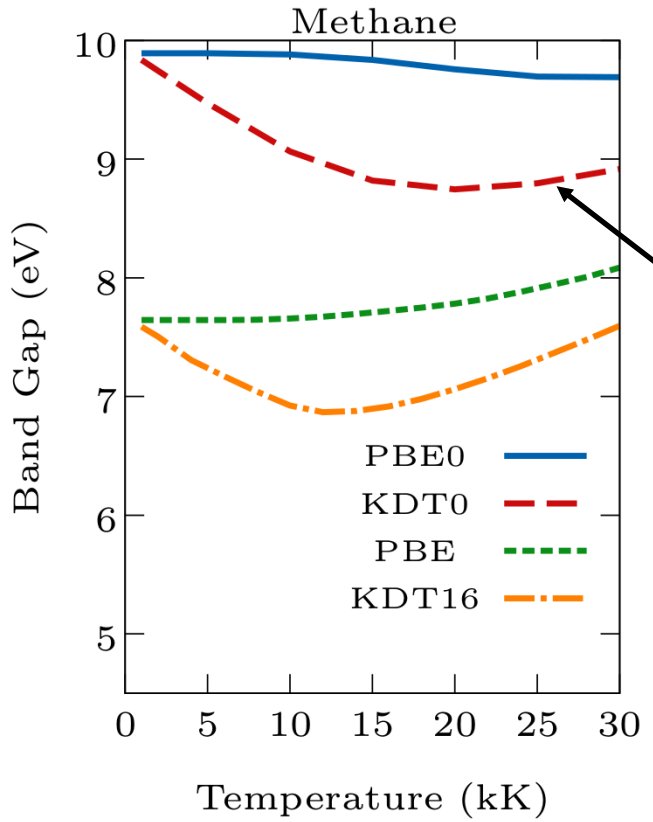
# Progress in Development of Thermal Hybrid Exchange-Correlation Density Functionals for Improving the Description of Warm Dense Matter

**Band gap as a function of electronic temperature**




**Improved description of the band gap at high temperatures.**


**D. Mihaylov**
**University of Rochester**
**Laboratory for Laser Energetics**



**APS Division of Plasma Physics**
**62nd Annual Meeting**
**9-13 November 2020**

# Collaborators

**V. V. Karasiev and S. X. Hu**

**University of Rochester**
**Laboratory for Laser Energetics**

**This material is based upon work supported by the Department of Energy National Nuclear Security Administration under Award Number DE-NA0003856, the University of Rochester, and the New York State Energy Research and Development Authority.**

**This material is based upon work supported by the U.S. National Science Foundation PHY Grant No. 1802964.**

Summary

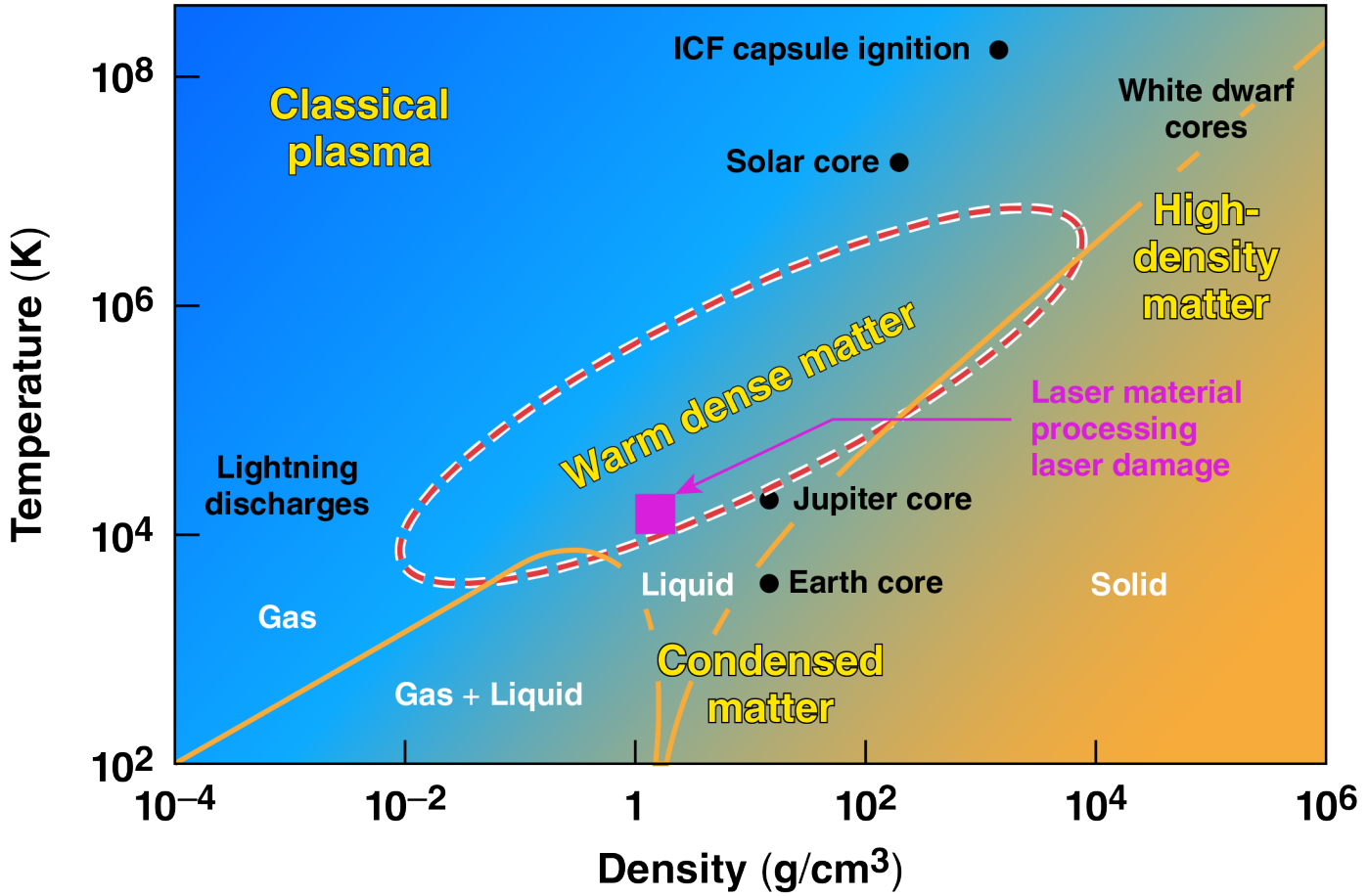
# We have developed an XC thermal density functional at the hybrid level of theory

- We have developed the KDT0 hybrid-level XC free-energy density functional, which is a finite-*T* version of the PBE0** functional.
- KDT0 reduces to PBE0** at *T* = 0 K, thus providing the high level of accuracy provided by hybrid functionals, especially in calculation of the electronic band gap.
- Preliminary calculations on various systems show that KDT0 provides an improved description of the band gap at high temperatures, evidenced by capturing the correct qualitative behavior as compared to finite-*T* GW***.

XC: exchange correlation
GGA: Generalized Gradient Approximation
PBE: Perdew-Burke-Ernzerhof

*V. V. Karasiev, J. W. Dufty, and S. B. Trickey, Phys. Rev. Lett. 120, 076401 (2018).
**J. P. Perdew, M. Ernzerhof, and K. Burke, J. Chem. Phys. 105, 9982 (1996).
***S. V. Faleev *et al.*, Phys. Rev. B 74, 033101 (2006).

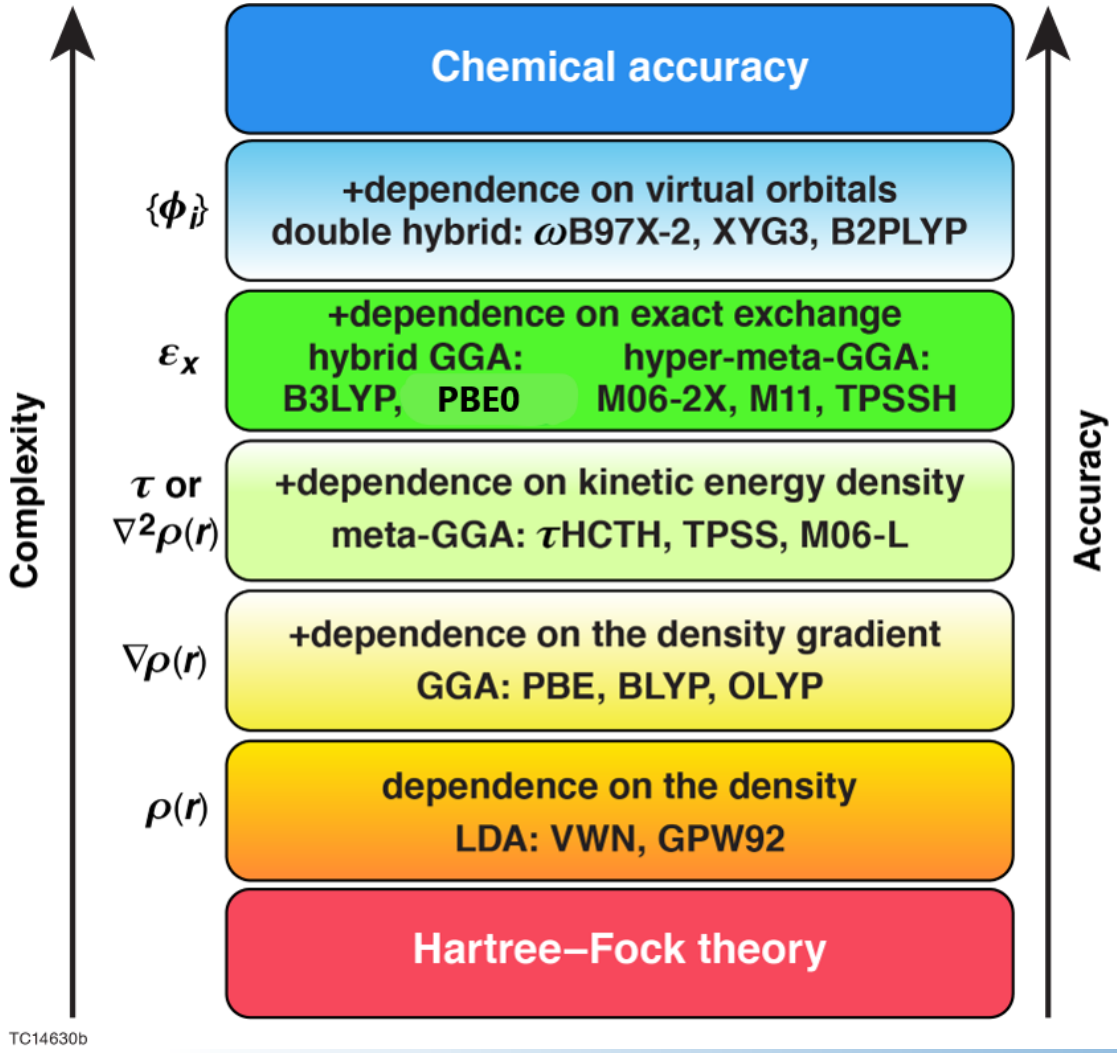
# Our goal is to develop more accurate XC free-energy density functionals for a better description of warm dense matter properties.




G11925a

ICF: inertial confinement fusion

# XC thermal functionals have previously been developed at the LDA and GGA levels. KDT0 is at the hybrid level of density functional approximation.




← KDT0† : finite-*T* extension to PBE0

← *T*-SCAN-L: finite-*T* extension to SCAN-L, the de-orbitalized version of SCAN

← Finite-temperature GGA (KDT16)*

← Finite-temperature LDA (KSDT)**, (corrKSDT)*

* V. V. Karasiev, J. W. Dufty, and S. B. Trickey, Phys. Rev. Lett. 120, 076401 (2018).
** V. V. Karasiev *et al.*, Phys. Rev. Lett. 112, 076403 (2014).
† D. Mihaylov, V. V. Karasiev, and S. X. Hu, Physical Review B 101 (24), 245141.

# KDT0 is a finite-*T* extension to PBE0 in a sense that it includes explicit *T* dependence in the GGA XC.

PBE0*: $$F_{\mathrm{xc}}^{\mathrm{PBE0}}[n,T] = E_{\mathrm{xc}}^{\mathrm{PBE}}[n] + \frac{1}{4}\left(F_x^{\mathrm{HF}}[n,T] - E_x^{\mathrm{PBE}}[n]\right)$$

KDT0**: $$F_{\mathrm{xc}}^{\mathrm{KDT0}}[n,T] = F_{\mathrm{xc}}^{\mathrm{KDT16}}[n,T] + \frac{1}{4}\left(F_x^{\mathrm{HF}}[n,T] - F_x^{\mathrm{KDT16}}[n,T]\right)$$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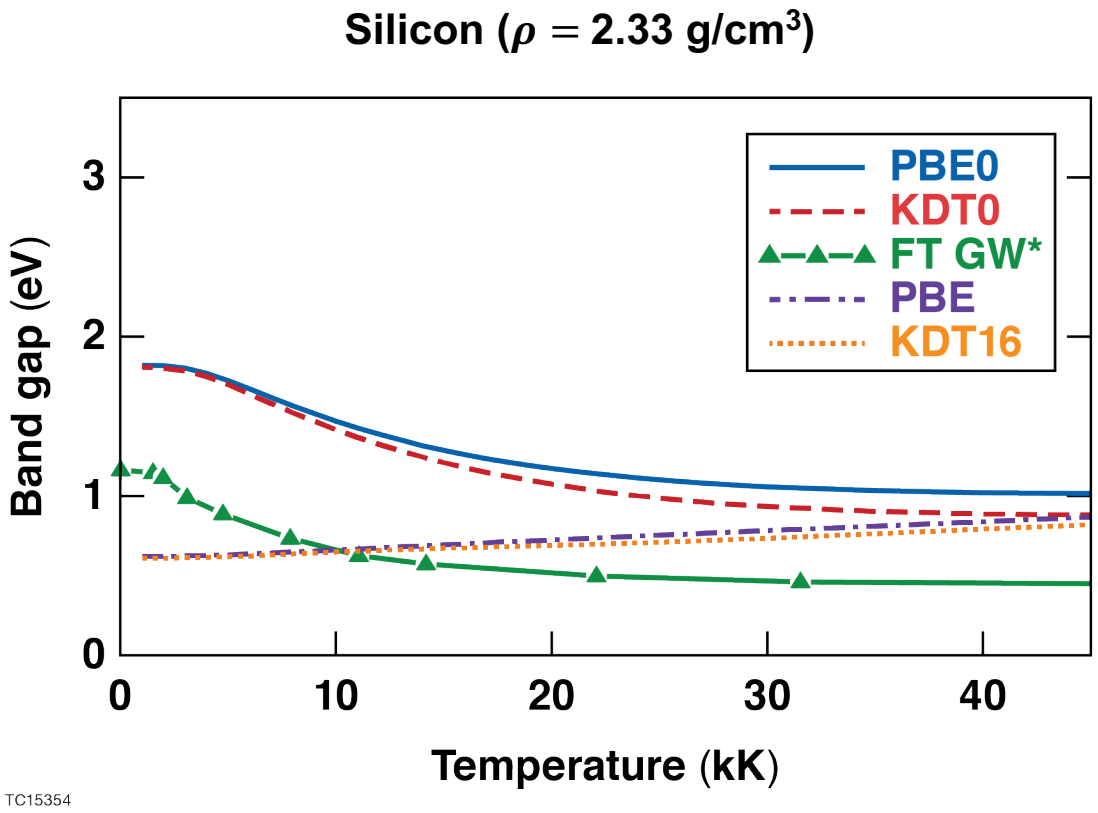
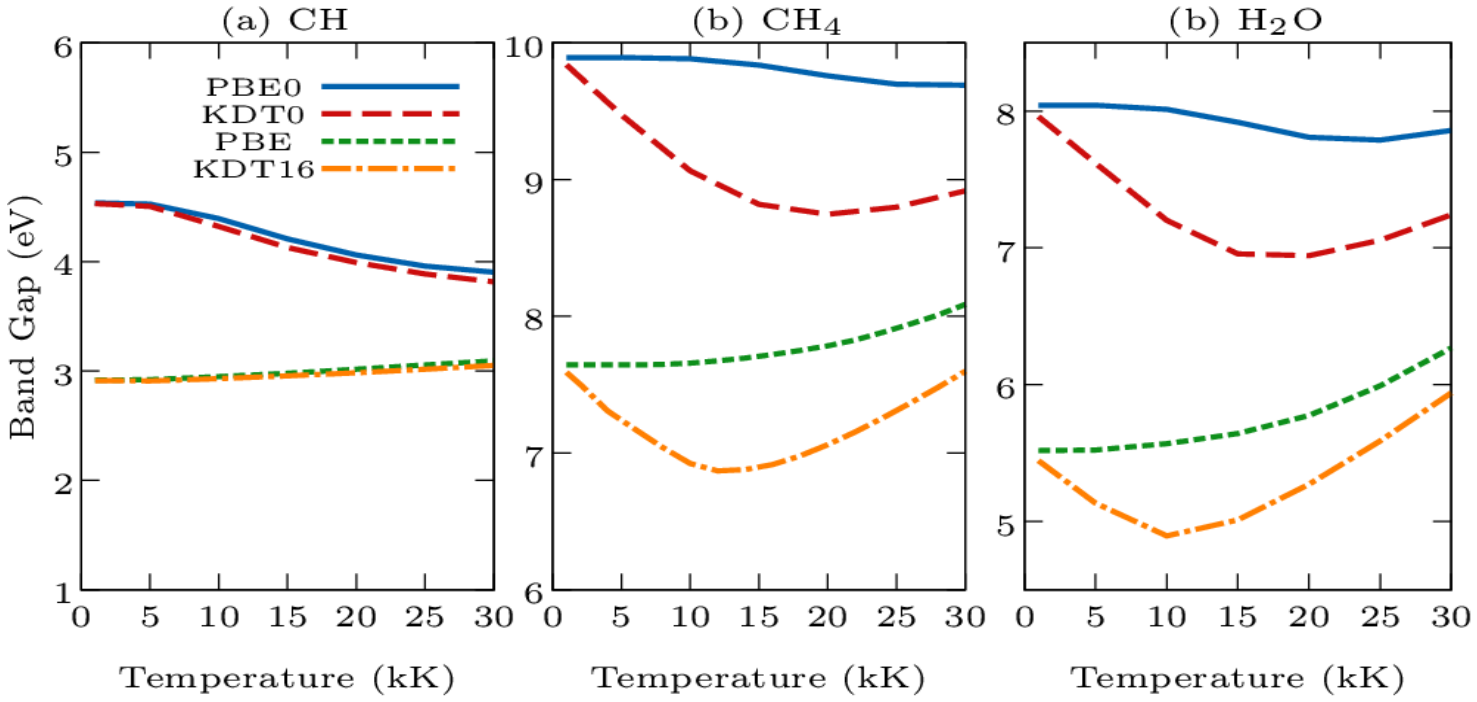
# Static calculations for band gap as a function of electronic *T* in Si show improved agreement with high-precision finite-*T GW* (FT *GW*) at high *T*




* S. V. Faleev *et al.*, Phys. Rev. B 74, 033101 (2006).

# Static calculations for band gap as a function of electronic *T* in CH, $CH_4$, $H_2O$ show that XC thermal effects in certain systems could be significant.

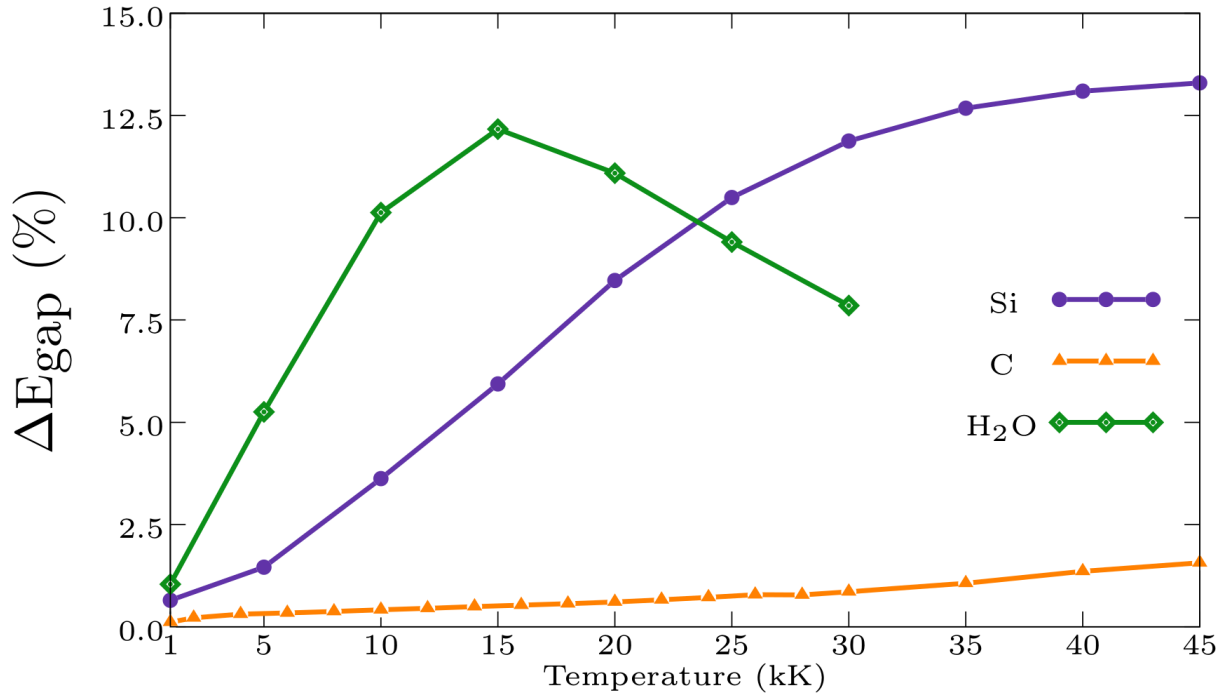



CH: $\rho = 1.06$ g/cm$^3$ $CH_4$: $\rho = 0.43$ g/cm$^3$ $H_2O$: $\rho = 0.96$ g/cm$^3$

**Strong localization around benzene ring means small XC and therefore, small XC thermal effects.**

# XC thermal effects could be strongly dependent on system and *T* range.

$$\Delta E_{gap} = \frac{E_{gap}^{PBE0} - E_{gap}^{KDT0}}{E_{gap}^{PBE0}} \times 100\%$$




**The relative corrections to bandgaps calculated with ground-state functionals vary strongly from system to system and peak at drastically different *T*.**

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# Static calculations of band structure at high *T* show that KDT0 predicts lower conduction band state energies resulting in a lower gap.