Understanding Properties of Materials under Extreme Conditions with *First-Principles* Methods for ICF/HED Applications

S. X. Hu (胡素兴)

Laboratory for Laser Energetics
University of Rochester

Seminar @ HEDS Center at LLNL ***Feb 7th, 2019***

A “startup” HEDP-theory group is being built recently at LLE

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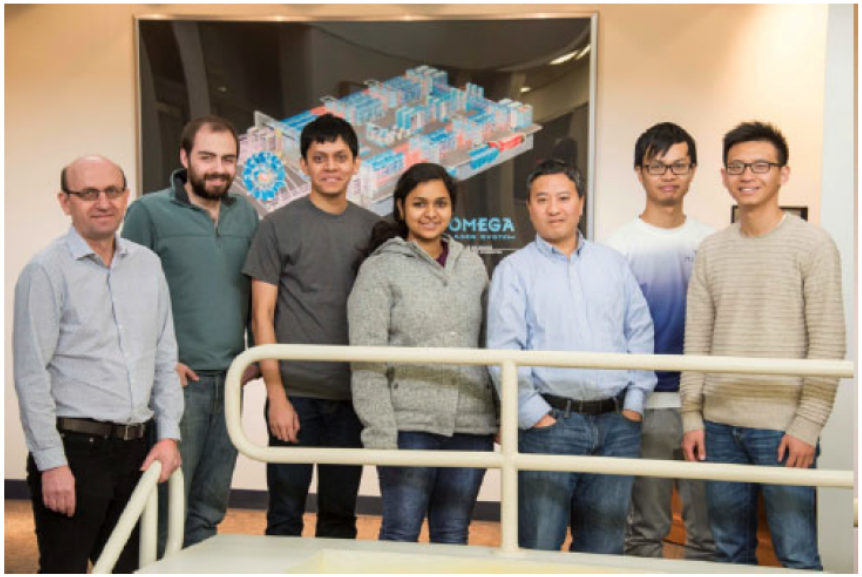
High-Energy-Density Physics (HEDP) Theory Group

Suxing Hu
Group Leader

Scientists
Valentin Karasiev

Contents

- What is HEDP/WDM?
- Why do we care about HEDP & WDM?
- Current Research Topics
- First-Principles/ *Ab-Initio* Methods for HEDP
- List of Selected Recent Publications and Preprints
- Opportunities & Contact information



Graduate Students
Yanhao Ding (~2021)
Maitrayee Ghosh (~2023)
Josh Hinz (~2022)
Reetam Paul (~2022)
Tian Tang (~2023)

Undergraduate/ High School Interns
Barry Xu
(Columbia University, 2010)
Jesse Pan
(Case Western, 2012)
Nathan Xu
(Univ. Pennsylvania, 2014)
Xilin Zhou
(Harvard, 2015)
Ryan Gao
(Princeton, 2016)

We are currently looking for two more scientists to join us!

Outline

- Introduction: *Why do we care about high-energy-density physics (HEDP) as ICF scientists?*
- What are our "*first-principles toolkits*" to understand HED matter as a *quantum many-body system*?
  - Density-Functional-Theory (DFT)
  - Path-integral Monte-Carlo (PIMC)
  - Quantum Monte-Carlo (QMC)
- *First-principles*-based and *self-consistent* material properties under extreme conditions for ICF/HED applications:
  - What have we learned so far?
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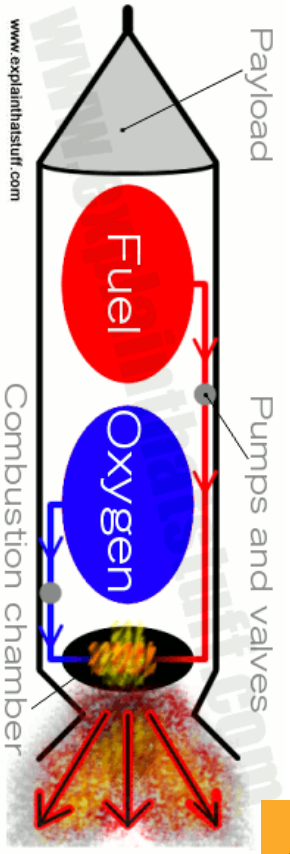
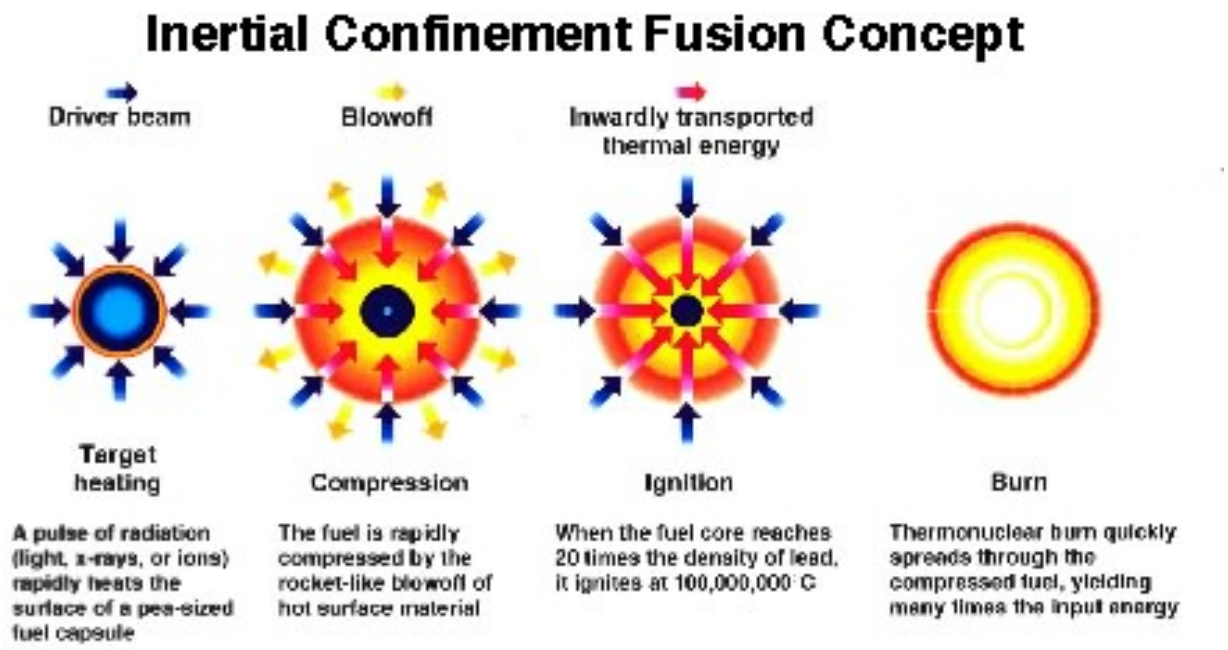
- Conclusion & Outlook

Why do we care about HEDP as ICF scientists?

How a rocket works?

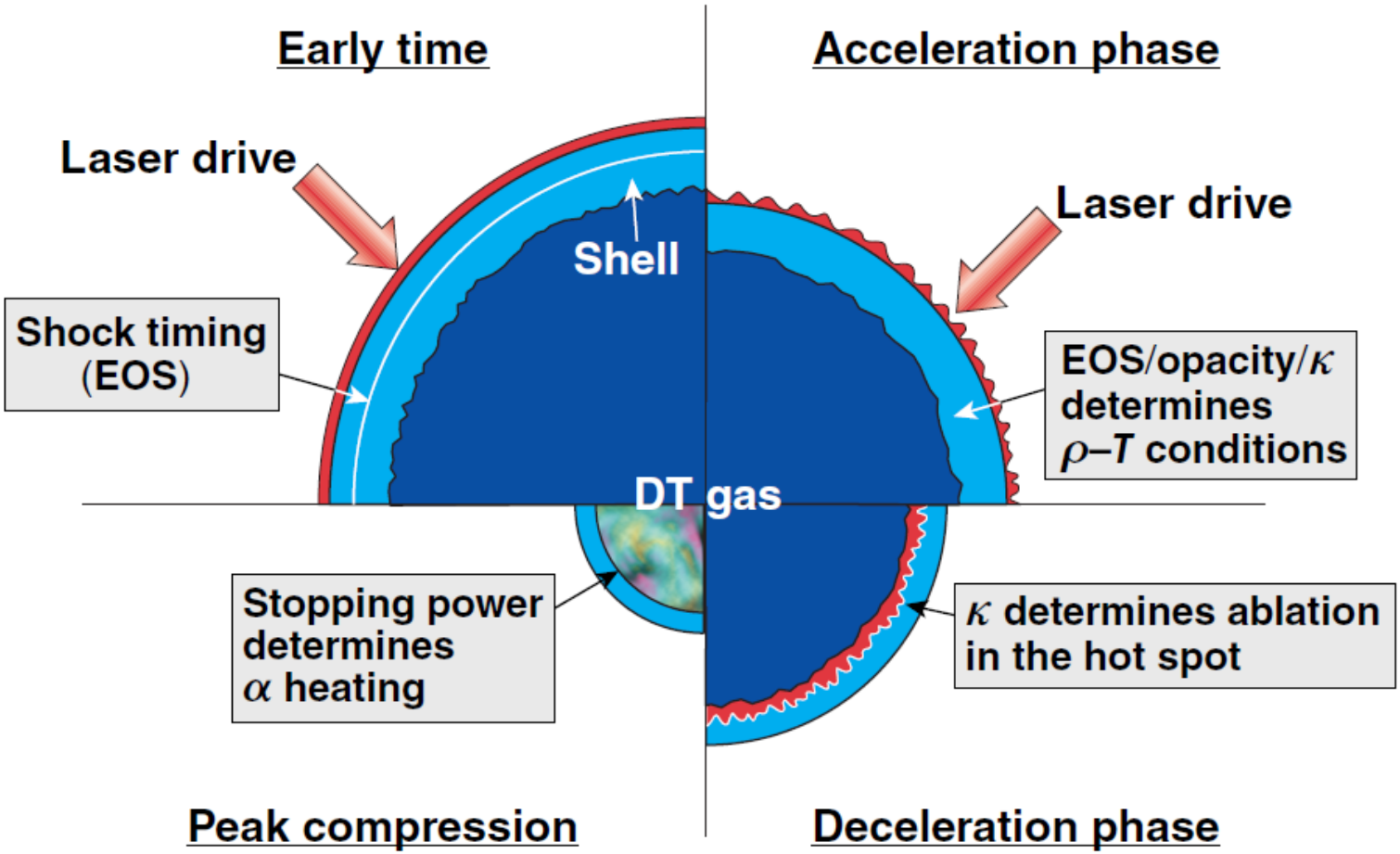


How ICF works?

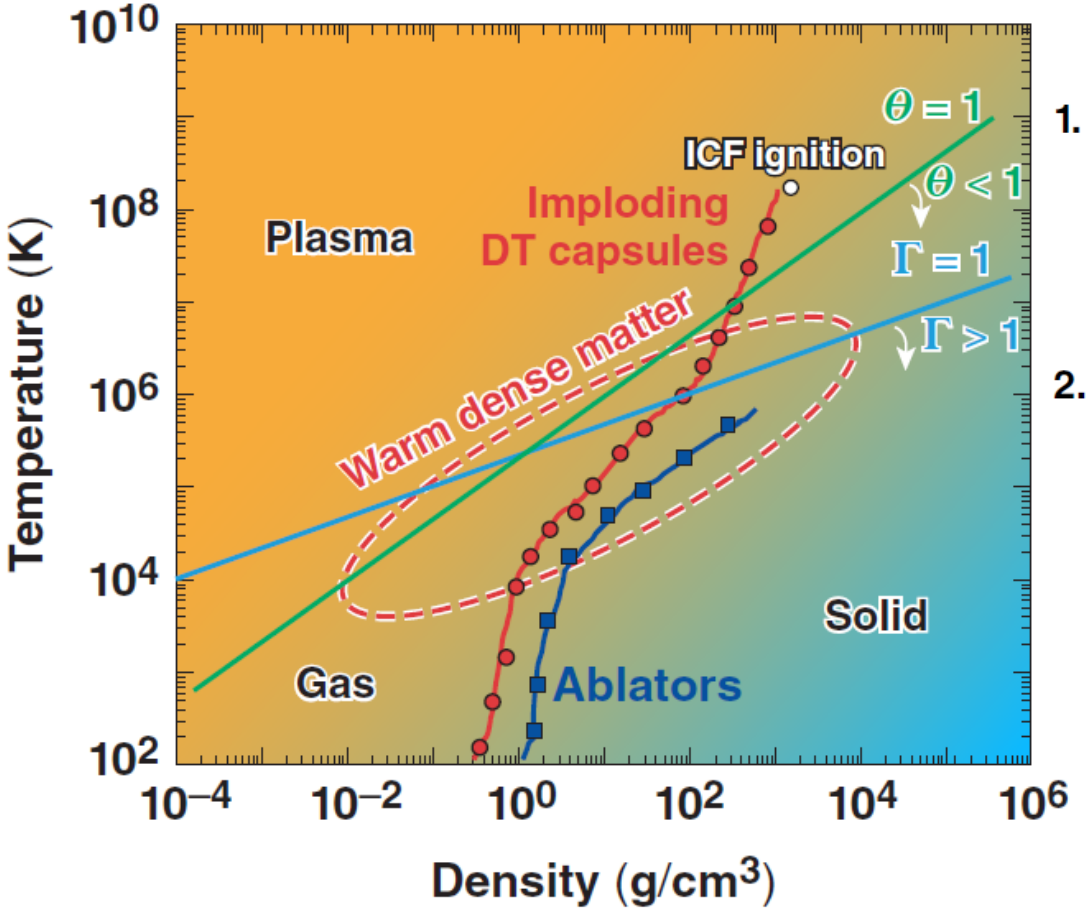


An ICF physicist is also a "rocket scientist"!

Accurate knowledge of *intrinsic* plasma properties (EOS,* opacity, thermal conductivity, and stopping power) of DT and ablators is required for ICF simulations



ICF implosions routinely access the WDM regime,* which demands a better understanding of material properties



1. The Coulomb coupling parameter:

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

2. The electron-degeneracy parameter:

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

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

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

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- **What are our "*first-principles toolkits*" to understand HED matter as a *quantum many-body system*?**
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  - **Quantum Monte-Carlo (QMC)**
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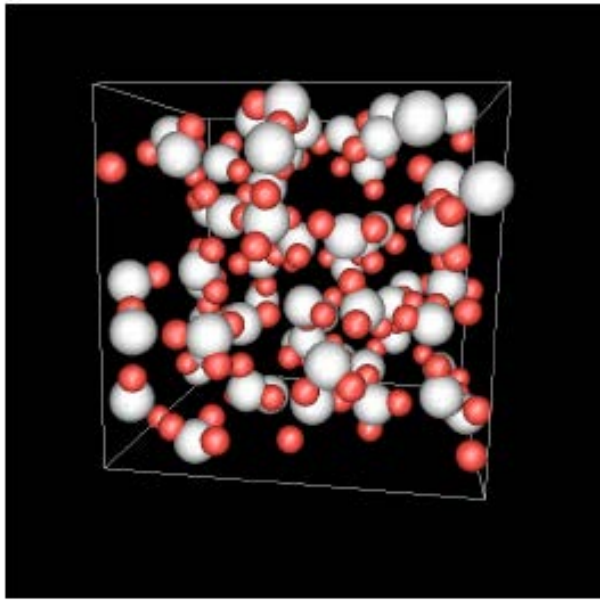
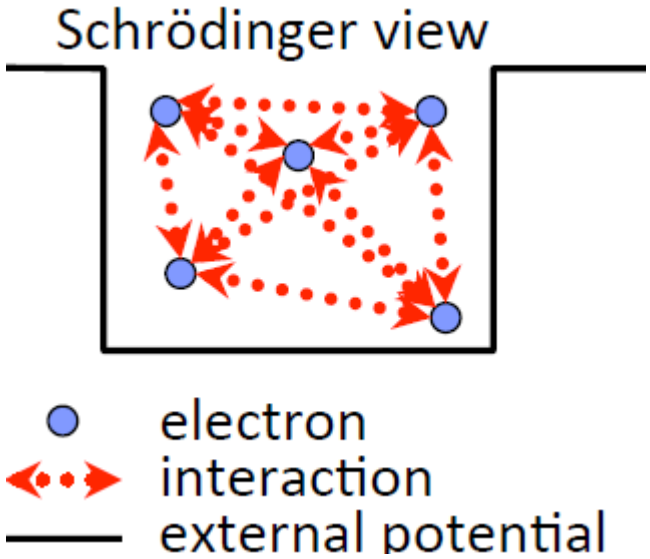
A view of an HEDP-theorist: Warm-dense matter (dense plasmas) as *quantum many-body systems*





Quantum many-body Schrödinger Equation

$$\left[-\frac{\hbar^2}{2m}\sum_i \nabla^2 + V(r_1, r_2, \ldots, r_n)\right]\Psi(r_1, r_2, \ldots, r_n) = E\Psi(r_1, r_2, \ldots, r_n)$$

Quantum many-body Schrödinger Equation:
Well-defined equation, but no easy solution

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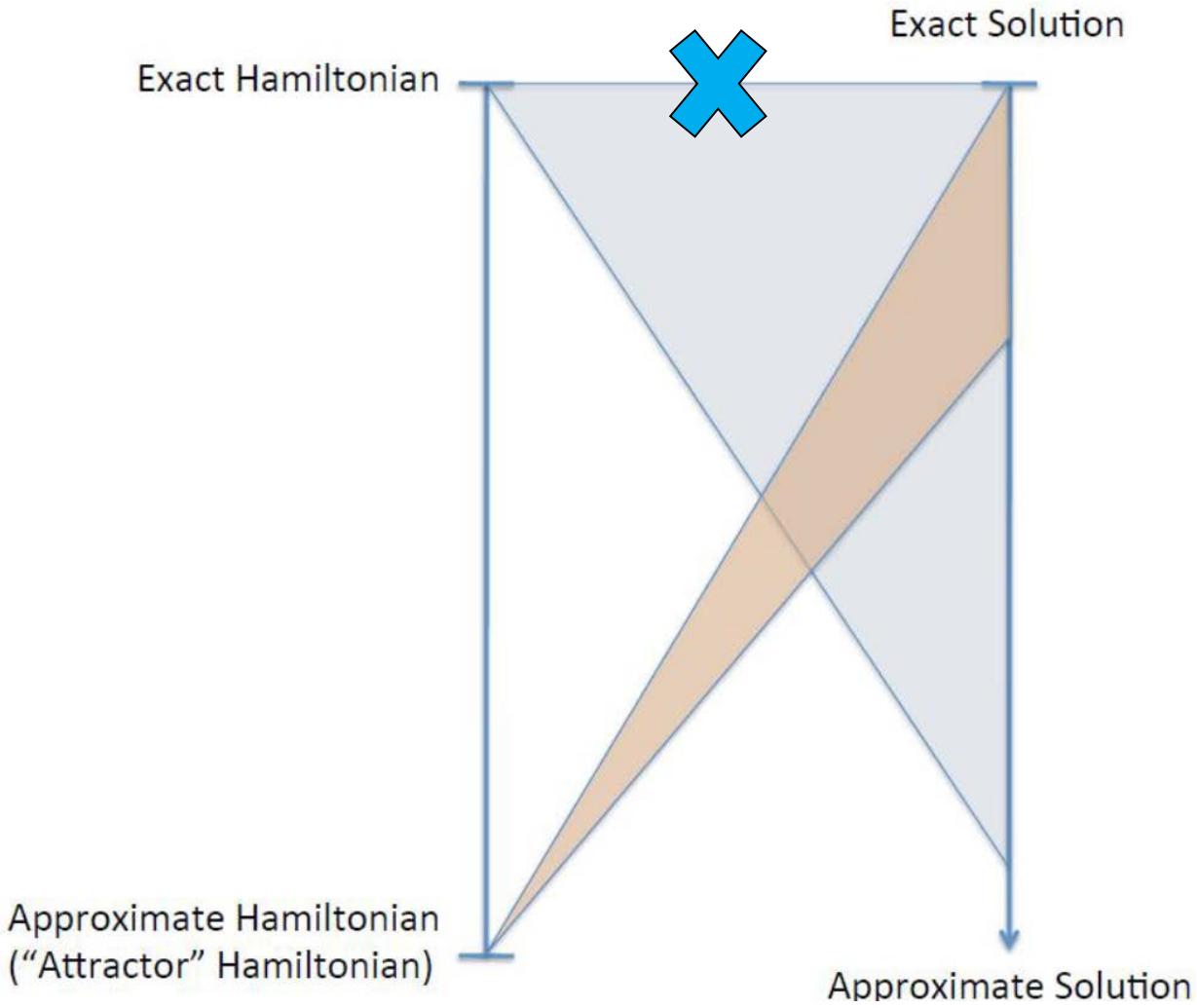
Quantum Mechanics

Dirac (1929)

" The general theory of quantum mechanics is now almost complete... The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble. "

P.A.M. Dirac, Proc. R. Soc. London Ser. A 123, 714 (1929).

How can we learn the many-body physics and chemistry from the Quantum Mechanics equations?



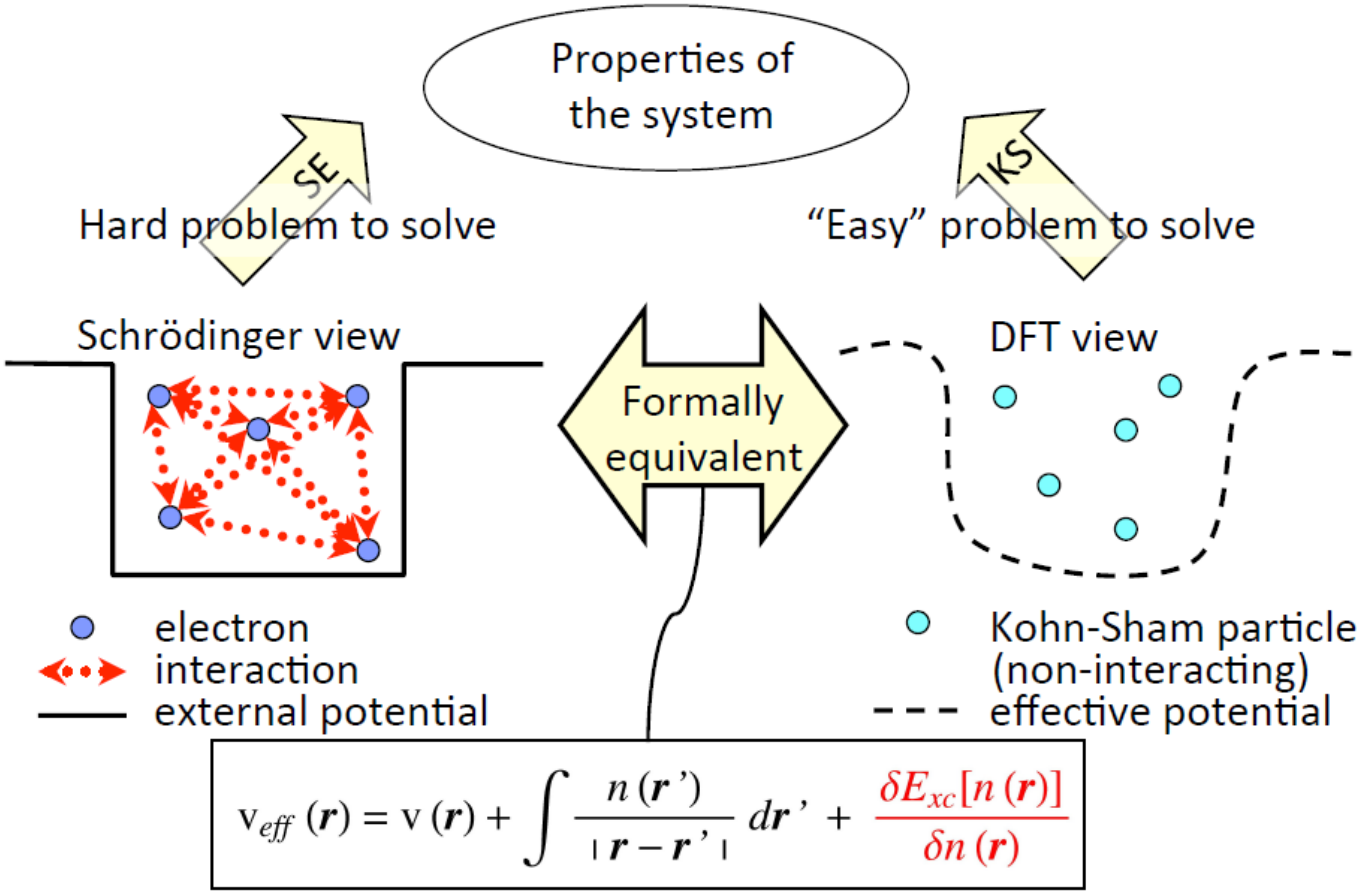
Our "*first-principles toolkits*" for quantum many-body systems

- Density-Functional-Theory (DFT)*
- Path-integral Monte-Carlo (PIMC)**
- Quantum Monte-Carlo (QMC)***

---

* W. Kohn and L. J. Sham, Phys. Rev. 140, A1133 (1965).
** D. M. Ceperley, Rev. Mod. Phys. 67, 279 (1995).
*** E. Fermi & R. D. Richtmyer (1948) and many papers afterwards [e.g., R. C. Clay, M. Holzmann, D. M. Ceperley, and M. A. Morales, Phys. Rev. B 93, 035121 (2016).]

DFT versus the Schrödinger Equation



$$v_{eff}(\boldsymbol{r}) = v(\boldsymbol{r}) + \int \frac{n(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|} d\boldsymbol{r}' + \frac{\delta E_{xc}[n(\boldsymbol{r})]}{\delta n(\boldsymbol{r})}$$

All many-body effects are included in the effective potential via the Exchange-Correlation functional, $E_{xc}[n(\boldsymbol{r})]$.

*Courtesy of Ann Mattsson

Kohn-Sham equations:

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + v_{eff}(\boldsymbol{r})\right)\psi_\nu(\boldsymbol{r}) = \epsilon_\nu \psi_\nu(\boldsymbol{r}) \quad \nu = 1, 2, \ldots, N$$

$$n(\boldsymbol{r}) = \sum_{\nu=1}^{N} |\psi_\nu(\boldsymbol{r})|^2$$

Seeking accurate ones for a long-time

$$v_{eff}(\boldsymbol{r}) = v(\boldsymbol{r}) + \int \frac{n(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|} d\boldsymbol{r}' + \frac{\delta E_{xc}[n(\boldsymbol{r})]}{\delta n(\boldsymbol{r})}$$

If we had the divine exchange-correlation functional, self-consistently solving these equations would give exactly the same density as the Schrödinger Equation, and thus via the HK theorem, we should be able to extract all information about the system.

Finding the best exchange-correlation functional is the key to have made DFT practical

LDA for V_{xc}

Alex Zunger

University of Colorado ,Boulder ,Colorado.Renewable and Sustainable Energy Institute

Physics
Material Science
nano science
photovoltaics

	All	Since 2013
Citations	88351	28397
h-index	136	77
i10-index	613	366

TITLE	CITED BY	YEAR
Self-interaction correction to density-functional approximations for many-electron systems JP Perdew, A Zunger Physical Review B 23 (10), 5048	18405	1981

GGA for V_{xc}

John P. Perdew

Temple University

density functional theory
materials theory
quantum chemistry

	All	Since 2013
Citations	234190	110367
h-index	103	65
i10-index	275	189

TITLE	CITED BY	YEAR
Generalized gradient approximation made simple JP Perdew, K Burke, M Ernzerhof Physical review letters 77 (18), 3865	86940	1996

The journey of searching for more and more accurate XC-functionals still continues: Meta-GGA, Hybrid, temperature-dependent,……

Quantum Molecular Dynamics (QMD) method is based on the thermal density-functional theory (DFT)*

- The thermal-DFT is a "mean-field" theory of many-electron system at finite temperatures:

$$\left\{-\frac{1}{2}\Delta + V_Z(r) + V_H[n](r) + V_{xc}[n](r)\right\}\psi_i = \epsilon_i\psi_i$$

$$\mathrm{n(r)} = \sum_{i=1}^{N} f_i|\psi_i(r)|^2,\ V_H[n](r) = \int \frac{n(r')}{|r-r'|}dr'$$

- Since V_H and V_{xc} terms depend on electron density n(r), which depends on the ψ_i, the thermal-DFT equation can be solved in a self-consistent (i.e., *iterative*) way, once the V_{xc} is known!

- The resulting electronic force together with ionic forces will drive the classical ions to move, through the Newton's equation, in the MD simulations.

*P. Hohenberg and W. Kohn, Phys. Rev. 136, B864 (1964).
W. Kohn and L. J. Sham, Phys. Rev. 140, A1133 (1965).
N. D. Mermin, Phys. Rev. 137, A1441 (1965).

A variety of material properties can be *self-consistently* calculated from QMD simulations

- **EOS are direct outputs 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/Electrical conductivities and optical absorption coefficients can be derived from these Onsager coefficients $L_{ij}(\omega)$:**

$$\sigma = L_{11};\ \kappa = \frac{1}{T}\left(L_{22} - {}^{L_{12}^2}/_{L_{11}}\right);\quad \alpha_m(\omega) = \frac{\alpha_K(\omega)}{\rho} = \frac{4\pi\bar{\sigma}_1(\omega)}{c\times\bar{n}(\omega)}\times\frac{1}{\rho}$$

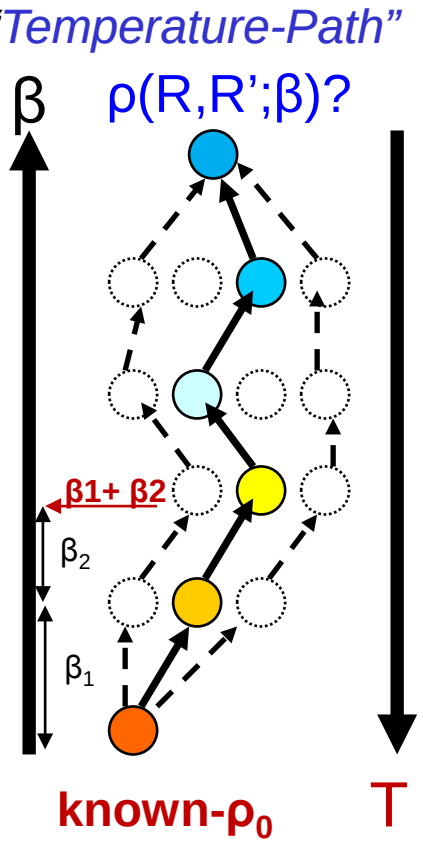
PIMC*, based on the convolution of density matrix, uses Monte-Carlo method to efficiently evaluate multi-dimensional integrations

- **Density-matrix ρ(R,R';T), introduced by John von Neumann in 1927, describes the statistical distribution of a quantum system in thermal equilibrium:**

$$\rho(R,R';T) = < R \mid e^{-\hat{H}/kT} \mid R' > = \sum_n \varphi_n(R)\varphi_n(R')e^{-E_n/kT}$$

- **The convolution property of ρ(R,R';β) can be written as:**

$$\rho(R,R';\beta_1+\beta_2) = < R \mid e^{-(\beta_1+\beta_2)\hat{H}} \mid R' >$$
$$= \int dR_1 \rho(R,R_1;\beta_1)\rho(R_1,R';\beta_2)$$
$$with \quad \beta_1 = 1/kT_1 \; and \; \beta_2 = 1/kT_2.$$



Difficult (if not impossible) to obtain transport and optical properties

*D. M. Ceperley, Rev. Mod. Phys. 67, 279 (1995).

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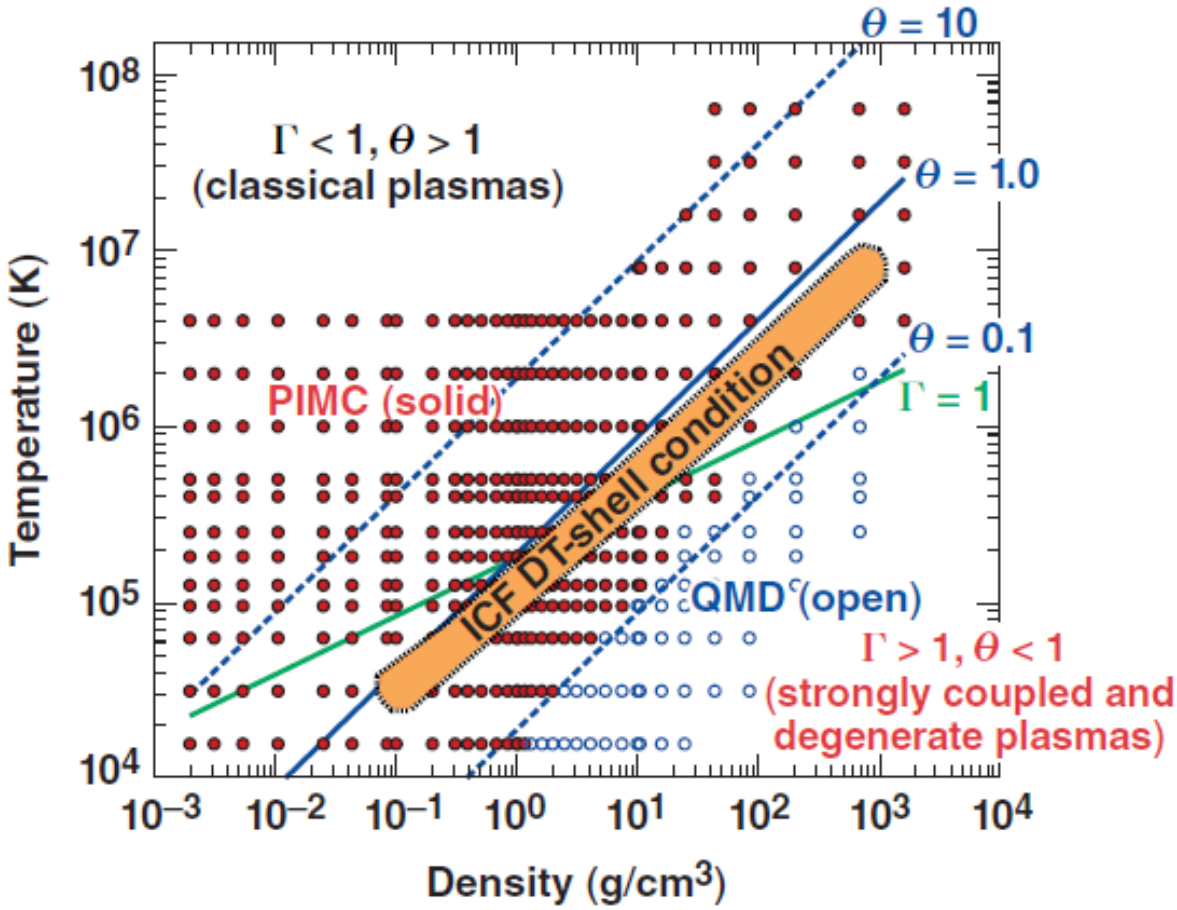
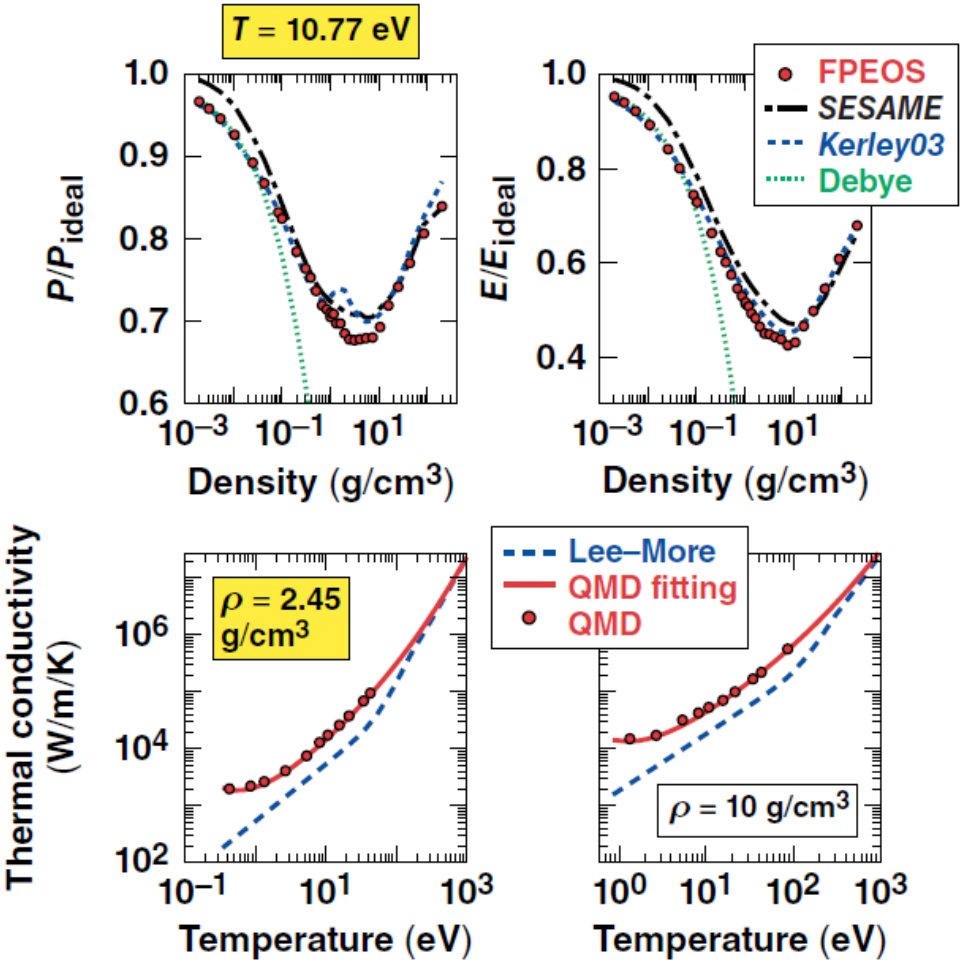
We studied the properties of deuterium* in a wide range of conditions by combining PIMC and QMD methods

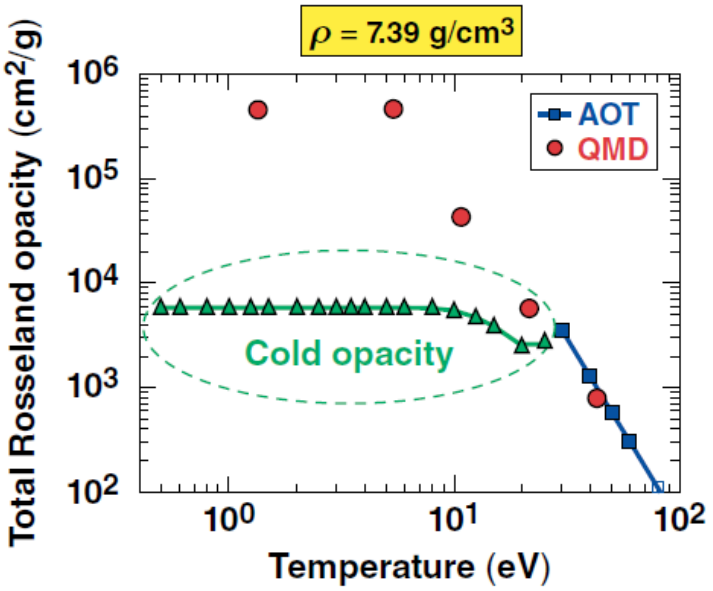


*S. X. Hu *et al.*, Phys. Rev. Lett. 104, 235003 (2010).

TC11442

Significant differences have been identified for warm dense deuterium when FPEOS,* κ_{QMD},** and FPOT† are compared with traditional models



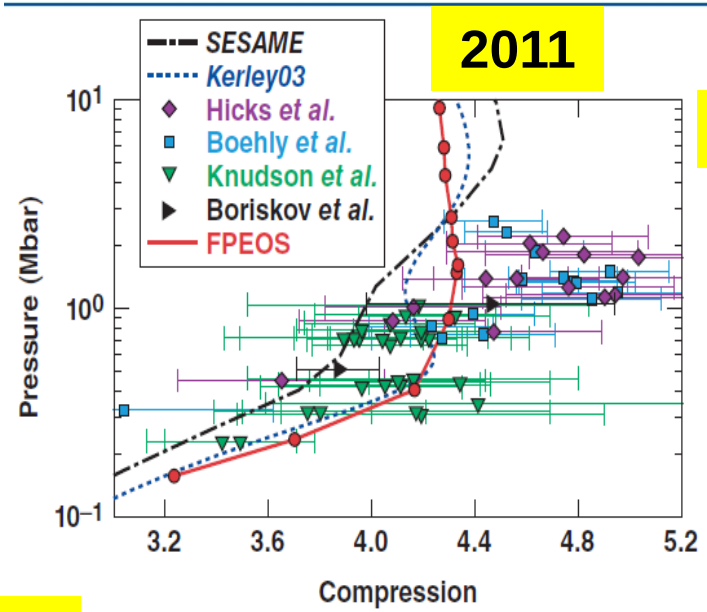


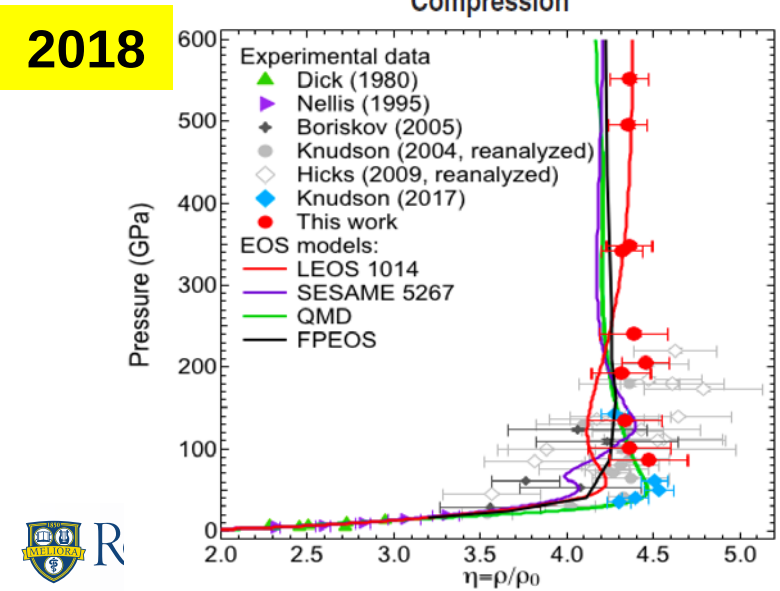
*FPEOS: first-principles equation of state; S. X. Hu *et al.*, Phys. Rev. B 84, 224109 (2011).

**κ_{QMD}: QMD-based thermal conductivity; S. X. Hu *et al.*, Phys. Rev. E 89, 043105 (2014).

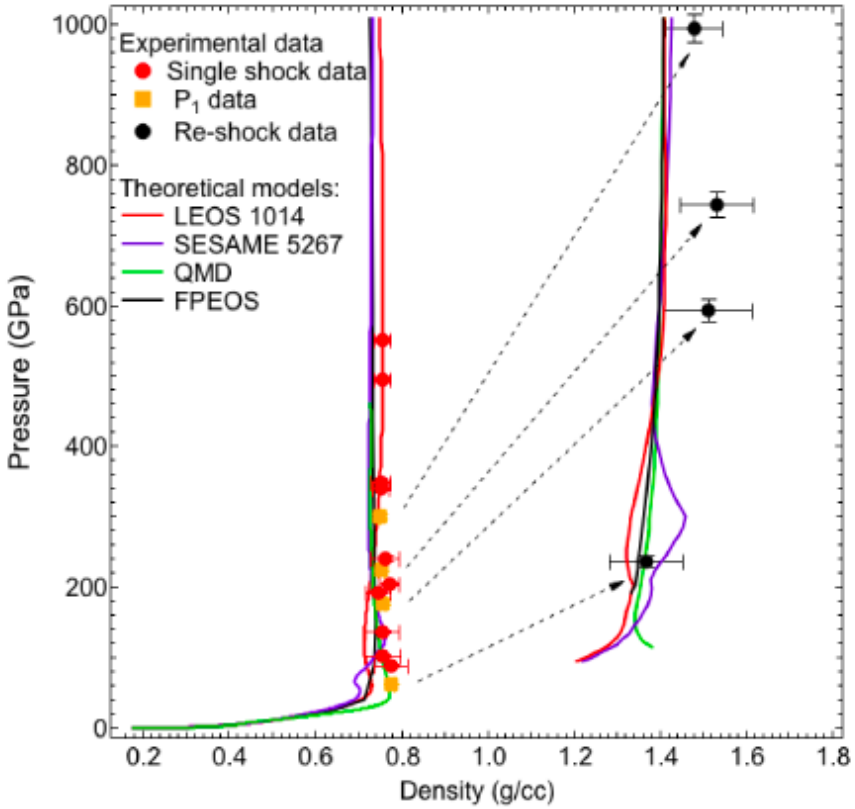
†FPOT: first-principles opacity table; S. X. Hu *et al.*, Phys. Rev. E 90, 033111 (2014).

New experiments* continue to challenge our understanding of the behavior of deuterium at WDM conditions





2018: more surprises for the double-shock data



*A. Fernandez-Panella *et al.*, Submitted (2018).

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

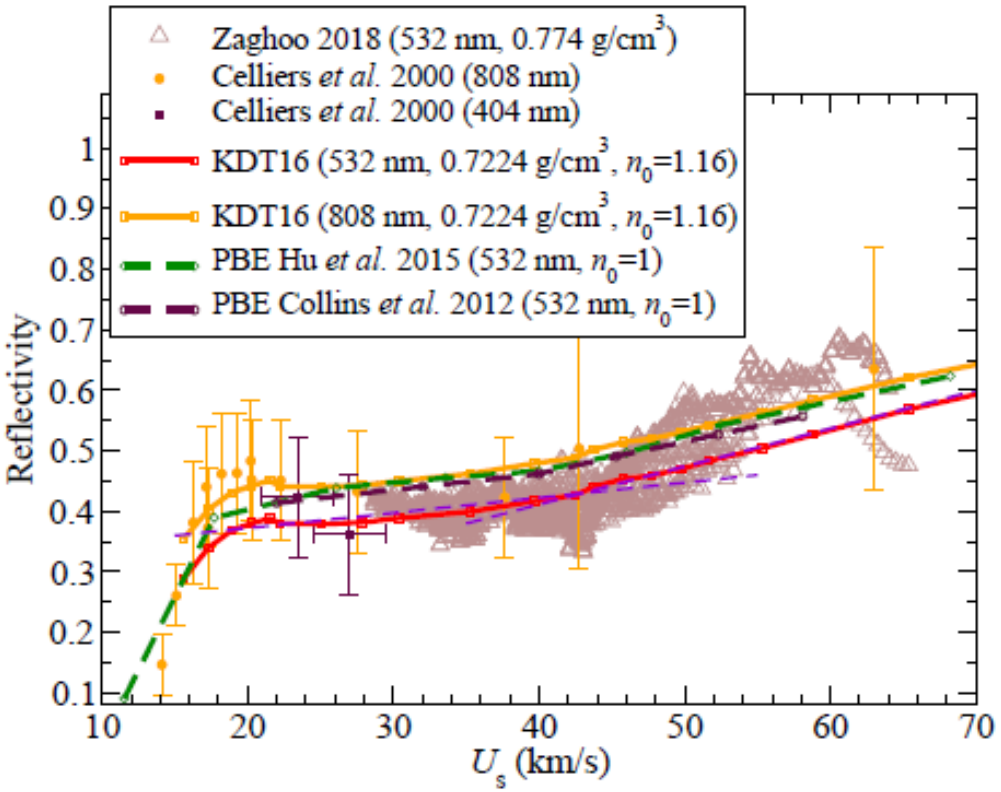
$$\sigma_1(\omega) = L_{11}(\omega);\ \sigma_2(\omega) = -\frac{2}{\pi} P\left(\int \frac{\omega \sigma_1(\omega')}{\omega'^2 - \omega^2} d\omega'\right).$$

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

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

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

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

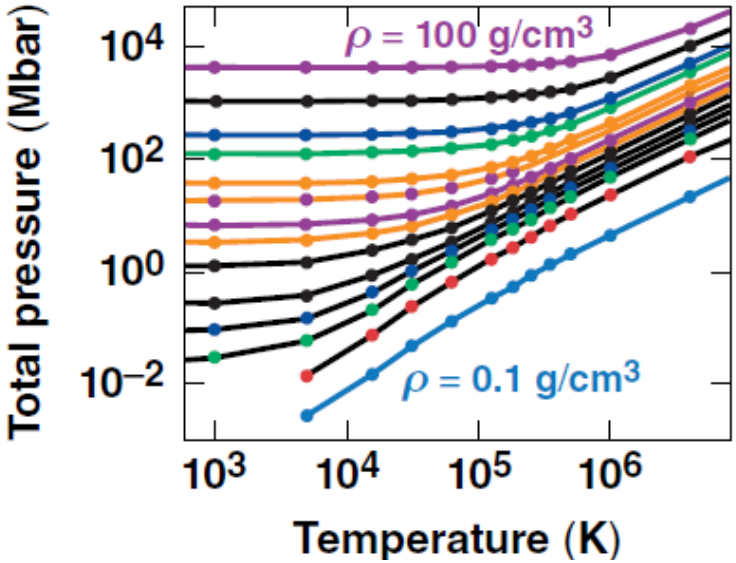


* S. X. Hu *et al.*, Phys. Plasmas 22, 056304 (2015).
V. V. Karasiev et al., Phys. Rev. B (to be submitted)

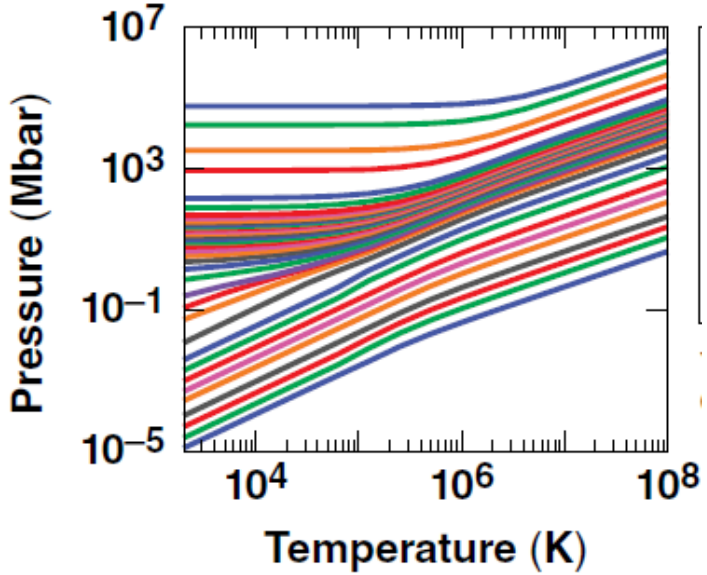
**P. M. Celliers *et al.*, Phys. Rev. Lett. 84, 5564 (2000).
T. R. Boehly *et al.*, Phys. Plasmas 16, 056302 (2009).
M. Zaghoo et al., Phys. Rev. Lett. (accepted, 2019).

A wide range of material conditions of ICF-relevant ablators* has also been studied by KSMD+OFMD calculations in their liquid phase

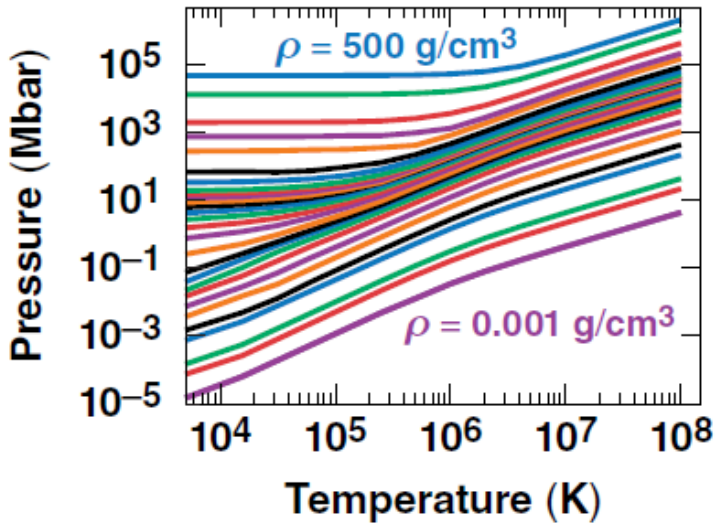
CH



Be

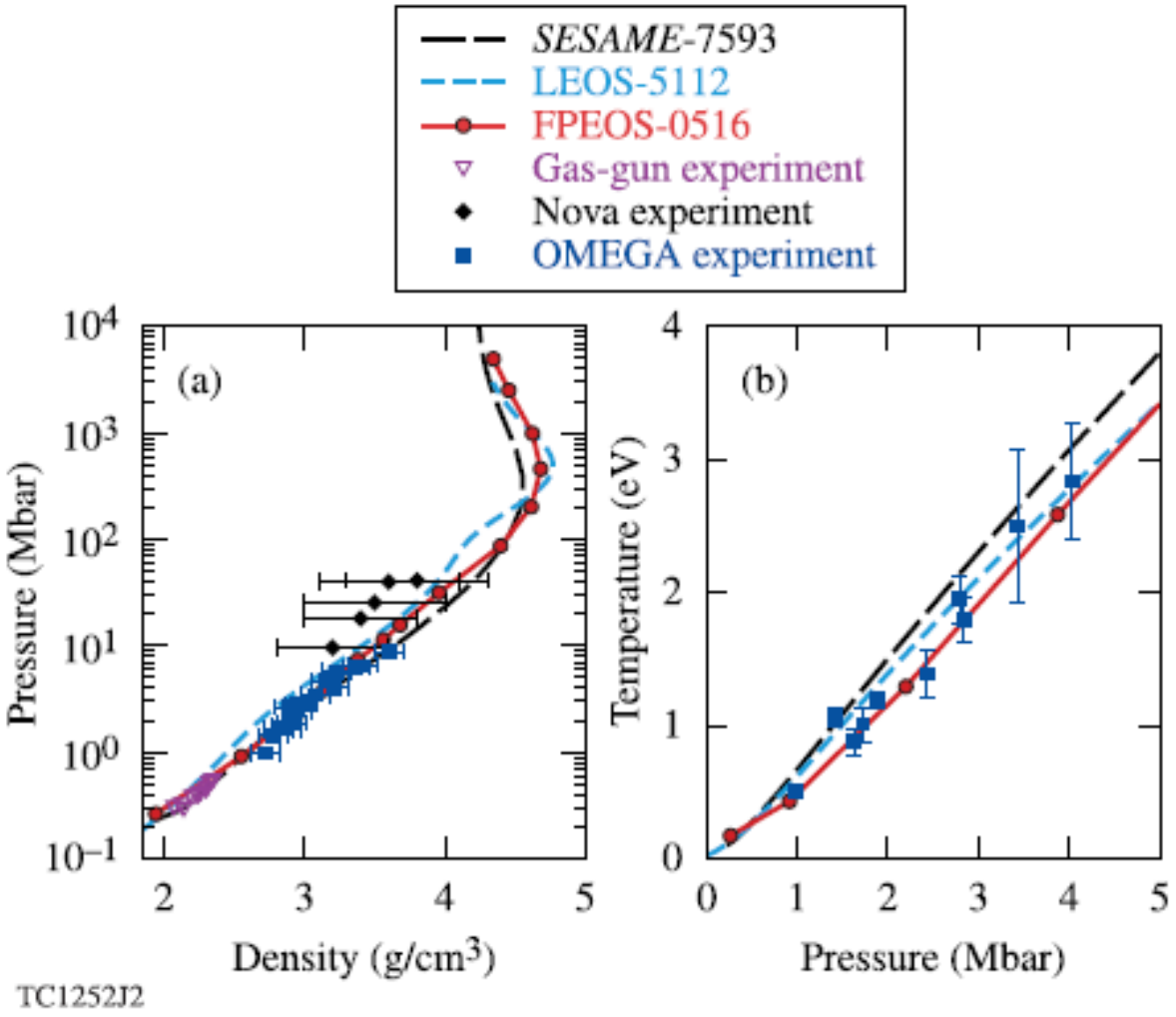


Si



*S. X. Hu *et al.*, Phys. Rev. E 92, 043104 (2015);
S. X. Hu *et al.*, Phys. Plasmas 23, 042704 (2016);
S. X. Hu *et al.*, Phys. Rev. B 94, 094109 (2016);
S. X. Hu *et al.*, Phys. Rev. E 95, 043210 (2017);
Y. H. Ding and S. X. Hu, Phys. Plasmas 24, 062702 (2017);
S. X. Hu, Phys. Rev. Lett. 119, 065001 (2017);
S. X. Hu *et al.*, Phys. Rev. B 96, 144203 (2017).

The calculated principal Hugoniot* of CH from FPEOS has been well compared with experiments



Recent EOS measurements at high pressures on NIF are in better agreement with FPEOS than SESAME-7592

PHYSICAL REVIEW LETTERS 121, 025001 (2018)

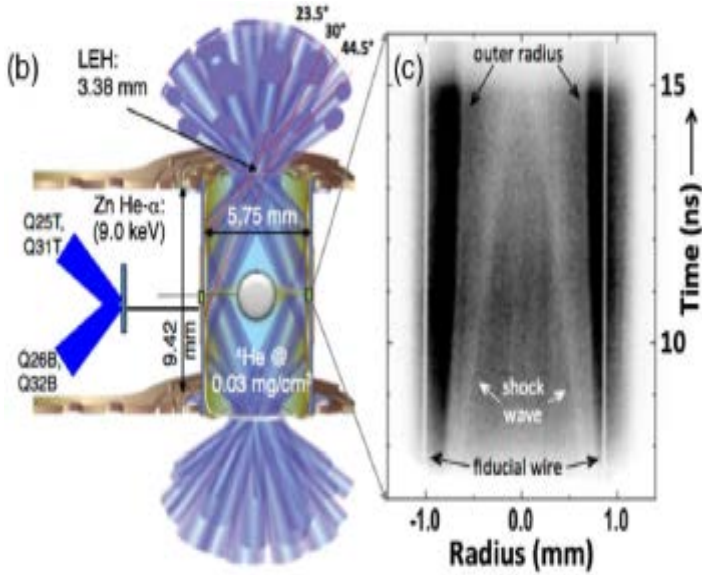
Absolute Equation-of-State Measurement for Polystyrene from 25 to 60 Mbar Using a Spherically Converging Shock Wave

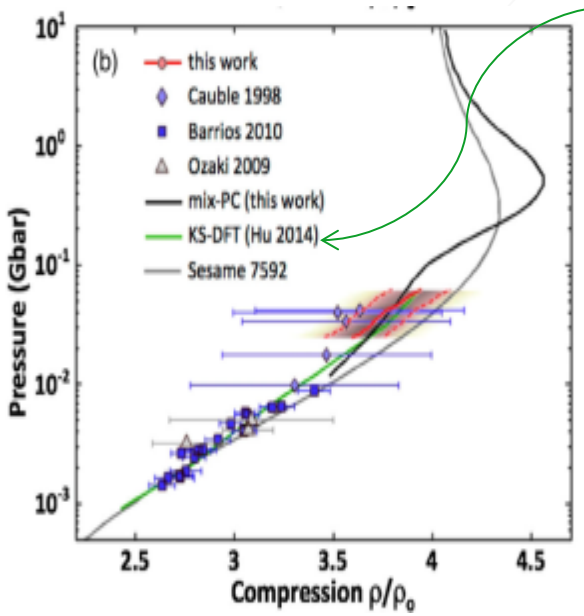
T. Döppner,[1,*] D. C. Swift,[1] A. L. Kritcher,[1] B. Bachmann,[1] G. W. Collins,[1,2] D. A. Chapman,[3] J. Hawreliak,[1] D. Kraus,[4,5] J. Nilsen,[1] S. Rothman,[3] L. X. Benedict,[1] E. Dewald,[1] D. E. Fratanduono,[1] J. A. Gaffney,[1] S. H. Glenzer,[6] S. Hamel,[1] O. L. Landen,[1] H. J. Lee,[6] S. LePape,[1] T. Ma,[1] M. J. MacDonald,[4] A. G. MacPhee,[1] D. Milathianaki,[6] M. Millot,[1] P. Neumayer,[7] P. A. Sterne,[1] R. Tommasini,[1] and R. W. Falcone[4]

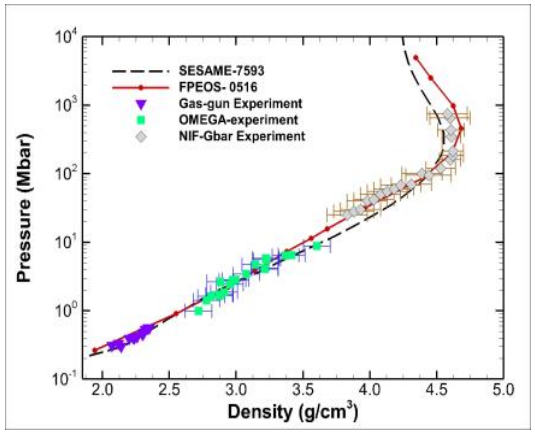
PHYSICAL REVIEW E 89, 063104 (2014)

Properties of warm dense polystyrene plasmas along the principal Hugoniot

S. X. Hu (胡素兴),[1,*] T. R. Boehly,[1] and L. A. Collins[2]
[1]Laboratory for Laser Energetics, University of Rochester, 250 East River Road, Rochester, New York 14623, US
[2]Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA
(Received 13 March 2014; published 30 June 2014)

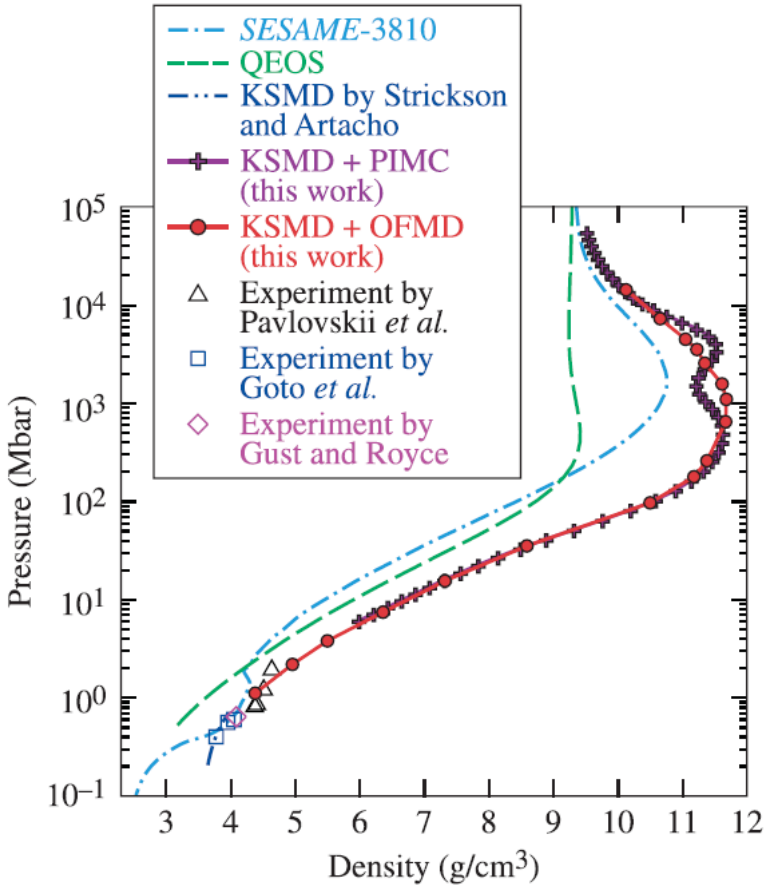




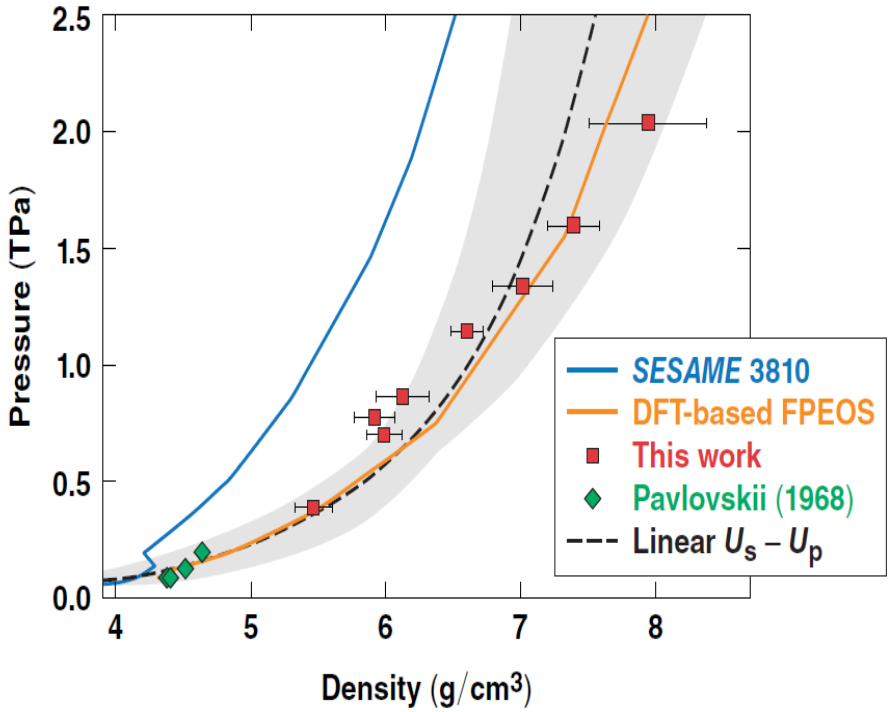


Thanks to Phil Sterne for file-format conversion, the FPEOS tables can now be accessed by HYDRA!

One more example: Our QMD study* has predicted a much softer Hugoniot of Si, which is proven to be true by recent experiments** on OMEGA-EP

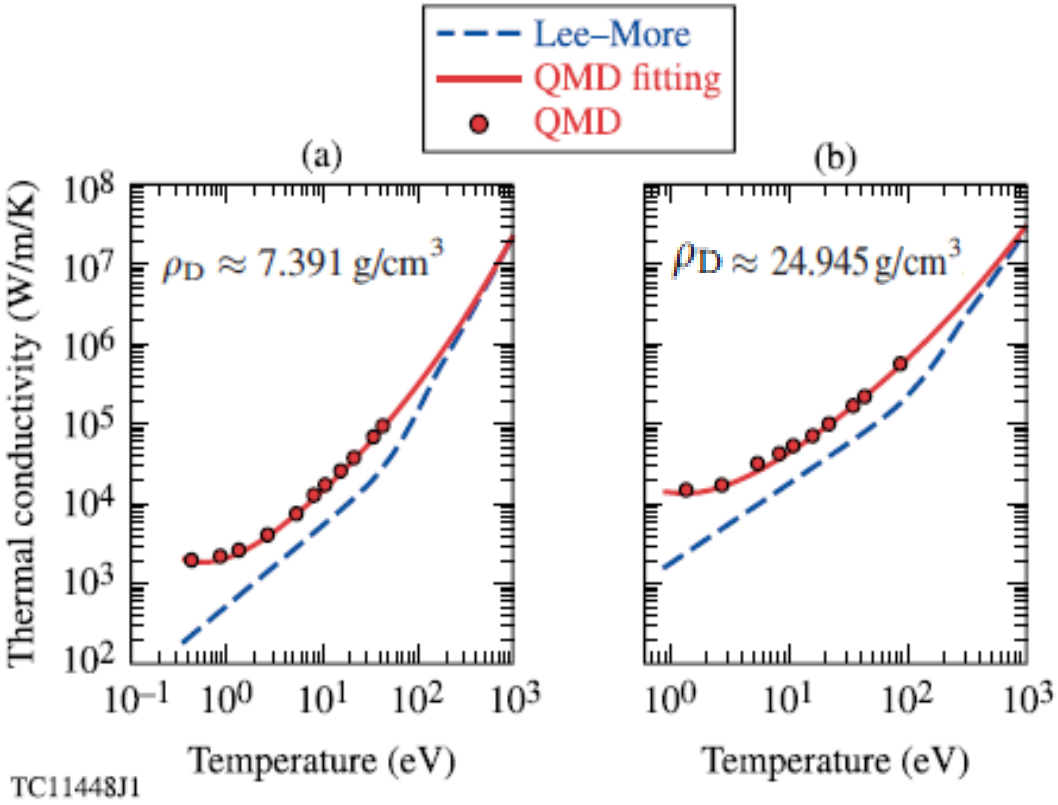


Recent experiments

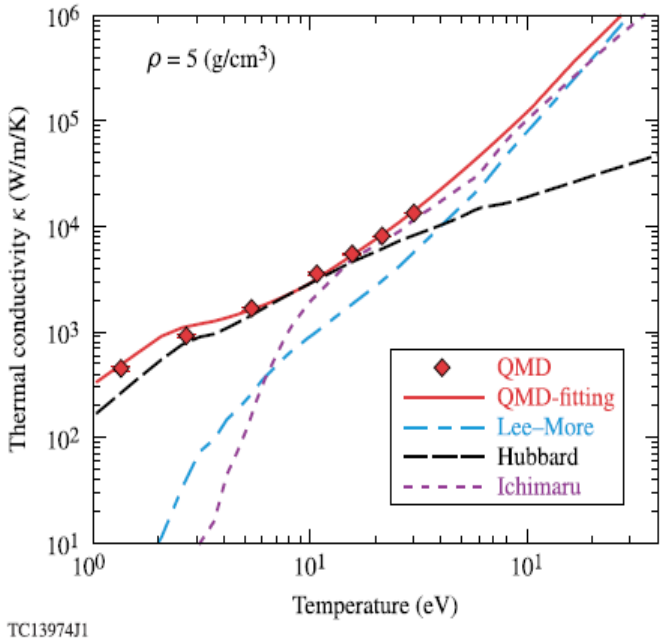


*S. X. Hu *et al.*, Phys. Rev. B 94, 094109 (2016).
** B. Henderson et al., talk at APS-DPP (2017).

Thermal conductivity models (κ_{QMD}) based on QMD calculations* has also been developed for D_2 and ablator materials [adopted into LANL's code: *Xrage***]



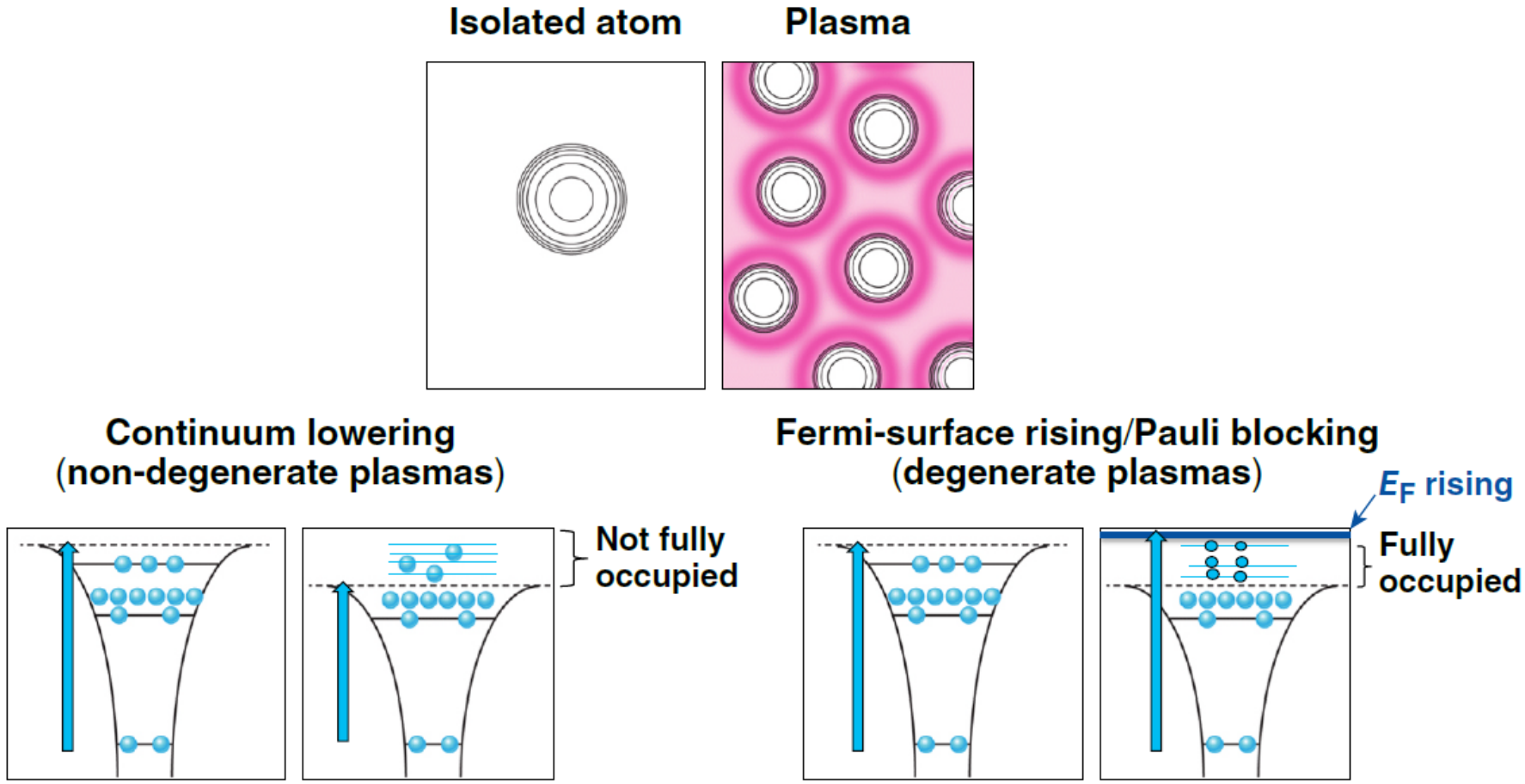
CH



The Coulomb-logarithm for electron-ion collisions is reduced in WDM condition

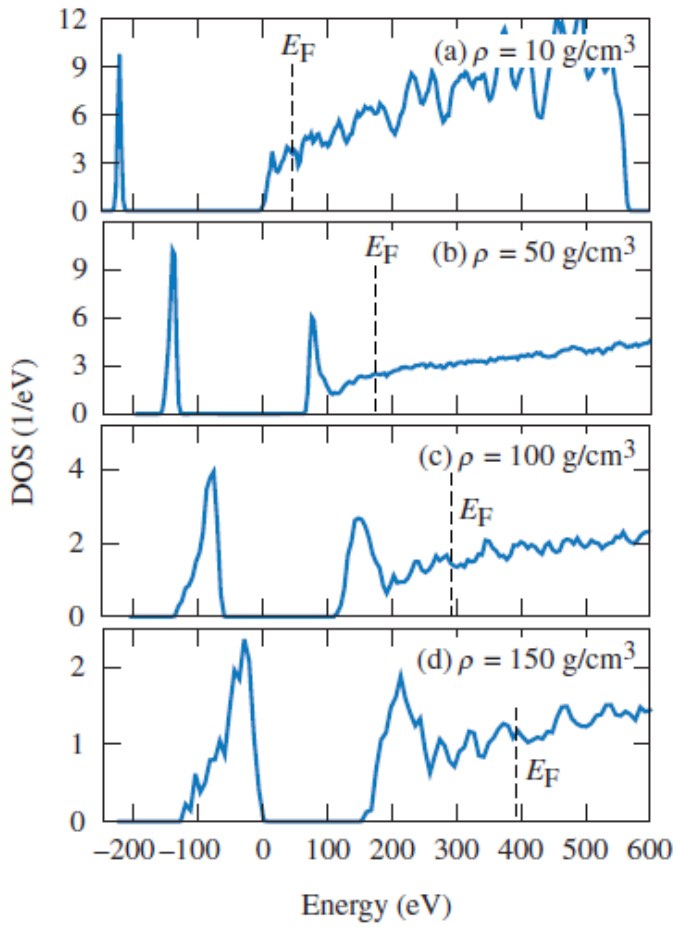
*S. X. Hu *et al.*, Phys. Plasmas 23, 042704 (2016).
** B. M. Haines *et al.*, Phys. Plasmas 26, 012707 (2019).

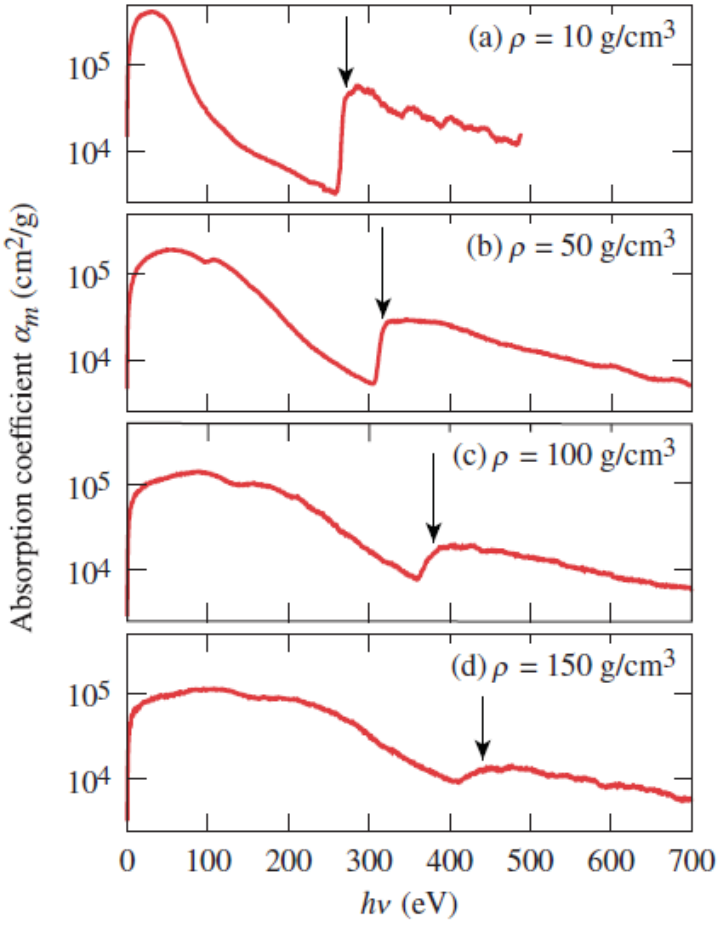
QMD calculations can also give us self-consistent optical properties of materials under HED conditions: *K-edge shifting as an example*



Both *continuum-lowering* and *Fermi-surface-rising* effects can be naturally included in QMD simulations

C at T = 1.35 eV



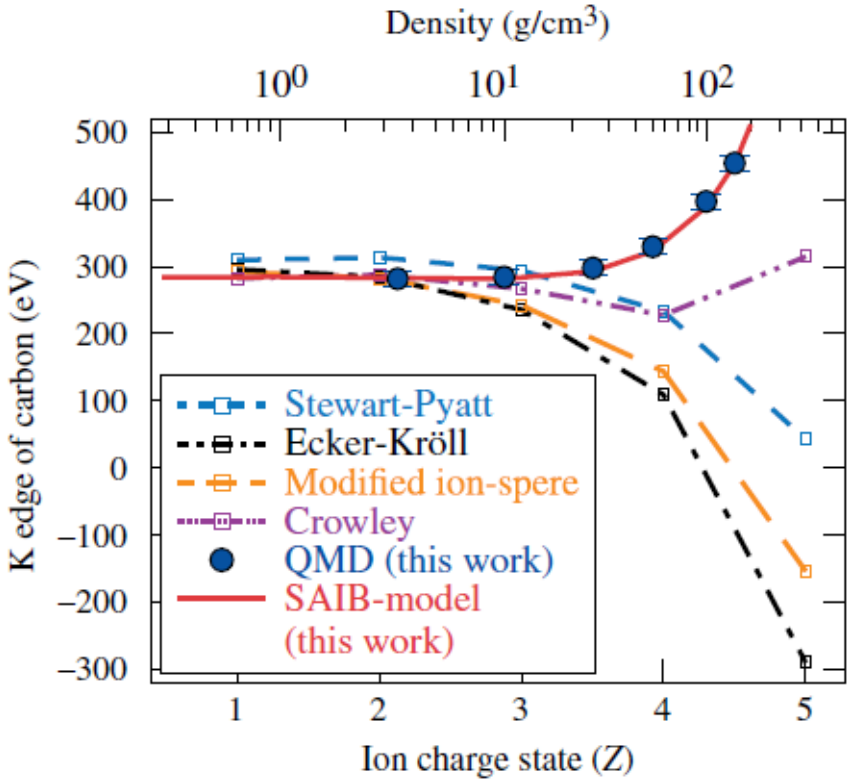


The *continuum-lowering* and *Fermi-surface-rising* (*Pauli-blocking*) can explain the K-edge up-shifting in strongly-coupled and degenerate dense plasmas

PRL 119, 065001 (2017) PHYSICAL REVIEW LETTERS week ending 11 AUGUST 2017

Continuum Lowering and Fermi-Surface Rising in Strongly Coupled and Degenerate Plasmas

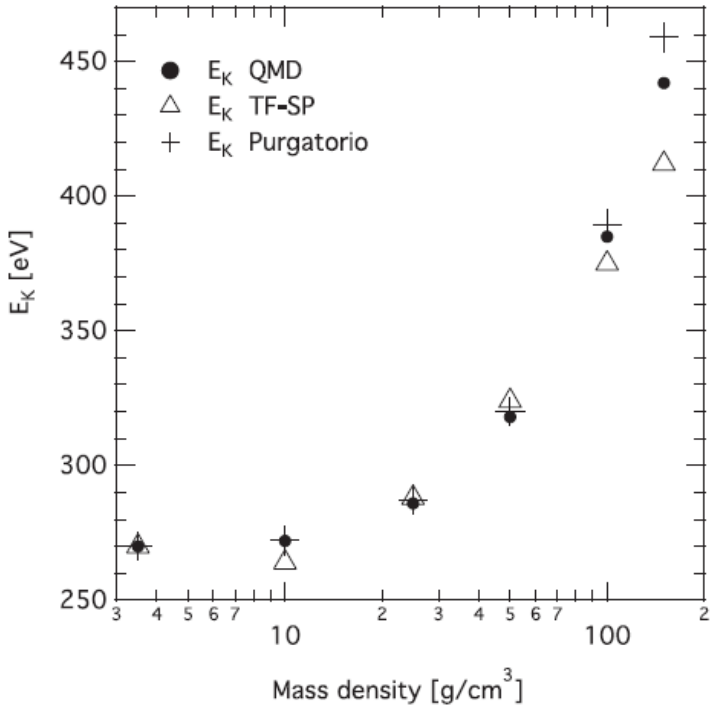
S. X. Hu (胡素兴)*
Laboratory for Laser Energetics, University of Rochester, 250 E. River Road, Rochester, New York 14623, USA
(Received 10 April 2017; published 10 August 2017)



PHYSICAL REVIEW LETTERS 120, 119501 (2018)

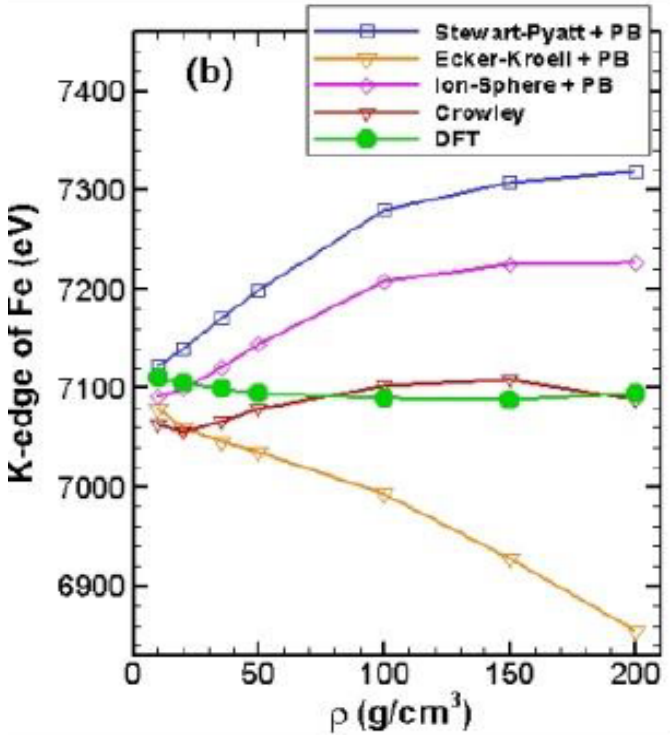
Comment on "Continuum Lowering and Fermi-Surface Rising in Strongly Coupled and Degenerate Plasmas"

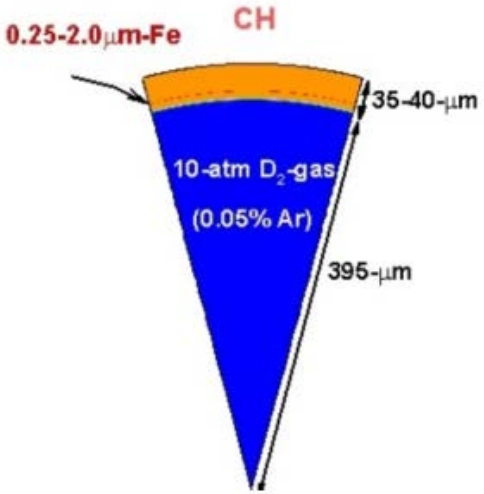
Carlos A. Iglesias and Philip A. Sterne
Lawrence Livermore National Laboratory

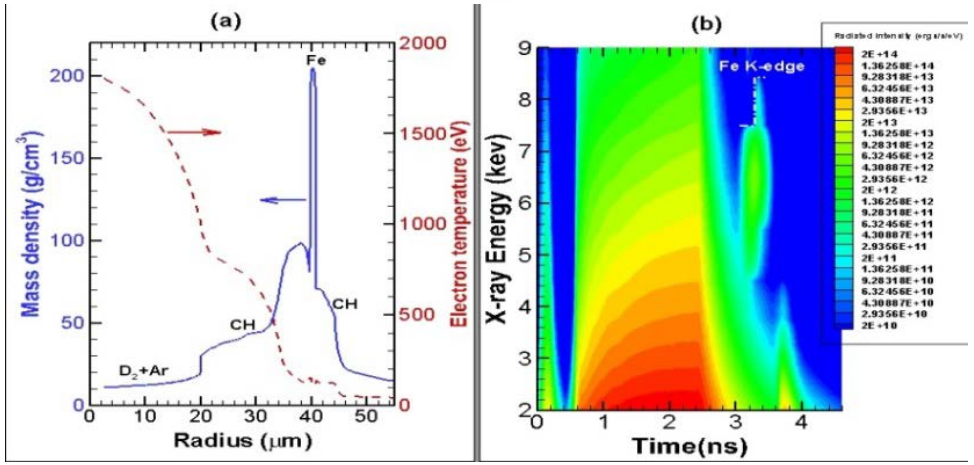


How our physics understanding may evolve for high-Z materials is waiting to be seen form our ExtremeDFT LBS campaigns

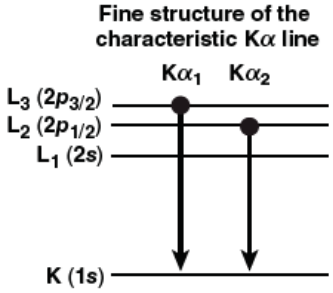
Experiments on iron K-edge shifting are proposed to test our DFT calculations



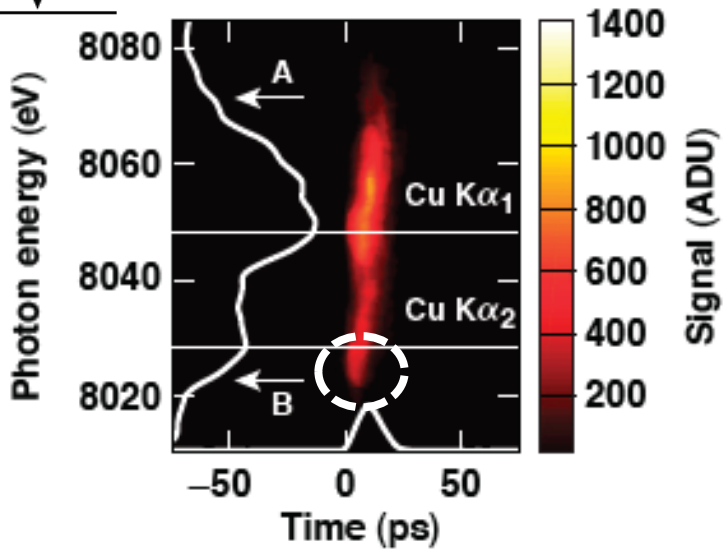




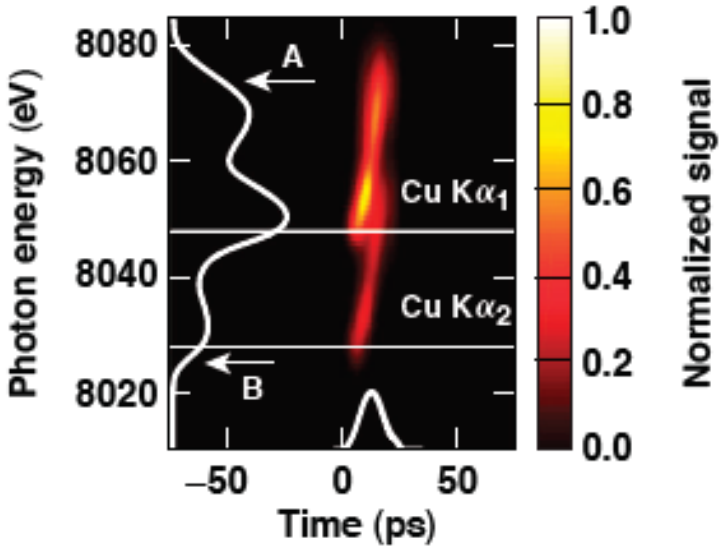
In addition, some existing experimental data* also indicated that traditional plasma-physics models do not catch all essential physics in HED conditions



K_α-emission from OMEGA-EP-heated solid-Cu targets



Laser: 905 J, 10 ps
Target: 250 × 250 × 10 μm Cu

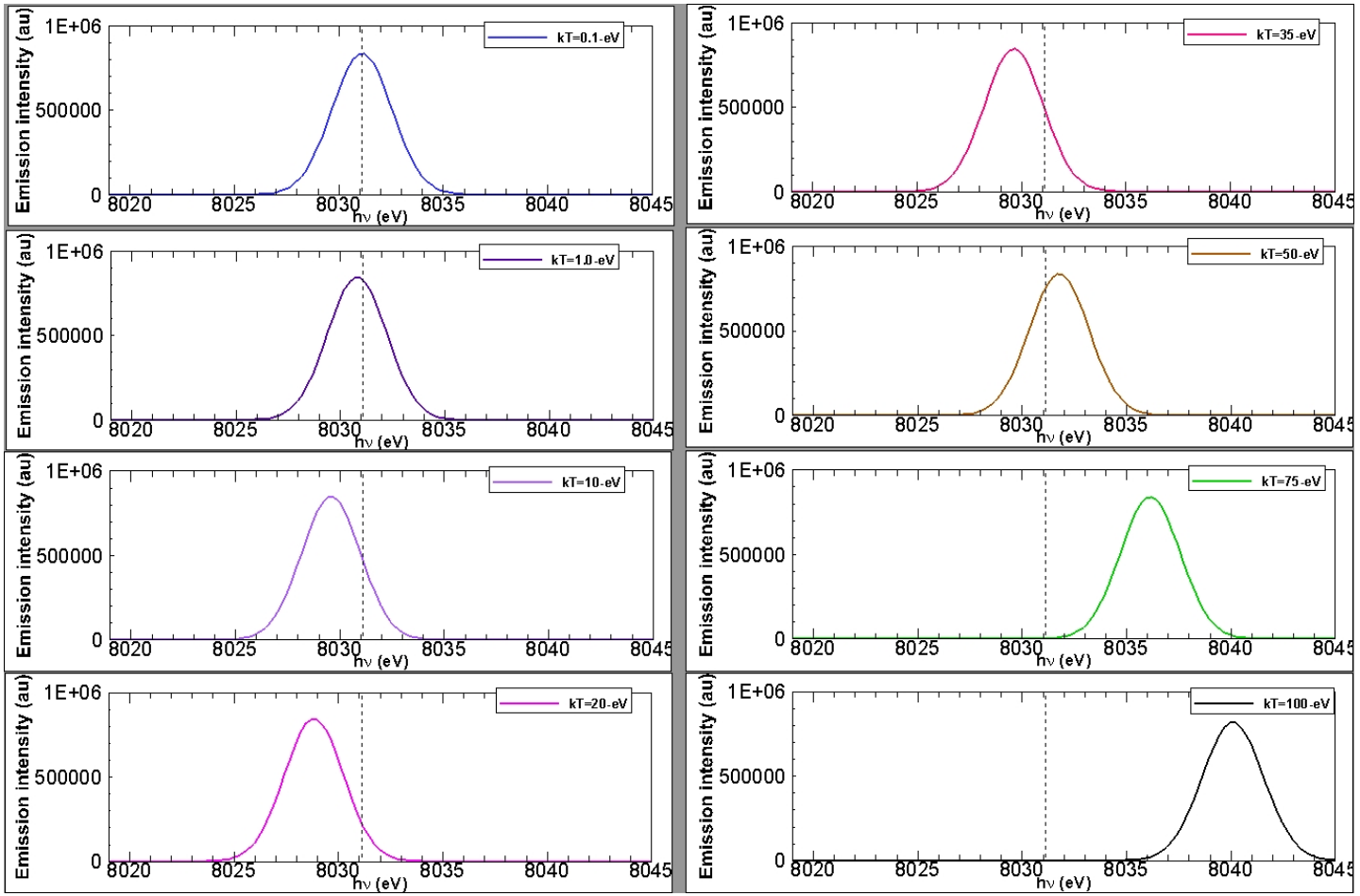


LSP/*PrismSPECT*
Stewart–Pyatt Model

*P. M. Nilson *et al.*, *APS-DPP Talk* (2018).

Preliminary DFT calculations show the red-shifts of Kα emission observed in experiment* when the target passes through warm-dense matter (WDM) regime

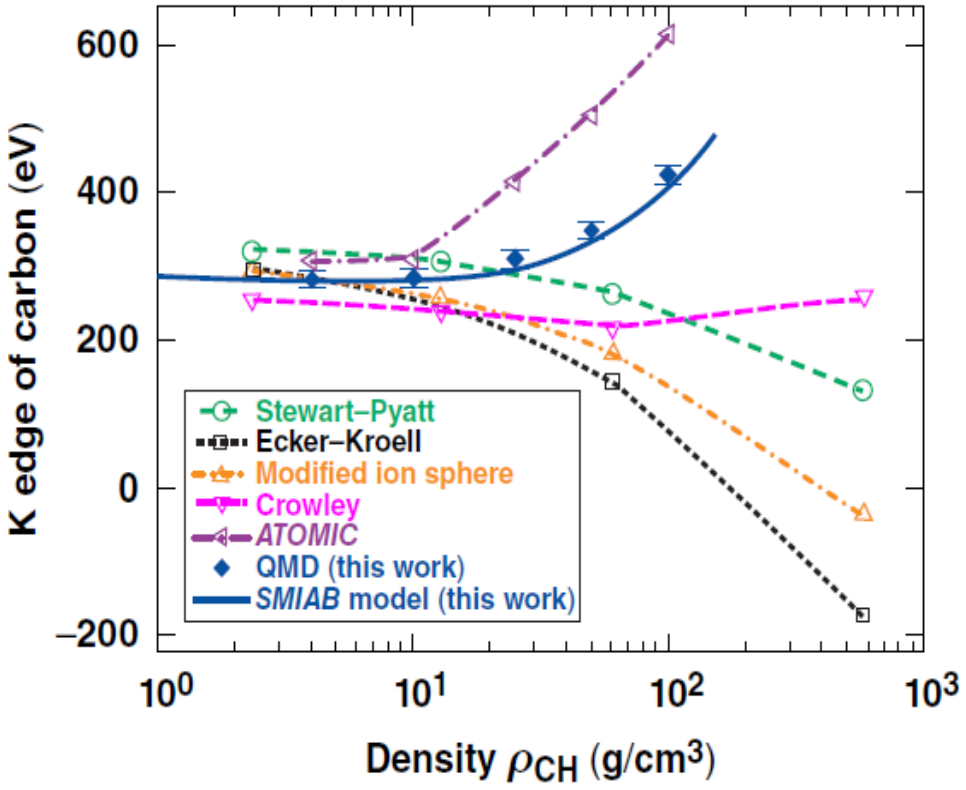
DFT-predicted K_α-line shifts in OMEGA-EP-heated solid-Cu target



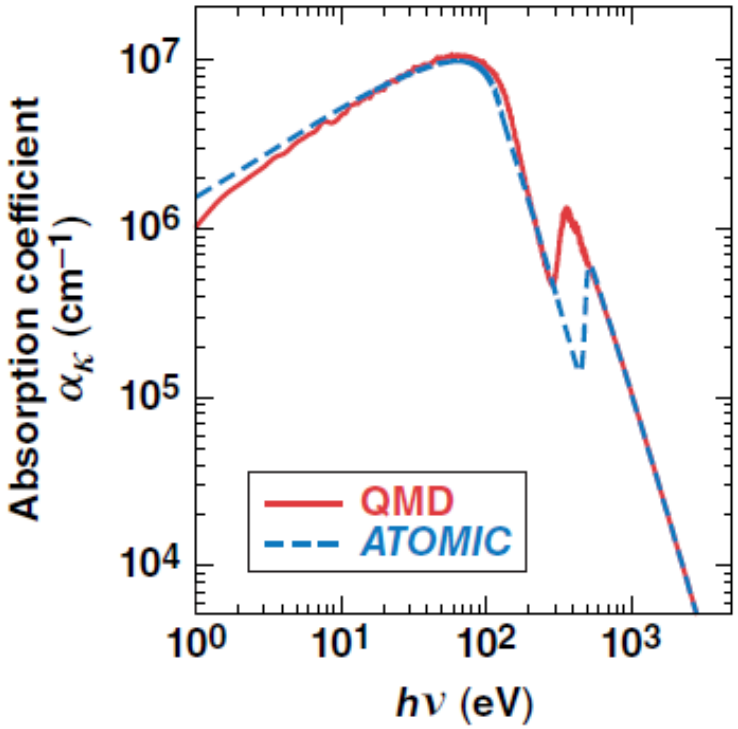
*P. M. Nilson *et al.*, *APS-DPP Talk* (2018).

Another challenge for traditional physics models is how to handle the mixture in dense plasmas (e.g., CH)

CH plasma at T = 10.77 eV



ρ = 50 g/cm^3 and T = 10.77 eV



*S. X. Hu *et al.*, Phys. Rev. B 96, 144203 (2017).
**N. R. Shaffer *et al.*, High Energy Density Phys. 23, 31 (2017).

Outline

- Introduction: *Why do we care about high-energy-density physics (HEDP) as ICF scientists?*
- What are our "*first-principles toolkits*" to understand HED matter as a *quantum many-body system*?
  - Density-Functional-Theory (DFT)
  - Path-integral Monte-Carlo (PIMC)
  - Quantum Monte-Carlo (QMC)

- ***First-principles*-based and *self-consistent* material properties under extreme conditions for ICF/HED applications:**
  - ❖ What have we learned so far?
  - ❖ **How do these knowledges impact on the ICF community?**
- Some recent focuses in a broad HEDS arena
- Conclusion & Outlook

Several different experimental observables show better agreement with FPEOS than *SESAME* EOS for CH

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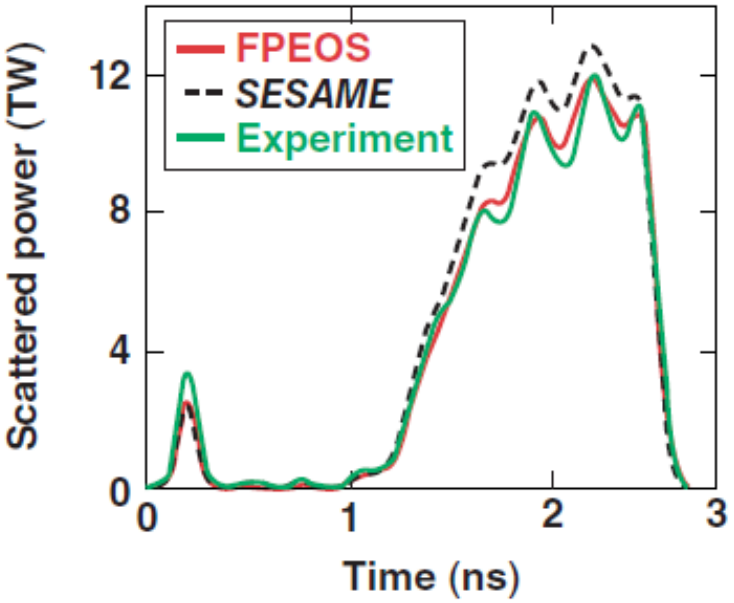
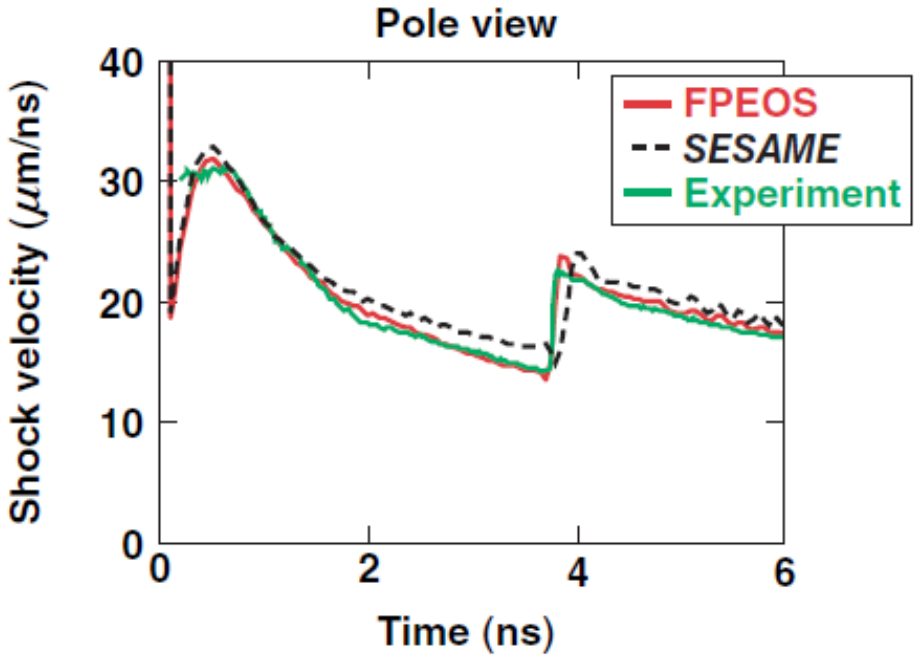
Time-resolved, scattered-light OMEGA implosion

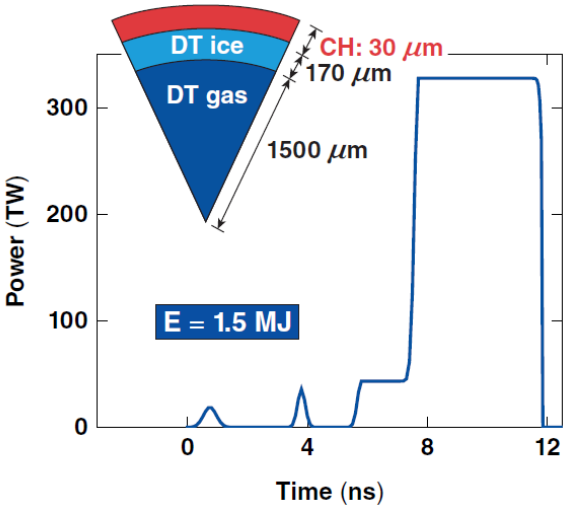


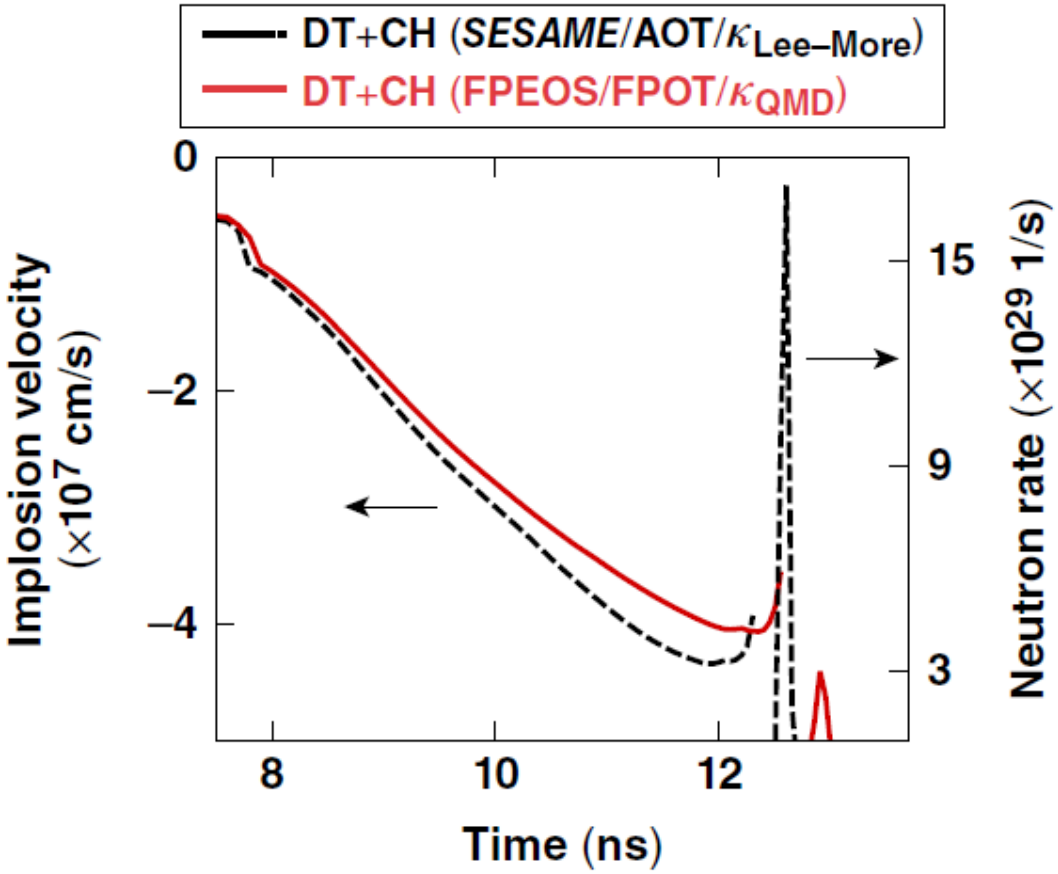
Low-intensity* NIF shock-timing experiment (N151025-001)



*P. B. Radha *et al.*, "Shock Velocity Measurements at the National Ignition Facility," to be submitted to Physical Review E.

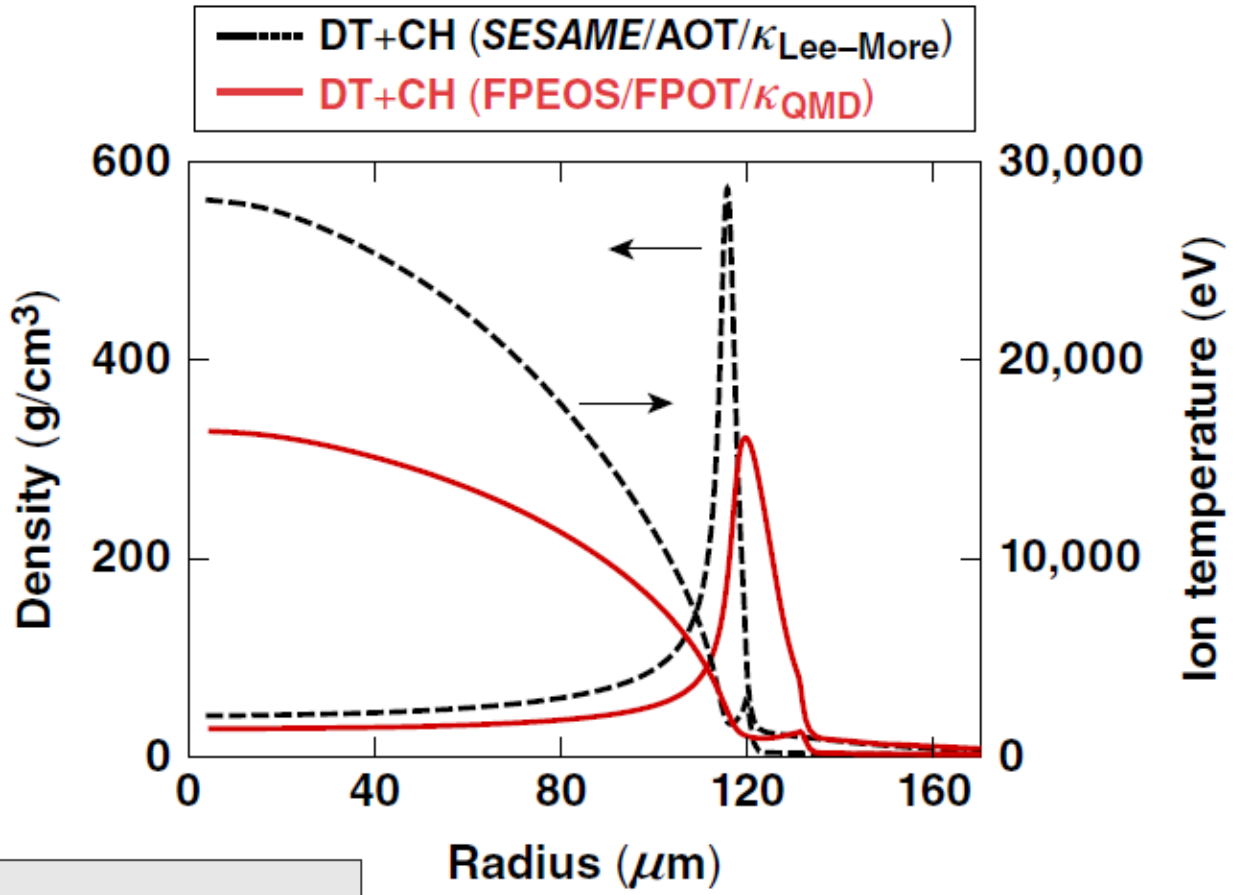
How did these first-principles properties of HED plasmas affect ICF target designs?





The major differences are due to: DT-EOS, DT-Opacity, and CH-EOS

Significant variations have been seen in direct-drive ICF target designs with first-principles plasma properties



1-D target gain:
G = 31 (*SESAME*/AOT/$\kappa_{Lee–More}$)
G = 8 (FPEOS/FPOT/κ_{QMD})

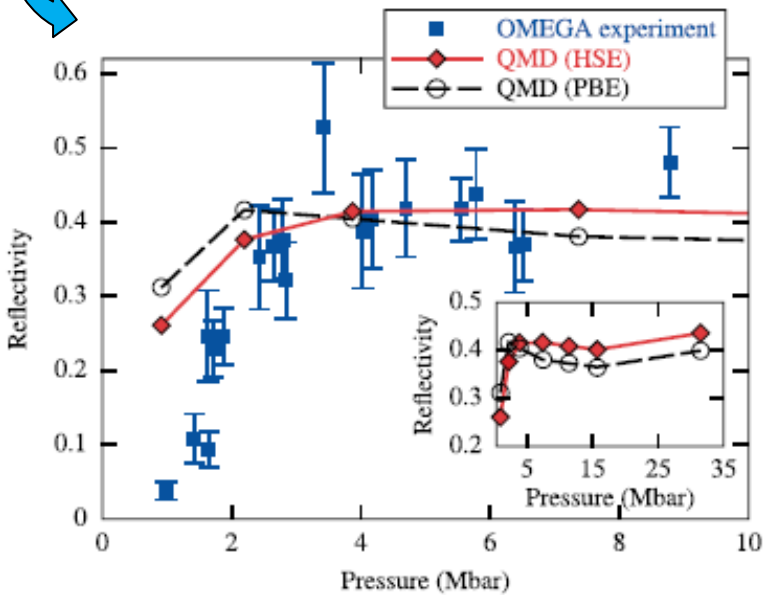
* S. X. Hu *et al.*, Phys. Plasmas 25, 056306 (2018).

Outline

- Introduction: *Why do we care about high-energy-density physics (HEDP) as ICF scientists?*
- What are our "*first-principles toolkits*" to understand HED matter as a *quantum many-body system*?
  - Density-Functional-Theory (DFT)
  - Path-integral Monte-Carlo (PIMC)
  - Quantum Monte-Carlo (QMC)
- *First-principles*-based and *self-consistent* material properties under extreme conditions for ICF/HED applications:
  - What have we learned so far?
  - How do these knowledge impact on the ICF community?
- **Some recent focuses in a broad HEDS arena**
- Conclusion & Outlook

What are the current limits of DFT? How can we improve it for better understanding HEDS?

- Most of the current exchange-correlation functionals underestimate band-gaps of materials*;
- Current exchange-correlation functionals do NOT have temperature dependence*;
- Current DFT implementations are using plane-wave basis and pseudopotentials, which have *frozen* core-electrons.



PHYSICAL REVIEW LETTERS 120, 076401 (2018)

Nonempirical Semilocal Free-Energy Density Functional for Matter under Extreme Conditions

Valentin V. Karasiev,[1,2,*] James W. Dufty,[3] and S. B. Trickey[1]
[1]*Quantum Theory Project, Department of Physics and Department of Chemistry, University of Florida, P.O. Box 118435, Gainesville, Florida 32611-8435, USA*
[2]*Laboratory for Laser Energetics, University of Rochester, 250 East River Road, Rochester, New York 14623, USA*
[3]*Department of Physics, University of Florida, P.O. Box 118435, Gainesville, Florida 32611-8435, USA*

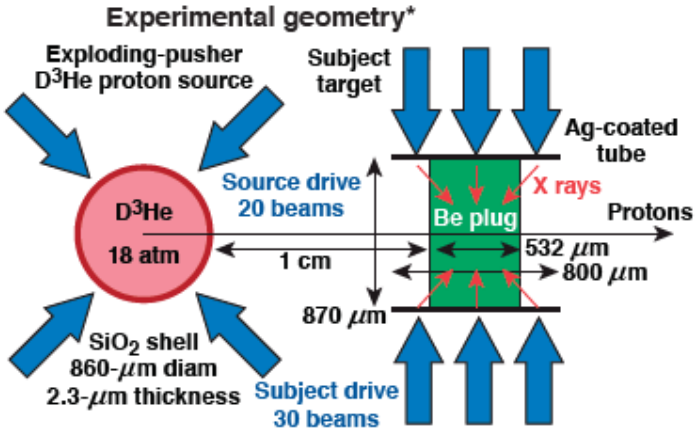
(Received 19 December 2016; revised manuscript received 30 August 2017; published 14 February 2018)

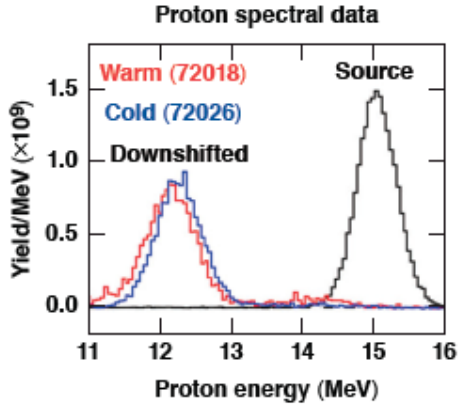
Realizing the potential for predictive density functional calculations of matter under extreme conditions depends crucially upon having an exchange-correlation (XC) free-energy functional accurate over a wide range of state conditions. Unlike the ground-state case, no such functional exists. We remedy that with systematic construction of a generalized gradient approximation XC free-energy functional based on rigorous constraints, including the free-energy gradient expansion. The new functional provides the correct temperature dependence in the slowly varying regime and the correct zero-T, high-T, and homogeneous electron gas limits. Its accuracy in the warm dense matter regime is attested by excellent agreement of the calculated deuterium equation of state with reference path integral Monte Carlo results at intermediate and elevated T. Pressure shifts for hot electrons in compressed static fcc Al and for low-density Al demonstrate the combined magnitude of thermal and gradient effects handled well by this functional over a wide T range.

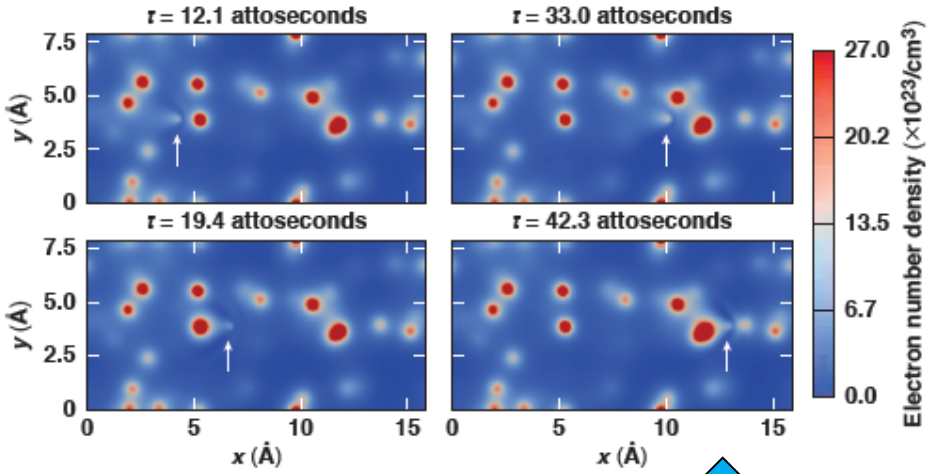
These efforts are also supported by an NSF grant

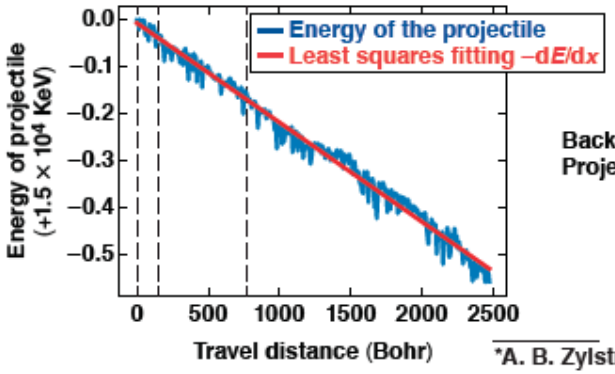
Time-Dependent Orbital-Free DFT (TD-OF-DFT)code has been developed in our group to understand stopping-power of warm-dense plasmas

proton stopping in warm-dense Be (solid @ kT=32-eV)









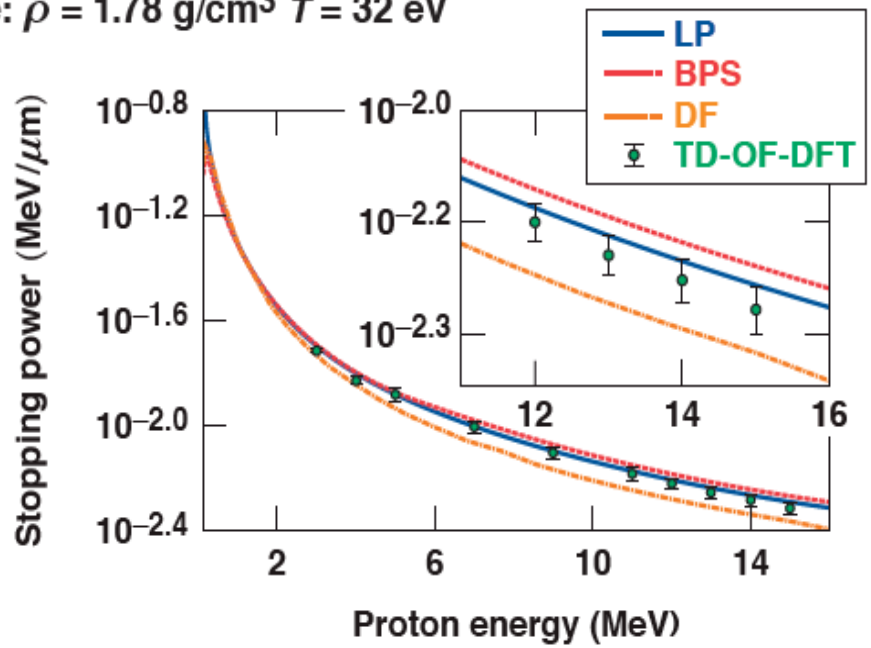
Background: Be plasma at 1.78 g/cm^3
Projectile: proton at 1 MeV

*A. B. Zylstra *et al.*, Phys. Rev. Lett. 114, 215002 (2015).

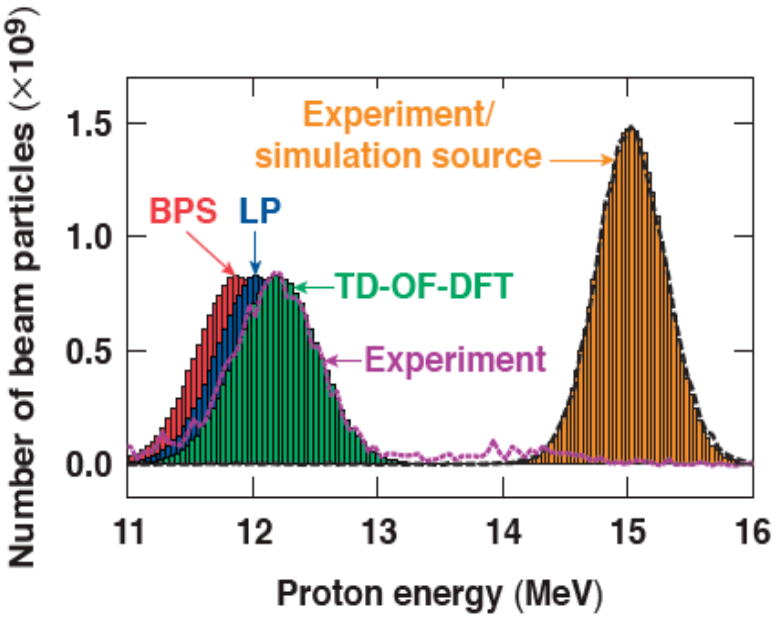
The TD-OF-DFT-calculated proton stopping power in high velocities in comparison with three stopping-power models

UR LLE

Be: $\rho = 1.78$ g/cm^3 $T = 32$ eV



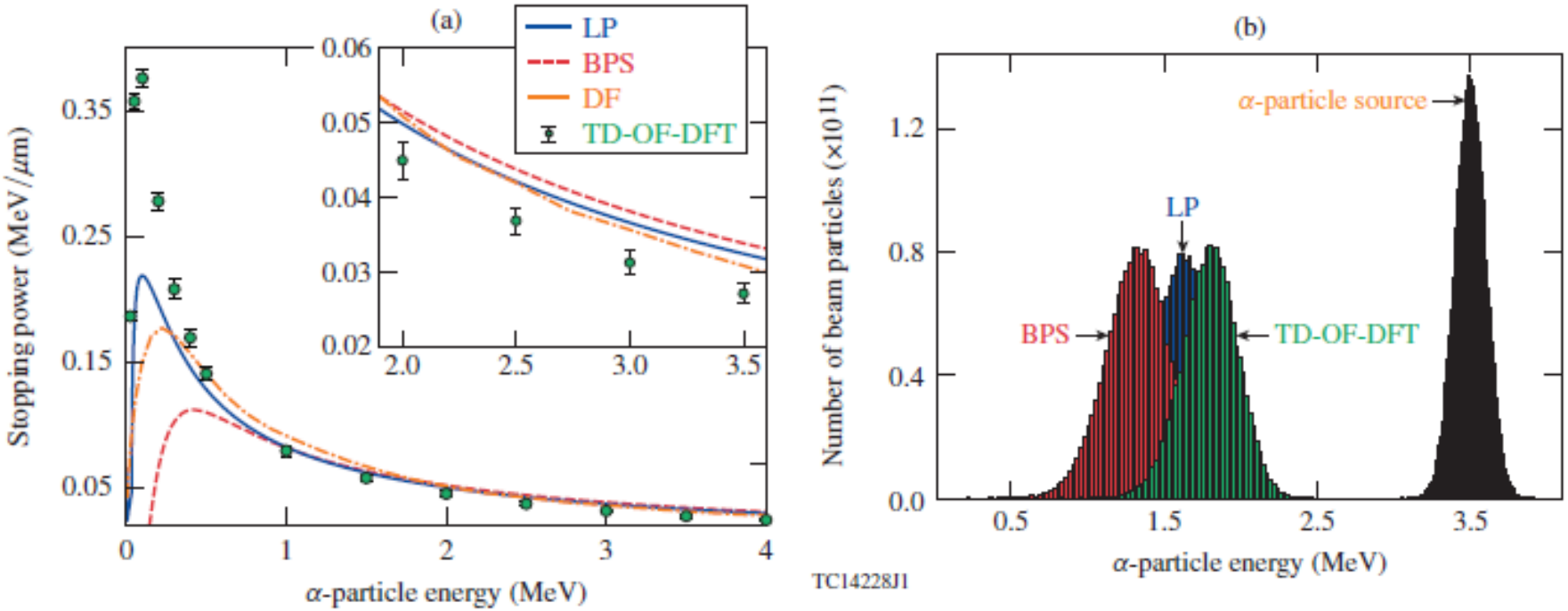
in comparison with experiment



The stopping power calculated by TD-OF-DFT is slightly lower than predictions of the LP and BPS models by ~5% and ~11%, respectively, and higher than predicted by DF by 20%.

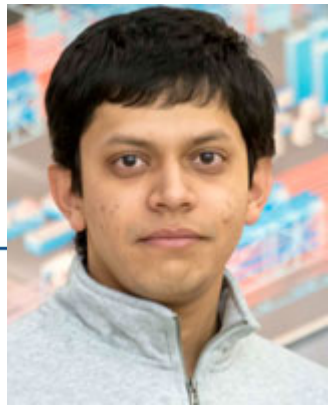
Ab-initio TD-OF-DFT calculations* indicated up to ~25% lower α-particle stopping-power in warm-dense DT than current models

α-particle stopping in warm-dense DT (solid @ kT=10-eV)

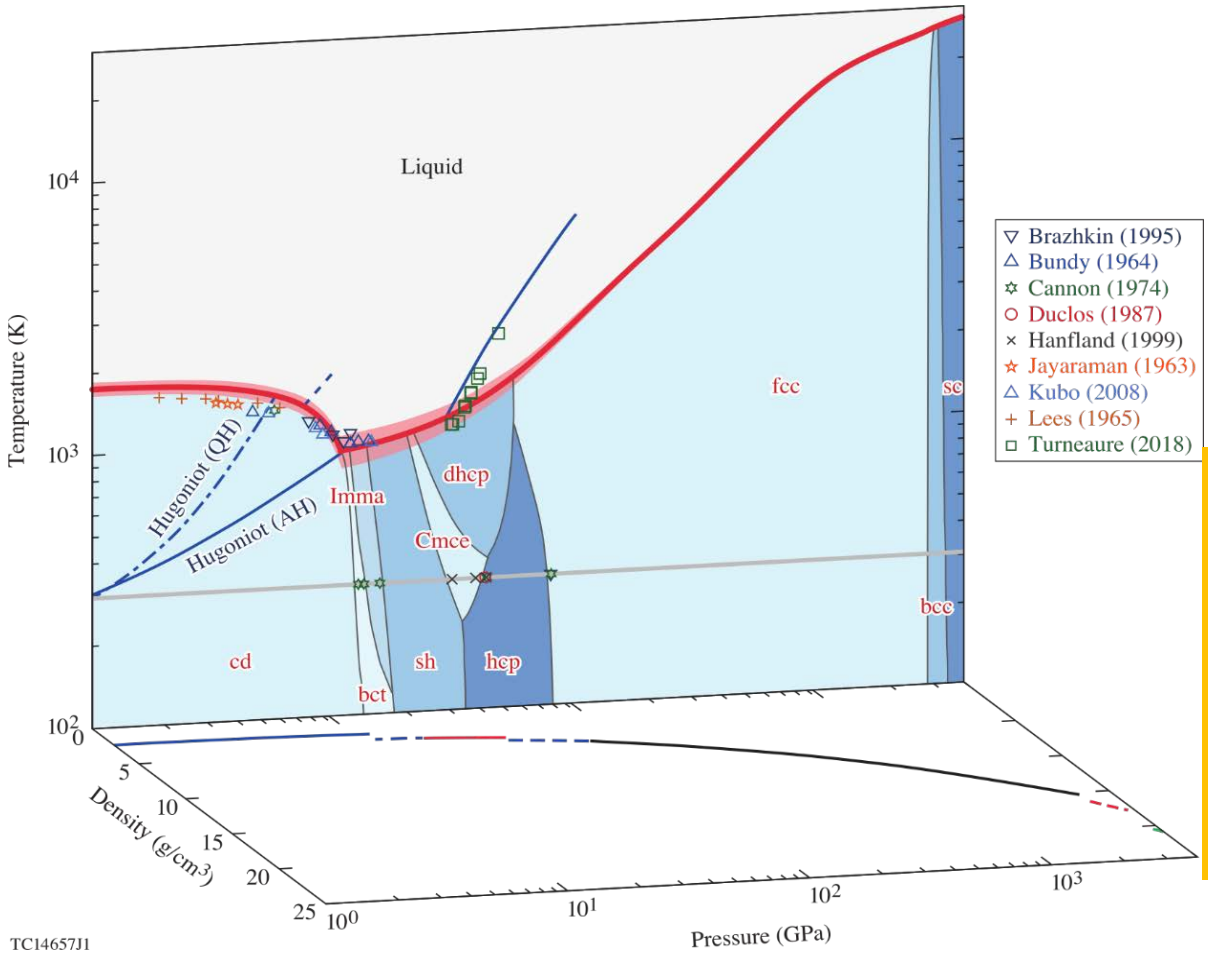


* Y. H. Ding , A. J. White, S. X. Hu, O. Certik, and L. A. Collins, Phys. Rev. Lett. 121, 145001 (2018).

High-pressure phase diagram of silicon up to ~4-TPa has been charted from *first-principles* DFT + Phonon-dynamics calculations*



Reetam Paul

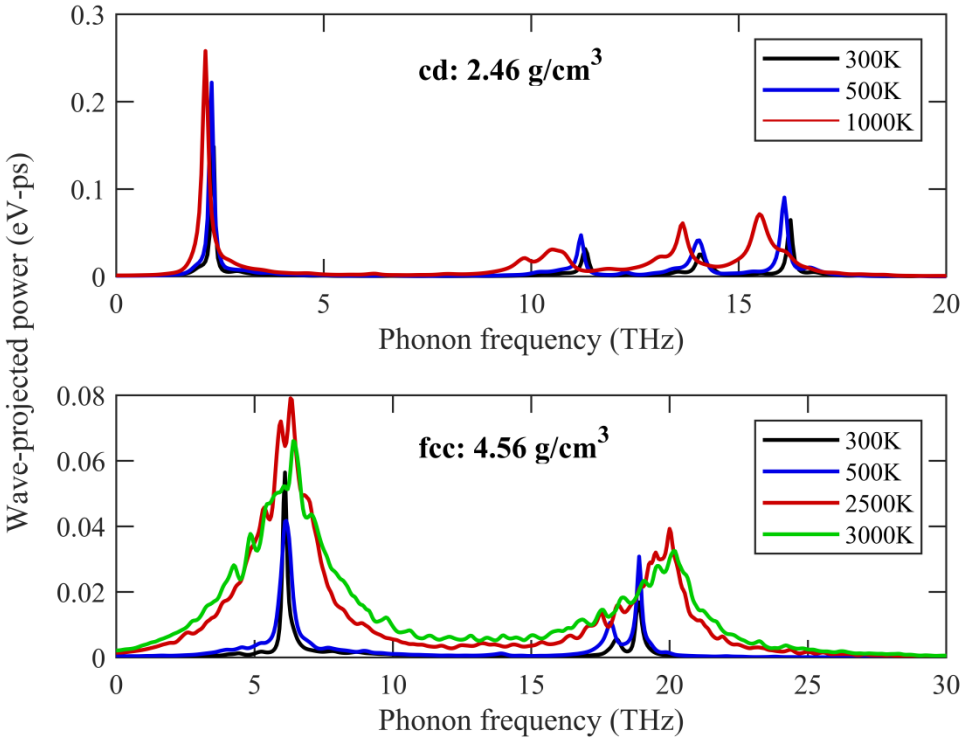


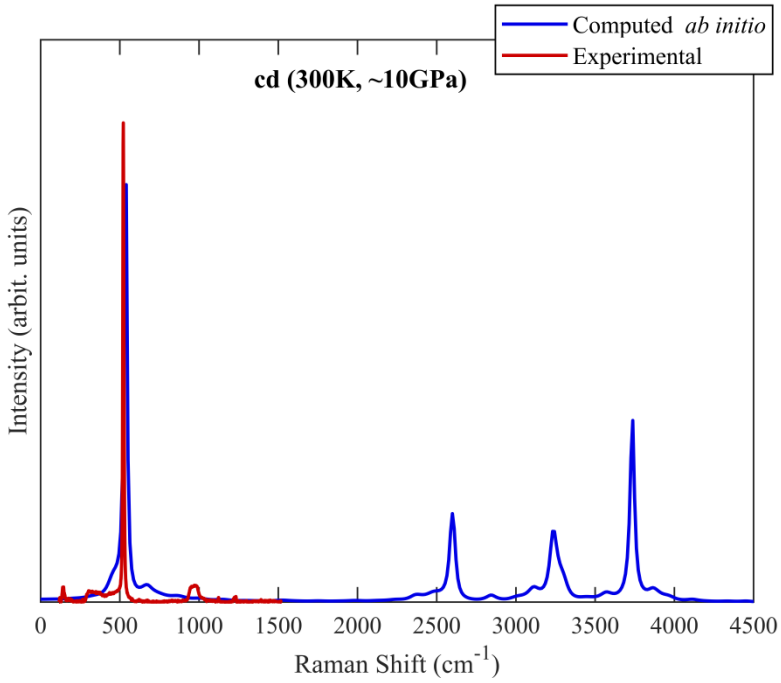
- **Anharmonic behavior of Si in the *cd* phase is important for properly predicting the shock Hugoniot at low pressures**
- **Two new phase transitions are predicted at ~2.8-/3.5-TPa: *fcc-to-bcc* & *bcc-to-sc***

*** R. Paul, S. X. Hu, V. V. Karasiev, Phys. Rev. Lett. (submitted)**

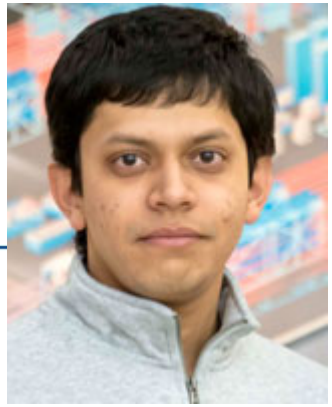
The phonon spectra (of ion vibration modes), a characteristic of different phases, can be picked up by Raman scattering measurements

Reetam Paul

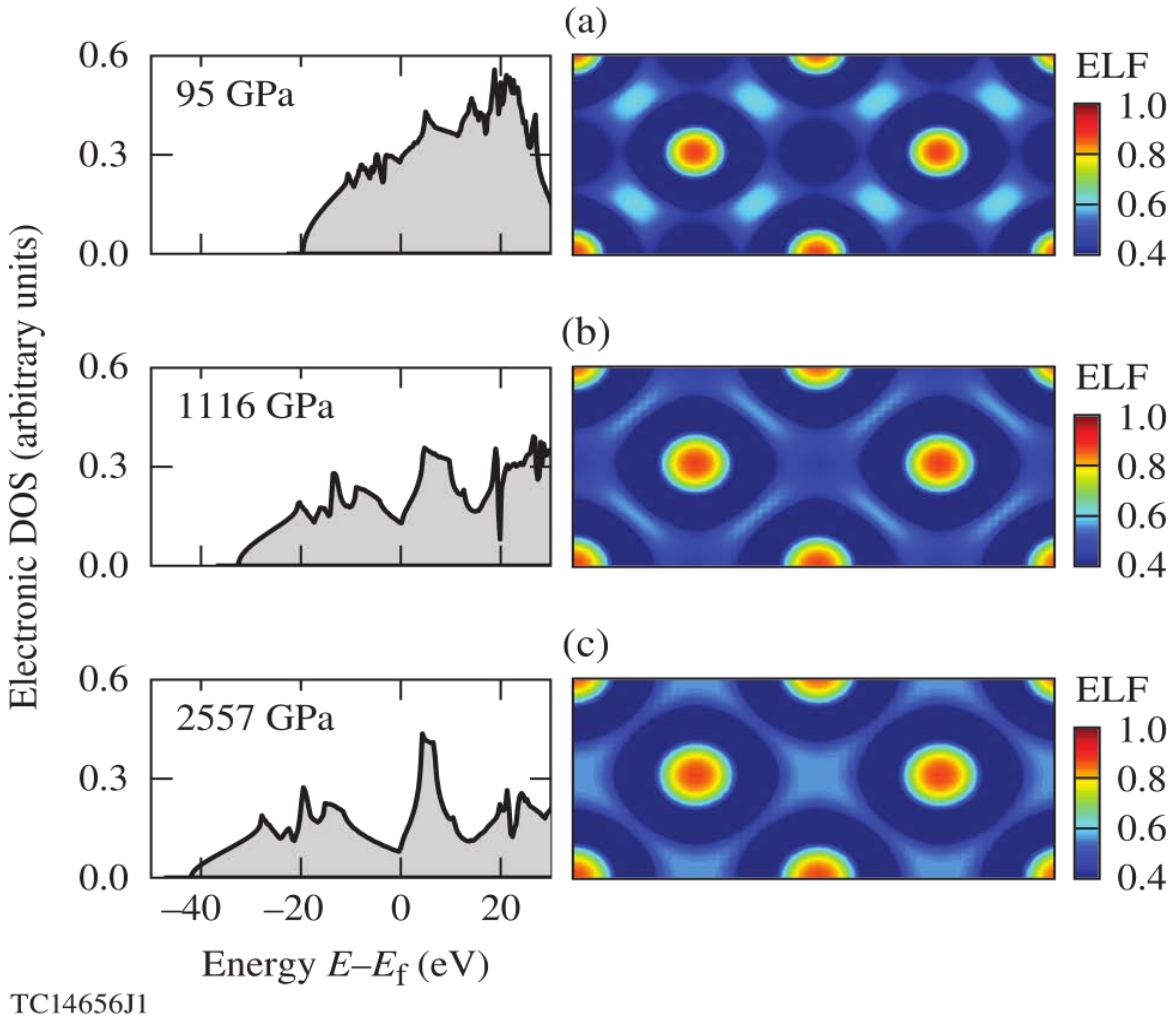




Under high pressures up to ~4-Tpa, silicon is still a metallic system even though interstitial electron localization appears (hydride-like)



Reetam Paul



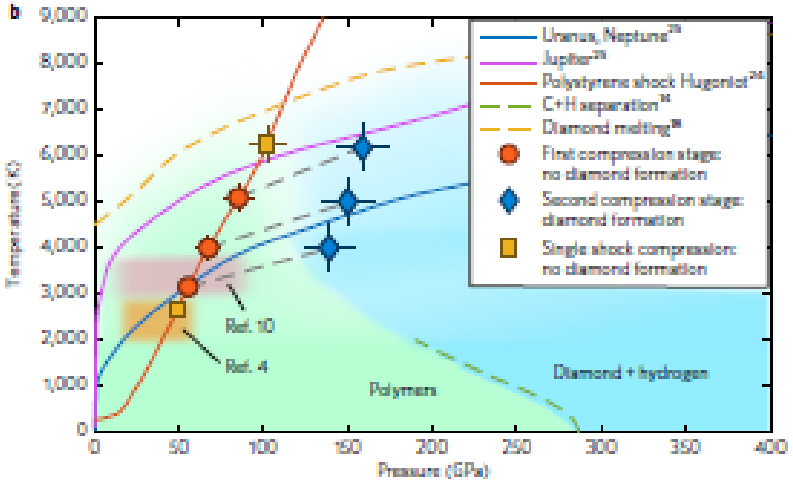
How can diamond be formed in polystyrene (CH), methane (CH_4), and other hydro-carbons under dynamic compression?

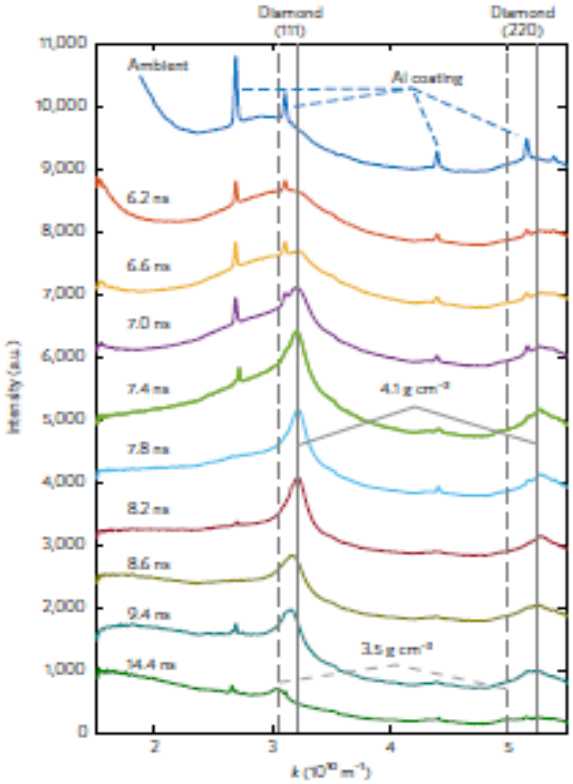
Maitrayee Ghosh

LETTERS
DOI: 10.1038/s41550-017-0219-9
nature astronomy

Formation of diamonds in laser-compressed hydrocarbons at planetary interior conditions

D. Kraus[1,2,3*], J. Vorberger[1], A. Pak[4], N. J. Hartley[1,5], L. B. Fletcher[6], S. Frydrych[4,7], E. Galtier[6], E. J. Gamboa[6], D. O. Gericke[8], S. H. Glenzer[6], E. Granados[6], M. J. MacDonald[6,9], A. J. MacKinnon[6], E. E. McBride[6,10], I. Nam[6], P. Neumayer[11], M. Roth[7], A. M. Saunders[2], A. K. Schuster[3], P. Sun[6,12], T. van Driel[6], T. Döppner[4] and R. W. Falcone[2,13]





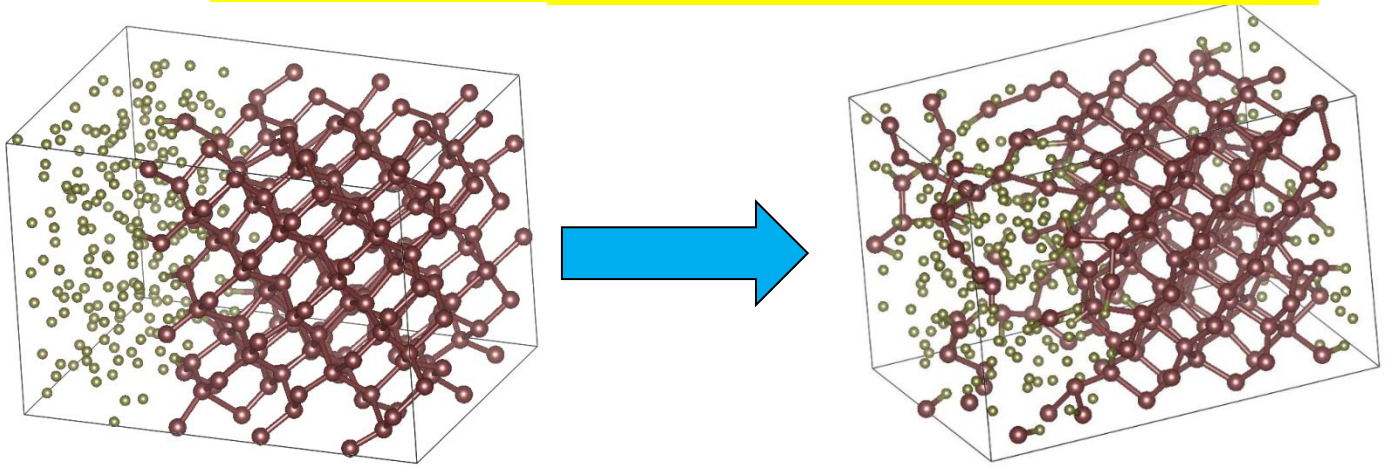
Questions remain: How did this happen? where are the hydrogen atoms? …

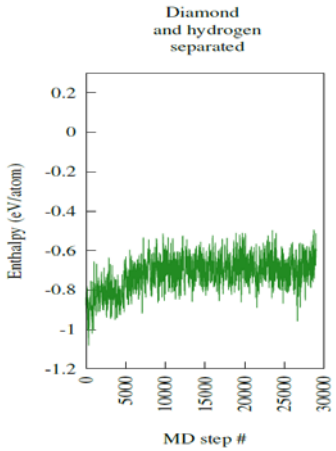
Where are the hydrogen atoms when diamond is formed?

Diamond+H ➔ CH-mixture @ ~150-Gpa?

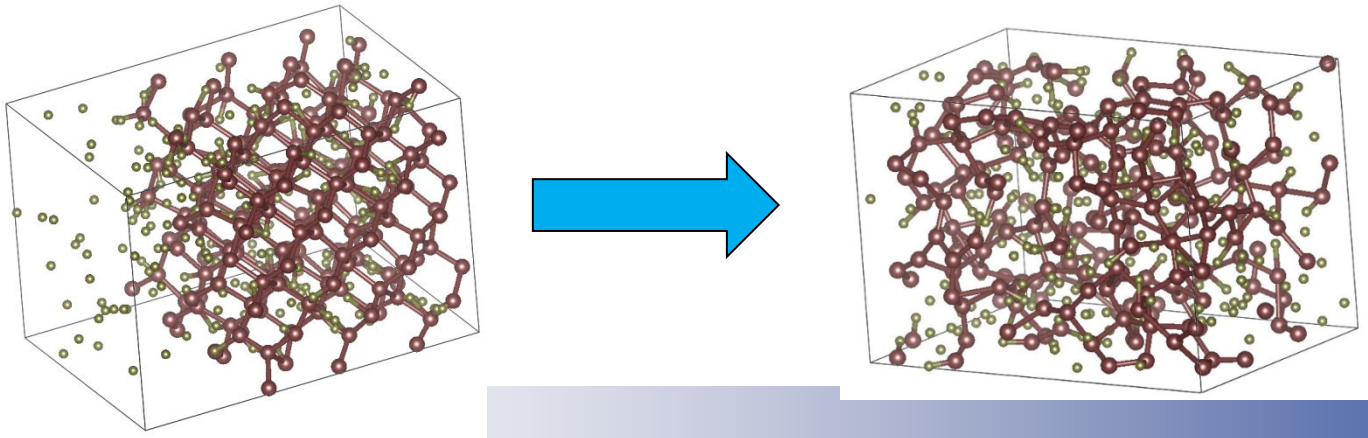
Maitrayee Ghosh

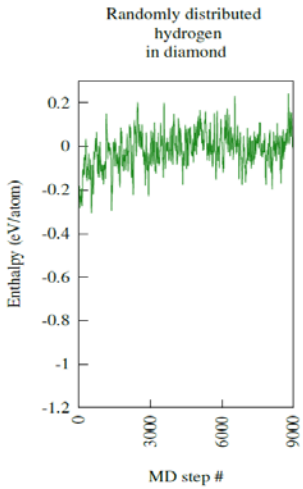
Case-1: Hydrogen sitting side-by-side with diamond





Case-2: Hydrogen randomly distributed in diamond





Back to the simplest element --- Hydrogen: The understanding of its optical property is still not complete ➔ better xc-functional? quantum-p?

Josh Hinz

PNAS

Conductivity and dissociation in liquid metallic hydrogen and implications for planetary interiors

Mohamed Zaghoo[a] and Isaac F. Silvera[a,1]

[a]Lyman Laboratory of Physics, Harvard University, Cambridge, MA 02138

Edited by Vladimir E. Fortov, Russian Academy of Sciences, Moscow, and approved September 7, 2017 (received for review May 12, 2017)

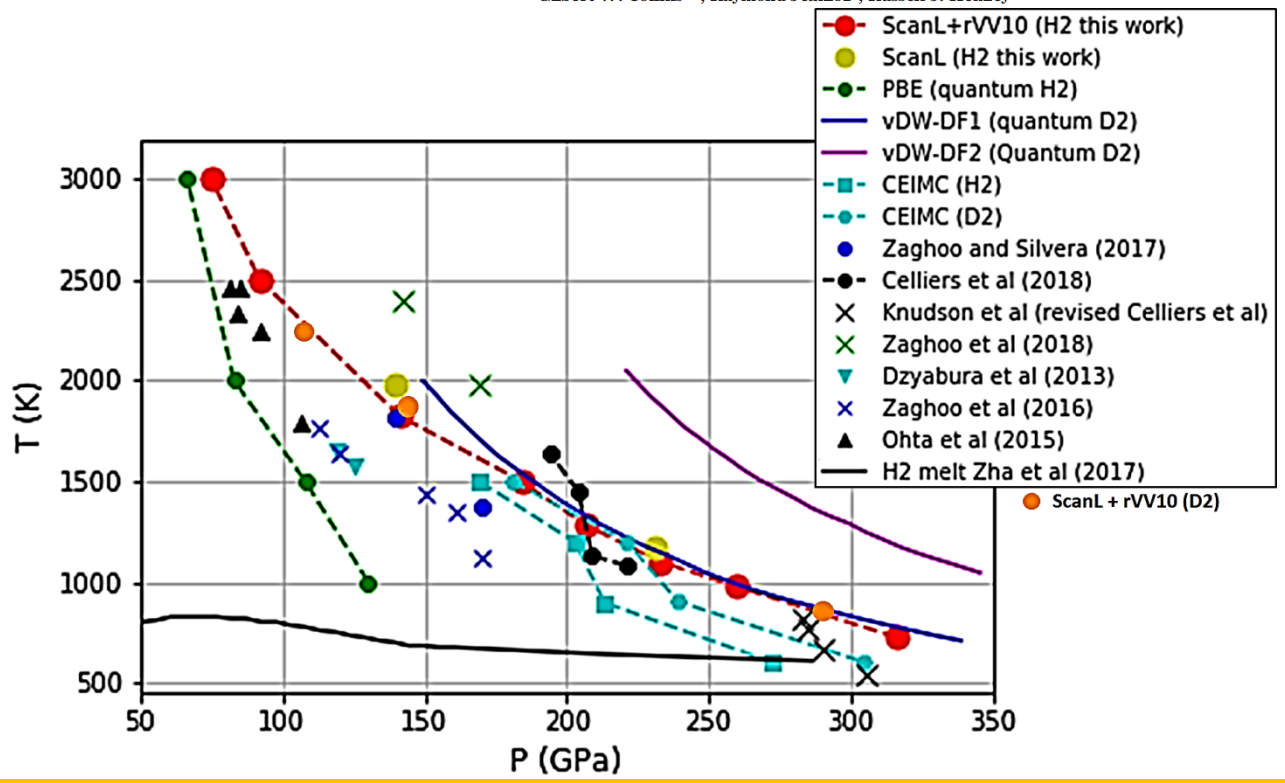
Liquid metallic hydrogen (LMH) is the most abundant form of condensed matter in our solar planetary structure. The electronic and thermal transport properties of this metallic fluid are of

plateauing of electrical conductivity at values around 2,0
the region 1.4–1.8 Mbar (6). It was argued that the
conductivity was due to thermal smearing of the band g

Celliers *et al.*, *Science* **361**, 677–682 (2018) 17 August 2018

Insulator-metal transition in dense fluid deuterium

Peter M. Celliers[1]*, Marius Millot[1], Stephanie Brygoo[2], R. Stewart McWilliams[3], Dayne E. Fratanduono[1], J. Ryan Rygg[1,4], Alexander F. Goncharov[5], Paul Loubeyre[2], Jon H. Eggert[1], J. Luc Peterson[1], Nathan B. Meezan[1], Sebastien Le Pape[1], Gilbert W. Collins[1,4], Raymond Jeanloz[6], Russell J. Hemley[7]



It looks like there is a winning xc-functional for hydrogen!

Conclusion & Outlook

- **First-principles methods developed for quantum many-body systems provide predictive capabilities for HED sciences (although limits exist);**
- **Significant improvements to current quantum many-body methods will be continuously made from our HEDS community;**
- **The HED-community efforts on seeking better understanding of the fundamental physics and chemistry at extreme conditions will make a difference to ICF, planetary science, astrophysics,…**
- **There are some urgent questions needed to be answered for communities of ICF and planetary science (*my personal list*):**
  - ✓ **What's the microphysics of non-uniform shock transition from ablator to DT? ➔ "*spall and ejecta*" ➔ mixing at the ablator/DT interface in ICF**
  - ✓ **What are the *true* α-particle stopping-power in ICF hot-spot and extremely-dense DT-shell?**
  - ✓ **Are there any "excessive" thermal conduction in ICF hot-spot?**
  - ✓ **What drives phase separation in hydrogen-helium mixture and hydro-carbons under WDM conditions?**
  - ✓ **……**

Acknowledge to collaborators

Y. H. Ding, V. V. Karasiev, R. Paul, M. Ghosh, J. Hinz, T. R. Boehly, P. B. Radha, V. N. Goncharov, S. Skupsky, J. R. Rygg, G. W. Collins, S. P. Regan, E. M. Campbell

Laboratory for Laser Energetics
University of Rochester

L. A. Collins, J. D. Kress, A. J. White, O. Certik

Theoretical Division, Los Alamos National Laboratory

B. Militzer

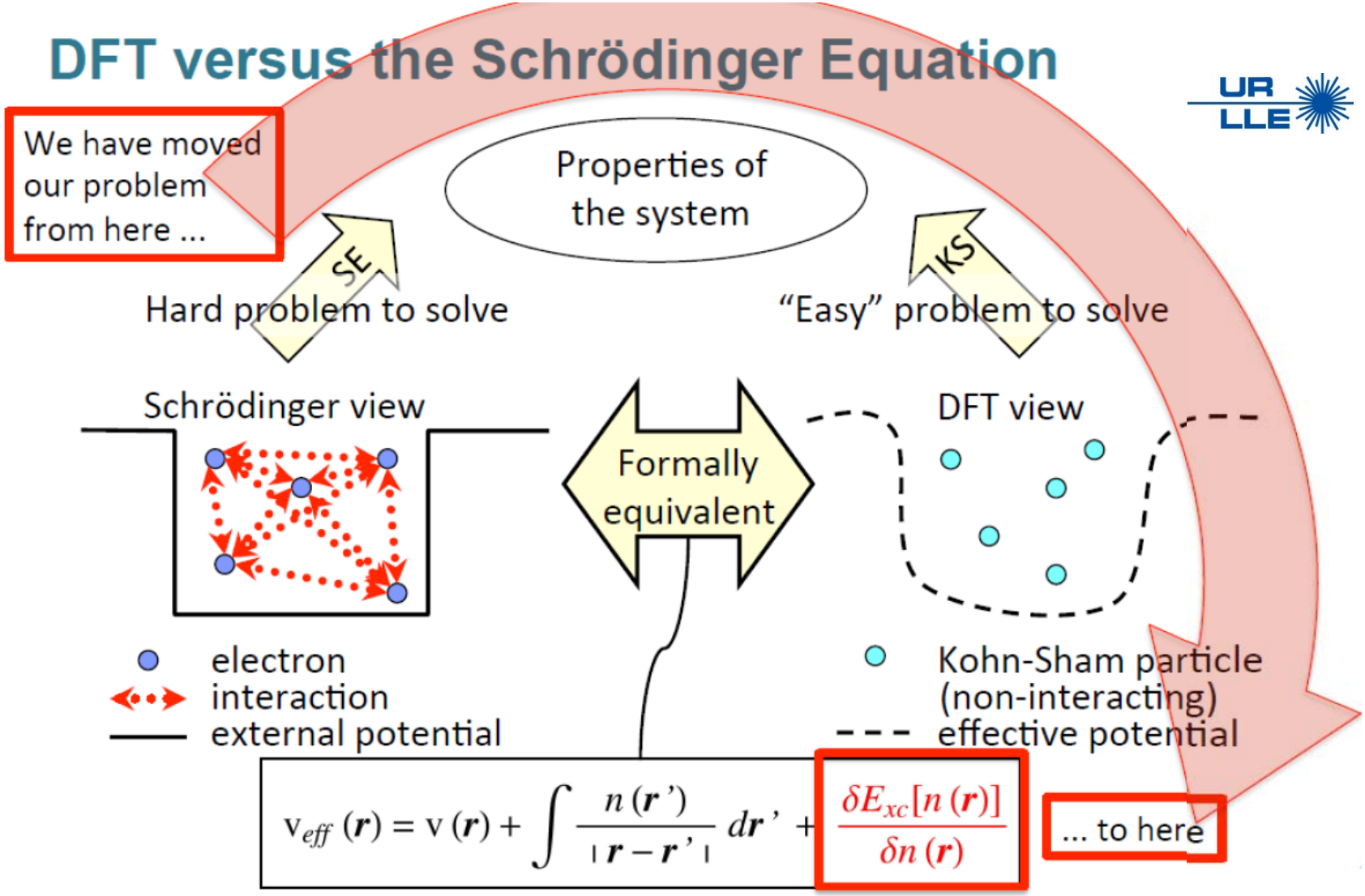
Department of Earth and Planetary Science and Astronomy
University of California – Berkeley

UR LLE

Thank you

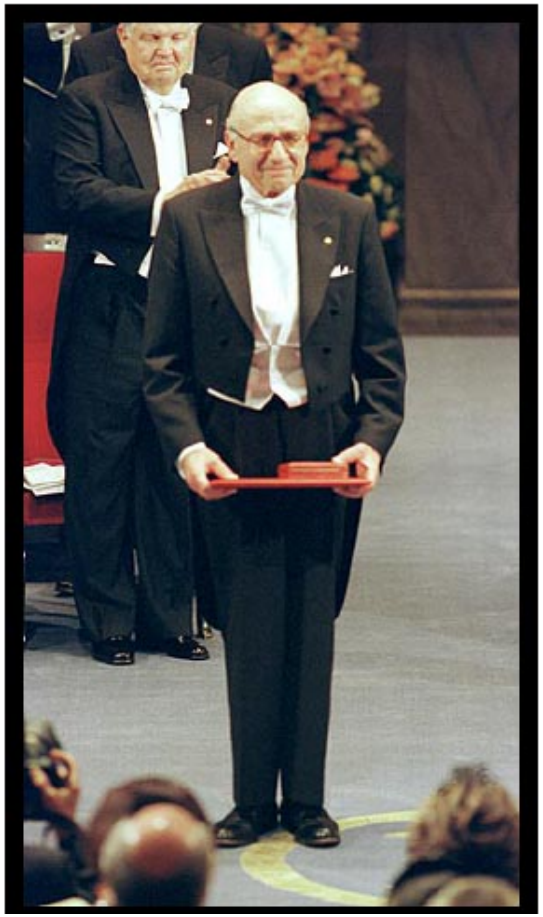
There is no free lunch!

DFT versus the Schrödinger Equation



All many-body effects are included in the effective potential via the Exchange-Correlation functional, $E_{xc}[n(\boldsymbol{r})]$.

Walter Kohn awarded the Nobel Prize in Chemistry 1998 for Density Functional Theory



Hohenberg-Kohn theorem:
Phys. Rev. 136, B864 (1964).
The electron density contains all information needed to determine ground state properties of a system.

Kohn-Sham equations:
Phys. Rev. 140, 1133 (1965).
Practical scheme for solving the quantum mechanical problem based on the HK theorem.

The effect of *Fermi-surface-rising* on K-edge shifting can be naturally accounted in QMD simulations