LA-UR-26-29649

Approved for public release; distribution is unlimited.

Title:	The Properties of Hot, Dense Plasmas
Author(s):	Starrett, Charles Edward
Intended for:	Other: For presentation to university collaborators and students
Issued:	2026-10-29

Los Alamos
NATIONAL LABORATORY







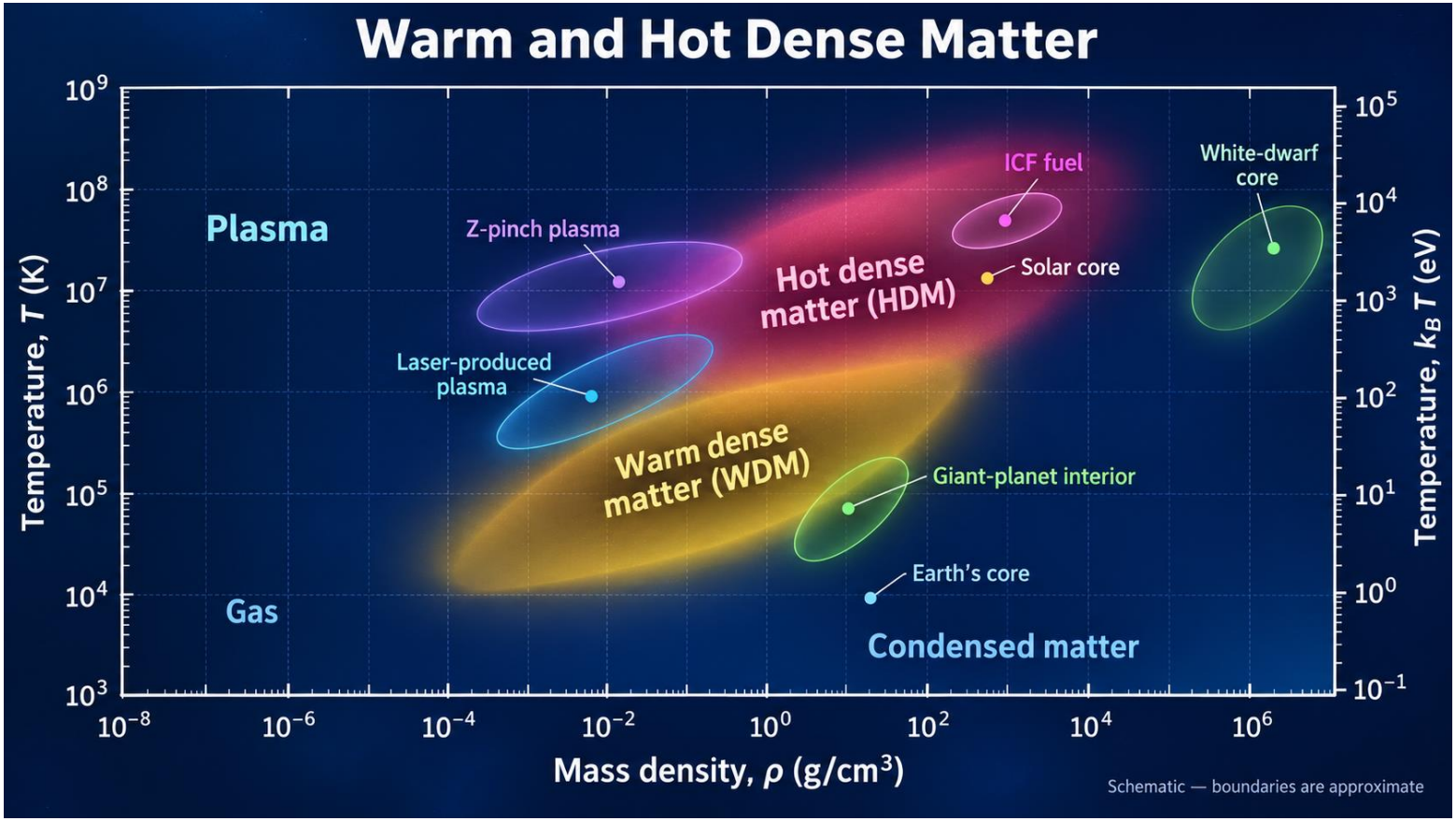
Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by Triad National Security, LLC for the National Nuclear Security Administration of U.S. Department of Energy under contract 89233218CNA000001. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

The Properties of Hot, Dense Plasmas

Charles Starrett

Los Alamos National Laboratory

Schematic of warm and hot dense matter



For accurate modeling of these real systems, we solve hydrodynamics equations

Conservation laws describe the flow. Material properties close the equations.

CONSERVATION EQUATIONS

Mass

$$D\rho/Dt = -\rho\,\nabla\cdot u$$

Momentum

$$\rho\,Du/Dt = -\nabla P + \nabla\cdot\tau + f_r$$

Internal energy

$$\rho\,De/Dt = -P\,\nabla\cdot u + \tau:\nabla u - \nabla\cdot q + Q_r$$

MATERIAL INPUTS

EOS P, e

$P(\rho,T)$ and $e(\rho,T)$

Pressure, temperature and compressibility

Opacity f_r, Q_r

Absorption and scattering

Radiation transport gives force and heating

Thermal conductivity q

$q = -\kappa_{th}\,\nabla T$

Heat flows down temperature gradients

Viscosity τ

Viscous stress from velocity gradients

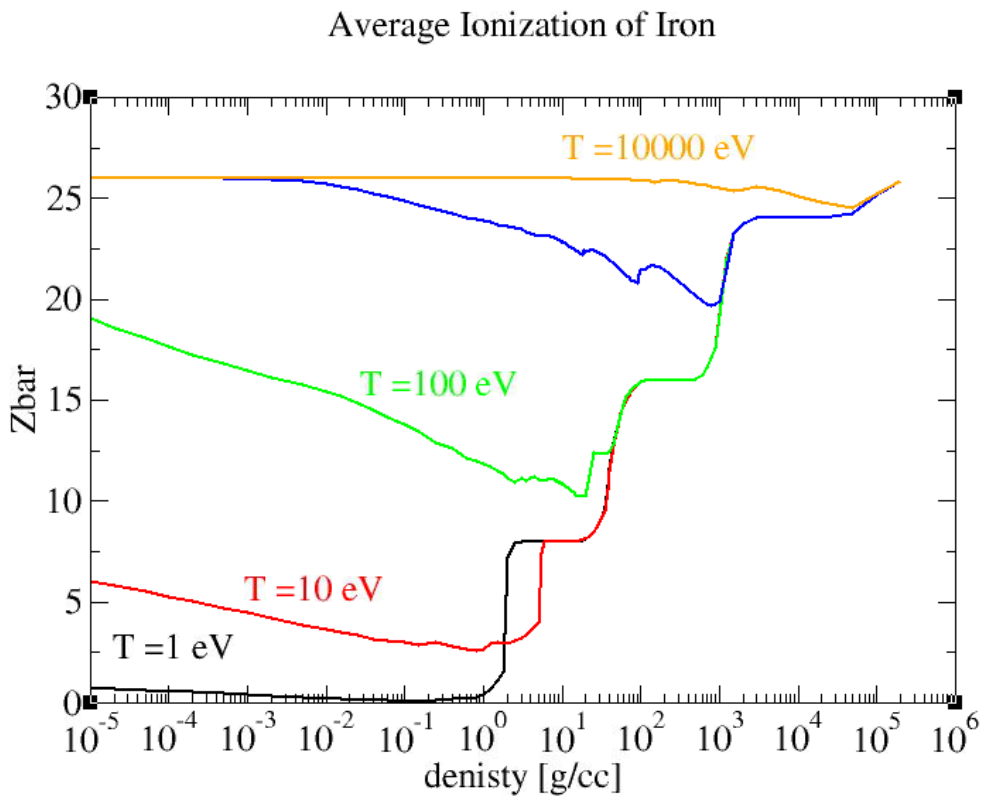
Momentum transport and viscous heating

$D/Dt = \partial/\partial t + u\cdot\nabla$ ρ: density u: velocity e: internal energy per unit mass

Single fluid with a common electron–ion temperature. Radiation requires its own transport equation.

But at these high temperatures (10 000 to 100 000 000 K), it's just an ideal gas, right?

Partial ionization, interactions and correlations distinguish this from ideal gas



A quantum mechanical treatment is necessary

Electronic structure underpins all of this

Time independent Dirac equation

$$(c\boldsymbol{\alpha}\cdot\boldsymbol{p}+\beta mc^2+V(\boldsymbol{r}))\psi_i=E_i\psi_i$$

V(r) contains the Coulomb interaction between all electrons and nuclei in the plasma

E_i, ψ_i are the energy and wave function for eigen state *i*

Boltzmann probability of excited states

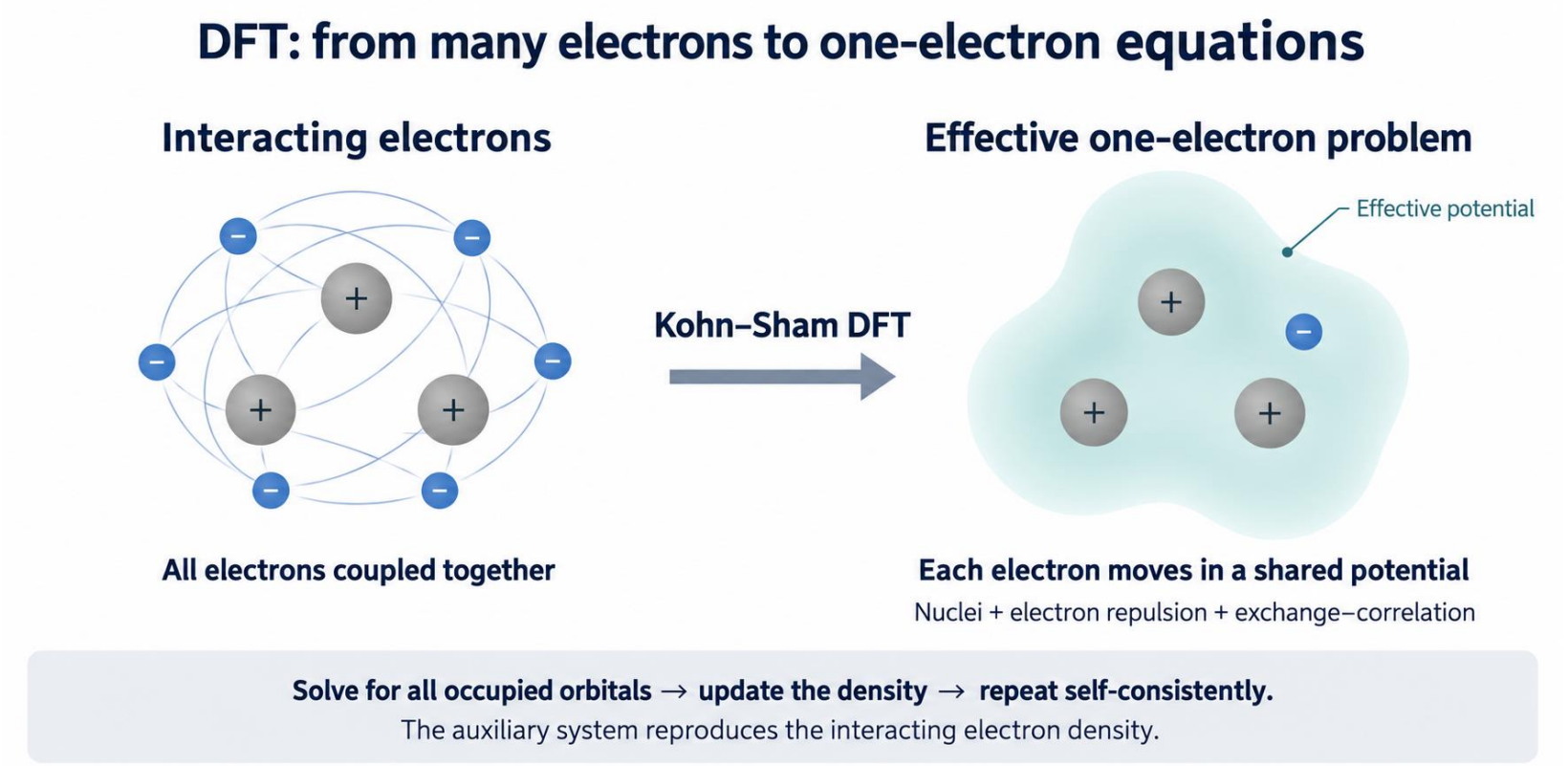
$$W_i=\frac{e^{-\beta F_i}}{Z}$$

This is a formidable challenge under normal conditions
In plasmas we need not just ground state, but many excited states!

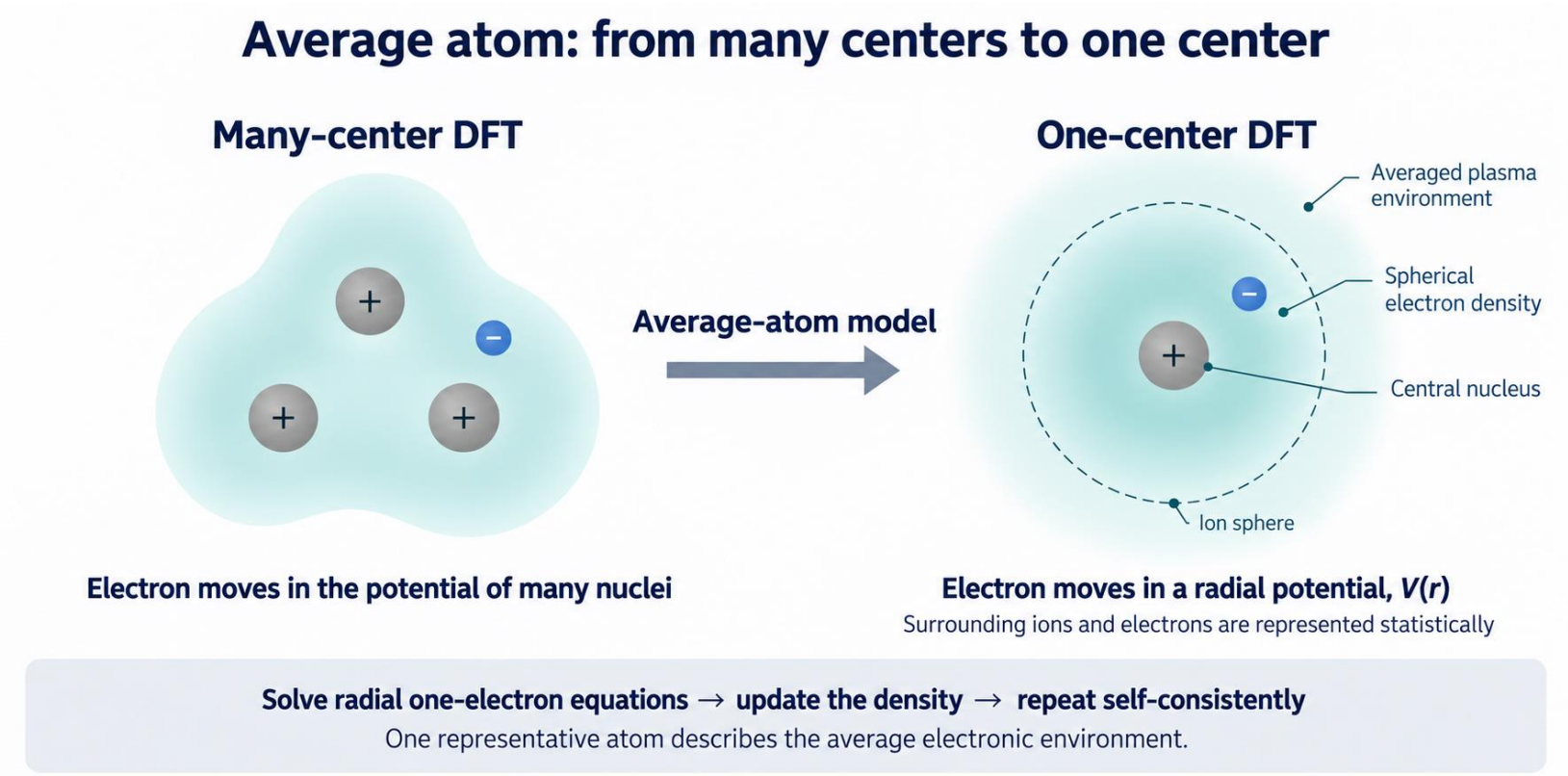
So where do you start?

Density Functional Theory is commonly used

→ DFT reduces the N body electronic problem to an effective one-body problem that you can solve

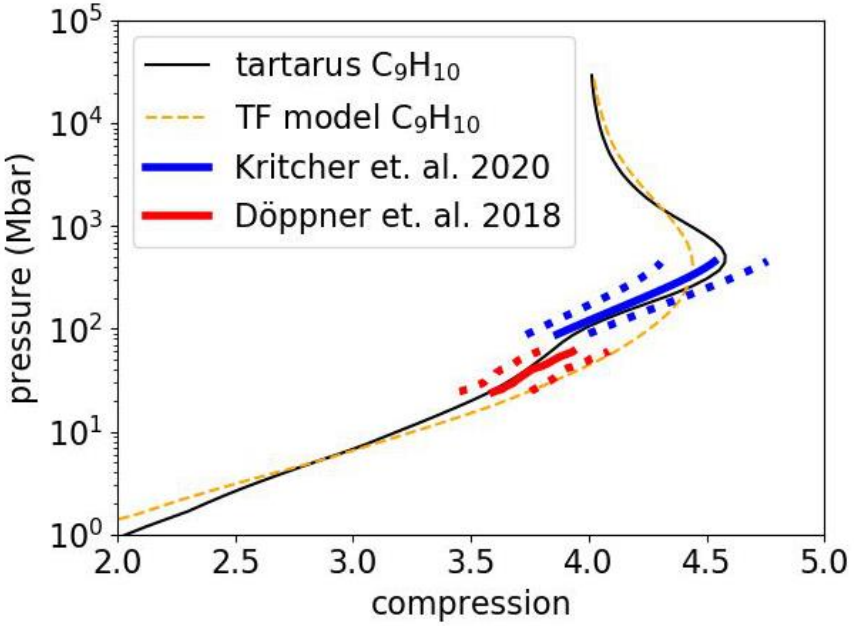


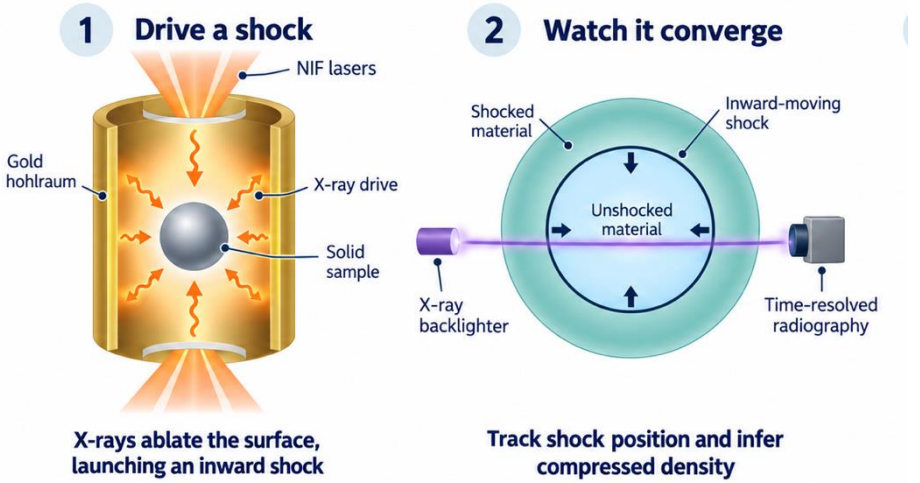
We can solve the equations of this model, but it is expensive. For wide ranging data we make the Average Atom approximation



This is much faster to solve, and for most cases of interest, is accurate enough

Tartarus AA model (Comp. Phys. Com. 2019)
A Relativistic DFT AA model



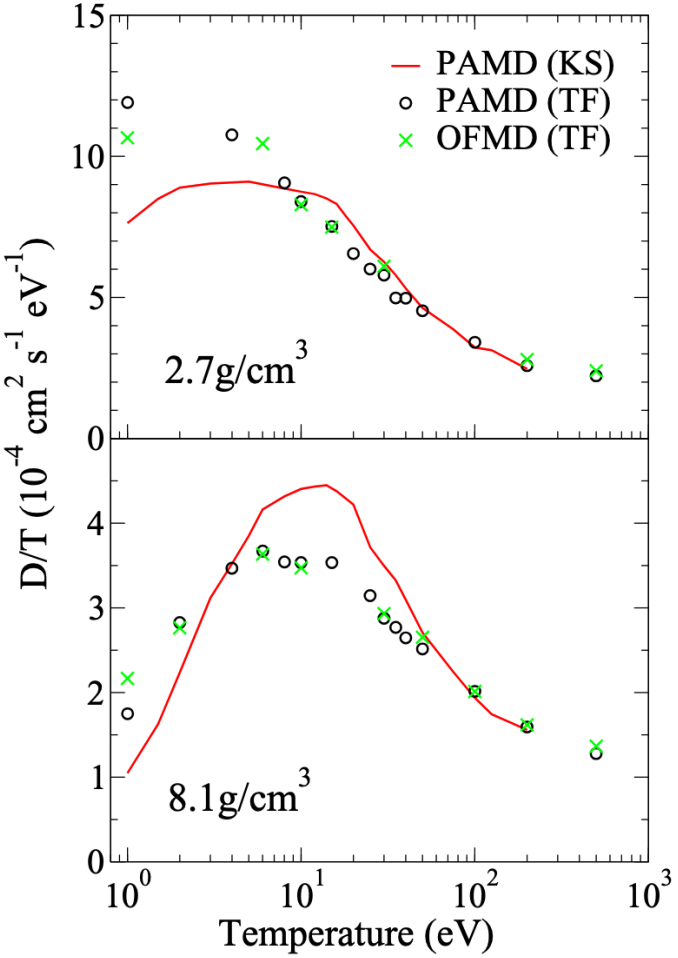


This compares the measured Hugoniot (using the NIF) to Tartarus

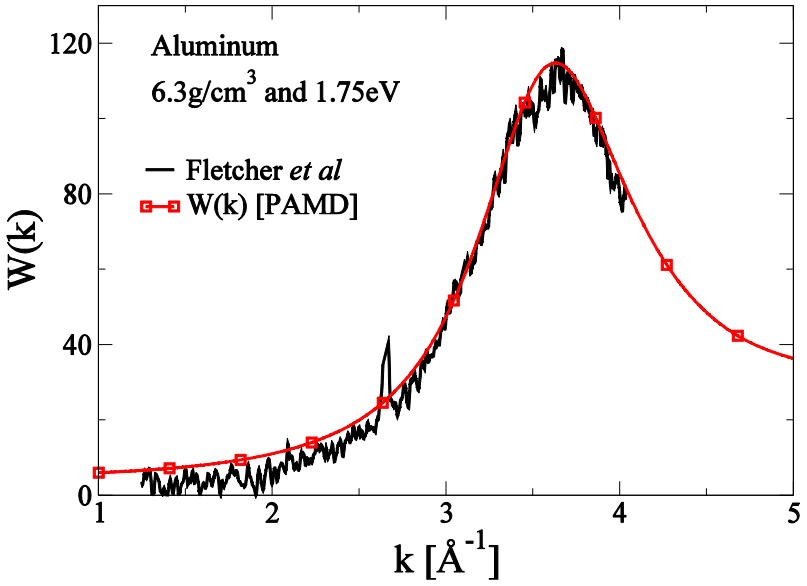
AA model agrees with data for EOS for this high-pressure environment

Comparison with experiment and many-ion DFT simulations tells us this physical model is reasonable

Diffusion in Aluminum



$$W(k) = n_e^{PA}(k)\, S_{II}(k)$$



Fletcher *et al* Nature Photonics (2015)
Starrett & Saumon PRE (2015)
Starrett & Saumon PRE (2013)

"Pseudoatom Molecular Dynamics"

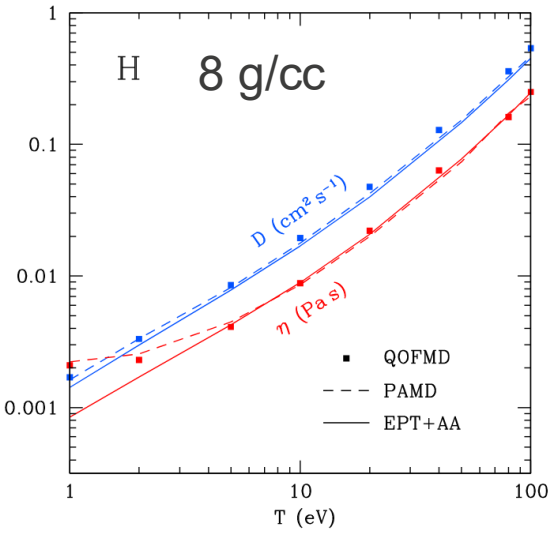
Ionic Transport without molecular dynamics

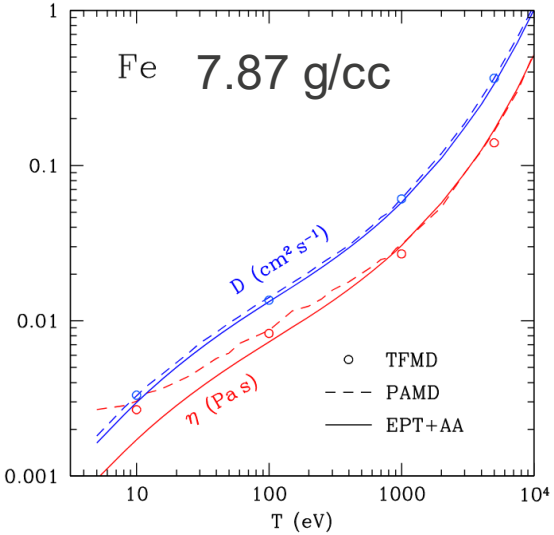
PRL 116, 075002 (2016) PHYSICAL REVIEW LETTERS week ending 19 FEBRUARY 2016

Ionic Transport Coefficients of Dense Plasmas without Molecular Dynamics

Jérôme Daligault,[1,*] Scott D. Baalrud,[2] Charles E. Starrett,[1] Didier Saumon,[1] and Travis Sjostrom[1]

This paper is part of a program led by Prof. Baalrud's group to develop a complete kinetic theory using this potential of mean force

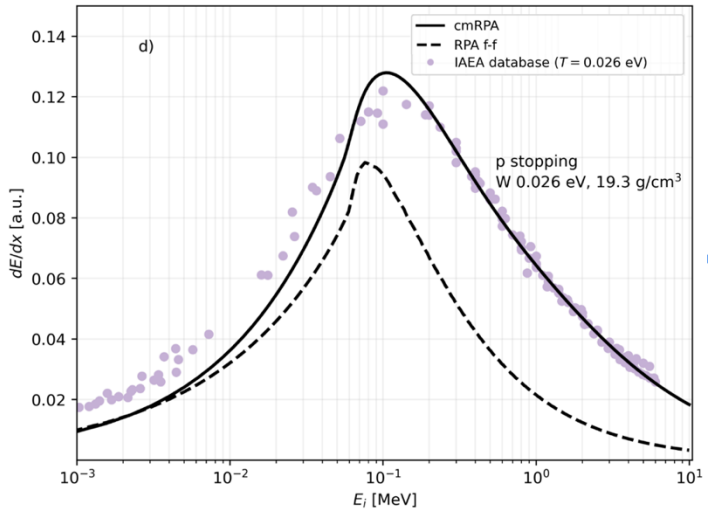




Agrees well with expensive ab initio simulations

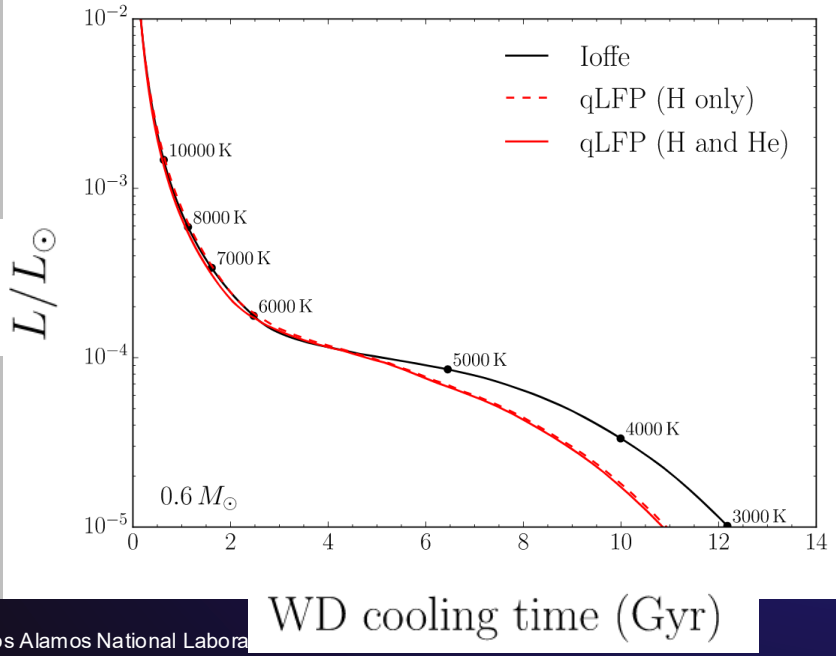
Note: ion-ion potentials are numerical, do not assume an analytic form

Many other applications: Stopping Power, electronic transport …



Proton stopping by Tungsten

Z. Johnson et al, under review



Cooling sequence for DA White Dwarfs is sensitive to hydrogen thermal conductivity

S. Blouin, **N. Shaffer** et al, ApJ 2020

AA model seems do do quite well so far..

Opacity, this is where things start to go wrong…

PHYSICAL REVIEW LETTERS **122,** 235001 (2019)

Editors' Suggestion | Featured in Physics

Systematic Study of *L*-Shell Opacity at Stellar Interior Temperatures

T. Nagayama,[1] J. E. Bailey,[1] G. P. Loisel,[1] G. S. Dunham,[1] G. A. Rochau,[1] C. Blancard,[2] J. Colgan,[3] Ph. Cossé,[2] G. Faussurier,[2] C. J. Fontes,[3] F. Gilleron,[2] S. B. Hansen,[1] C. A. Iglesias,[4] I. E. Golovkin,[5] D. P. Kilcrease,[3] J. J. MacFarlane,[5] R. C. Mancini,[6] R. M. More,[1,*] C. Orban,[7] J.-C. Pain,[2] M. E. Sherrill,[3] and B. G. Wilson[4]

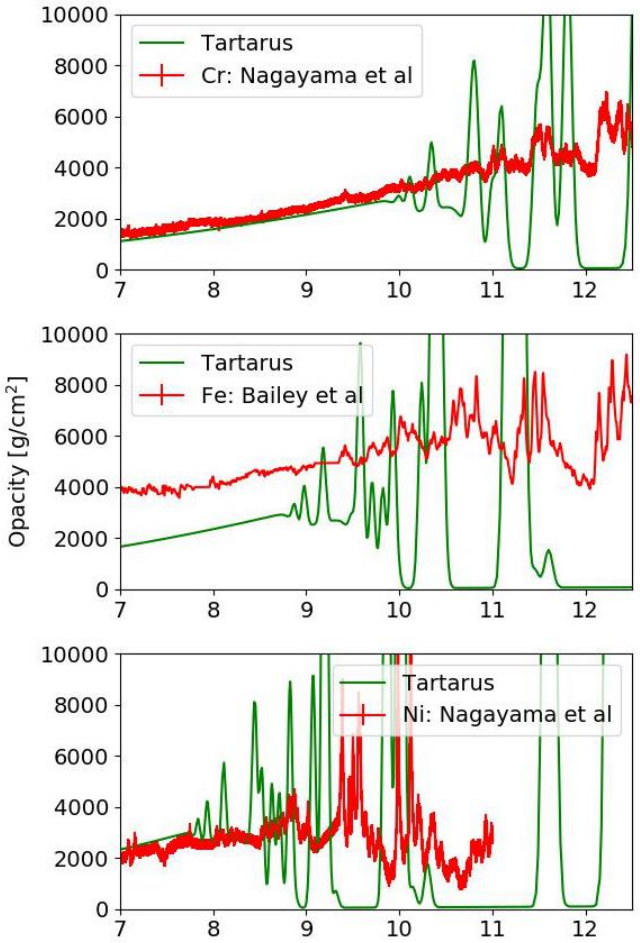
LETTER

doi:10.1038/nature14048

A higher-than-predicted measurement of iron opacity at solar interior temperatures

J. E. Bailey[1], T. Nagayama[1], G. P. Loisel[1], G. A. Rochau[1], C. Blancard[2], J. Colgan[3], Ph. Cosse[2], G. Faussurier[2], C. J. Fontes[3], F. Gilleron[2], I. Golovkin[4], S. B. Hansen[1], C. A. Iglesias[5], D. P. Kilcrease[3], J. J. MacFarlane[4], R. C. Mancini[6], S. N. Nahar[7], C. Orban[7], J.-C. Pain[2], A. K. Pradhan[7], M. Sherrill[3] & B. G. Wilson[5]

~ 180 eV, 0.16 g/cc



Why so poor? Could it be … Time dependent effects

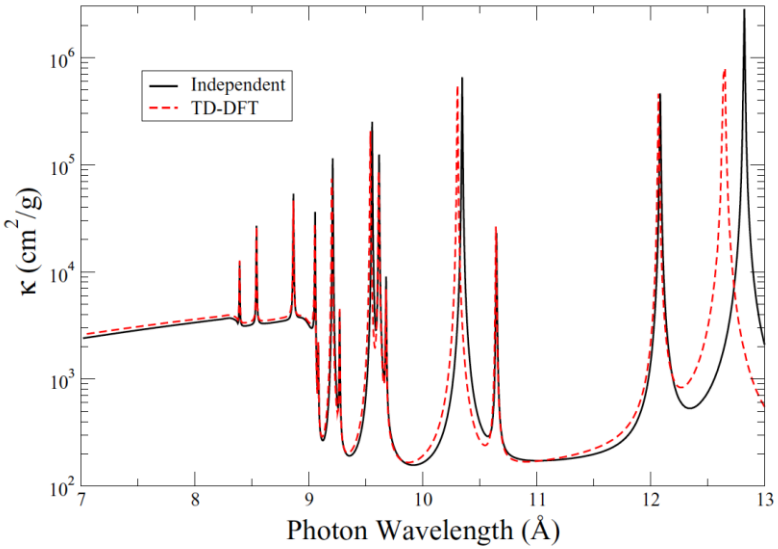
1) Independent particle approximation for opacity

We checked with time-dependent DFT

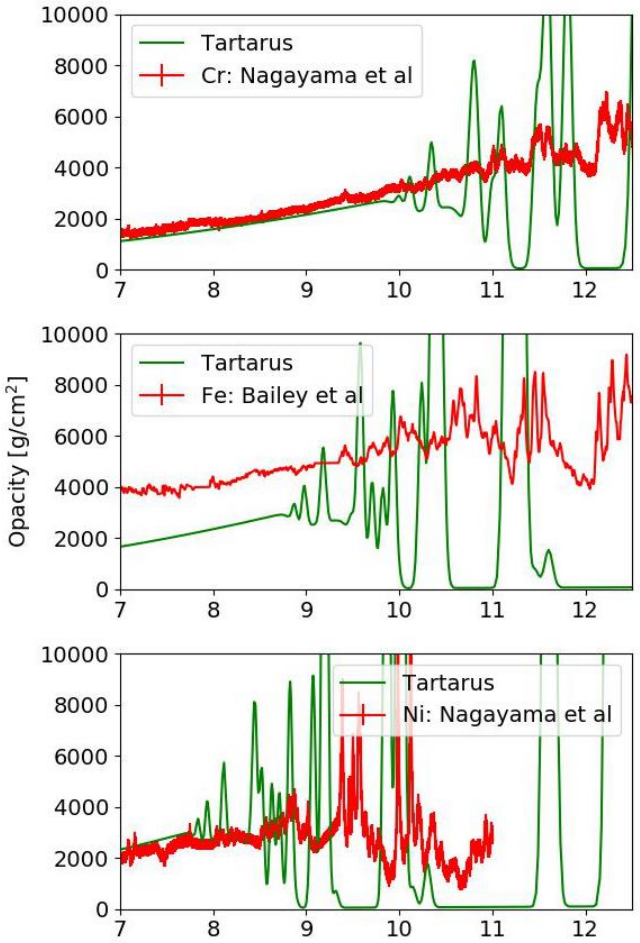
PHYSICAL REVIEW E **103**, 043206 (2021)

Time-dependent density functional theory applied to average atom opacity

N. M. Gill,* C. J. Fontes, and C. E. Starrett
Los Alamos National Laboratory, P.O. Box 1663, Los Alamos, New Mexico 87545, USA



~ 180 eV, 0.16 g/cc



Why so poor? Could it be …
Multi-center effects

2) Crude plasma physics (Average atom approx.)

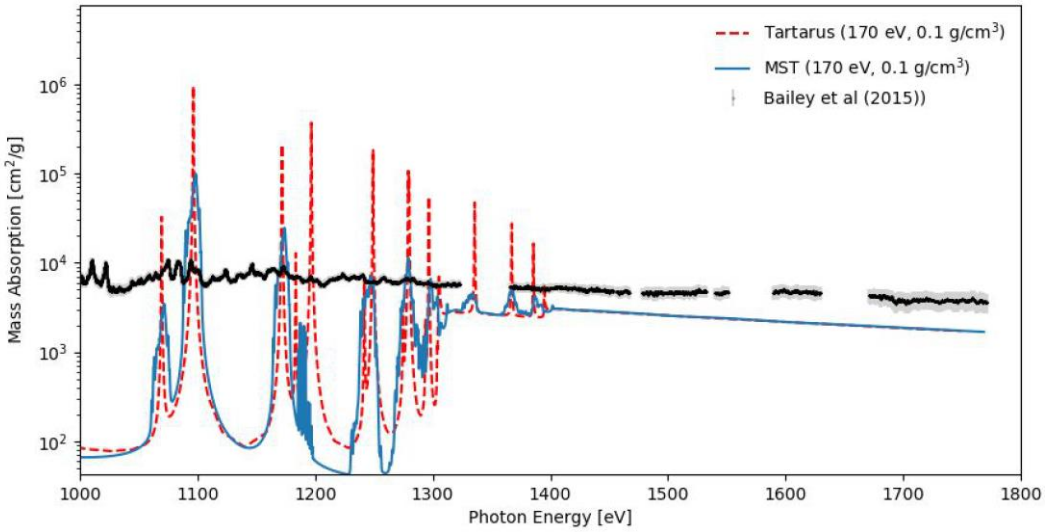
We checked by developing multicenter model

PHYSICAL REVIEW E **105**, 015203 (2022)

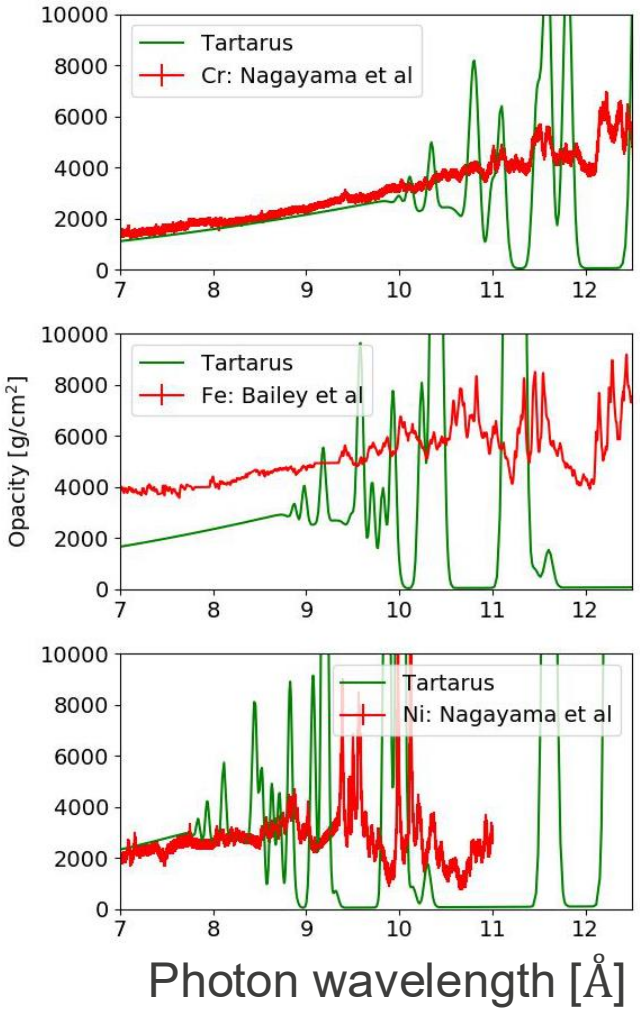
Dense plasma opacity via the multiple-scattering method

Nathaniel R. Shaffer*
Los Alamos National Laboratory, P.O. Box 1663, Los Alamos, New Mexico 87545, USA
and Laboratory for Laser Energetics, University of Rochester, 250 East River Road, Rochester, New York 14623, USA

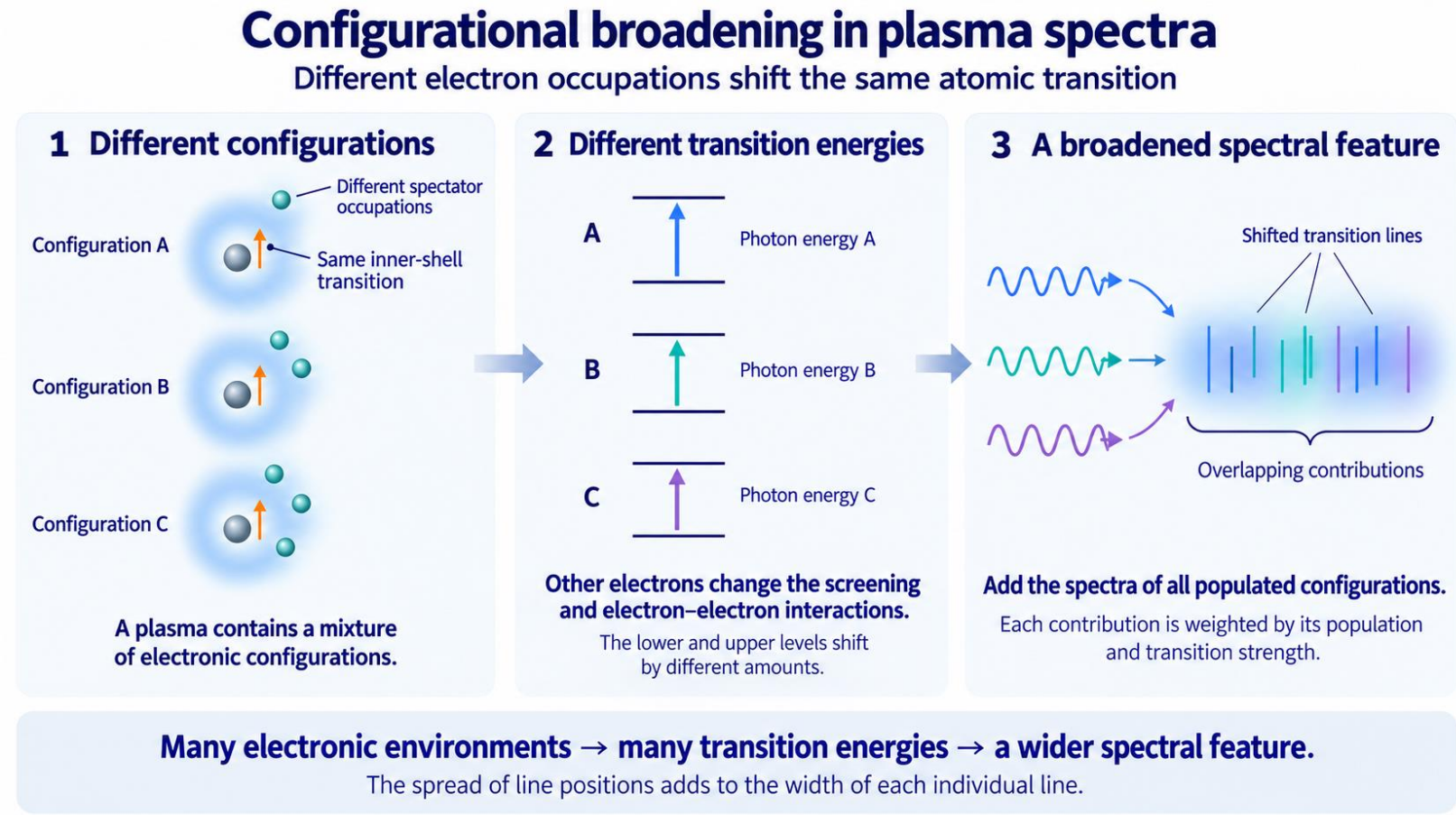
Charles E. Starrett
Los Alamos National Laboratory, P.O. Box 1663, Los Alamos, New Mexico 87545, USA



~ 180 eV, 0.16 g/cc



The problem lies with finite temperature DFT
In practice, it is too crude for opacity of WDM/HDM



In DFT, configurational broadening is missing, or rather, it should be in the exchange and correlation term (it isn't!)

The solution: Go beyond DFT
A Variational Model of excited states

In DFT, the free energy is

$$F = E - TS$$

Energy is approximated with effective one-electron model including XC
Uses Fermi-Dirac (fractional) occupations of orbitals

In our new excited states method:

$$F = \sum_x W_x [E_x - TS_x] + T \sum_x W_x \ln W_x,$$

Population

Free energy for excitation *x*

Entropy due to energy degeneracy

Each excited state, *x*, is approximated by an effective one-electron model (inc. XC)
Uses integer occupation factors for orbitals, these define the excited state

Minimize Constrained Free Energy Ω

$\frac{d\Omega}{dn_{e,x}(\vec{r})} = 0$ Leads to DFT-like equation for each excited state

$$\left[-\tfrac{1}{2}\nabla^2 + V_x^{\mathrm{el}}(\boldsymbol{r}) + V_x^{\mathrm{xc}}(\boldsymbol{r}) - \gamma \right]\psi_{x,i}(\boldsymbol{r}) = \epsilon_{x,i}\psi_{x,i}(\boldsymbol{r})$$

$$n_x(\boldsymbol{r}) = \sum_i f_{x,i}|\psi_i(\boldsymbol{r})|^2$$

integer occupations

$$n(\boldsymbol{r}) = \sum_x W_x n_x(\boldsymbol{r})$$

ESM

$$n(\boldsymbol{r}) = \sum_i f_i|\psi_i(\boldsymbol{r})|^2$$

Fermi-Dirac occupation factors

DFT

$$\frac{d\Omega}{dW_x} = 0 \qquad W_x = \frac{e^{-\beta F_x}}{Z}$$

Variational, Excited State Method (ESM)

PHYSICAL REVIEW E **109**, 035201 (2024)

Excited states in warm and hot dense matter

C. E. Starrett,* T. Q. Thelen, C. J. Fontes, and D. A. Rehn
Los Alamos National Laboratory, P.O. Box 1663, Los Alamos, New Mexico 87545, USA

PHYSICAL REVIEW E **110**, 015207 (2024)

Predicting excitation energies in warm and hot dense matter

T. Q. Thelen, D. A. Rehn, C. J. Fontes, and C. E. Starrett*
Los Alamos National Laboratory, P.O. Box 1663, Los Alamos, New Mexico 87545, USA

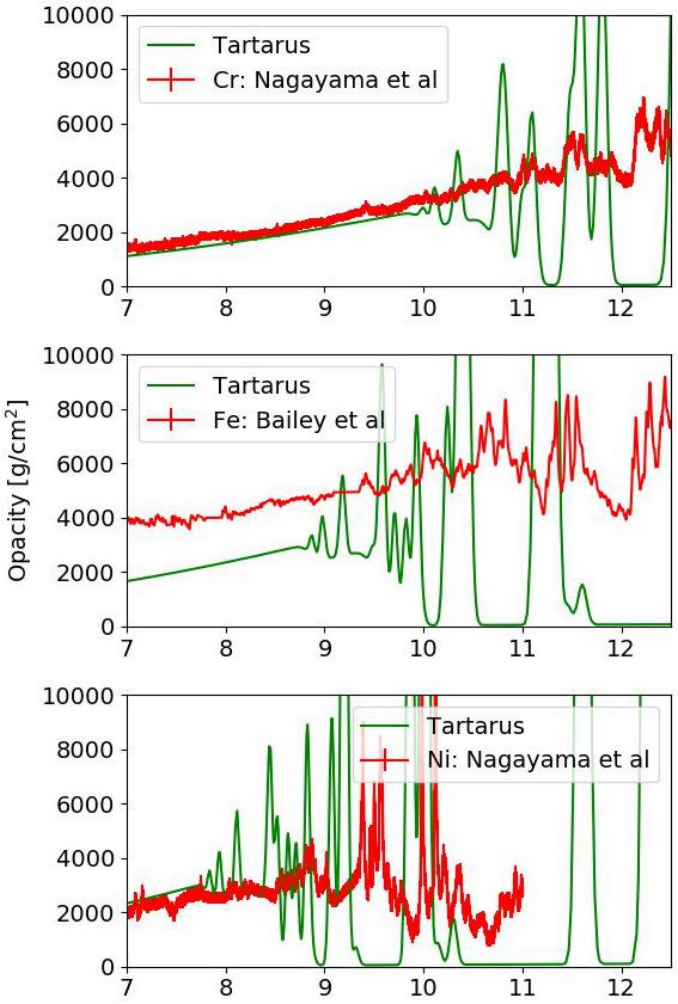
PHYSICAL REVIEW E **110**, 045208 (2024)

Dense plasma opacity from excited states method

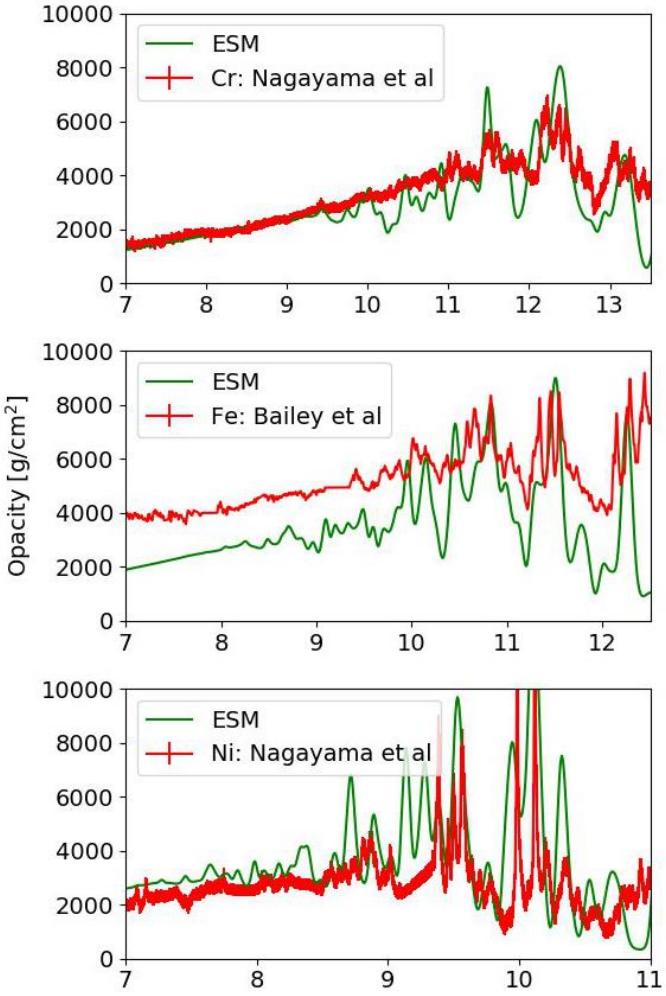
C. E. Starrett,[1,*] C. J. Fontes,[1] H. B. Tran Tan,[1] J. M. Kasper,[1] and J. R. White[1,2]
[1]*Los Alamos National Laboratory, P.O. Box 1663, Los Alamos, New Mexico 87545, USA*
[2]*Department of Astronomy, University of Texas at Austin, Austin, Texas 78712, USA*

Opacity Experiments

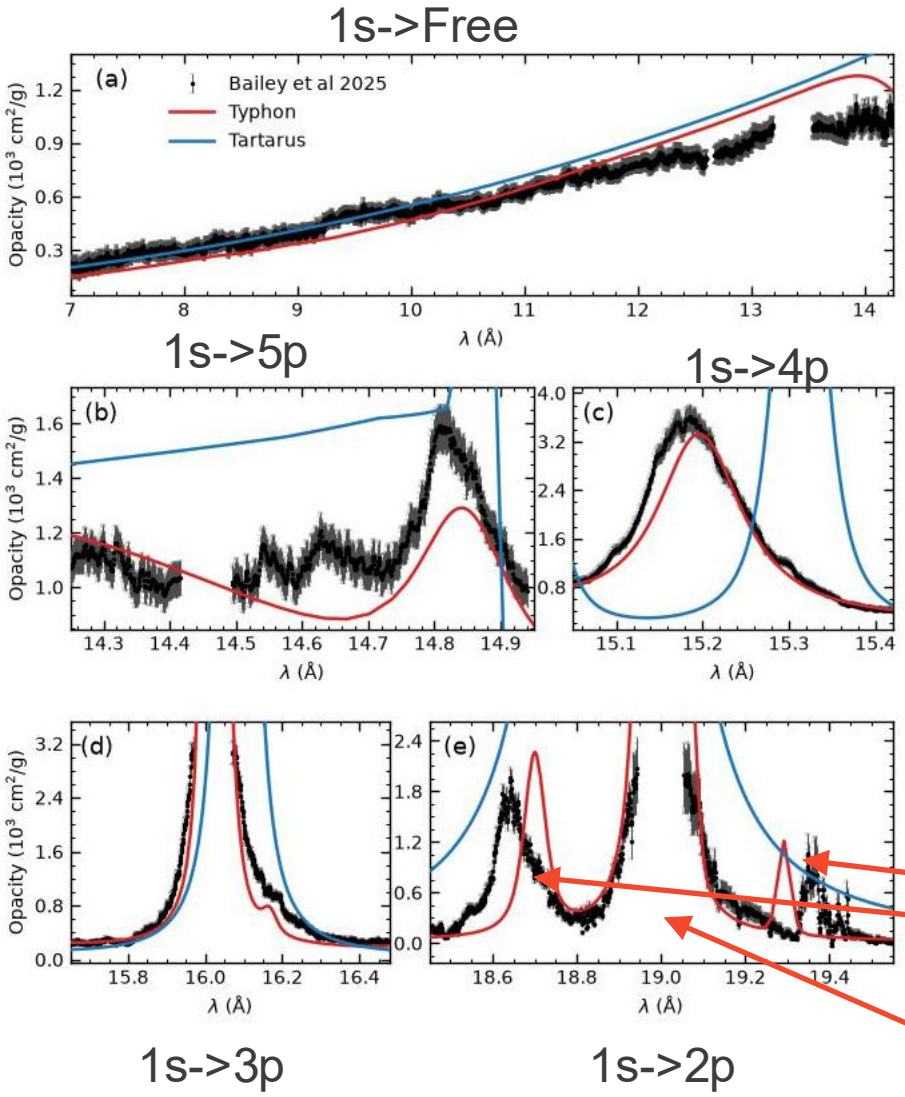
Average Atom



Excited State model



Opacity Experiments on Oxygen



Oxygen at 148 eV, 0.033 g/cc

Generally good agreement with our ESM code Typhon

Bound-Free threshold error is presumably due to crude plasma physics

Can the multi-center model do better?

He-like lines

H-like lines

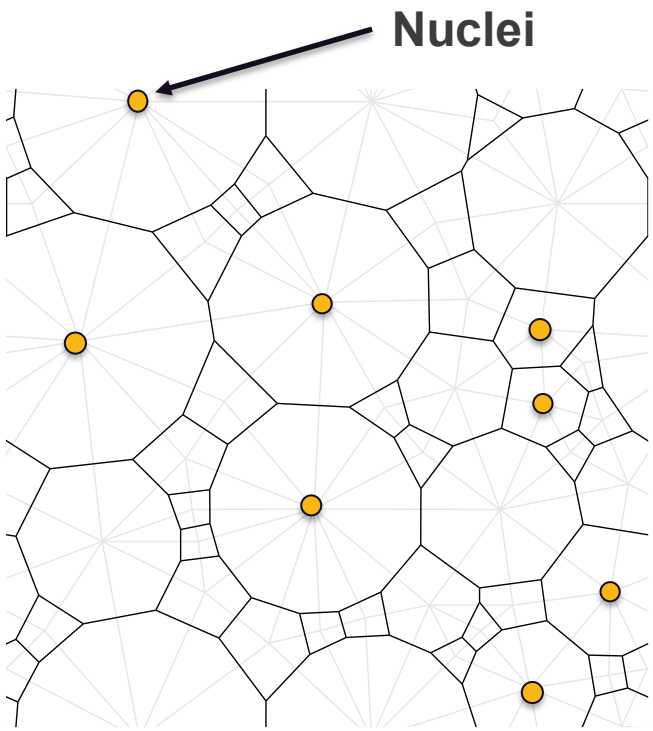
Multi-center model improvements Ongoing…

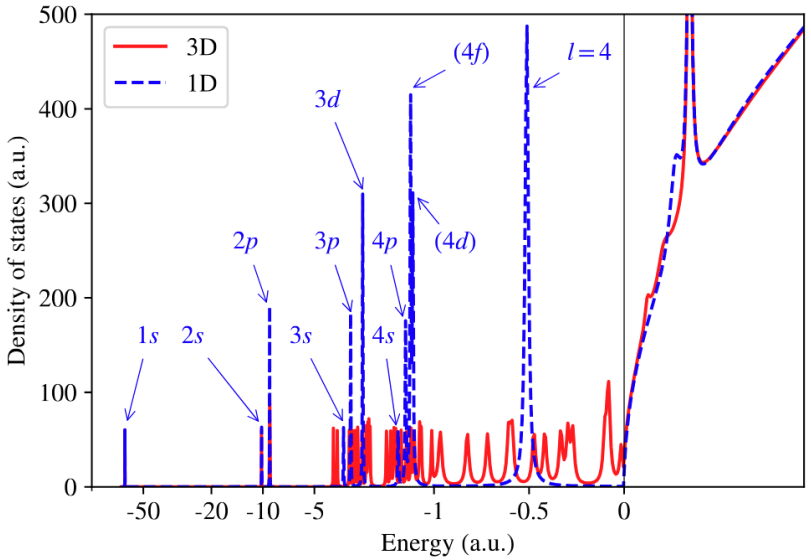
Currently we use the muffin-tin approximation which makes the one-electron potential spherically symmetric in each cell.

We have found a new way to solve the 3-D potential problem

$$G = G^0 + G^0 T G^0$$

$$T = V + V G^0 T = V + T G^0 V$$





Finite-basis method for full-potential Green's functions in density functional theory

H. B. Tran Tan,[1] J. R. White,[1,2] Z. A. Johnson,[1] R. J. Fish,[3,1] C. J. Fontes,[1] and C. E. Starrett[1]
[1]*Los Alamos National Laboratory, P.O. Box 1663, Los Alamos, New Mexico 87545, USA*
[2]*Department of Astronomy, University of Texas at Austin, Austin, Texas 78712, USA*
[3]*Department of Applied Mathematics and Statistics, Colorado School of Mines, Golden, Colorado 80401, USA*

(Received 13 April 2026; revised 17 August 2026; accepted 2 September 2026; published 15 September 2026)

Improvements in Line Shapes

Quantum fluctuations in dense plasma simulations

Cite as: Phys. Plasmas **33**, 032701 (2026); doi: 10.1063/5.0312332
Submitted: 15 November 2025 · Accepted: 19 February 2026 ·
Published Online: 17 March 2026

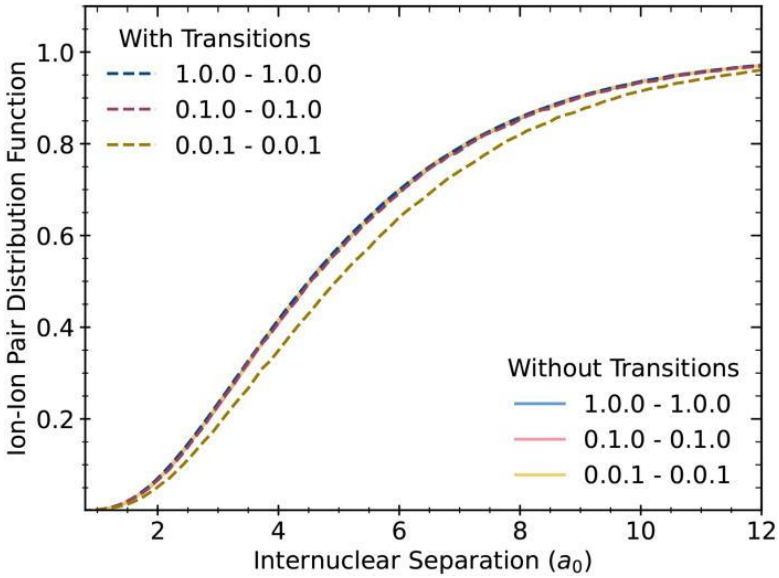
View Online Export Citation

J. R. White,[1,2,a)] C. E. Johnson,[3] K. S. Davis,[4,5,b)] H. B. Tran Tan,[1] C. J. Fontes,[1] and C. E. Starrett[1]

This work introduces the idea that the pair distribution function for an ion is affected by the lifetime of that ion

→ More highly excited states generally live for less time that less energetic state

→ This changes their pair distribution function, and in turn, the line-shape



Conclusions and Outlook

Dense Plasma physics (Warm and hot dense matter) is an exciting field to work in!

Applications to fusion energy facilities like NIF and Pacific Fusion, as well as astrophysics (e.g., White Dwarfs)

We have made progress but there is still much to be done…

If you are a student or postdoc and interested in working with us, reach out to us
starrett@lanl.gov

Collaborators at LANL involved with this effort:
C. Fontes
J. Kasper
J. Leveillee
A. White
J. Daligault
B. Tran
J. White
Z. Johnson

LANL Computational Physics Workshop

Los Alamos has a computational Physics summer student workshop

Aimed at undergraduate and graduate students

There are a wide range of projects

Just search for the website to see examples from this year.

Applications for next summer (2027) will open usually around thanksgiving time.



Sponsored by the Los Alamos National Laboratory Advanced Scientific Computing (ASC) Program

June 1, 2026 - August 7, 2026

Applications are currently closed

Los Alamos National Laboratory's Computational Physics Division, in cooperation with Advanced Simulation and Computation Program is pleased to sponsor the 2026 Computational Physics Student Summer Workshop. The workshop seeks to bring to the Laboratory a diverse group of exceptional graduate and advanced undergraduate students from within the United States for enriching lectures and to work with the staff scientists for 10 weeks on exciting and relevant projects that may culminate in articles or conference presentations.

Workshop Overview

Teams of two participants work under the guidance of one or more mentors. A fellowship is awarded to each participant and typically ranges from $9,000 to $17,000, based on academic rank. Lectures, teamwork, and mentoring help students learn about computational physics and enhance their careers. Shared technical goals help students build future connections. Social events and tours enhance the workshop experience, promoting team-building and creating lasting memories and professional relationships.