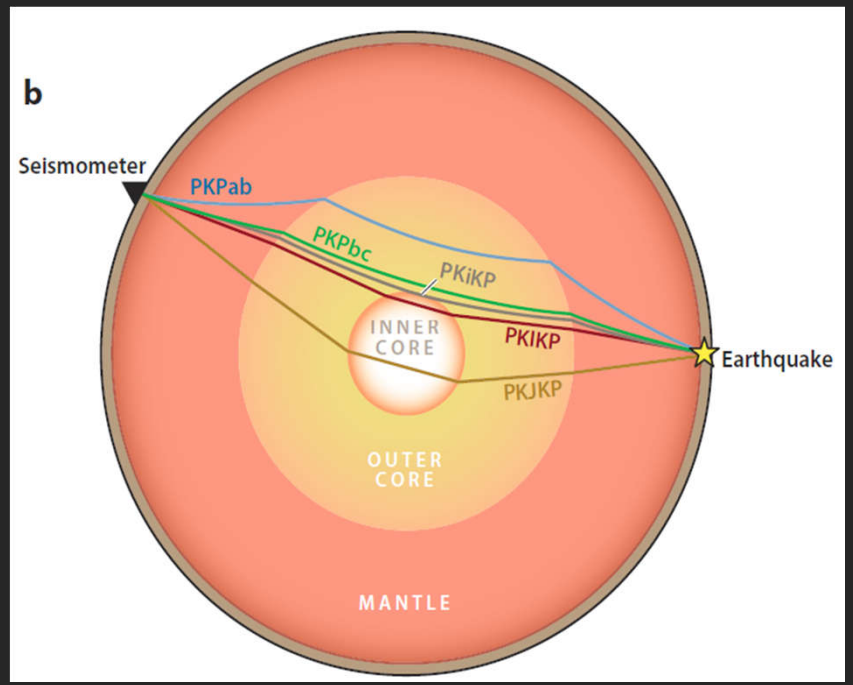
OUTLINE

- Inner core of Earth: iron alloy at extreme conditions
- Electronic correlations in the 3 phases of iron
- Fermi-liquidness and transport in hcp-Fe at Earth core conditions
- Lattice distorsions, correlations and transport in bcc-Fe

Solid inner core of Earth





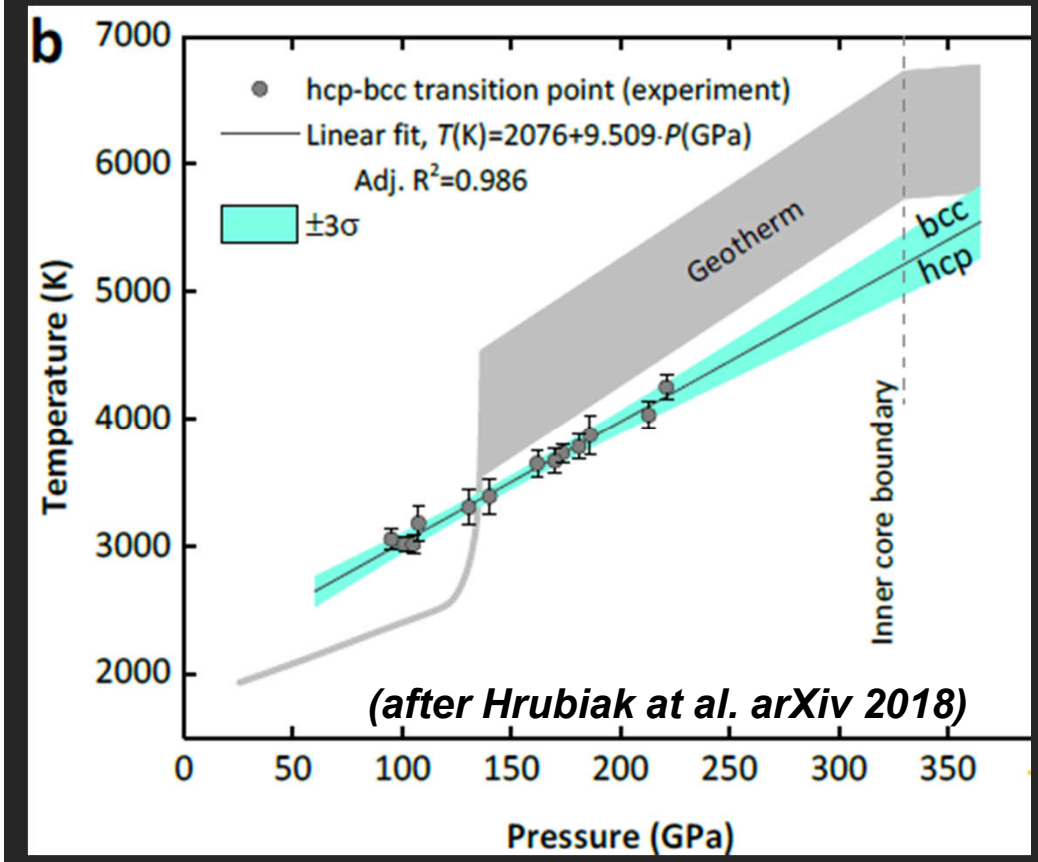
after Deuss Ann. Rev. Ear. Pl. Sci. 2014

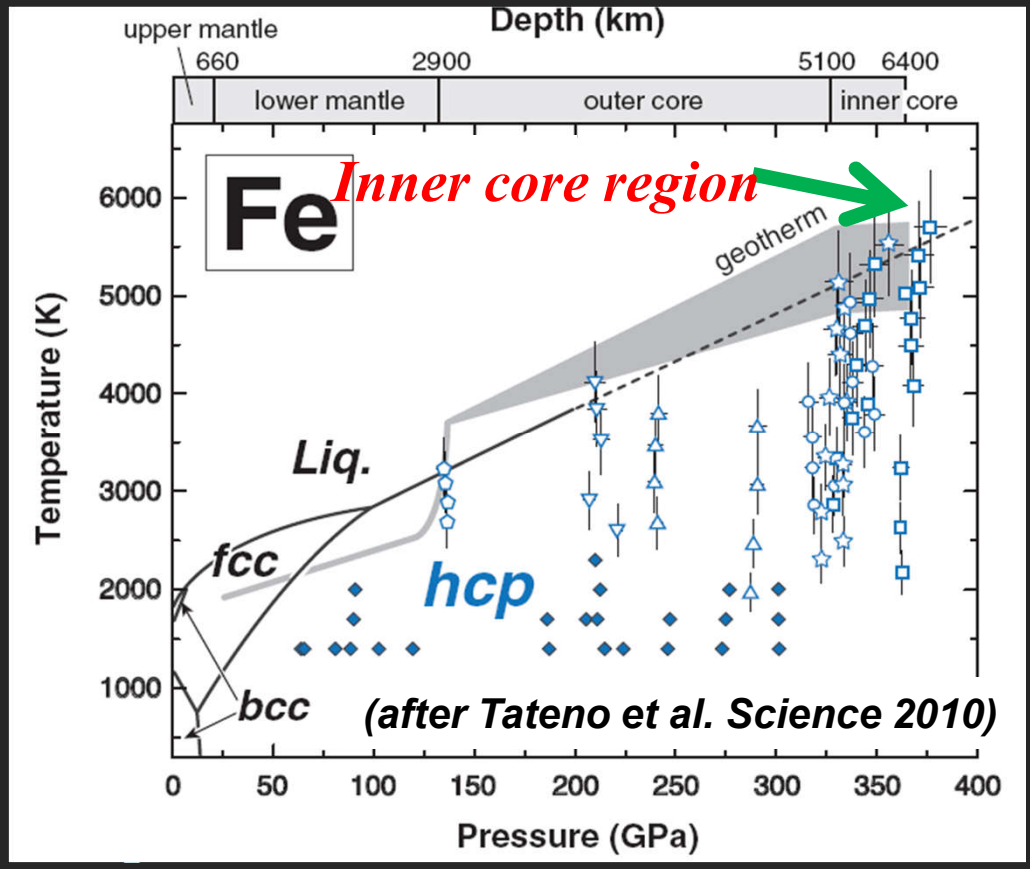
- radius ≈ 1200 km
- density ≈ 13 g/cm^3
- composition:
  mainly Fe+(~5-10% Ni, Si, S, O…)
- temperature 5200÷6500 K (uncertain)
- pressure 330÷370 Gpa
- age: may be < 1 bY
- anisotropy in seismic wave propagation:
- 3-4% faster $\vec{v}$ along spin axis
  (Creager Nature 1992)
  - strong anisotropy (different Fe phases?) in the inner part R < 500 km
  - weak anisotropy in the outmost part; different $\vec{v}$ in hemispheres

Hirose *et al*. Annu. Rev. Earth Planet. Sci. 2013

Tkalčić Rev. of Geophys. 2015

State of iron in the inner core of Earth





Density functional theory (DFT):

bcc α: Belonoshko *et al.* Nature 2004
Luo *et al.* PNAS 2010
Belonoshko *et al.* Nat. Geo. 2017

fcc γ: Mikhaylushkin *et al.* PRL 2007

hcp ε: Vočadlo *et al.*, Nature 2003

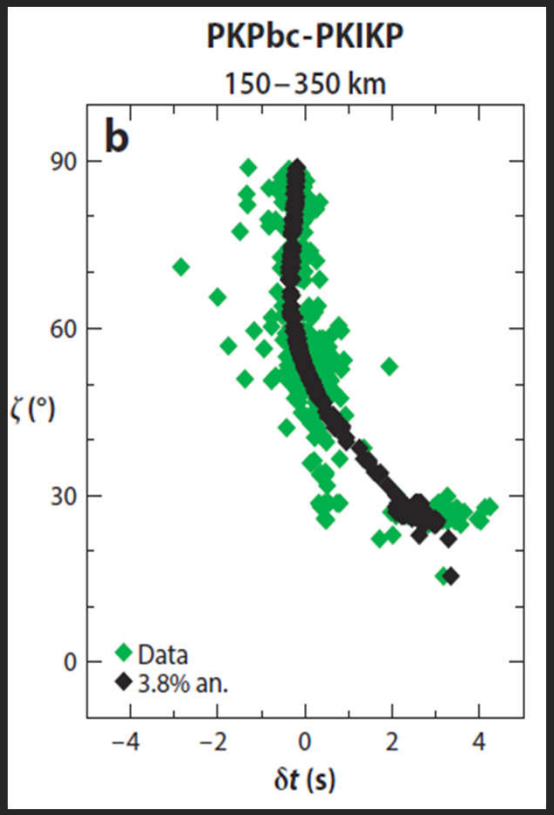
Diamond anvil cell experiments:

bcc ***Fe*** Hrubiak et al. arXiv 2018
$Fe_{0.9}Ni_{0.1}$: Dubrovinsky *et al.* Science 2007

hcp: Tateno *et al.*
Fe *(370 GPa, 5800 K)* : Science 2010
$Fe_{0.9}Ni_{0.1}$: Geophys. Res. Lett . 39 L12305 (2012)

Anisotropy of Fe inside the inner core

Relative velocity vs. angle to the rotation axis

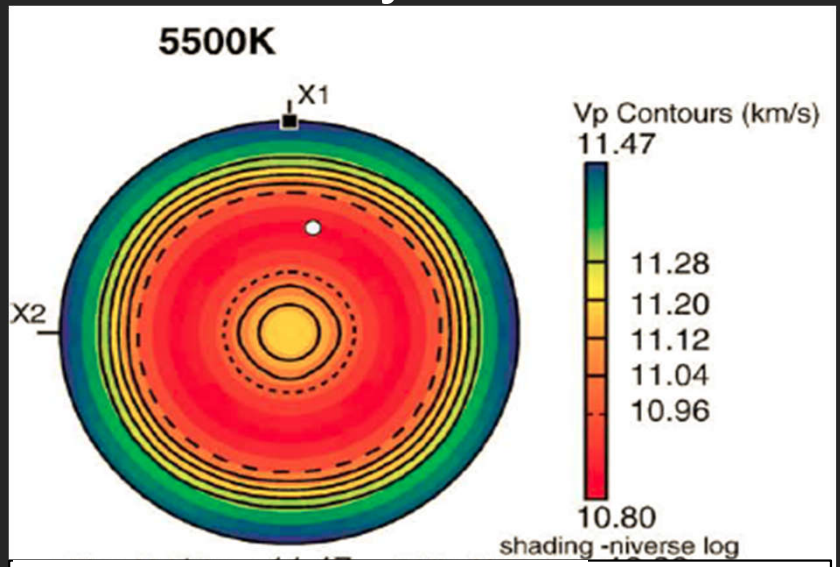


Deuss Ann. Rev. Ear. Pl. Sci. 2014

DFT ab initio molecular dynamics

Vočaldo et al.
Earth. Pl. Sci. Lett. 2009

hcp-Fe: velocity anisotropy sensitive to c/a ratio (hence, T)



Largest velocity in *ab* plain

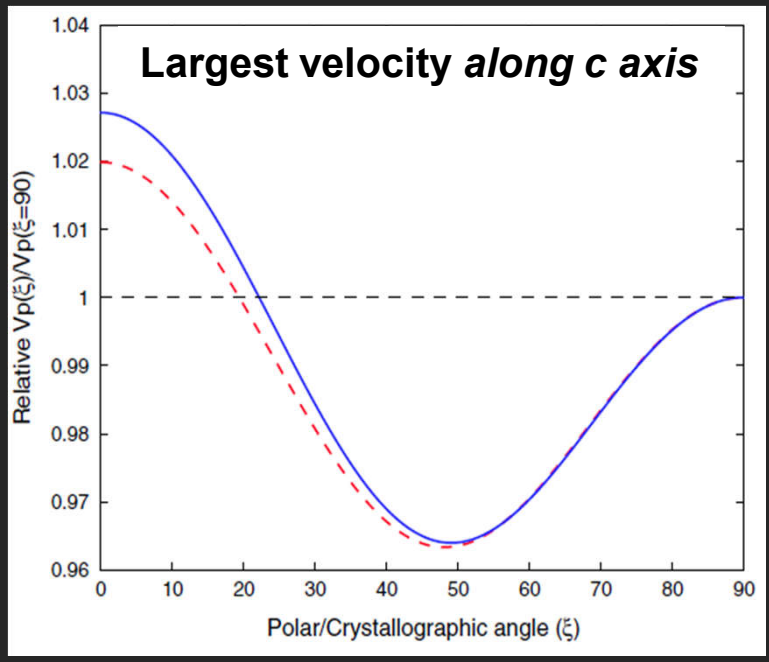
Belonoshko et al. Nature 2004,
Science 2008
Mattesini PNAS 2010

hcp-Fe:

low anisotropy in hcp (high-T c/a ~1.633)

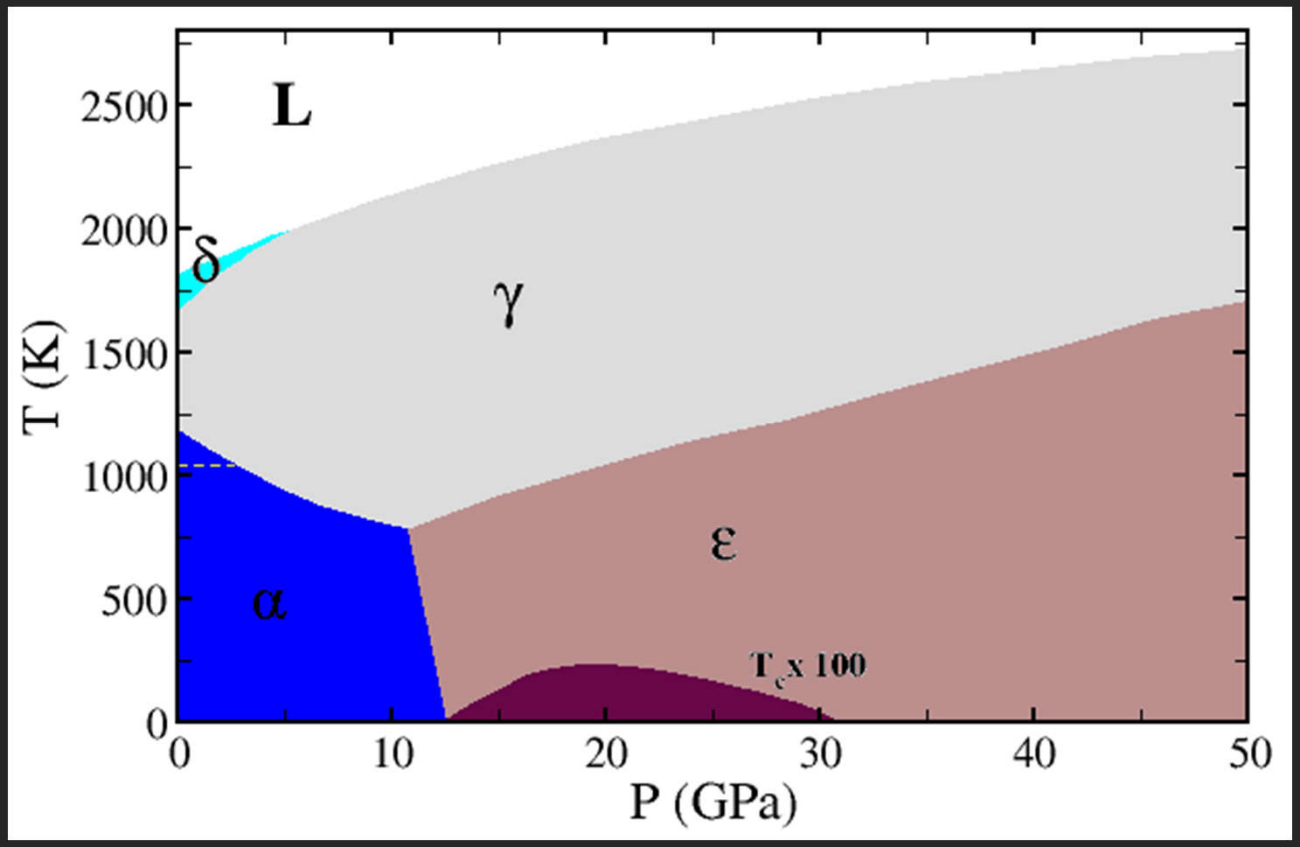
bcc-Fe:

large anisotropy [100] vs. [111]



Iron metal at low P-T and electronic correlations

Low P-T phase diagram of Fe



- α bcc, ground state, FM
- γ fcc, T> 1185 K (P=0)
- δ bcc, T > 1667 K (P=0)
- ε hcp, P-stabilized, paramagnetic, superconducting

- narrow (***W***~6 eV) 3d band hybridized with wide 4s
- ***U*(3d)**≈3-5 eV < ***W*** but large J_H~0.9 eV

α-Fe: moderate QP renormalization (**Z~0.5**) in ARPES and theory

Schäfer et al. 2005
Sànchez-Barriga et al. 2009
, Sànchez-Barriga et al., 09, Sponza et al., PRB 17, Hausoel et al., Nat. Com. 17

PM α-Fe and α→γ transition phonon spectra of PM α and γ

Leonov et al. PRL 11, SciRep. 14, Han et al. PRL 17

FM α-Fe → ε-Fe transition

Pourovskii et al. PRB 2014

Are correlations still relevant at high P and T?

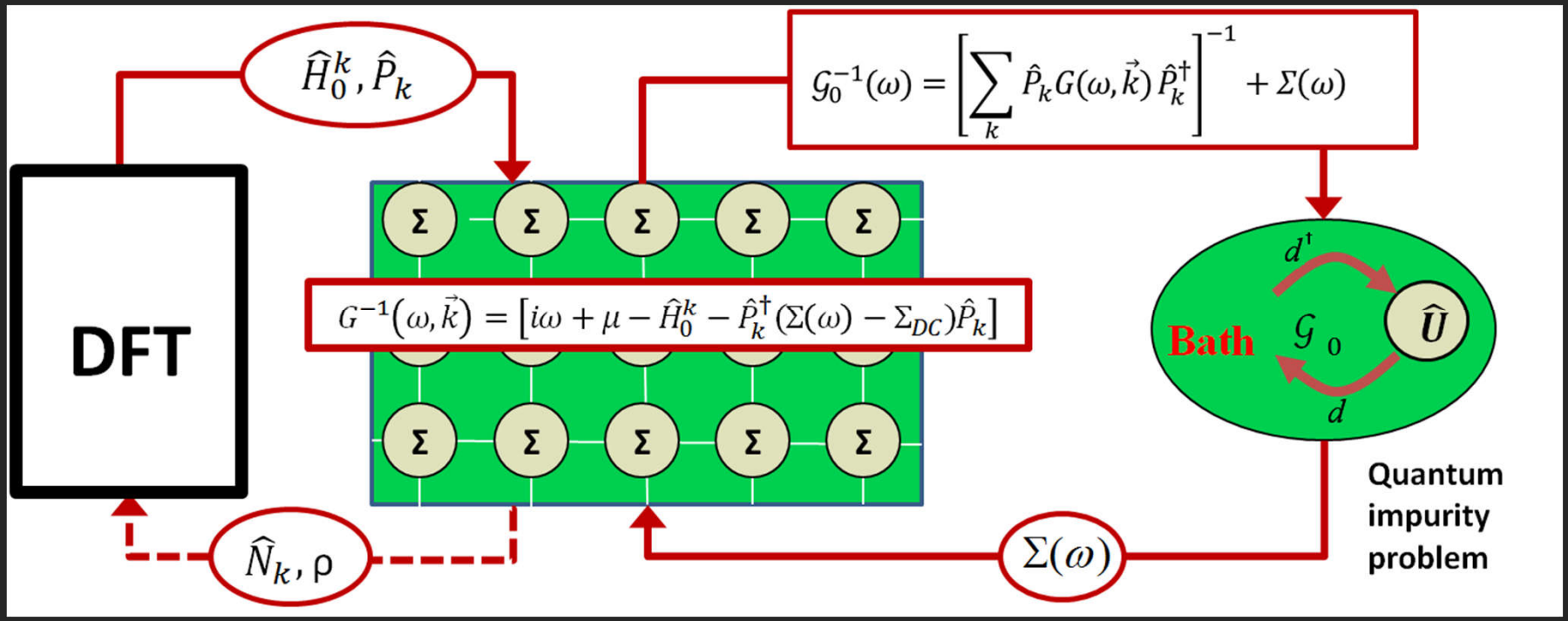
$P\uparrow \Rightarrow V\downarrow \Rightarrow W\uparrow$ and $U/W\downarrow$

at high pressure correlation effects can be ignored

?

- $U/W < 1$ in Fe even at P=0 (but J_H is more important)
- high T stabilizes high-entropy (local moment) phases
- for metals el.-el. scattering $\sim T^2 \rightarrow$ significant at high T

self-consistent DFT+DMFT method



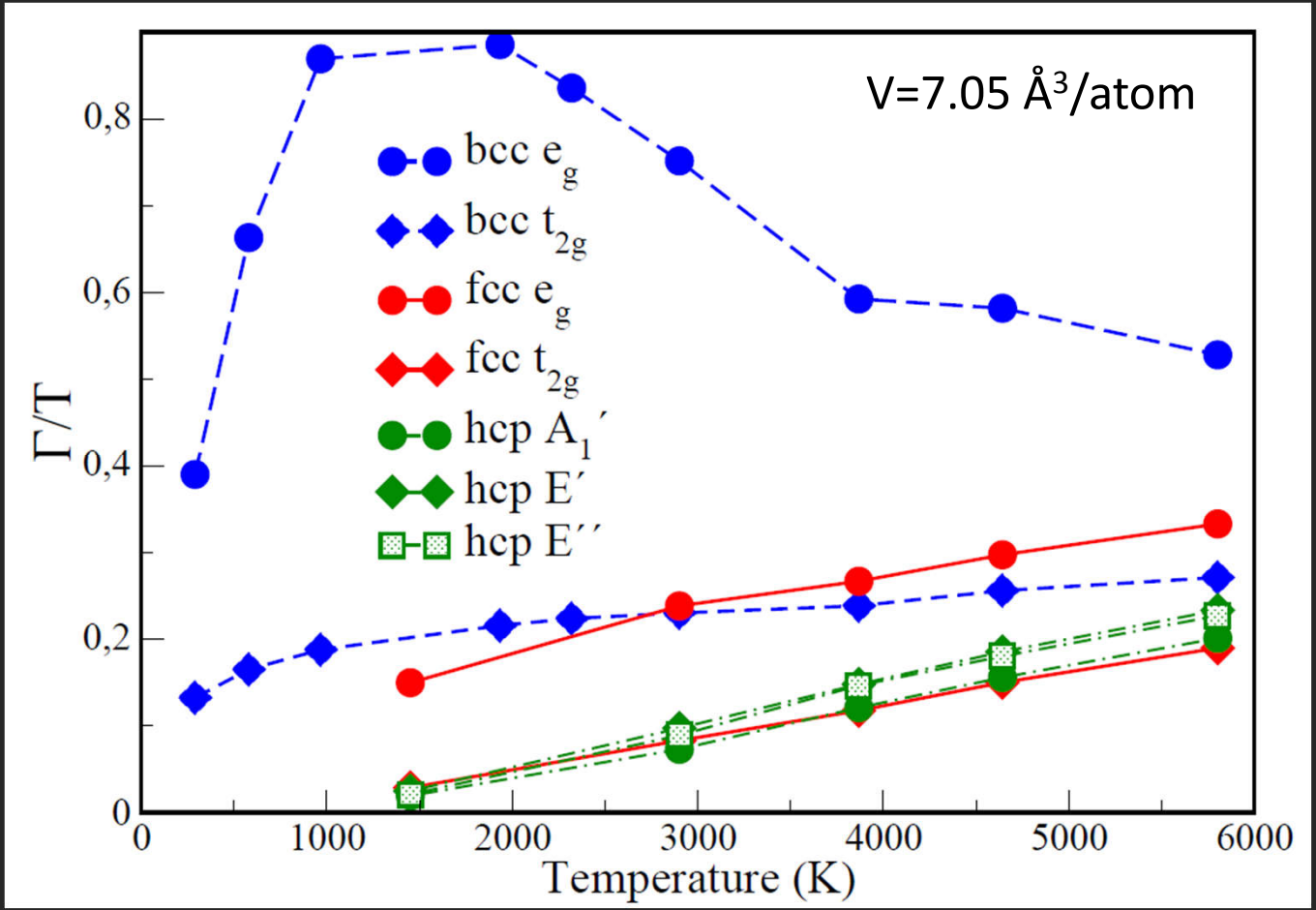
- **hybridization-expansion CT-QMC:** segment picture (mostly),
  full U: Seth *et al.* Comp. Phys. Comm. 2016
- self-consistency over the charge density ρ
- conductivity: Kubo formula neglecting vertex corrections
- Calculation for the Earth core atomic volume 7.05 $\text{Å}^3/\text{atom}$
- U in the range 3.3÷5 eV, J_H~0.9 eV

Fermi-liquid vs. non-Fermi liquid behavior of bcc, fcc and hcp-Fe at extreme conditions

Inverse quasiparticle lifetime:

$\Gamma = Z\, Im[\Sigma(0)] \sim T^2$
in Fermi-liquid (FL) regime

Hence $\Gamma/T \sim T$ in FLs



hcp ε-Fe: Fermi-liquid behavior in the full T range up to 6000 K

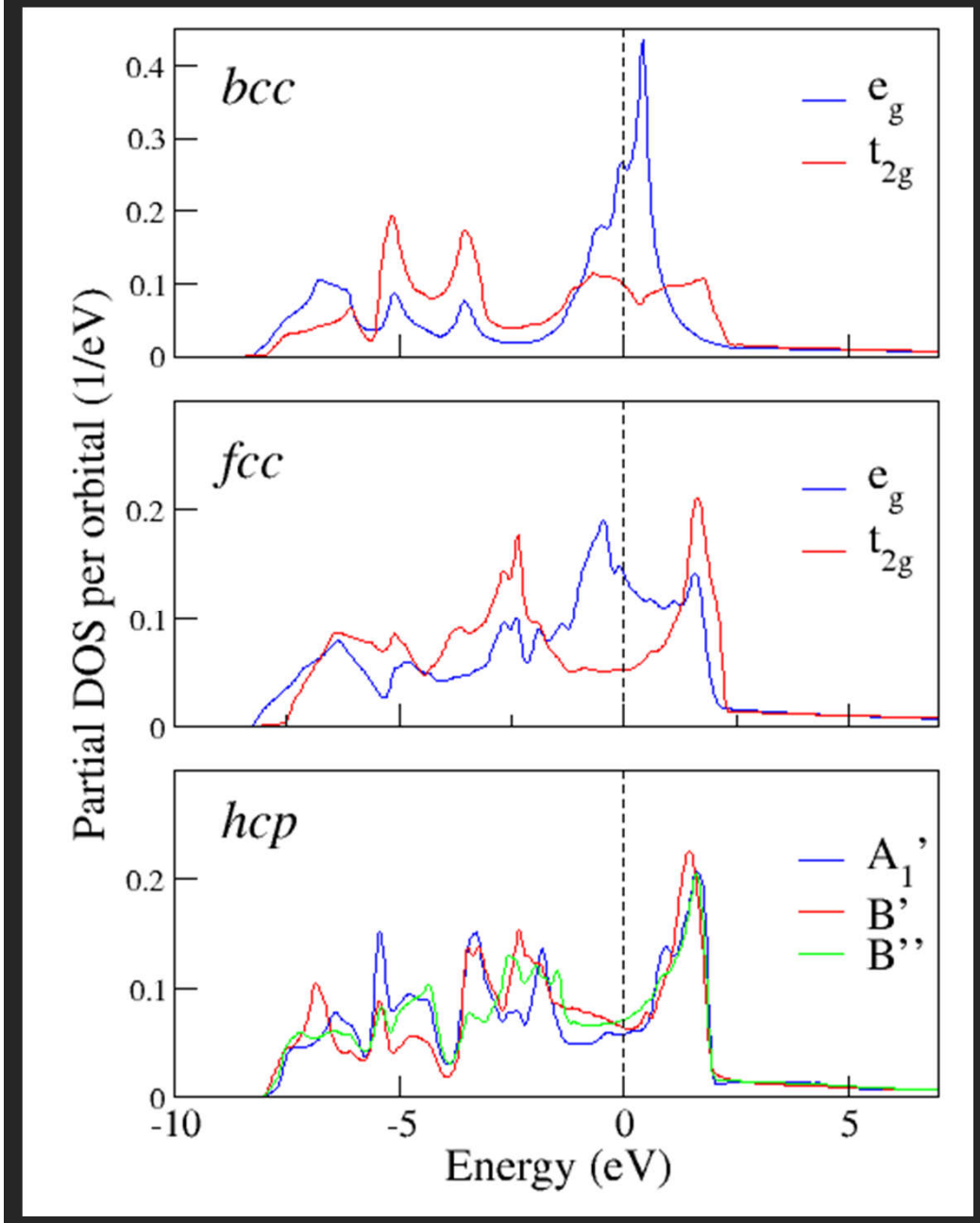
bcc α-Fe: a strongly non-FL behavior for T > 1000 K

fcc γ-Fe: Fermi-liquid in t2g, an intermediate case for eg

Pourovskii *et al.* PRB 2013

Why is the bcc phase more correlated?

DFT DOS



Large peak in bcc DOS due to a Van-Hove singularity

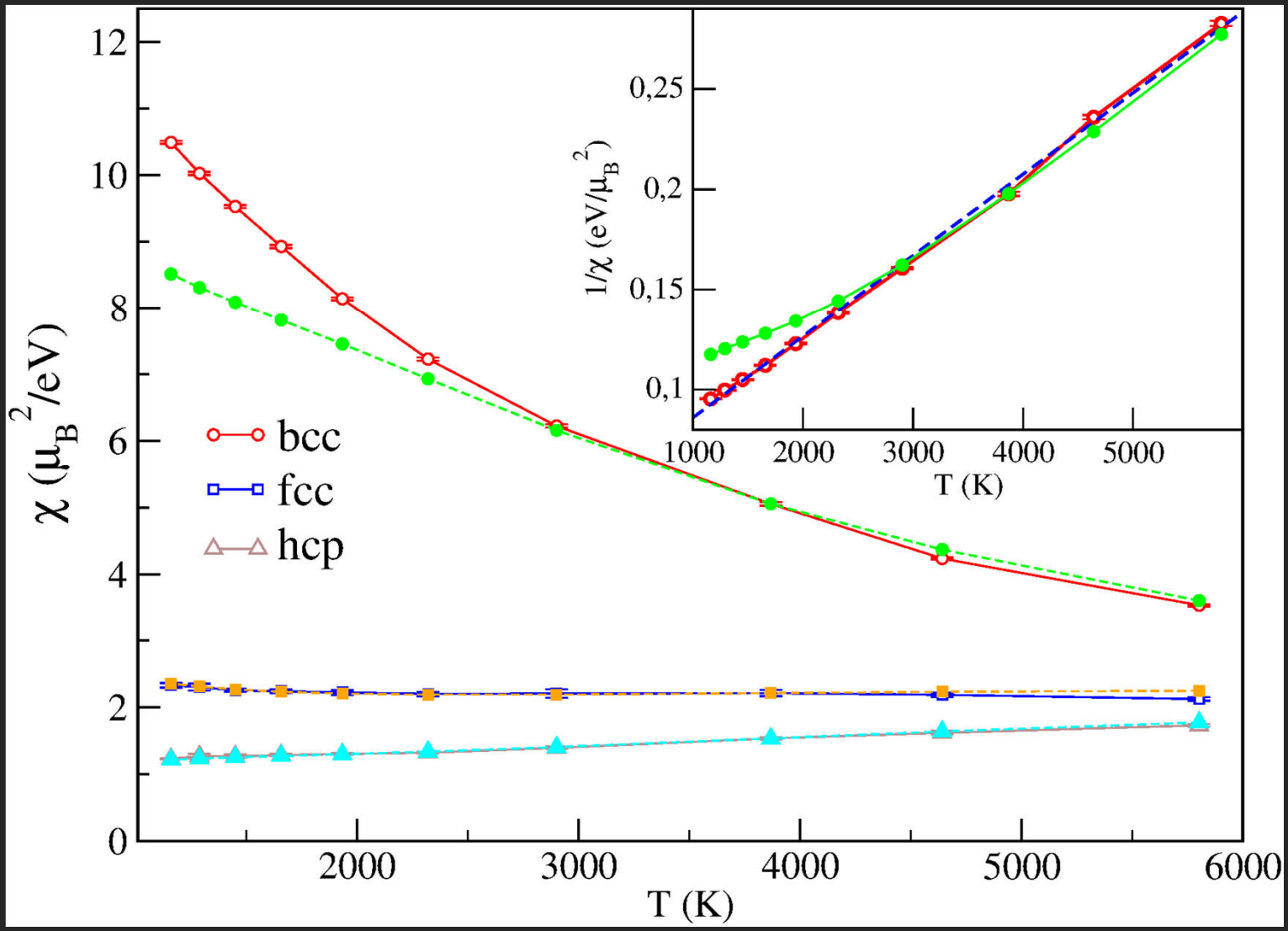
Suppression of hybridization at low E:

$$\mathrm{Im}[\ \Delta(E_F)] \approx -[\pi D(E_F)]^{-1}$$

Enhancement of correlations

Mravlje *et al.* PRL 2011
Leonov *et al.* PRL 2015

Uniform magnetic susceptibility in applied field



- **Pauli behavior**
  fcc and **hcp**
- **Curie-Weiss χ** in **bcc**
  due to a local moment

Earth core thermal conductivity “puzzle”

Low thermal conductivity is necessary to sustain the convection

For the geodynamo (liquid iron)

extrapolation of shock-wave results

Stacey&Andereson Phys. Earth Planet. Inter. 2001

about **30-50 W/(m·K)**

***ab initio* DFT calculations:**

thermal conductivity in liquid Fe:
> 200 W/(m·K)

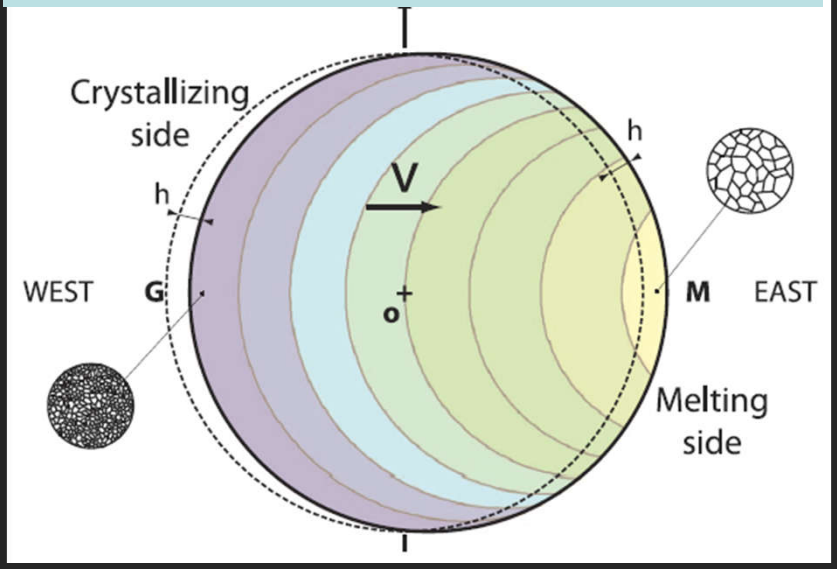
in iron-rich Fe-(Ni)-(Si)-(O):
~ 150 W/(m·K)

DFT calculations of el.-ph. electrical and thermal conductivities:

Pozzo *et al.* Nature 2012, PRB 2013
Earth Planet. Sci. Lett. 2014
de Koker *et al.* PNAS 2012
Shi *et al.* J. Phys. Condens. Matter 2011

Formation of solid core anisotropy

e. g., Monnereau *et al.* Science **2010**



requires κ well below 200 W/(m·K)

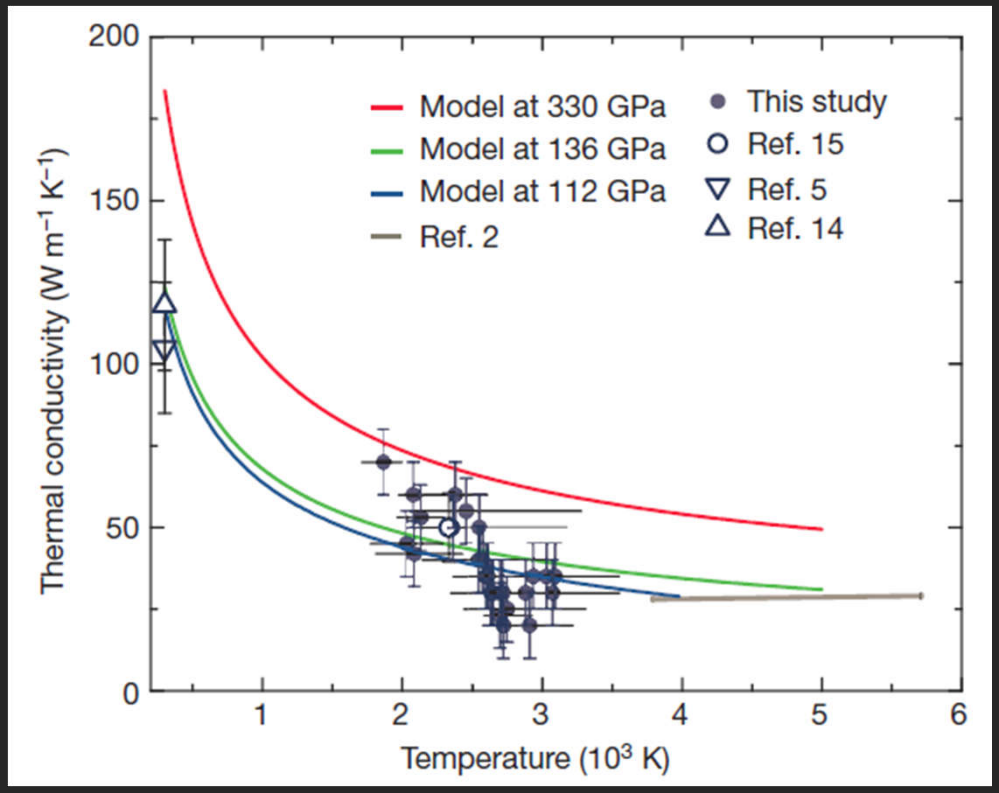
see B. Buffet Nature 2012

***ab initio* DFT value for el-ph κ:**

pure ε-Fe ~300 W/(m·K)
Fe-Si alloy ~235 W/(m·K)

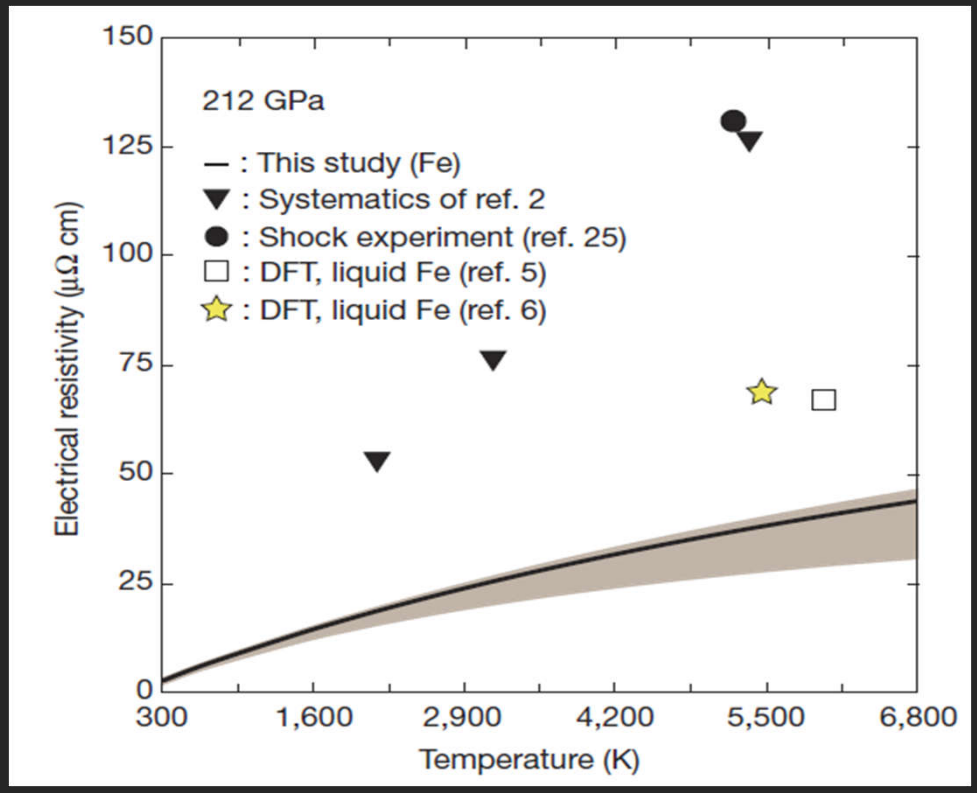
Inconclusive experiments in DAC

Konôpková *et al.* Nature 2016
direct measurements of κ +extrapolation



κ~ 33-50 W/(m·K) for pure ε-Fe at outer core conditions

Ohta *et al.* Nature 2016
direct measurements of ρ +WF law



κ> 200 W/(m·K) for pure ε-Fe at outer core conditions

Theory:

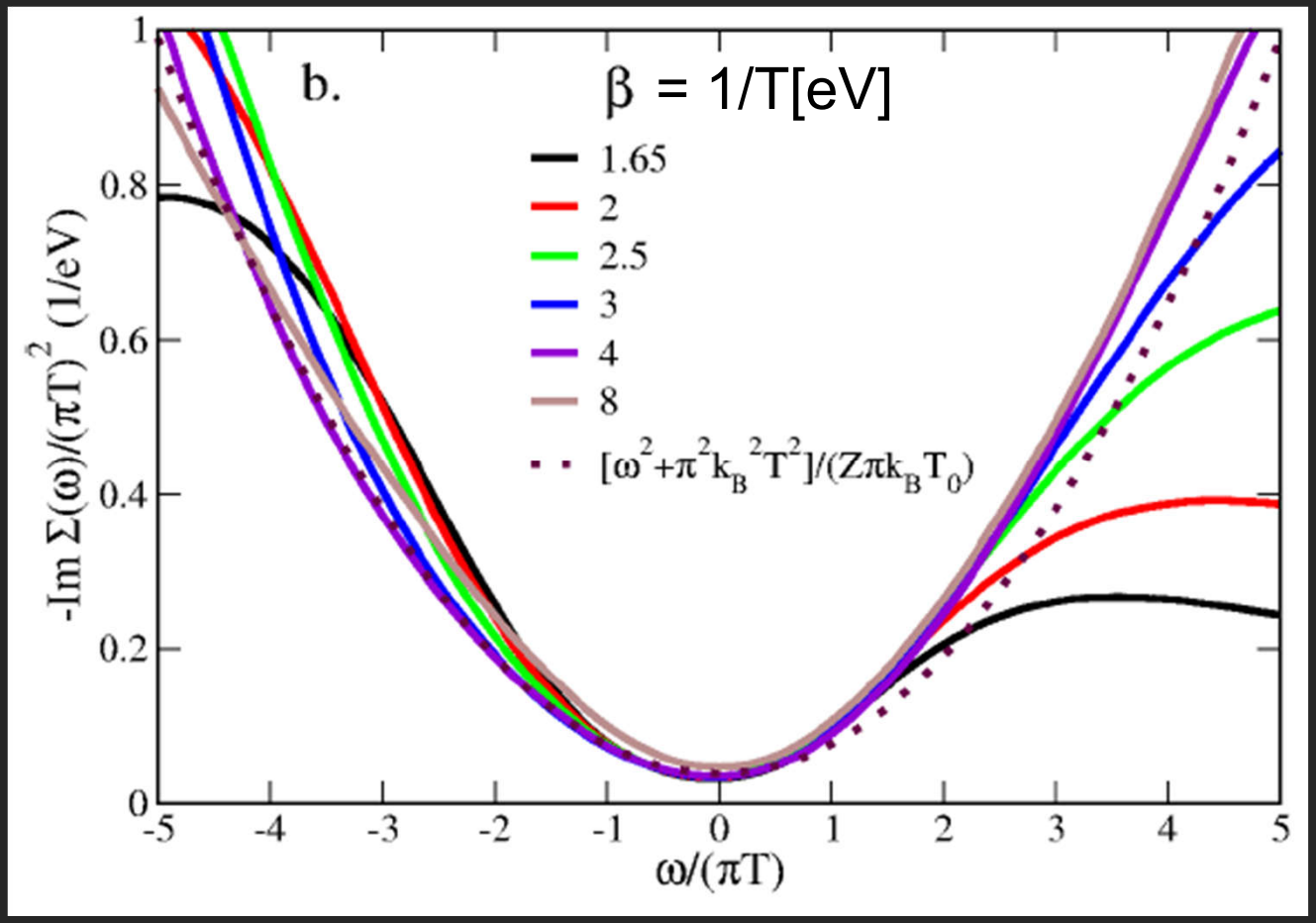
previous *ab initio* DFT calculations: only **electron-phonon scattering** included

what is the contribuiton of **electron-electron scattering**?

Fermi-liquid behavior of ε-Fe: DMFT self-energy at real frequencies

Fermi-liquid behavior of Γ stems from $Im[\Sigma(\omega,T)] = const * (\omega^2 + \pi^2 T^2)$

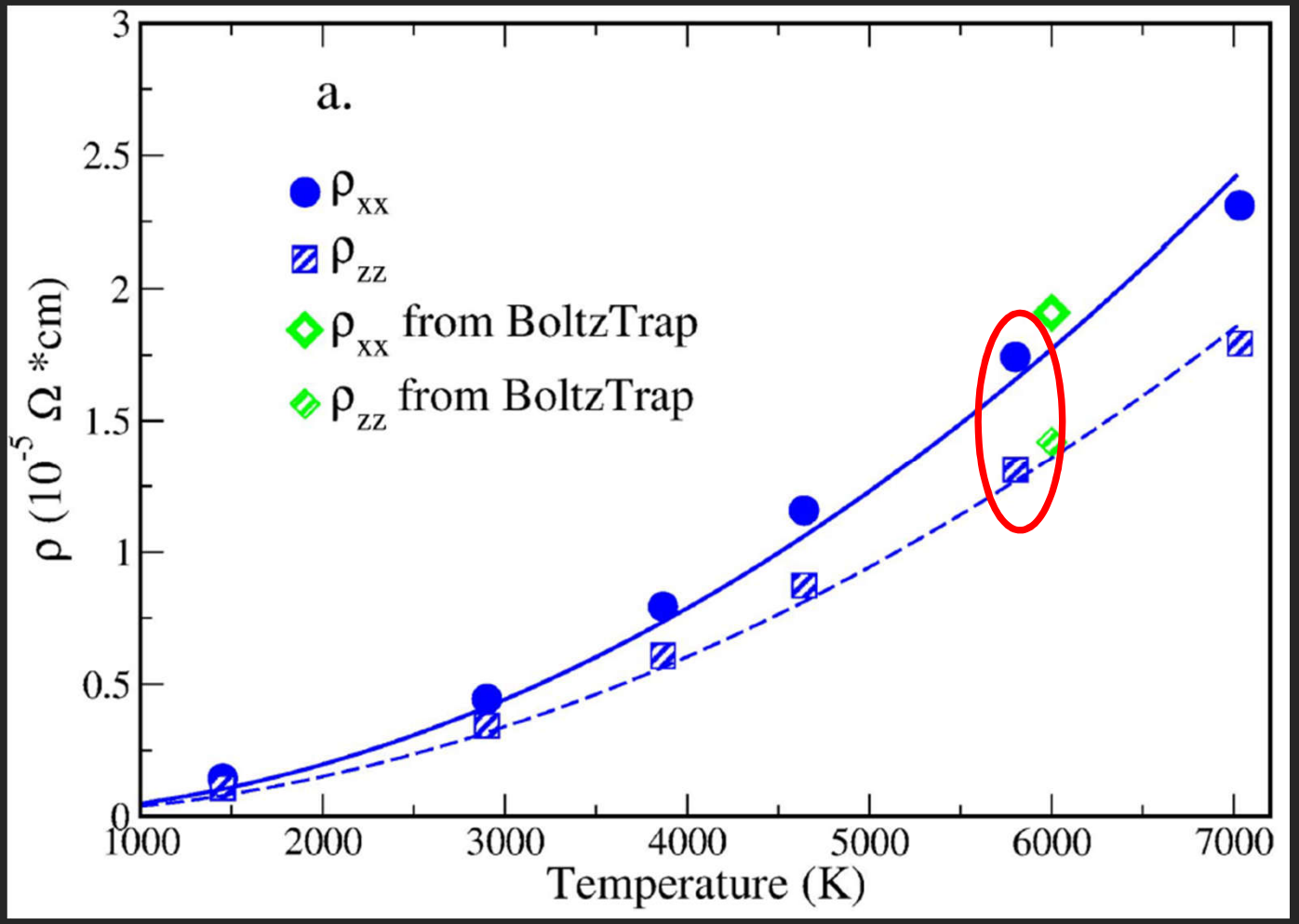
Therefore $\frac{Im[\Sigma(\omega,T)]}{\pi^2 T^2} = const * \left(\left(\frac{\omega}{\pi T} \right)^2 + 1 \right)$



Fermi-liquid temperature scale $T_{FL} \approx 0.1 T_0 = 14\,000$ K

Electron-electron contribution to **electrical** resistivity of ε-Fe: **weak**

Fermi-liquid
$\rho_{ee} \sim T^2$



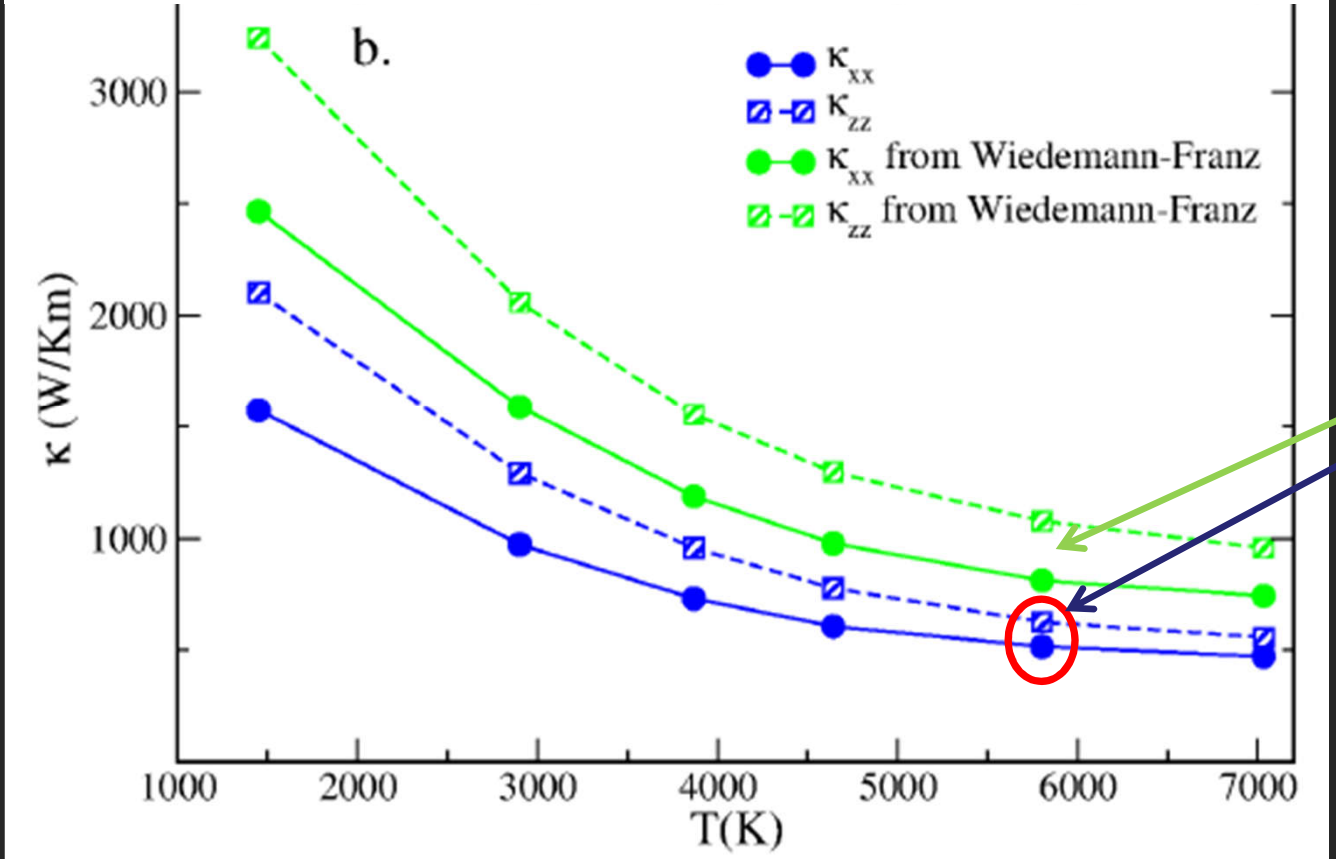
At T~6000 K ρ_{ee} is about 1.6 ·10^{-5}Ω·cm

The electron-phonon $\rho_{e\text{-}ph}$ is about 5.3 ·10^{-5}Ω·cm

from Pozzo *et al.* Earth & Pl. Sci. Let. 2014

Electron-electron contribution to **thermal** resistivity of ε-Fe: **significant**

Thermal conductivity κ_{ee} calculated within DFT+DMFT



Smaller than predicted by Wiedemann-Franz with standard Lorenz number

$$L = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2$$

At T~6000 K $\kappa_{ee} \approx$ **540 W/(m·K)**

Electron-phonon $\kappa_{e\text{-}ph} \approx$ **300 W/(m·K)** **from Pozzo *et al.* Earth & Pl. Sci. Let. 2014**

Total $\kappa_{tot} = \left(1/\kappa_{e-ph} + 1/\kappa_{ee}\right)^{-1} \approx$ **190 W/(m · K)**

Reduction of the Lorenz number in Fermi liquids

In the semi-classical Boltzmann formalism:

$$\sigma = e^2 \int d\epsilon \Phi(\epsilon)(-f'(\epsilon))\tau(\epsilon)$$

$$\kappa = \frac{1}{T} \int d\epsilon \epsilon^2 \Phi(\epsilon)(-f'(\epsilon))\tau(\epsilon)$$

and $\kappa/(\sigma T) = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2 = L$, in SI units $2.44 \cdot 10^{-8} W\Omega K^{-2}$

assuming frequency-independent lifetime τ

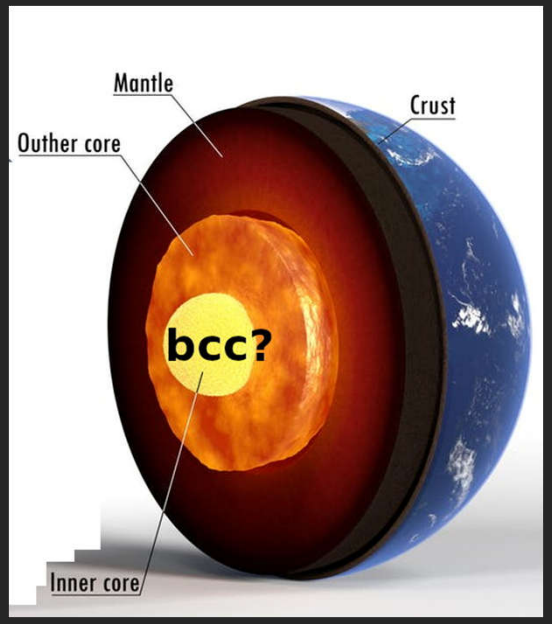
But in Fermi liquids frequency dependence of τ_{ee}~1/Im[Σ(ω)] is strong

$$1/\tau(\epsilon) = 1/\tau(\epsilon = 0) \cdot (1 + \epsilon^2/\pi^2 T^2 k_B^2)$$

and additional ϵ^2 in κ enhances contributions of high frequencies.

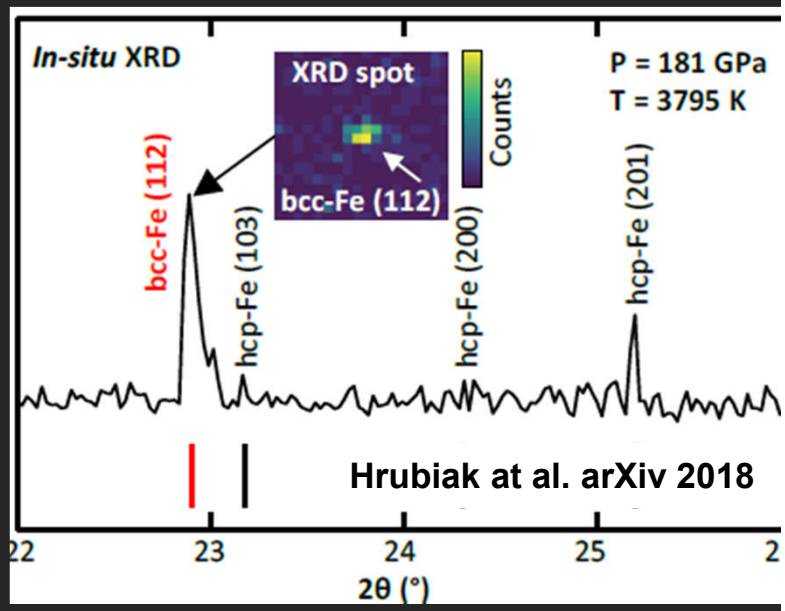
One obtains $\kappa/(\sigma \cdot T) = L/1.54 = L_{FL}$ **thus significanlty reducing** κ

Electron correlations and conductivity in bcc-Fe



- bcc-Fe observed(?) in anvil cell experiments
  Dubrovinsky et al. Science 2008
  Hrubiak et al. arXiv:1804.05109
- dynamically unstable in the harmonic approximation at high P
- **can be stablized by unharmonic vibrations**

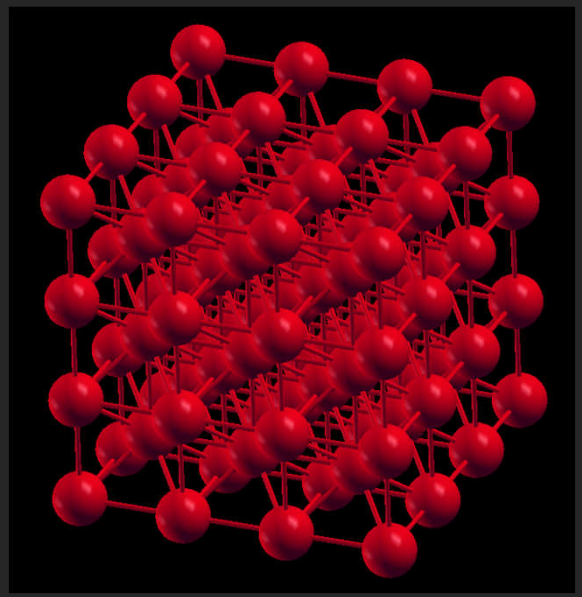
Belonoshko et al. Nat. Geo 2018



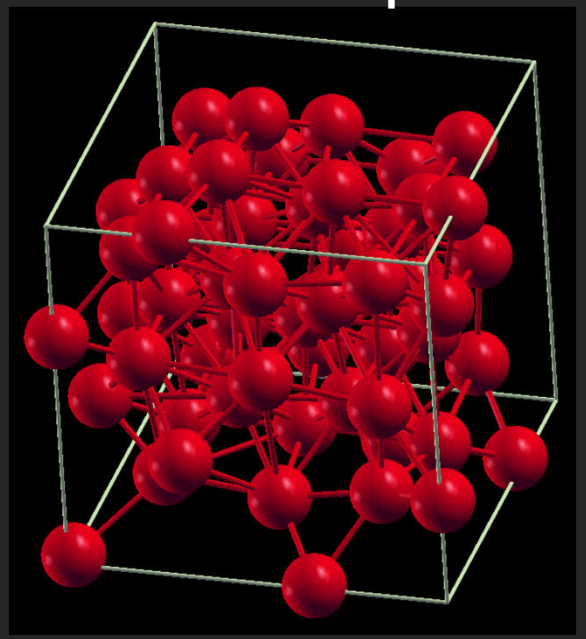
fixed lattice calculations not reliable for bcc!

1. **perform *ab initio* DFT mol. dynamics (MD) simulations**
2. **run DFT+DMFT for a set of MD snapshots**

3x3x3 undistorted



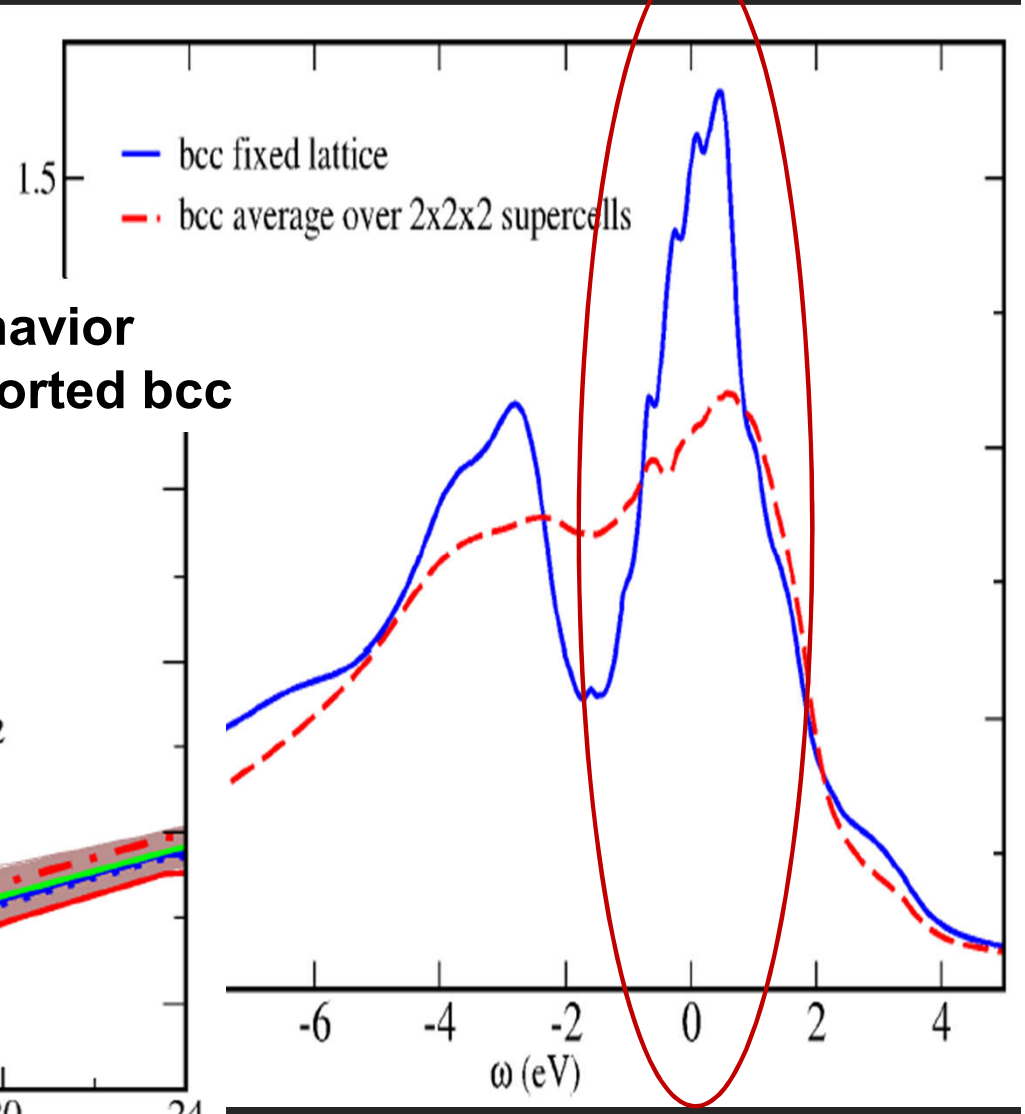
3x3x3 MD snapshot



non-Fermi-liquid effects in bcc washed away by lattice distorsions!

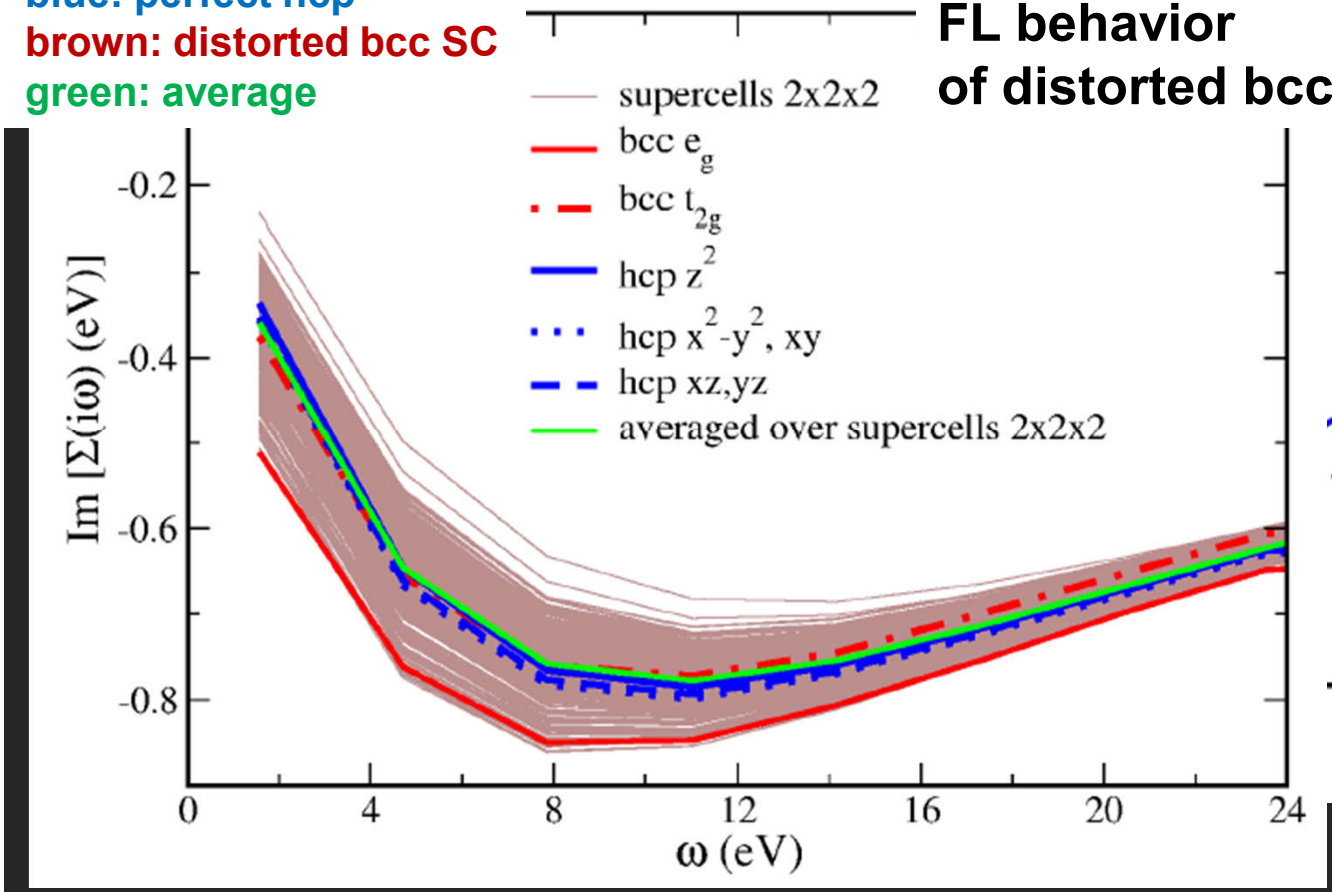
bcc-Fe DFT DOS at EIC volume

- van Hove singularity due to drives nonFL behavior of **e_g orbitals**
- it's almost washed away by lattice vibrations

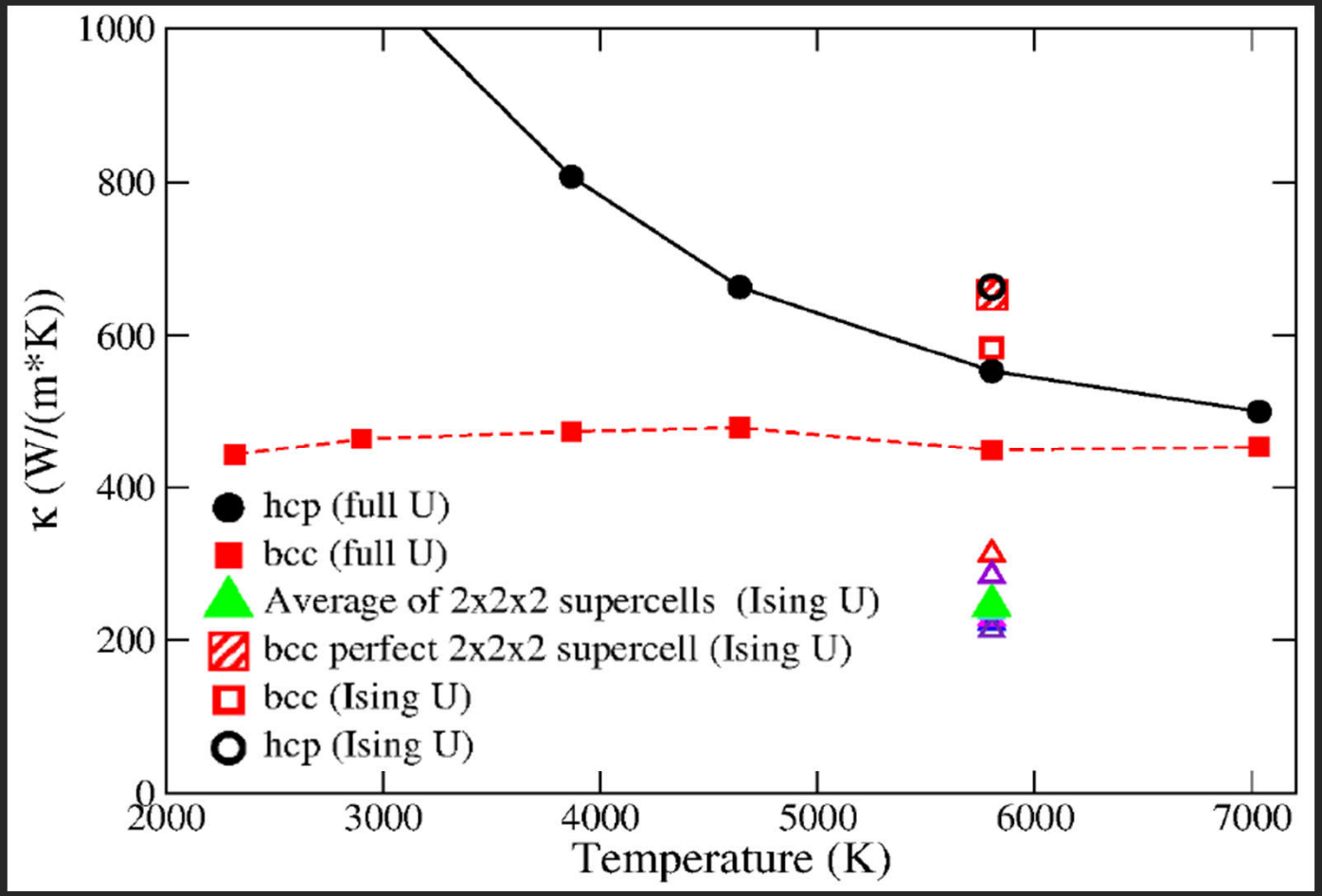


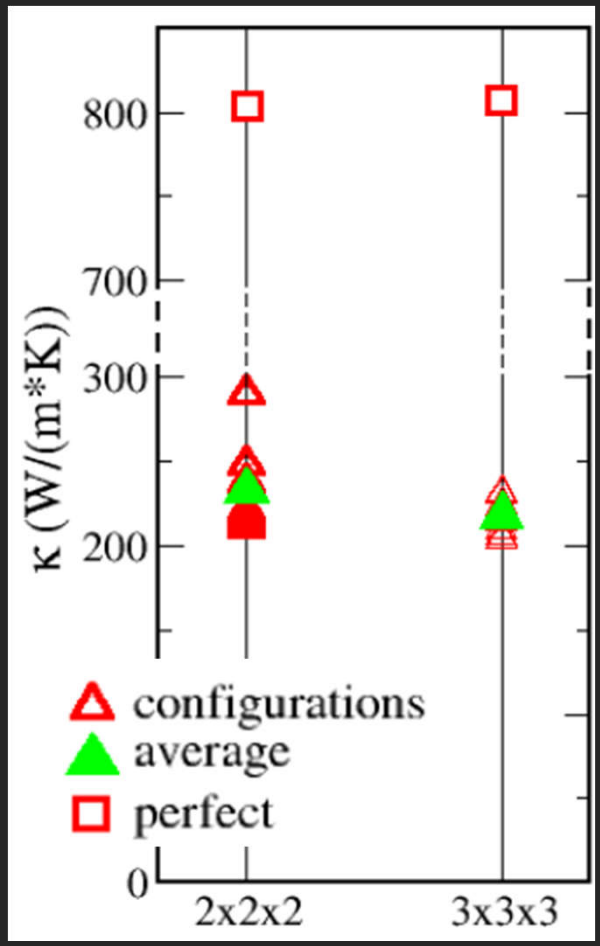
red: perfect bcc
blue: perfect hcp
brown: distorted bcc SC
green: average

FL behavior of distorted bcc



bcc-Fe: Suppression of conductivity by distortions



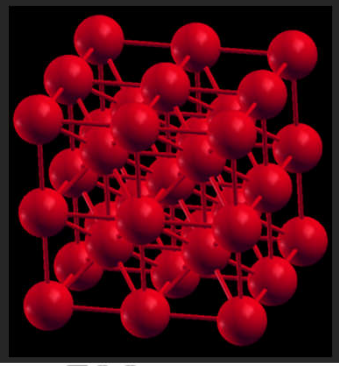


thermal conductivity of fully distorted cells **~4 times lower** than in perfect bcc

can be understood $\frac{1}{\kappa_{tot}} = \frac{1}{\kappa_{latt}} + \frac{1}{\kappa_{el.-el.}}$

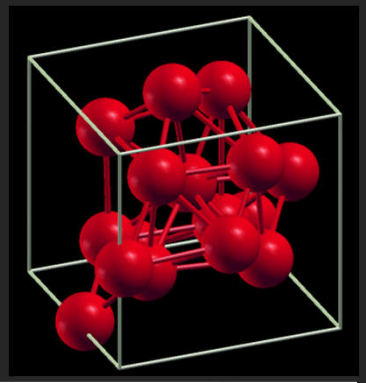
where κ_{latt} ≈280 W/(m·K), $\kappa_{el.-el.}$ ≈800 W/(m·K)

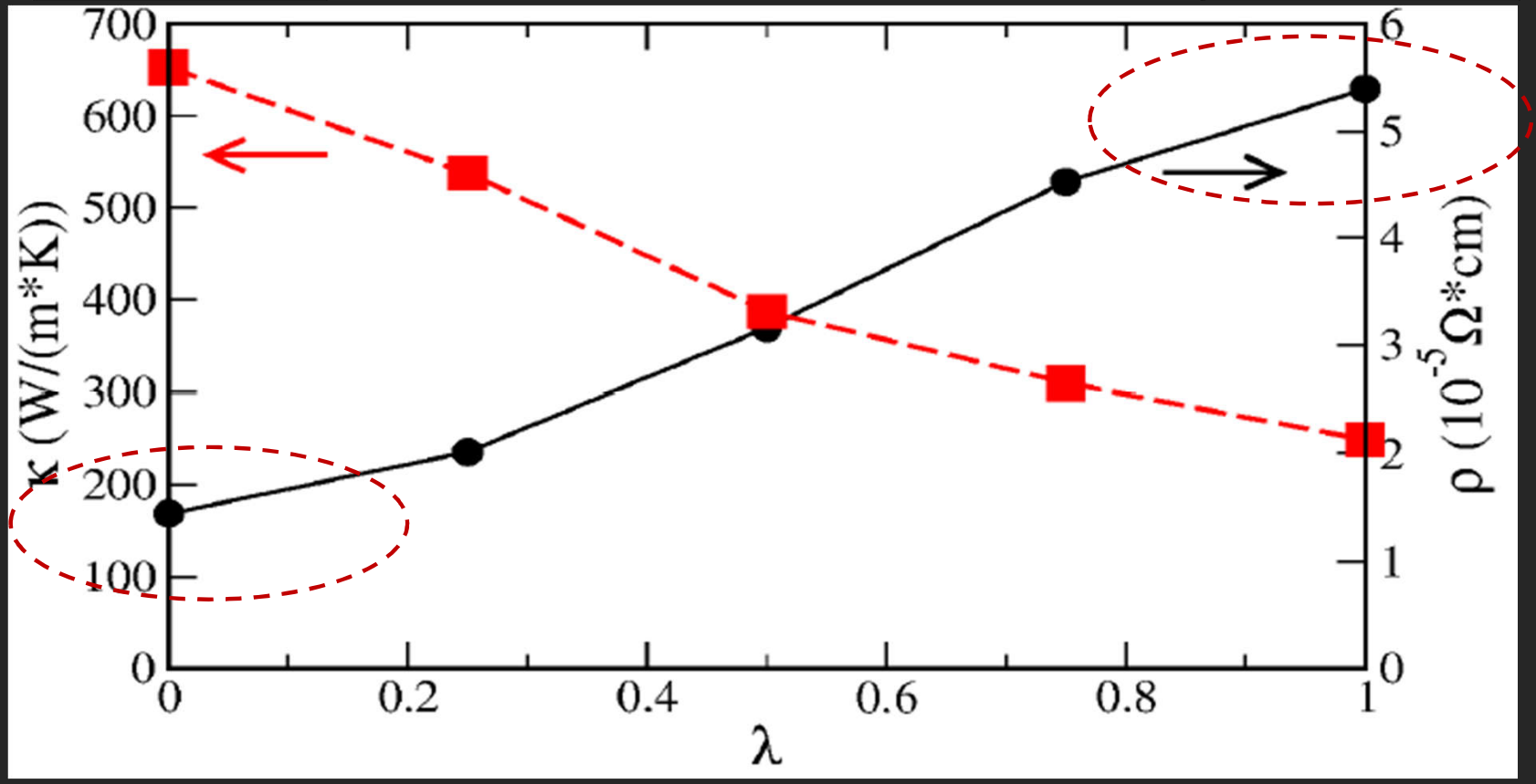
Electrical and thermal resistivity vs. distorsions



distorsion level defined by $\lambda \in [0:1]$

λ



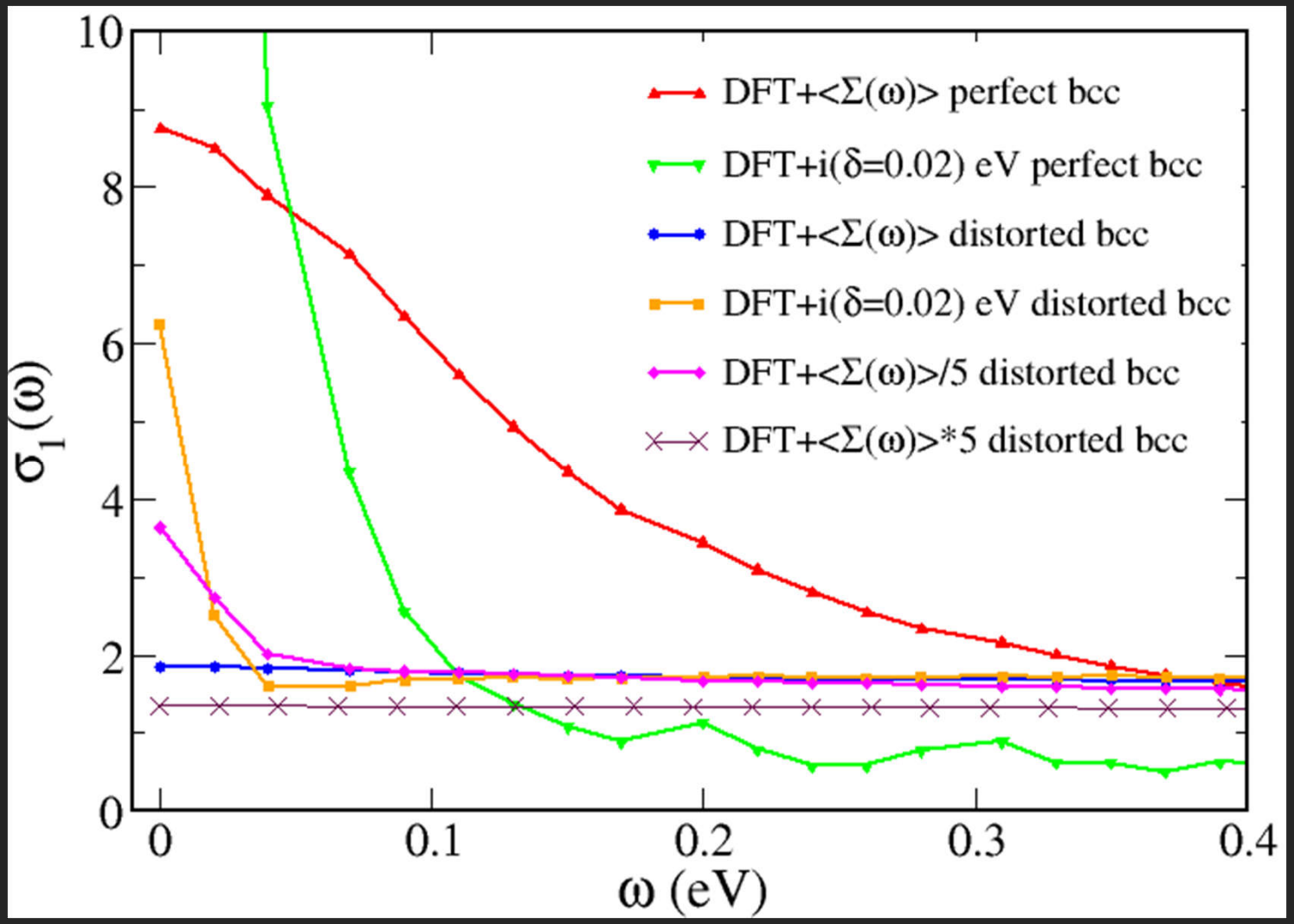


$\lambda = 0$: transport is determined by electron-electron scattering

$\lambda = 1$: **what determines the conductivity?**

Optical conductivity vs. distorsions in bcc Fe

optical conductivity for perfect and fully distorted case **for different $\Sigma(\omega)$**:



- small flat Im Σ
- supercell $\langle\Sigma(\omega)\rangle$
- $\langle\Sigma(\omega)\rangle$ scaled up or down

In the distorted limit enhancing $\langle\Sigma(\omega)\rangle$ seems to have little impact

the conductivity is fixed by the distorsion levels

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  J. Mravlje
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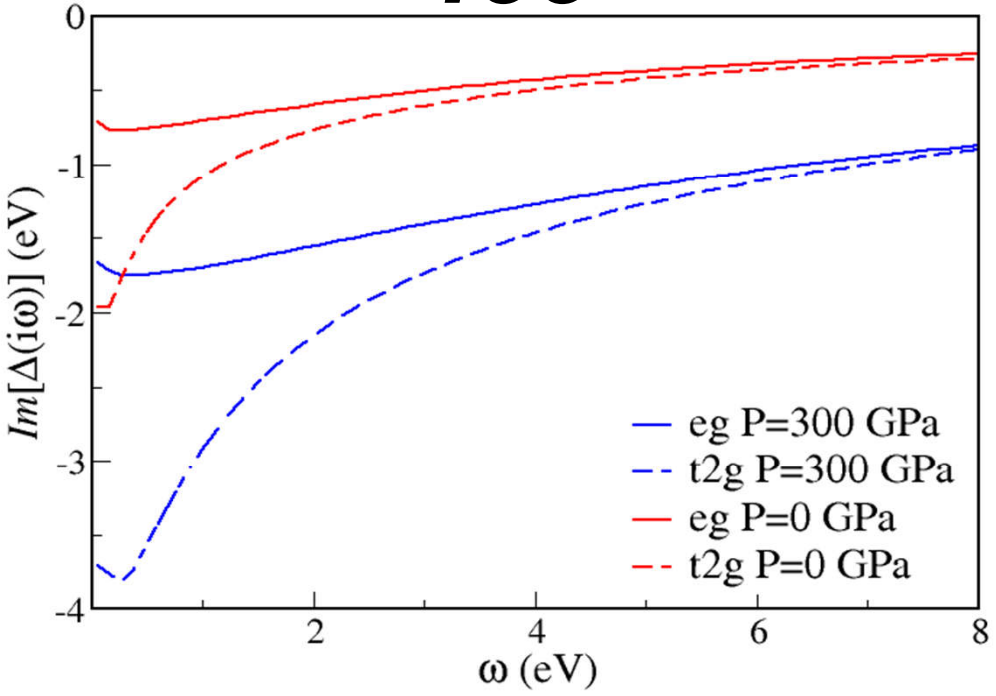
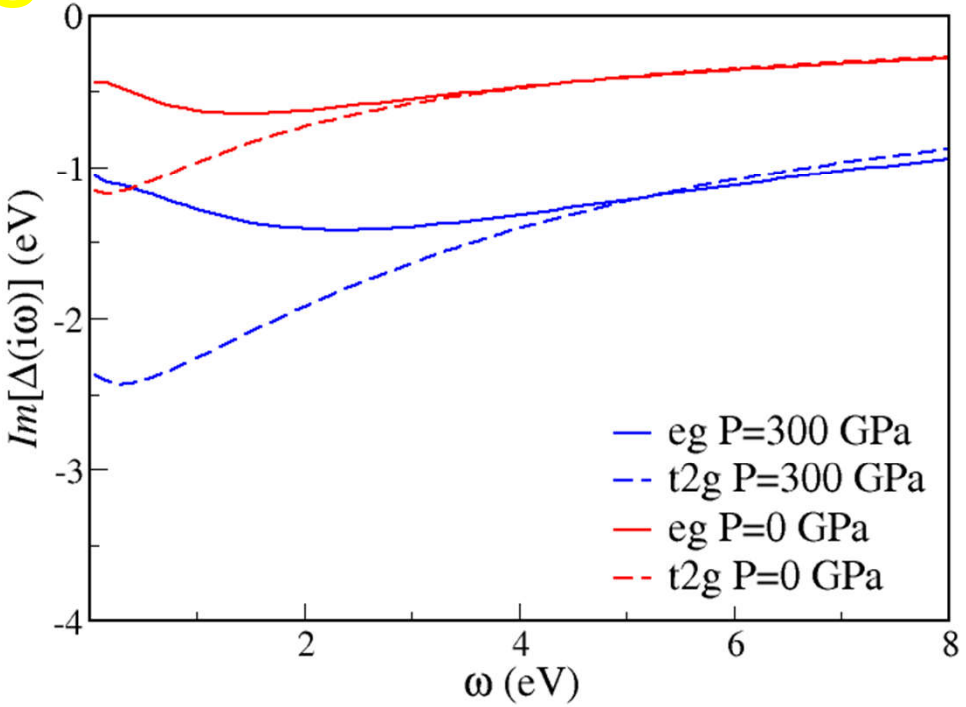
References

LP, Miyake, Simak, Ruban, Dubrovinsky, Abrikosov PRB **87,** 115130 (2013)
Vekilova, LP, Abrikosov, Simak, PRB **91,** 245116 (2015)
LP, Mravlje, Georges, Simak, Abrikosov, New J. Phys. **19,** 073022 (2017)
LP, Mravlje, Alfe … (in preparation)

review: LP Ψ_k Highlight 11/2018 & Topical Review JPCM (in press)

bcc Fe: hybridization suppression at low energies





Large peak in bcc DOS due to a Van-Hove singularity

Suppression of hybridization at low

$$\mathrm{Im}[\ \Delta(E_F)] \approx -[\pi D(E_F)]^{-1}$$