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# Stopping Powers from Average Atom and TD-DFT Models

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# The simplest Self-Consistent Field models find the distribution of fluid electrons in a muffin-tin potential

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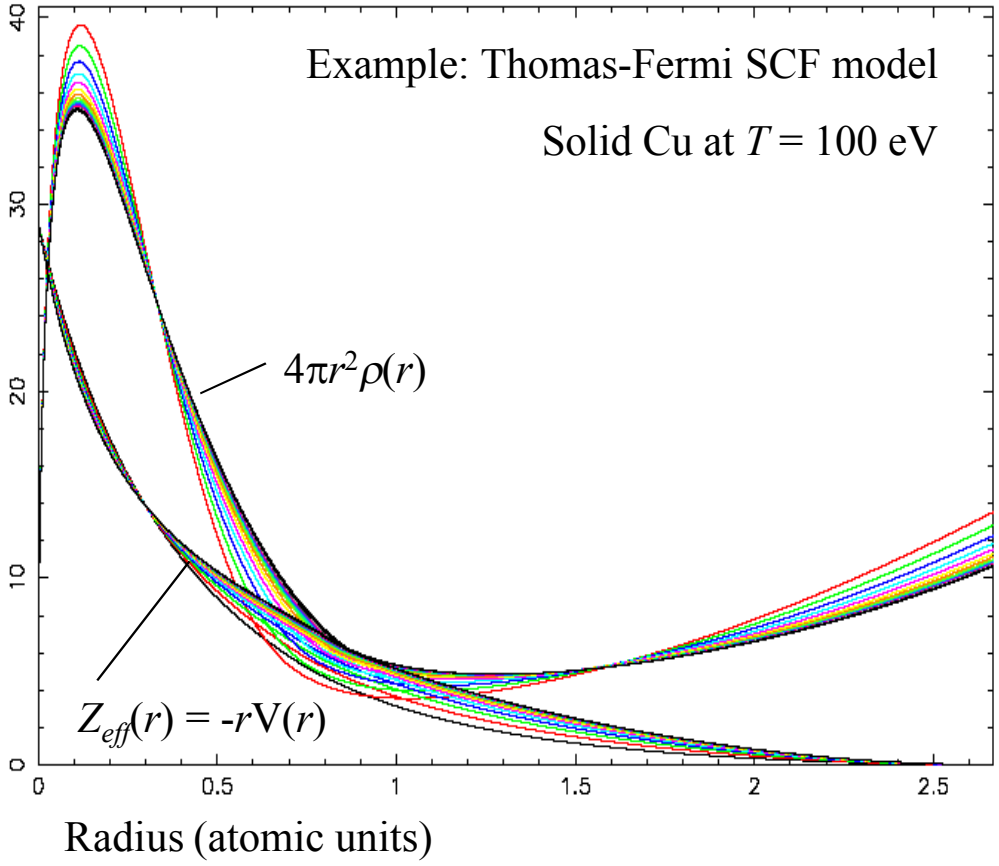
A representative ion is taken to exist in a Wigner-Seitz sphere with radius $R_0 = (3\Omega/4\pi)^{1/3}$, where $\Omega$ is the volume taken by an atom or ion in an isotropic medium at a given material density.

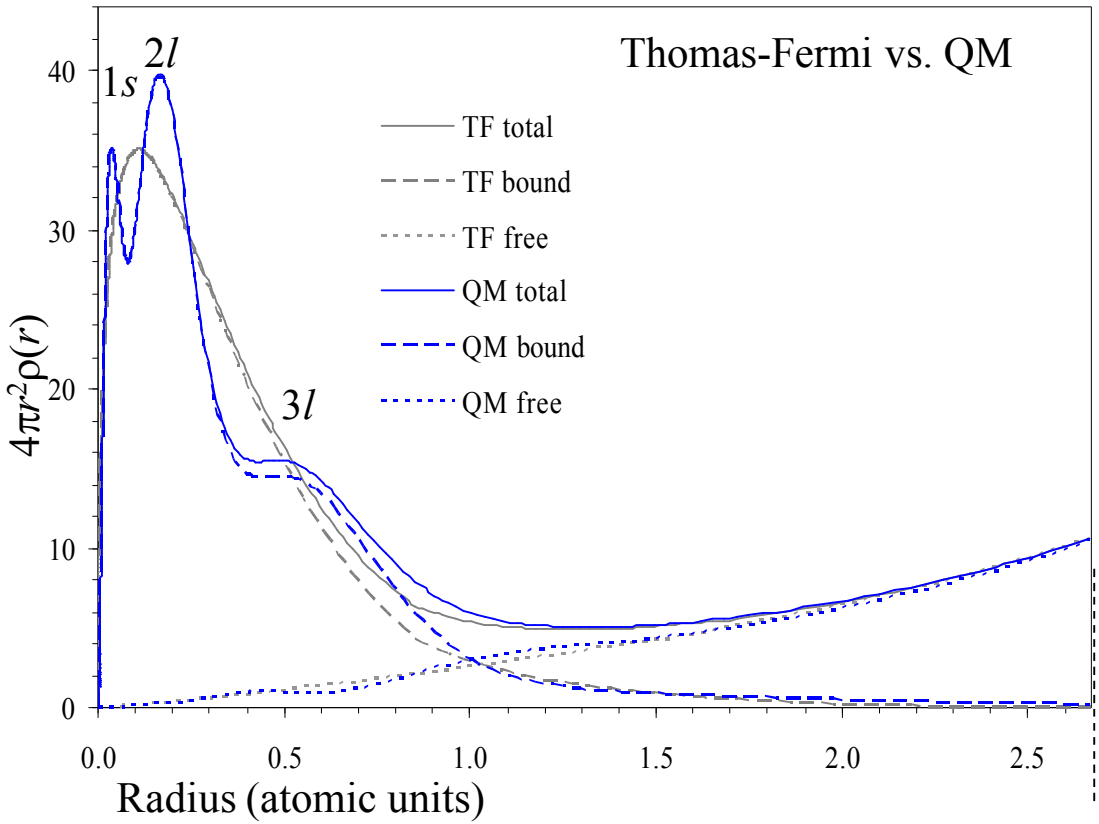



An initial guess is made for the electrostatic potential $V(r)$ in the ion sphere. This potential is used to determine an electron density distribution $\rho(r)$, which is in turn used to generate a new potential.

The procedure is iterated until self-consistent $V(r)$ and $\rho(r)$ are obtained, giving also $Z_i$ and $\mu$.

Thomas-Fermi models treat electrons as a fluid. "Muffin-tin" models force the potential to zero at the ion-sphere boundary

# Quantum Mechanical SCF models treat all electrons with wavefunctions




QMAA models* use bound and free wave functions to determine

$$\rho(r) = \rho_{\text{bound}} + \rho_{\text{continuum}}$$

$$4\pi r^2 \rho_{bound}(r) = \sum_{nlj} f(\varepsilon_{nlj}, \mu)(2l+1)\left\{P^2_{nlj}(r)\right\}$$

$$4\pi r^2 \rho_{continuum}(r) = \int_0^\infty d\varepsilon f(\varepsilon, \mu) \sum_l (2l+1)\left\{P^2_{\kappa,\varepsilon}(r)\right\}$$

QM models capture bound-state shell structure and Freidel oscillations in the continuum, but may still force the potential to zero at the ion-sphere boundary

*D. A. Liberman, Phys. Rev. B **20**, 4981 (1979)

# Stopping Powers are calculated following Wang et al. (cf. Faussurier) using data from Average Atom model MUZE

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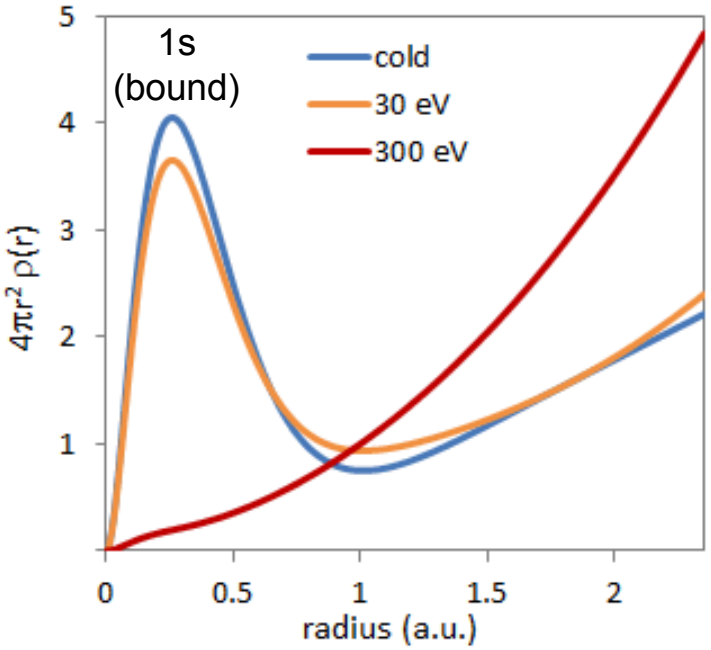
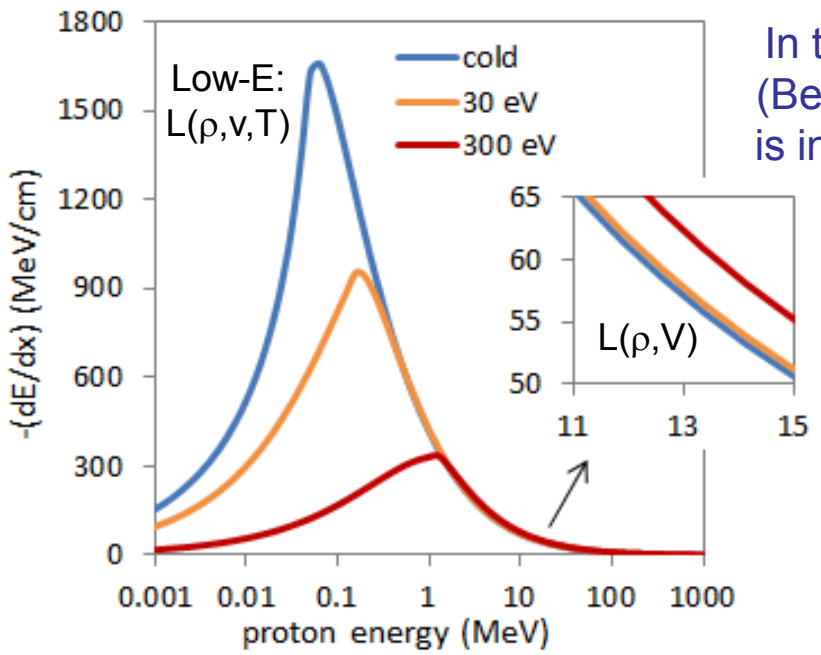
Stopping power is the integral of stopping number L(ρ,V) over average-atom electron density ρ(r):

$$\left(\frac{dE}{dx}\right) = -\frac{4\pi}{m}\left(\frac{Ze^2}{V}\right)^2 \int_0^\infty \rho(r) L(\rho,V) 4\pi r^2 dr$$

The stopping number is related to the dielectric -- currently using RPA L(ρ,V) from Arista & Piriz, PRA 35, 3450 (1987)

$$L(\rho,V) = \frac{i}{\pi\omega_0^2}\int_0^\infty \frac{dk}{k}\int_{-kV}^{kV} \omega dw \left(\frac{1}{\varepsilon(k,\omega)} - 1\right)$$




In the high-energy (Bethe) limit, L(ρ,v) is independent of T → dE/dx increases with Z*

**These all-electron calculations take about a minute for a single ρ,T point**

*Wang, et al., Phys Plas 5, 2977 (1998); Faussurier et al., Phys Plas 17, 052707 (2010)

# These stopping powers (AA-LDA) described Zylstra's recent measurements of 14 MeV proton stopping reasonably well

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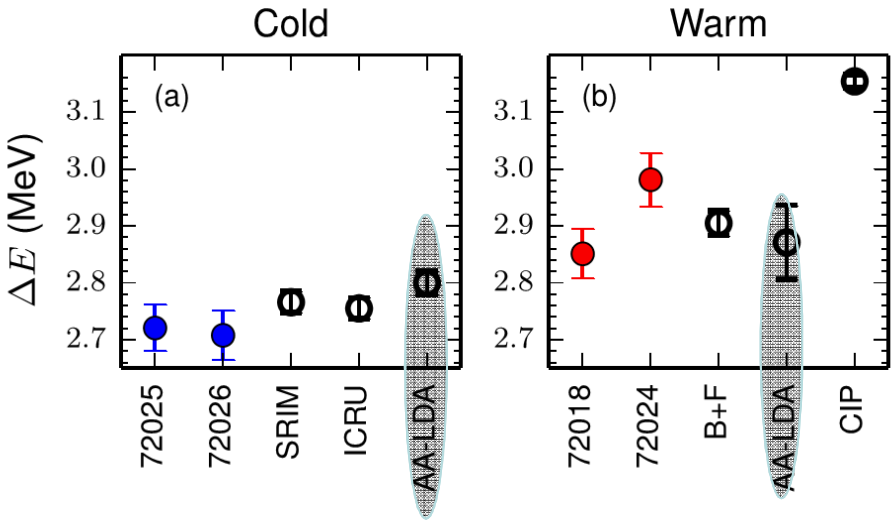



FIG. 4 (color online). Downshift ($\Delta E$) for cold (a) and warm (b) shots compared to theory. The solid points are data (denoted by shot number), and theories are hollow points. The uncertainties in theoretical calculations are due to uncertainties in $\rho L$ and plasma conditions.

The downshift of 14 MeV protons is determined by integrating calculated dE/dx over measured path length

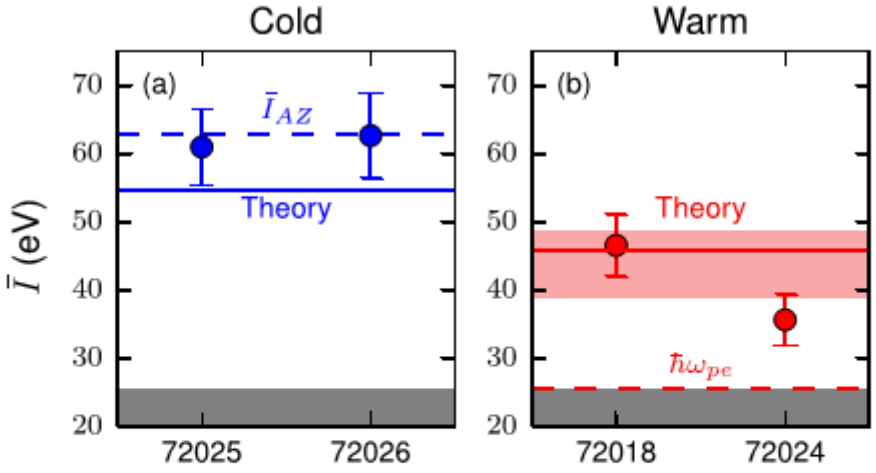
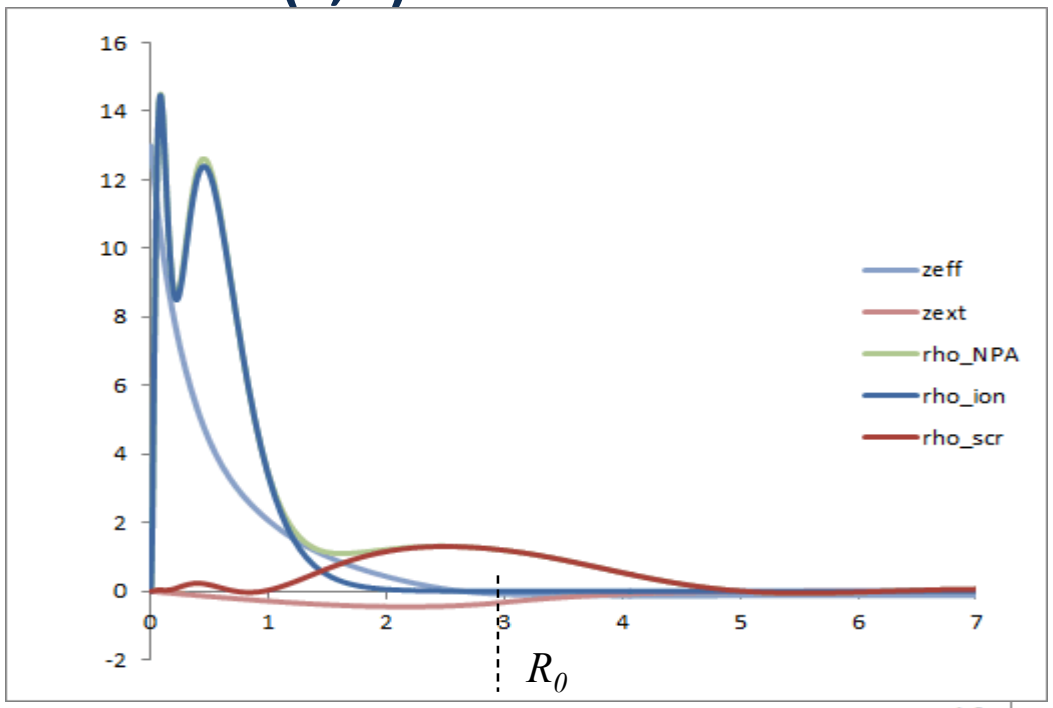



FIG. 5 (color online). Mean ionization potential ($\bar{I}$) inferred from the stopping-power data in the cold (a) and warm (b) cases compared to the Andersen-Ziegler empirical fits ($\bar{I}_{AZ}$), the ideal plasma case ($\hbar\omega_{pe}$), and electronic structure theory.

Mean ionization potential can be calculated simply by averaging $E_{binding} + E_{Fermi}$ for all electrons in the Average Atom calculation

From Zylstra et al., Phys Rev Lett 114, 215002 (2015)

# Future work: use neutral pseudo-atom (NPA) model that captures ion structure beyond the muffin-tin approximation, and refine $\varepsilon(k,\omega)$ used for calculation of $L(\rho,v,T)$



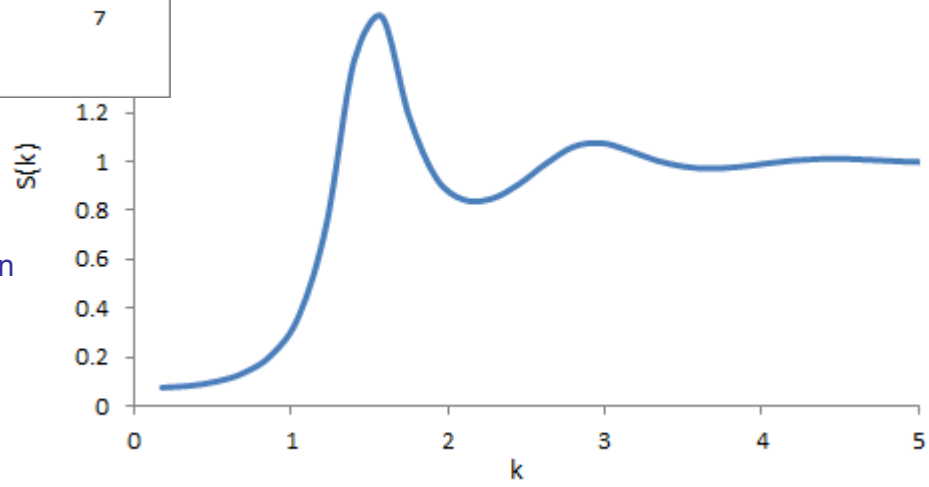

The potential does not vanish at the ion sphere boundary, and a neutral pseudo-atom can be defined with

$\int_{\text{all R}} \rho^{NPA}\, dr = Z_{nuc}$

This is distinct from the muffin-tin average atom with

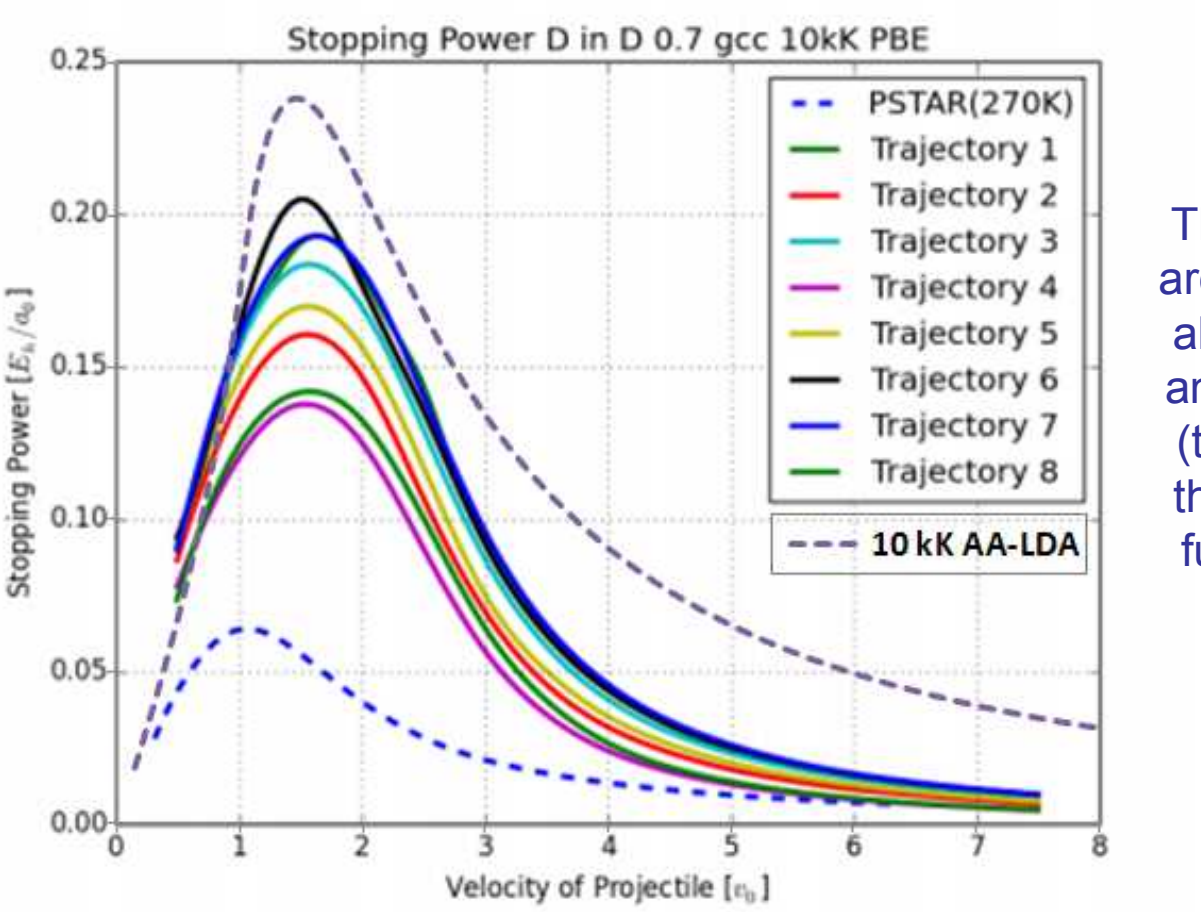
$\int_{r< Ro} \rho^{AA}\, dr = Z_{nuc}$

With a suitable definition of $\rho^{ion}$ , a self-consistent screening density $\rho^{scr} = \rho^{NPA} - \rho^{ion}$ can be determined and used with Quantum Ornstein-Zernike relations to find $g_{ii}(r)$ and $S_{ii}(k)$, along with the dielectric $\varepsilon(k,\omega)$




*Starrett and Saumon, HEDP 10, 35 (2014)

# In parallel with the Average-Atom based work (Hansen), Magyar *et al*. are investigating a TD-DFT-based approach




**(T = 10 kK)**

Figure 2: The Stopping of Deuterium in Deuterium ($\rho$= 0.7 gcc). Several curves represent different trajectories through the disordered supercell.

The TD-DFT calculations are free from assumptions about the collision model and the dielectric function (they remain sensitive to the exchange-correlation functional and trajectory averaging)

*Magyar, Shulenburger, and Baczewski, in preparation

# Conclusions

- We are calculating stopping powers using both Average-Atom-LDA and TD-DFT approaches; both depend on exchange-correlation functionals
- The Average-Atom approach has additional dependence on dielectric and collision models; we are working to increase self-consistency by incorporating ideas from Starrett and Saumon (this will reduce “knobs”)
- Both approaches generate XRTS scattering signals in addition to dE/dx – these two observables sample electronic response and together offer a powerful way to discriminate among self-consistent quantum models
- We urgently need precise experimental data from quiescent, uniform samples in the warm and hot dense matter regimes – the most useful comparisons will be of direct observables (e.g. XRTS and self-emission signals) rather than scalar values interpreted through (possibly inconsistent) models