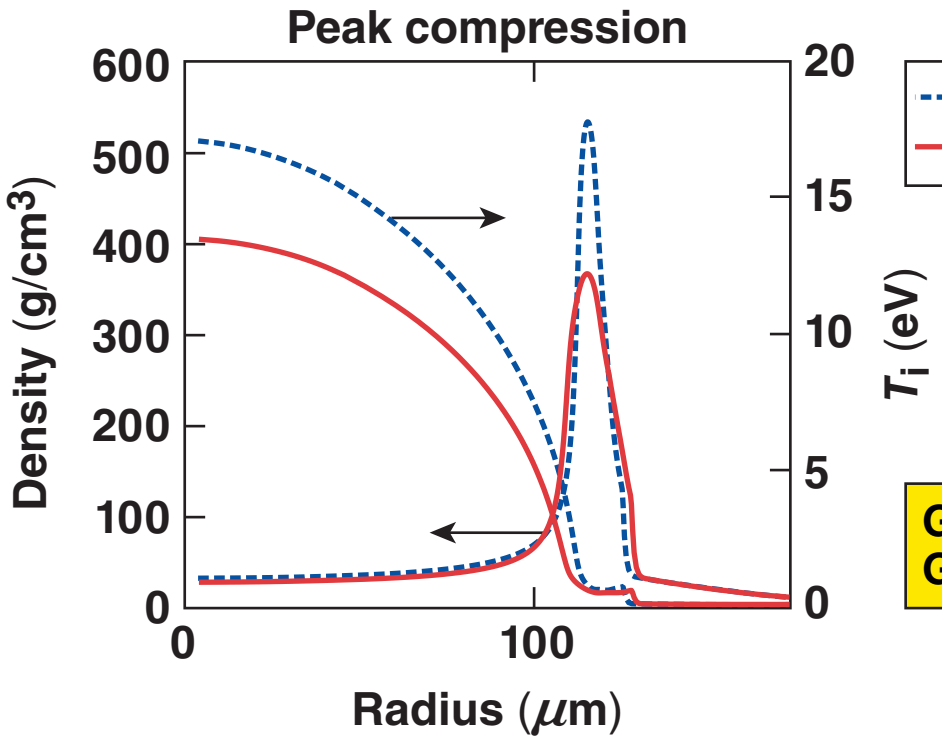
Impact of First-Principles Calculated Properties of Warm-Dense Deuterium–Tritium on Inertial Confinement Fusion Target Designs



Gain = 40.0 (*SESAME*/AOT/κ_{LM})
Gain = 23.8 (FPEOS/FPOT/κ_{QMD})

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Summary

Accurate properties of deuterium–tritium (DT) fuel from first-principles calculations are crucial to inertial confinement fusion (ICF) target designs

UR LLE

- First-principles (FP) methods, including path-integral Monte Carlo (PIMC) and quantum molecular dynamics (QMD), are used to self-consistently calculate the properties of DT fuel for ICF applications
- Significant differences are identified when comparing FP-based equation of state (FPEOS), opacity table (FPOT), and thermal conductivity (κ_{QMD}) with models adopted in hydrocodes
- Hydro simulations using FP-based properties of DT have shown a factor of ~2 difference in ICF neutron yield compared to model simulations
- The lower the adiabat (α = 1.5 to 3.0), the larger the differences are in predicting ICF target performance

Collaborators

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Outline

- Introduction: warm dense matter (WDM)
- First-principles methods for studying WDM
  - path-integral Monte Carlo (PIMC)
  - quantum molecular dynamics (QMD)
- Properties of warm dense DT: FPEOS/FPOT/κ_{QMD} compared to model predictions
- Impact of first-principles properties of DT fuel on ICF implosions
- Conclusions

Accurate knowledge of DT properties [equation of state (EOS), opacity, κ, stopping power] is required to simulate ICF implosions

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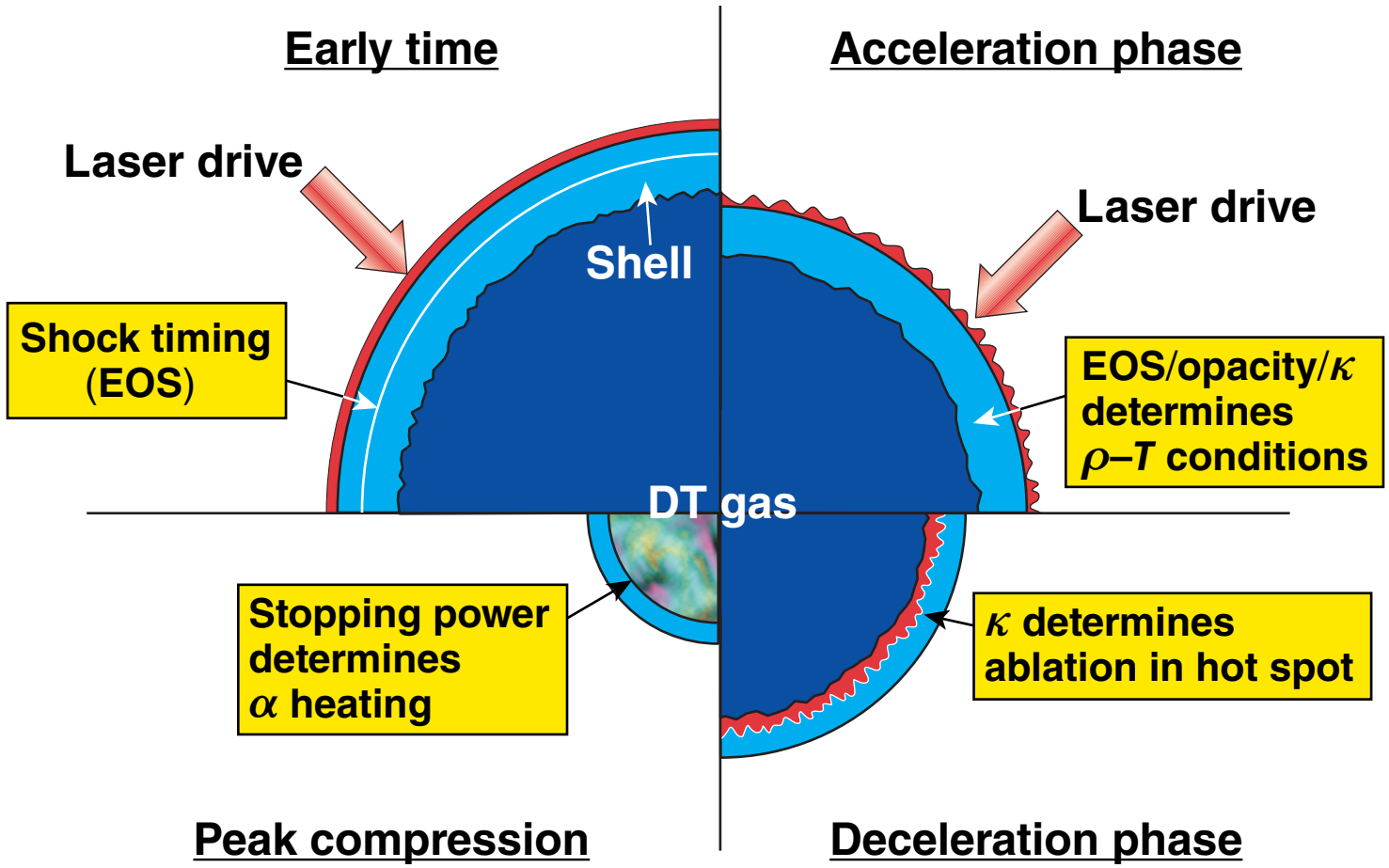
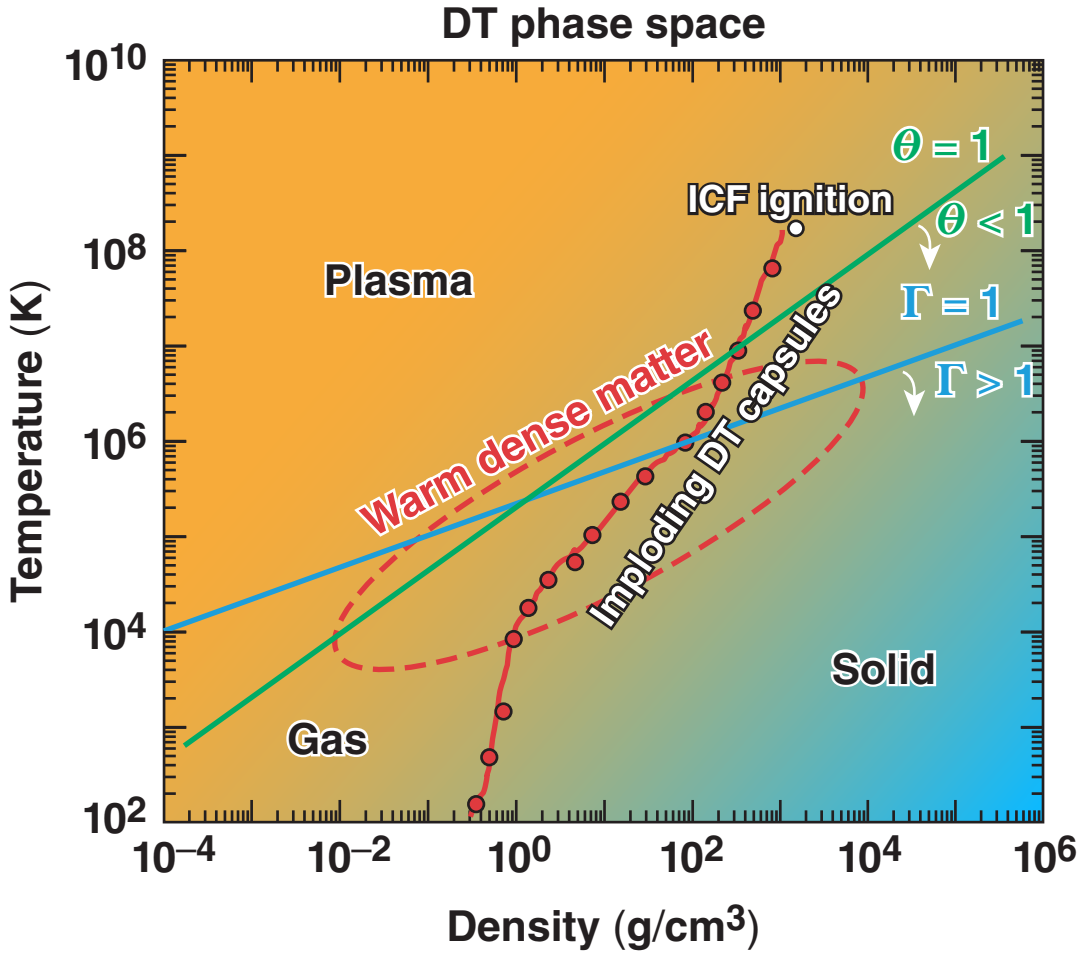
EOS is needed to close the hydrodynamics equations.



TC5723c

Coupled and degenerate warm dense matter are routinely accessed by imploding DT shells in ICF



The Coulomb coupling parameter:

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

The electron-degeneracy parameter:

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

WDM:

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

TC11490

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 PIMC and QMD provide self-consistent and accurate properties of WDM.

* G. I. Kerley, Phys. Earth Planet. Inter. 6, 78 (1972); G. I. Kerley, "Equations of State for Hydrogen and Deuterium," Sandia National Laboratory, 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).

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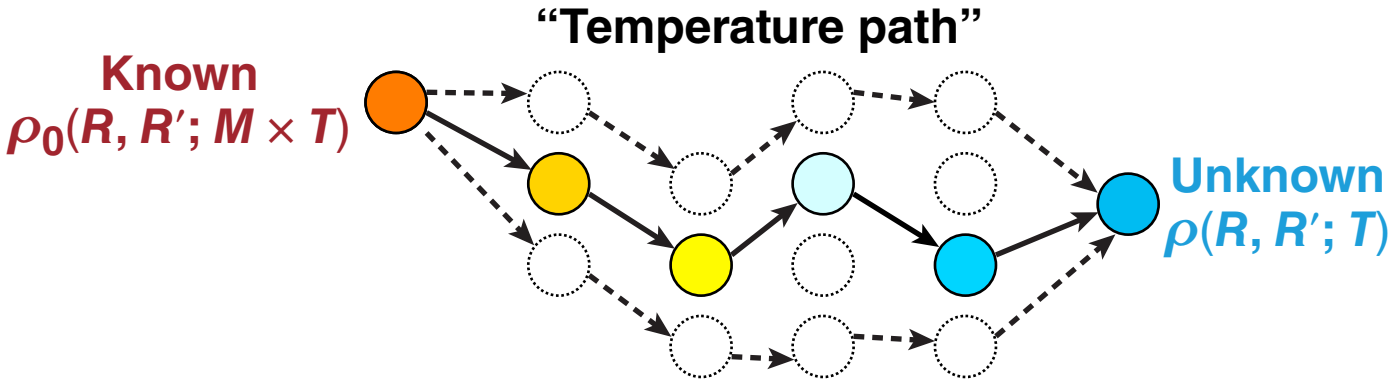
PIMC,* based on the convolution of the density matrix, uses the Monte Carlo method to efficiently evaluate multidimensional integrations

- The density matrix $\rho(R, R'; T)$, introduced by J. von Neumann in 1927, describes the statistical distribution of a quantum system in thermal equilibrium

$$\rho(R,R';T) = \left\langle R \left| e^{-\vec{H}/kT} \right| R' \right\rangle = \sum_n \varphi_n(R)\varphi_n(R')e^{-E_n/kT}$$

- The convolution property of $\rho(R, R'; T)$ can be written as

$$\rho(R,R';T) = \left\langle R \left| e^{-\vec{H}/KT} \right| R' \right\rangle = \int dR_1 \rho(R,R_1;2T)\rho(R_1,R';2T)$$



*D. M. Ceperley, Rev. Mod. Phys. 67, 279 (1995);
B. Militzer, Ph.D. thesis, University of Illinois at Urbana-Champaign, 2000.

The QMD method is based on the Kohn–Sham density functional theory (DFT)*

UR LLE

- EOS is a direct output from QMD simulations
- Transport properties can be calculated using the Kubo–Greenwood formalism**

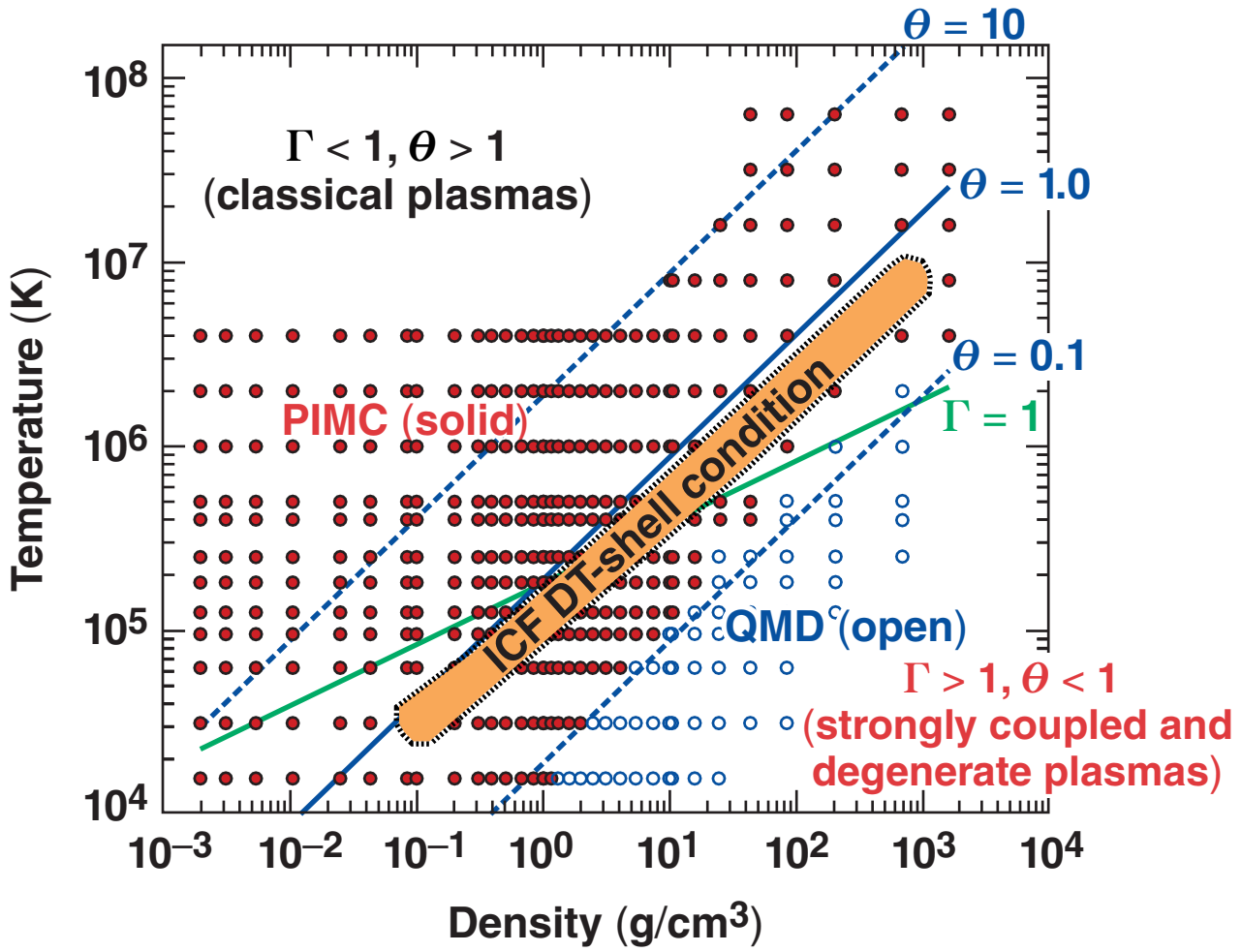
$$L_{ij}(\omega) = \frac{2\pi(-e)^{4-i-j}}{3Vm_e^2\omega}\sum_{mn} F_{mn}\left|D_{mn}\right|^2 \times \left(\frac{E_m + E_n}{2} - H\right)^{i+j-2} \delta(E_m - E_n - \hbar\omega)$$

- Thermal conductivity and optical absorption coefficients can be derived from these Onsager coefficients $L_{ij}(\omega)$

* W. Kohn and L. J. Sham, Phys. Rev. 140, A1133 (1965).
** R. Kubo, J. Phys. Soc. Jpn. 12, 570 (1957);
D. A. Greenwood, Proc. Phys. Soc. Lond. 71, 585 (1958).

TC11493

Coupled and degenerate WDM conditions* are studied by PIMC and QMD methods



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

TC11442

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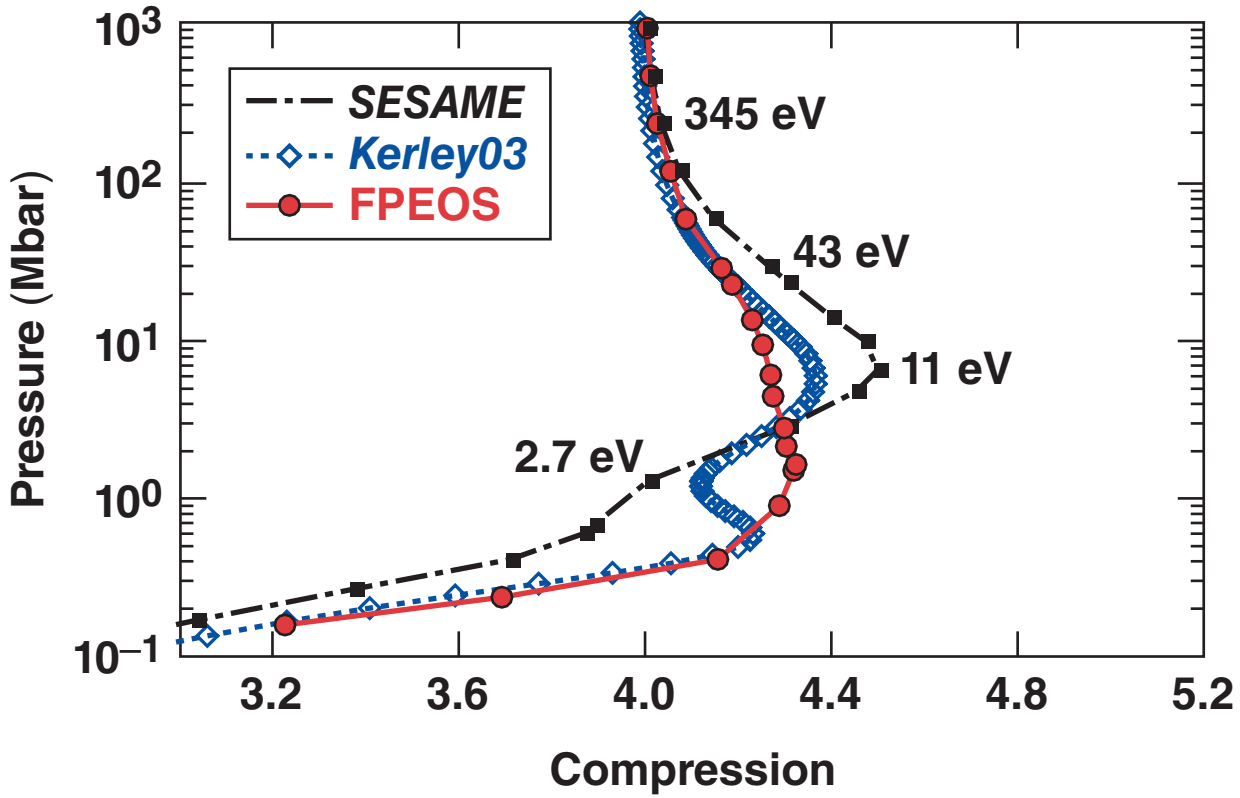
Differences in the principal Hugoniot of deuterium are identified between the FPEOS and EOS models

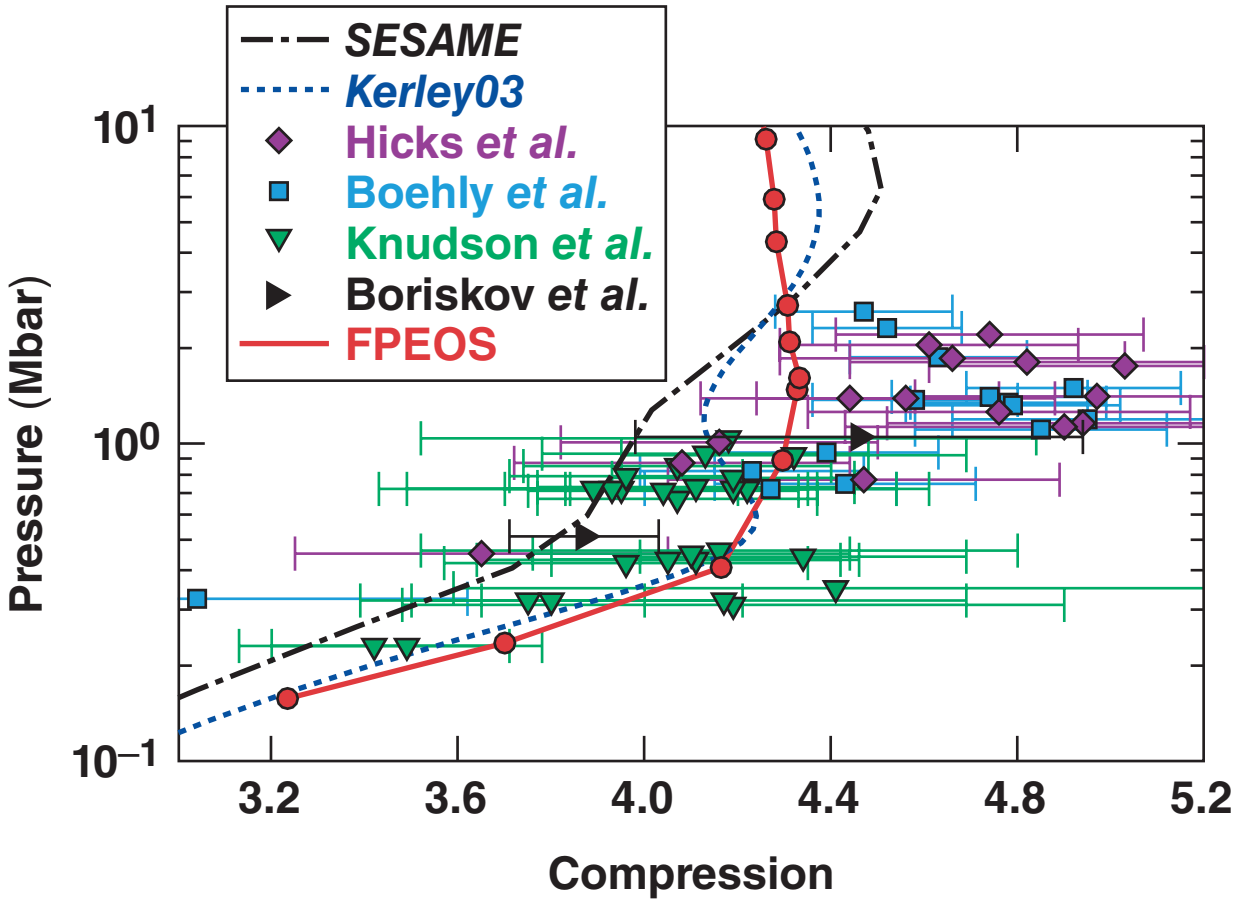


Calculations of deuterium Hugoniot using QMD have been previously studied.*

*L. A. Collins *et al.*, Phys. Rev. B 63, 184110 (2001); M. P. Desjarlais, Phys. Rev. B 68, 064204 (2003); B. Holst *et al.*, Phys. Rev. B 77, 184201 (2008); S. X. Hu *et al.*, Phys. Rev. B 84, 224109 (2011); L. Caillabet, S. Mazevet, and P. Loubeyre, Phys. Rev. B 83, 094101 (2011); C. Wang and P. Zhang, Phys. Plasmas 20, 092703 (2013).

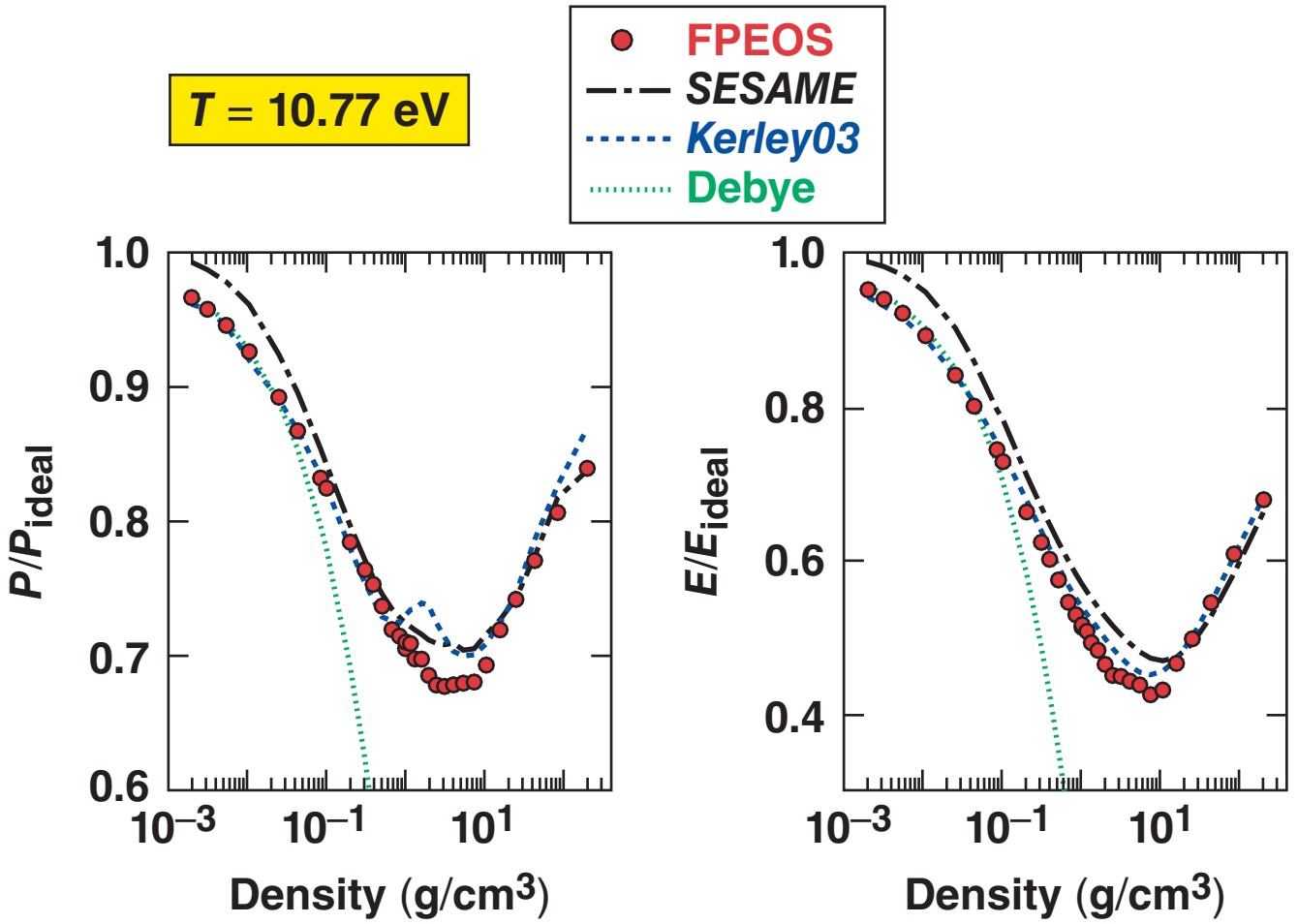
TC11444

The FPEOS-predicted Hugoniot of deuterium is better compared with experiments



TC11494

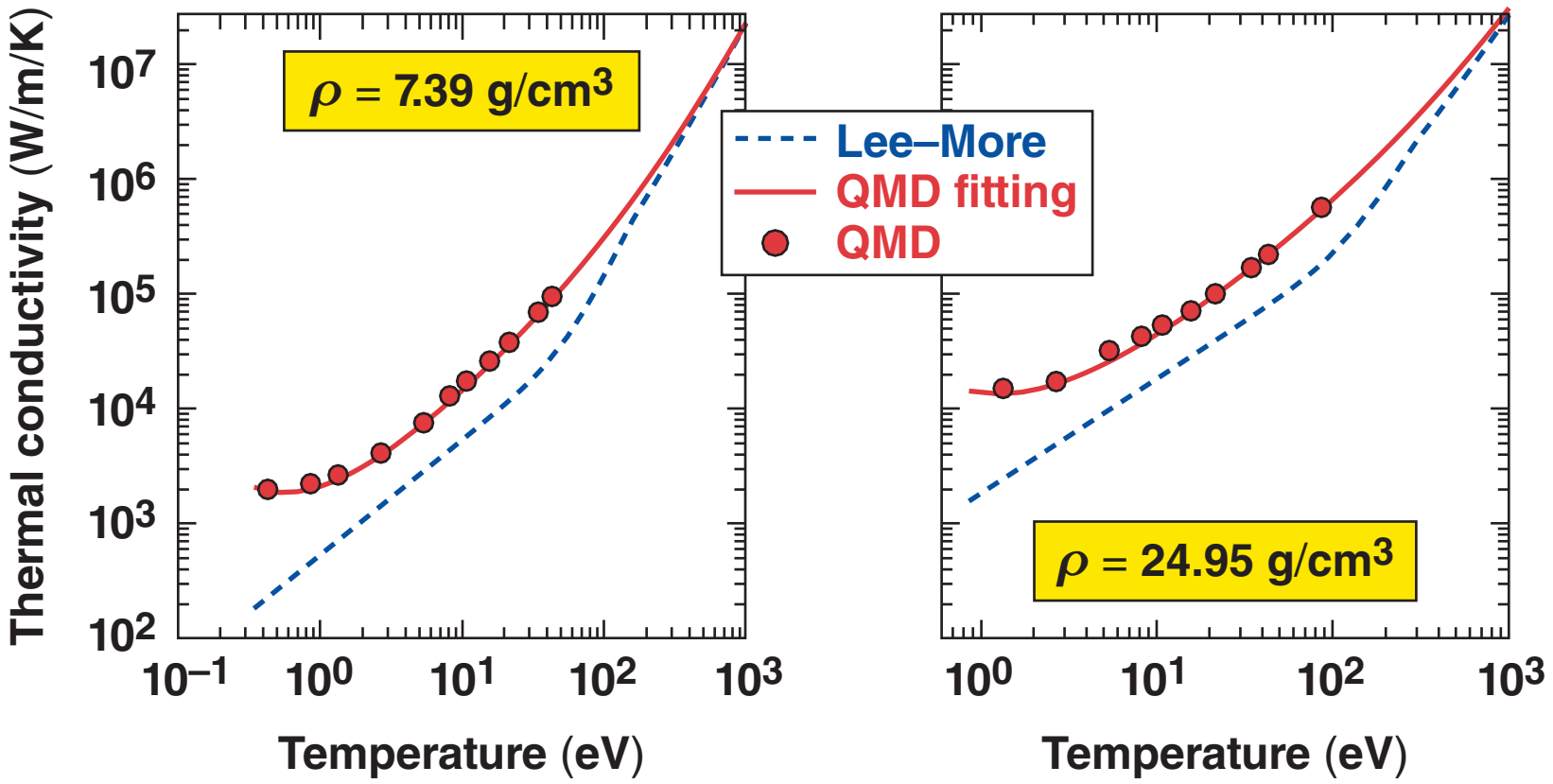
Differences have been identified for warm dense deuterium between FPEOS* and EOS models



*S. X. Hu *et al.*, Phys. Rev. B 84, 224109 (2011).

TC11445

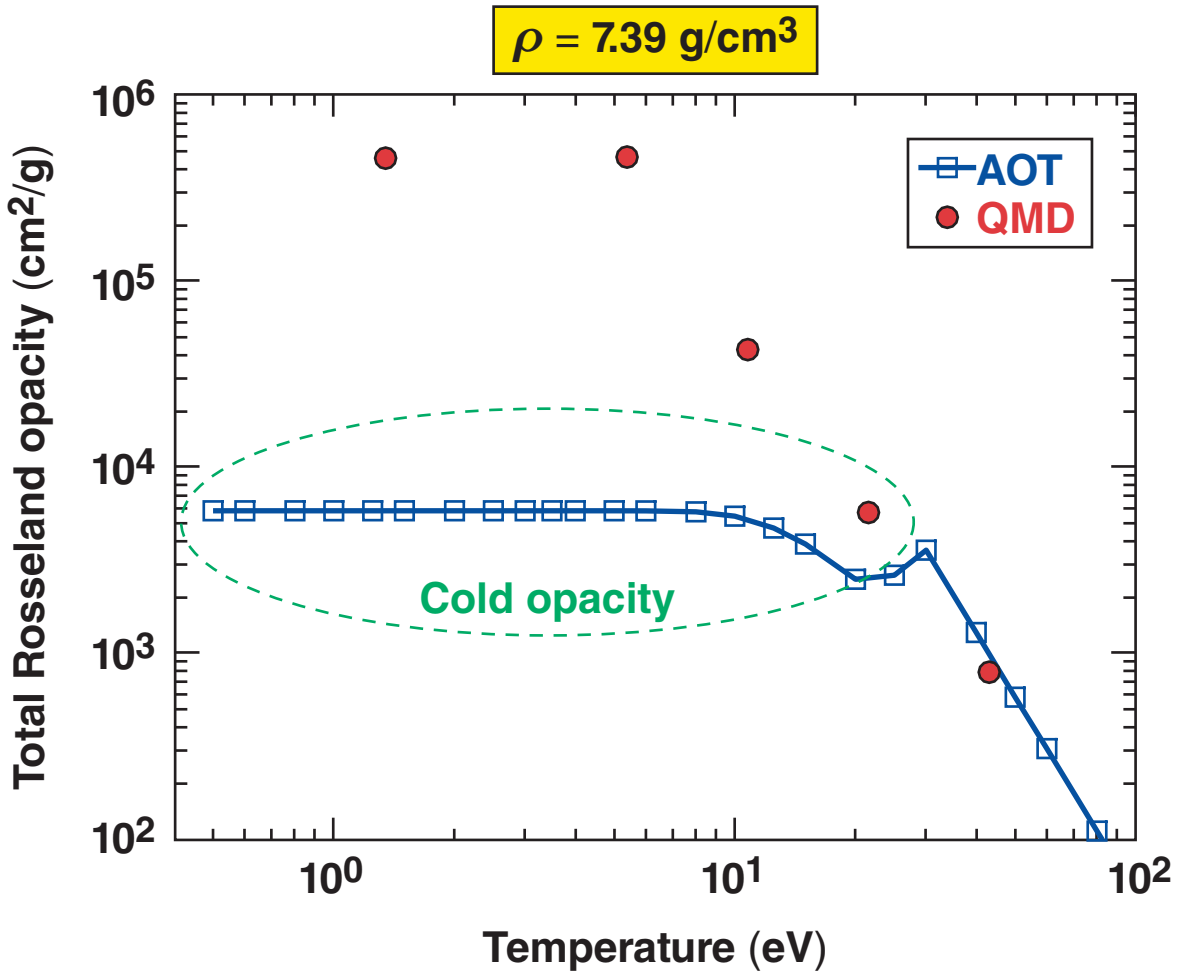
The QMD thermal conductivity* of warm dense deuterium is 3 to 10× higher than the Lee–More model**



* S. X. Hu *et al.*, Phys. Rev. E 89, 043105 (2014).
** Y. T. Lee and R. M. More, Phys. Fluids 27, 1273 (1984).

TC11448

The QMD opacities* show a large difference in the WDM regime when compared to the cold-opacity–patched AOT



Enhanced opacity is caused by

- **35× compression**
- **Temperature increase**

TC11449

*S. X. Hu *et al.*, Phys. Rev. E 90, 033111 (2014).

The QMD-predicted reflectivity along the Hugoniot of deuterium agreed with Nova and OMEGA experiments*

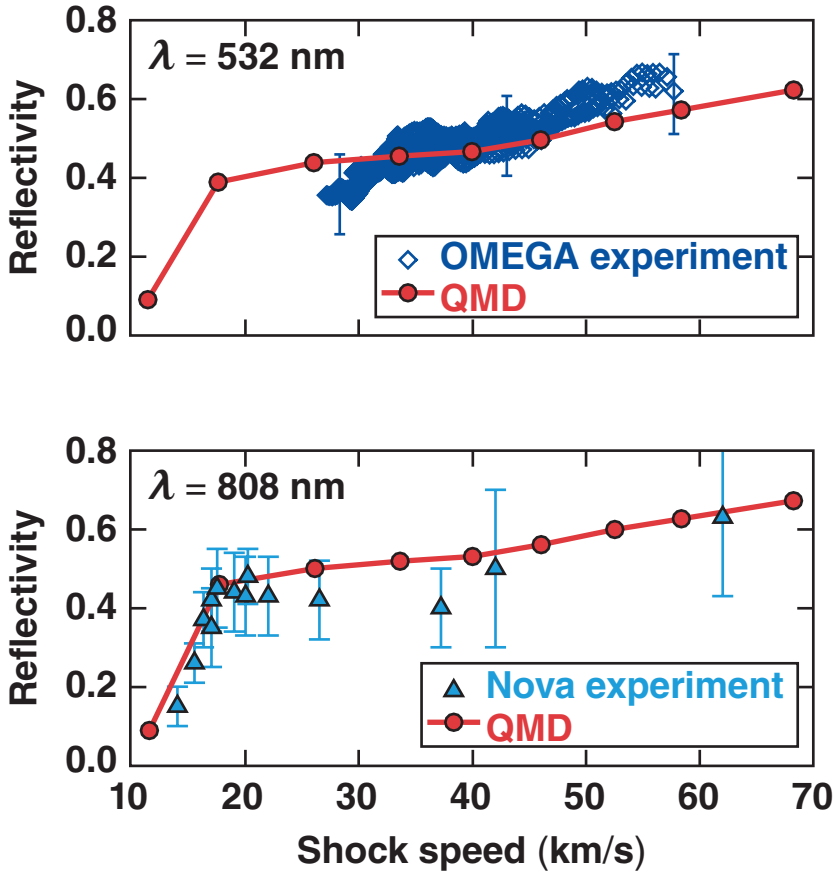
$$\sigma_1(\omega) = L_{11}(\omega);\ \sigma_2(\omega) = -\frac{2}{\pi} P\left(\int \frac{\omega \sigma_1(\omega')}{\omega'^2 - \omega^2} d\omega'\right)$$

$$\varepsilon_1(\omega) = 1 - \frac{4\pi}{\omega}\sigma_2(\omega);\ \varepsilon_2(\omega) = \frac{4\pi}{\omega}\sigma_1(\omega)$$

$$n(\omega) = \sqrt{\frac{|\varepsilon(\omega)| + \varepsilon_2(\omega)}{2}};\ k(\omega) = \sqrt{\frac{|\varepsilon(\omega)| - \varepsilon_1(\omega)}{2}}$$

$$R(\omega) = \frac{[n(\omega) - n_0]^2 + k(\omega)^2}{[n(\omega) + n_0]^2 + k(\omega)^2}$$

$$\alpha_m(\omega) = \frac{\alpha_K(\omega)}{\rho} = \frac{4\pi\overline{\sigma}_1(\omega)}{c \times \overline{n}(\omega)} \times \frac{1}{\rho}$$



*P. M. Celliers *et al.*, Phys. Rev. Lett. 84, 5564 (2000); T. R. Boehly *et al.*, Phys. Plasmas 16, 056302 (2009).

TC11447

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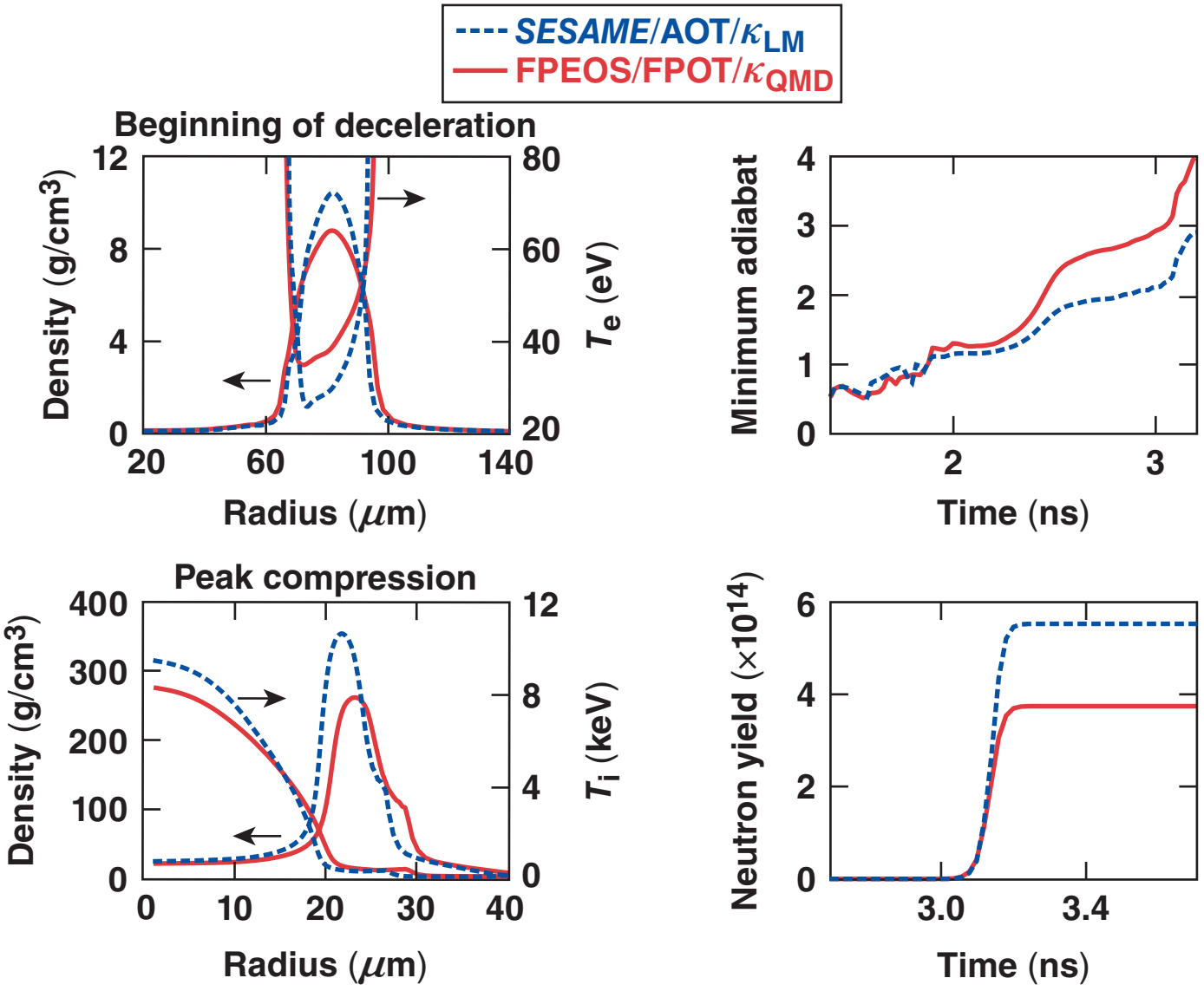
For a direct-drive OMEGA target ($\alpha \approx 2$), a higher *adiabat* in DT was predicted in FP simulations of ICF implosions



TC11452

A factor of ~2 difference in direct-drive target performance has been predicted between FPEOS/FPOT/κ_{QMD} and typical simulations for a National Ignition Facility (NIF) target

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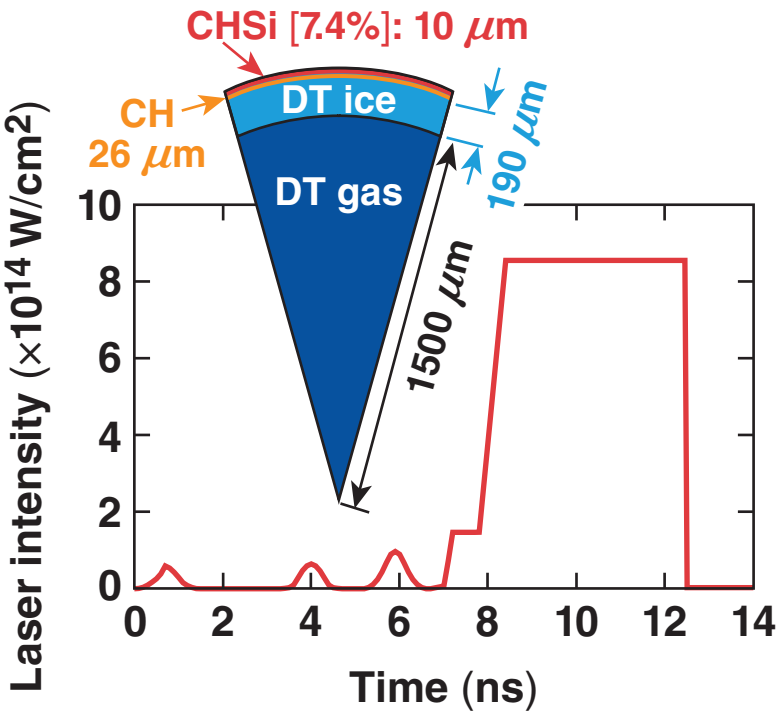
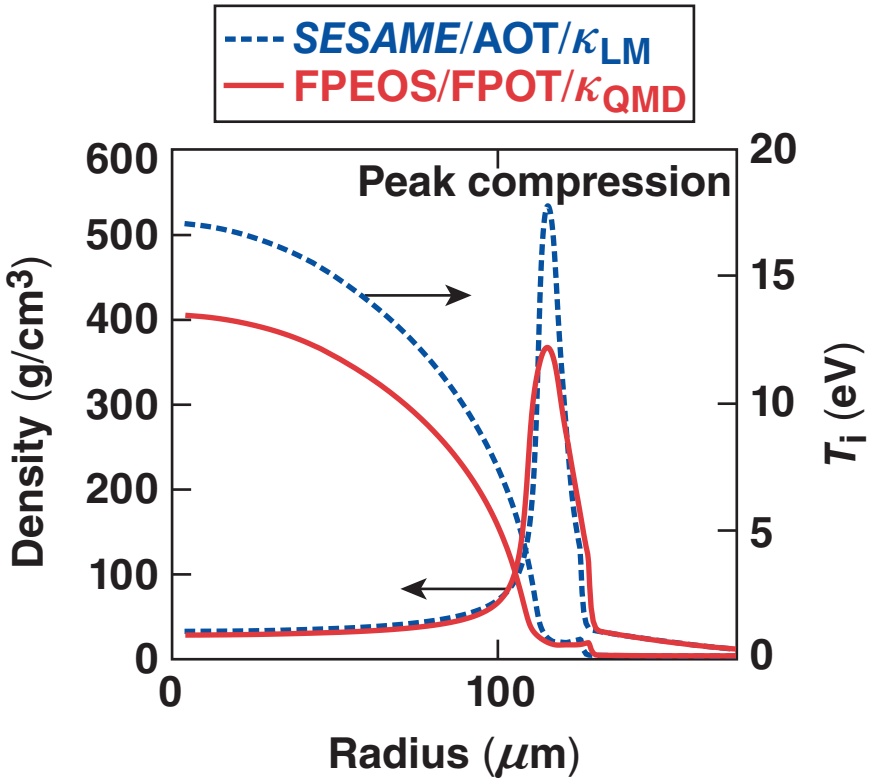
Si-doped CH is used to reduce laser imprint*



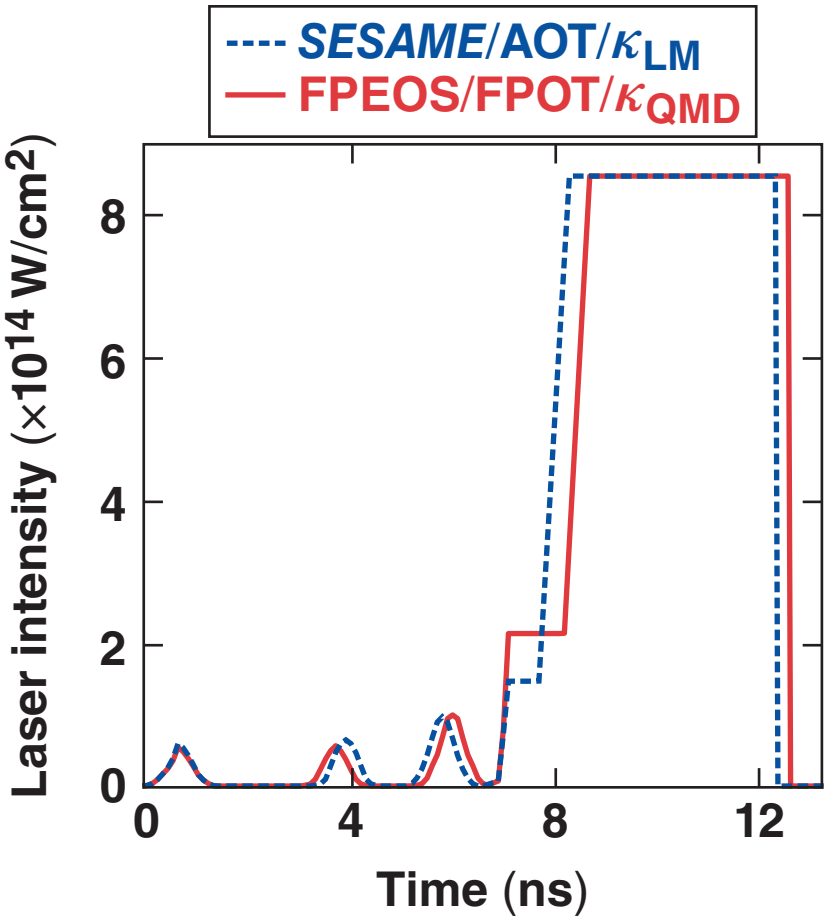


Gain = 40 (*SESAME*/AOT/κ_{LM})
Gain = 23 (FPEOS/FPOT/ κ_{QMD})

*G. Fiksel *et al.*, Phys. Plasmas 19, 062704 (2012); S. X. Hu *et al.*, Phys. Rev. Lett. 108, 195003 (2012).

TC11454

High gain ($G \sim 40$) can be recovered for the same NIF target by retuning the laser pulse shape using FPEOS/FPOT/κ_{QMD}



Gain = 40 (*SESAME*/AOT/κ_{LM})
Gain = 40 (FPEOS/FPOT/ κ_{QMD})

TC11457

Future work will test these effects beyond 1-D as well as extend such FP studies to ablator materials

- Two-dimensional simulations with FPEOS/FPOT/κ_{QMD} will show how these FP-based properties of DT may affect target performance (beyond 1-D)
- First-principles calculations for ablator materials have begun with studying the CH Hugoniot*

Consistent properties (FPEOS/FPOT/κ_{QMD}) of ablator materials in WDM conditions can be established with such first-principles calculations.

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

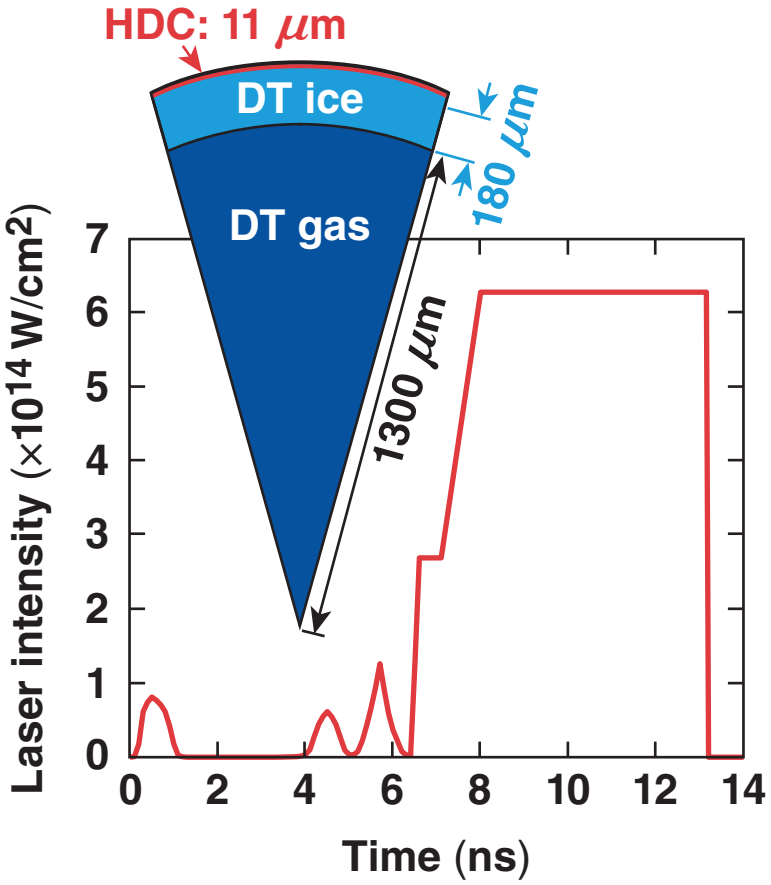
Summary/Conclusions

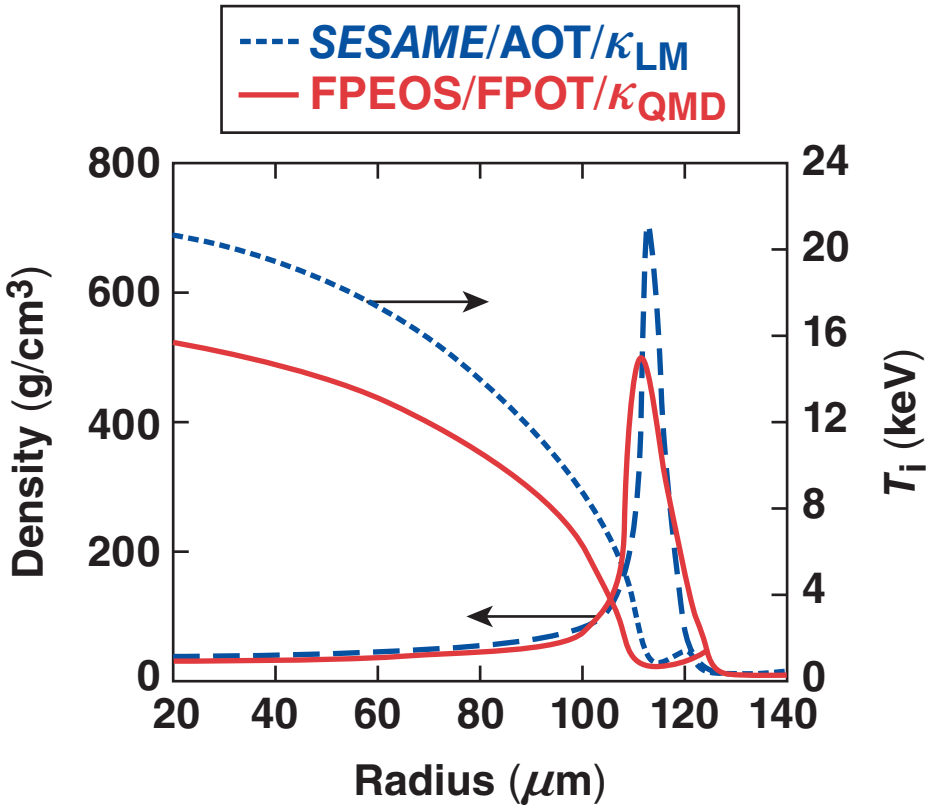
Accurate properties of deuterium–tritium (DT) fuel from first-principles calculations are crucial to inertial confinement fusion (ICF) target designs

UR LLE

- First-principles (FP) methods, including path-integral Monte Carlo (PIMC) and quantum molecular dynamics (QMD), are used to self-consistently calculate the properties of DT fuel for ICF applications
- Significant differences are identified when comparing FP-based equation of state (FPEOS), opacity table (FPOT), and thermal conductivity (κ_{QMD}) with models adopted in hydrocodes
- Hydro simulations using FP-based properties of DT have shown a factor of ~2 difference in ICF neutron yield compared to model simulations
- The lower the adiabat (α = 1.5 to 3.0), the larger the differences are in predicting ICF target performance

The lower the adiabat becomes ($\alpha \approx 2.2 \rightarrow 1.5$), the larger the variations (>2) in target performance are observed*





Gain = 28 (*SESAME*/AOT/κ_{LM})
Gain = 11 (FPEOS/FPOT/κ_{QMD})

*S. X. Hu *et al.*, "Impact of First-Principles Property Calculations of Warm-Dense Deuterium-Tritium on Inertial Confinement Fusion Target Designs," to be submitted to Physics of Plasmas.

TC11458