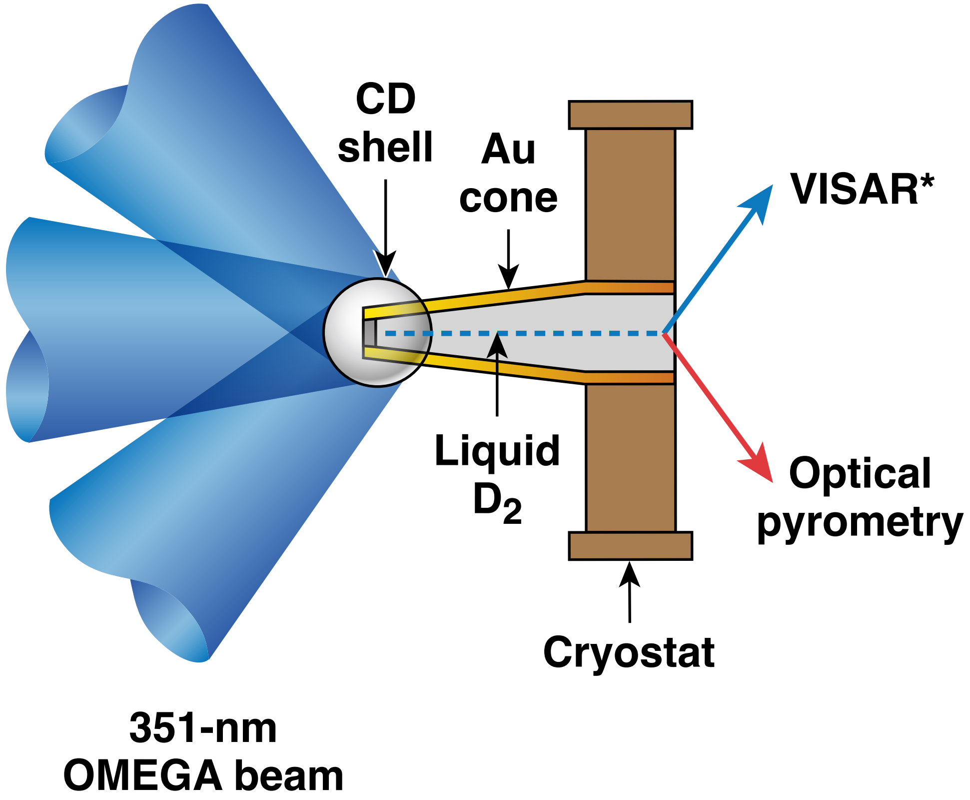
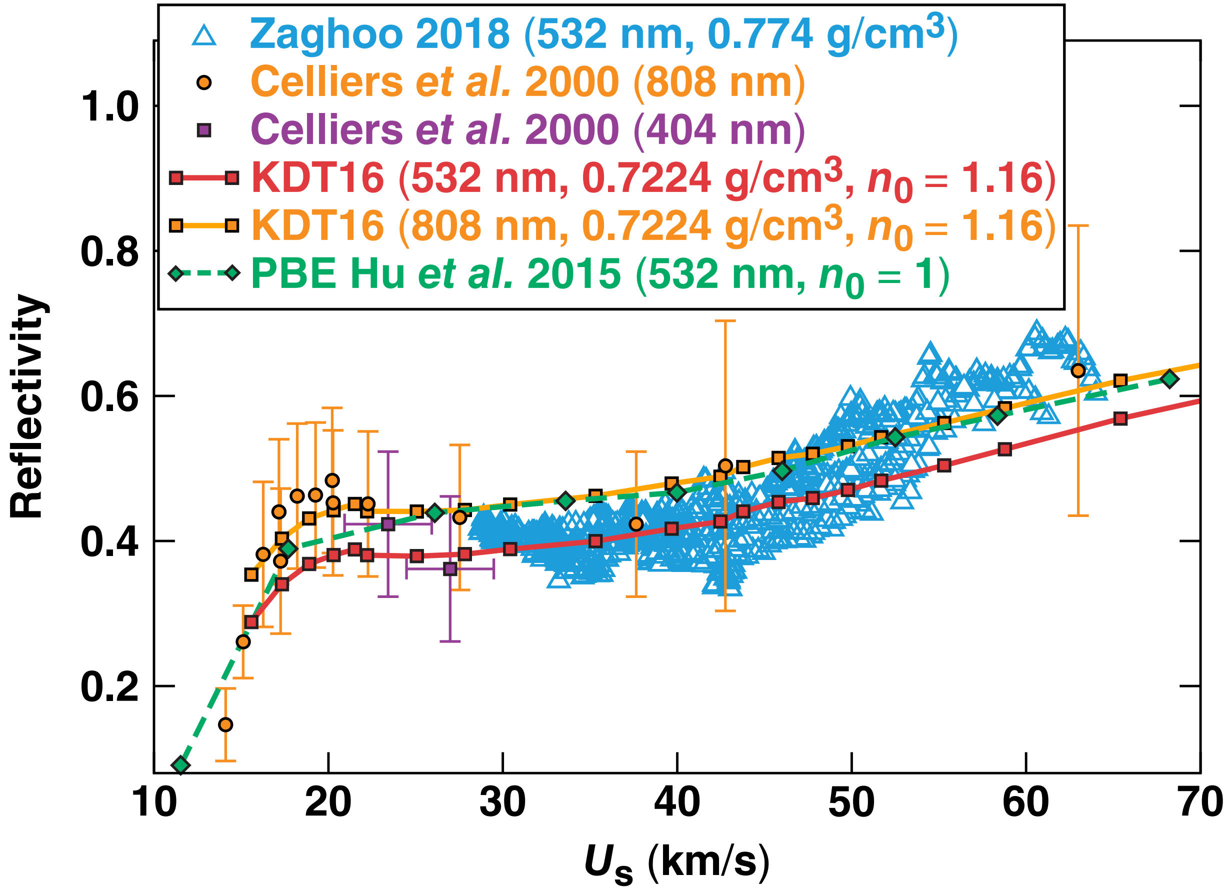
Study of the Exchange-Correlation Thermal Effects for Transport and Optical Properties of Shocked Deuterium

CD shells filled with liquid D_2 ρ_0 = 0.172 g/cm^3





V. V. Karasiev
University of Rochester
Laboratory for Laser Energetics

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Summary

Exchange-correlation (XC) thermal effects have an impact of up to 5% on the calculated properties of D_2 and must be taken into account for accurate predictions

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- XC thermal effects account for the softening of the deuterium Hugoniot at $P > 300$ GPa in agreement with recent experimental measurements
- The calculated reflectivity of shocked deuterium is in a good agreement with experimental measurements for shock speeds up to 50 km/s
- The deuterium system along the Hugoniot transforms from a semiconducting *molecular liquid* to an *atomic-poor metallic liquid* and finally to a *nondegenerate plasma*

Collaborators

S. X. Hu, M. Zaghoo, and T. R. Boehly

University of Rochester
Laboratory for Laser Energetics

Funding Acknowledgments:

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We are developing temperature-dependent XC functionals to improve density functional theory (DFT) predictions

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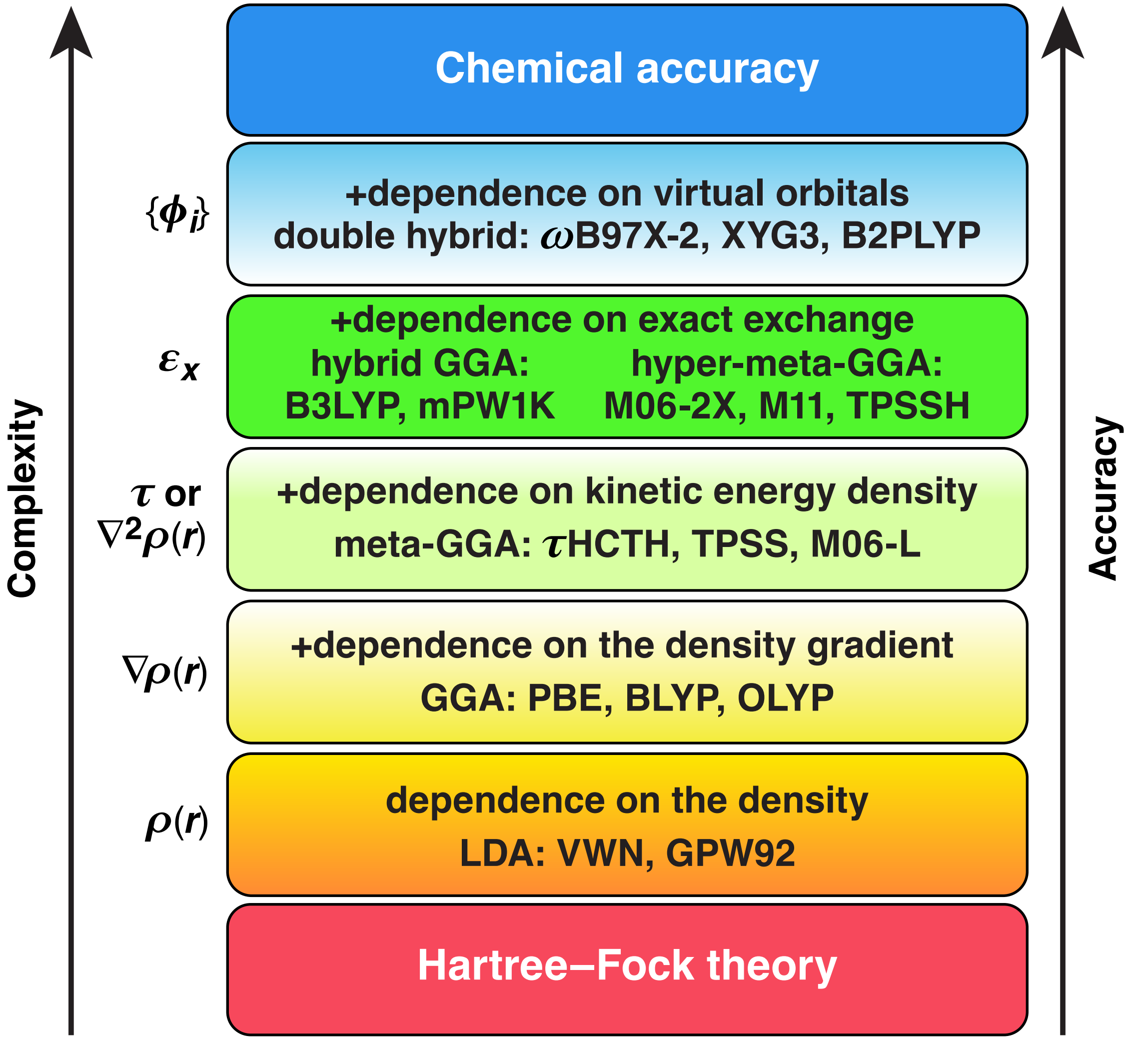
Jacob's ladder* of the zero-temperature XC functional approximations



← Finite-temperature Hybrids: project funded by NSF

← Finite-temperature metaGGA: finite-temperature version of SCAN (work in progress)

← Finite-temperature GGA (KDT16): Karasiev *et al.*, PRL 120, 076401 (2018)

← Finite-temperature LDA (KSDT): Karasiev *et al.*, PRL 112, 076403 (2014)

Development has to start from the lowest rung because low-rung functionals are used as ingredients for higher rungs

TC14630

PBE/GGA: J. P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. 77, 3865 (1996); 78, 1396(E) (1997).
PZ/LDA: J. P. Perdew and A Zunger, Phys. Rev. B 23, 5048 (1981).
*J. P. Perdew and K. Schmidt, AIP Conf. Proc. 577, 1 (2001).

The XC thermal effects for the homogeneous electron gas (HEG) are significant in warm-dense-matter (WDM) regime*

f_{xc} = XC free energy per particle

ε_{xc} = XC energy per particle at $T = 0$

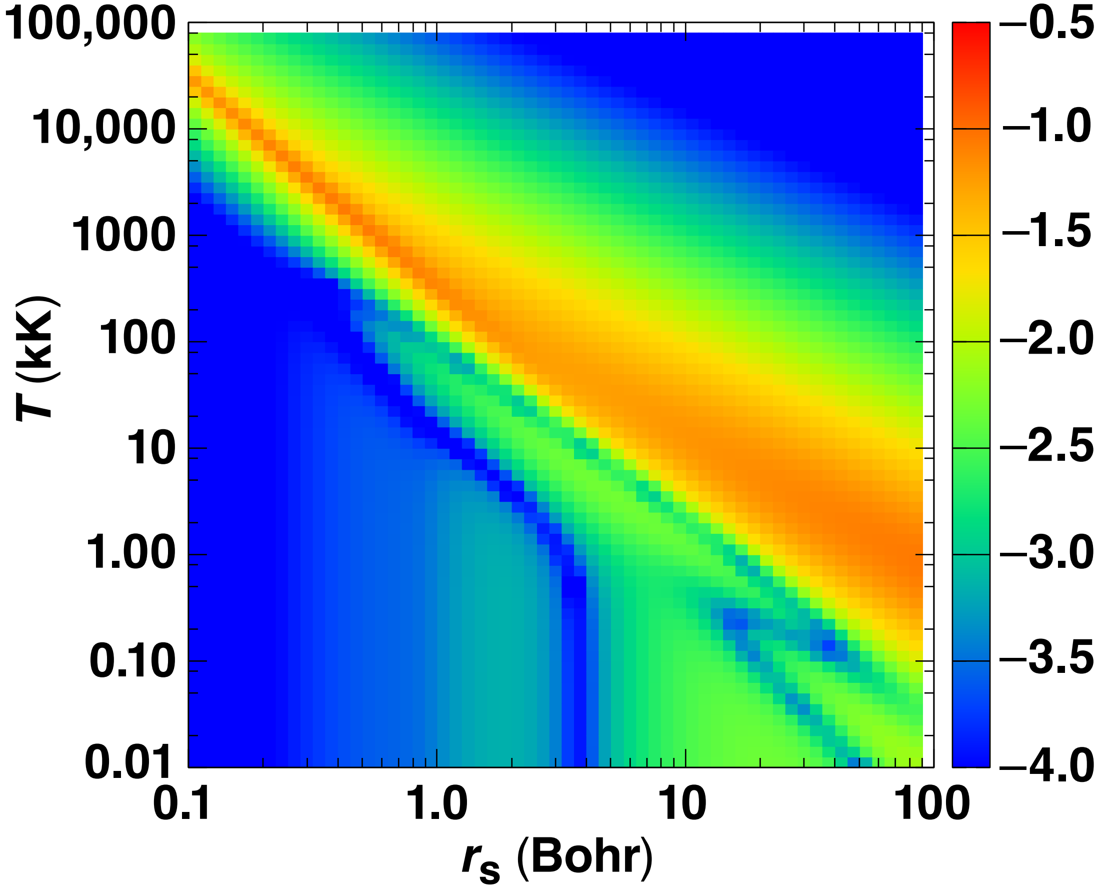
f_s = non-interacting free energy

- At low temperature the XC thermal effects are negligible
- In high temperature limit the free-energy is dominated by the noninteracting part → XC is negligible and does not play a role

In this work we use Karasiev–Dufty–Trickey (KDT16) GGA-level XC free-energy functional to address the issue of thermal effects
See details in:
Karasiev *et al.*, Phys. Rev. Lett. 120, 076401 (2018).

Measure of relative importance of thermal effects

$$A = \log_{10} \frac{\left| f_{xc}(r_s, T) - \varepsilon_{xc}(r_s) \right|}{\left| f_{xc}(r_s, T) \right| + \left| \varepsilon_{xc}(r_s) \right|}$$



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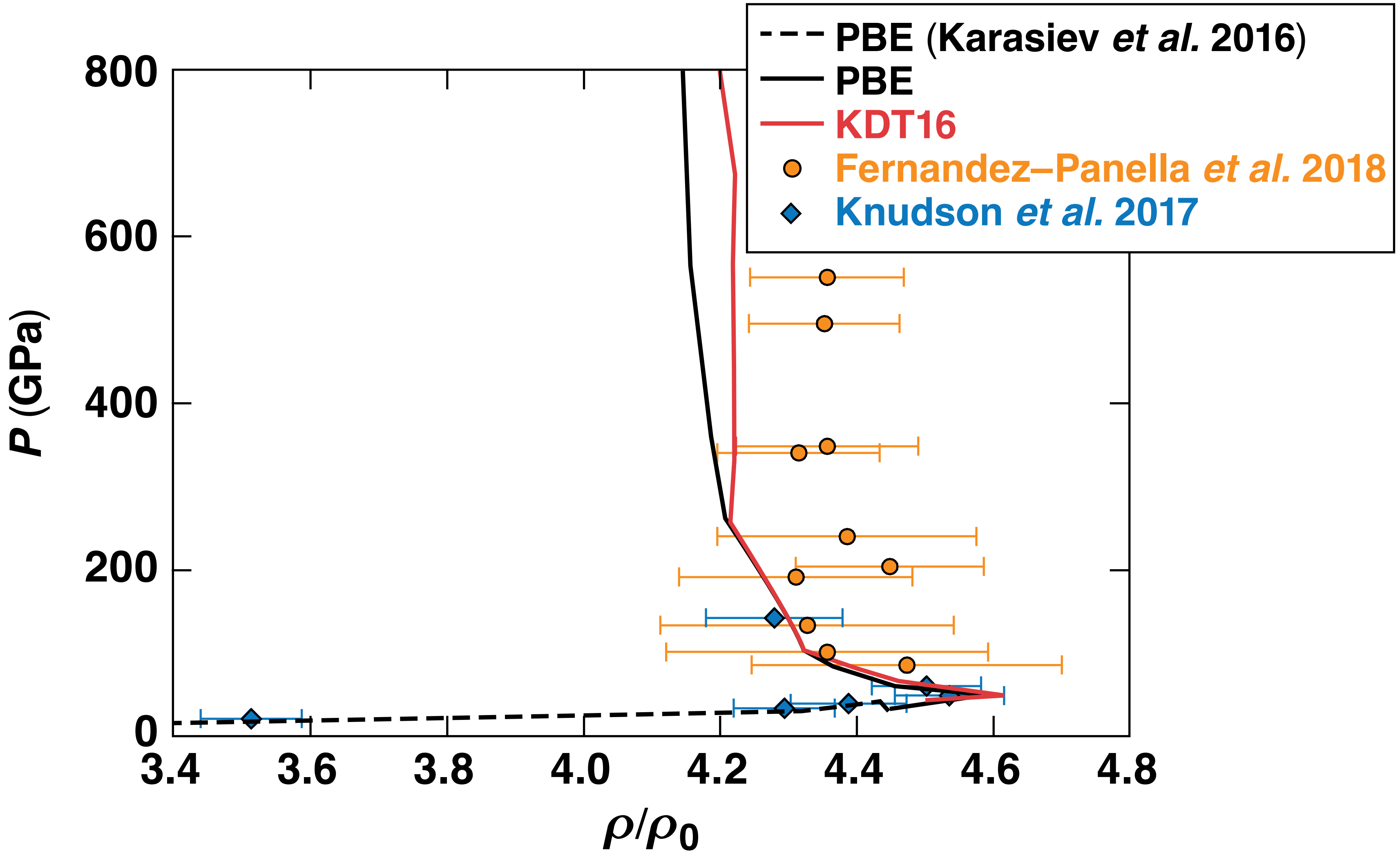
*V. V. Karasiev, L. Calderín, and S. B. Trickey, Phys. Rev. E 93, 063207 (2016).

Results

The D_2 Hugoniot becomes ~2% softer at high pressure ($P > 300$ GPa) as a result of thermal XC effects; agreement with recent experimental measurements is improved



- Energy ΔE and pressure ΔP corrections caused by the thermal XC effects are larger than 4% but have the same sign
- There is some cancellation between ΔE and ΔP corrections in the Hugoniot relation*

$$E - E - \frac{1}{2}(P - P_0)\left(\frac{1}{\rho} - \frac{1}{\rho_0}\right) = 0$$

Fernandez-Pañella *et al.*, (submitted) (2018);
Knudson, Desjarlais PRL, 118 035501 (2017).
*V. V. Karasiev, L. Calderín, and S. B. Trickey, Phys. Rev. E 93, 063207 (2016).

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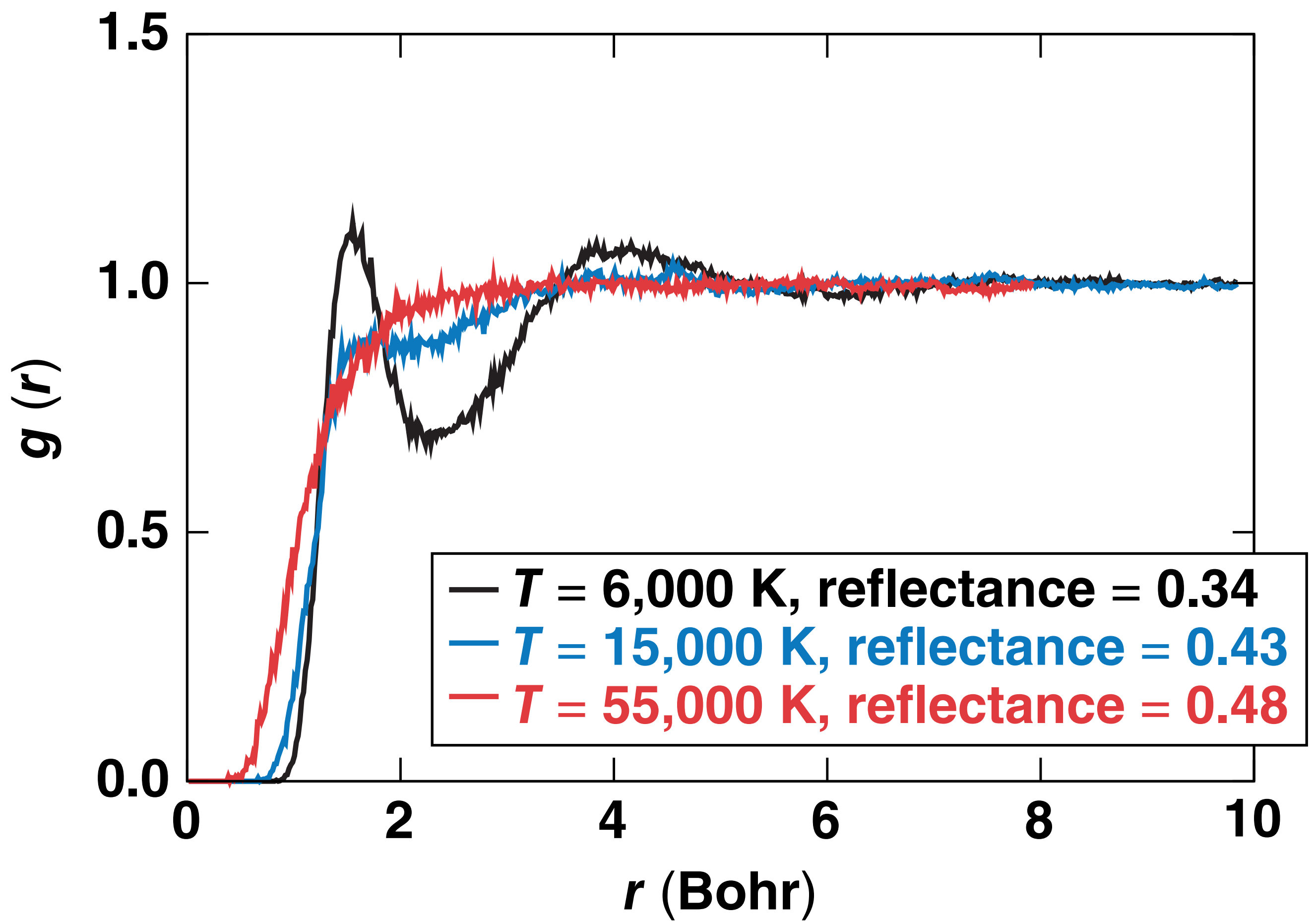
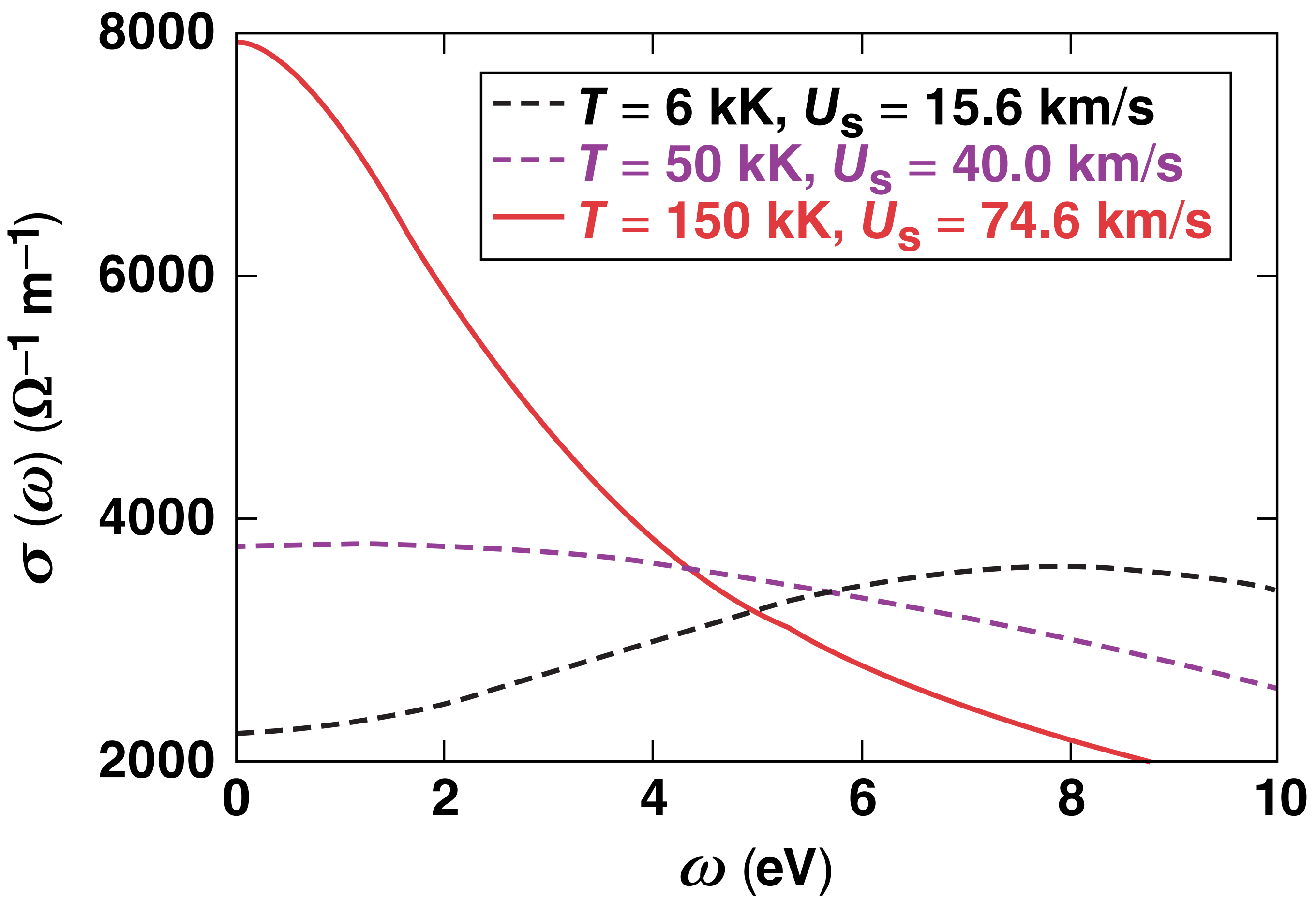
Results

Shocked D_2 along the principal Hugoniot changes from molecular semiconducting liquid to atomic metallic liquid and finally to nondegenerate plasma



Radial D–D distribution function for three selected temperatures



Frequency-dependent electrical conductivity

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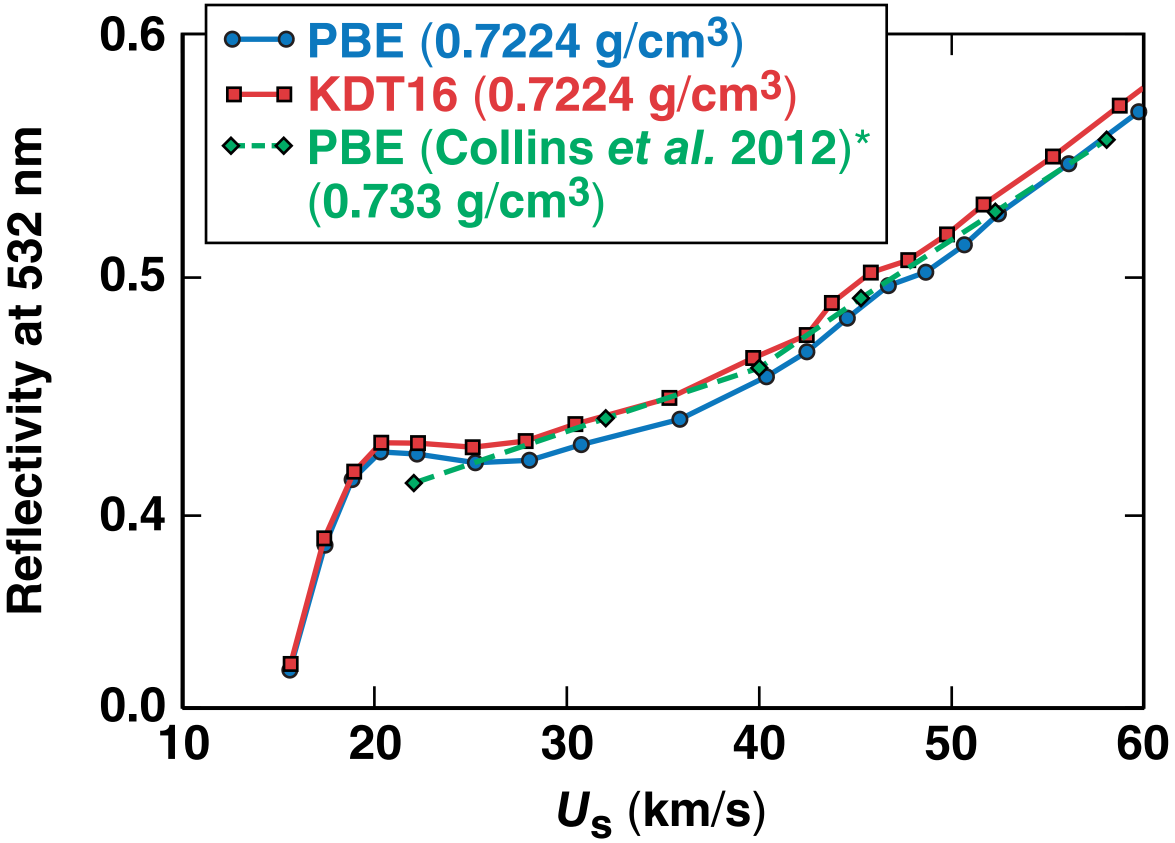
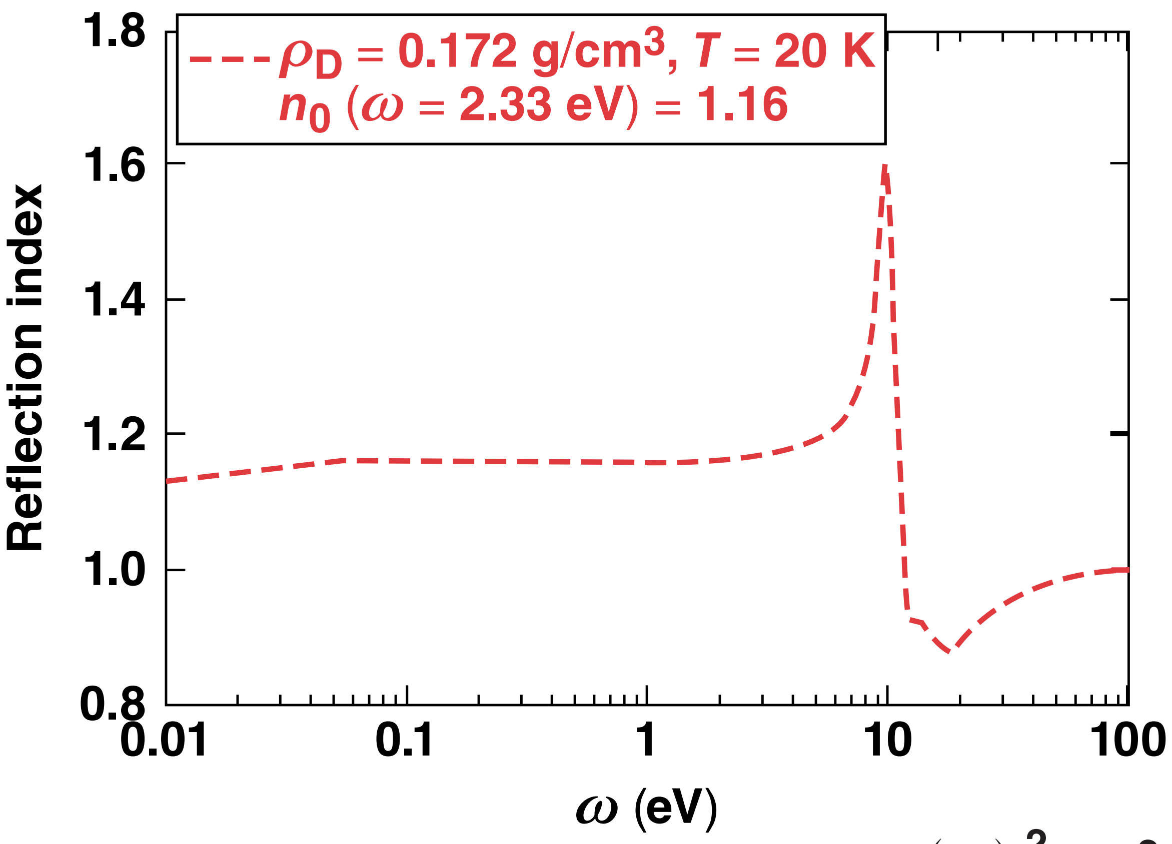
As a result of thermal XC effects, the reflectivity of D_2 along the Hugoniot is increased by about 4% for shock speeds above 20 km/s



Reflectivity of deuterium as a function of shock speed along the principal Hugoniot



Reflectivity is defined as: $$r(\omega) = \frac{[n_0 - n(\omega)]^2 + k^2(\omega)}{[n_0 + n(\omega)]^2 + k^2(\omega)}$$

n_0 (532 nm) = 1.16 – calculated value

n_0 = 1.14 – experimental value**

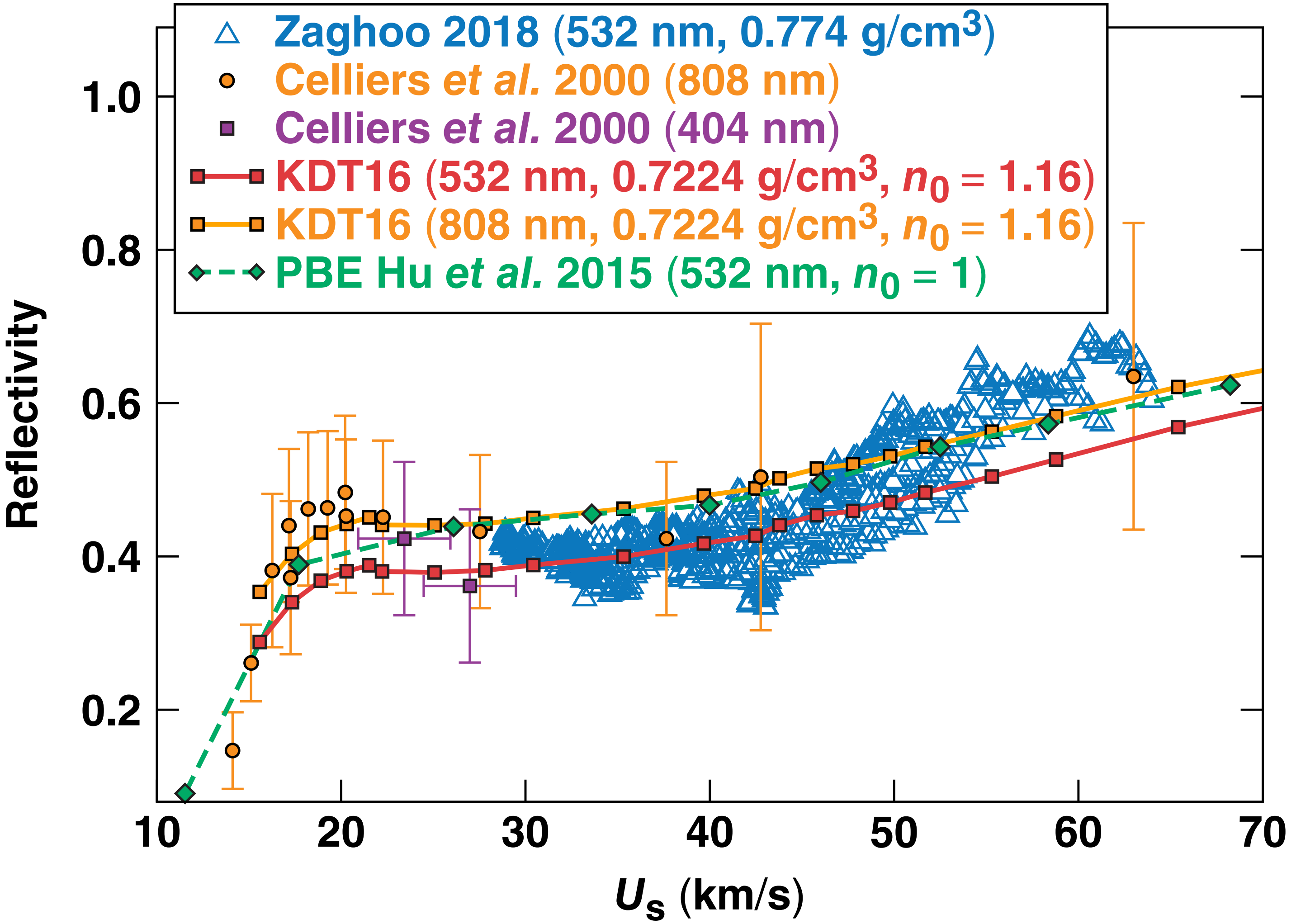
*L. A. Collins, J. D. Kress, and D. E. Hanson, Phys. Rev. B 85, 233101 (2012).

**P. C. Souers, *Hydrogen Properties for Fusion Energy* (University of California, Berkeley, CA, 1986).

TC14634

Results

There is good agreement with recent experimental measurements on OMEGA by M. Zaghoo



Recent experimental measurements on OMEGA: see M. Zaghoo *et al.*, "Breakdown of Fermi Degeneracy in the Simplest Liquid Metal," to be submitted to Physical Review Letters

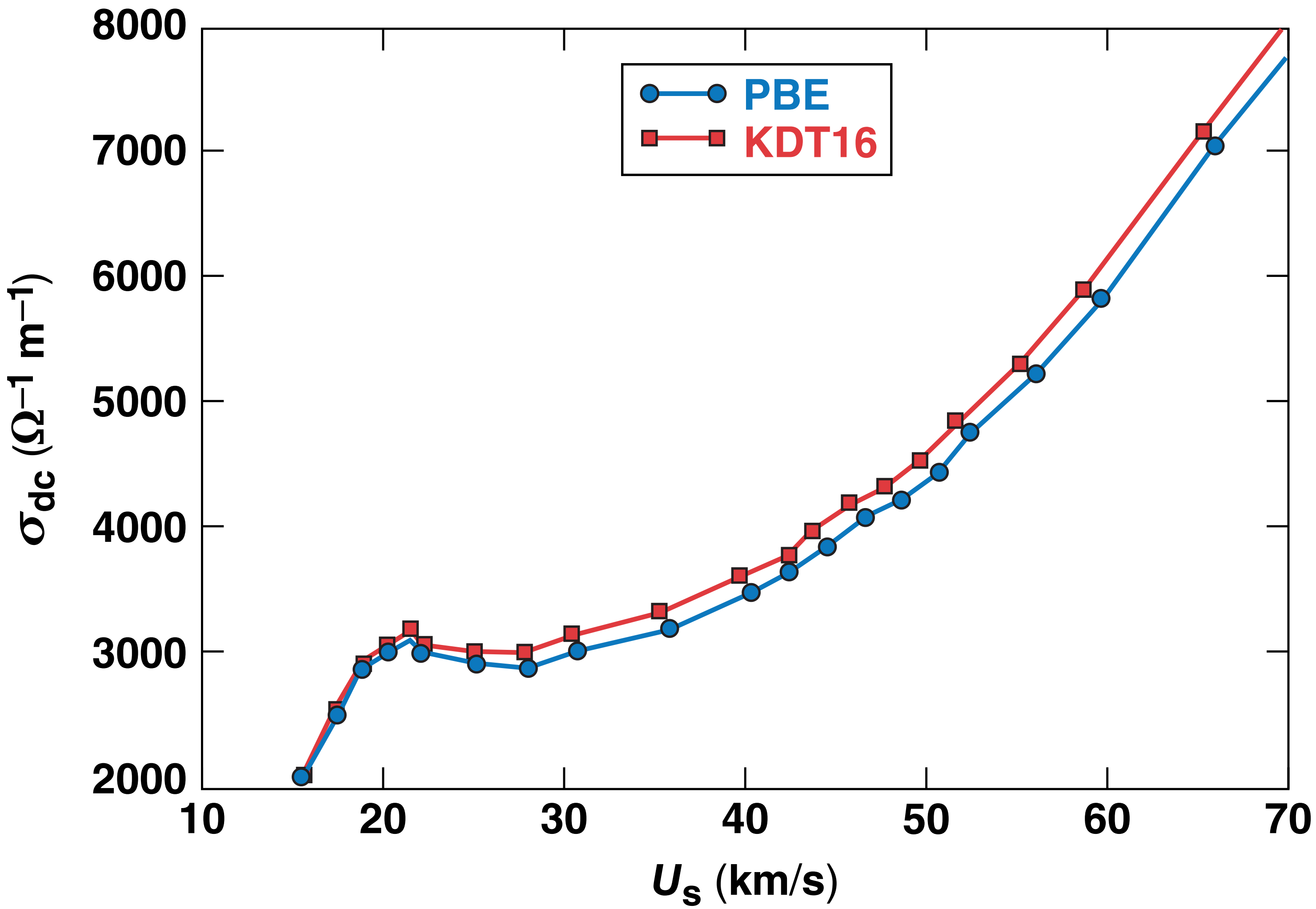
- Our calculations with KDT16 XC functional take into account the refraction index $n_0 = 1.16$ of liquid deuterium in its initial state $\rho_D = 0.172$ g/cm^3 and $T = 20$ K

M. Zaghoo, QI3.00001, this conference (invited);
P. M. Celliers *et al.*, Phys. Rev. Lett. 84, 5564 (2000);
S. X. Hu *et al.*, Phys. Plasmas 22, 056304 (2015).

TC14635

Results

Due to thermal XC effects the dc conductivity of D_2 along the Hugoniot is increased by about 5%



- dc conductivity is quickly increased between U_s = 15 and 20 km/s
- The system behaves as a *liquid metal* between U_s = 20 and 30 km/s: σ_{dc} decreases as T increases
- The system behaves as *plasma* for $U_s > 40$ km/s: σ_{dc} increases as T increases

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