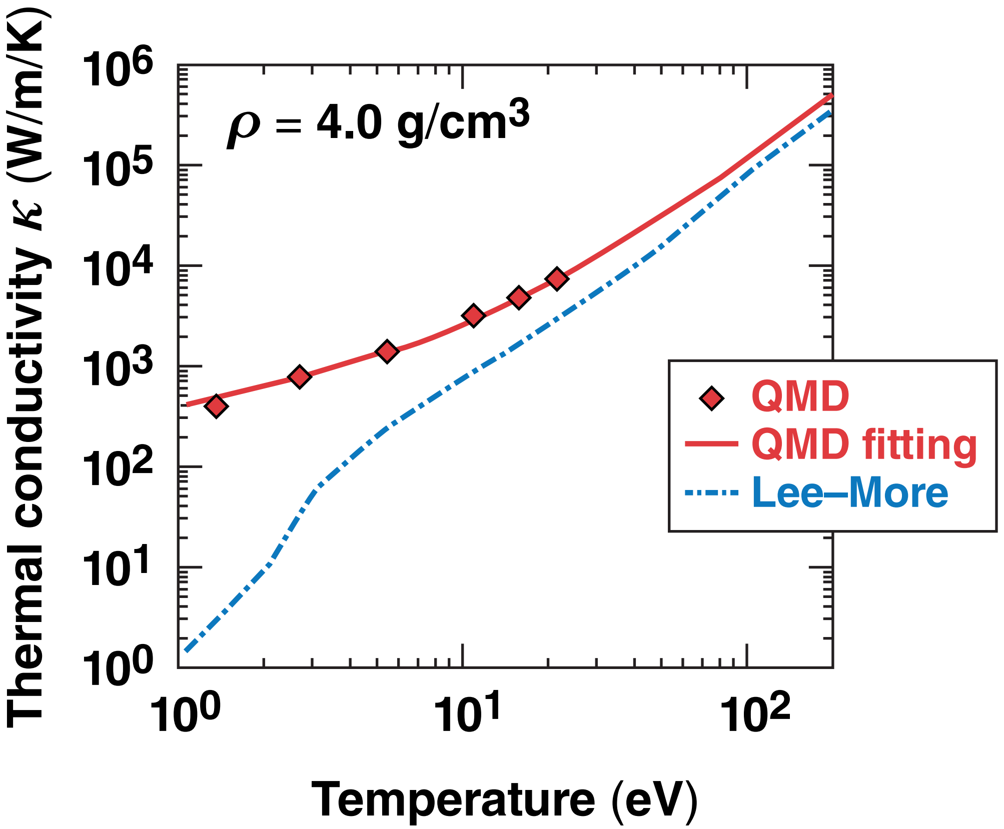
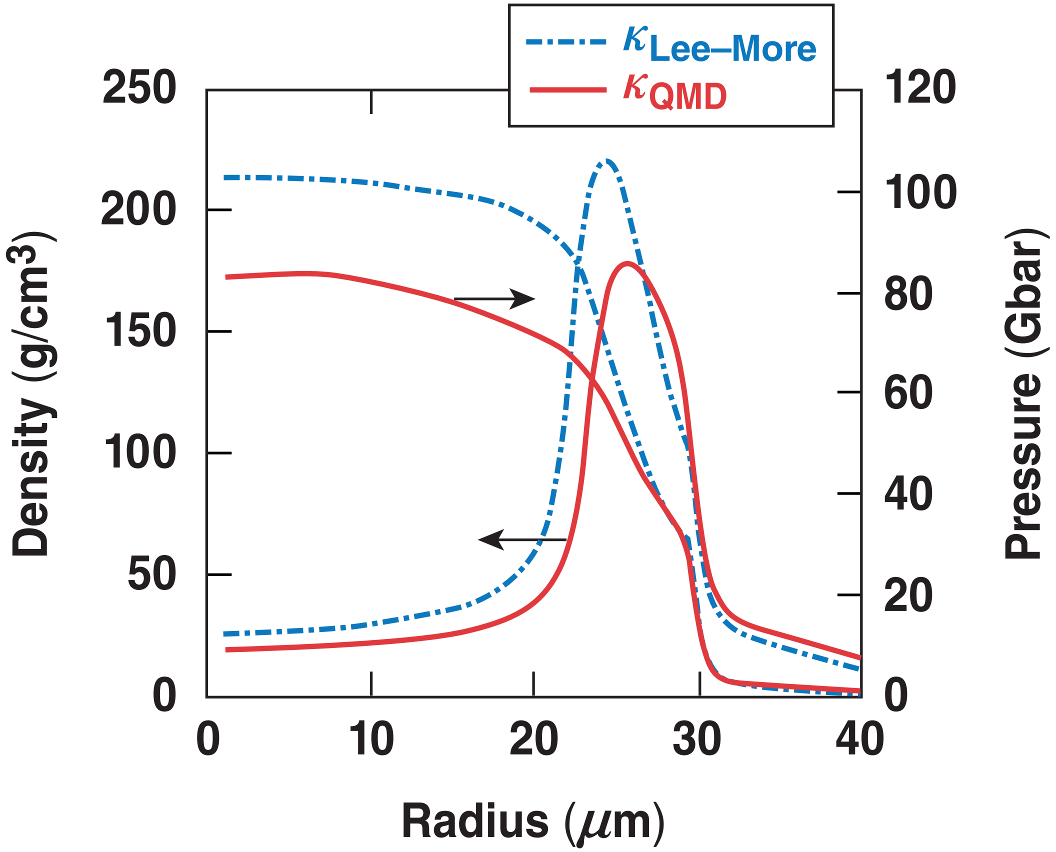
First-Principles Investigations on Thermal Conductivity and Average Ionization of Polystyrene (CH) Ablators Under Extreme Conditions





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Summary

The quantum-molecular-dynamics (QMD) method, based on density-functional theory (DFT), has been used to study thermal conductivity and ionization of CH ablators under inertial confinement fusion (ICF) conditions

- The resulting thermal conductivity of CH (κ_{QMD}) is 2 to 10× higher than the traditional Lee–More model predictions in warm dense plasmas
- The average ionization $\langle Z \rangle_{\mathrm{QMD}}$ of warm dense CH is larger than the astrophysics model predictions
- Hydro simulations using these κ_{QMD} and $\langle Z \rangle_{\mathrm{QMD}}$ have shown differences in target performance relative to traditional model simulations

Collaborators

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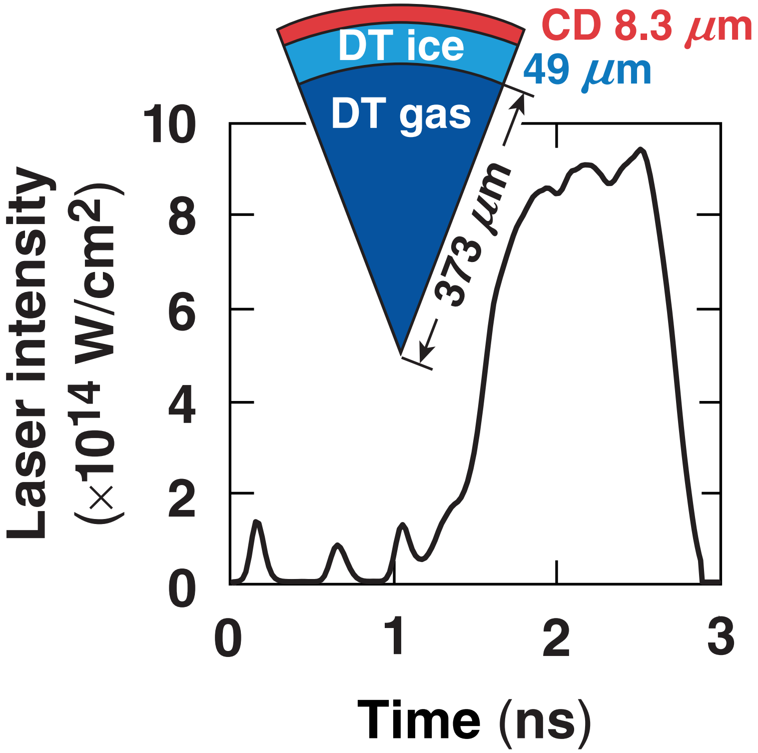
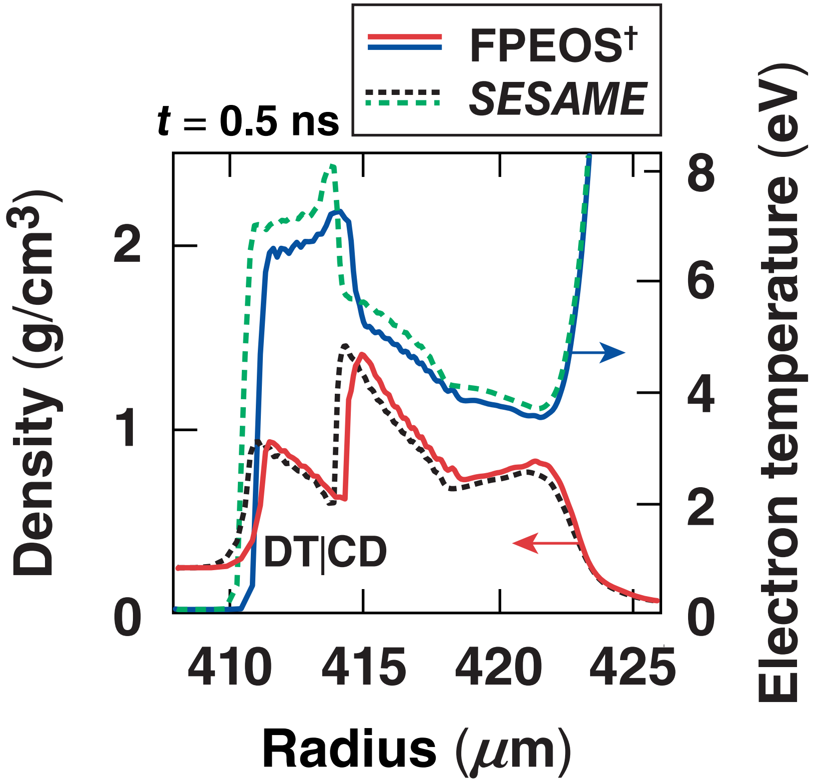
Warm dense CH plasmas (ρ = 0.5 to 10 g/cm^3 and T = 1 to 20 eV) are routinely accessed in ICF implosions





† First-principles equation of state

Approximated physics models, such as the Lee–More model* for κ and the astrophysics model for $\langle Z \rangle$ have been used to estimate these plasma properties in hydrocodes for ICF simulations.**

TC12155b

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*Y. T. Lee and R. M. More, Phys. Fluids 27, 1273 (1984).

**W. F. Huebner *et al.*, Los Alamos National Laboratory, Los Alamos, NM, Report LA-6760-M (1977).

QMD combines Kohn–Sham molecular dynamics (KSMD)* and orbital-free molecular dynamics (OFMD)** to study warm dense CH plasmas

- Both methods are based on DFT: KSMD (orbital based) and OFMD (orbital free)
- The KSMD method can handle plasma temperatures up to T_F, while the OFMD can be used for high-temperature (as well as low-density) plasmas
- A full range of density-temperature conditions of CH plasmas can be investigated with the combined KSMD–OFMD method

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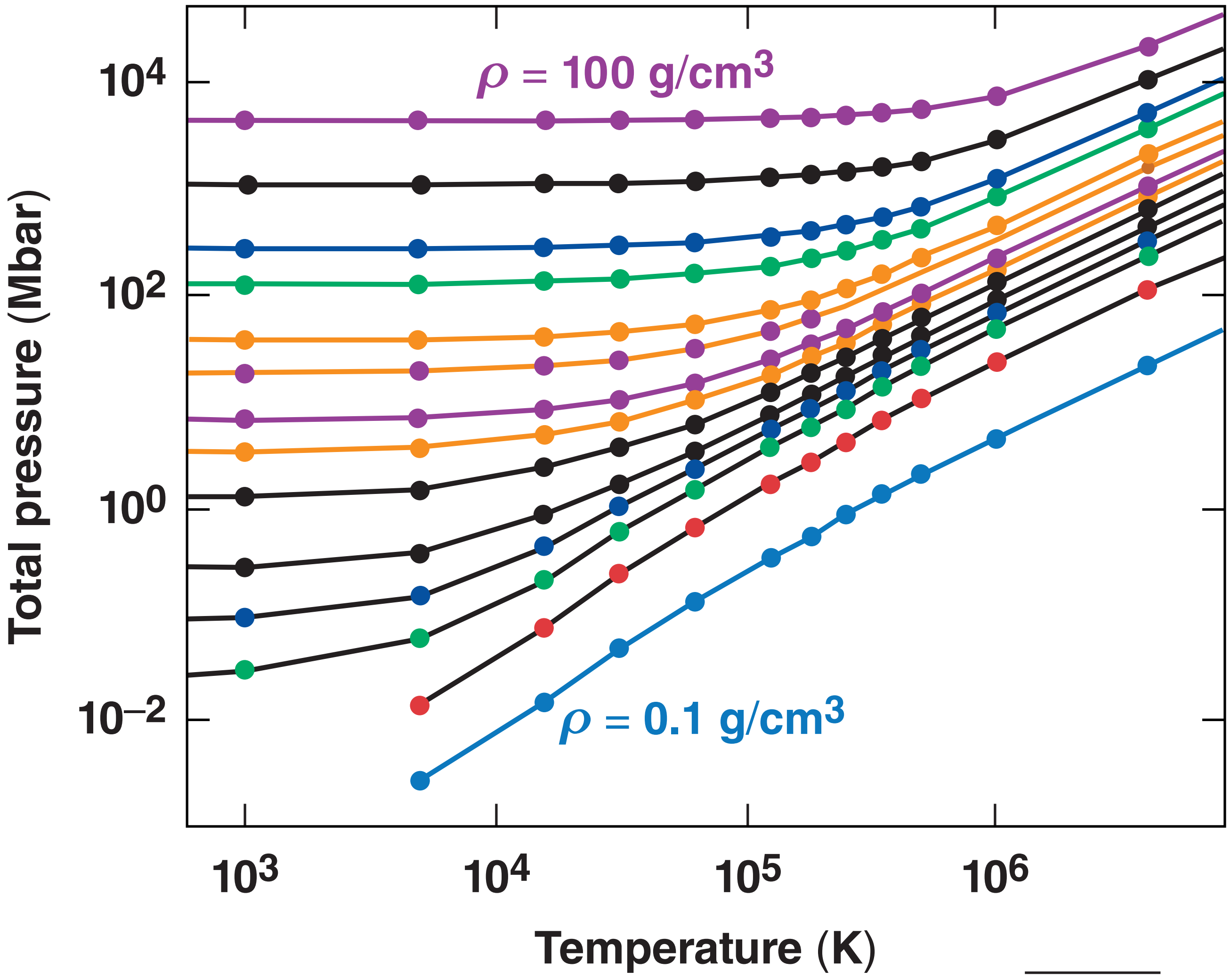
*W. Kohn and L. J. Sham, Phys. Rev. 140, A1133 (1965).

**F. Lambert, J. Clerouin, and G. Zerah, Phys. Rev. E 73, 016403 (2006).

A wide range of CH plasma conditions have been investigated with the QMD method

CH-FPEOS*



- The thermal conductivity** of CH can be calculated in KSMD using the Onsager coefficients L_{ij}:

$$\kappa = \frac{1}{T}\left(L_{22} - L_{12}^2/L_{11}\right)$$

- The average ionization $\langle Z \rangle$ can be derived from the pressure-matching mixing rule between C and H in OFMD

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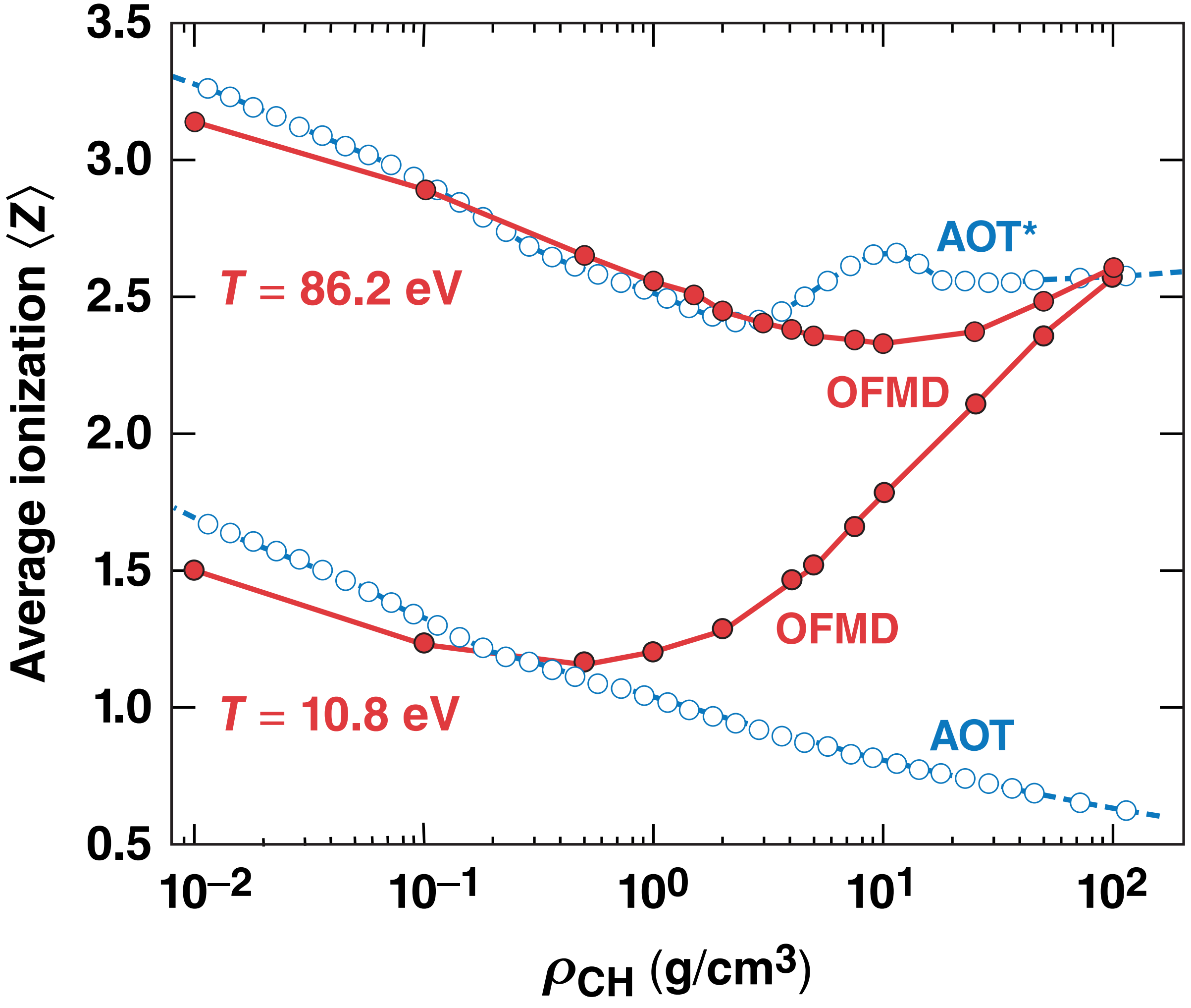
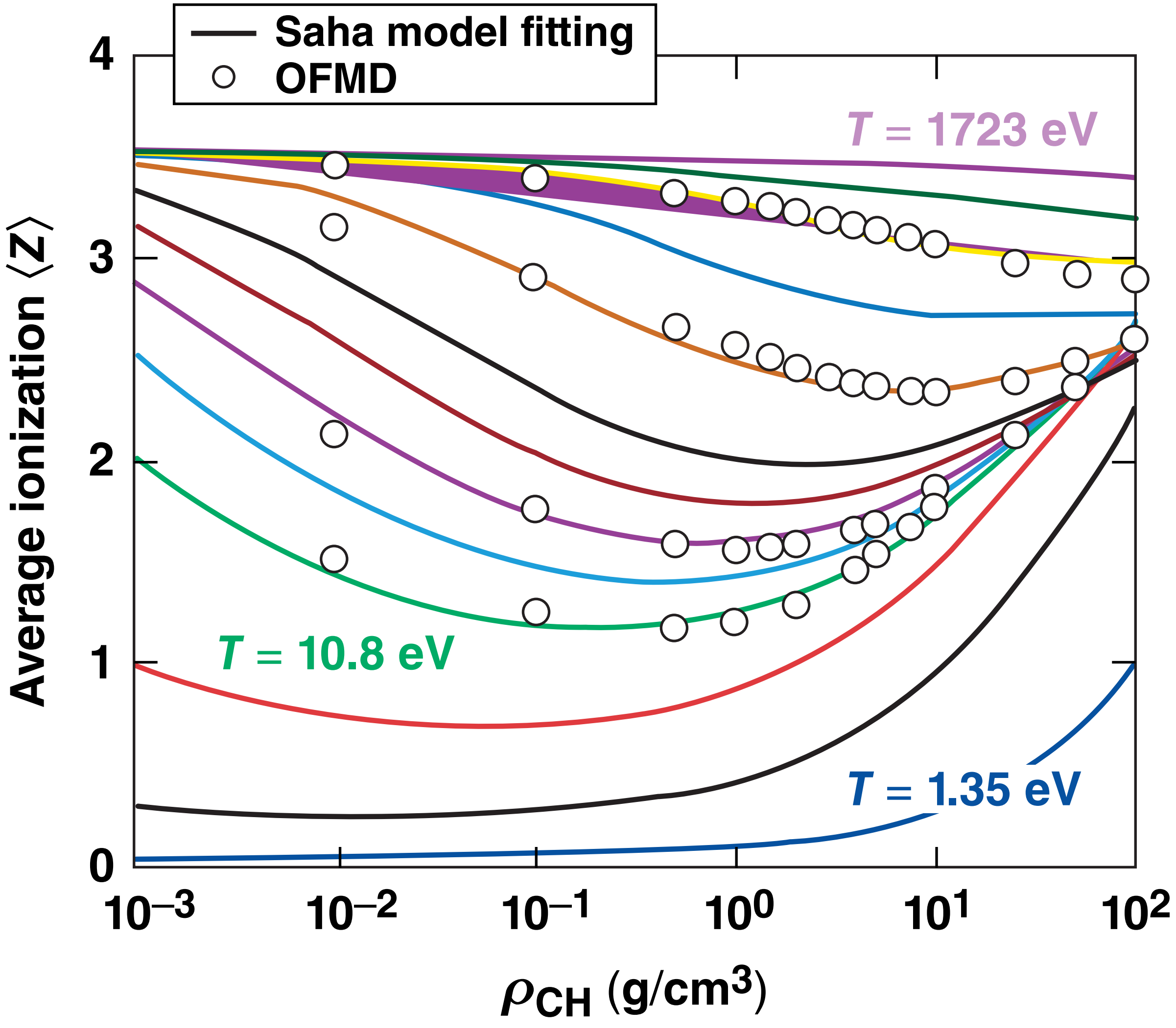
*S. X. Hu *et al.*, Phys. Rev. E 92, 043104 (2015).

**S. X. Hu *et al.*, "First-Principles Investigations on Ionization and Thermal Conductivity of Polystyrene (CH) for Inertial Confinement Fusion Applications," to be submitted to Physical Review E.

TC12151a

The OFMD-predicted average ionization ⟨Z⟩ is higher than the astrophysics model for warm dense CH plasmas





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*AOT: astrophysics opacity table

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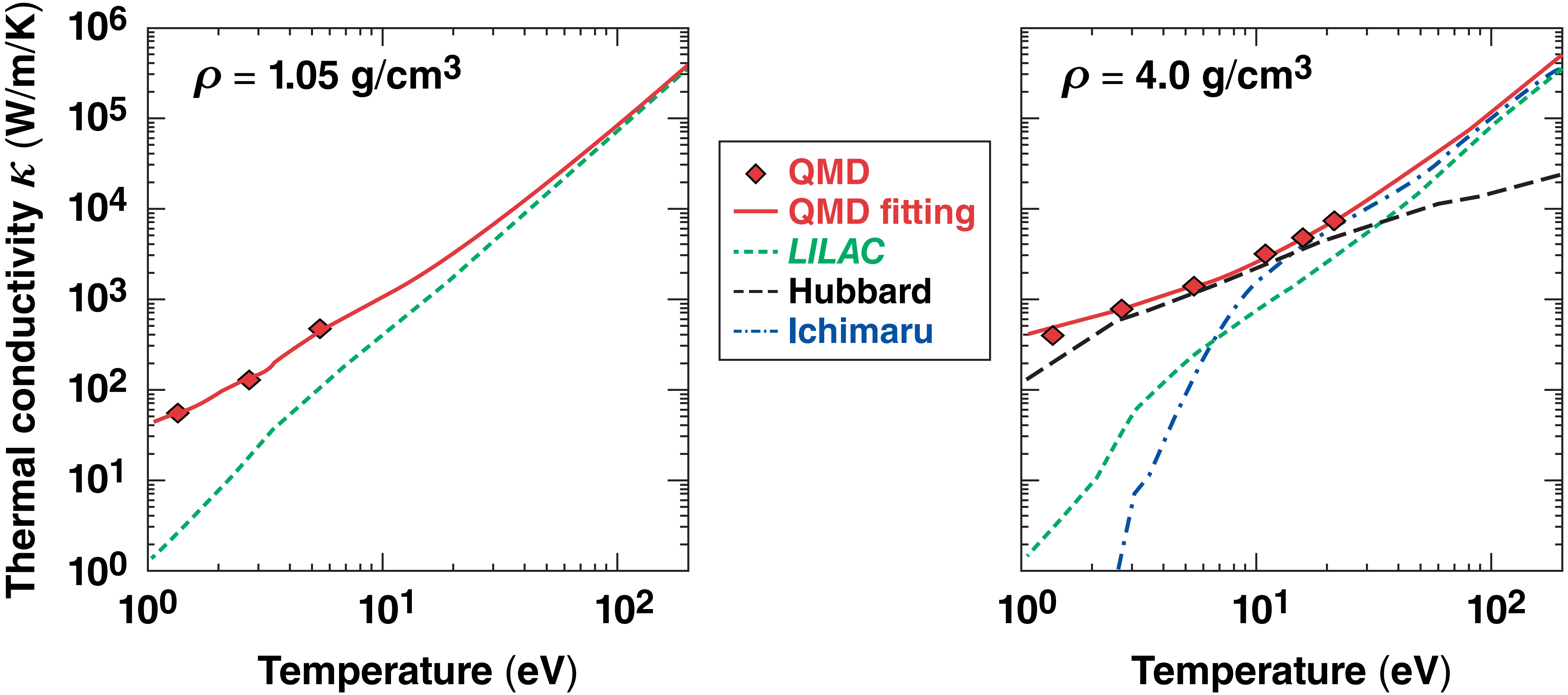
QMD-predicted thermal conductivities are 2 to 10× higher than the Lee–More model predictions currently used in our hydrocode *LILAC*



The resulting κ_{QMD} is fitted with a generalized Coulomb logarithm $(\ln\Lambda)_{QMD}$ for hydrocodes.

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With $Z_{\mathrm{eff}} = \langle Z^2 \rangle / \langle Z \rangle$ obtained in OFMD, we can fit the QMD-derived thermal conductivity κ with a generalized Coulomb logarithm for CH plasmas

$$\kappa_{\text{QMD fitting}}(\rho, T) = \underbrace{\frac{20 \times \left(\frac{2}{\pi}\right)^{3/2} k_{\mathrm{B}}^{7/2}\, T^{5/2}}{\sqrt{m} \times Z_{\mathrm{eff}} \times e^4} \times \frac{0.095\,(Z_{\mathrm{eff}} + 0.24)}{1 + 0.24 \times Z_{\mathrm{eff}}}}_{\text{Spitzer prefactor}} \frac{1}{(\ln\Lambda)_{\mathrm{QMD}}}$$

- The generalized Coulomb logarithm is a function of the ion-coupling parameter $\left[\Gamma_i = \frac{\langle Z \rangle^2 e^2}{r_0 kT}\right]$ and the electron-degeneracy parameter $\left(\theta_{\mathrm{e}} = \frac{T}{T_{\mathrm{F}}}\right)$:

$$(\ln\Lambda)_{\mathrm{QMD}} = \exp\left\{\gamma_0 + \sum_{i=1}^{6} \left[\gamma_{\mathrm{i}} \times (\ln\Gamma_{\mathrm{i}})^i + \sigma_{\mathrm{i}} \times (\ln\theta_{\mathrm{e}})^i\right]\right\}$$

with fitting parameters of γ_{i} and σ_{i}

In contrast to $\kappa_{\text{QMD fitting}}$, κ_{LILAC} is a hybrid model that uses the Lee–More Coulomb logarithm $[(\ln\Lambda)_{\mathrm{LM}}]$ with the same Spitzer prefactor.

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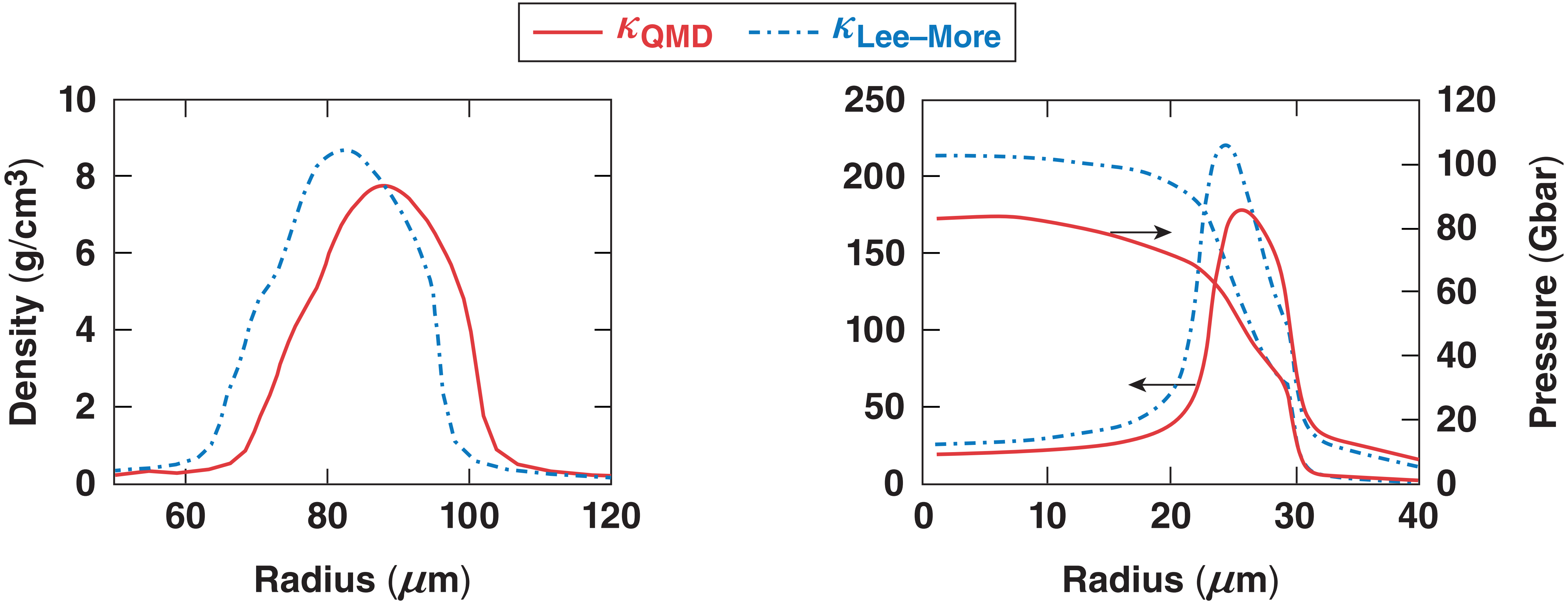
Hydro simulations using fitted κ_{QMD} and $\langle Z \rangle_{\mathrm{QMD}}$ for CH have predicted a slower implosion velocity and ~20% lower pressure in the hot spot



κ_{LILAC}: Yield = 1.9×10^{14}, $\langle T_{\mathrm{i}} \rangle$ = 4.17 KeV, P_{peak} = 100 Gbar
κ_{QMD}: Yield = 1.6×10^{14}, $\langle T_{\mathrm{i}} \rangle$ = 4.07 KeV, P_{peak} = 80 Gbar

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*S. X. Hu *et al.*, "First-Principles Investigations on Ionization and Thermal Conductivity of Polystyrene (CH) for Inertial Confinement Fusion Applications," to be submitted to Physical Review E.

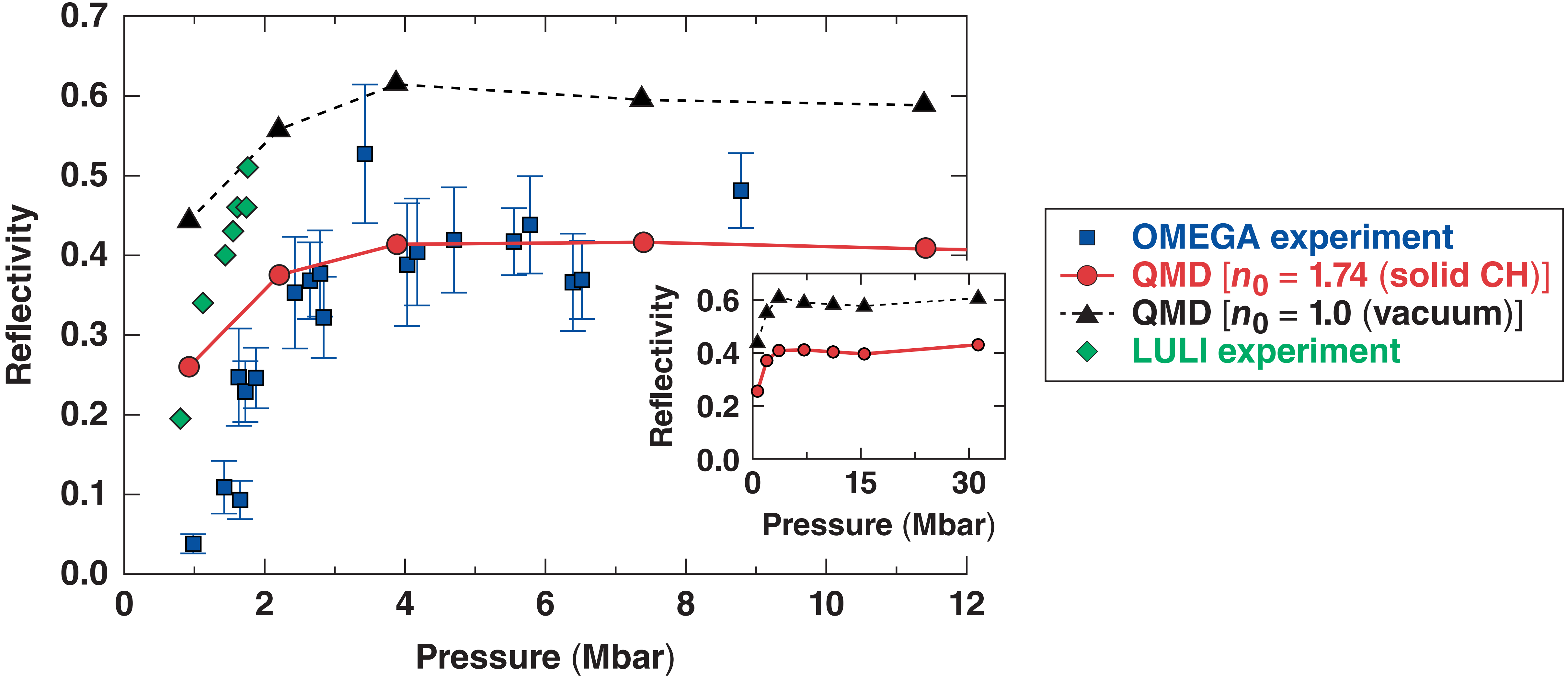
TC12418

Summary/Conclusions

The quantum-molecular-dynamics (QMD) method, based on density-functional theory (DFT), has been used to study thermal conductivity and ionization of CH ablators under inertial confinement fusion (ICF) conditions

- The resulting thermal conductivity of CH (κ_{QMD}) is 2 to 10× higher than the traditional Lee–More model predictions in warm dense plasmas
- The average ionization $\langle Z \rangle_{\mathrm{QMD}}$ of warm dense CH is larger than the astrophysics model predictions
- Hydro simulations using these κ_{QMD} and $\langle Z \rangle_{\mathrm{QMD}}$ have shown differences in target performance relative to traditional model simulations

QMD-predicted reflectivity* of shocked CH compares well with experiments in the saturation level



TC11155a

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

First-principles calculations of average ionization and thermal conductivity for CH under extreme conditions

- **Using the QMD methods (KSMD and OFMD), we have performed first-principles calculations of $\langle Z \rangle$, Z_{eff}, and κ for the ICF ablator material CH**

$$\kappa_{\text{QMD fitting}}(\rho, T) = \underbrace{\frac{20 \times \left(\frac{2}{\pi}\right)^{3/2} k_B^{7/2} T^{3/2}}{m \times Z_{\text{eff}} \times e^4} \times \frac{0.095\,(Z_{\text{eff}} + 0.24)}{1 + 0.24 \times Z_{\text{eff}}}}_{\text{Spitzer prefactor}} \times \frac{1}{(\ln \Lambda)_{\text{QMD}}}$$

- **The thermal conductivity κ depends on the effective charge Z_{eff}, which is defined as**

$$\boxed{Z_{\text{eff}} = \frac{\langle Z^2 \rangle}{\langle Z \rangle};\ \langle Z \rangle = f_C \times 6 + f_H \times 1;\ \langle Z^2 \rangle = f_C \times 36 + f_H \times 1}$$

Saha-type fitting of $\langle Z \rangle$ for hydrocode:

$$\frac{\xi^2}{1-\xi} = \frac{\alpha_0}{n_i \Lambda_e^3} \exp\left[-\frac{f_z(\rho, T)}{kT}\right] \quad \boxed{\langle Z \rangle = Z_{\max} \times \xi,\ \text{with } Z_{\max} = 3.5 \text{ for } C_1 H_1}$$

$$f_z(\rho, T) = \alpha_1 + \alpha_2 \cdot kT\left[\left(1 + \sqrt{3\Gamma_0}\right)^{1/4} - 1\right] + \alpha_3 \cdot (kT)^{0.9} + kT \times \left(\frac{\alpha_4}{r_0} + \frac{\alpha_5}{r_0^2} + \frac{\alpha_6}{r_0^3}\right)$$

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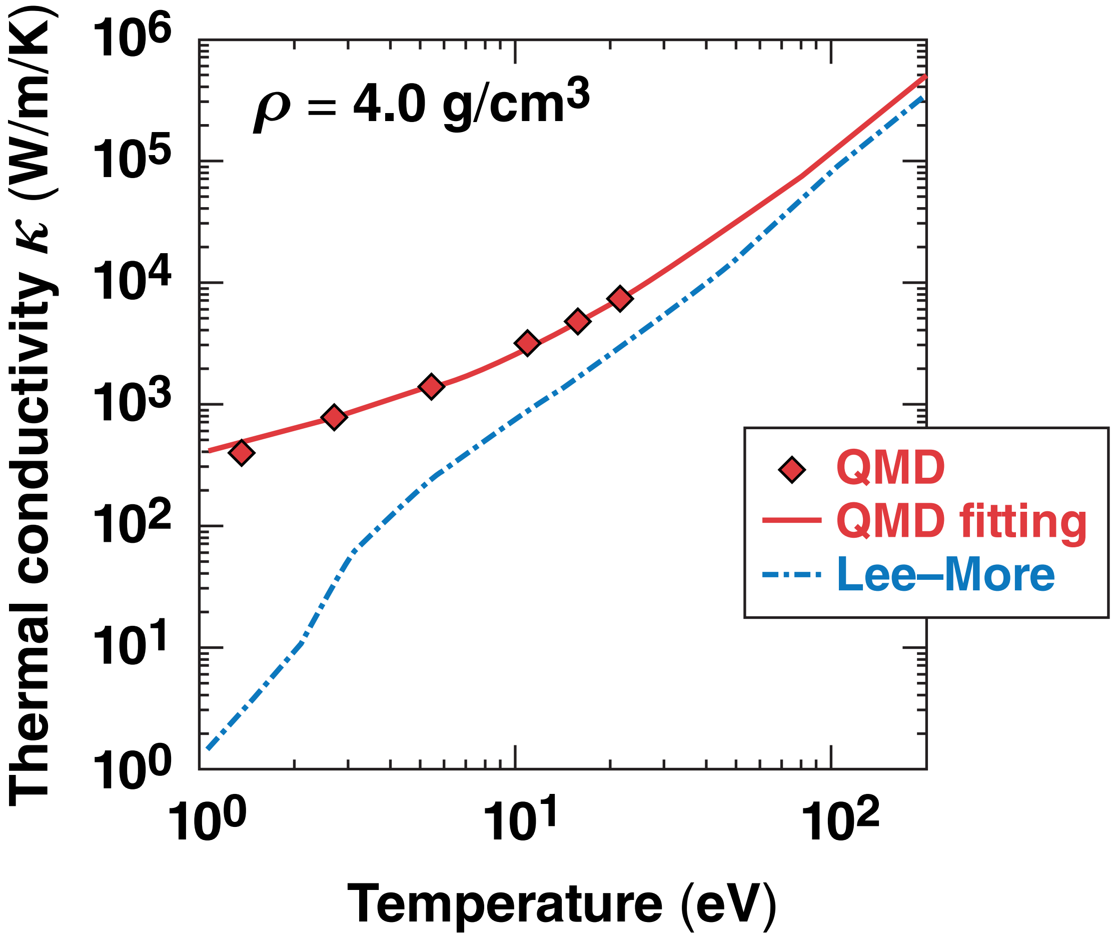
QMD-predicted thermal conductivities are 2 to 10× higher than the Lee–More model predictions currently used in our hydrocode *LILAC*



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

The resulting κ_{QMD} is fitted for hydrocodes with a generalized Coulomb logarithm $(\ln\Lambda)_{\mathrm{QMD}}$.