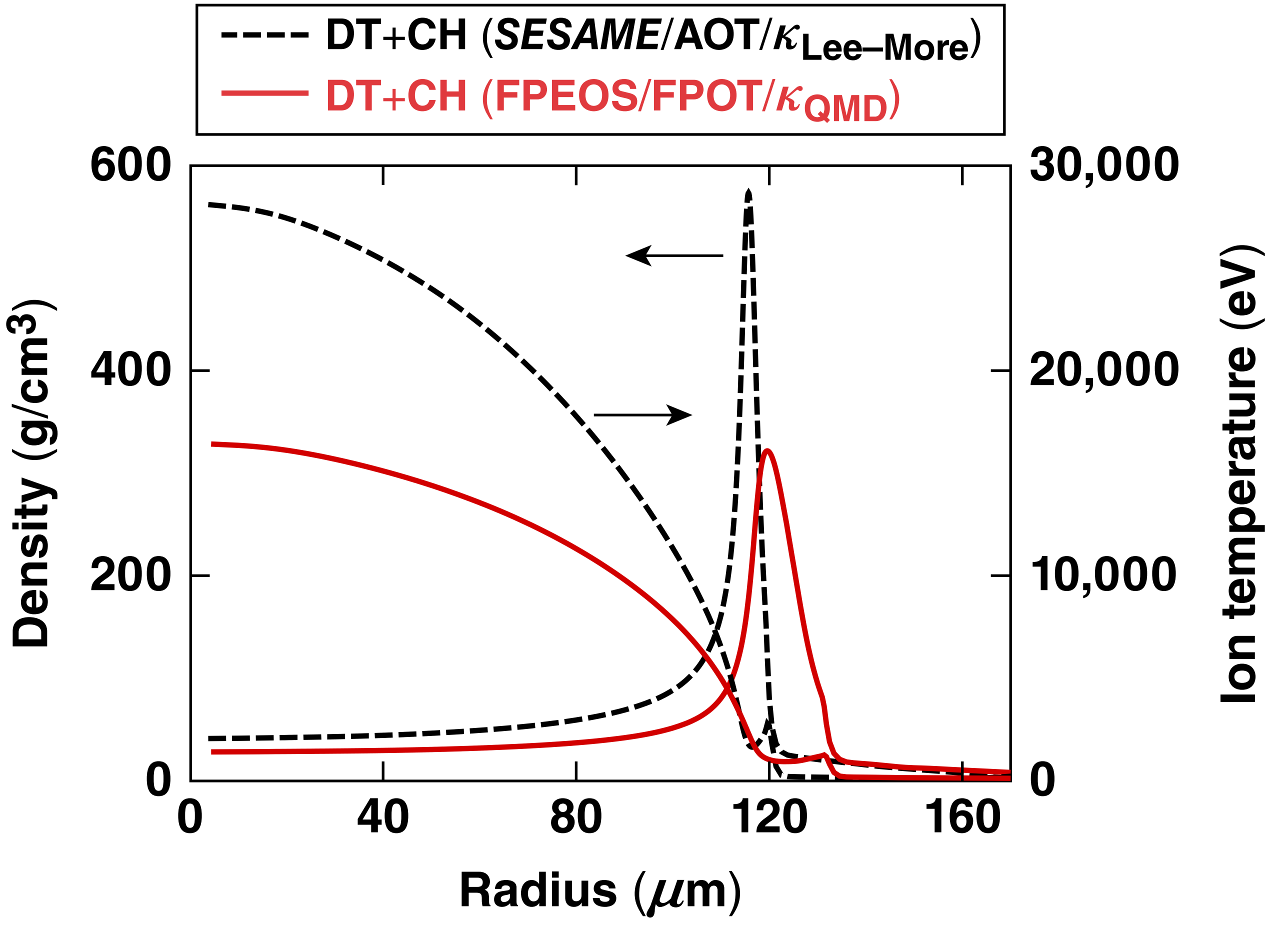
High-Energy-Density–Physics Studies for Inertial Confinement Fusion Applications



1-D target gain:
G = 31 (*SESAME*/AOT/$\kappa_{\text{Lee–More}}$)
G = 8 (FPEOS/FPOT/κ_{QMD})

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59th Annual Meeting of the
American Physical Society
Division of Plasma Physics
Milwaukee, WI
23–27 October 2017

Summary

Accurate intrinsic properties of plasmas under extreme conditions are essential for reliable inertial confinement fusion (ICF) target designs

- *First-principles* methods have been used to self-consistently calculate intrinsic properties of DT and ablators under extreme conditions
- These *ab initio* results, which can significantly differ from the predictions of traditional plasma models in the warm-dense-matter (WDM) regime, compared well with experiments
- Hydro simulations using these *first-principles* properties of DT and ablators have shown a significant difference in predicting target performance when compared with traditional model simulations

Knowing material properties better would result in a more-reliable understanding and designing of ICF implosions.

TC13827

Collaborators

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University of Rochester
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Outline

- Introduction: Why should we care about material properties under extreme conditions?
- *First-principles* methods and their applications to DT properties at high-energy-density (HED) conditions
- *Ab-initio* studies on ablator materials at HED conditions: How do they compare with traditional plasma models and experiments?
- Impact of these *first-principles* properties of both DT and ablators on ICF implosions
- Conclusions

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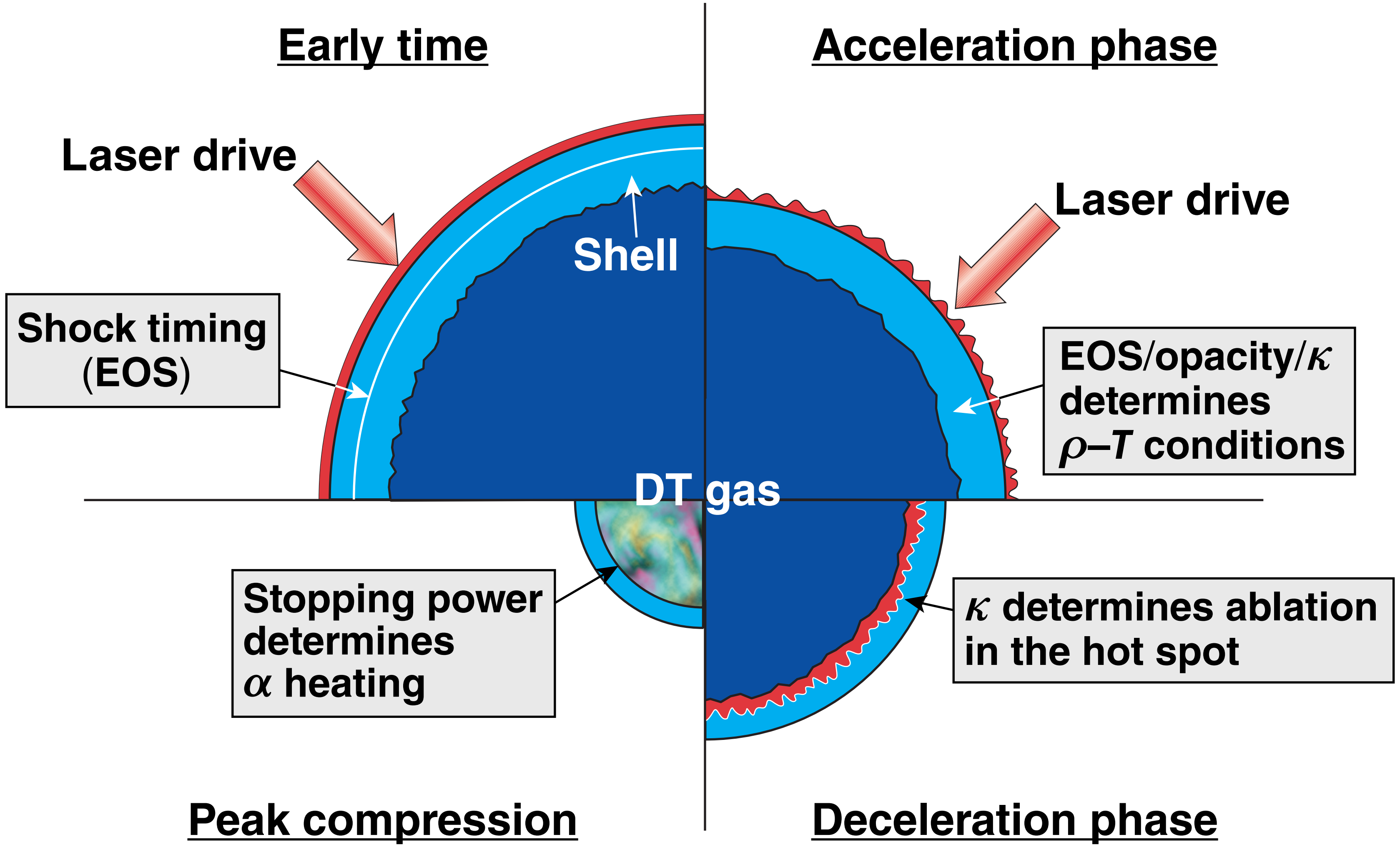
TC13828a

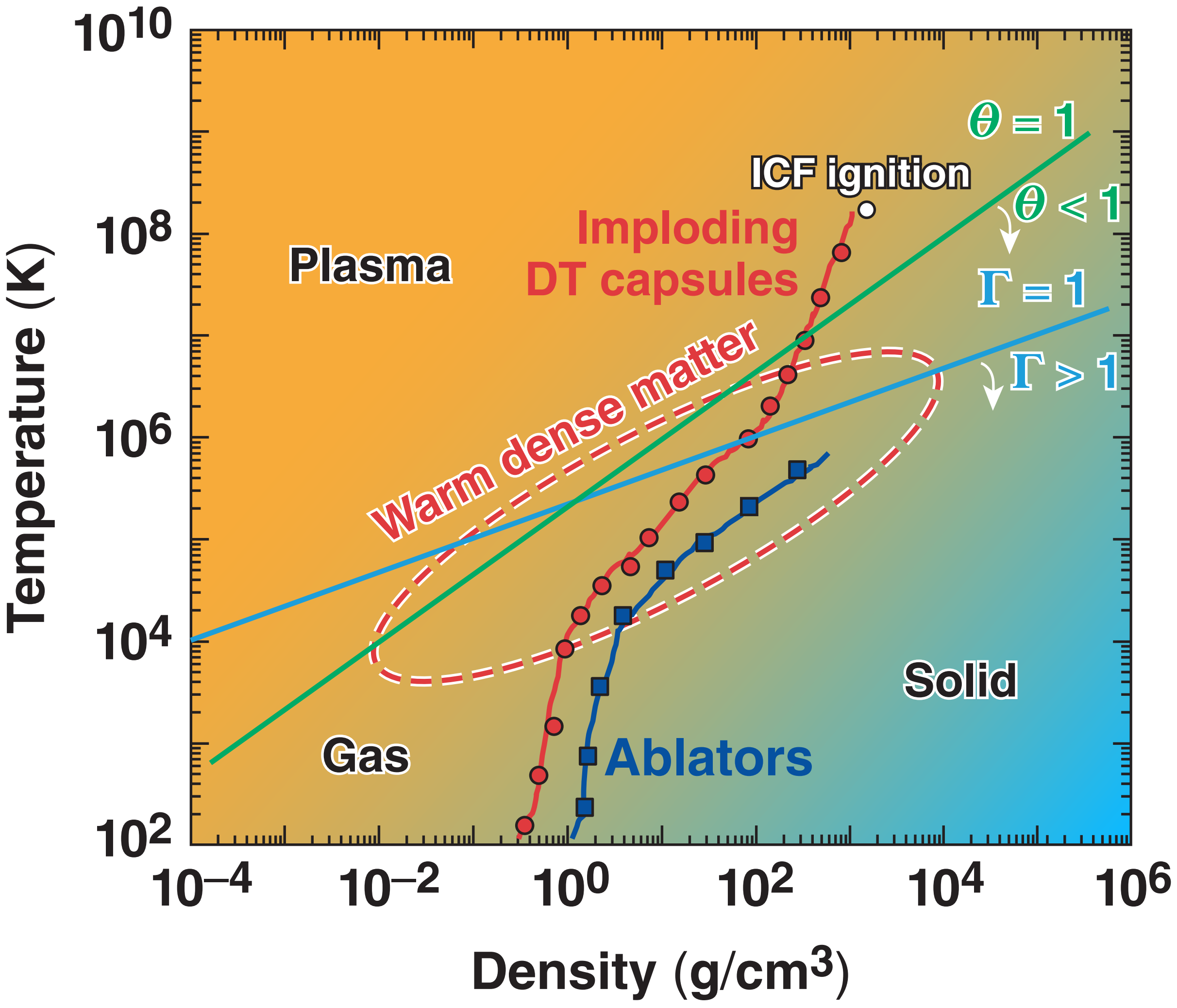
Accurate knowledge of *intrinsic* plasma properties (EOS,* opacity, thermal conductivity, and stopping power) of DT and ablators is required for ICF simulations



*EOS: equation of state

TC5723f

ICF implosions routinely access the WDM regime,* which demands a better understanding of material properties



1. **The Coulomb coupling parameter:**

$$\Gamma = \frac{q^2}{r_s k_B T},\ r_s = (3/4\pi n)^{1/3}$$

2. **The electron-degeneracy parameter:**

$$\theta = \frac{T}{T_F}$$

WDM: $\Gamma \geq 1; \theta \leq 1$

*S. X. Hu *et al.*, Phys. Rev. Lett. 104, 235003 (2010).

TC11490t

A variety of models have been adopted in ICF hydrocodes to estimate the properties of WDM

- Equation of state
  - *SESAME*/*Kerley03** based on the chemical model of matter, with perturbations of many-body coupling and electron degeneracy
- Thermal conductivity (κ)
  - the Lee–More model** was based on the first-order approximation to the Boltzmann equation, while the *Purgatorio*† (LLNL) is an average-atom model
- Opacity
  - the astrophysics opacity table (AOT)‡ has no available data in the WDM regime

First-principles calculations using path-integral Monte Carlo (PIMC) and quantum molecular dynamics (QMD) can provide self-consistent and accurate properties of WDM.

*G. I. Kerley, Phys. Earth Planet. Inter. 6, 78 (1972); G. I. Kerley, Sandia National Laboratories, Albuquerque, NM, Report SAND2003-3613 (2003).
**Y. T. Lee and R. M. More, Phys. Fluids 27, 1273 (1984).
†P. Sterne, Lawrence Livermore National Laboratory, Livermore, CA, Report UCRL-PROC-227242 (2006).
‡W. F. Huebner *et al.*, Los Alamos National Laboratory, Los Alamos, NM, Report LA-6760-M (1977).

TC11491c

Outline

- Introduction: Why should we care about material properties under extreme conditions?
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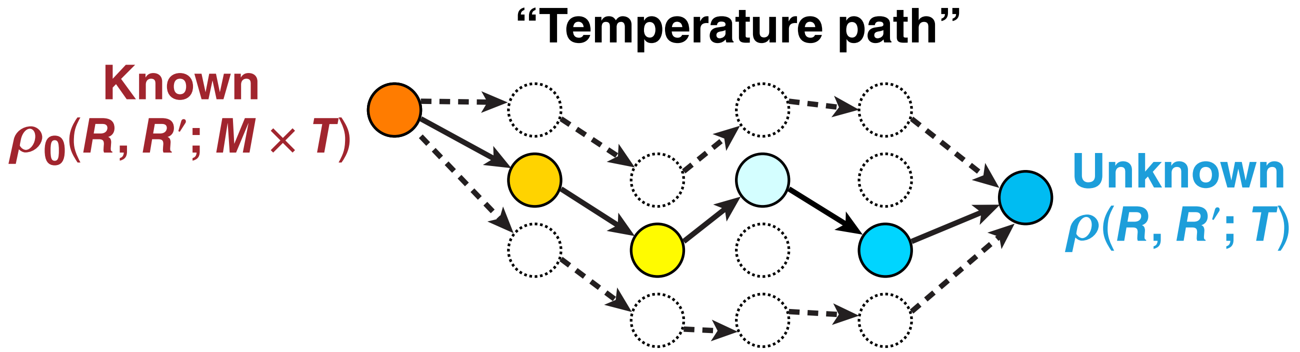
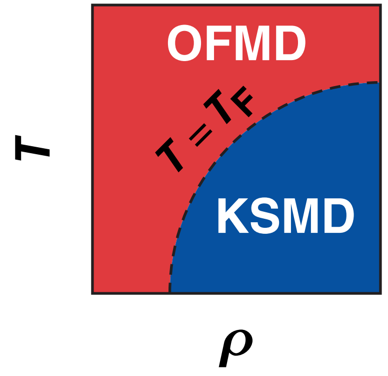
TC13828b

Both PIMC and QMD methods have been used to self-consistently calculate intrinsic plasma properties under extreme conditions

- **PIMC is based on the density-matrix representation of a quantum many-body system***

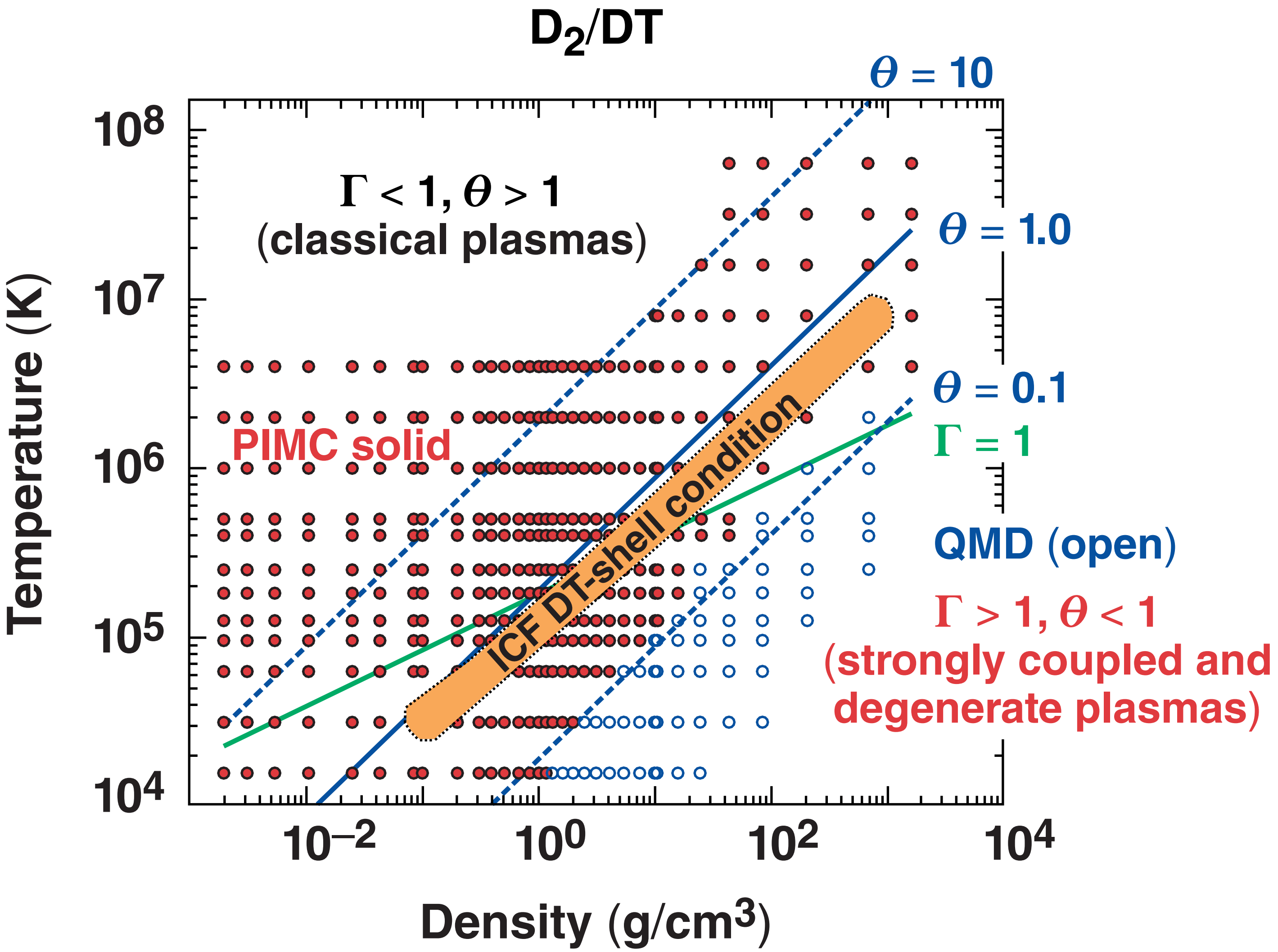


- **QMD uses the density-functional theory** to simulate dense plasmas in two "flavors": [Kohn–Sham molecular dynamics (KSMD, orbital based) and orbital-free molecular dynamics (OFMD†)]**



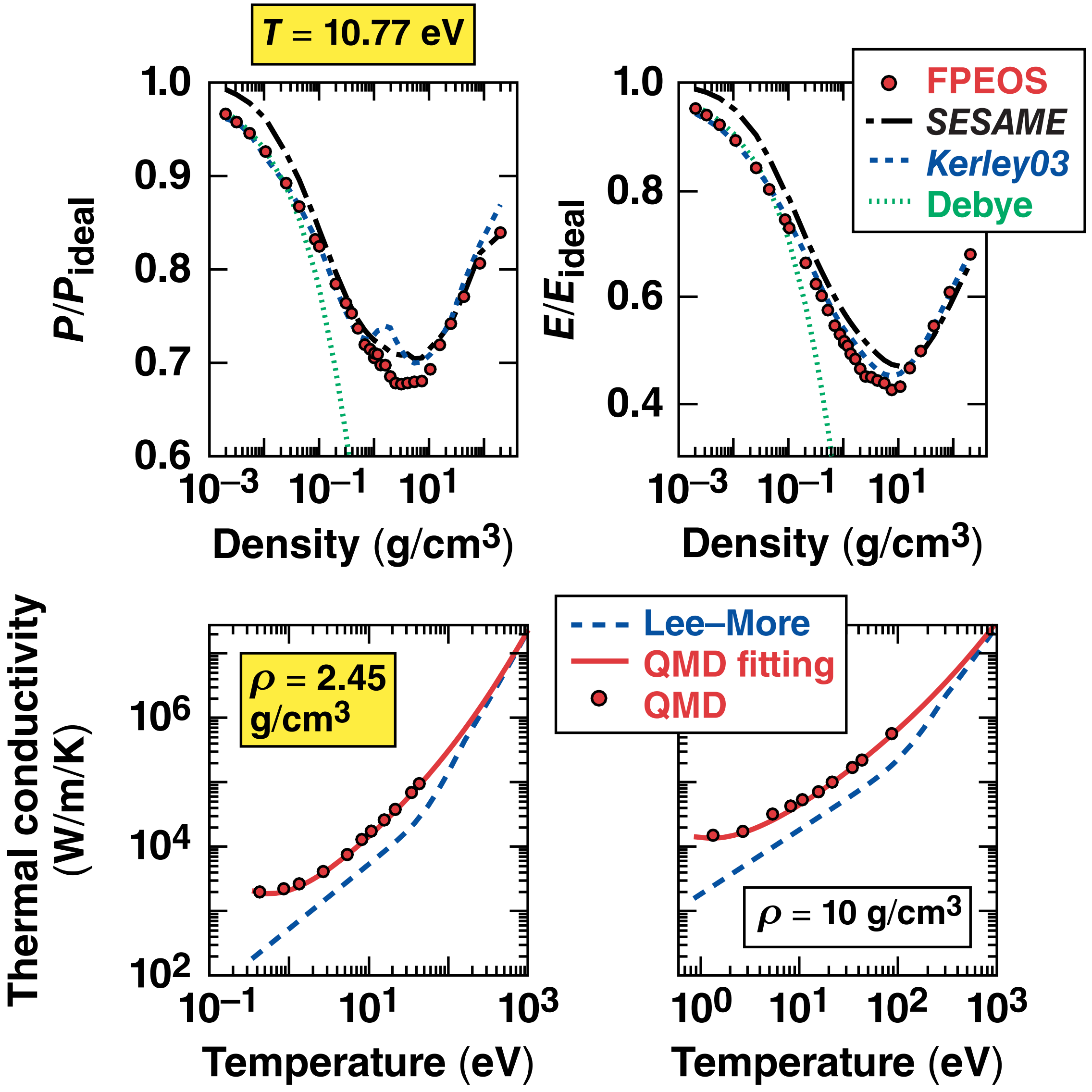
*D. M. Ceperley, Rev. Mod. Phys. 67, 279 (1995).
**W. Kohn and L. J. Sham, Phys. Rev. 140, A1133 (1965).
†F. Lambert, J. Clérouin, and G. Zérah, Phys. Rev. E 73, 016403 (2006).

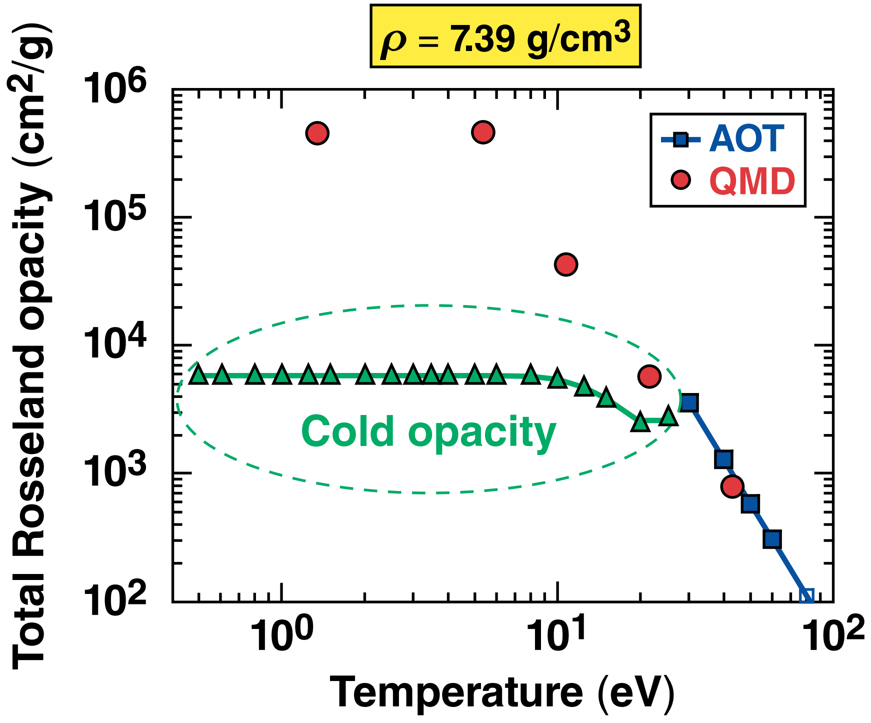
A wide range of DT plasma conditions has been investigated previously by PIMC and QMD methods



TC12246a

Significant differences have been identified for warm dense deuterium when FPEOS,* κ_{QMD},** and FPOT† are compared with traditional models





*FPEOS: first-principles equation of state; S. X. Hu *et al.*, Phys. Rev. B 84, 224109 (2011).

**κ_{QMD}: QMD-based thermal conductivity; S. X. Hu *et al.*, Phys. Rev. E 89, 043105 (2014).

†FPOT: first-principles opacity table; S. X. Hu *et al.*, Phys. Rev. E 90, 033111 (2014).

TC11448d

Outline

- Introduction: Why should we care about material properties under extreme conditions?
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- ***Ab-initio*** **studies on ablator materials at HED conditions: How do they compare with traditional plasma models and experiments?**
- Impact of these *first-principles* properties of both DT and ablators on ICF implosions
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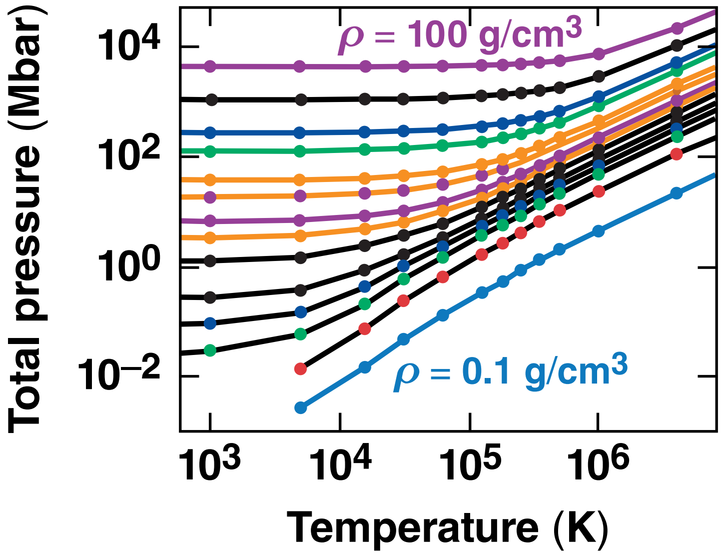
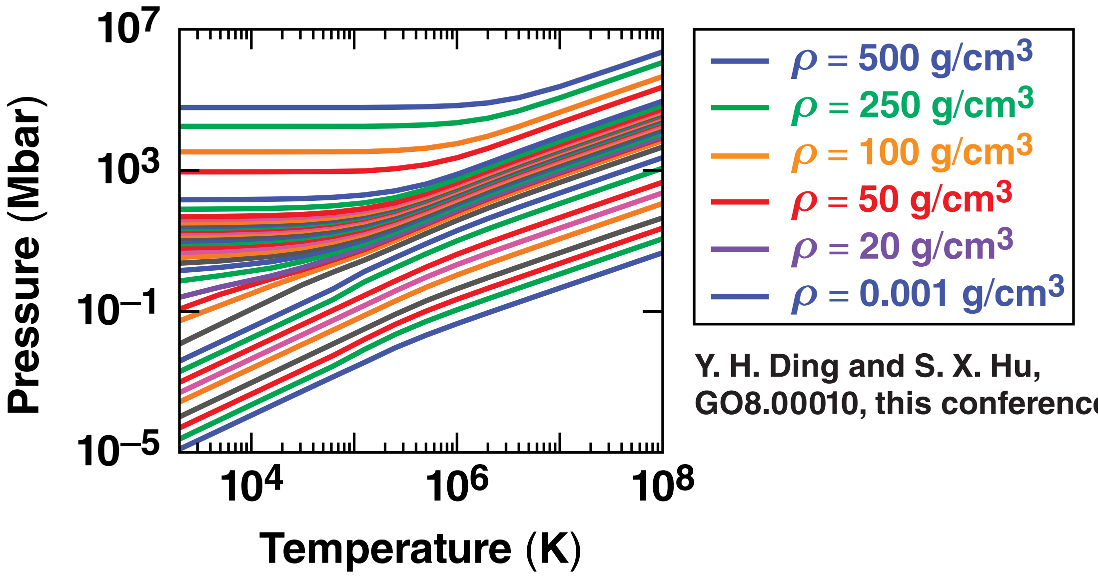
A wide range of plasma conditions of various ablators* are investigated by PIMC and QMD methods

CH

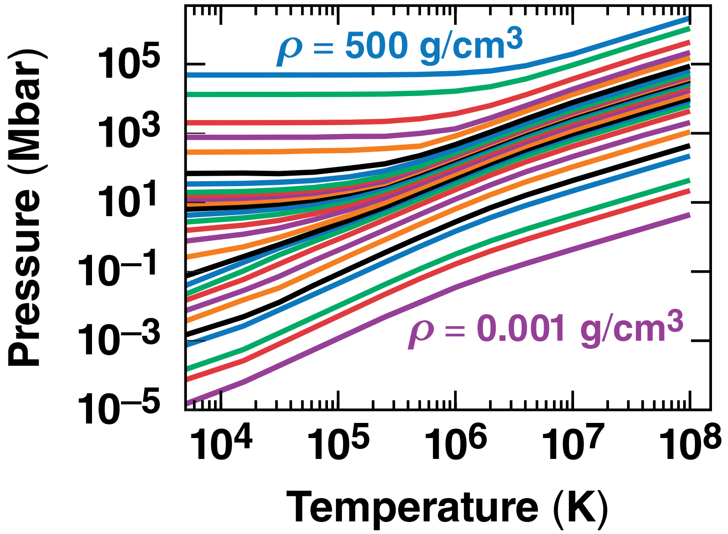


Be



Y. H. Ding and S. X. Hu, GO8.00010, this conference.

Si



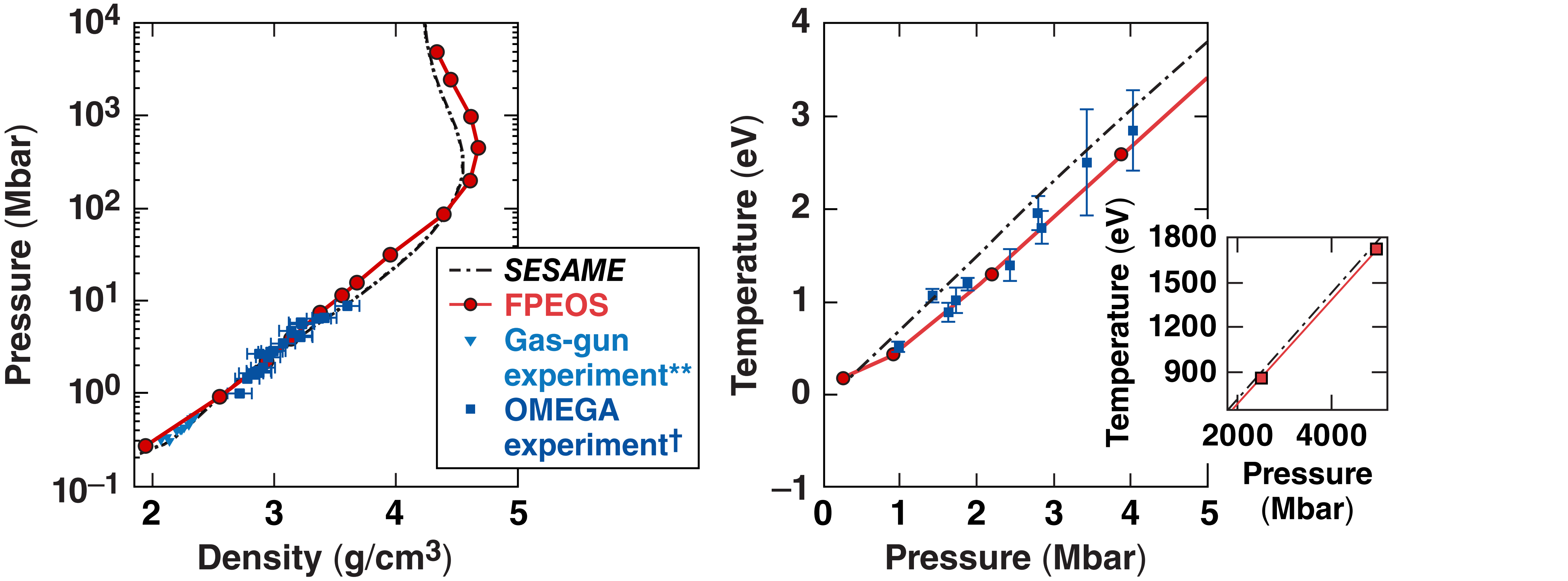
B. Henderson *et al.*, JO8.00003, this conference.

This talk will focus on CH properties, although Be and Si have been used for multilayer target designs.**

*S. X. Hu *et al.*, Phys. Rev. E 92, 043104 (2015);
S. X. Hu *et al.*, Phys. Plasmas 23, 042704 (2016);
S. X. Hu *et al.*, Phys. Rev. B 94, 094109 (2016);
S. X. Hu *et al.*, Phys. Rev. E 95, 043210 (2017);
Y. H. Ding and S. X. Hu, Phys. Plasmas 24, 062702 (2017);
S. X. Hu, Phys. Rev. Lett. 119, 065001 (2017);
S. X. Hu *et al.*, Phys. Rev. B 96, 144203 (2017).
**V. N. Goncharov *et al.*, Phys. Plasmas 21, 056315 (2014).

TC13613a

The calculated principal Hugoniot* of CH from FPEOS has been well compared with experiments



The Hugoniot temperature predicted by FPEOS is in better agreement with the experiment!

*S. X. Hu, T. R. Boehly, and L. A. Collins, Phys. Rev. E 89, 063104 (2014).

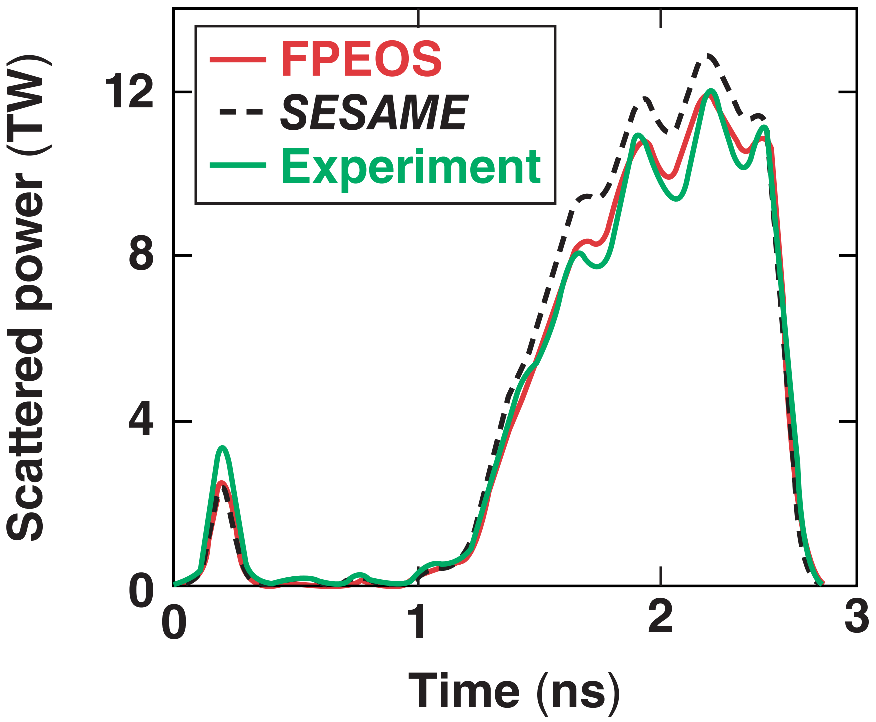
**S. P. Marsh, ed. LASL Shock Hugoniot Data, Los Alamos Series on Dynamic Material Properties (University of California Press, Berkeley, CA, 1980).

†M. A. Barrios *et al.*, Phys. Plasmas 17, 056307 (2010).

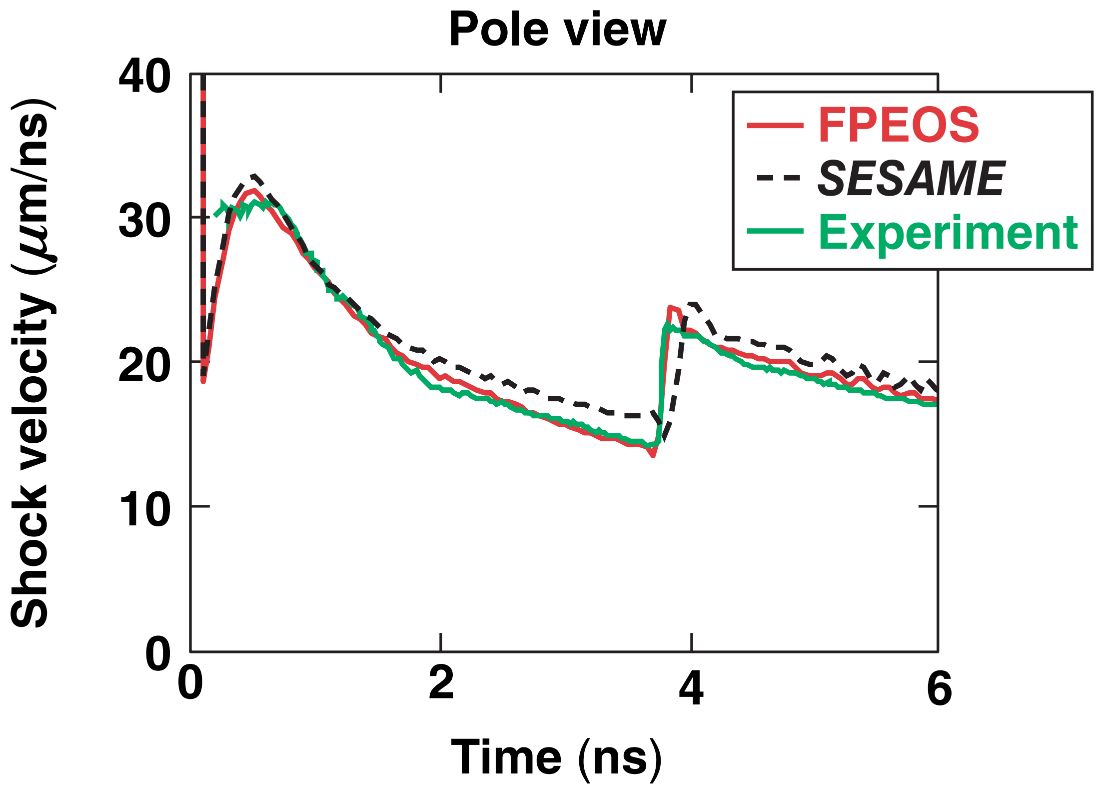
TC12152t

Several different experimental observables show better agreement with FPEOS than *SESAME* EOS for CH

Time-resolved, scattered-light OMEGA implosion



Low-intensity* NIF shock-timing experiment (N151025-001)

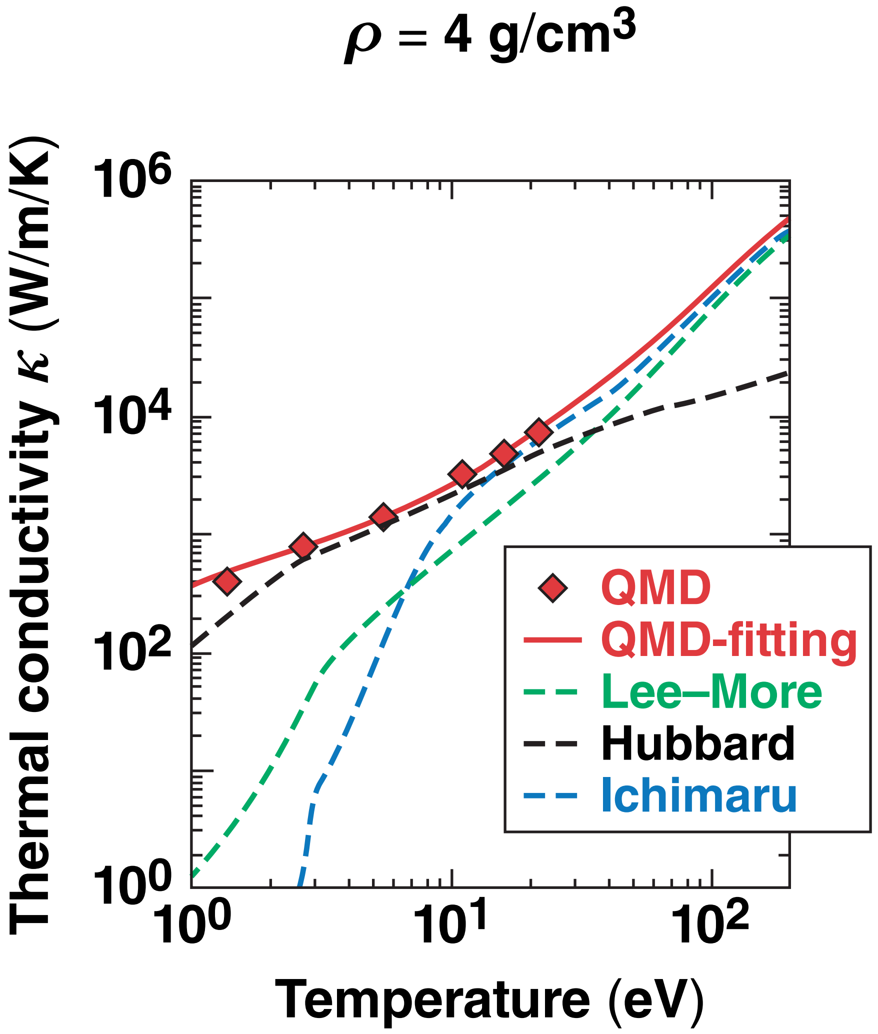


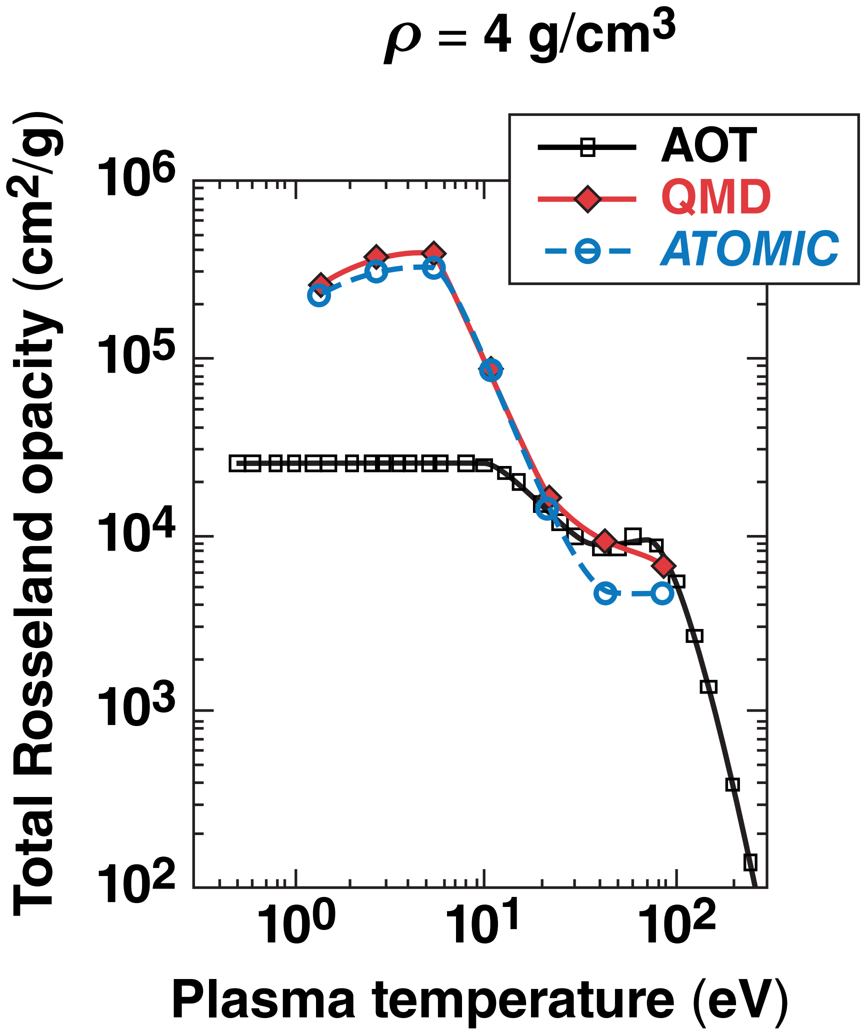
See T. R. Boehly talk at this conference, JO8.00007, for FPEOS comparison with sound-speed and Grüneisen parameter measurements in shocked CH.

*P. B. Radha *et al.*, "Shock Velocity Measurements at the National Ignition Facility," to be submitted to Physical Review E.

TC13614a

QMD predicted larger thermal conductivity* and opacity** in warm dense CH plasmas when compared to the models used in our hydrocodes



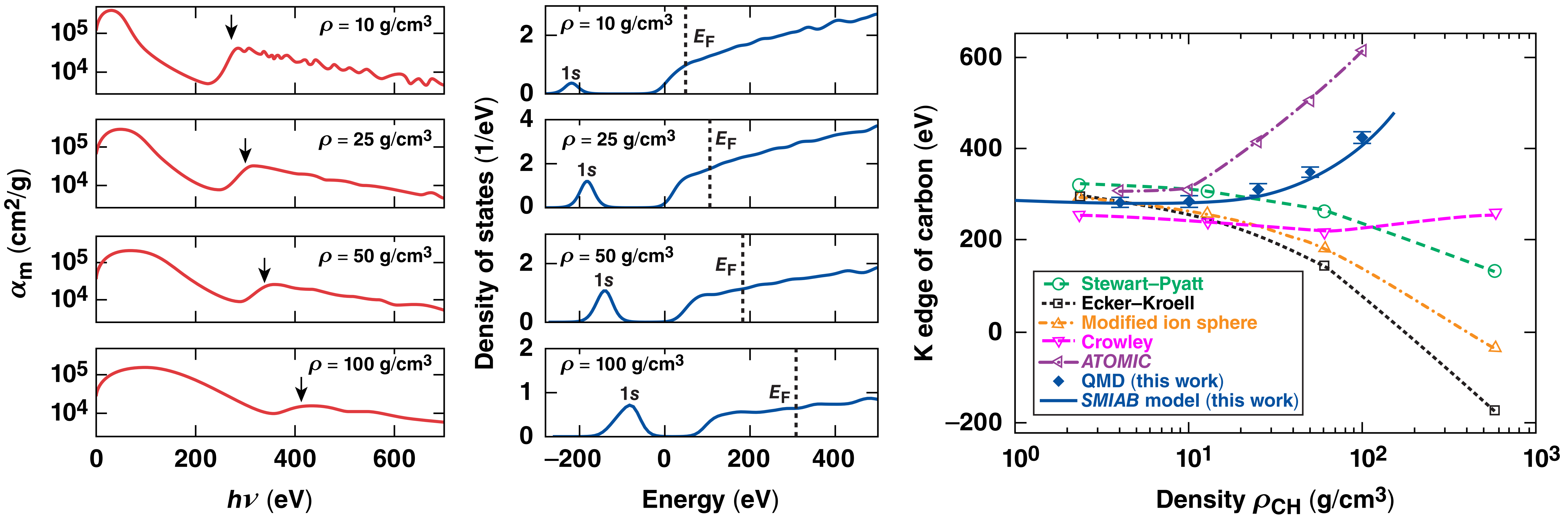


*S. X. Hu *et al.*, Phys. Plasmas 23, 042704 (2016).
**S. X. Hu *et al.*, Phys. Rev. B 96, 144203 (2017).

TC13615a

The QMD-predicted carbon K-edge shifting in extremely dense and warm C* and CH** plasmas cannot be explained by plasma models

CH plasma at T = 10.77 eV

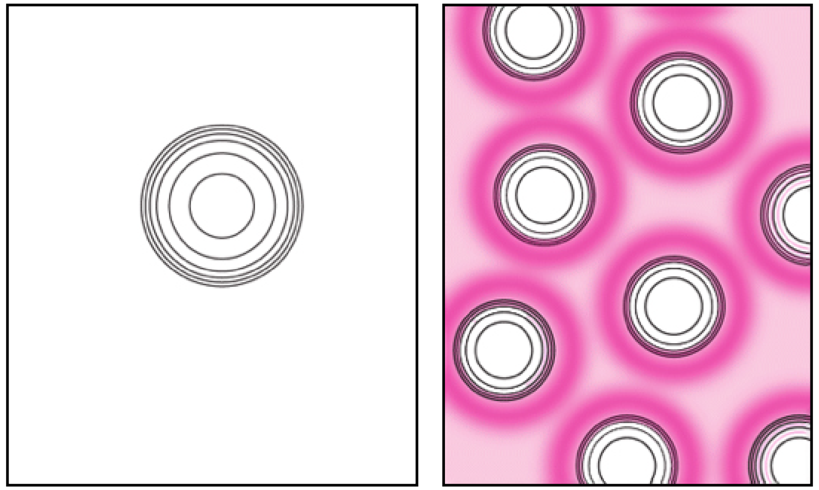


*S. X. Hu, Phys. Rev. Lett. 119, 065001 (2017);
**S. X. Hu *et al.*, Phys. Rev. B 96, 144203 (2017).

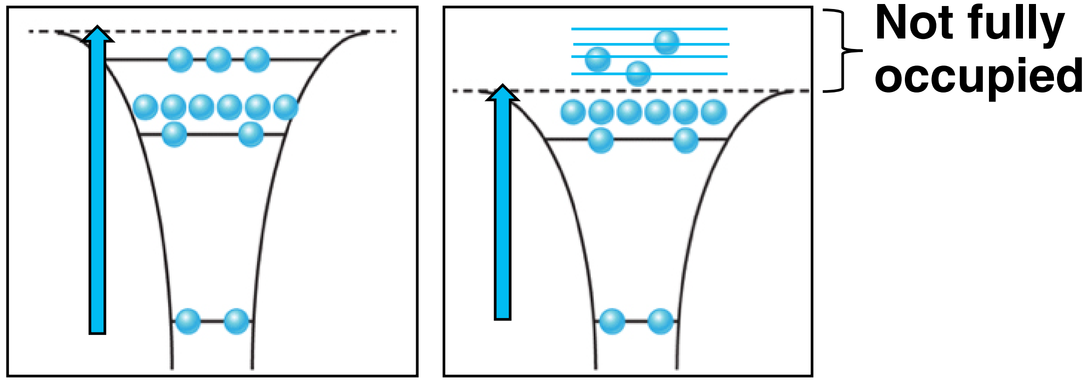
TC13616a

The physics picture of x-ray-absorption K-edge shifting in extremely dense and warm plasmas are different from classical plasma models

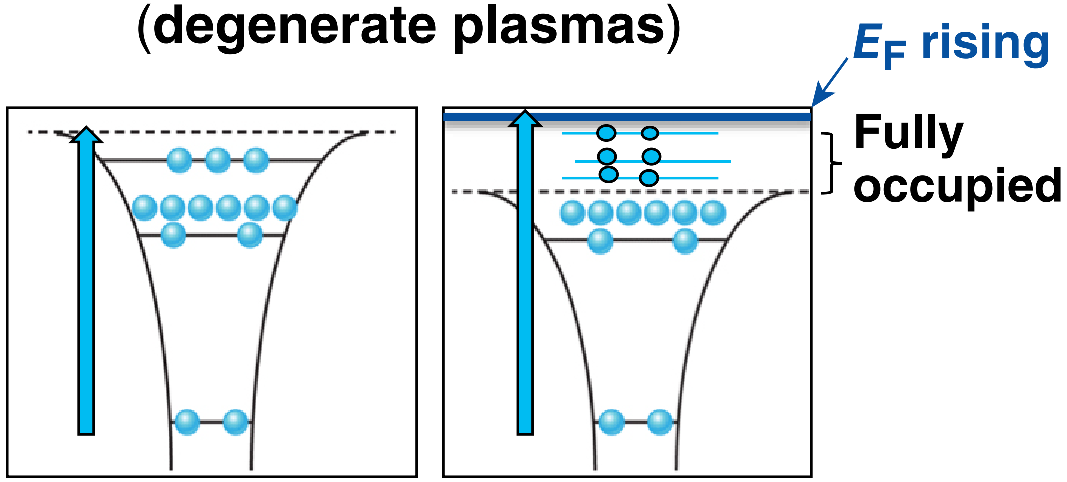
Isolated atom | **Plasma**



Continuum lowering
(non-degenerate plasmas)



Fermi-surface rising/Pauli blocking
(degenerate plasmas)



TC13830

Our quantum-physics–based models can explain the unusual K-edge shifting in extremely dense and warm plasmas

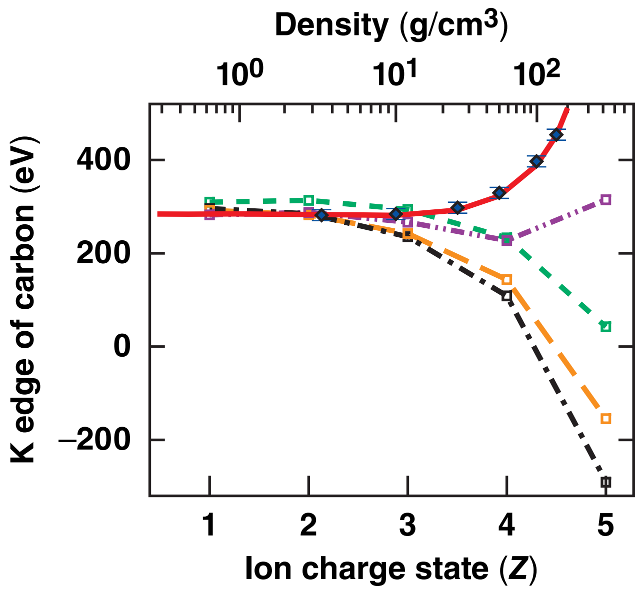
- **Single atom in a box (SAIAB)/single mixture in a box (SMIAB) model (putting a single atom or mixture into a cubic box of $V = \rho/A$, with the periodic boundary condition)**
  - **solving the Kohn–Sham equation to determine E_{1s}**

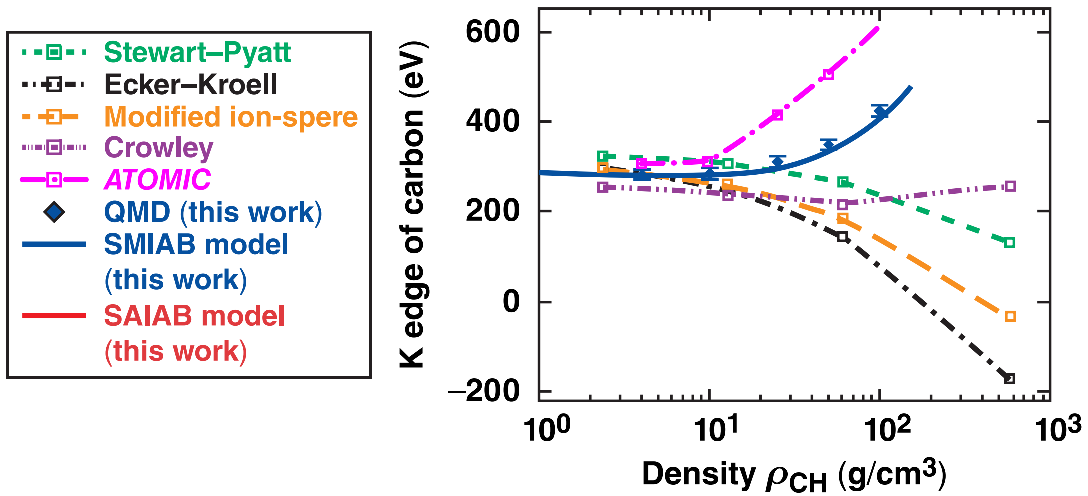
$$\left\{-\frac{1}{2}\nabla^2 - \frac{Z}{r} + \int \frac{\rho_e(r')}{|r - r'|} dr' + V_{XC}[\rho_e](r)\right\}\varphi_i = E_i\varphi_i;\ \rho_e = \sum_i |\varphi_i|^2$$

  - **using the average-atom model to gauge ionization $\langle Z \rangle$ for (ρ, T)**
  - **calculating the Fermi surface: $E_F = \frac{\hbar^2}{2m}\left[3\pi^2 \rho Z/A\right]^{2/3}$ for degenerate plasmas**

$$E_{K\ edge} = E_F - E_{1s}$$

C at T = 1.35 eV



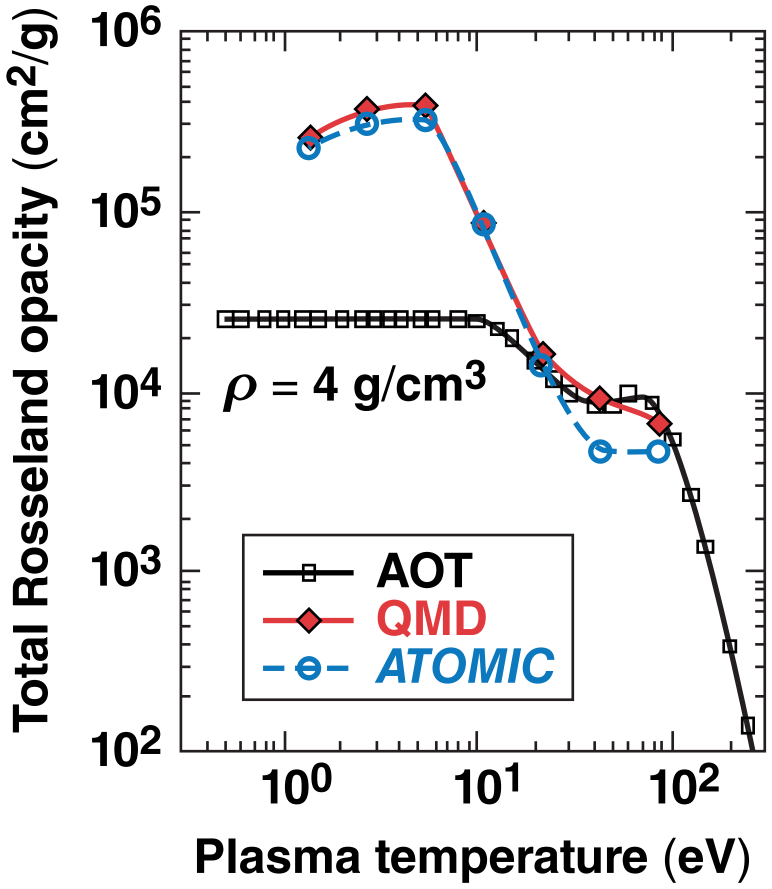


CH at T = 10.77 eV

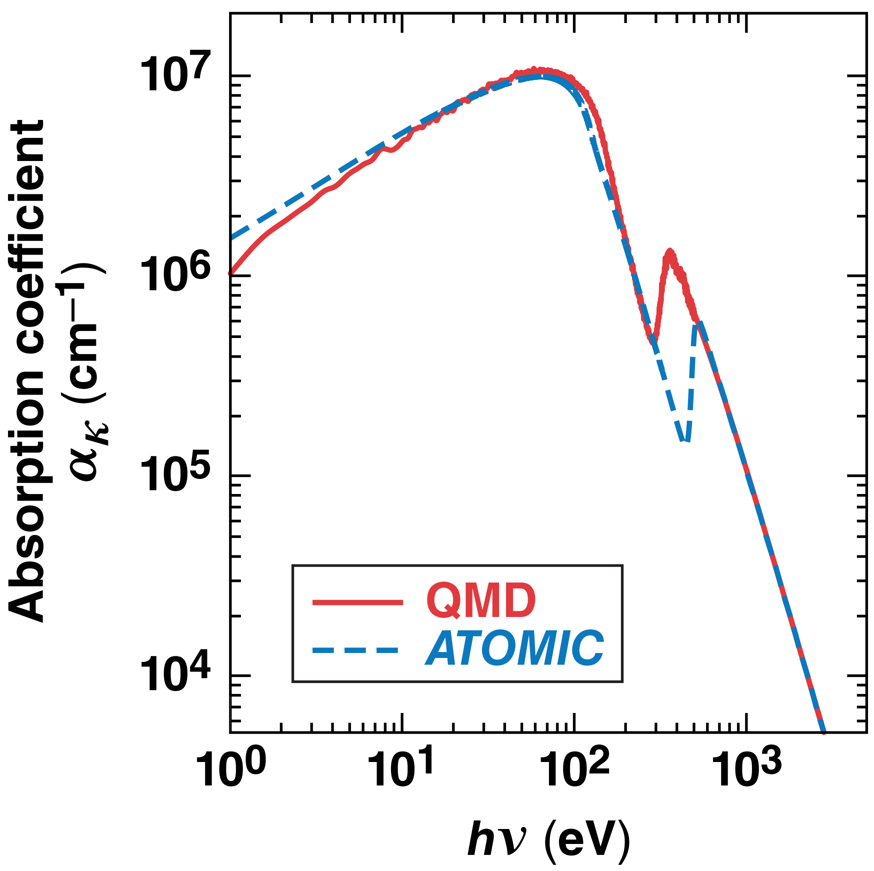
TC13831

At very high densities, a factor of ~2 difference in CH opacity between QMD* and LANL's *ATOMIC*** model is attributed to the different K-edge shifting

ρ = 50 g/cm^3



ρ = 50 g/cm^3 and T = 10.77 eV



*S. X. Hu *et al.*, Phys. Rev. B 96, 144203 (2017).
**N. R. Shaffer *et al.*, High Energy Density Phys. 23, 31 (2017).

TC13832

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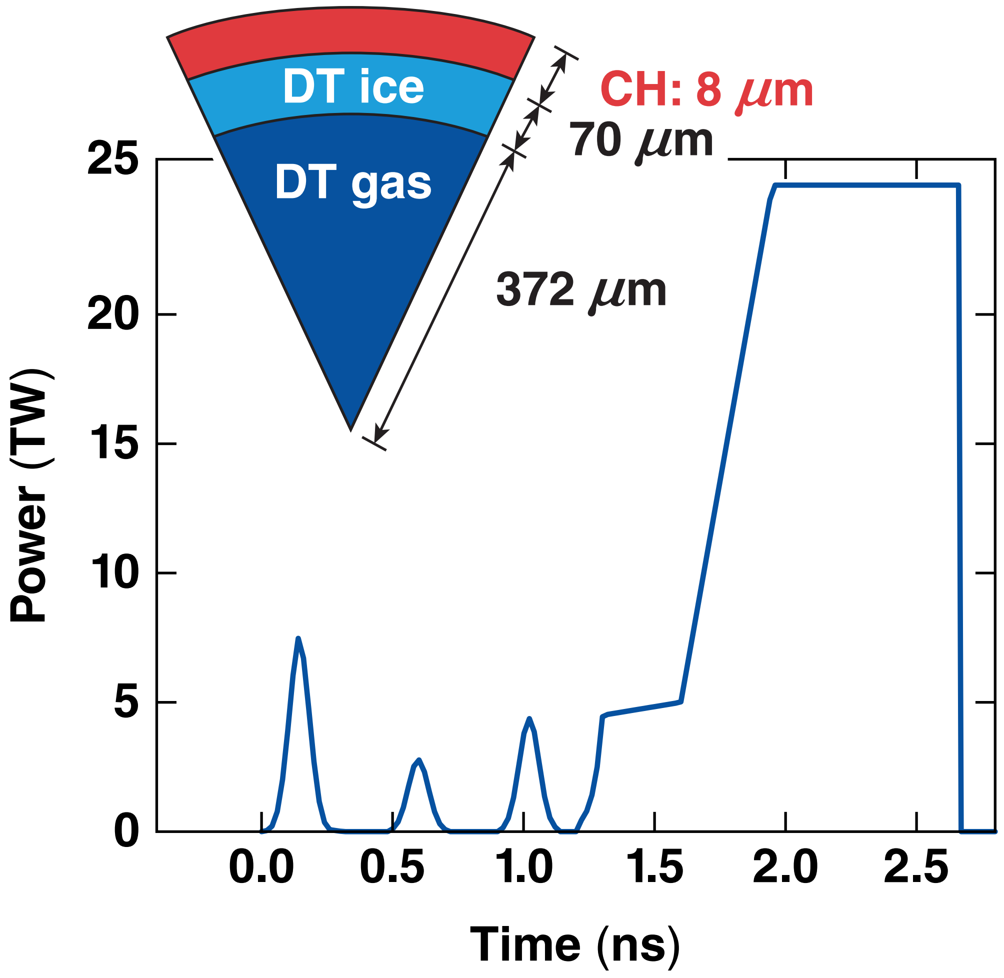
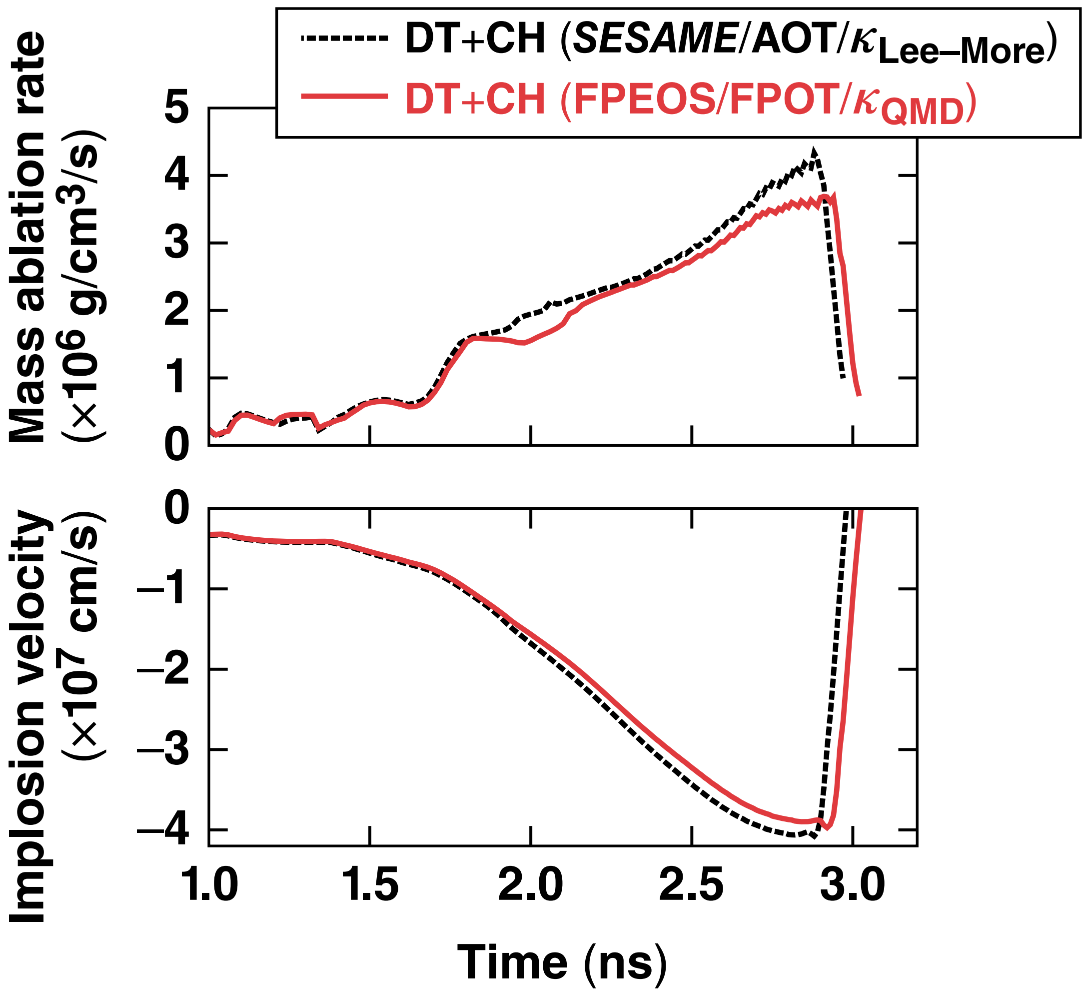
- **Impact of these *first-principles* properties of both DT and ablators on ICF implosions**
- Conclusions

TC13828d

The effects of accurate intrinsic properties of DT and CH on ICF implosions have been studied through radiation–hydrodynamic simulations for 100-Gbar targets on OMEGA*

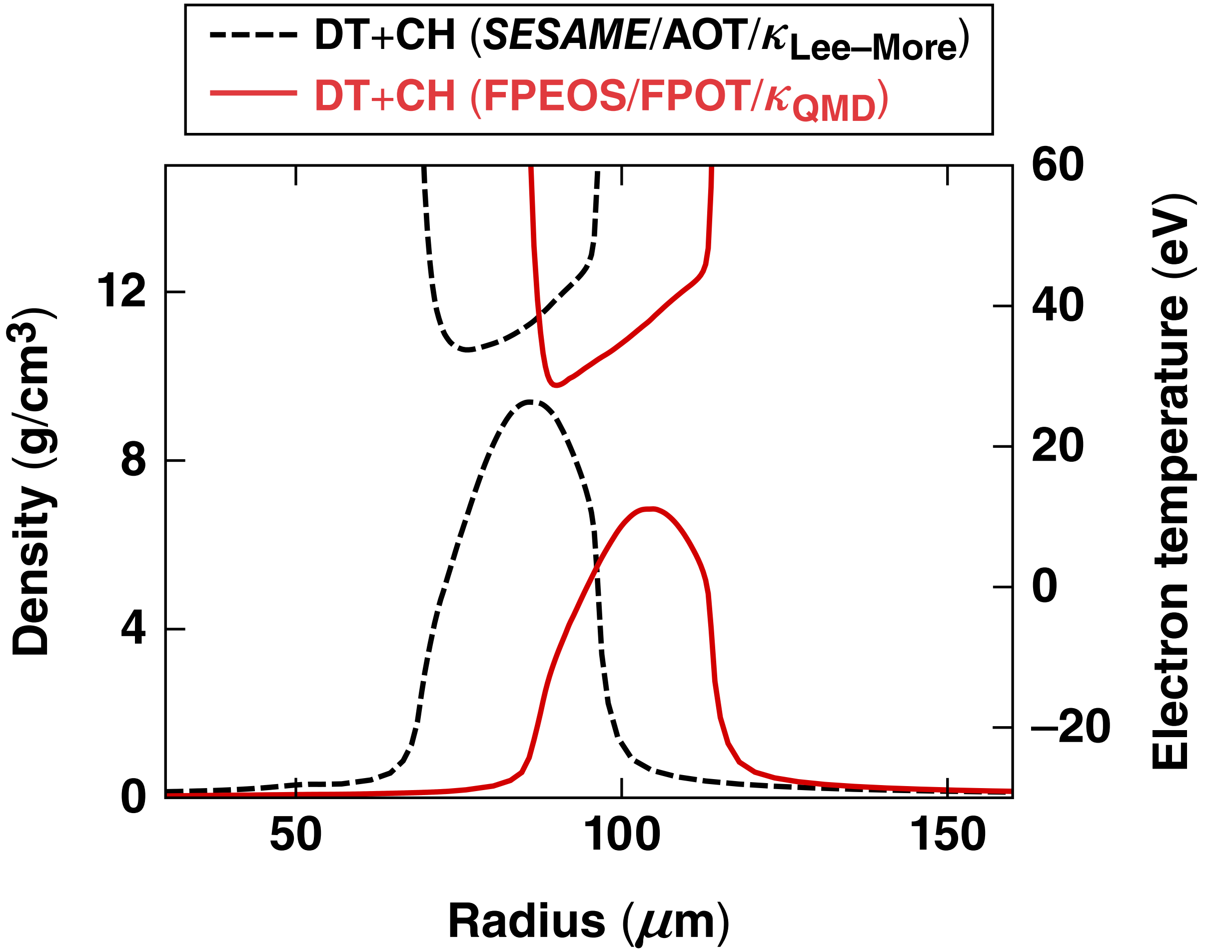


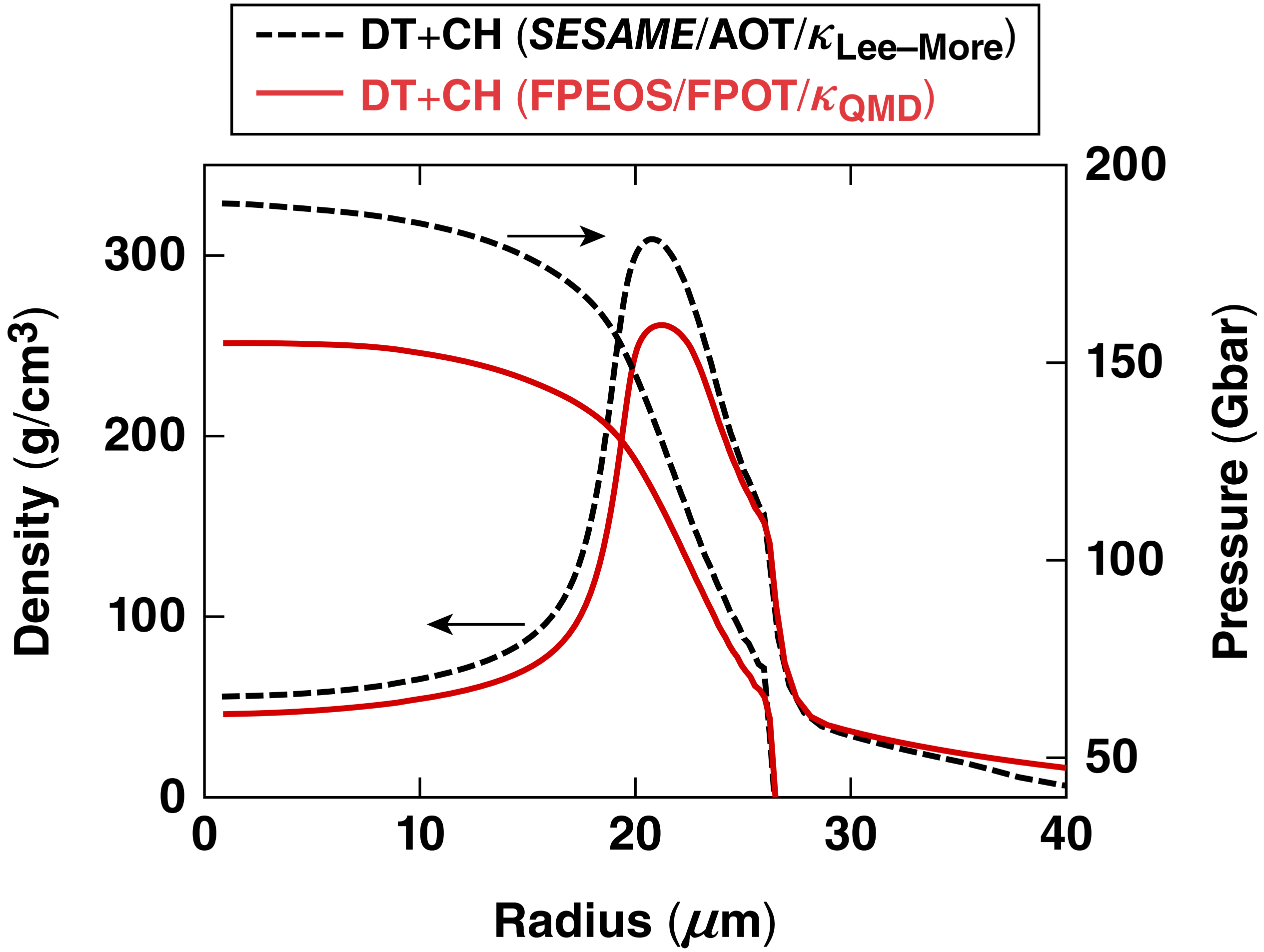


TC13833

* S. P. Regan *et al.*, YO7.00007, this conference.

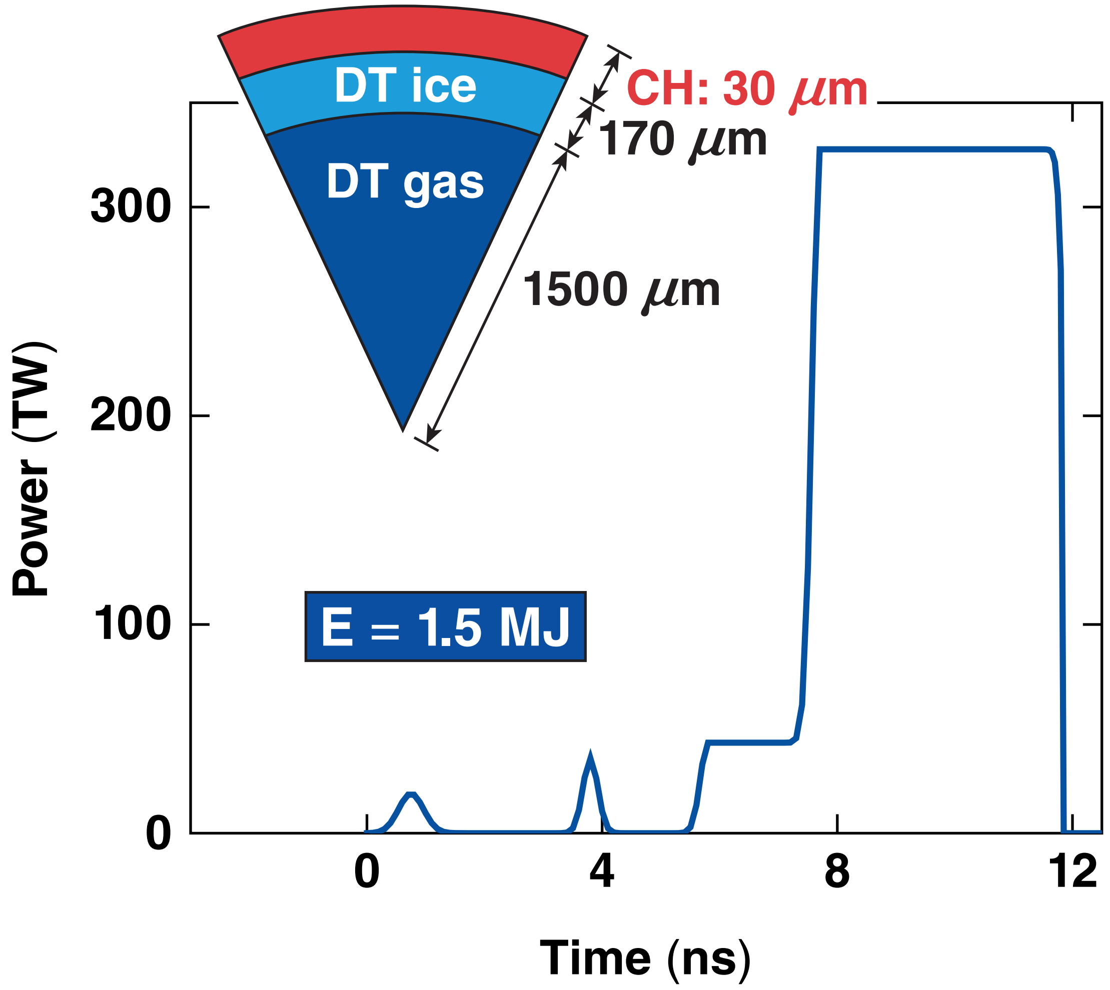
Differences in target performance are predicted between the *first-principles*–based new models and the old plasma models for cryo DT targets on OMEGA

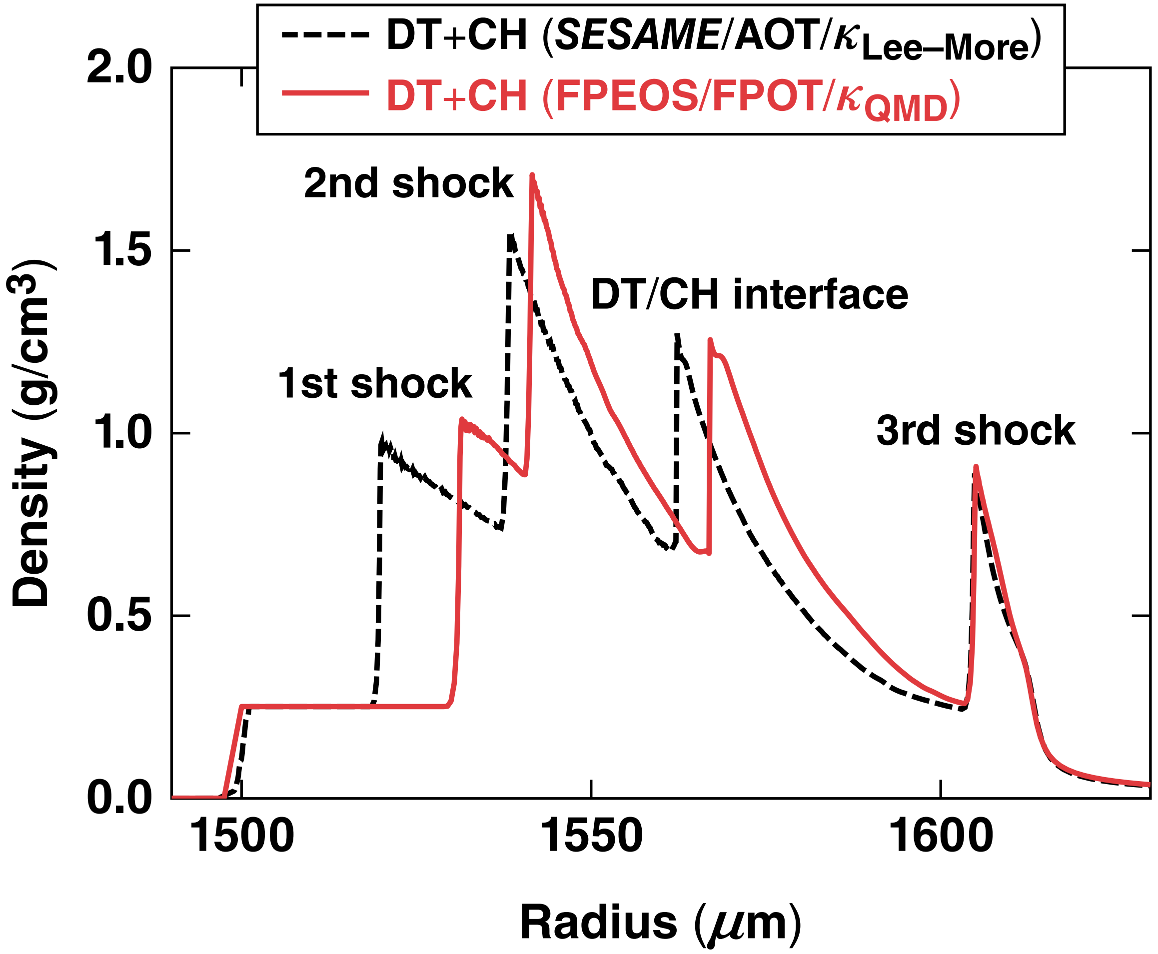




TC13834

The effects of accurate intrinsic properties of DT and CH on direct-drive NIF* designs have also been tested



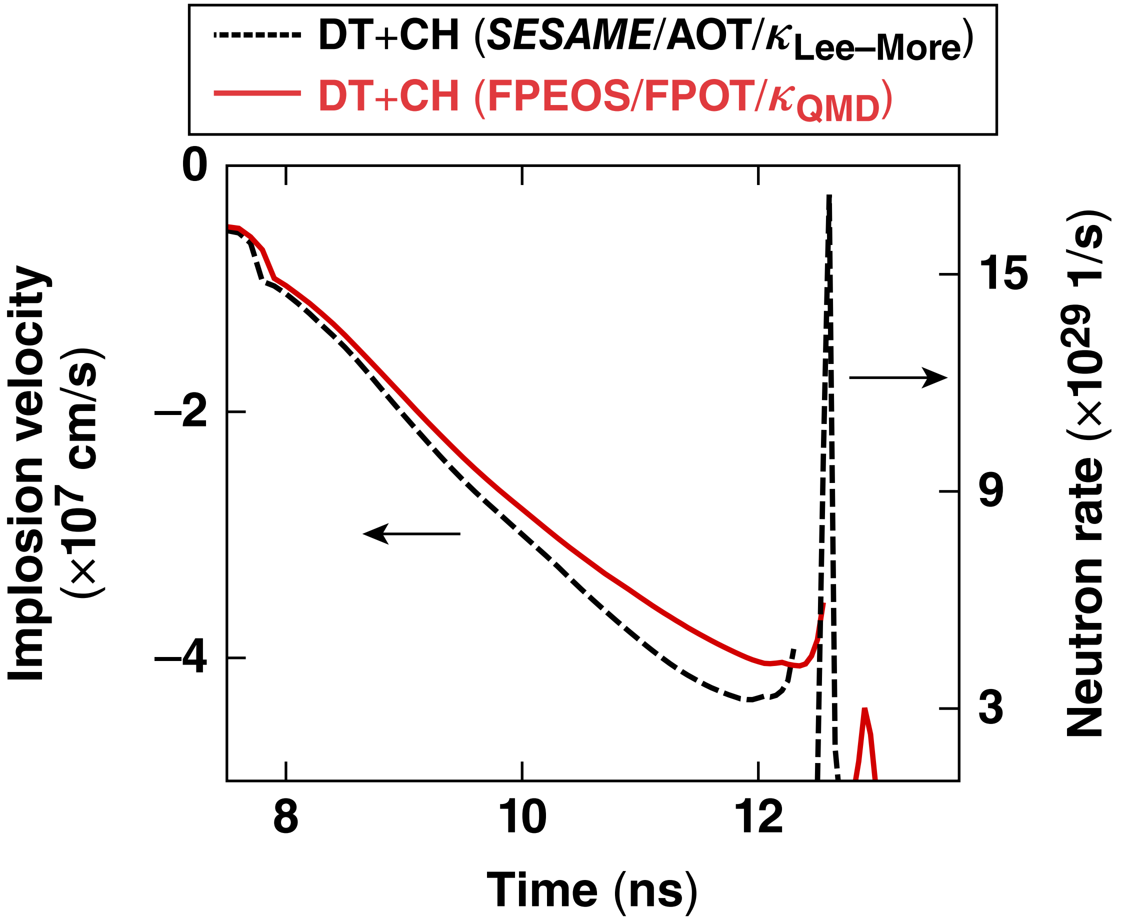


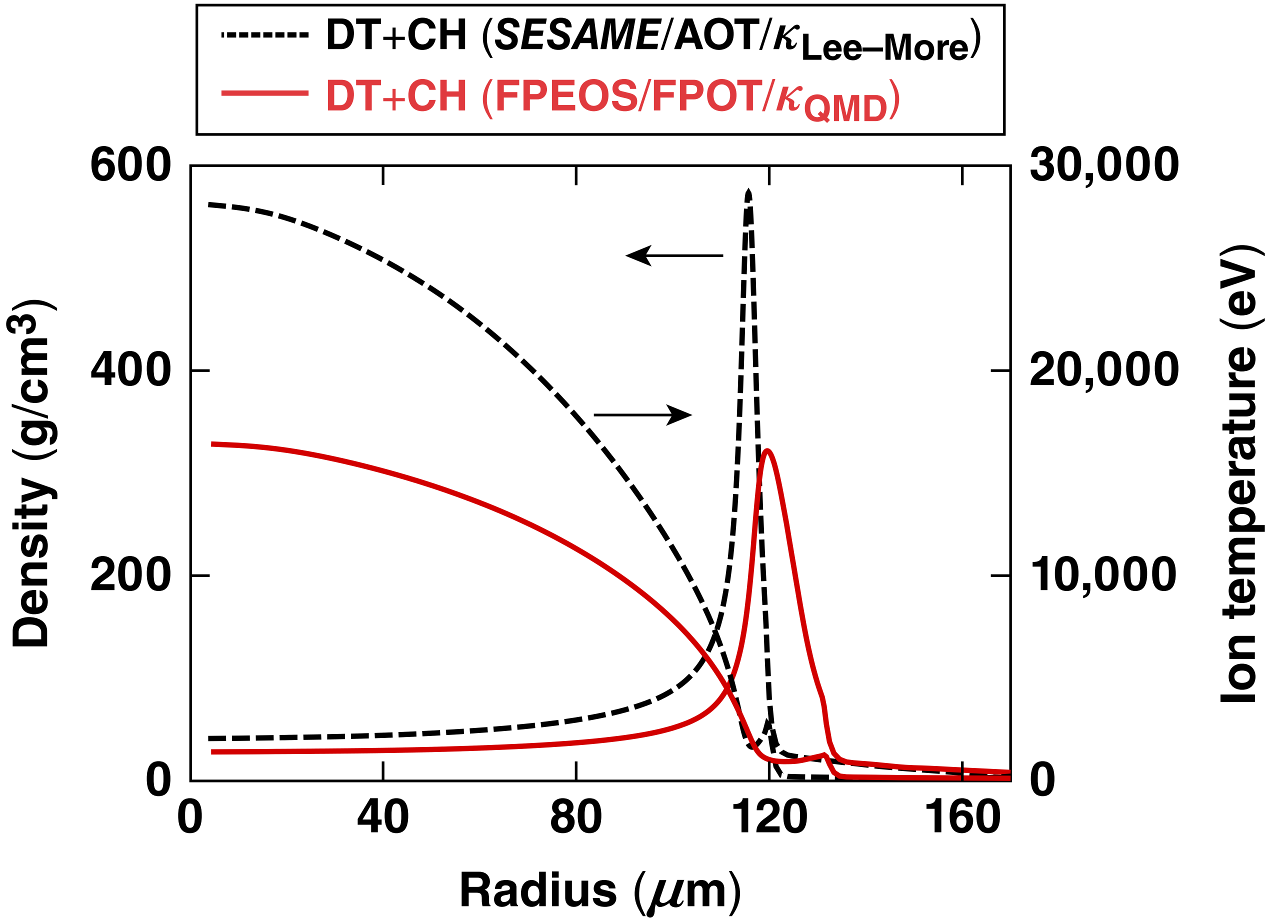
Shock timing is affected by the FPEOS of the CH ablator.

*NIF: National Ignition Facility

TC13835

Significant variations in NIF target performance have been predicted using first-principles properties when compared to traditional plasma-model simulations





The lower ablation rate of CH could mean that we may need either more laser energy or thinner shells for ICF implosions.

TC13836

A factor of ~3 to 4 difference in ICF target gain is predicted using new *first-principles* properties versus old plasma-model simulations

Target performance	DT+CH (*SESAME*/AOT/$\kappa_{\text{Lee–More}}$)	DT+CH (FPEOS/FPOT/κ_{QMD})
$\langle \rho R \rangle_n$	0.807 g/cm^2	0.654 g/cm^2
$\langle T_i \rangle_n$	22.8 keV	11.2 keV
$\langle P \rangle_n$	999 Gbar	342 Gbar
$\langle \rho \rangle_{\text{peak}}$	602.9 g/cm^3	322.7 g/cm^3
$R_{\text{hot spot}}$	64.2 μm	87.6 μm
$C_{\text{hot spot}}$	26.5	19.4
Yield	1.66×10^{19}	4.26×10^{18}
Gain	31.3	8.0

High gain may be recovered by using the *first-principles*–based material properties to retune target designs.

TC13837

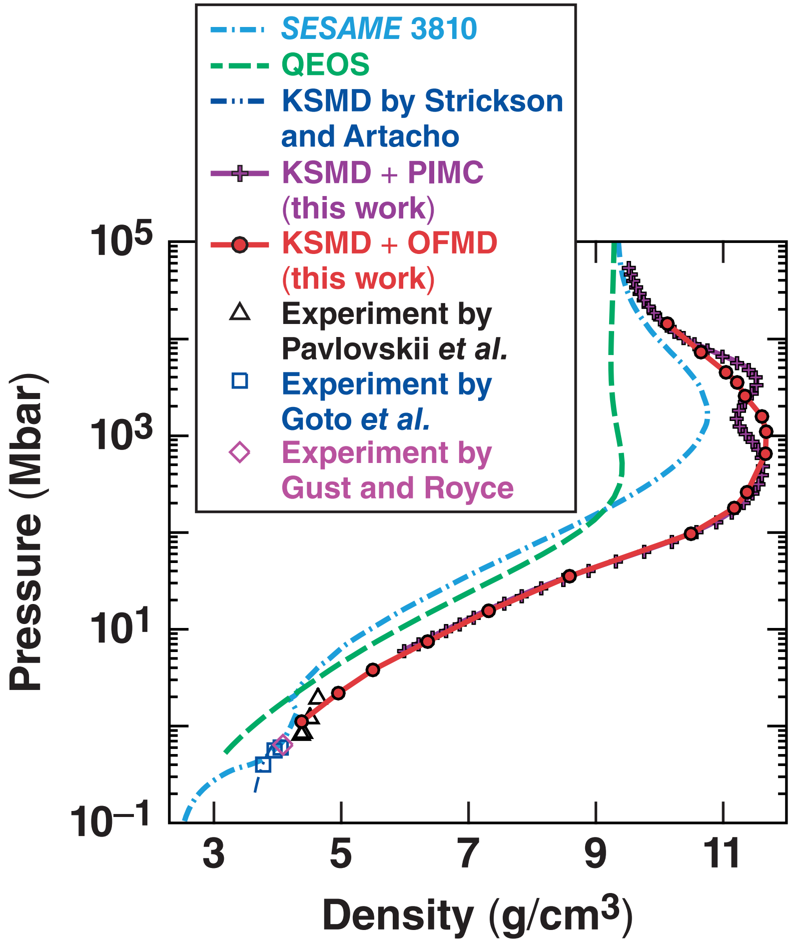
Accurate intrinsic properties of plasmas under extreme conditions are essential for reliable inertial confinement fusion (ICF) target designs

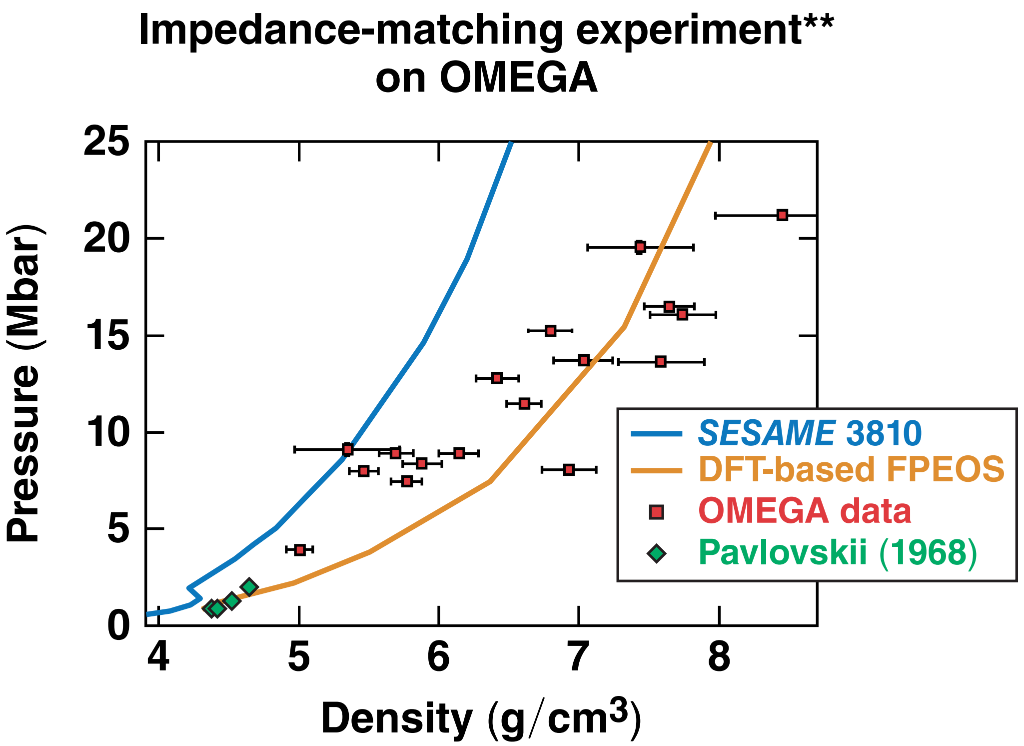
- *First-principles* methods have been used to self-consistently calculate intrinsic properties of DT and ablators under extreme conditions
- These *ab initio* results, which can significantly differ from the predictions of traditional plasma models in the warm-dense-matter (WDM) regime, compared well with experiments
- Hydro simulations using these *first-principles* properties of DT and ablators have shown a significant difference in predicting target performance when compared with traditional model simulations

Knowing material properties better would result in a more-reliable understanding and designing of ICF implosions.

Backup

For silicon, our first-principles calculations predicted a much softer Hugoniot than traditional EOS models,* which seems consistent with preliminary experiments





*S. X. Hu *et al.*, Phys. Rev. B 94, 094109 (2016).
**B. Henderson *et al.*, presented at the 20th Biennial Conference of the APS Topical Group on Shock Compression of Condensed Matter, St. Louis, MO, 9–14 July 2017 (Abstract T6.00002).

TC13619a