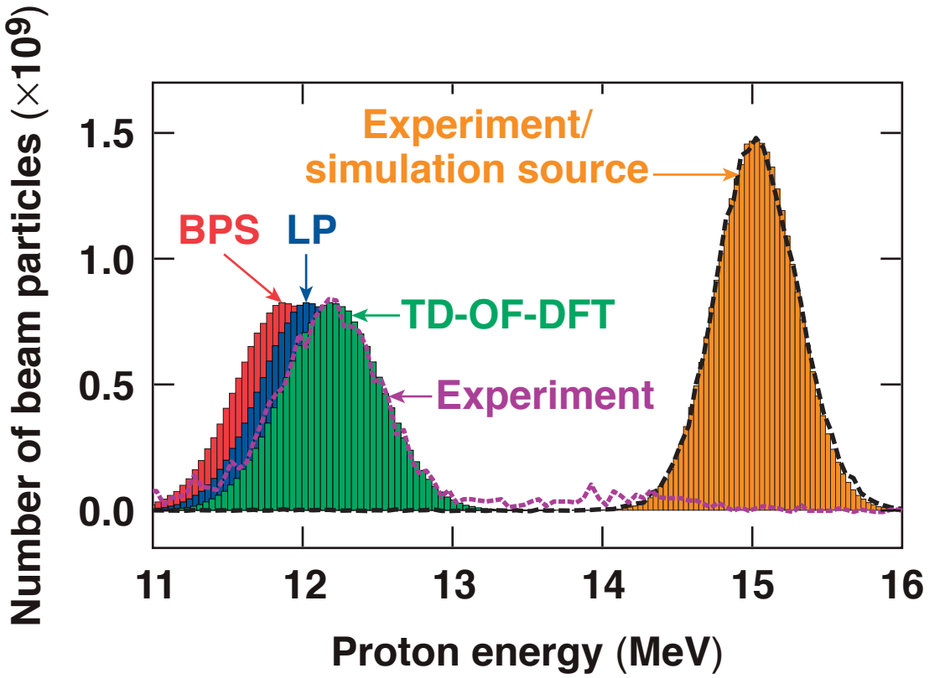
Ab Initio Studies on Stopping Power of Warm Dense Matter with Time-Dependent Orbital-Free Density Functional Theory



Y. H. Ding
University of Rochester
Laboratory for Laser Energetics
Department of Mechanical Engineering

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Summary

A time-dependent orbital-free density functional theory (TD-OF-DFT) code has been developed for *ab initio* investigations of transport properties of warm dense plasmas

- The electron dynamic has been implemented to OF-DFT for first-principles simulations of the transport properties of dense plasma
- Our current-dependent TD-OF-DFT calculations have reproduced the recently well-characterized stopping-power experiment in warm dense beryllium
- For α-particle stopping in warm and solid-density DT plasmas, the *ab initio* TD-OF-DFT shows a lower stopping power (up to 25%) in comparison with three stopping-power models often used in the high-energy-density physics community

TC14490

* Y. H. Ding , A. J. White, S. X. Hu, O. Certik, and L. A. Collins, Phys. Rev. Lett. 121, 145001 (2018).

Collaborators

S. X. Hu

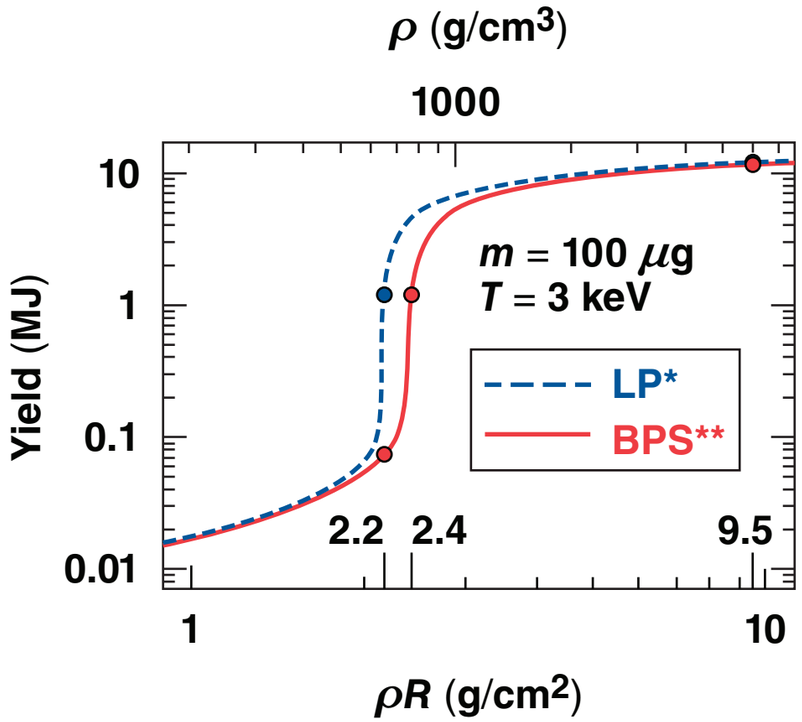
University of Rochester
Laboratory for Laser Energetics
and Department of Mechanical Engineering

A. J. White, O. Certik, and L. A. Collins

Los Alamos National Laboratory

Motivation

Transport properties (thermal/electrical conductivity and stopping power) of dense plasmas are crucial for accurately modeling ICF and HED experiments

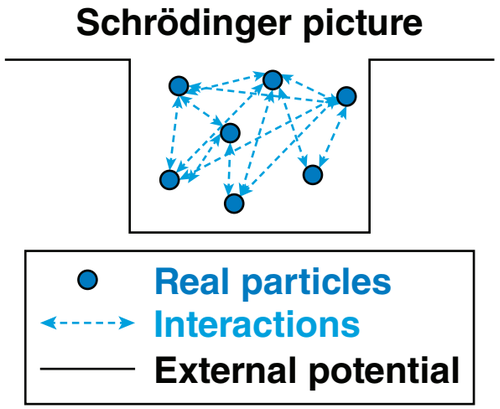


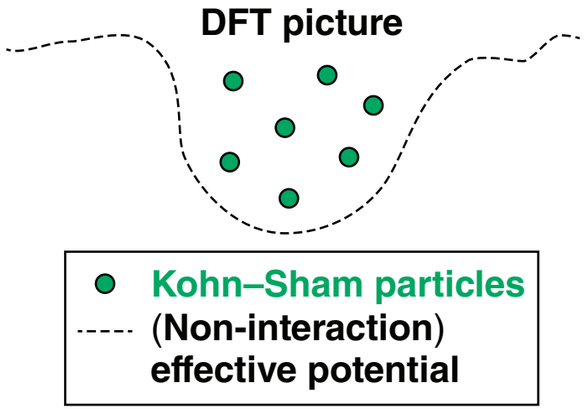
Differences in stopping power will influence energy delivered from α particles to the dense shell, which will also influence the yield

ICF: inertial confinement fusion
HED: high-energy density
LP: Li–Petrasso
BPS: Brown–Preston–Singleton

*C. K. Li and R. D. Petrasso, Phys. Rev. Lett. 70, 3059 (1993); 114, 199901(E) (2015).
**L. S. Brown, D. L. Preston, and R. L. Singleton, Jr., Phys. Rep. 410, 237 (2005); R. L. Singleton, Jr., Phys. Plasmas 15, 056302 (2008).
†S. X. Hu *et al.*, Phys. Plasmas 23, 042704 (2016).

Orbital-free DFT can be used to investigate relatively high-temperature and dense plasmas





$$n(\vec{r}) = \sum_{i=0}^{N} \left| \phi_i(\vec{r}) \right|^2$$ **Simplify to** $$n(\vec{r}) = \left| \phi(\vec{r}) \right|^2$$

OF-DFT: only one orbital basis

The transport properties of warm dense plasmas can be studied by the time-dependent OF-DFT code

The split-operator (SO) scheme is used to solve the TD-OF-DFT equation

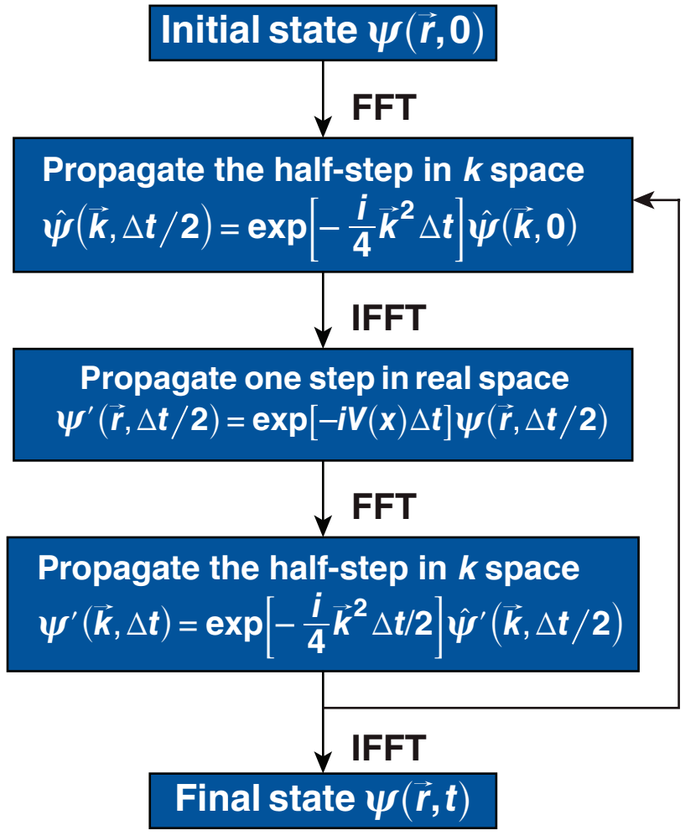
TD-OF-DFT equation:

$$i\frac{\partial\psi(\vec{r},t)}{\partial t}=\left[-\frac{1}{2}\nabla^2+V_{\text{eff}}(\vec{r},t)+V_{\text{dyn}}(\vec{r},t)\right]\psi(\vec{r},t)$$

To capture the low-frequency, long-wavelength current response, we introduce a current-dependent* (CD) dynamic kinetic energy potential (functional derivative)

$$V_{\text{dyn}}(\vec{r},t)=\frac{\pi^3}{2k_F^2(\vec{r},t)}\mathcal{F}^{-1}\left[i\vec{q}\cdot\vec{J}(\vec{q},t)/\left|q\right|\right](\vec{r})$$

derived using the Lindhard response function match method



FFT: fast Fourier transform
IFFT: inverse fast Fourier transform

*A. J. White *et al.*, Phys. Rev. B 98, 144302 (2018).

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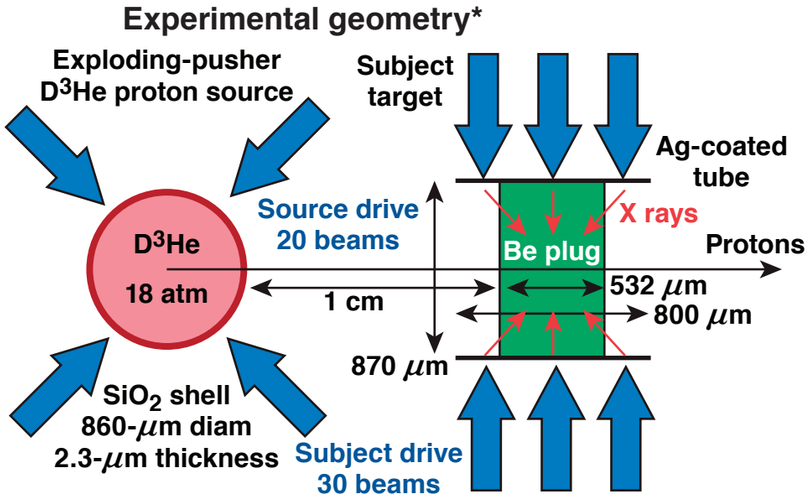
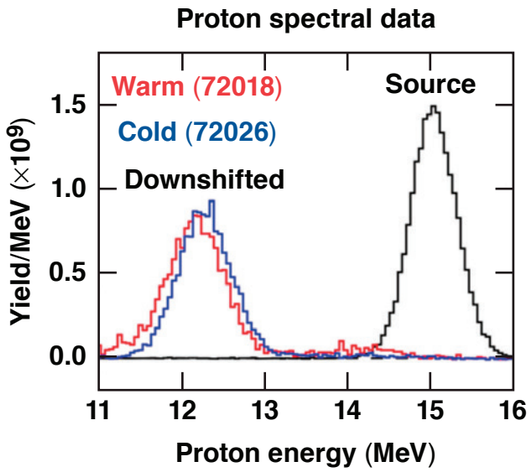
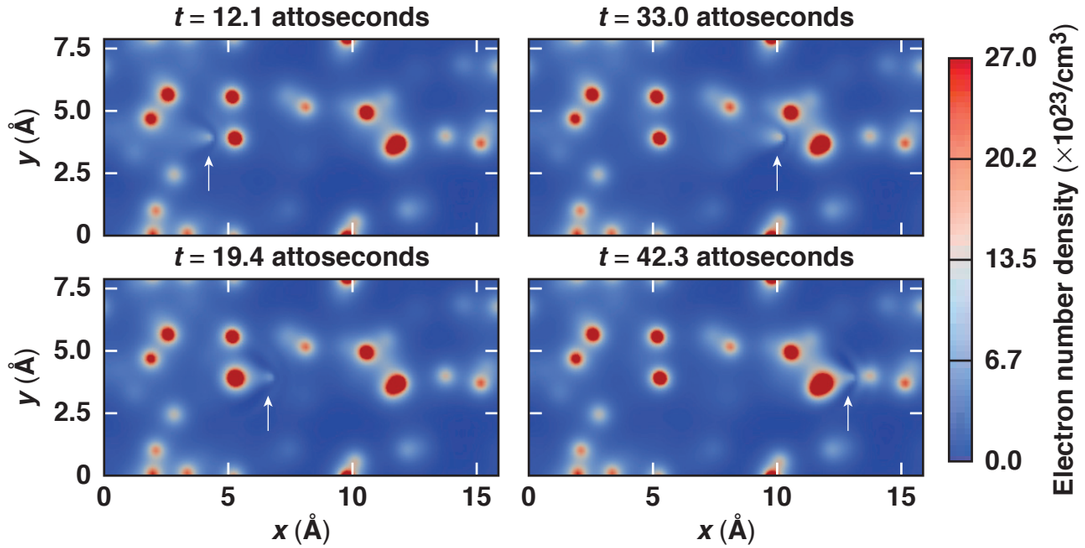
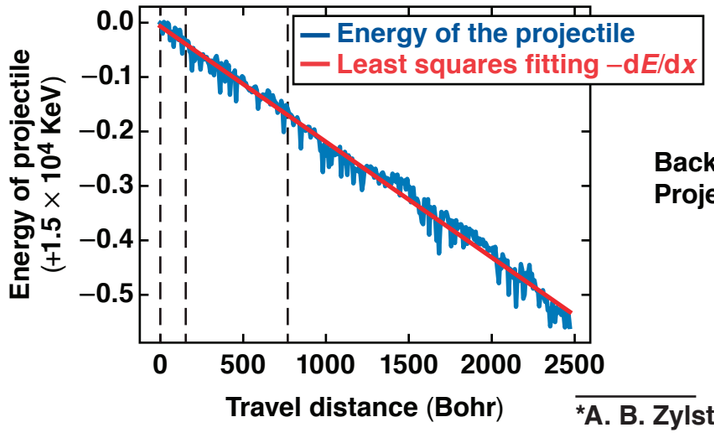
We first simulate the recent stopping-power measurement in warm dense Be conducted on OMEGA









Background: Be plasma at 1.78 g/cm^3
Projectile: proton at 1 MeV

*A. B. Zylstra *et al.*, Phys. Rev. Lett. 114, 215002 (2015).

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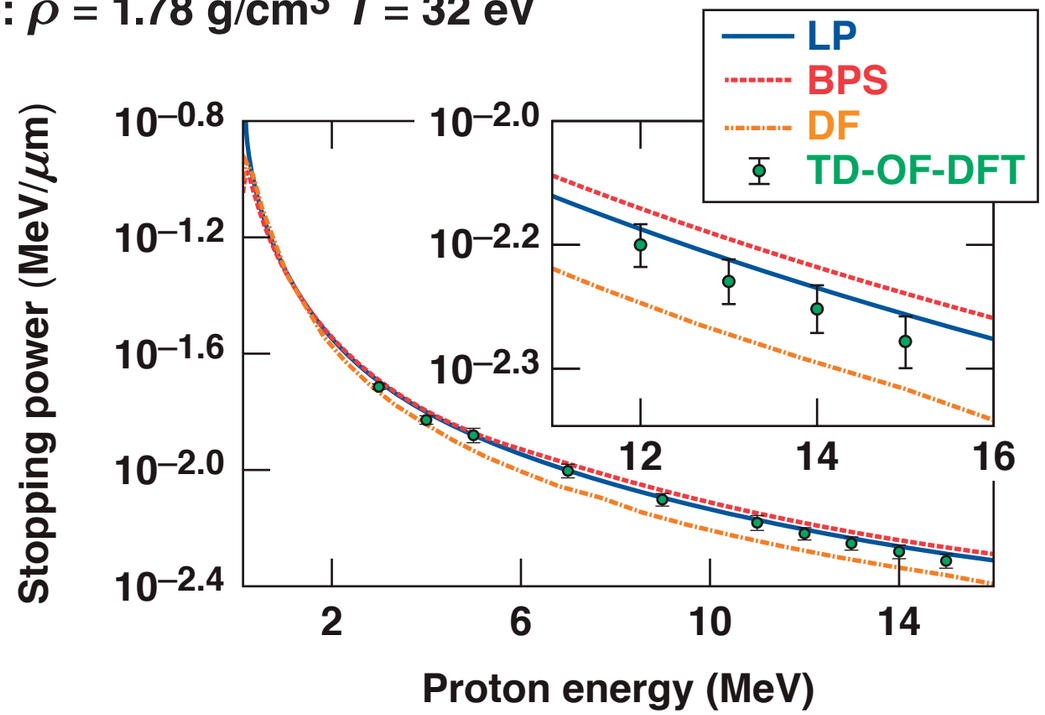
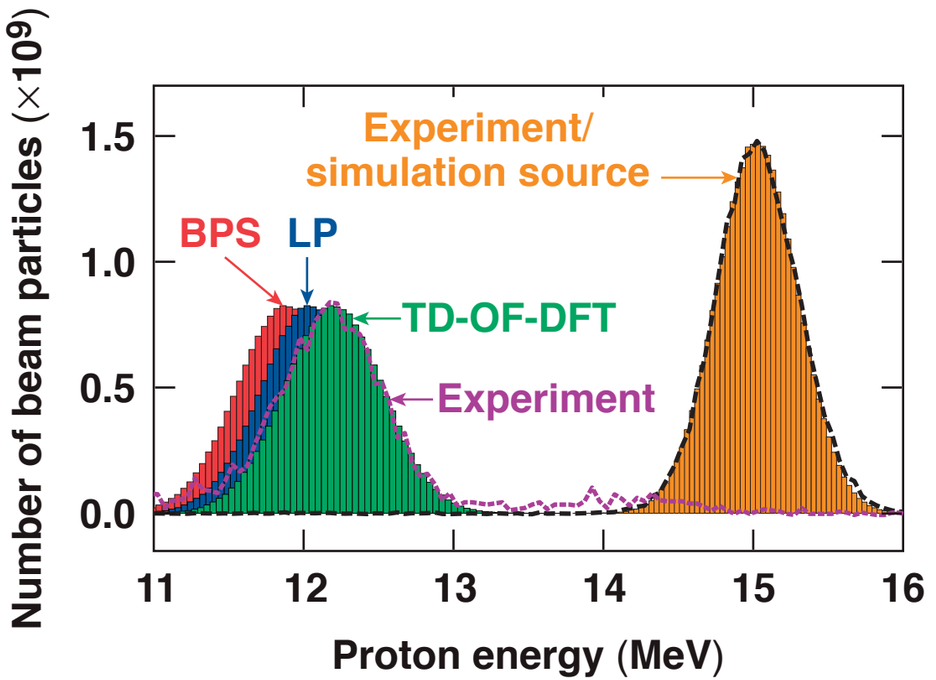
The TD-OF-DFT-calculated proton stopping power in high velocities in comparison with three stopping-power models

Be: $\rho = 1.78$ g/cm^3 $T = 32$ eV





The stopping power calculated by TD-OF-DFT is slightly lower than predictions of the LP and BPS models by ~5% and ~11%, respectively, and higher than predicted by DF by 20%.

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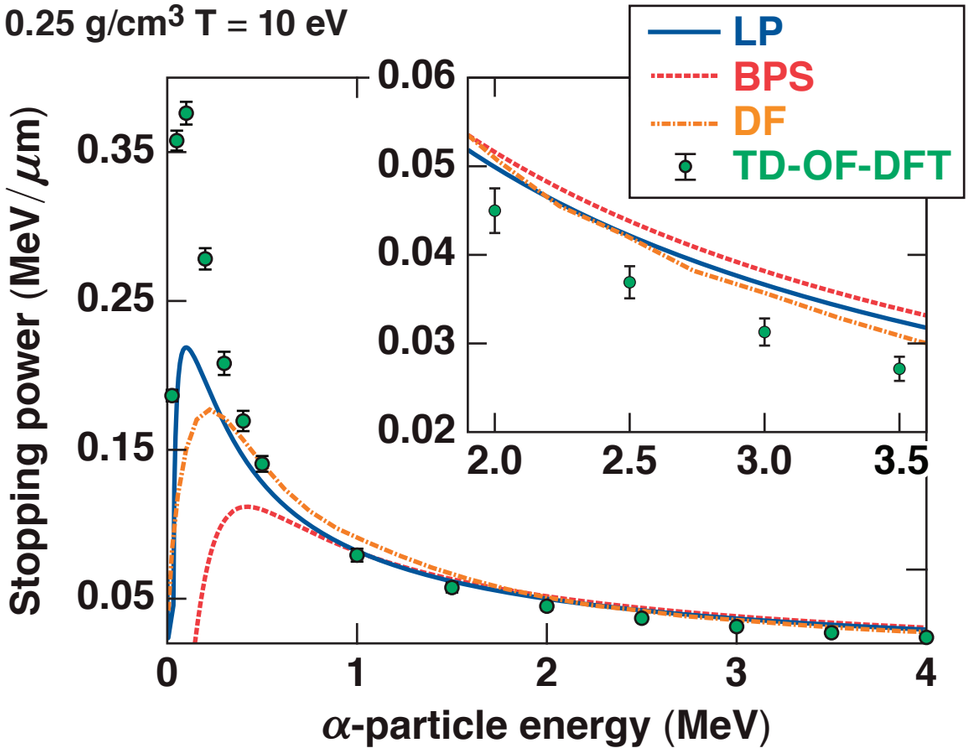
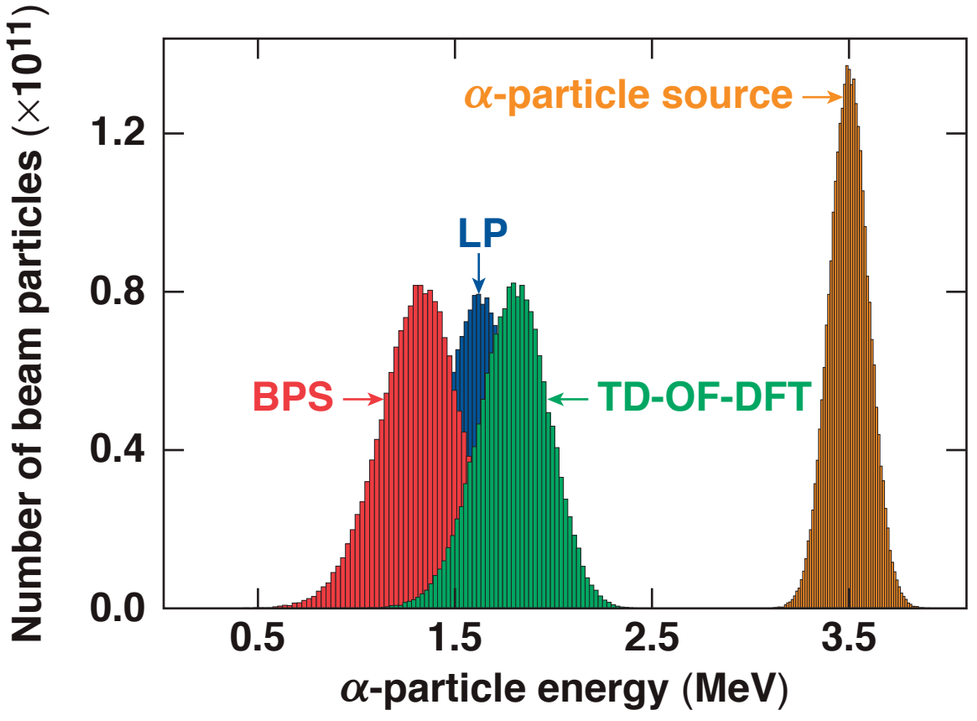
*A. B. Zylstra *et al.*, Phys. Rev. Lett. 114, 215002 (2015).

DF: dielectric function

TD-OF-DFT calculations indicate that the α-particle stopping power of warm dense DT is less than the LP and BPS models by ~15% to 25% in the ICF-relevant regime

DT: ρ = 0.25 g/cm^3 T = 10 eV





The comparison shows the stopping power from TD-OF-DFT calculations is smaller overall than LP, BPS, and DF models by ~16%, ~25%, and 15%, respectively. TD-OF-DFT predicts greater stopping from TD-OF-OF-DFT than all the models near the Bragg peak.

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Summary/Conclusions

A time-dependent orbital-free density functional theory (TD-OF-DFT) code has been developed for *ab initio* investigations of transport properties of warm dense plasmas

- We have presented a time-dependent orbital-free density-functional-theory formulation to investigate charged-particle stopping power of warm-dense plasmas
- Our comparison to recently measured downshifted spectra of energetic protons passing through the warm dense beryllium plasma agrees to within ~20 keV, while the LP and BPS models somewhat overestimated downshift by ~100 keV and ~200 keV, respectively
- Moreover, our TD-OF-DFT calculations indicate that the α-particle stopping power of warm dense DT is less than the LP, BPS, and DF models by ~15% to 25% in the ICF-relevant regime

TC14490

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