Finite-temperature Exchange-Correlation Functionals: Developments and Implications

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HiPerGator RESEARCH COMPUTING

Publications, preprints, local pseudopotentials, and codes at
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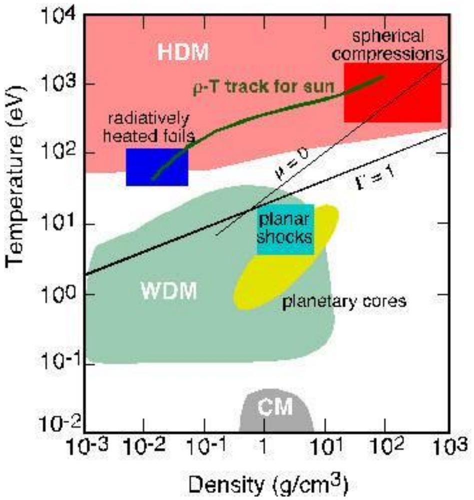
Warm Dense Matter (WDM)

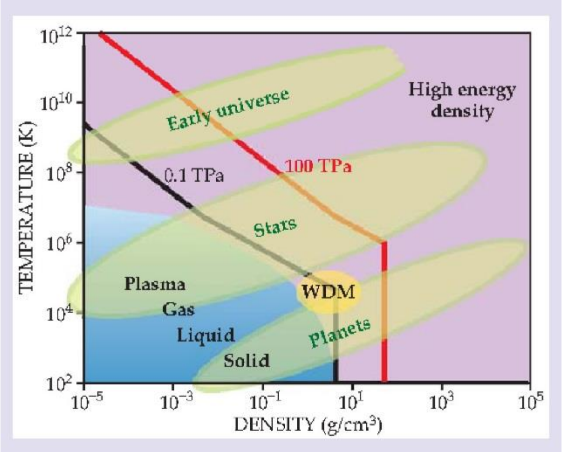
- **Challenging region *between* normal condensed matter and plasmas:**
  T < 100eV (≈1,100,000 K)
  Densities: from gas to ≈100 × equilibrium density
  (*i.e. P* → thousands of GPa).
- **Inertial confinement fusion pathway; interiors of giant planets & exo-planets, shock compression experiments**

- **Both the Coulomb coupling constant** $\Gamma = e^2 / r_s k_B \mathrm{T}$
  and the Fermi-degeneracy parameter $t = \theta := k_B \mathrm{T} / E_F$
  are in the intermediate region ⇒
  no perturbation expansion.

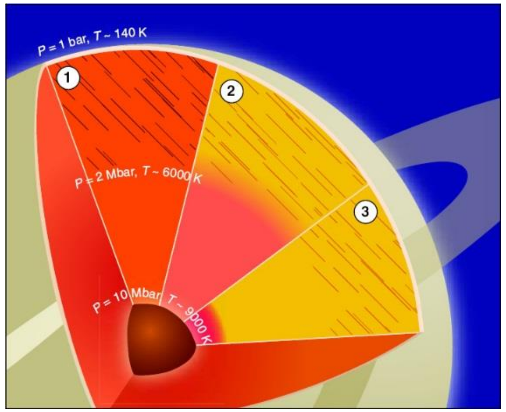
- **Methods developed for WDM regime also work well for high-energy density physics and dense plasmas.**

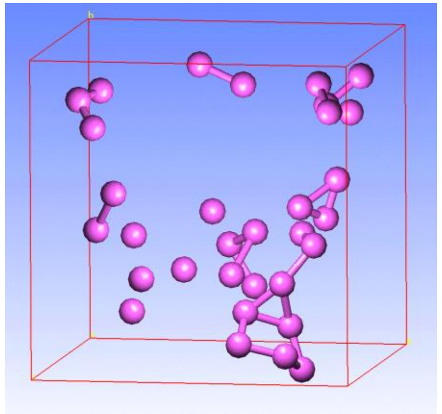
Warm Dense Matter (WDM)





Schematic temperature-density diagrams -
Left: Hydrogen [from R. Lee, LLNL**]**
Right: Aluminum [Phys. Today <u>63</u>(6), 28 (2010)**]**





<u>Left:</u> Interior of Saturn [J.J. Fortney, Science <u>305</u>, 1414 (2004)**]:**

(1) At an age of ≈ 1.5 billion years

(2) The current Saturn according to previous H-He phase diagram

(3) The current Saturn according to new evolutionary models

<u>Right:</u> ab initio MD snapshot of *<u>low</u>* *<u>density</u>* Al (0.20 g/cm^3) at T=5 kK. Shows complexity of WDM regime, formation of ions, molecules, and clusters.

Ab initio Molecular Dynamics (AIMD)

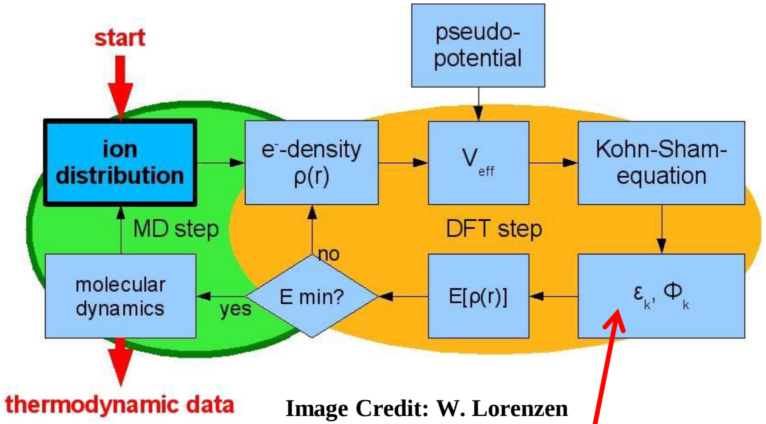


Image Credit: W. Lorenzen

Molecular dynamics

$$m_I \ddot{\mathbf{R}}_I = -\vec{\nabla}_I V(\mathbf{R}_1, \mathbf{R}_2, \cdots, \mathbf{R}_N)$$

Computational Load: the Born-Oppenheimer free- energy surface

$$V(\{\mathbf{R}\}) = F(\{\mathbf{R}\}) + E_{ion-ion}(\{\mathbf{R}\})$$

Current best practice uses Free Energy Density Functional Theory with explicit Kohn-Sham orbitals - cost scales as cube of the number of occupied levels.

$$\Omega[n] = F[n] + \int d\mathbf{r}\,(v_{ext}(\mathbf{r}) - \mu)\,n(\mathbf{r})$$ **Grand potential**

$$F[n] = F_s[n] + F_H[n] + F_{xc}[n]$$ **Universal free energy functional**

$F_H[n]$ = Hartree free energy , $F_s[n]$ = Non-interacting (KS) free energy,

$F_{xc}[n]$ = XC free energy

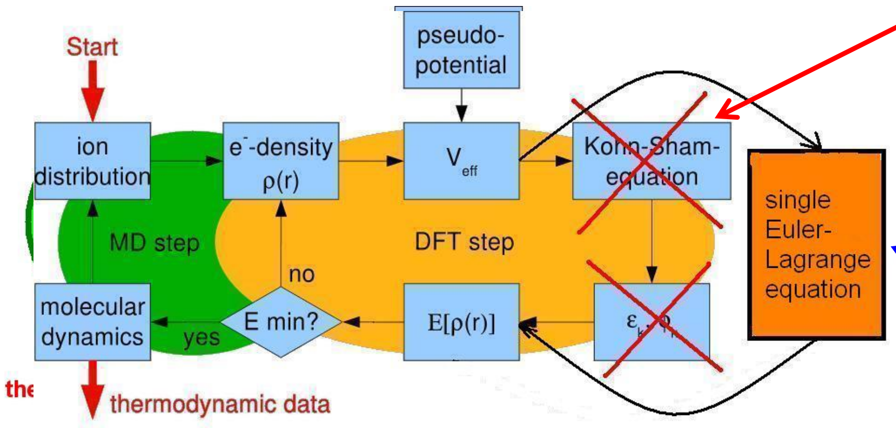
Kohn-Sham problem scales as N^3 at best = orbitals are the problem

“Ab Initio” is an old Latin phrase that means expensive” – J.W.D. Connolly (circa 1975)

$$\left\{-\tfrac{1}{2}\nabla^2_{r_1} + v_H(\mathbf{r}_1;\{\mathbf{R}\}) + v_{xc}(\mathbf{r}_1;\{\mathbf{R}\};\beta) + v_{ext}(\mathbf{r}_1;\{\mathbf{R}\})\right\}\varphi_j(\mathbf{r}_1;\{\mathbf{R}\}) = \varepsilon_j\,\varphi_j(\mathbf{r}_1;\{\mathbf{R}\})$$

$$n(\mathbf{r}_1;\{\mathbf{R}\}) = \sum_j f(\varepsilon_j;\beta)\left|\varphi_j(\mathbf{r}_1;\{\mathbf{R}\})\right|^2 \quad ; \quad v_{xc}[n] = \frac{\delta F_{xc}}{\delta n} \quad ; \quad \beta = 1/k_B T$$

Computational Challenge of ab-initio MD



KS computational cost scales as cube of the number of occupied levels. Scaling worsens with increasing T (non-integer occupation).

Orbital-free Free Energy DFT – *No* explicit KS orbitals . Scales with system size.

Mermin, Hohenberg-Kohn DFT

$$\Omega\,[n] = F[n] + \int d\mathbf{r}\ (v_{\rm ext}(\mathbf{r}) - \mu)\, n(\mathbf{r})$$ Grand potential

$$F[n] = F_{\rm s}[n] + F_{\rm H}[n] + F_{\rm xc}[n]$$ Universal free energy functional

$F_{\rm H}[n]$ = Hartree free energy , $F_{\rm s}[n]$ = Non-interacting (KS) free energy,

$F_{\rm xc}[n]$ = eXchange-Correlation (XC) free energy

KS equation

$$\left\{ -\tfrac{1}{2}\nabla^2_{r_1} + v_{\rm H}\left(\mathbf{r}_1;\{\mathbf{R}\}\right) + v_{\rm xc}\left(\mathbf{r}_1;\{\mathbf{R}\};\beta\right) + v_{\rm ext}\left(\mathbf{r}_1;\{\mathbf{R}\}\right)\right\}\varphi_j\left(\mathbf{r}_1;\{\mathbf{R}\}\right) = \varepsilon_j\,\varphi_j\left(\mathbf{r}_1;\{\mathbf{R}\}\right)$$

$$n\left(\mathbf{r}_1;\{\mathbf{R}\}\right) = \sum_j f(\varepsilon_j;\beta)\left|\varphi_j\left(\mathbf{r}_1;\{\mathbf{R}\}\right)\right|^2 \quad ; \quad v_{\rm xc}[n] = \frac{\delta F_{\rm xc}}{\delta n}$$

Electrons Nuclei

Original Image: W. Lorenzen

Finite-Temperature OF-DFT Basics

OF-DFT requirements: reliable, orbital-free approximations for

$F_s[\{\varphi\}] = T_s[\{\varphi\}] - \mathrm{T} S_s[\{\varphi\}]$ ← **Non-interacting (Kohn-Sham) free energy**

$F_{xc}[n] = (T[n] - T_s[n]) - \mathrm{T}(S[n] - S_s[n]) + (U_{ee}[n] - F_H[n])$ ← **Exchange-Correlation free energy; REQUIRED for BOTH standard KS and OF-DFT**

$\frac{\delta F_s[n]}{\delta n(r)} + v_s([n];r) = \mu, \quad \text{where} \quad v_s = v_{ext} + v_H + v_{xc}$ ← **Single Euler equation solver**

Partial history of finite-T functional development:

- **(1949) Feynman, Metropolis: finite-T Thomas-Fermi:** $F_s^{TF}[n]$
- **(1979) Perrot: Gradient corrections to TF:** $F_s^{SGA}[n]$
- **(2012) Karasiev, Sjostrom, Trickey: Finite-T GGA formalism:** $F_s^{GGA}[n]$ Phys. Rev. B **86**, 115101 (2012)
- **(2013) Karasiev, Chakraborty, et al.: Non-empirical GGA:** $F_s^{GGA}[n]$ Phys.Rev. B **88**, 161108(R) (2013)

- **(1979-2000) finite-T XC based on different many-body models:** $F_{xc}[n]$
- **(2014) Karasiev, Sjostrom, Dufty, Trickey: finite-T LDA XC** $F_{xc}^{LDA}[n]$ Phys. Rev. Lett. **112**, 076403 (2014)
- **(2017) Karasiev, Dufty, Trickey: finite-T GGA XC** $F_{xc}^{GGA}[n]$ Phys. Rev. Lett. (submitted) (2017)

Results, then Methods

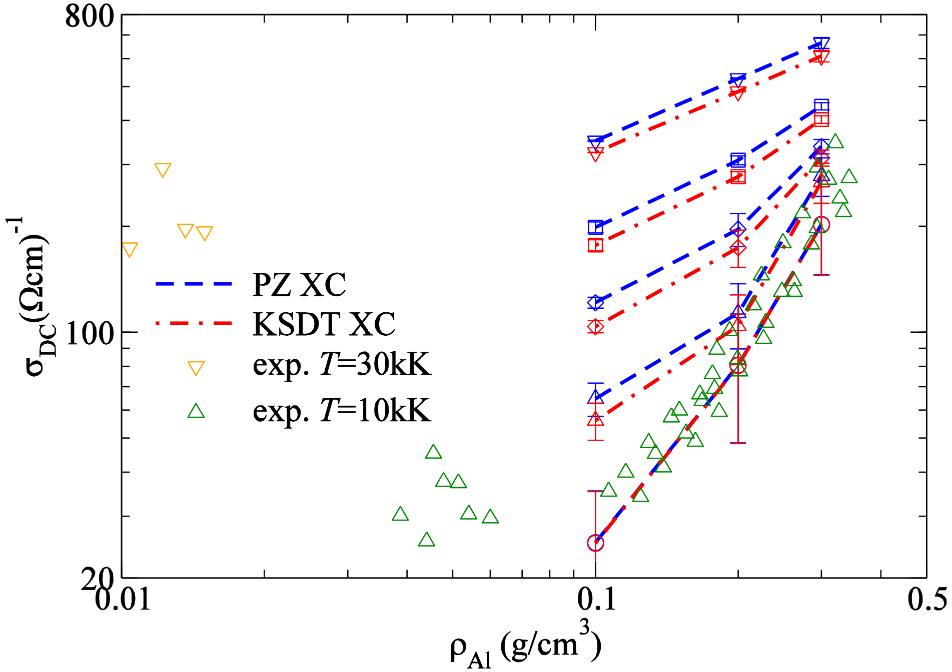
RESULTS

1. DC conductivity of low density Al; ground-state LDA XC vs. genuine F_{xc}
2. Band-structure effects of genuine LDA F_{xc} in Al
3. Hugoniot effects of genuine F_{xc} in Deuterium
4. Finite-T Generalized Gradient Approximation (GGA) F_{xc} effects on calculated Pressures
5. Liquid-vapor phase transition in Al

METHODS

1. Tunable F_s functionals to treat regions otherwise inaccessible (at present) to OF-DFT
2. Finite-T LDA F_{xc} and calibration to QMC data
3. Finite-T GGA F_{xc} construction
4. New Kubo-Greenwood code for Quantum Espresso

Optical Conductivity & LDA F_{xc} thermal effects

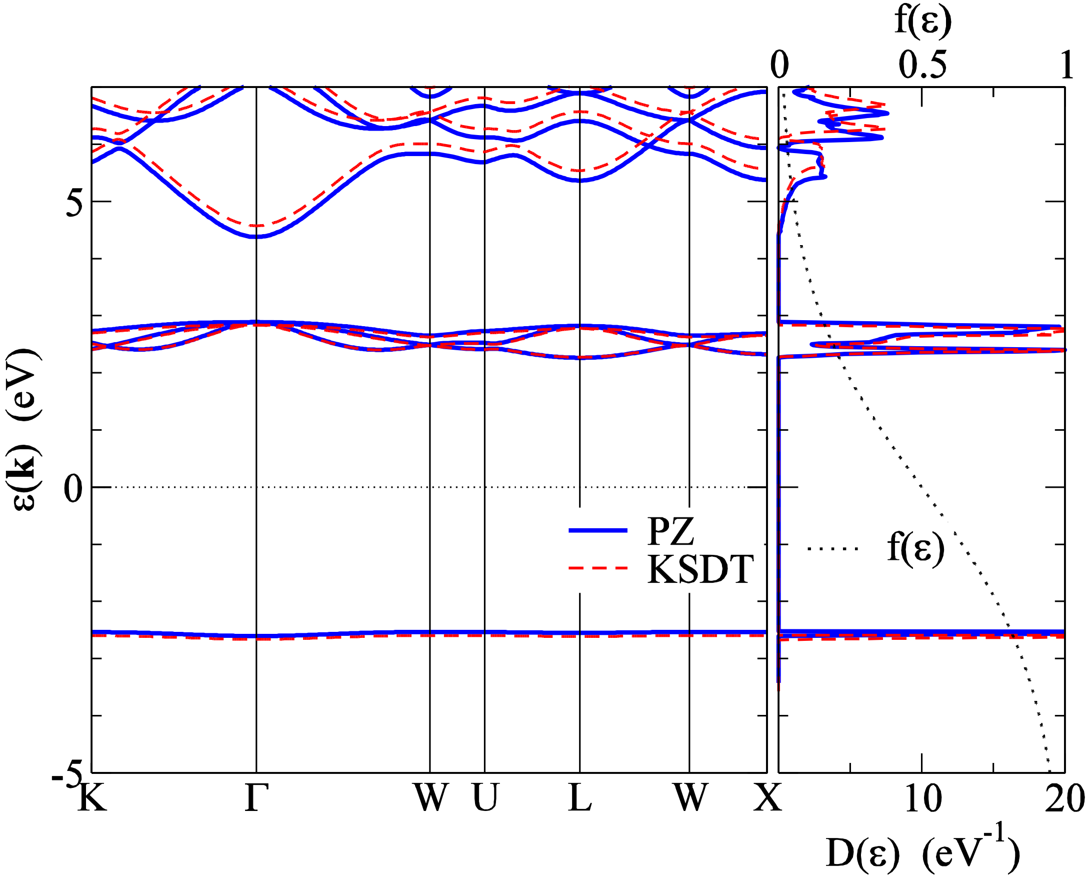


Aluminum DC conductivity as a function of material density from calculations with T-dependent KSDT (dot-dashed) and ground state PZ (dashed) XC functionals for five isotherms: 5, 10, 15, 20, and 30 kK (bottom to top).

Use of explicitly T-dependent LDA XC lowers the DC conductivity of low-density Al, yielding improved agreement with experiment.

[Karasiev, Calderín, Trickey, Phys. Rev. E 93, 063201 (2016)]

LDA F_{xc} thermal effects, fcc Al band structure

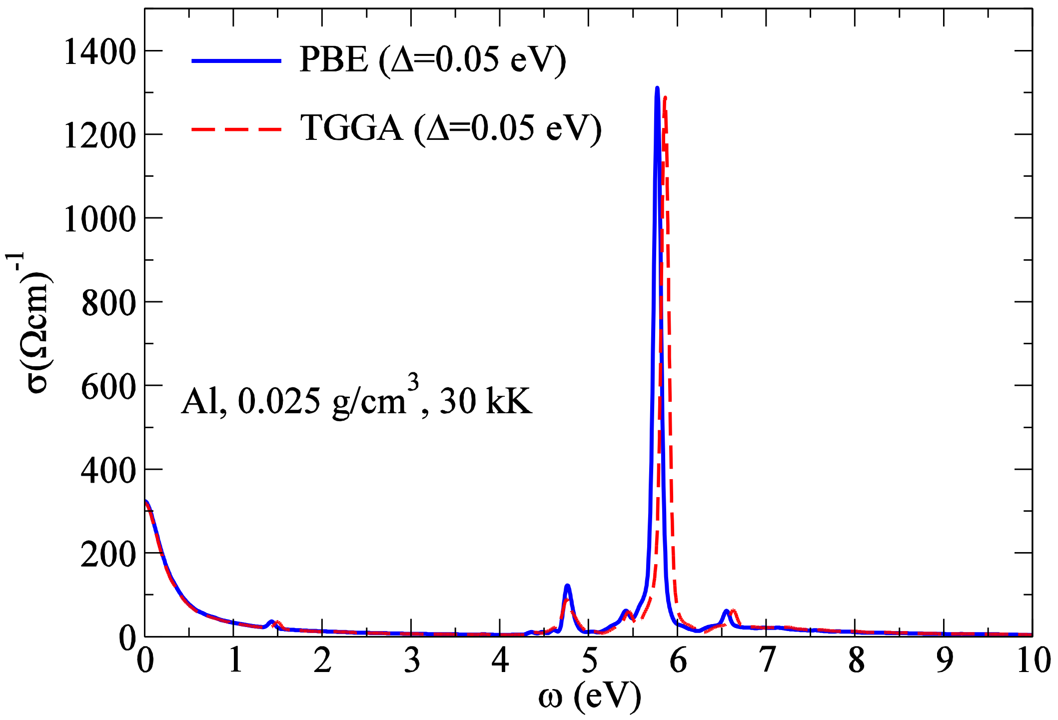


KS band structure for fcc Al at ρ=0.2 g/cm³ and T=20 kK calculated with ground state (PZ, blue) and finite-*T* (KSDT, red) XC functionals.

[Karasiev, Calderín, Trickey, Phys. Rev. E 93, 063201 (2016)]

LDA XC thermal effects increase the inter-band separation
⇒ Fermi-Dirac occupations above the Fermi level are decreasd
⇒ the DC conductivity is lowered

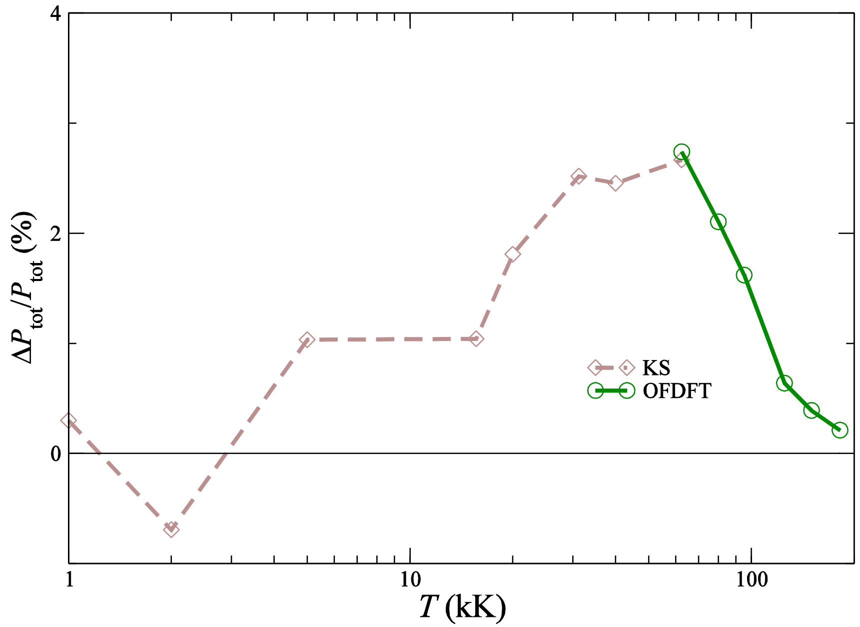
GGA F_{xc} optical conductivity effects in low-density Al



Optical conductivity of low-density Al (0.025 g/cm³) at T=30,000K with new KDT GGA F_{xc}

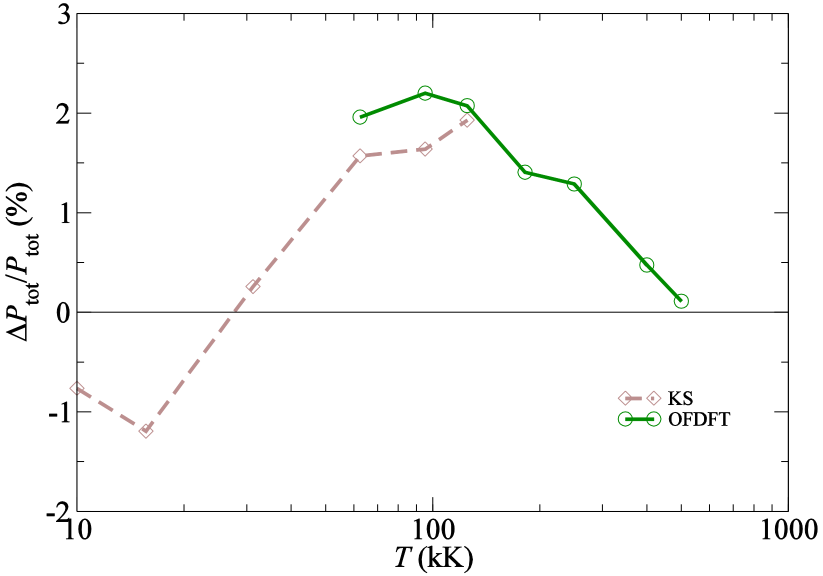
- **Drude-like behavior for small-ω**
- **Blue shift (sharp peak at ≈ 5.7 eV) due to XC thermal effects at the GGA level of refinement (explained by increased gap in calculations with thermal XC)**

Deuterium Eq. of State ; OF-DFT-AIMD
(VT84F F_s, KSDT TLDA F_{xc})



Deuterium <u>total</u> pressure (includes ionic KE contribution) percentage error as a function of T

$$\Delta P = \left(P_{tot}^{LDA} - P_{tot}^{TLDA} \right) / \, P_{tot}^{TLDA}$$



Above: $\rho_D = 0.20$ g/cm^3
Right : $\rho_D = 1.964$ g/cm^3

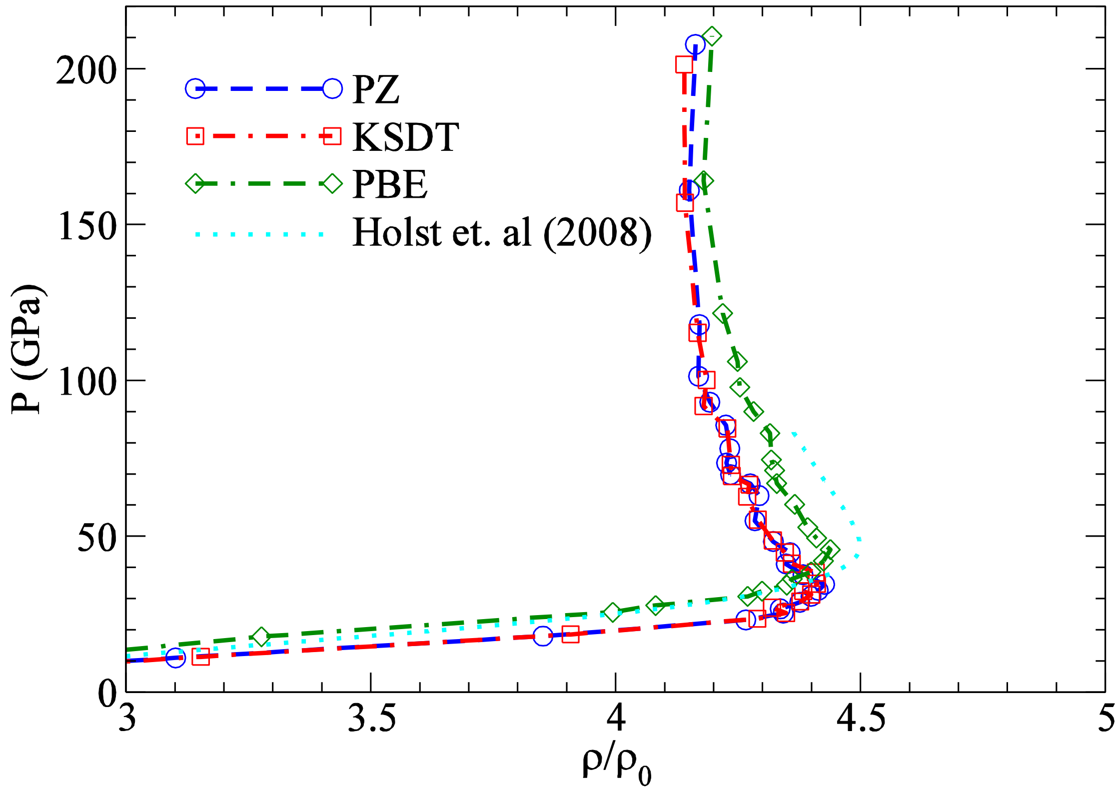
Karasiev, Calderín, Trickey,
Phys. Rev. E <u>93</u>, 063201 (2016)

UF UNIVERSITY of FLORIDA

Hugoniots seem comparatively insensitive to F_{xc}

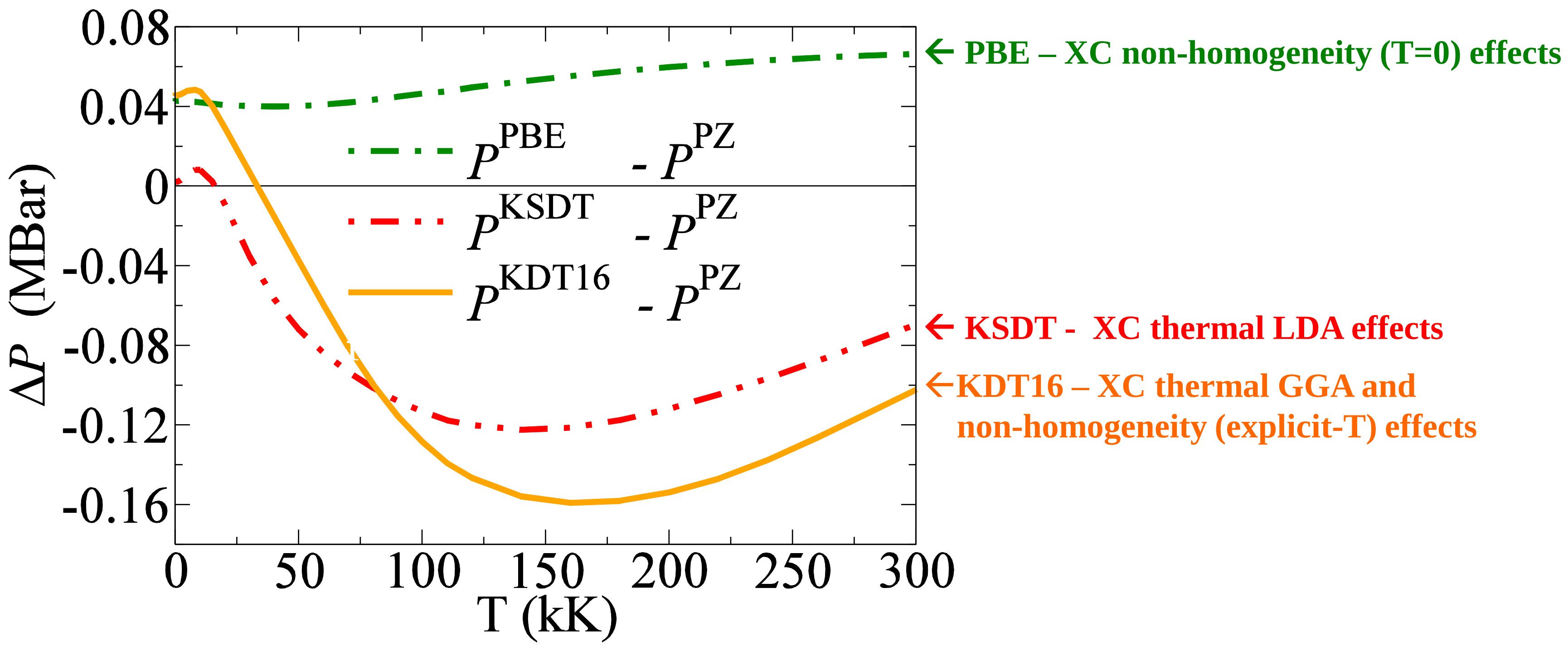
Hydrogen principal Hugoniot; Initial density ρ_0=0.0855 g/cm^3

$$E - E_0 = \frac{1}{2}(P + P_0)\left(\frac{1}{\rho} - \frac{1}{\rho_0}\right)$$



Two issues: (1) Large error bars on most experimental data (not shown). (2) Cancellation between internal energy difference and PV work difference terms in Rankine–Hugoniot equation. [Karasiev, Calderín, Trickey, Phys. Rev. E 93, 063201 (2016)]

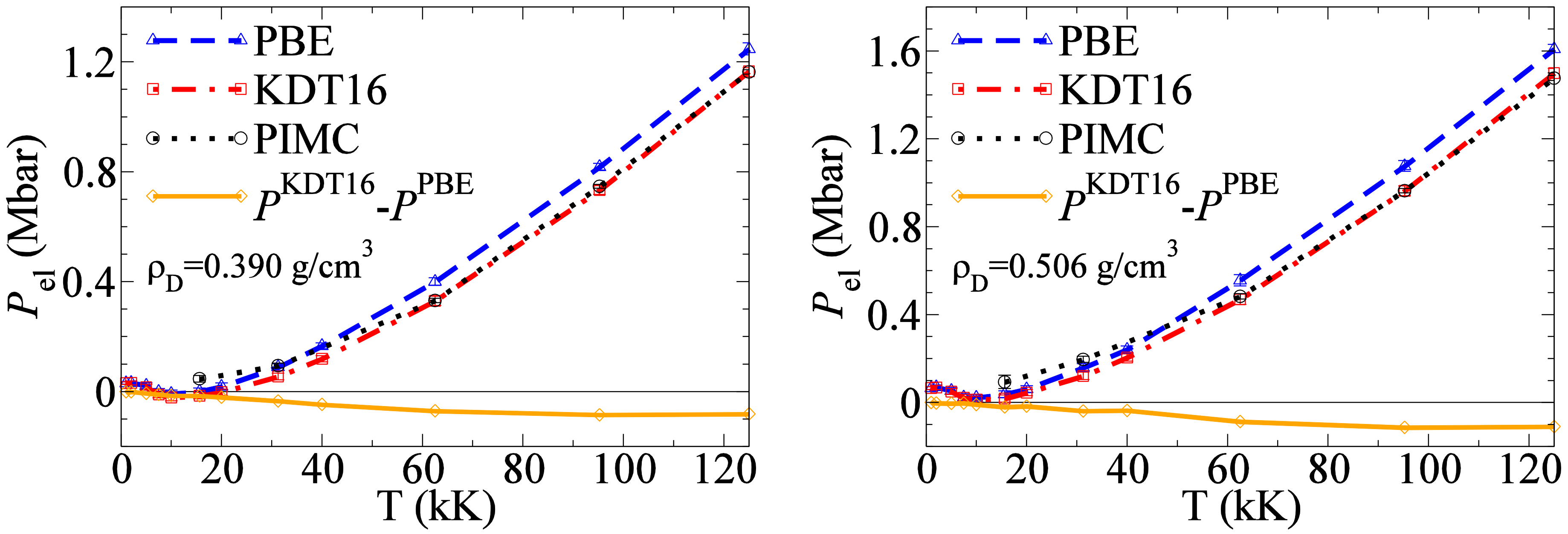
Thermal GGA XC results on fcc-Al model system



Electronic pressure differences vs. T for the new finite-T GGA ("KSDT16"), KSDT LDA, and ground-state PBE XC functionals, all referenced to PZ ground-state LDA values. Static lattice fcc Aluminum at 3.0 g/cm^3.

Karasiev, Dufty, & Trickey, Phys. Rev. Lett. (submitted) arXiv 1612.06266

Thermal GGA XC results on Deuterium EOS



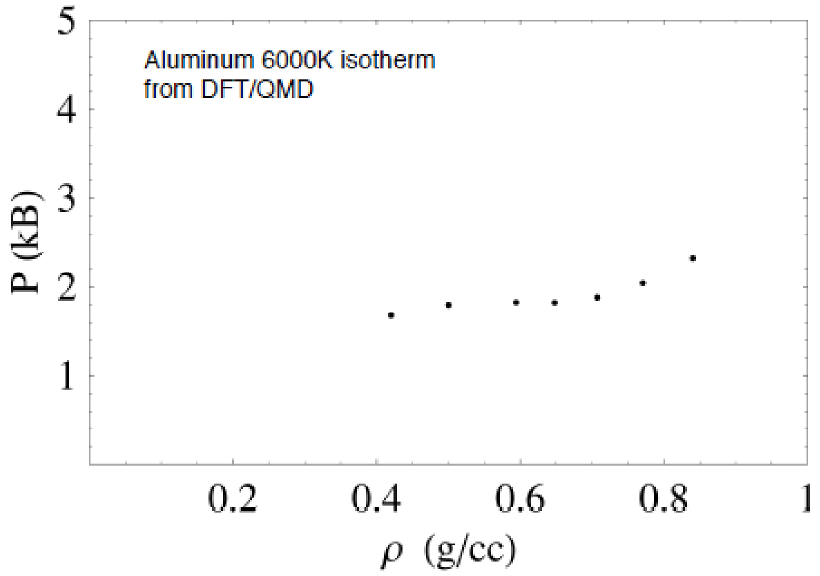
Deuterium electronic pressure vs. T for the finite-T GGA ("KDT16") and ground-state PBE XC functionals, as well as PIMC reference results.

AIMD super-cell simulations, Γ-point only, for 128 atoms (8500 steps, T ≤ 40 kK) or for 64 atoms (4500 steps, *T* ≥ 62 kK

Karasiev, Dufty, & Trickey, Phys. Rev. Lett. (submitted) arXiv 1612.06266

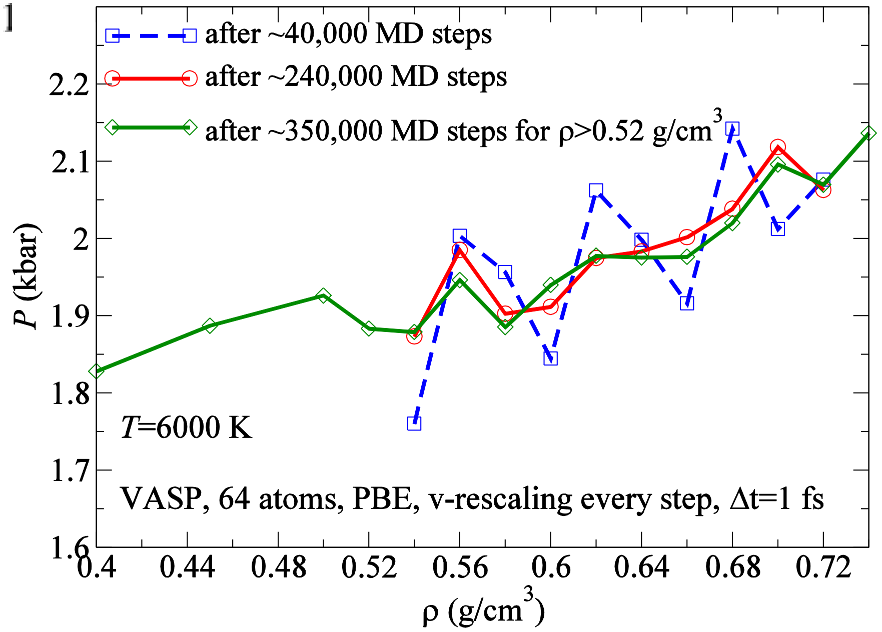
PIMC results: S.X. Hu, B. Militzer, V.N. Goncharov, and S. Skupsky, Phys. Rev. B 84 224109 (2011).

Low-density System Challenge: Liquid-vapor transition in Al

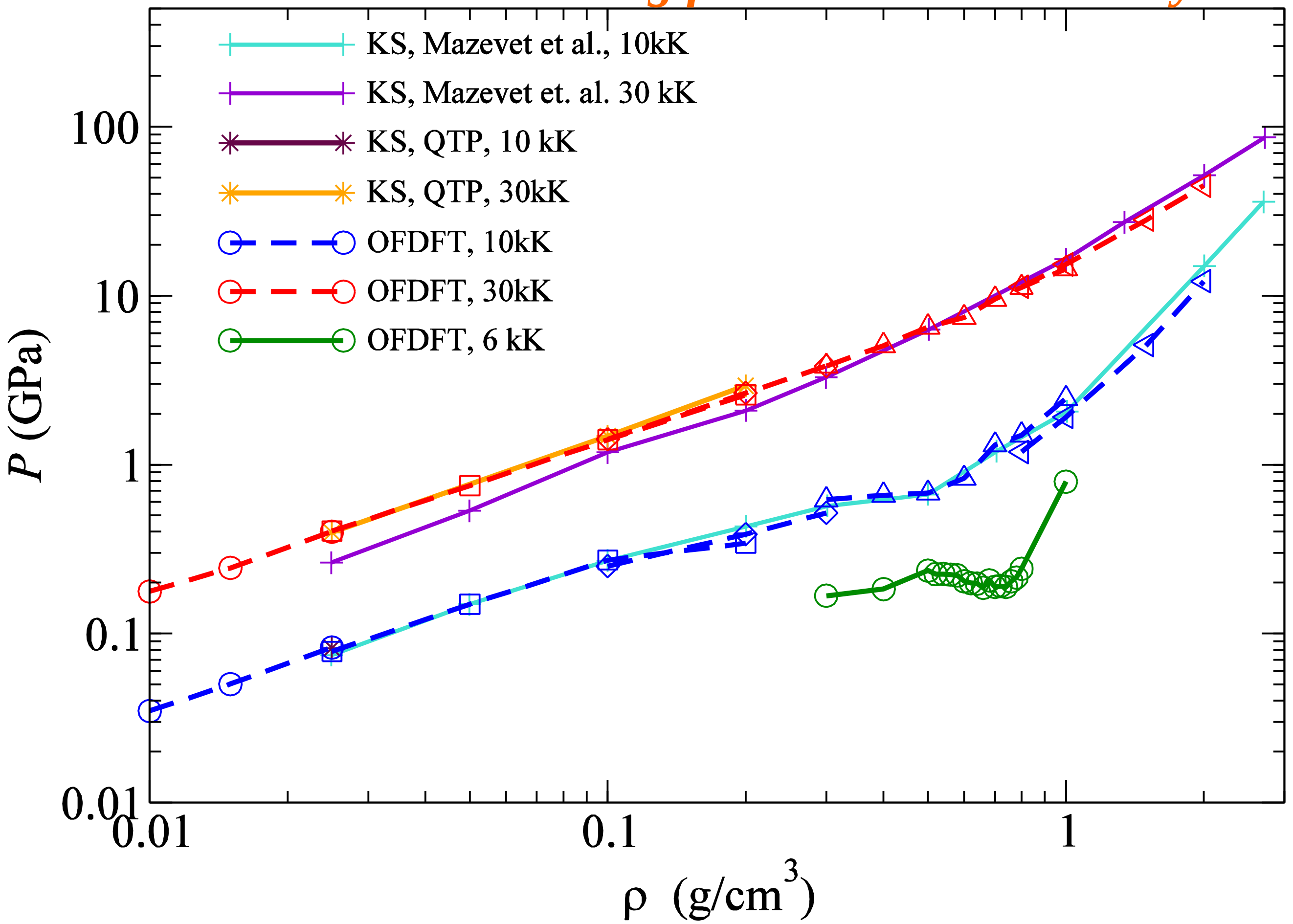


M.P. Desjarlais [Atom. Proc. Plasmas CP-1161, 32 (2009)] **"very tedious" KS-MD calculations**

Low-density Al EOS at T=6 kK; pure KS AIMD.



Tunable OF Non-interacting functional: Low density Al



Low-density Al EOS at T=10 kK and 30 kK; tunable OF-DFT functional compared to KS. Tuned at T_m = 8kK & three ρ_m (1.0, 1.5, 2.0 g/cm^3)

Number of atoms in simulation cell: 8 → 108.

10 kK. 30 kK OF-DFT ≈ 12,000 steps
6 kK ≈ 6,000 steps

Liquid-vapor critical point -

- **Does not model two phases (phase separation or co-existence)**
- **Searches for the diverging isothermal compressibility** $\kappa = \left(n \left. \frac{\partial P}{\partial n} \right|_T \right)^{-1}$
- **Requires very long MD due to slow convergence of averages over MD steps.**

Methods: Low-density System Challenge & Tunable Functionals

Challenge to OF-DFT bypass of Kohn-Sham bottleneck: all known orbital-free non-interacting functionals (including ours) are grossly inaccurate for low density Al.

Pragmatic response: Develop tunable OF-DFT functionals to work with particular system at relevant thermodynamic conditions.

Tuning: Adopt a functional form with parameters, set most of them to match exact conditions, set the rest to match reference Kohn-Sham calculations at some matching temperatures T_m and material densities ρ_m .

Build transferability to higher $T > T_m$ by incorporating exact high-T limit by construction.

Orbital-free tunable non-interacting functional

1) *Zero-T kinetic energy GGA enhancement factor*

$$F_t(s) = \frac{1 + a_2 s^2 + a_4 s^4 + a_5 s^5 + a_6 s^6}{1 + b_2 s^2 + b_4 s^4} \qquad s(n, \nabla n) = \frac{|\nabla n|}{2(3\pi^2)^{1/3} n^{4/3}}$$

2) *Apply the finite-T GGA framework* [*Karasiev, Sjostrom, Trickey, PRB 86, 115101 (2012)*] **:**

$$F_\tau(s_\tau) = F_t(s_\tau); \quad F_\sigma(s_\sigma) \approx 2 - F_t(s_\sigma)$$

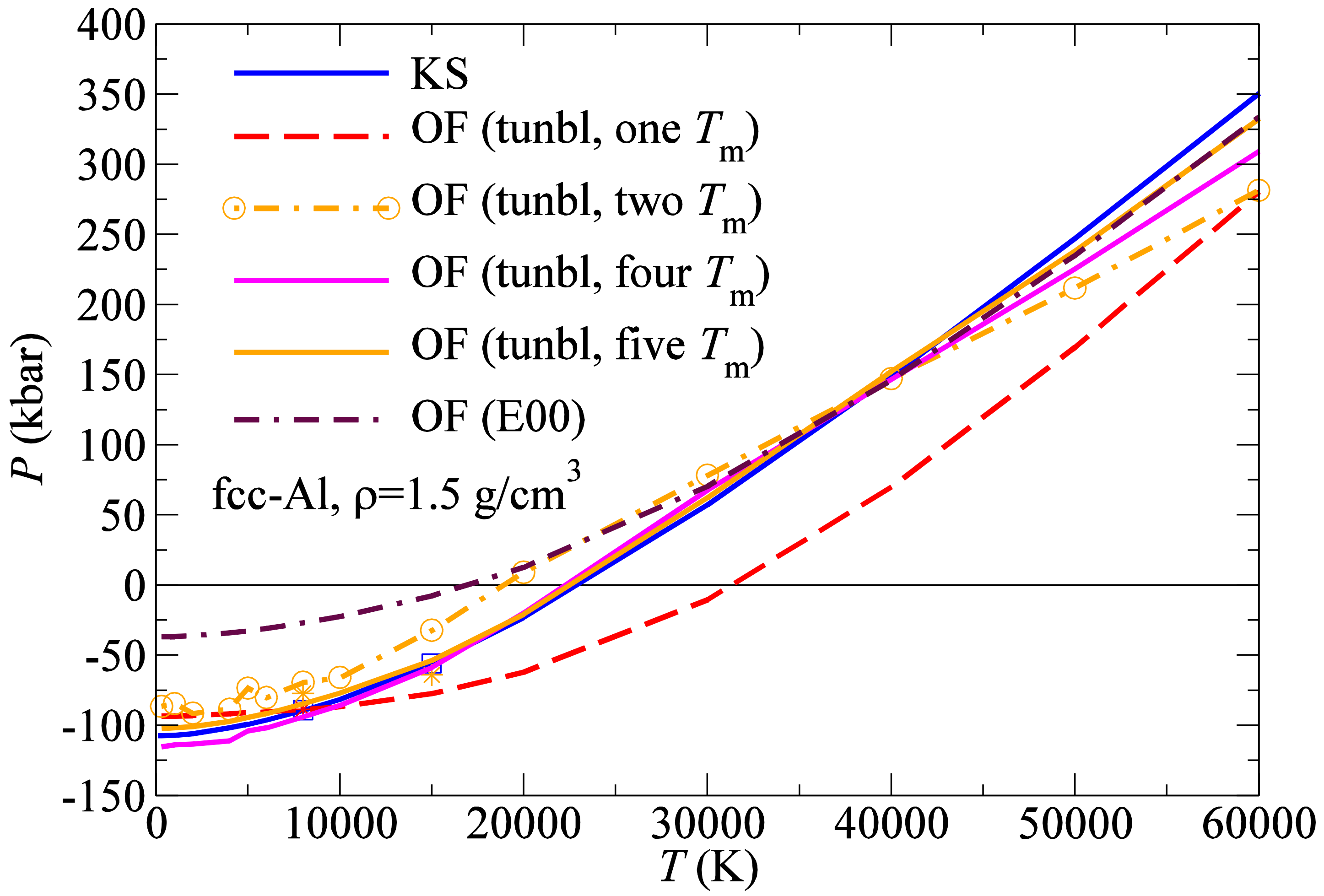
$$F_{\mathrm{s}}^{\mathrm{GGA}}[n, \mathrm{T}] = \int d^3 r \tau_0^{\mathrm{TF}}(n) \{\xi(t) F_\tau(s_\tau) - \varsigma(t) F_\sigma(s_\sigma)\}$$

$$s_\tau(n, \nabla n, \mathrm{T}) := s(n, \nabla n) \sqrt{\frac{\tilde{h}(t) - t(\mathrm{d}\tilde{h}/\mathrm{d}t)}{\xi(t)}} \qquad s_\sigma(n, \nabla n, \mathrm{T}) := s(n, \nabla n) \sqrt{\frac{t(\mathrm{d}\tilde{h}/\mathrm{d}t)}{\zeta(t)}} \qquad t = \mathrm{T}/\mathrm{T}_F$$

3) *Most parameters determined from constraints; leave a few free.*

4) *Tune free parameters to match the KS static lattice hot curve (pressure vs. volume), not KS AIMD, at T=$\mathrm{T_m}$ and relevant bulk density regime.*

Tuning – At how many Temperatures?



T_m sets = {8 kK}; {8, 15 kK}; {8, 15, 30, 60 kK}; {8, 15, 30, 40, 60 kK}

ρ_m set = {1.0, 1.5, 2.0} g/cm^3

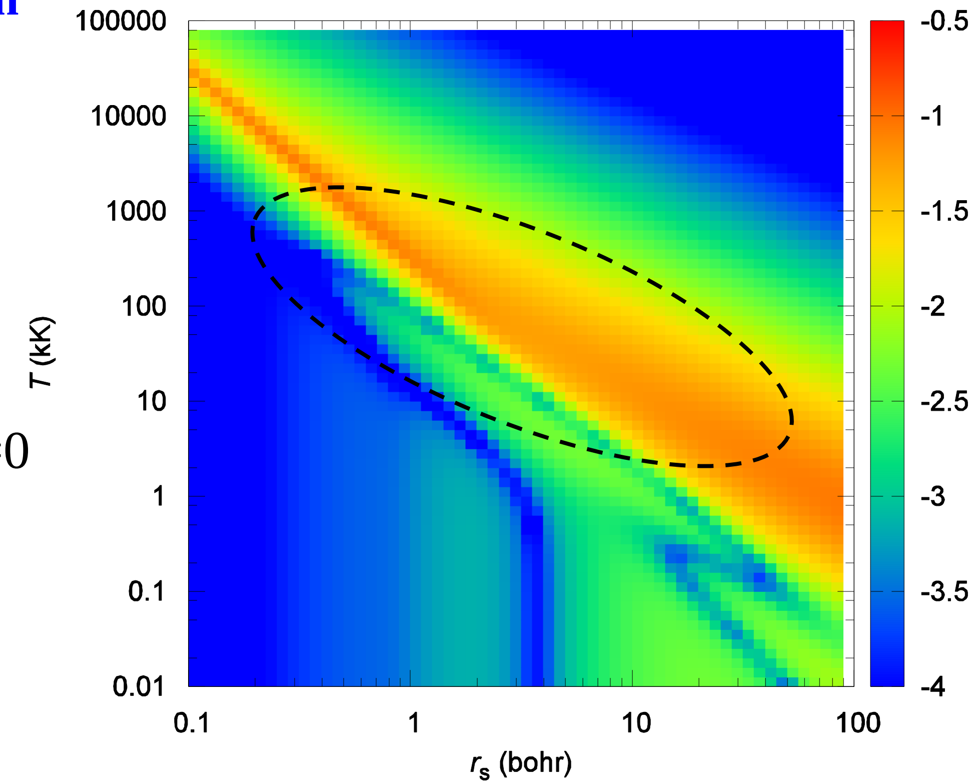
XC thermal effects for the homogeneous electron gas (HEG)

XC thermal effects are significant in WDM regime:

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

f_{xc} = XC free energy per particle
ε_{xc}= XC energy per particle at T=0
f_s = non-interacting free energy

Rough WDM region in ellipse.



Common practice is to use a T=0 XC functional:

$$F_{xc}[n, T] \approx E_{xc}[n(T)]$$

May not be accurate in WDM regime

Local spin density approximation (LSDA) F_{xc} [n]

$$F_{xc}[n(T),T] \approx \int d\mathbf{r}\, n(\mathbf{r},T)\, f_{xc}^{HEG}(n(\mathbf{r},T),T)$$

- **Note: no gradient or higher derivative dependence**
- **Determine f_{xc}^{HEG} from fit to restricted path integral Monte Carlo (RPIMC) data [Brown et al., Phys. Rev. Lett. 110, 146405 (2013)]**
- **Fit must extrapolate smoothly to correct large-T, T=0, and small r_s limits**
- **Fit must be augmented with T-dependent interpolation to intermediate spin polarization**
- **Procedural issue: Four formally equivalent thermodynamic relationships between XC internal energy density ε_{xc} and XC free energy density f_{xc} are not computationally equivalent. Detailed study led to use of**

"Fit A" -- $$f_{xc}(r_s,t) - t\frac{\partial f_{xc}(r_s,t)}{\partial t}\bigg|_{r_s} = \varepsilon_{xc}(r_s,t).$$

"Fit B" if you have only the potential energy -- $$2f_{xc}(r_s,t) + r_s\frac{\partial f_{xc}(r_s,t)}{\partial r_s}\bigg|_t = u_{ee}(r_s,t).$$

Karasiev, Sjostrom, Dufty, & Trickey; Phys. Rev. Lett. 112, 076403 (2014)

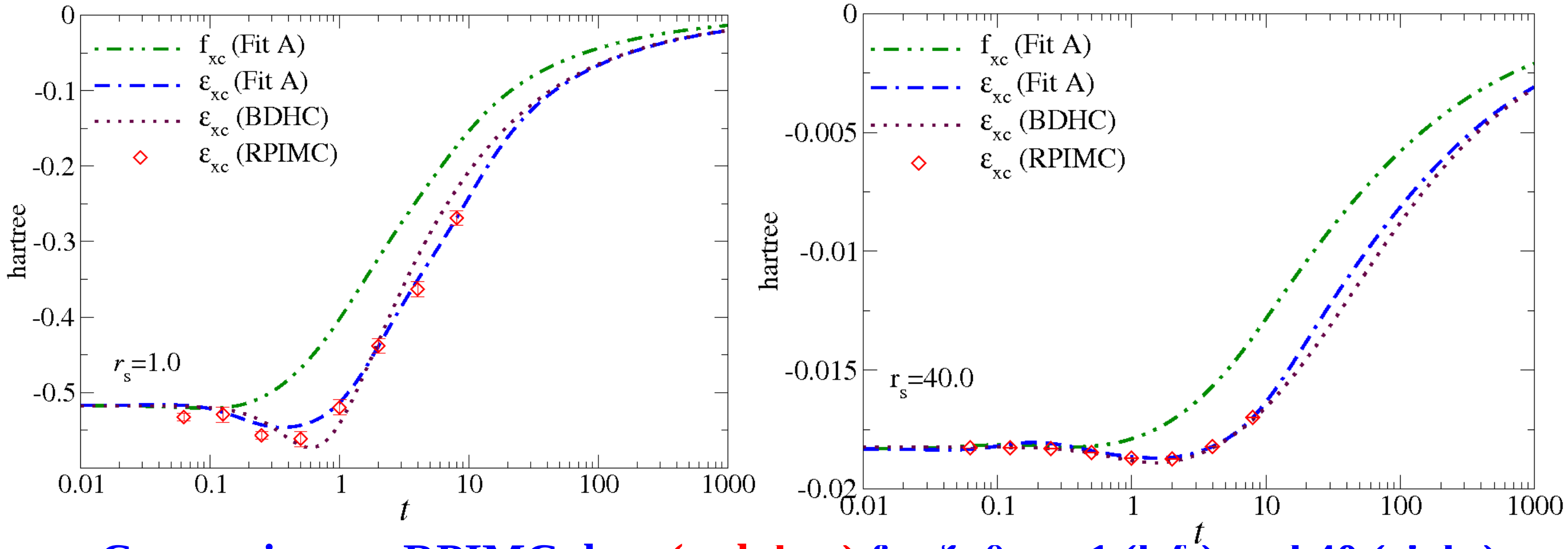
LSDA F_{xc} [n]

Fitted solution to thermodynamic differential relation

$$f_{xc}^{\zeta}(r_s,t) = -\frac{1}{r_s}\frac{\omega_\zeta a(t) + b_\zeta(t) r_s^{1/2} + c_\zeta(t) r_s}{1 + d_\zeta(t) r_s^{1/2} + e_\zeta(t) r_s}$$

$$\zeta = (n_\uparrow - n_\downarrow)/n; \quad \omega_{\zeta=0} = 1; \quad \omega_{\zeta=1} = 2^{1/3}$$

a(t), b(t), c(t), d(t), e(t) **are functions of *t*=T/T_F with tabulated coefficients.**



Comparison to RPIMC data (red dots) for ζ=0, r_s=1 (left) and 40 (right) for ε_{xc} and resulting f_{xc}.

Phys. Rev. Lett. 112, 076403 (2014)

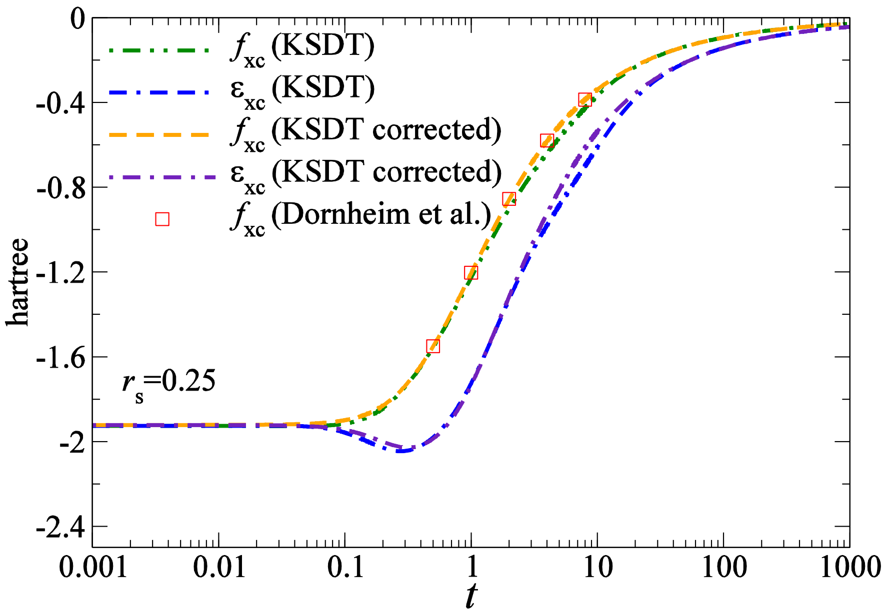
Note: we had a bit of trouble regarding the low r_s, low t data

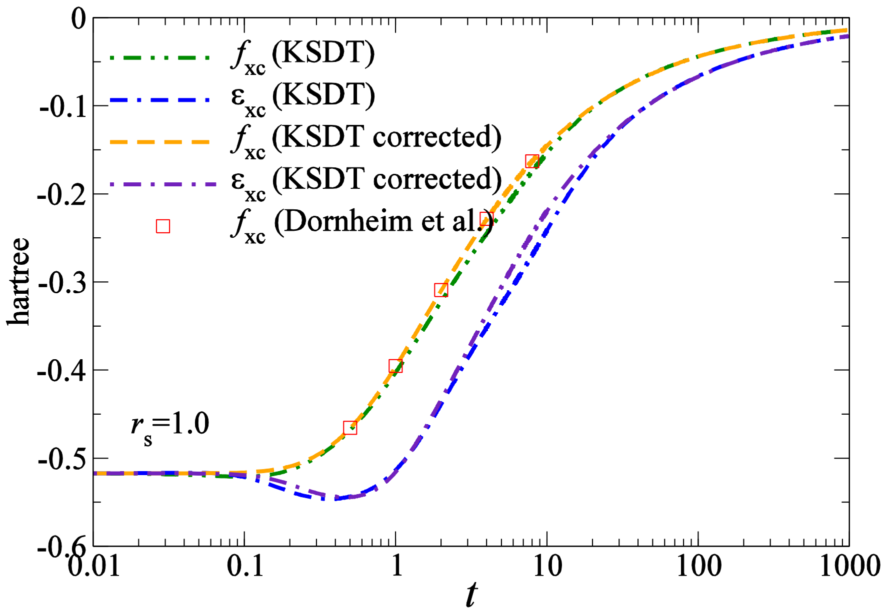
LSDA $F_{xc}[n]$ – small refinements and fixes

K. Burke, J. C. Smith, P. E. Grabowski, and A. Pribram-Jones,
Phys. Rev. B 93, 195132 (2016): $S < 0$ **for r_s > 10, t < 0.1 (by < 100 μH/electron)**

T. Dornheim, S. Groth, T. Sjostrom, F.D. Malone , W.M.C. Foulkes, and M. Bonitz
PRL <u>117</u>, 156403 (2016) QMC on HEG, new finite size corrections on $0.1 \leq r_s \leq 10.0$
and t > 0.5 "…reveals ~~significant~~ deviations…" with respect to KSDT.
In fact, we very recently discovered a tiny T=0K fitting error in KSDT that causes most of the problem.

Correcting KSDT to fix both issues is straightforward and changes virtually nothing:

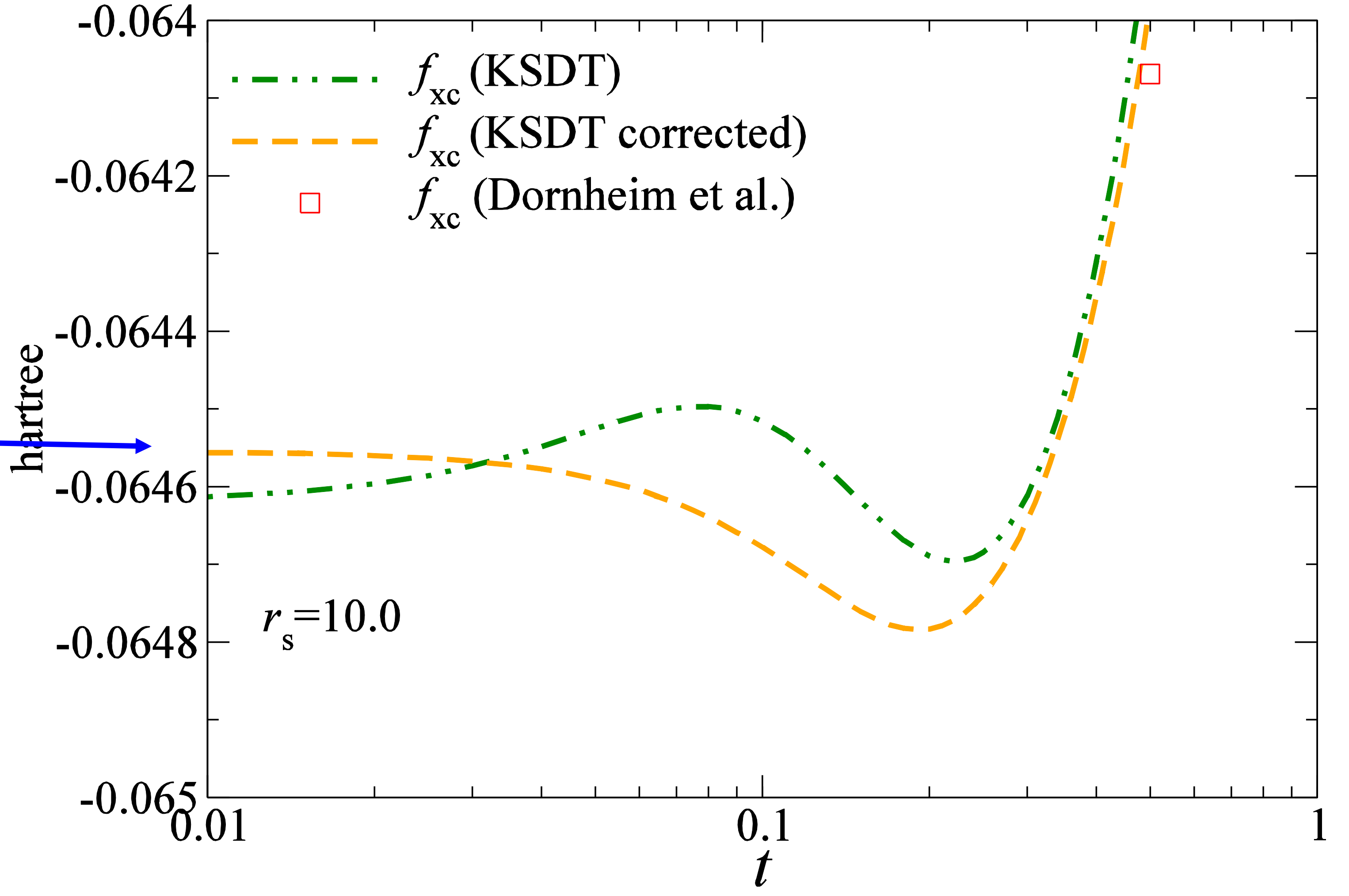




LSDA $F_{xc}[n]$ – small refinements and fixes

T=0 data set error corrected

(≈30 microH)



Karasiev, Dufty, & Trickey, unpublished; "Fit B" identity

Dornheim et al. = Phys. Rev. Lett. 117, 156403 (2016)

Framework for GGA XC free-energy functional development

A Practical, Non-empirical, Free-Energy Density Functional for Warm Dense Matter

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(Dated: REV-v4; 04 Apr. 2017)

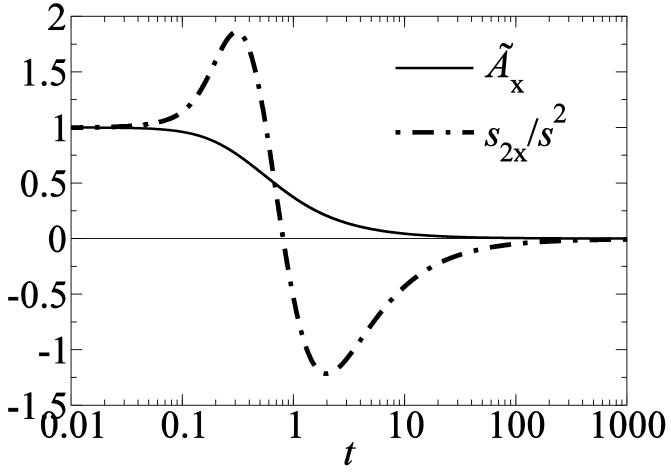
- **Identify T-dependent gradient variables for X and C free-energies**
- **Identify relevant finite-T constraints**
- **Use our finite-T LDA XC as an ingredient**
- **Propose appropriate analytical forms, incorporate constraints**
- **Implementation, tests, applications**

Karasiev, Dufty, Trickey, Phys. Rev. Lett. (submitted, 2016) arXiv: 1612.06266

T-dependent GGA for eXchange

Finite-T reduced density gradient variable for X from finite-T gradient expansion for X: $s_{2x}(n,\nabla n,T) \equiv s^2(n,\nabla n)\tilde{B}_x(t)$

Combination of F-D integrals



$\tilde{A}_x(t)$ **t-dependence of LDA X**

$\tilde{B}_x(t) = s_{2x}/s^2$ **t-dependence of GGA X**

Enhancement factor constraints:

- **Reproduce finite-T small-s grad. expansion**
- **Satisfy Lieb-Oxford bound at T=0**
- **Reduce to appropriateT=0 limit (here PBE X)**
- **Reduce to correct high-T limit**

$$F_x^{GGA}[n,T] = \int n\, f_x^{LDA}(n,T)\, F_x(s_{2x})\, d\mathbf{r}$$

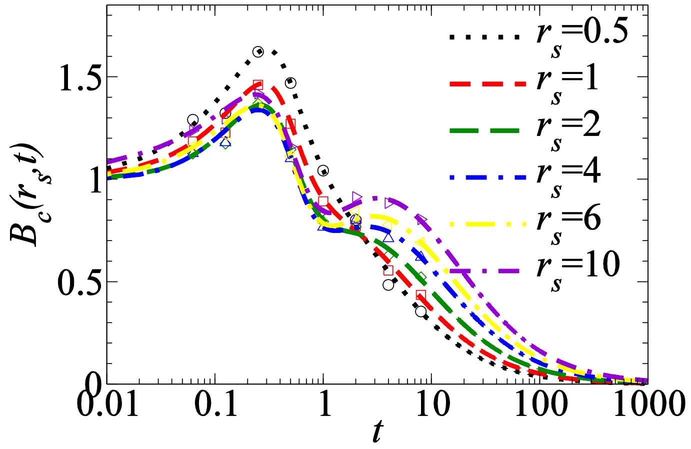
$$F_x(s_{2x}) = 1 + \frac{\nu_x s_{2x}}{1+\alpha|s_{2x}|}$$

T-dependent GGA for Correlation

Finite-T reduced density gradient variable for C from T-dependent gradient expansion -

$$n^{1/3} s^2(n,\nabla n)\tilde{B}_c(n,t) \propto q^2 \tilde{B}_c(n,t)$$

$$q_c(n,\nabla n,T) \equiv q(n,\nabla n)\sqrt{\tilde{B}_c(n,t)}$$



q **is a ground-state reduced density gradient for C**
$\tilde{B}_C(n,\mathrm{T})$ **is an analytic expression found from FD integrals and numerical QMC data. Its T-dependence is shown at right.**

$$f_c^{GGA}(n,\nabla n,\mathrm{T}) = f_c^{LDA}(n,\mathrm{T}) + H(f_c^{LDA}, q_c)$$

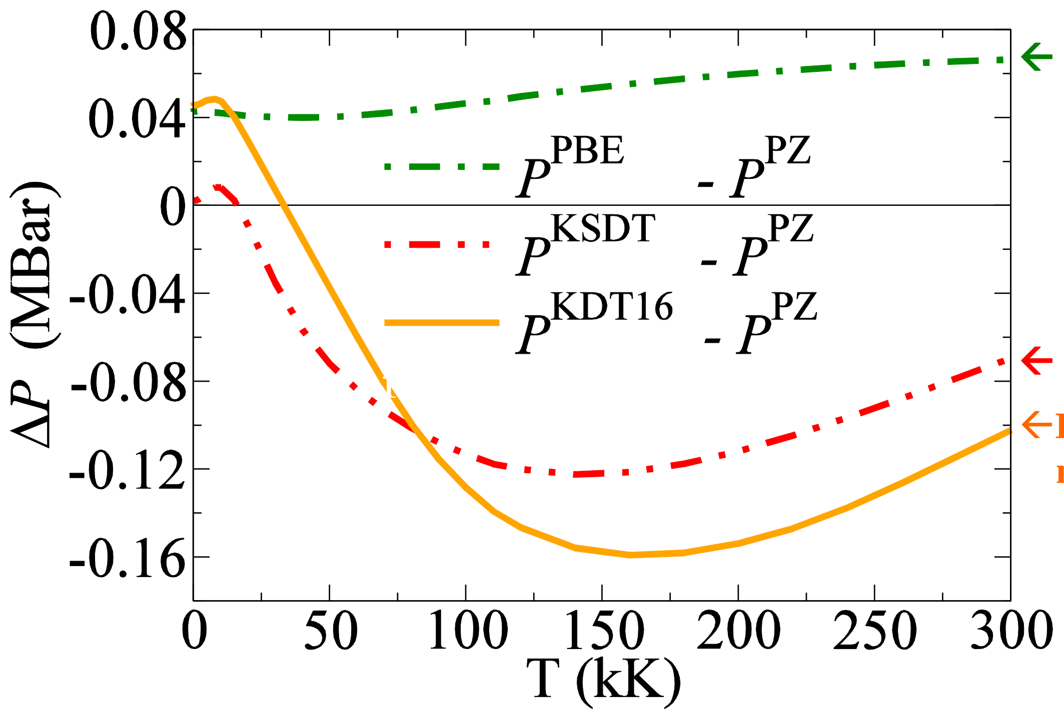
where the function $H(f_c^{LDA},q_c)$ **is defined by the ground-state PBE functional to achieve a widely used zero-T limit.**

Constraints on f_c^{GGA}**:**

- **Reproduce finite-T small-s grad. expansion**
- **Reduce to correct T=0 limit**
- **Reduce to correct high-T limit**

$$F_c^{GGA}[n,T] = \int n\, f_c^{GGA}(n,\nabla n,T)\,d\mathbf{r}$$

Result is Thermal GGA XC shifts shown before (fcc-Al model system)



Electronic pressure differences vs. T for the new finite-T GGA ("KSDT16"), KSDT LDA, and ground-state PBE XC functionals, all referenced to PZ ground-state LDA values. Static lattice fcc Aluminum at 3.0 g/cm^3.

Karasiev, Dufty, & Trickey, Phys. Rev. Lett. (submitted) arXiv 1612.06266

PROFESS@Quantum-Espresso package

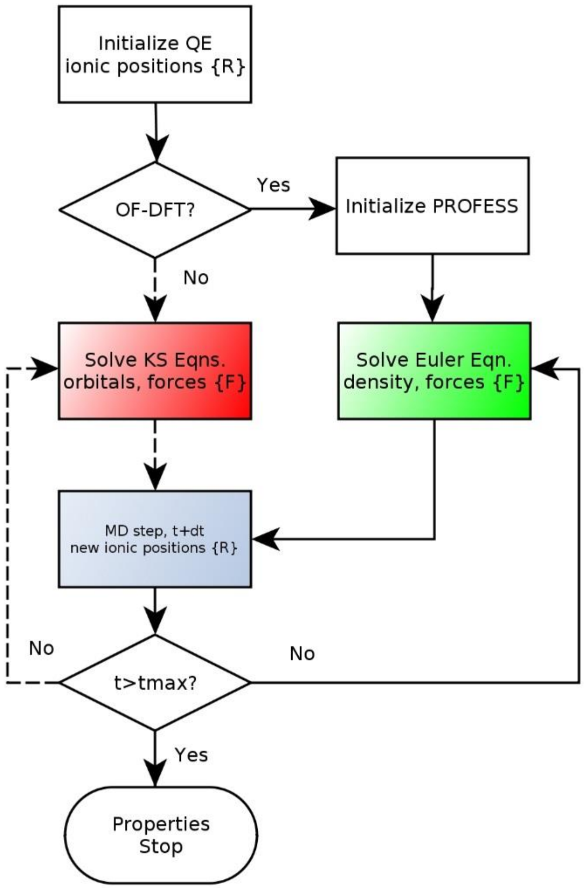
- **Finite-T OF-DFT functionals are implemented in the PROFESS code.**

- **T-dependent XC implemented in PROFESS and Q-Espresso**

- **Our analytical representations of Fermi-Dirac integral combinations are implemented**

- **PROFESS@Q-Espresso interface gives Quantum-Espresso MD driven by OF-DFT forces**

- **Vers. 2.0 was released recently – go to http://www.qtp.ufl.edu/ofdft**



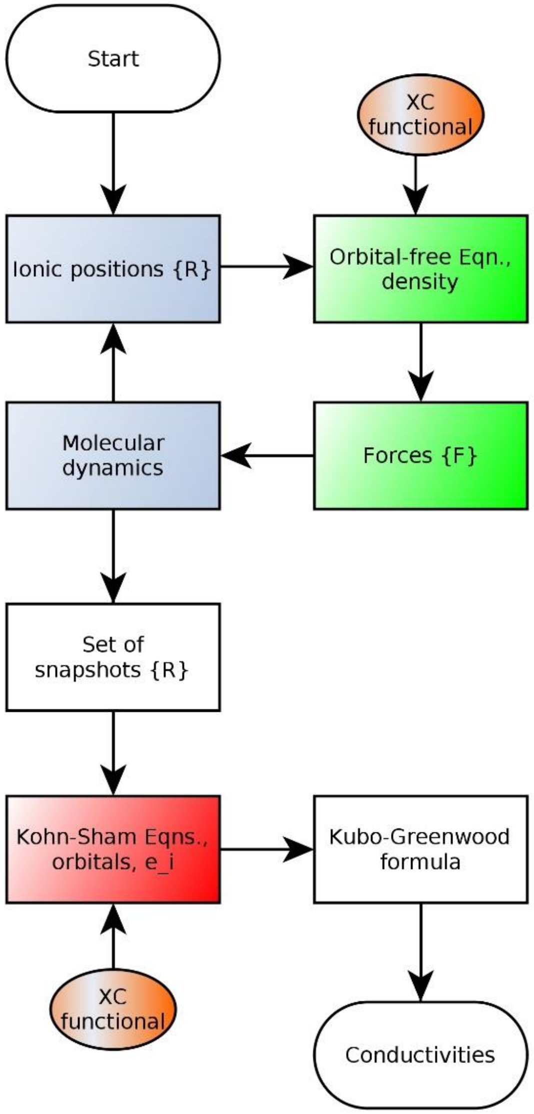
Flow chart for MD simulation with PROFESS@Q-Espresso

Karasiev, Sjostrom, Trickey, Comput. Phys. Commun. 185, 3240 (2014)

Optical Conductivity & XC thermal effects

OF-DFT MD and subsequent Kohn-Sham and Kubo-Greenwood conductivity calculations -

- **Non-interacting free-energy functional is a critical input to OF-DFT MD**
- **2 to 10 “snapshots”; explicit KS to get orbitals and eigenvalues**
- **XC free-energy functional is a critical input for both OF-DFT MD and snapshot KS**



Kubo-Greenwood Electron Conductivity Expression and Implementation for Projector Augmented Wave Datasets

L. Calderín, V. Karasiev, S.B. Trickey; QTP, Physics and Chemistry, Univ. Florida

2 Mar 2017; version 3; not for circulation outside UF WDM/OFDFT group

Paper & code in preparation for GPL release.

Summary

- **Real progress on orbital-free DFT (both T = 0 K and T > 0 K):**
  *** Finite-T GGA formalism (for the non-interacting free-energy)**
  *** First non-empirical GGAs for non-interacting free-energies**
  *** Tunable non-interacting functional enables far-reaching extension of static KS calculations into OF-DFT MD**

- **Real progress on finite-T XC:**
  *** "KSDTcorr" LSDA XC based on parametrization of quantum Monte-Carlo data**
  *** Non-empirical "KDT16" GGA XC free-energy (submitted)**

- **Software:**
  *** Profess@QuantumEspresso orbital-free package**
  *** Kubo-Greenwood post-pocessing transport properties package for QE (soon)**

- **Everything downloadable from www.qtp.ufl.edu/ofdft**