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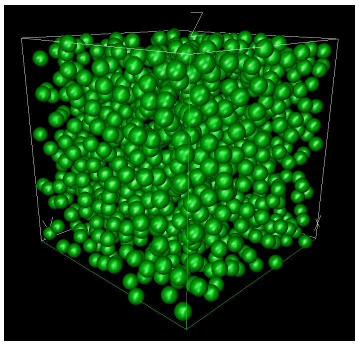

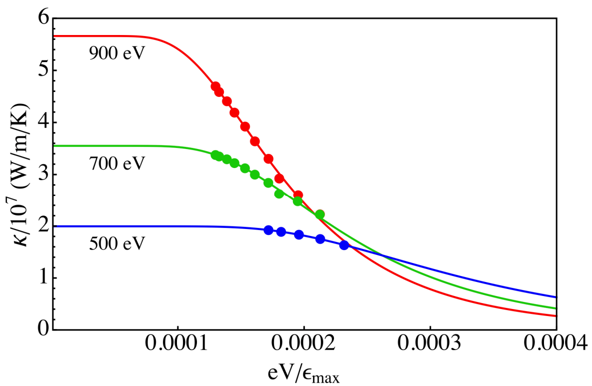

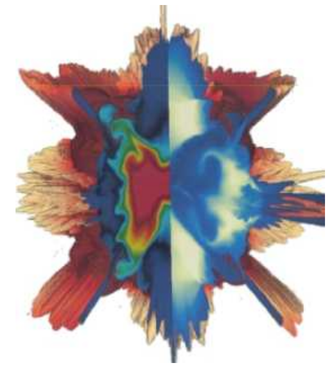

Development of a wide-range electrical and thermal conductivity model for ICF applications

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Cimarron

WDM 2017

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Simulations of ICF capsule implosions have reached a high level of sophistication

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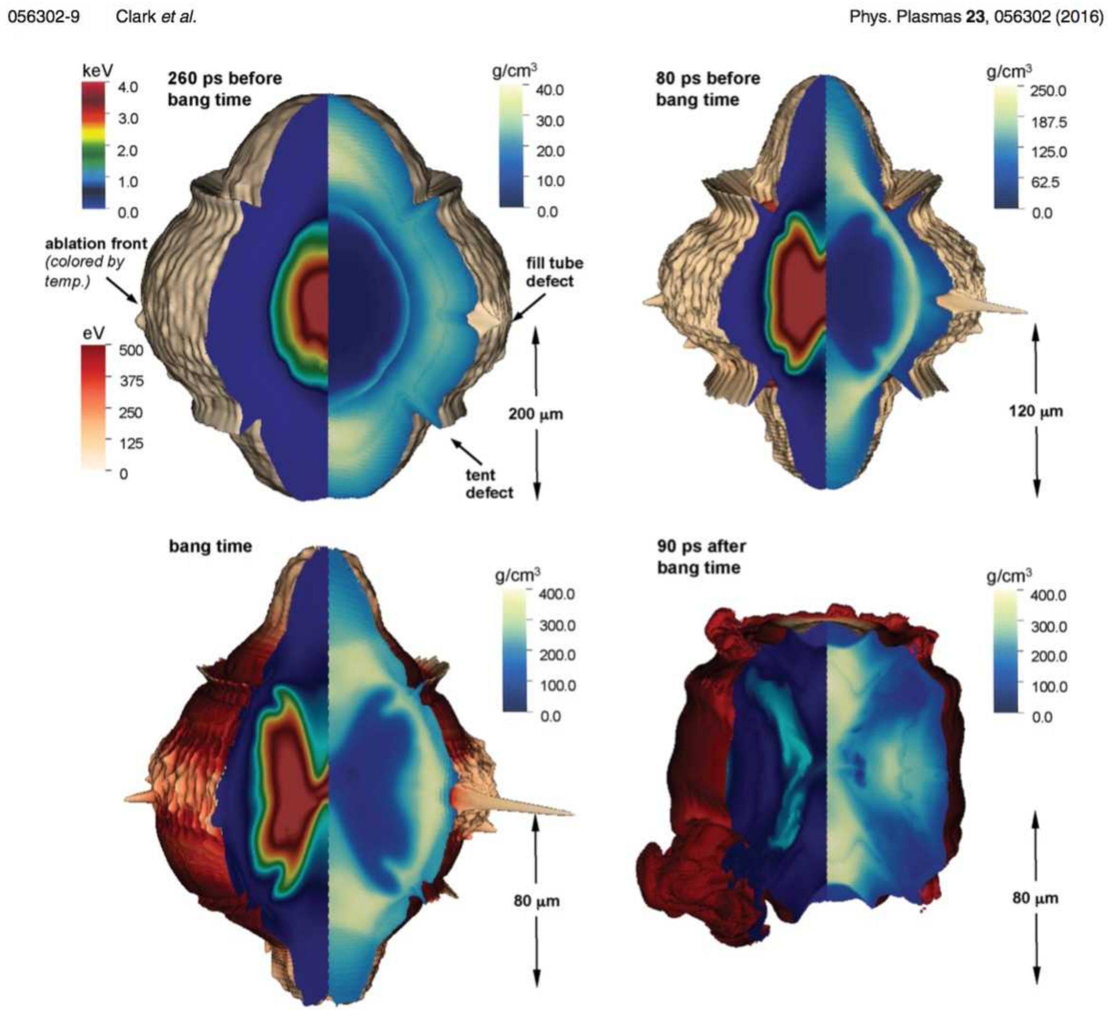
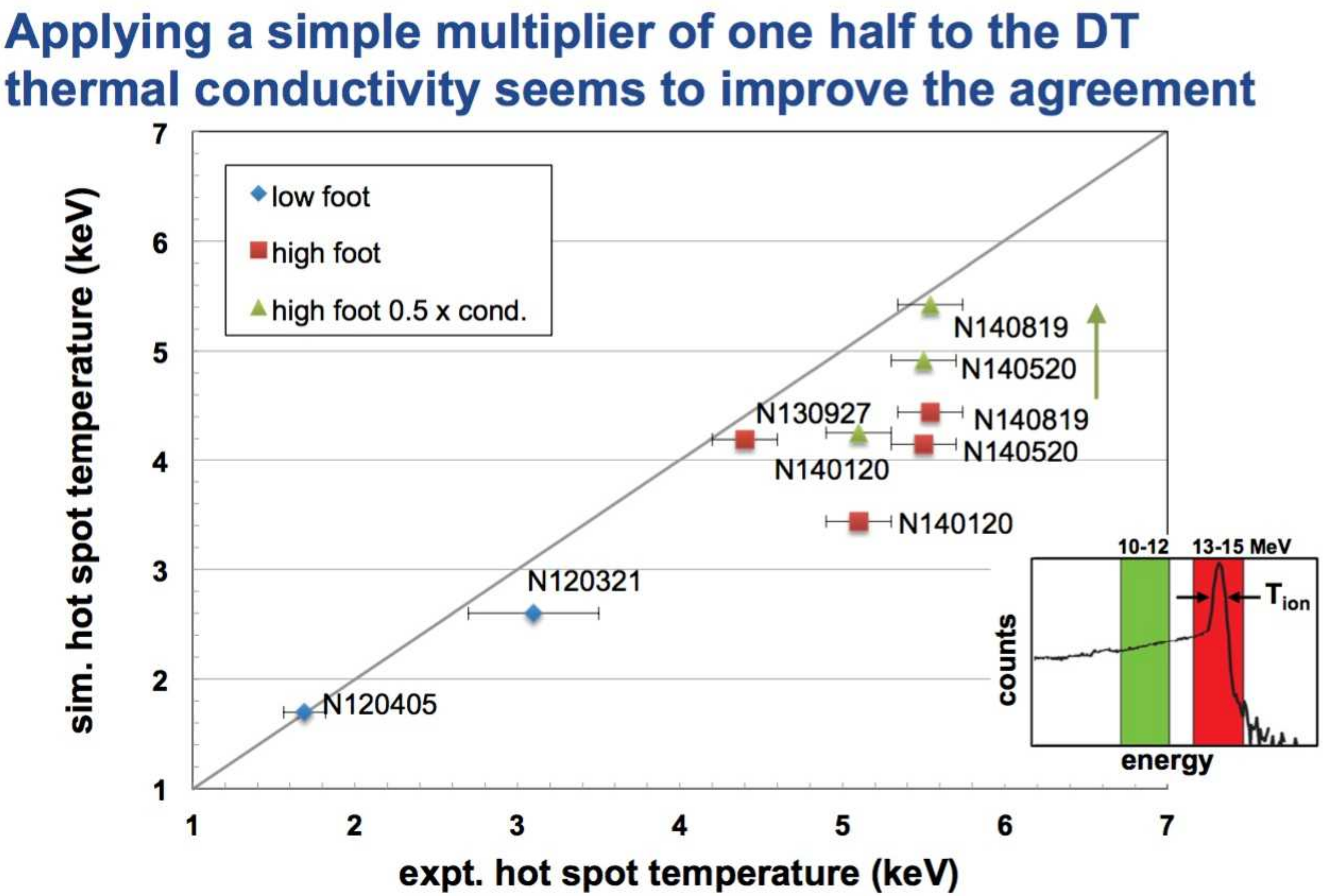
3D HYDRA simulation of a high-foot ICF capsule implosion



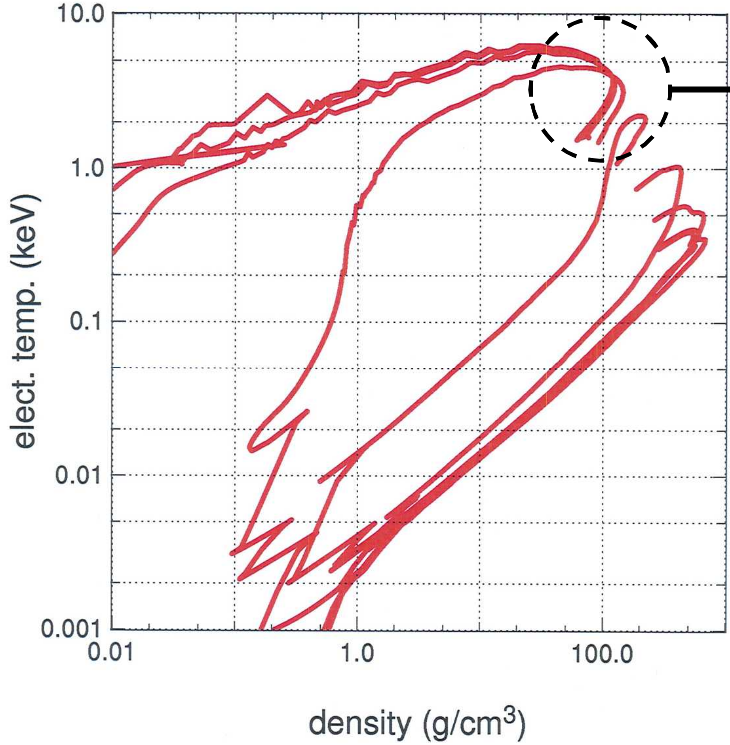
Dan Clark, *et al.*, Phys Plasmas **23**, 056302 (2016)

Simulations of NIF high-foot capsule implosions with lowered thermal conductivity are in better agreement with experiment



Slide courtesy of Dan Clark (LLNL)

ICF capsule implosions traverse a broad region of phase space, from condensed matter to WDM to ideal plasma



Hot spot boundary – region of greatest yield sensitivity to thermal conductivity (Steve Hahn)

Capsule phase space trajectories courtesy of Dan Clark (LLNL)

We appeal to three different computational frameworks for a wide-range description of hydrogen transport

- First-principles calculations with DFT-MD and Kubo-Greenwood transport calculations
  - No assumption of ionization level or electron distribution
  - Bare proton potential – no pseudopotential issues
  - Particularly well suited to warm dense matter
  - Very high temperatures are computationally difficult – must resort to extrapolations for converged quantities
- Quantum Lenard-Balescu calculations*
  - Particularly well suited to the ideal plasma limit: weak coupling, small angle scattering
  - Includes electron diffraction and dynamic screening
  - Does not include electron degeneracy – no Pauli blocking
  - Assumes full ionization

* See Whitley, Scullard, Benedict, *et al.*, Contrib. Plasma, Phys. **55**, 192 (2015).

We appeal to three different computational frameworks for a wide-range description of hydrogen transport (cont.)

- Linear response theory in the Zubarev framework*
  - Boltzmann collision operator
  - Particularly well suited to the expanded, partially ionized plasma
  - T-matrix scattering cross sections – strong and weak scattering
  - Pauli blocking included
  - Static screening lengths for ion and electron potentials are assumed
  - Ionization state provided by auxiliary models

* See H. Reinholz, R. Redmer, and S. Nagel, Phys. Rev. E **52**, 5368 (1995)

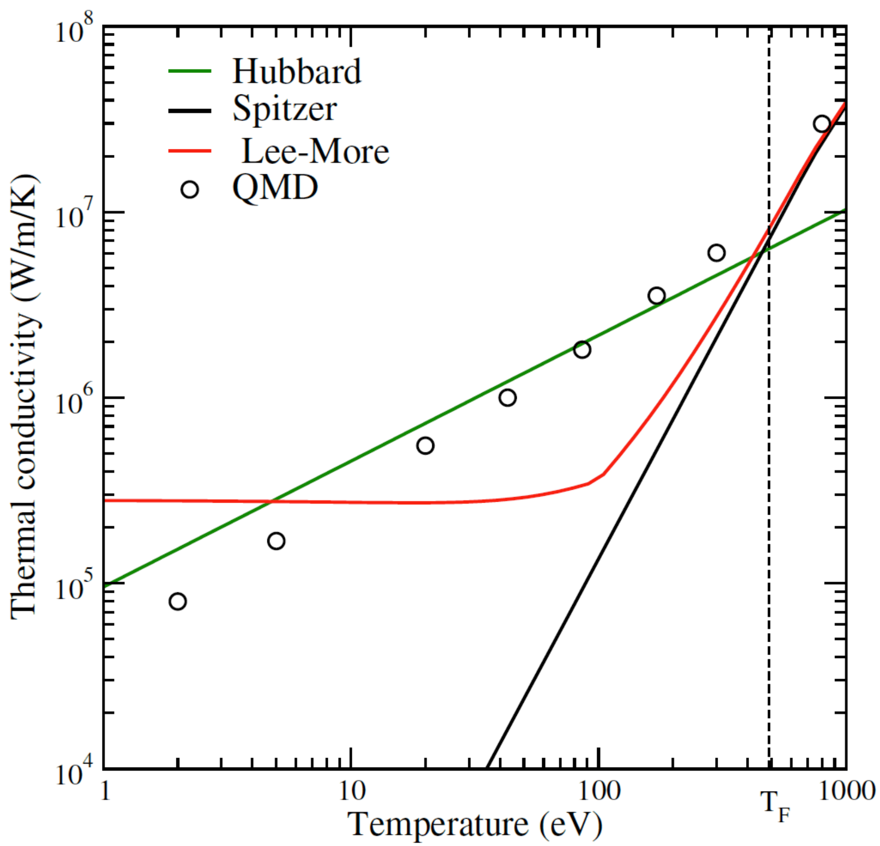
All calculations and results in this talk are for pure hydrogen (H)

The CEA group demonstrated the viability of *ab initio* thermal conductivity calculations for very dense hydrogen

PRL **102,** 075002 (2009) PHYSICAL REVIEW LETTERS week ending 20 FEBRUARY 2009

Ab Initio Determination of Thermal Conductivity of Dense Hydrogen Plasmas

Vanina Recoules, Flavien Lambert, Alain Decoster, Benoit Canaud, and Jean Clérouin
CEA, DAM, DIF, F-91297 Arpajon, France
(Received 4 November 2008; published 20 February 2009)



First-principles calculations of transport quantities are carried out in the Kubo – Greenwood / Chester – Thellung formalism

- For these dense conditions we abandon the pseudopotential approach and use a bare proton (this forces high plane wave cutoff energies)
- We calculate the full set of Onsager transport coefficients and calculate the thermal conductivity directly (no Wiedemann-Franz law assumptions)

Fermi weights

Dipole matrix elements

$$L_{mn}\left(\omega\right) = \frac{2\pi q^{4-m-n}}{3Vm_e^2\omega}\sum_{\mathbf{k}\nu\mu}\left(f_{\mathbf{k}\nu}-f_{\mathbf{k}\mu}\right)\langle\mathbf{k}\nu|\hat{\mathbf{p}}|\mathbf{k}\mu\rangle\langle\mathbf{k}\mu|\hat{\mathbf{p}}|\mathbf{k}\nu\rangle$$

$$\cdot\left(\frac{E_{\mathbf{k}\nu}+E_{\mathbf{k}\mu}}{2}-h\right)^{m+n-2}\delta\left(E_{\mathbf{k}\mu}-E_{\mathbf{k}\nu}-\hbar\omega\right) \quad .$$

Onsager weights

Energy conservation

$$\omega \rightarrow 0 \qquad K = \frac{1}{T}\left(\mathcal{L}_{22}-\frac{\mathcal{L}_{12}^2}{\mathcal{L}_{11}}\right),$$

Larger boxes (more atoms) are necessary to converge the degenerate limit

1024 H atoms

0.0208 Å^3/atom

0.14 a_B^3 /atom

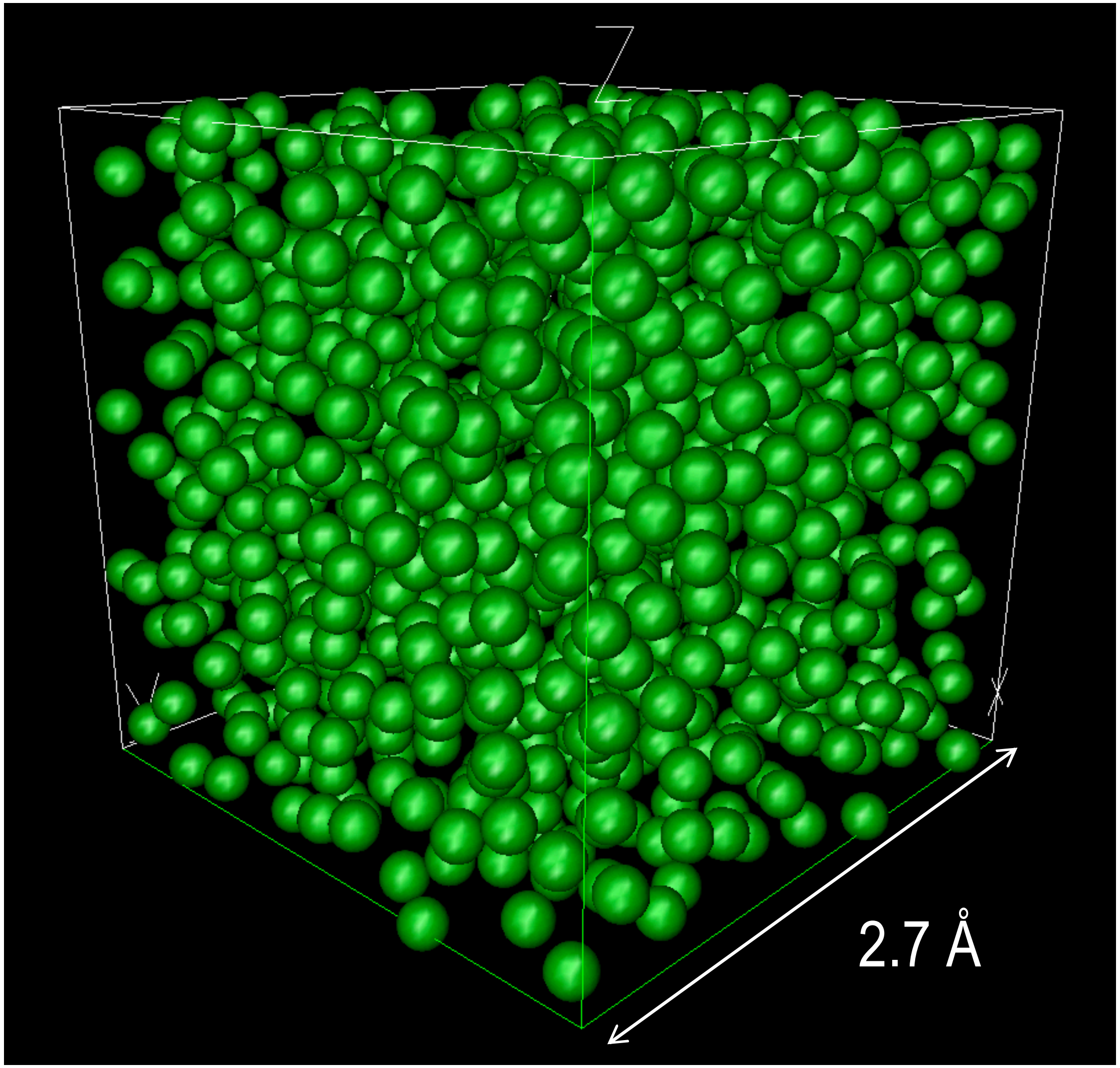
T = 10 eV

80 g/cc H

or

200 g/cc DT

P = 13 Gbar



The transport properties are also difficult to converge in the high temperature limit, particularly the thermal conductivity

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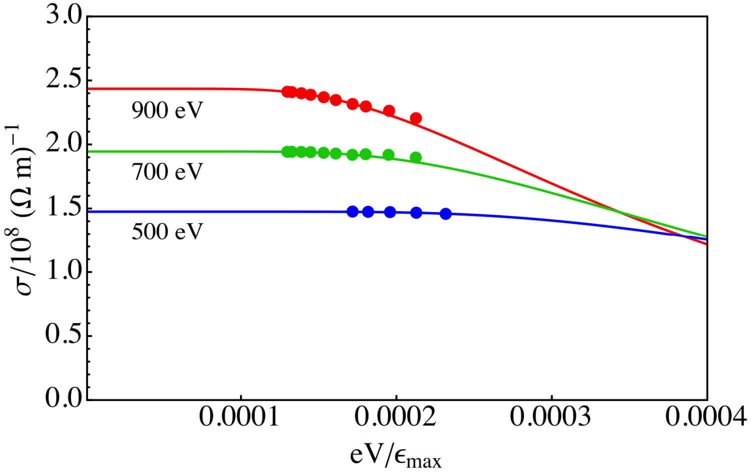
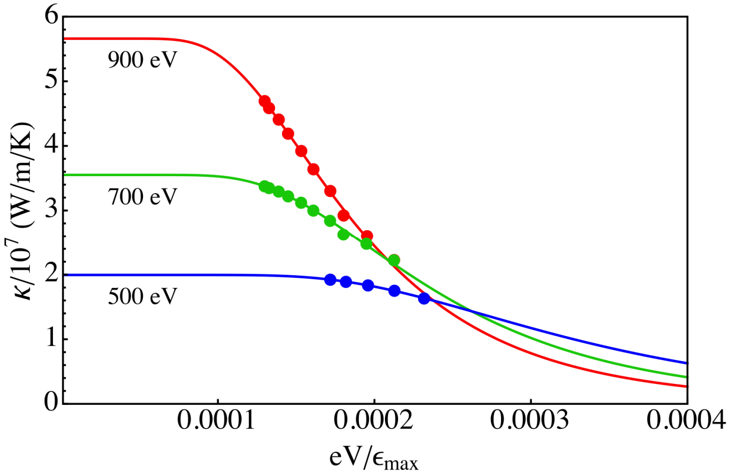
ρ = 40 g/cm³



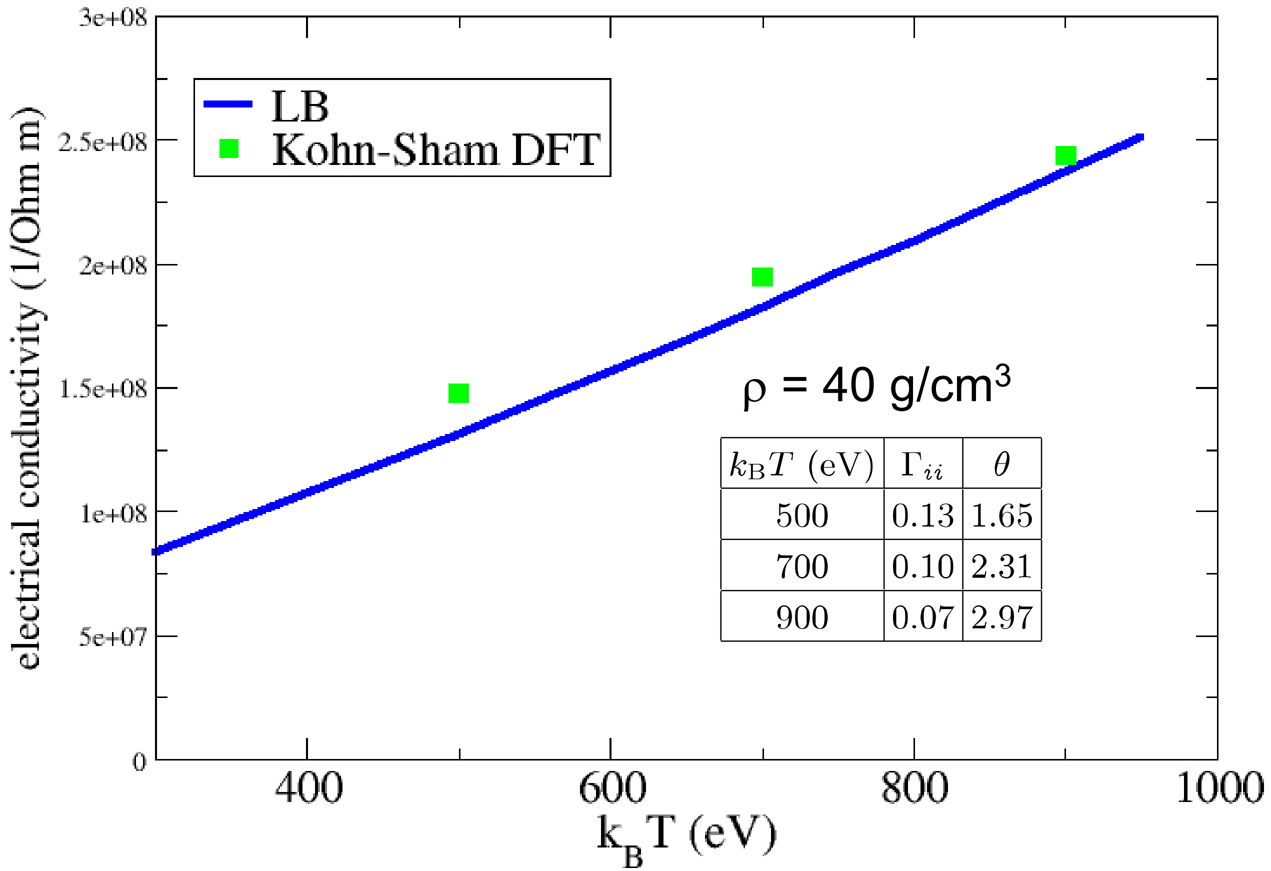


$$\kappa(\epsilon_{\max}) = \kappa_\infty \frac{\int_{-\infty}^{\epsilon_{\max}} E^2 E^\gamma \frac{\partial f}{\partial E} dE}{\int_{-\infty}^{\infty} E^2 E^\gamma \frac{\partial f}{\partial E} dE}$$

We extrapolate to infinite bands through the assumption of a power law scaling of the dipole matrix elements

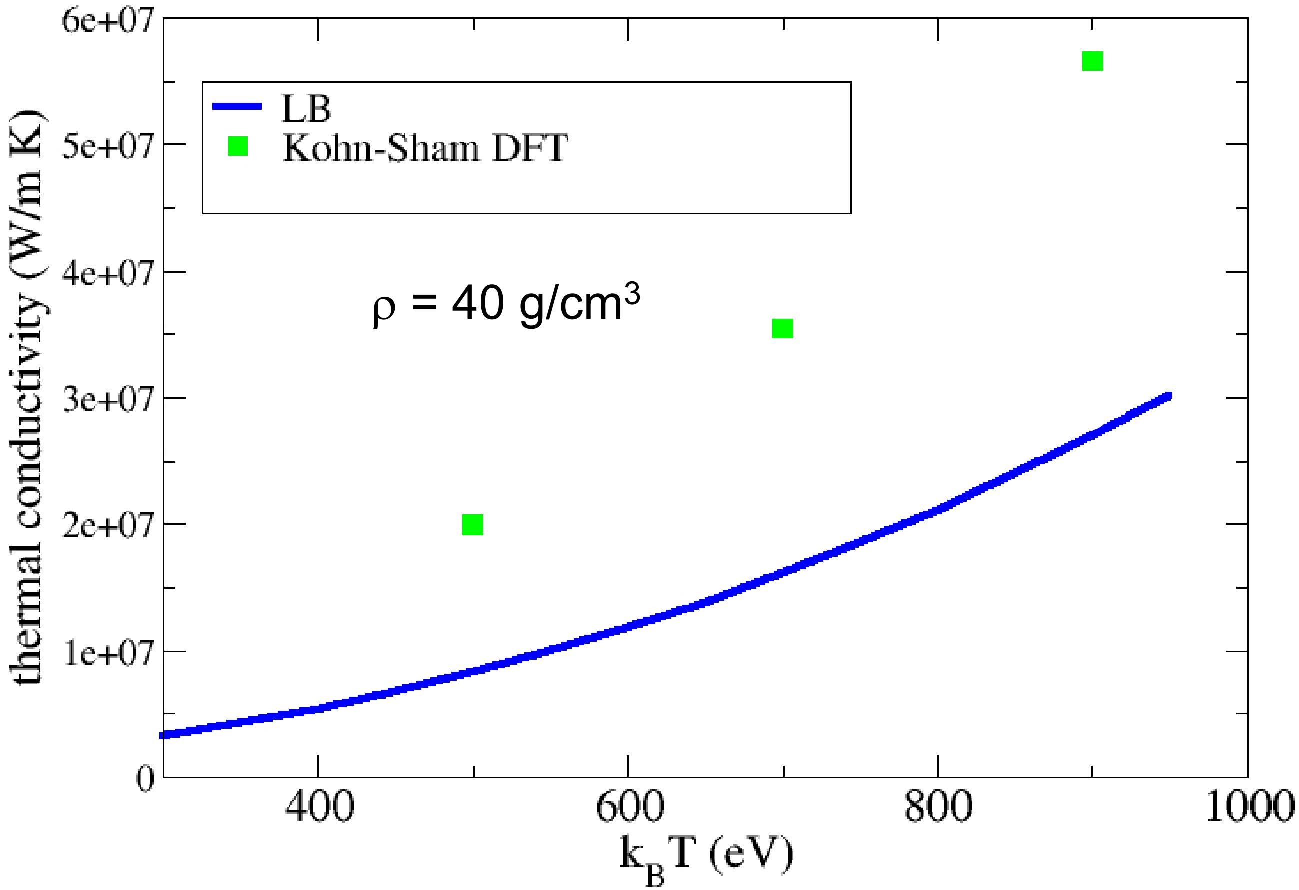
Desjarlais, Scullard, Benedict, Whitley, and Redmer, Phys. Rev. E **95**, 033203 (2017)

The electrical conductivities from the Kubo-Greenwood calculations agree well with our quantum Lenard-Balescu results



Residual differences are due to small degeneracy effects included in the DFT but not the QLB. The sum rule on $\sigma(\omega)$ is well satisfied.

The thermal conductivities from the Kubo-Greenwood calculations (■) do not agree with our quantum Lenard-Balescu results



Density functional theory provides an accurate description of the electrical conductivity in the non-degenerate limit, but only partially captures the thermal transport

No momentum transport for e-e

$$\frac{1}{\sigma} = \frac{1}{S_\sigma \sigma_{ei}} + \cancel{\frac{1}{\sigma_{ee}^{\mathrm{OCP}}}} = \frac{1}{S_\sigma \sigma_{ei}},$$

DFT

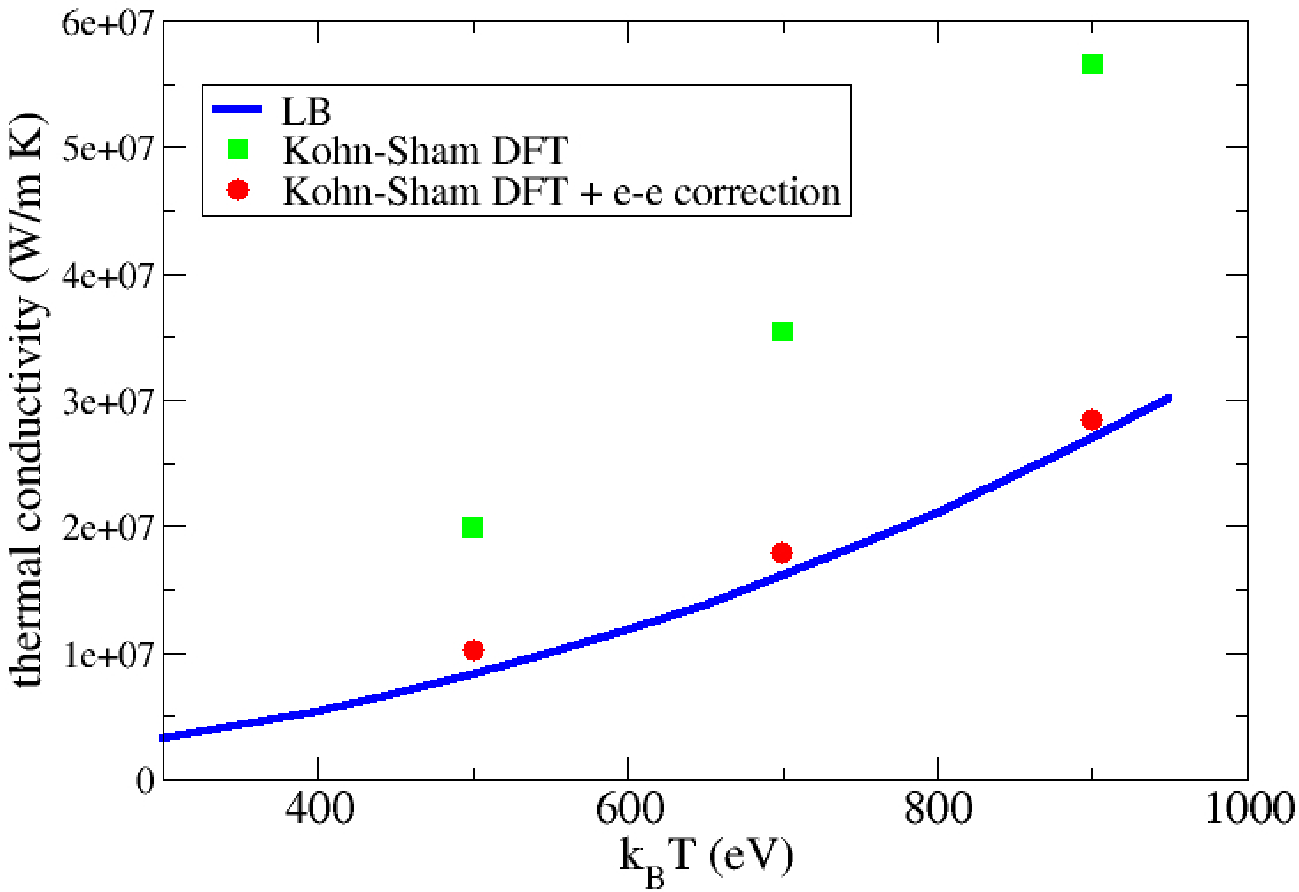
$$\frac{1}{\kappa} = \frac{1}{S_\kappa \kappa_{ei}} + \boxed{\frac{1}{\kappa_{ee}^{\mathrm{OCP}}}}.$$

DFT

Explicit e-e collisions, missing from DFT

See: Desjarlais, Scullard, Benedict, Whitley, and Redmer, Phys. Rev. E **95**, 033203 (2017)

The thermal conductivities from the Kubo-Greenwood calculations with an e-e correction (•) agree with our quantum Lenard-Balescu results



The red points show the agreement when an explicit e-e scattering correction, calculated in the Zubarev formalism (T-matrix, Boltzmann collision operator) is added to the thermal.

Small differences due to the treatment of degeneracy remain

We build a wide-range model with a suite of semi-classical algorithms tuned to the results of our calculations

- Lee-More-Desjarlais algorithms*
  - Non-ideal Saha ionization model
  - Electron-ion and electron-neutral scattering
  - Degeneracy dependent reduction factors for electron-electron scattering
  - Wide-range Coulomb logarithm model
    - Depends on Γ_{ii} in the degenerate limit
    - Includes b_{minC}, b_{minQ} for the classical or quantum minimum impact parameter in the plasma limit
    - Includes b_{max} tuned to capture effects of dynamic screening
  - Several additional minor tuning parameters

* MPD, Contrib. Plasma Phys. **41**, 267 (2001)

The plasma literature suggests a variety of choices for the minimum impact parameter in the quantum limit

$b_{minQ} = \frac{h}{2m_e\bar{V}_e}$ e.g. Lee-More

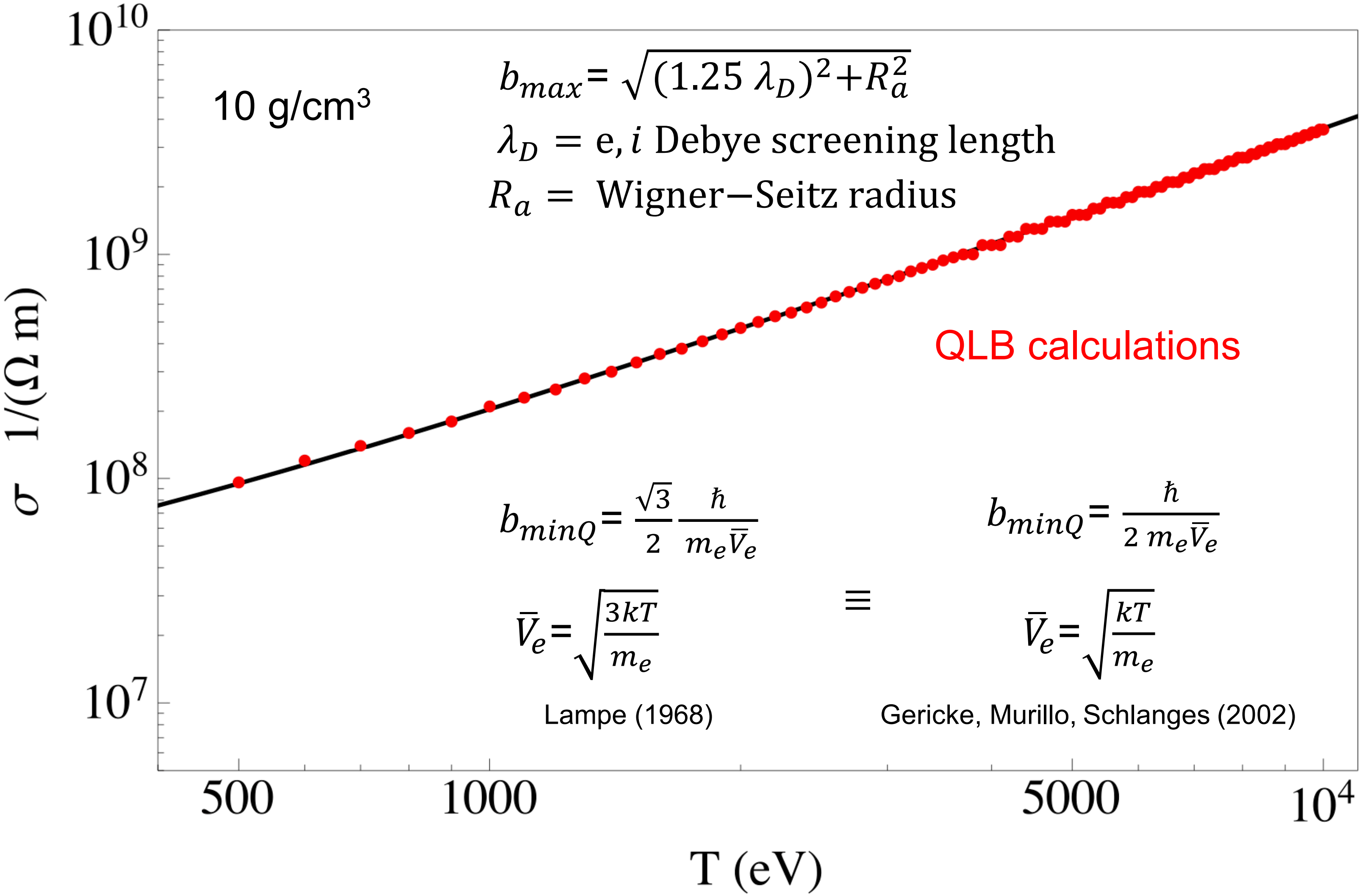
$b_{minQ} = \frac{\hbar}{m_e\bar{V}_e}$ e.g. Jackson

$b_{minQ} = \frac{\hbar}{2\, m_e\bar{V}_e}$ e.g. Brysk

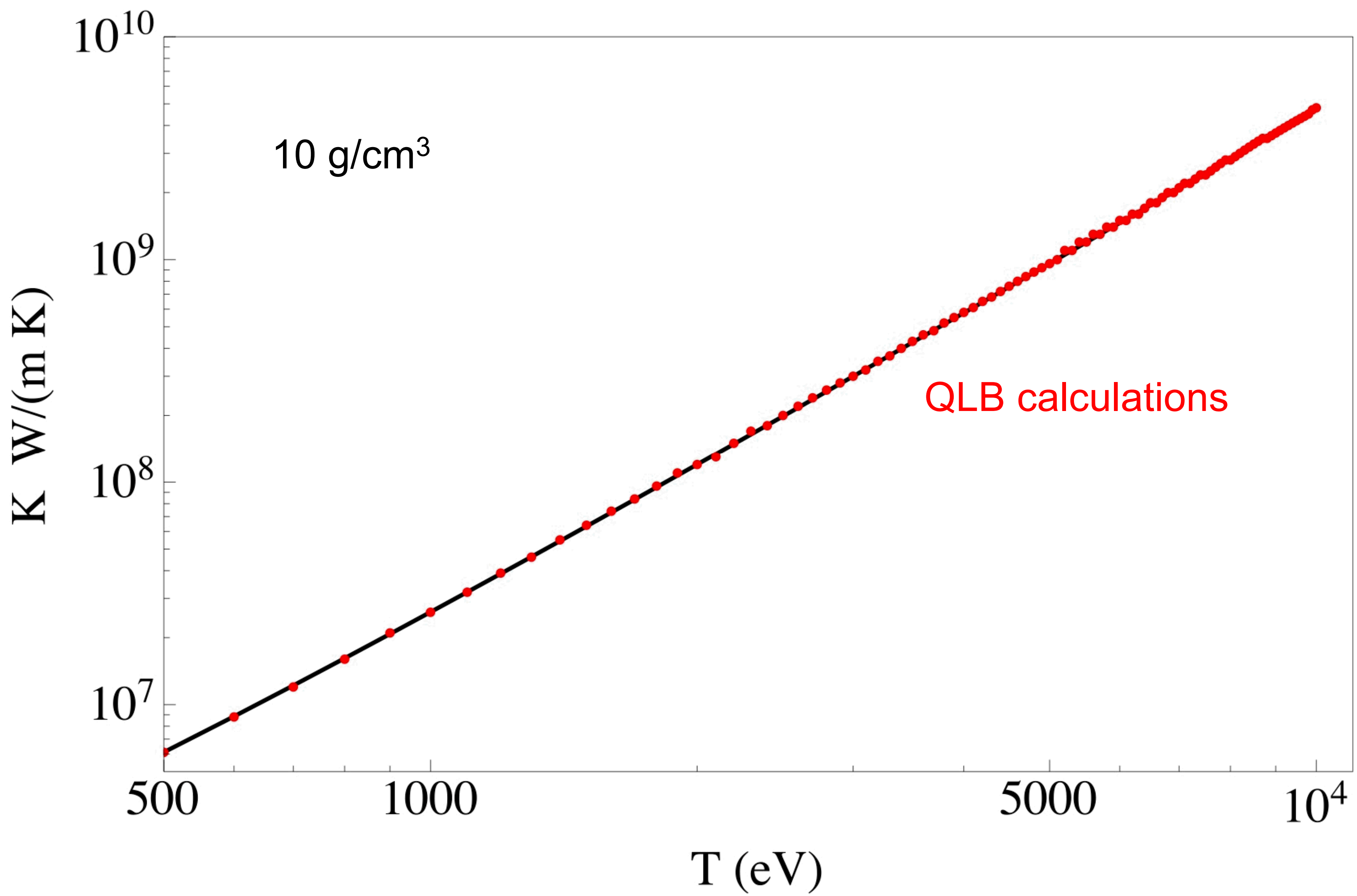
$b_{minQ} = \frac{\sqrt{3}}{2}\frac{\hbar}{m_e\bar{V}_e}$ e.g. Lampe

Combined with $\bar{V}_e = \sqrt{\frac{3kT}{m_e}}$ or in some cases $\bar{V}_e = \sqrt{\frac{kT}{m_e}}$ or $\bar{V}_e = \sqrt{\frac{2kT}{m_e}}$

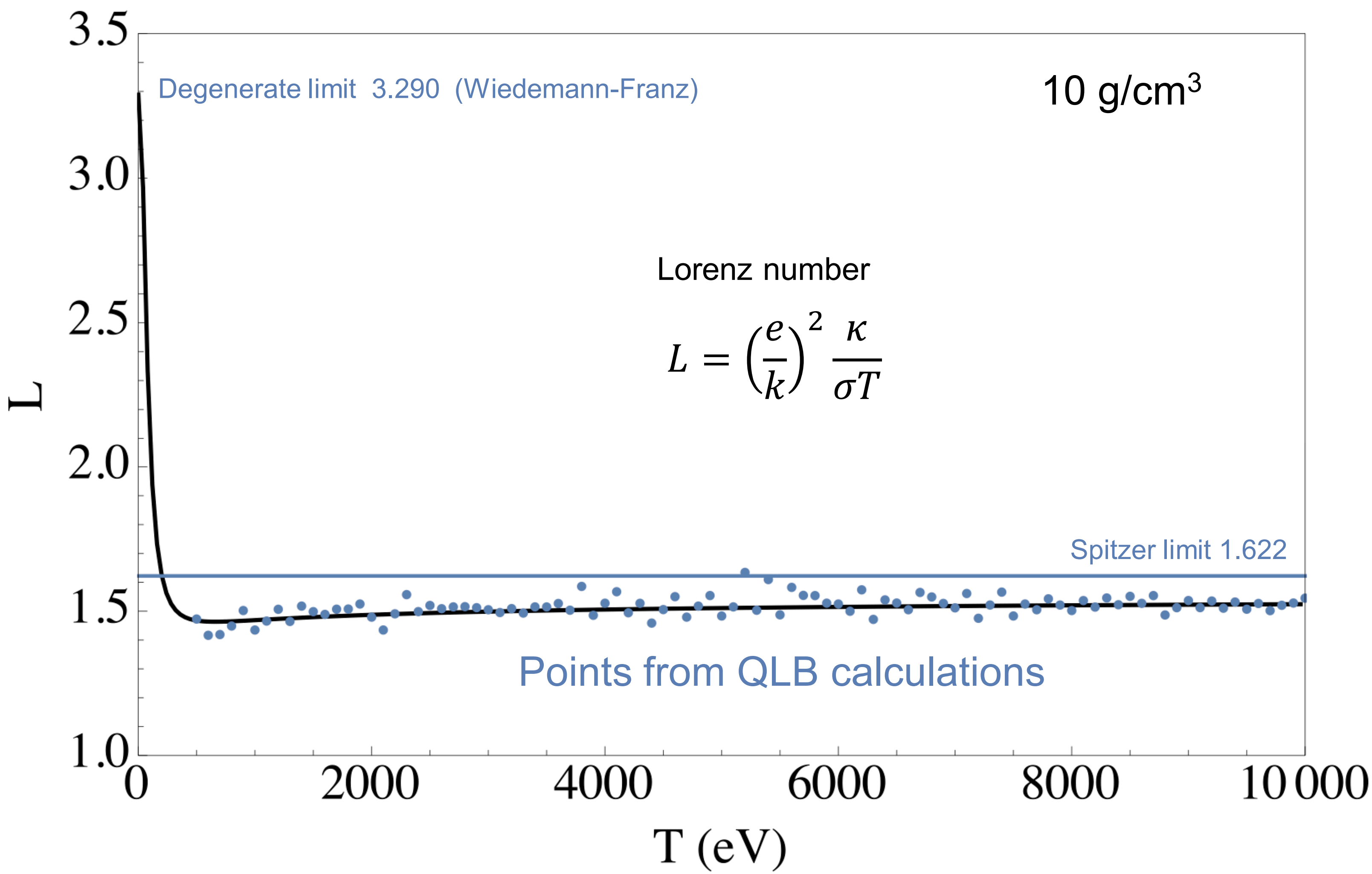
We found optimum choices of b_{max} and b_{minQ}



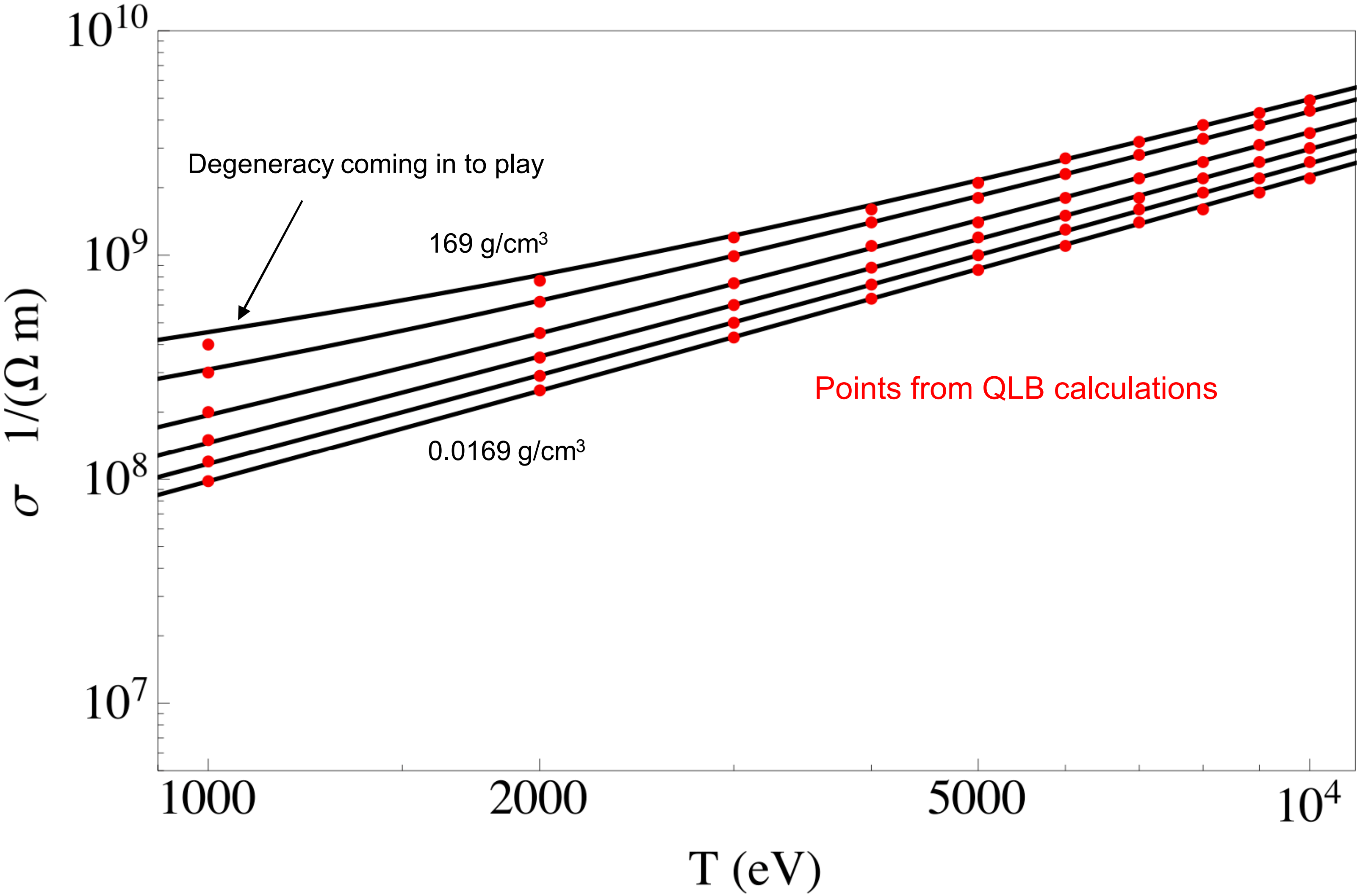
The thermal conductivity is equally well fit with the same parameters



Dynamic screening has a greater effect in reducing the thermal conductivity, pushing L below the Spitzer limit



The model accurately represents the QLB electrical conductivity results over many decades of ρ and T



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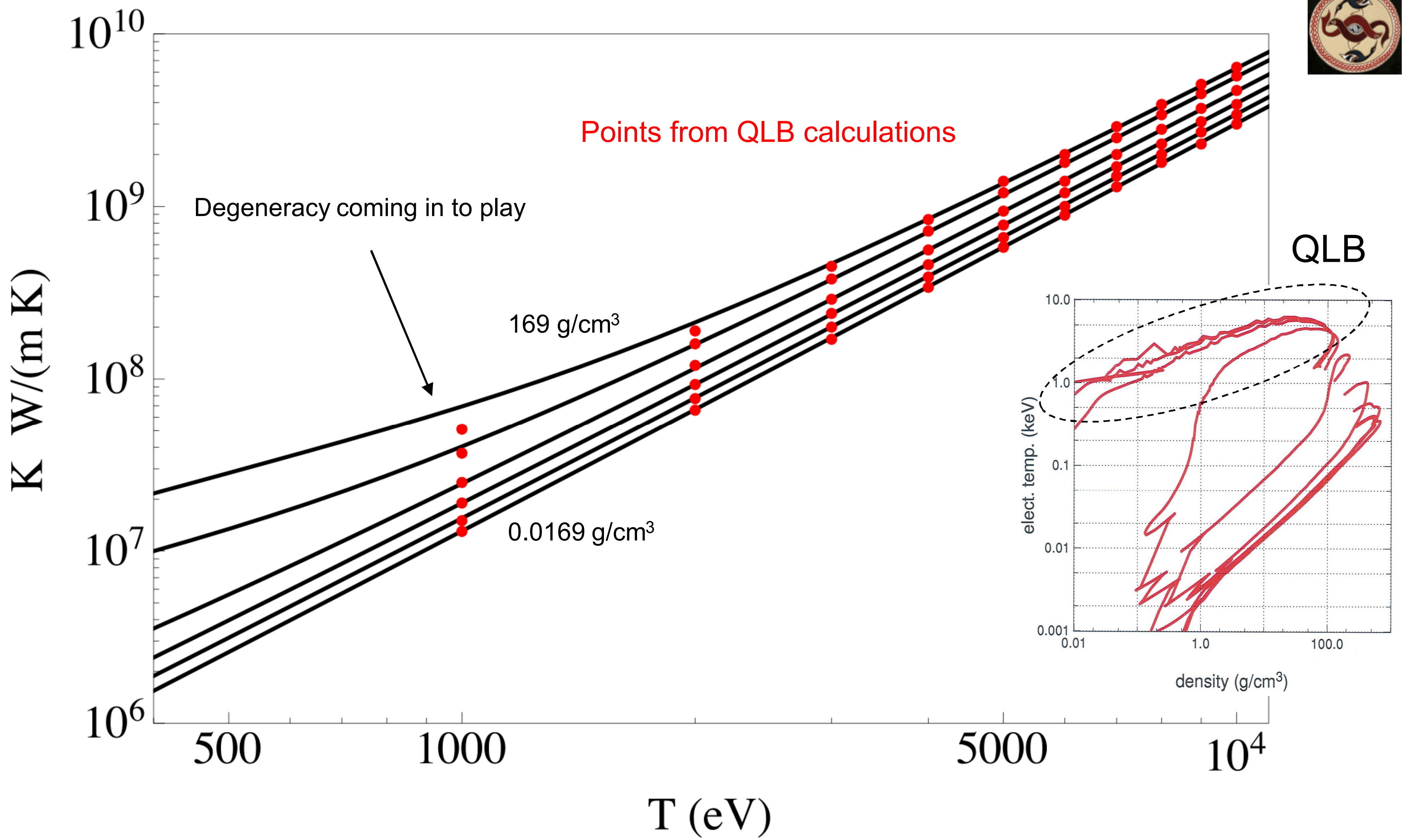
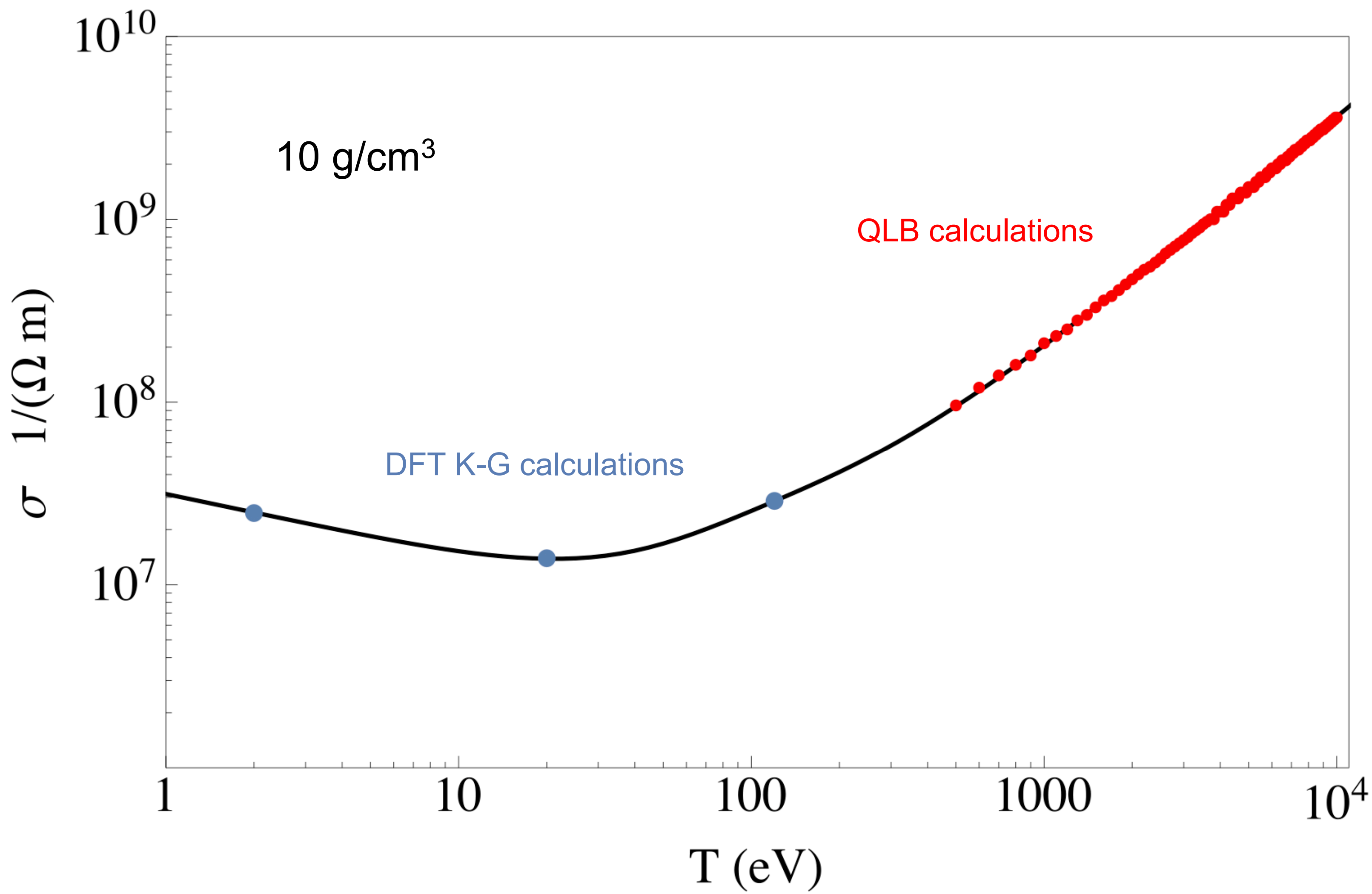


These QLB results are lower than the current LLNL thermal conductivity model by about 15%

The model is tuned to our DFT Kubo-Greenwood electrical conductivity calculations in the degenerate limit



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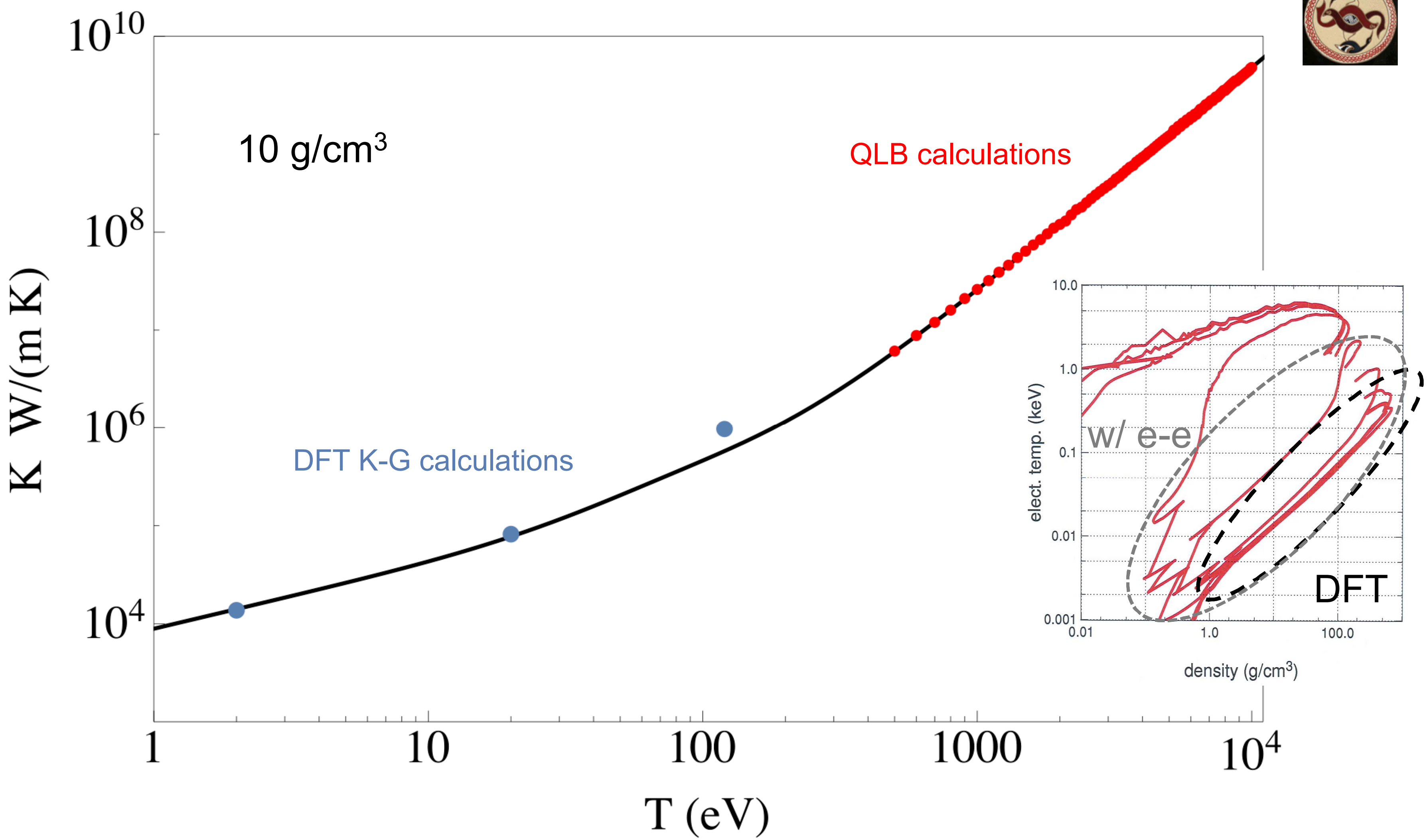
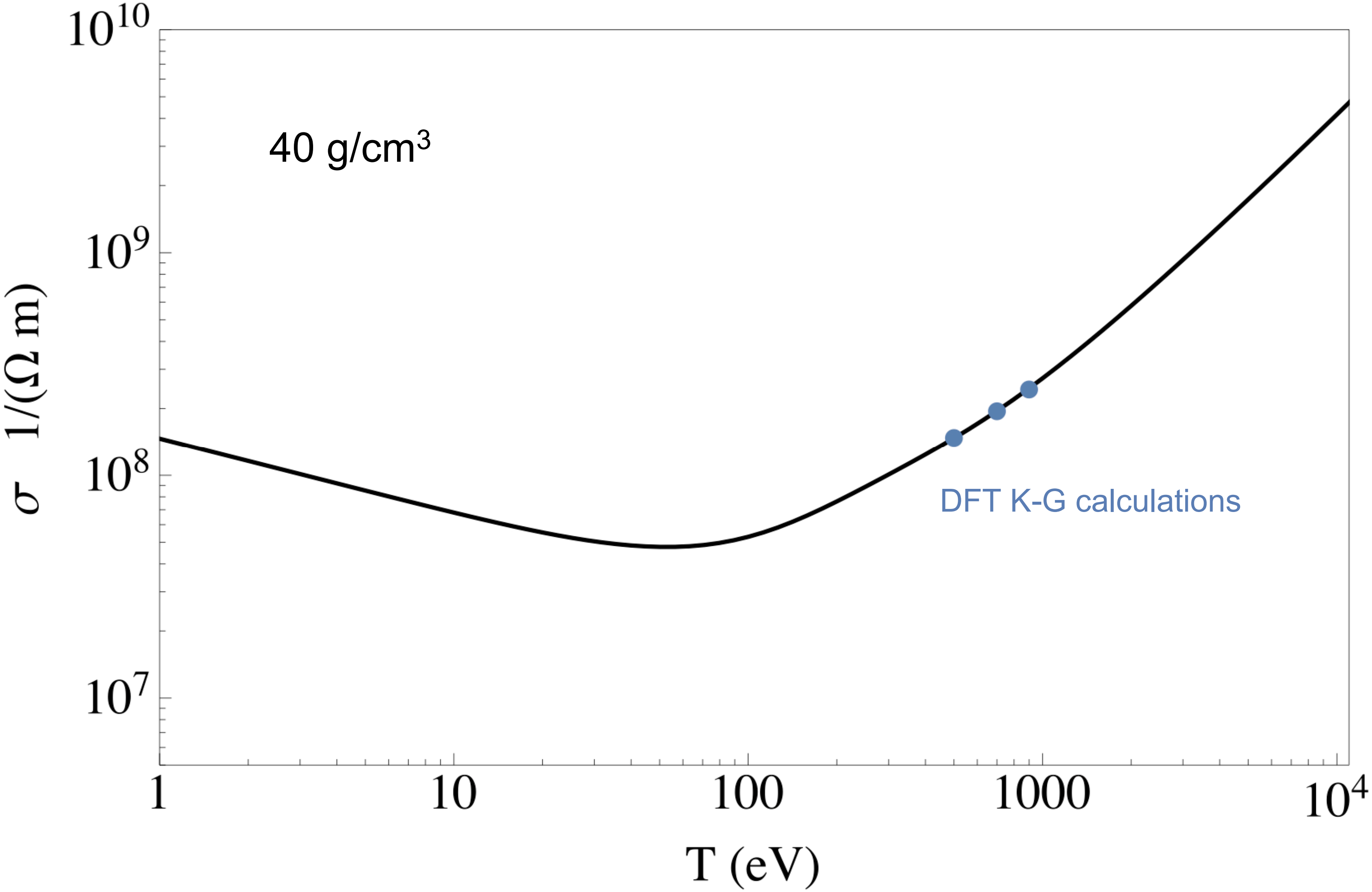
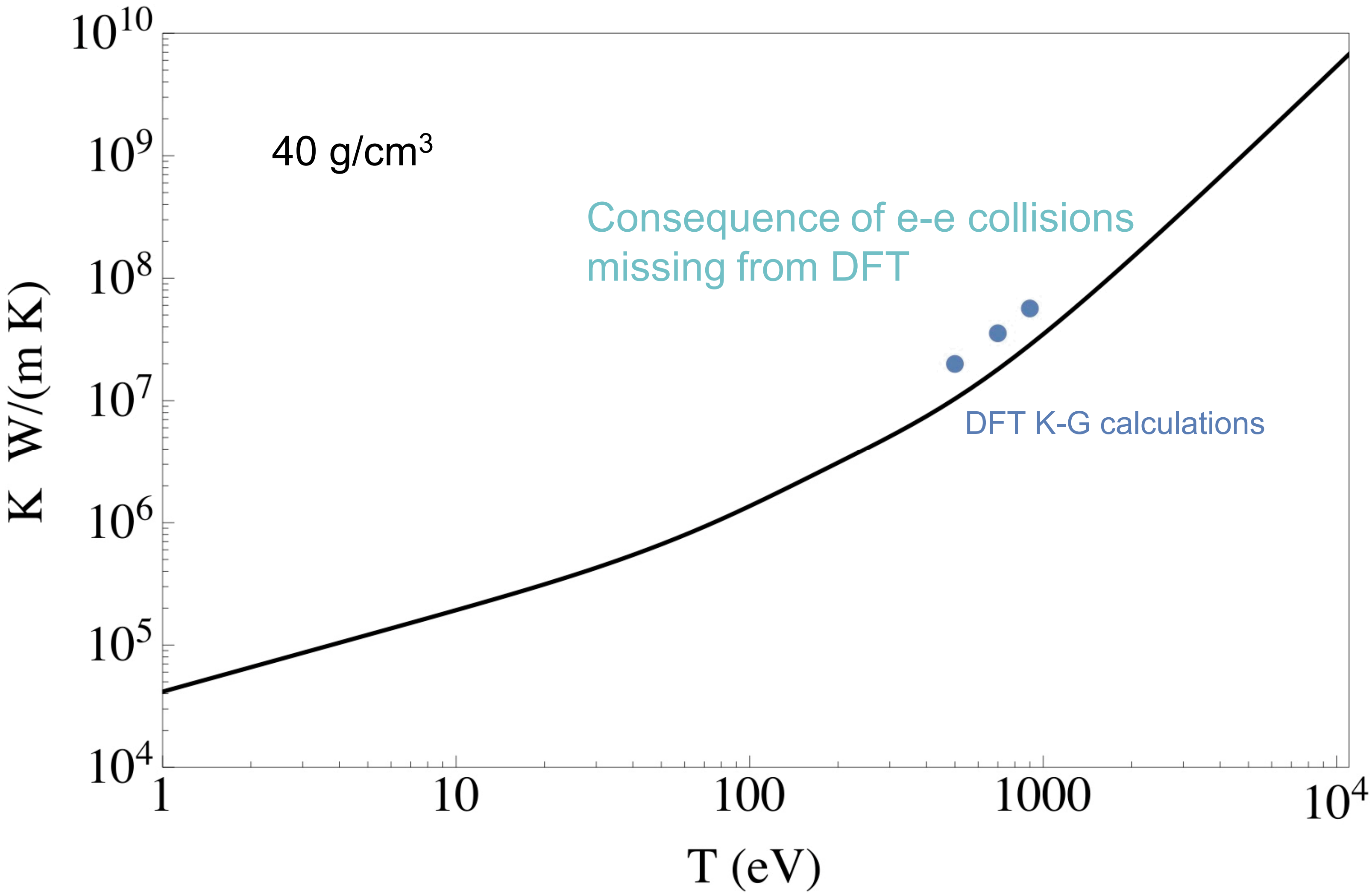


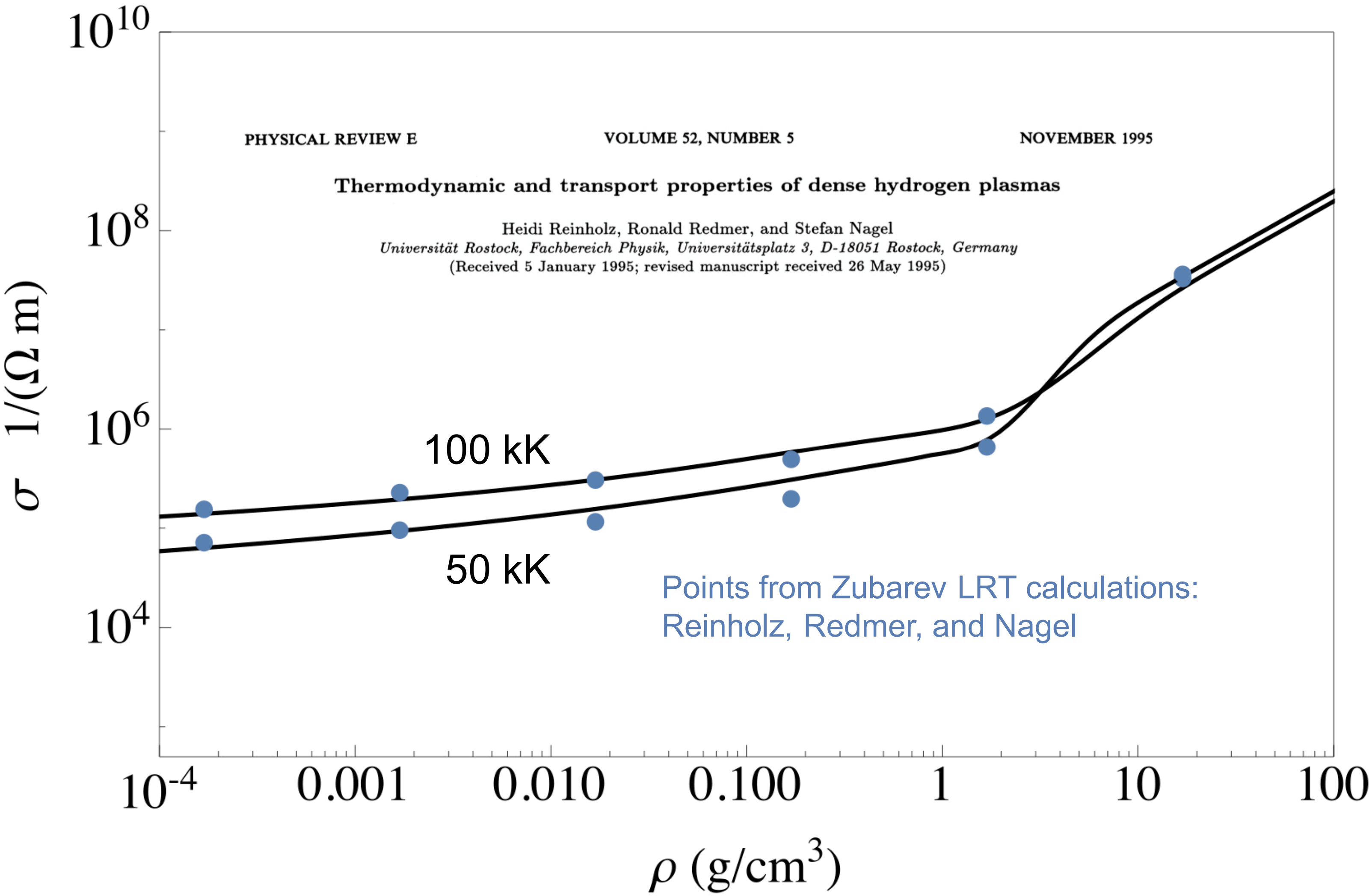
We accurately fit DFT-KG electrical conductivities calculated at higher density in the non-degenerate limit



The DFT-KG thermal conductivities in the non-degenerate limit are missing the explicit e-e scattering contribution



The wide-range model is in good agreement with Zubarev electrical conductivity calculations for hot expanded plasmas



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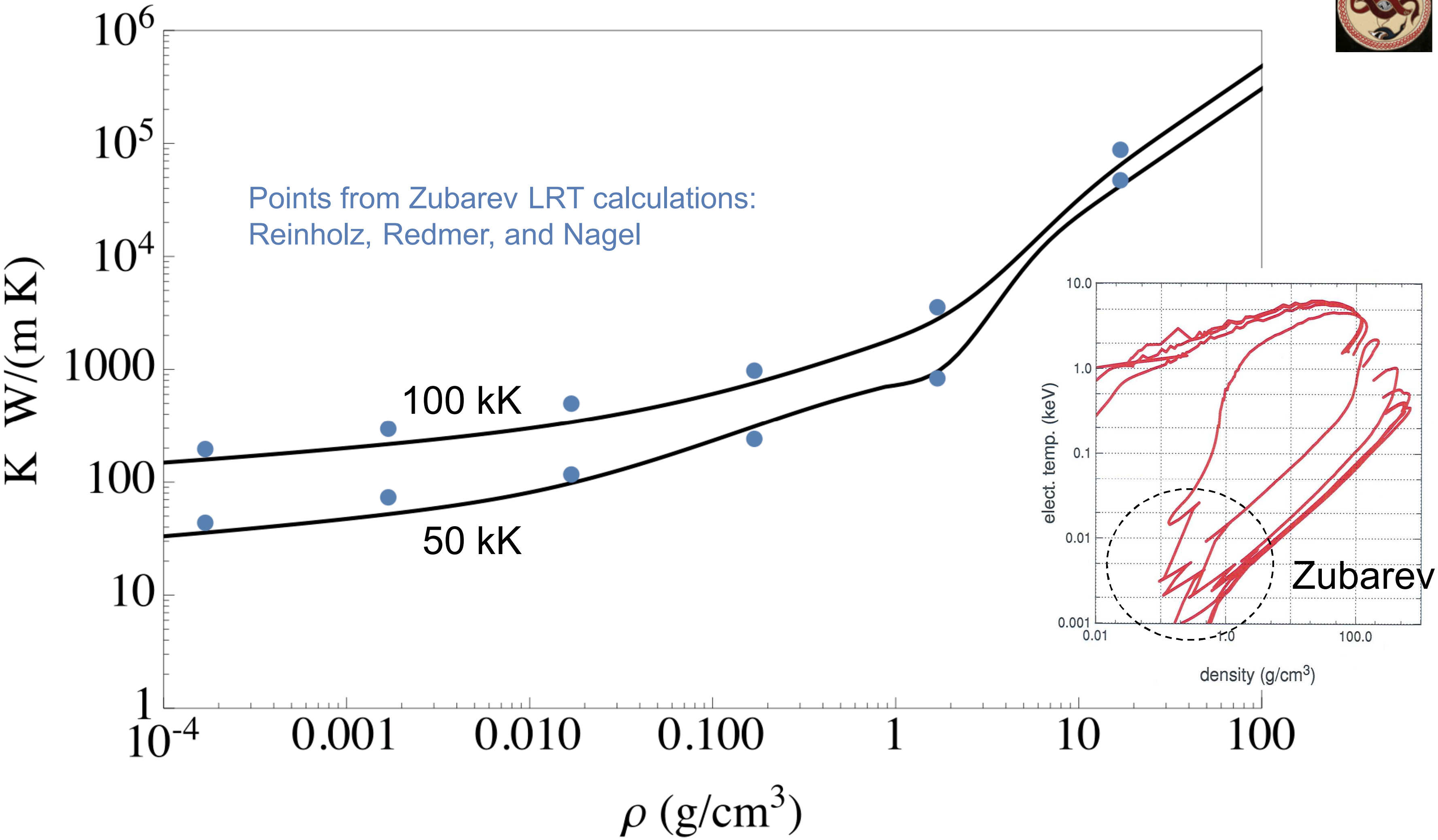

We will revisit the Zubarev calculations with static screening lengths matched to dynamic screening

Summary

- Comparisons between state-of-the-art 3D simulations and data from NIF experiments are in better agreement when the current model for thermal conductivity is reduced
- We have combined results from 3 different calculational frameworks to tune a wide-range model for the electrical and thermal conductivity of hydrogen emphasizing ICF conditions
- The model accurately captures the results of the calculations, particularly in the region of the hot-spot boundary where sensitivity is greatest, and provides for a 15% lower thermal conductivity