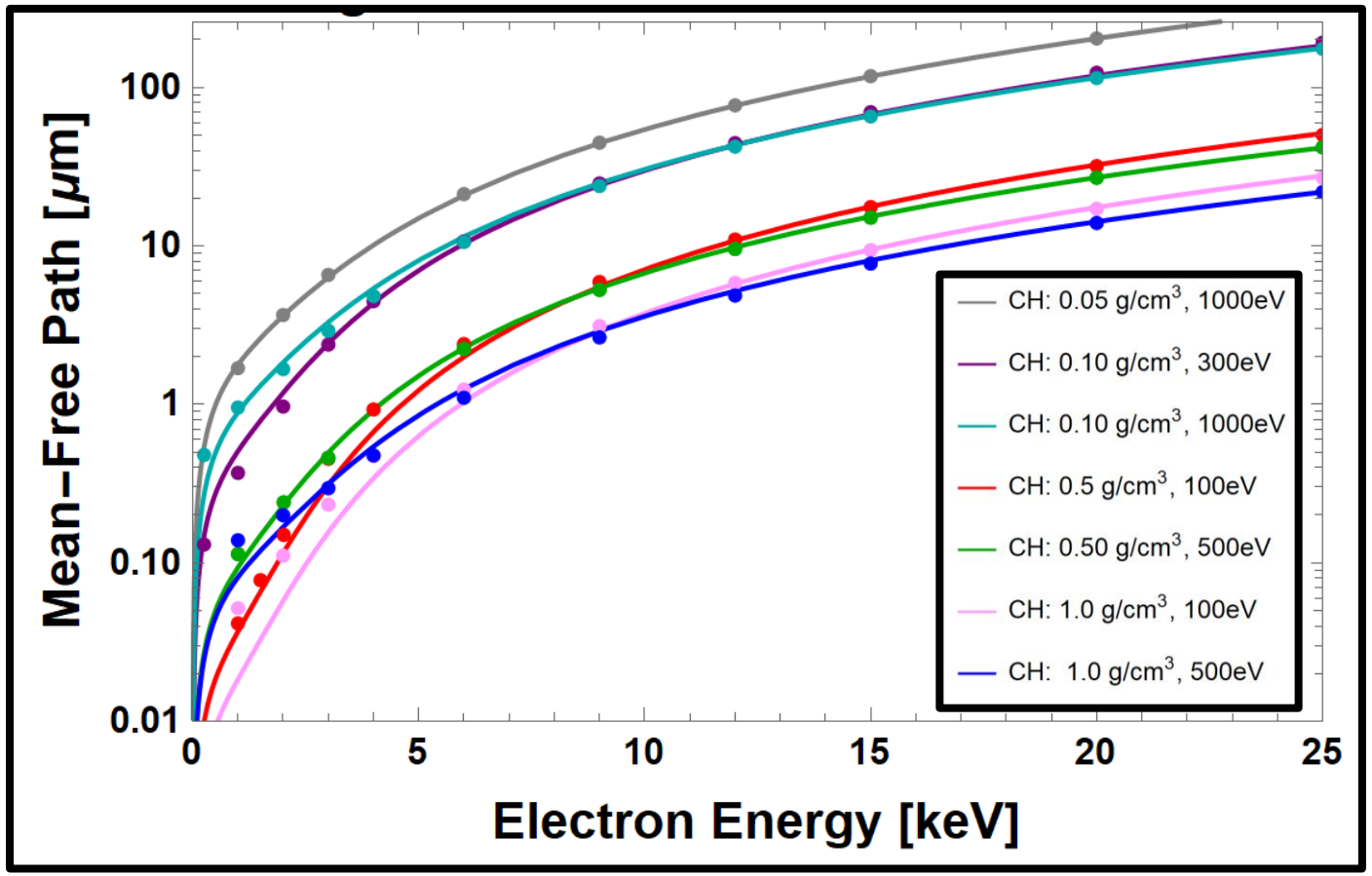
Investigation of Nonlocal Electron Transport in High-Energy-Density Plasmas using *Ab Initio* Methods



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Collaborators

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Summary

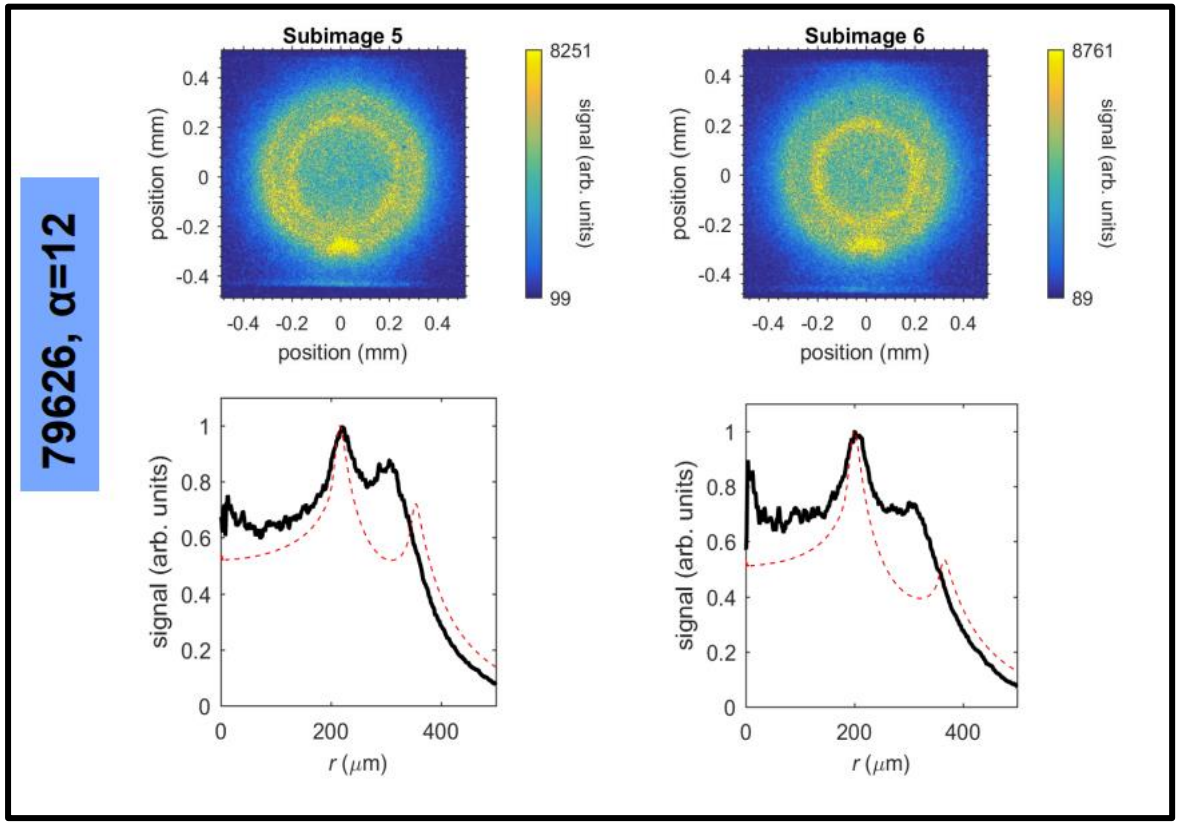
TD-DFT calculations of electron stopping range in “conduction zone” plasmas are used to improve the modeling accuracy for laser-target coupling in LDD

- **Modeling the non-local electron transport is important for simulating LDD ICF experiments**
- **The current modified Lee-More model for nonlocal mean free path used in LDD hydrocodes, shows discrepancy when compared to experimental observations**
- **The preliminary stopping power results can be used for developing a global analytical/numerical model for the MFP in both CH and DT plasmas, which is expected to improve the hydrocode simulations for LDD implosions**

TD-DFT: Time-Dependent Density Functional Theory
LDD: Laser Direct Drive
ICF: Inertial Confinement Fusion
MFP: Mean Free Path

There is a clear distinction between simulation and experiment for x-ray self emission corresponding to ICF experiments

- ICF target: solid DT covered with ablator layer (CH)[3, 4]
- Laser energy transported to ablation surface by electrons - through the conduction zone (CZ)[3,4]
- Electron thermal transport: way that energy flows through the CZ – modeled in rad-hydro codes[1,2, 3]
- As electrons travel through plasma, they lose energy and are deposited in CH or DT [2, 3]
- The current model for electron MFP inaccurate predicts the path length and causing other systematic inaccuracies for quantities (such as the emission spectrum) in the hydrocode[1, 5, 6,7]



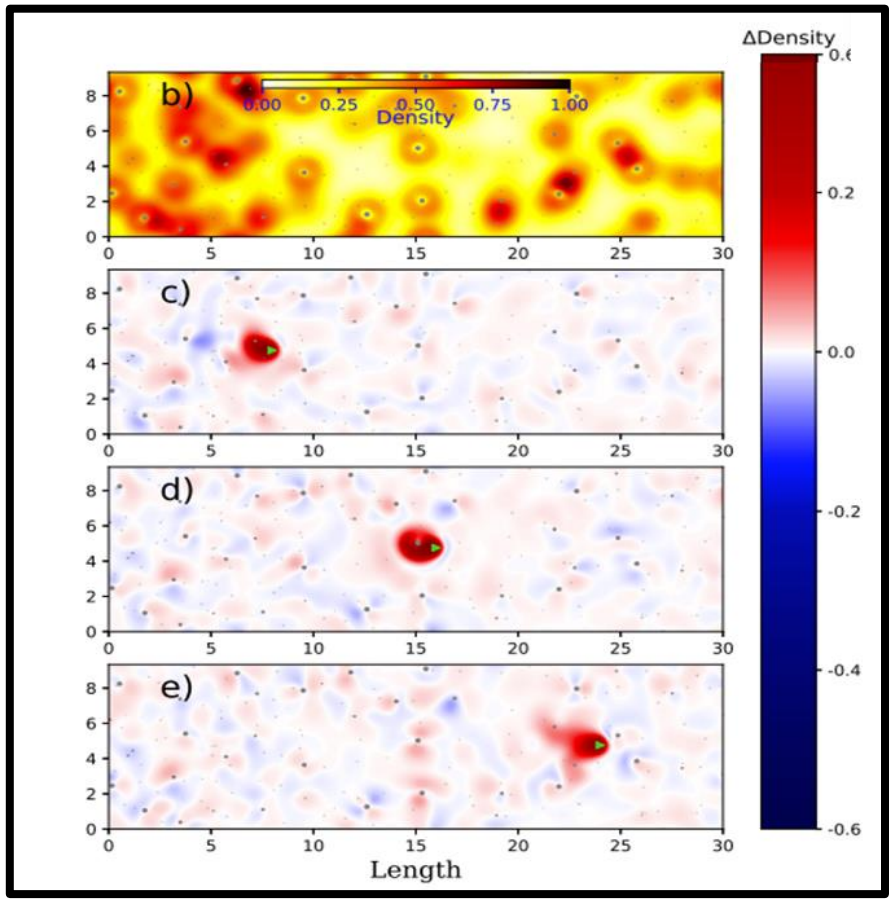
[1] V. N. Goncharov, O. V. Gotchev, E. Vianello, et al. Phys. Plasmas 13, 012702 (2006)
[2] Duc Cao, Gregory Moses and Jacques Delettrez Phys. Plasmas 22, 082308 (2015)
[3] S. X. Hu, D. T. Michel, A. K. Davis, et al , Understanding the effects of laser imprint on plastic-target implosions on OMEGA, Phys. Plasmas 23, 102701 (2016)
[4] D. T. Michel, S. X. Hu, et. Al., Measurement of the shell decompression in direct-drive inertial-confinement-fusion implosions (2017)
[5] S. X. Hu, L. A. Collins, V. N. Goncharov, et al. Phys. Plasmas 23, 042704 (2016)
[6] R. Shah et al., Observations of anomalous x-ray emission at early stages of hot-spot formation in deuterium-tritium cryogenic implosions Phys. Rev. E 103, 023201 (2021)
[7] R. Shah et al. (in preparation)

TD-DFT *ab initio* calculations of stopping power will improve the calculation for electron MFP in ICF relevant conditions

- **Many analytical methods for SP/ MFP fall short**
  - **Use TD-DFT to obtain ESP calculations – relate to MFP and globally fit the MFP**
- **Use SHRED* to probe a variety of density/temperature conditions relevant to ICF experiments**
  - **Take a high energy electron and probe a box of CH plasma**
  - **Measure average force against the electron:**

$$S_p(v_p) = < \frac{dE_{KS}}{dx(t)} >$$

The stopping power calculations are allowed to run for the time it takes for the electron through the box 10x, the final measurement is the SP



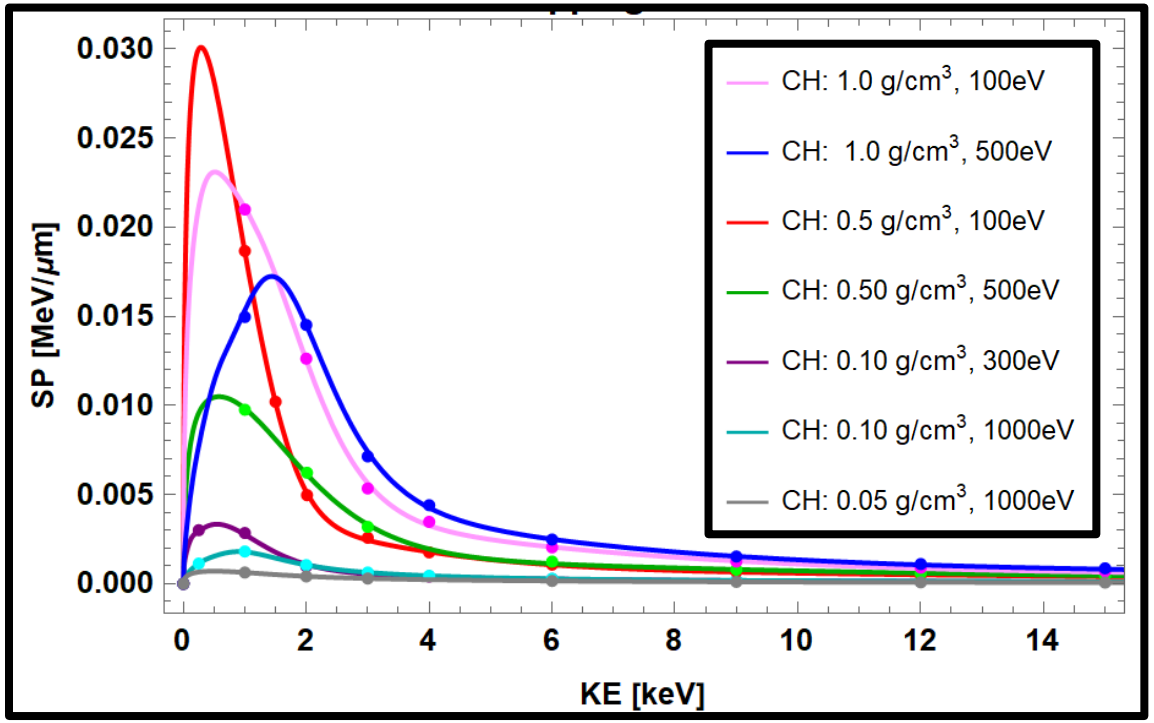
*SHRED: Stochastic and Hybrid Representation Electronic structure by Density functional theory

[1] A. White, L. A. Collins, K. Nichols, S. X. Hu, 2022 *J. Phys.: Condens. Matter* 34 174001
[2] A. White and L. A. Collins, Phys. Rev. Lett. 125, 055002 (2020).
[3] Y. H. Ding, A. J. White, S. X. Hu, O. Certik, and L. A. Collins, Phys. Rev. Lett. 121, 145001 (2018)
[4] R. J. Magyar, L. Shulenburger, and A. D. Baczewski, Contrib. Plasma Phys. 56, 459 (2016).

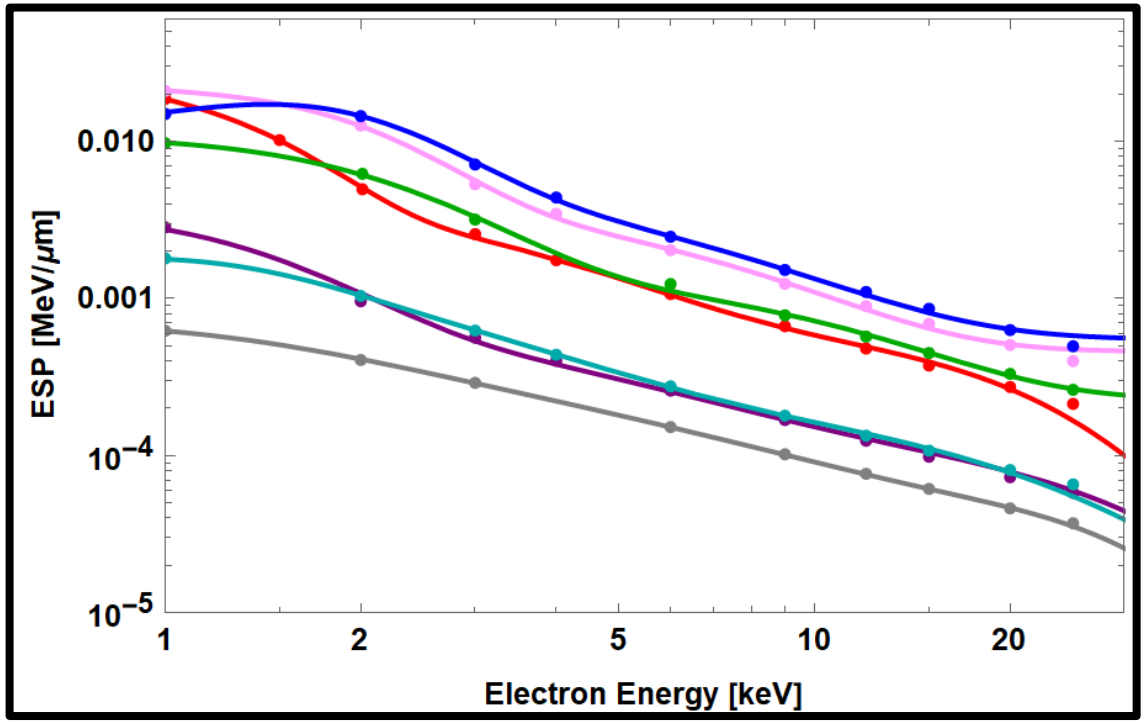
Stopping Power Data

The stopping power of a high energy electron in a CH plasma is calculated for many plasma density and temperature conditions and over many velocity values

SP with respect to Electron Energy



Log – Log SP with respect to Electron Energy

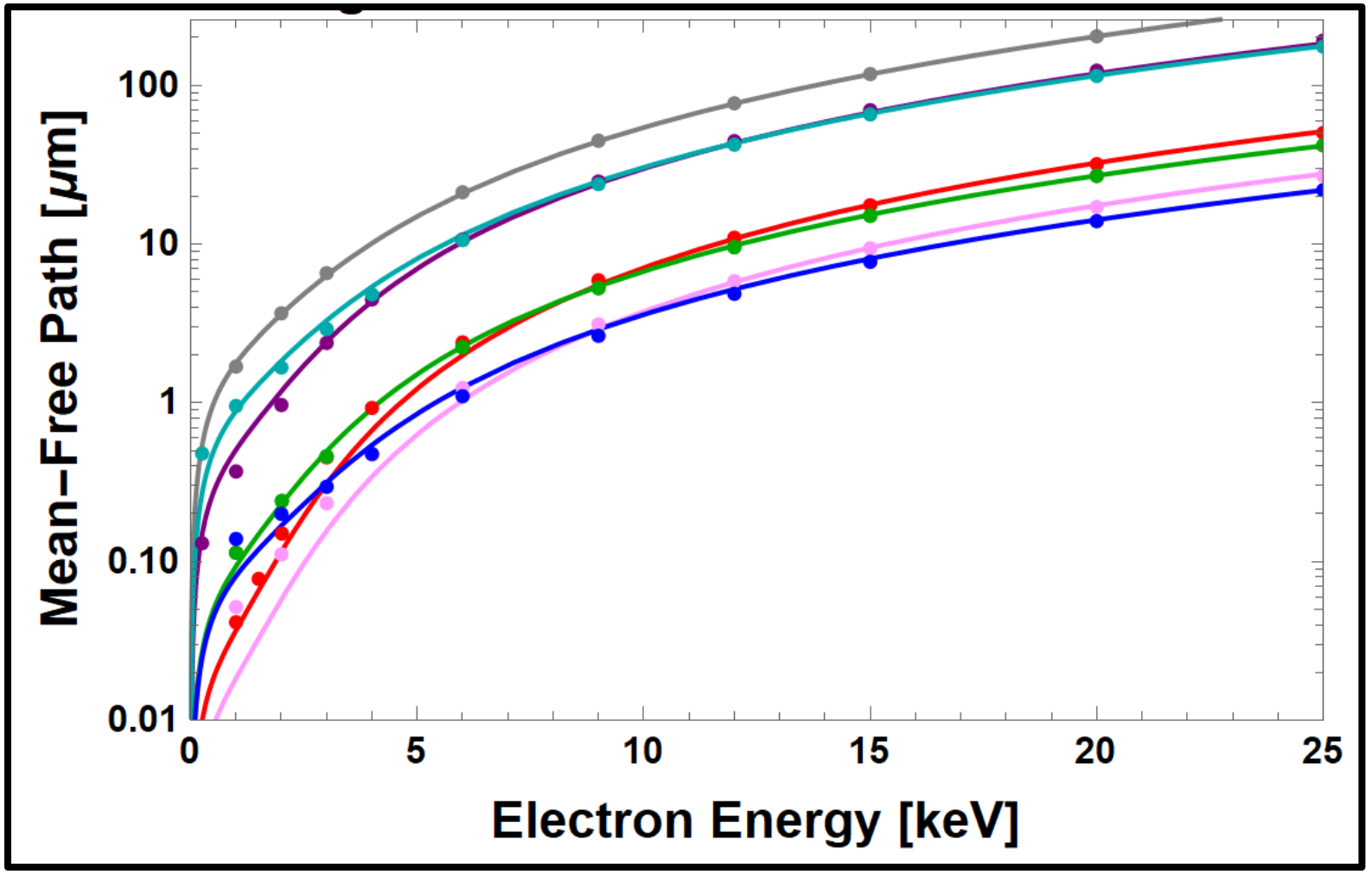


For each stopping power calculation, we take the average of two independent OFMD snapshots

[1] A. White, L. A. Collins, K. Nichols, S. X. Hu, 2022 *J. Phys.: Condens. Matter* 34 174001

[2] A. White and L. A. Collins, Phys. Rev. Lett. 125, 055002 (2020).

Using the TD-DFT calculations for the non-local electron MFP, a global analytical model can fit the data as a function of temperature, density, and electron energy



$$\lambda_e = \int_0^{v_p} \frac{mv}{ESP(v)} dv$$

- CH: 0.05 g/cm^3, 1000eV
- CH: 0.10 g/cm^3, 300eV
- CH: 0.10 g/cm^3, 1000eV
- CH: 0.5 g/cm^3, 100eV
- CH: 0.50 g/cm^3, 500eV
- CH: 1.0 g/cm^3, 100eV
- CH: 1.0 g/cm^3, 500eV

MFP Model Formula

The non-local electron MFP in CH can be fit by a global analytical / numerical model that is dependent on the CH density/temperature and the electron energy

$$\lambda_k = \left(\frac{k^2}{4\pi e^4 n_i} \cdot \frac{1}{(Z \cdot \Lambda_{DFT} + < Z > \cdot \Lambda_C)}\right) + L$$

Mean free path

$$\Lambda_{DFT} = a_0 \cdot \left(\frac{k}{Z_{eff}}\right)^{-\alpha} \cdot \left(d_0 \cdot (1 + b_0 \cdot Z_{eff}) + c_0 \cdot \epsilon_f \cdot \left(\frac{T}{450}\right)^{\beta} \cdot \left(\frac{\rho}{0.450}\right)^{\gamma} \cdot k^{1.5}\right)$$

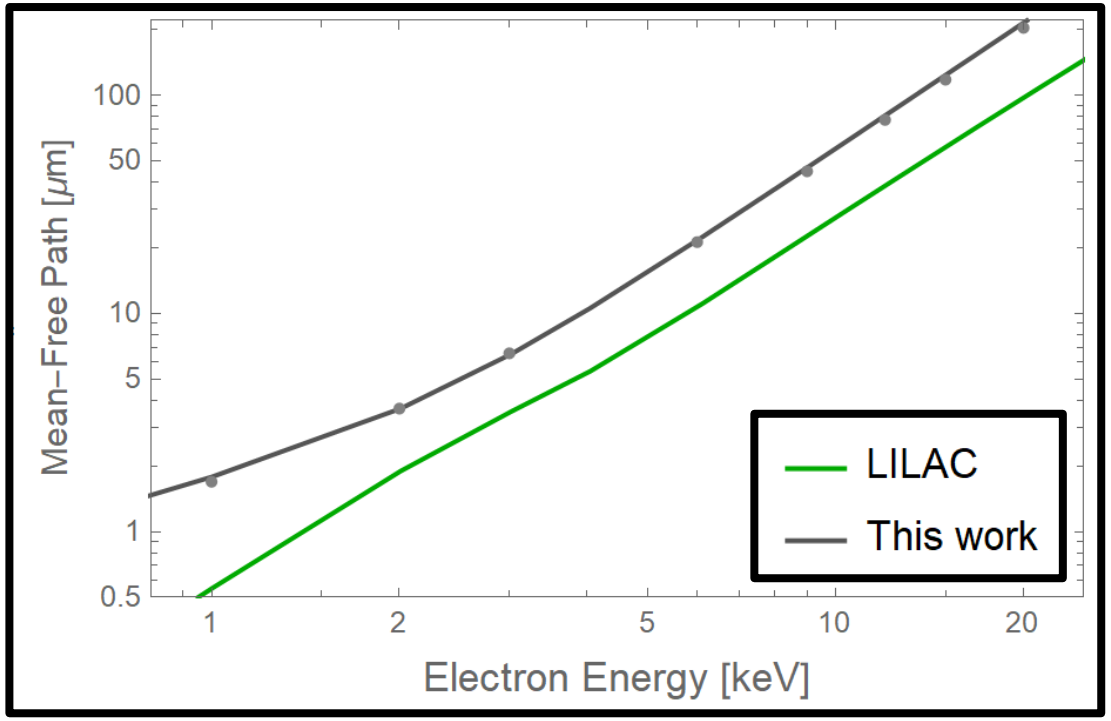
Coulomb Logarithm

- Additional Term: $L = \frac{c_1 T}{\rho} Log(k+1)$
- Electron energy in keV: k
- CH density in g/cc: ρ
- CH temperature in eV: T
- The fermi energy in eV: $\epsilon_F(\rho)$:
- Effective charge: $Z_{eff}(\rho, T) = \frac{<Z^2>}{<Z>}$ [1]
- Fitting Parameters: $\alpha, \beta, \gamma, a_0, b_0, c_0, d_0, c_1$
- Collective effects: $\Lambda_C = Log\left(\frac{1.123 \cdot v}{\omega_p \cdot b_{max}}\right)$ [2]
- Max Impact Parameter $b_{max} = max(R_i, \lambda_D)$
- Plasma frequency: ω_p
- Interparticle distance R_i:
- Debye Length: λ_D

[1] V. N. Goncharov, O. V. Gotchev, E. Vianello, et al. Phys. Plasmas 13, 012702 (2006)
[2] S.X. Hu, et al. Physics of Plasmas **23**, 042704 (2016)
[3] Wolfram Research, Inc., Mathematica, Version 12.1, Champaign, IL (2020).

Our newly developed model for MFP can be compared to the current model for the MFP used in hydrodynamic codes at the LLE

CH : $0.05\ g/cm^3, 1000\ eV$



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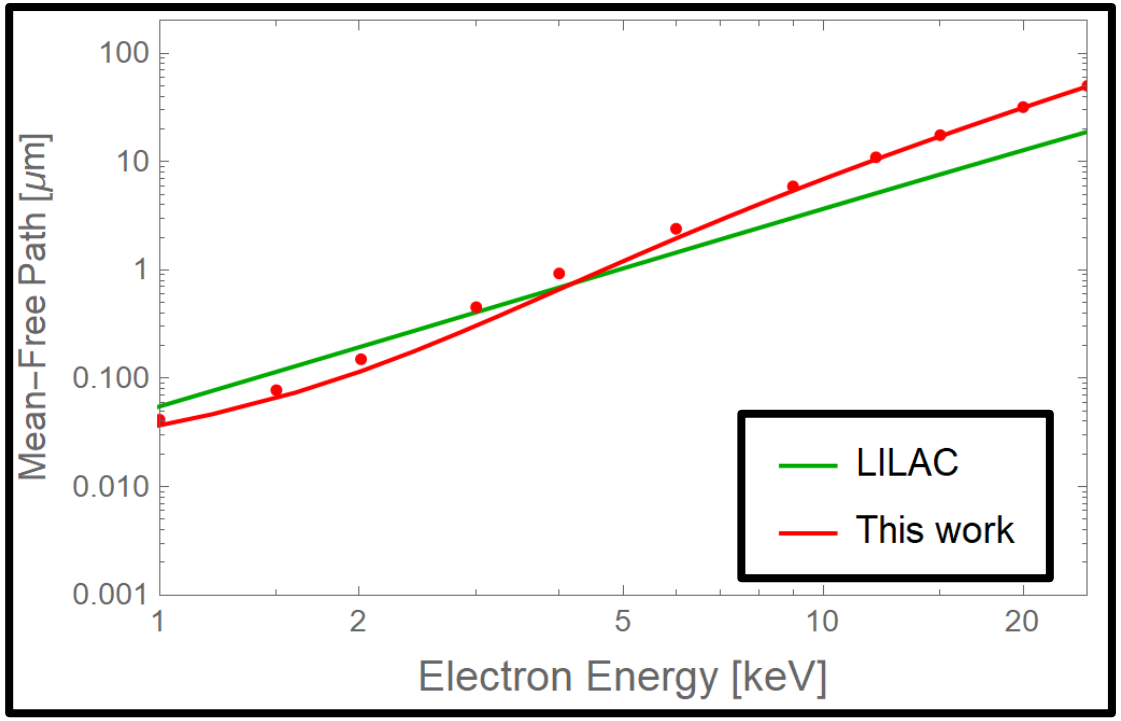

We see a clear distinction between the current method for mean free path used in LILAC and the method discussed here

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[2] S.X. Hu, et al. Physics of Plasmas 23, 042704 (2016)
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Thank You!