SAND2019-4880C

Electronic Transport Properties of Warm Dense Matter from Time-Dependent Density Functional Theory

Sandia National Laboratories

PRESENTED BY

Attila Cangi

10th International Workshop on Warm Dense Matter 2019
Travemünde, Germany

Collaborators

Andrew. D. Baczewski, Stephanie. B. Hansen

Tuesday, May 7, 2019

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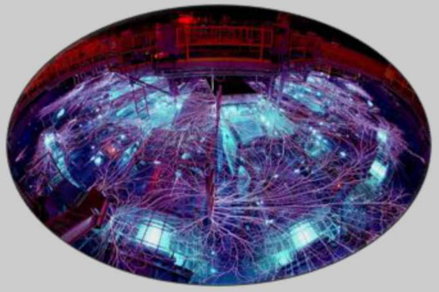
Overview and Goal of this Talk

Characterization of HED phenomena is challenging.



Modeling landscape is a blend of **various disciplines** (plasma, atomic, condensed matter physics) and **methods** (magnetohydrodynamics, particle-in cell, molecular dynamics average-atom, DFT-MD, TDDFT).

Persistence of electron correlation and non-LTE conditions are the greatest challenges for numerical modeling.

Ultimately want to avoid empiricism and a **self-consistent, first-principles method** for the prediction of WDM/HED phenomena.

Compare prediction of HED **transport phenomena** within various methods (average atom, Kubo-Greenwood) with TDDFT.

Stopping power

$$\frac{\partial E}{\partial x} = \frac{1}{v}\frac{\partial}{\partial t}\langle E \rangle$$

Electrical conductivity

$$\sigma(\omega) = \frac{\mathbf{J}(\omega)}{\mathbf{E}(\omega)}$$

Dynamic structure factor

$$S(\mathbf{q},\omega) = -\frac{1}{\pi}\frac{\Im[\chi(\mathbf{q},-\mathbf{q},\omega)]}{1 - e^{-\omega/k_B T}}$$

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Coupled Electron-Ion Many-Body Problem

$$i\hbar\frac{\partial}{\partial t}\Psi(\{\mathbf{R}\},\{\mathbf{r}\},t) = \hat{H}\Psi(\{\mathbf{R}\},\{\mathbf{r}\},t)$$

Time-dependent (non-relativistic) Schrödinger equation for the many-particle (molecular) Hamiltonian.

$$\hat{H} = \hat{T}^n + \hat{W}^{nn} + \boxed{\hat{T}^e + \hat{W}^{ee} + \hat{W}^{en}} + \hat{V}^n + \boxed{\hat{V}^e}$$

$$\hat{T}^n = \sum_{\alpha}^{N^n} -\frac{1}{2M_\alpha}\nabla_\alpha^2 \qquad \hat{W}^{nn} = \frac{1}{2}\sum_{\alpha,\beta,\alpha\neq\beta}^{N^n}\frac{Z_\alpha Z_\beta}{|\mathbf{R}_\alpha - \mathbf{R}_\beta|}$$

Kinetic energy and interaction of ions.

$$\hat{T}^e = \sum_{\alpha}^{N^e} -\frac{1}{2}\nabla^2 \qquad \boxed{\hat{W}^{ee} = \frac{1}{2}\sum_{i,j,i\neq j}^{N^e}\frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}}$$

Kinetic energy and interaction of electrons.

$$\hat{W}^{ne} = -\sum_{i}^{N^e}\sum_{\alpha}^{N^n}\frac{Z_\alpha}{|\mathbf{r}_i - \mathbf{R}_\alpha|}$$

Electron-ion interaction.

$$\hat{V}^n = \sum_{\alpha}^{N^n} v^n(\mathbf{R}_\alpha) \qquad \hat{V}^e = \sum_{i}^{N^e} v^e(\mathbf{r}_i)$$

External potential.

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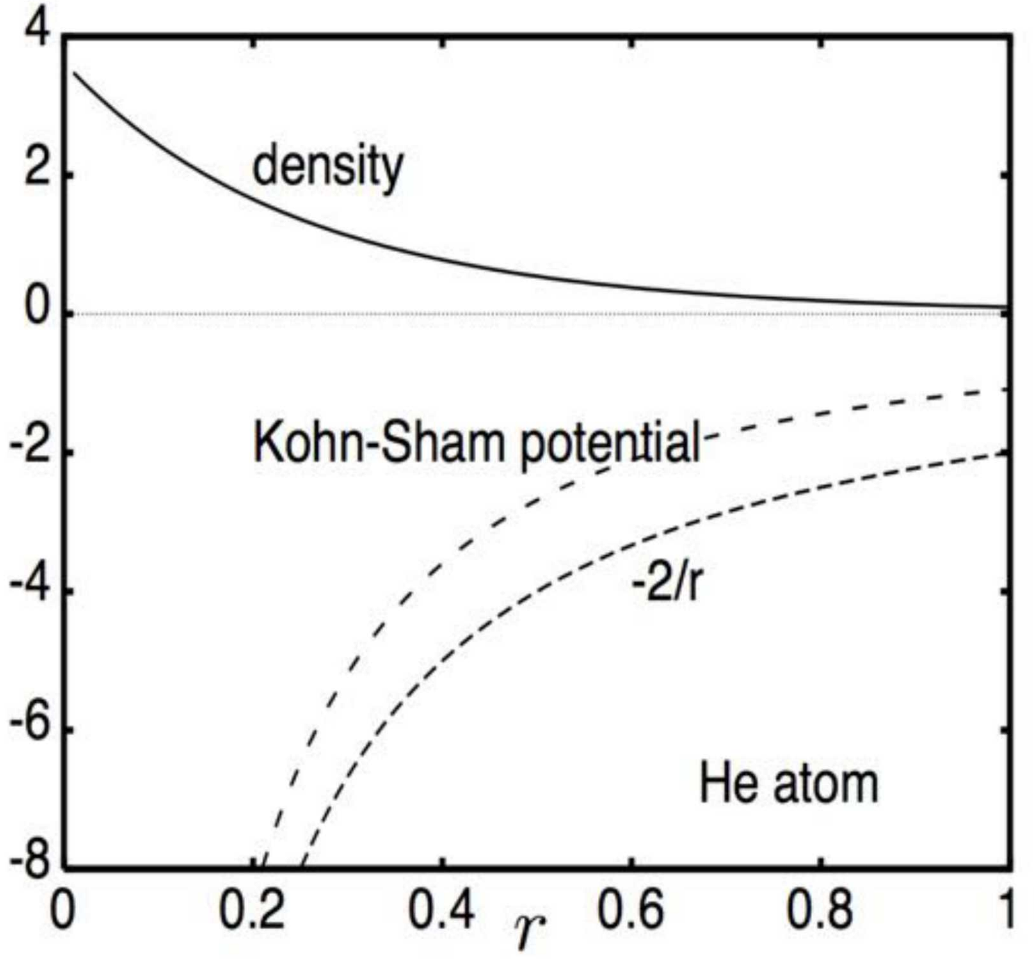
Introduction to Density Functional Theory (DFT)

$$\left[-\frac{\nabla^2}{2} + v_S(\mathbf{r})\right]\phi_j(\mathbf{r}) = \epsilon_j \phi_j(\mathbf{r}) \qquad \text{(Kohn-Sham equations)}$$

$$v_S(\mathbf{r}) = v(\mathbf{r}) + \frac{\delta U}{\delta n(\mathbf{r})} + \boxed{\frac{\delta E_{XC}}{\delta n(\mathbf{r})}} \qquad \text{(Kohn-Sham potential)}$$

$$n(\mathbf{r}) = \sum_i \phi_i^*(\mathbf{r})\phi_i(\mathbf{r}) \qquad \text{(Electronic density)}$$



The ABC of DFT (dft.uci.edu/doc/g1.pdf).

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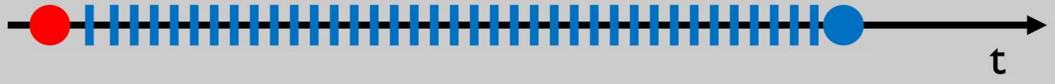
Introduction to Time-dependent DFT

Real-time propagation



1. Prepare initial state from a static DFT calculation

$$\left[-\frac{\nabla^2}{2} + v_{\rm S}(\mathbf{r})\right]\phi_j(\mathbf{r}) = \epsilon_j \phi_j(\mathbf{r})$$

2. Solve the TD Kohn-Sham equations

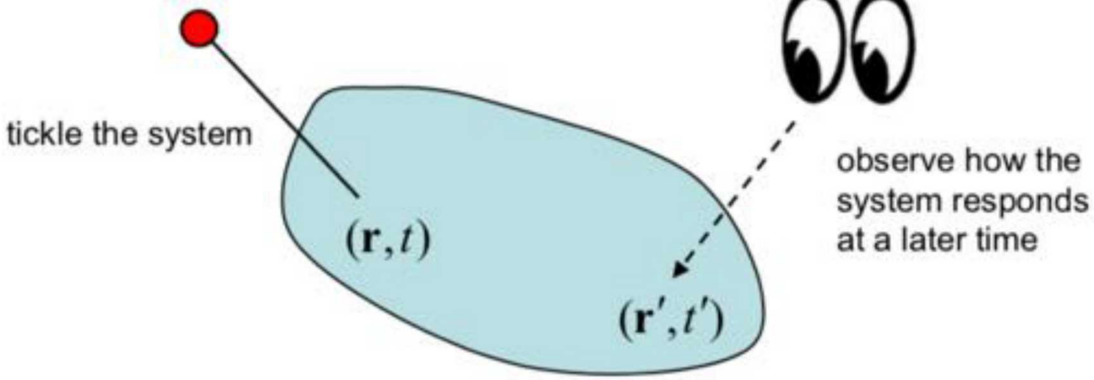
$$i\frac{d\phi_j(\mathbf{r})}{dt} = \left[-\frac{\nabla^2}{2} + v_{\rm S}(\mathbf{r})\right]\phi_j(\mathbf{r})$$

$$v_{\rm S}(\mathbf{r},t) = v(\mathbf{r},t) + v_{\rm H}(\mathbf{r},t) + v_{\rm XC}(\mathbf{r},t) \approx v_{\rm S}^{gs}[n(\mathbf{r},t)](\mathbf{r})$$

3. Compute observables in terms of time-dependent density

$$n(\mathbf{r},t) = \sum_i \phi_i^*(\mathbf{r},t)\phi_i(\mathbf{r},t)$$

Linear response



Courtesy of N. Maitra and C. Ullrich (2018).

$$\delta n(\mathbf{q},t) = \int_0^\infty d\tau\ \chi(\mathbf{q},-\mathbf{q},\tau)\, v_0\, f(t-\tau)$$

$$\epsilon^{-1}(\mathbf{r},\mathbf{r}',\omega) = \delta(\mathbf{r}-\mathbf{r}') + \int d\mathbf{r}''\frac{\chi(\mathbf{r}'',\mathbf{r}',\omega)}{|\mathbf{r}-\mathbf{r}''|}$$

Compute various transport properties (stopping power, conductivity, dynamical structure factor).

Sandia's Implementation of TDDFT

Implementation of TDDFT-Ehrenfest MD in VASP

- Andrew D. Baczewski et al., PRL **116**, 115004 (2016)
- Plane wave basis
- Projector-augmented wave (PAW) formalism
- Crank-Nicolson time integration (unitary)
- Generalized minimal residual method

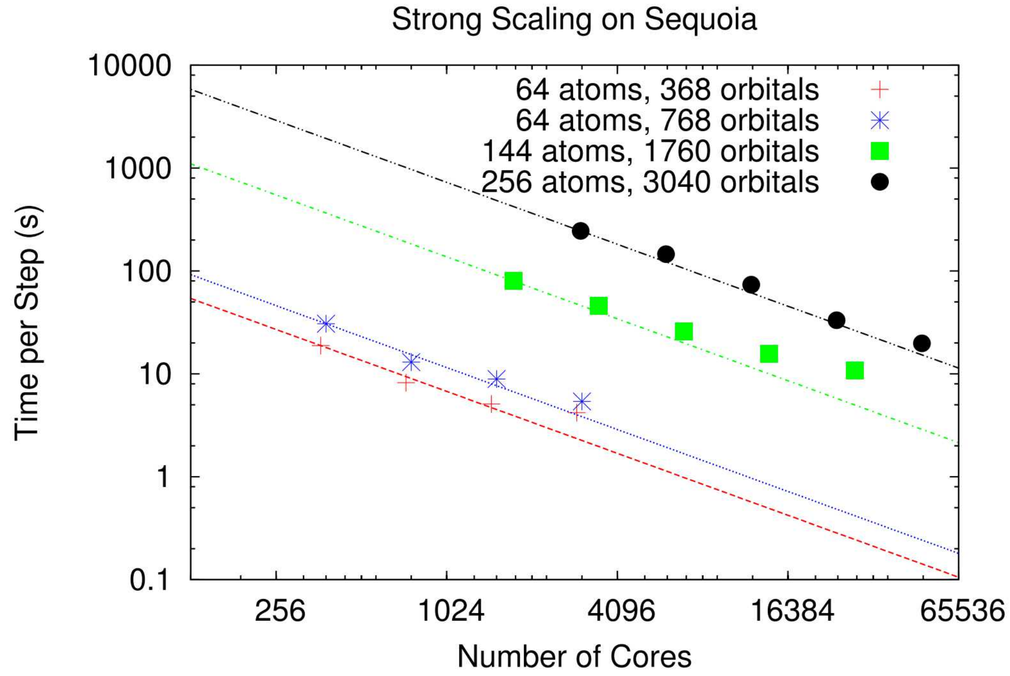
Coupled electron-ion equations of motion

$$i\frac{\partial}{\partial t}\phi_i(\mathbf{r},t) = \left\{-\frac{1}{2}\nabla^2 + v_{\mathrm{S}}(\mathbf{r},t)\right\}\phi_i(\mathbf{r},t)$$

$$M_\alpha \frac{\partial^2 \mathbf{R}_\alpha}{\partial t^2} = -\nabla_{R_\alpha} E[R_\alpha, n(\mathbf{r},t)]$$

Scales well on DOE machines

- Typically 100s of cores, a few hours
- No "free" parameters
- takes mass density
- # of electrons
- exchange-correlation functional



Elk code

QUANTUMESPRESSO

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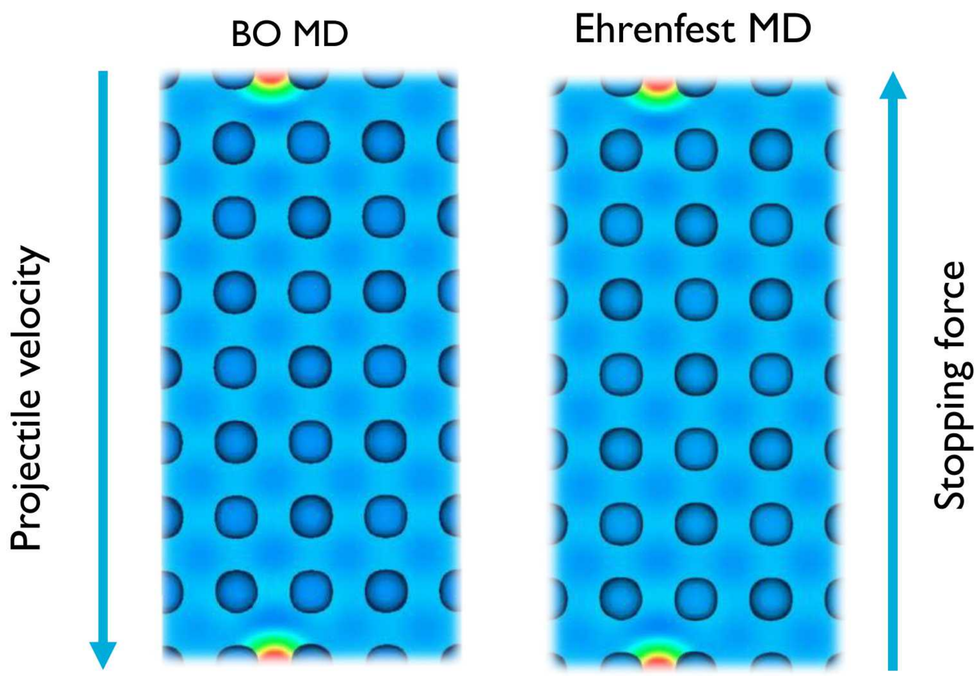
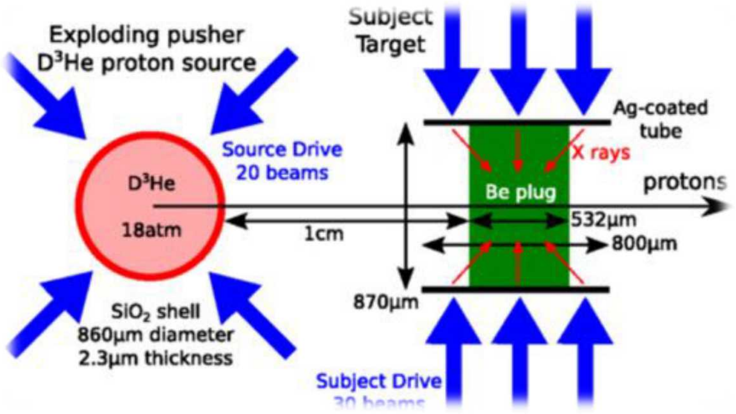
Example: Hydrogen moving through cold, bulk aluminum in a channeling trajectory

$$\frac{\partial E}{\partial x} = \frac{1}{v}\frac{\partial}{\partial t}\langle E \rangle$$



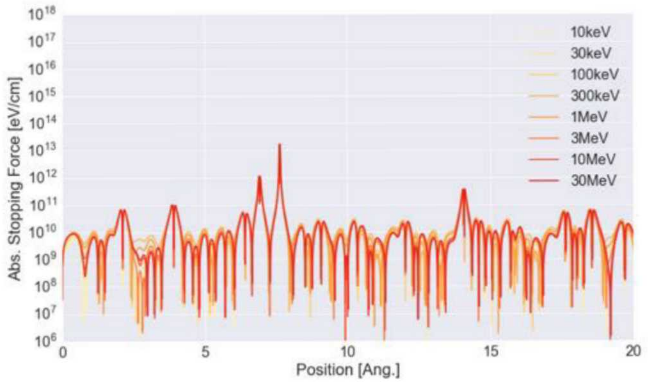
Stopping mechanisms
- Nuclear stopping (lattice vibrations)
- Electronic stopping (electronic excitations)

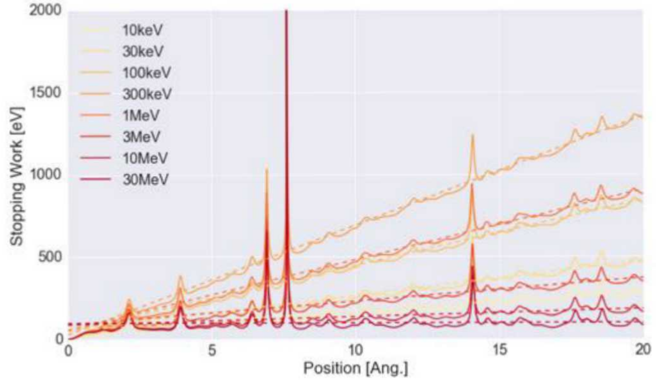
Large body of literature for cold targets
- Empirical approximations (Rutherford, Thomson, Bohr, Bethe)
- Parameter-free atomistic simulations
- Electronic structure coupled to molecular dynamics
- Cold stopping power (Echenique, Correa, Artacho, Schleife)

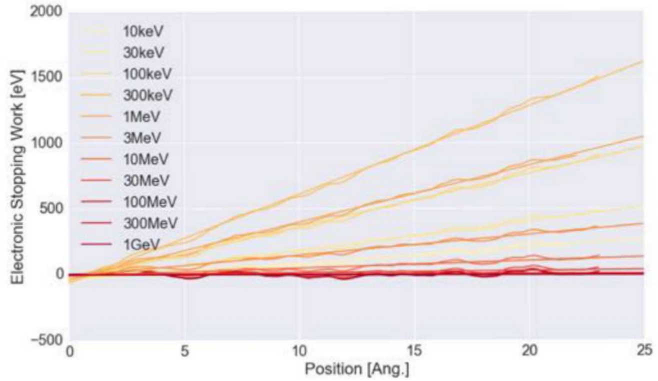


Zylstra et al., Phys. Rev. Lett. 114, 215002 (2015).

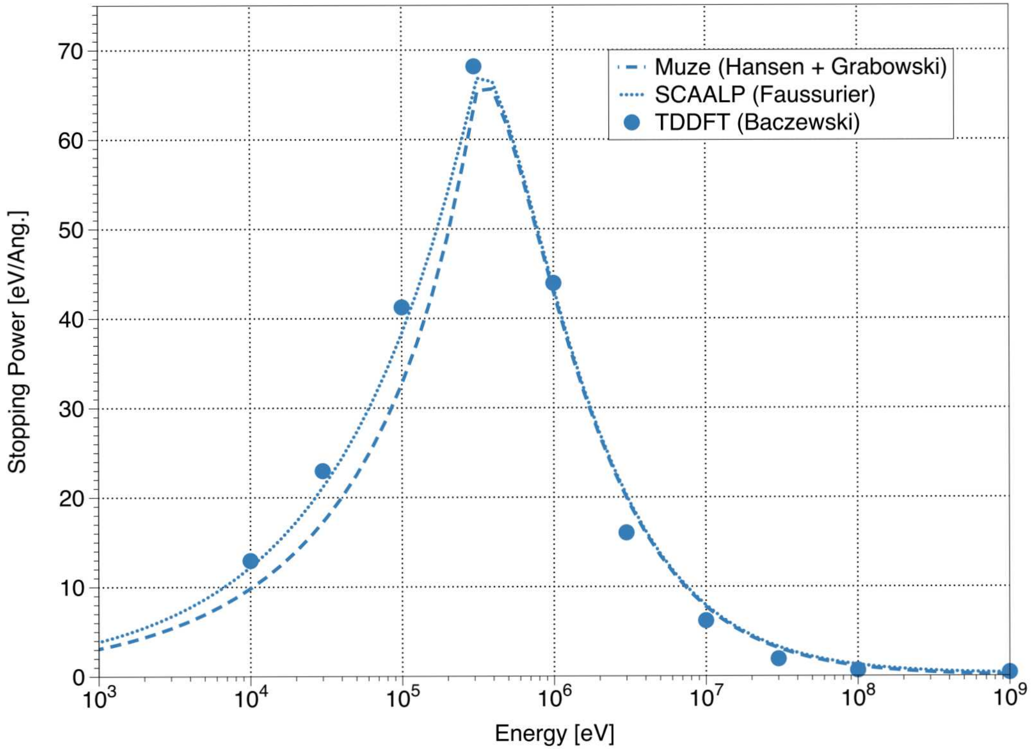
Stopping Power in Warm Dense Targets



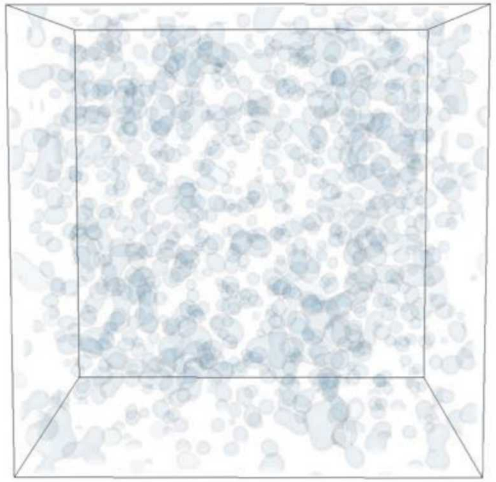




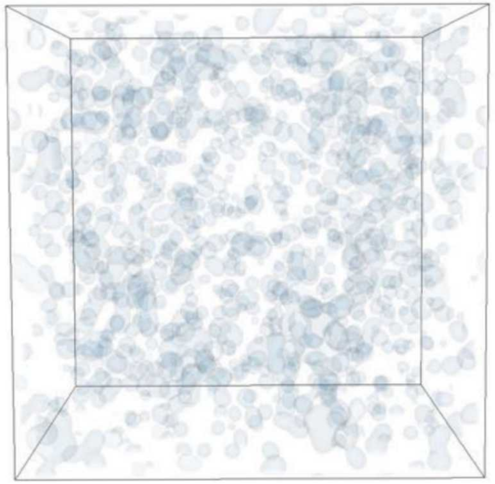
- Stopping at 10 g/cc (mass density) and 2 eV (temperature)
- **Force vs. projectile distance:** Similar across velocities
- **Work vs. projectile distance:** Spikes represent ions
- **Electronic work vs. projectile distance:** Slope represents stopping power



Projectile at 300 keV



Projectile at 30 MeV



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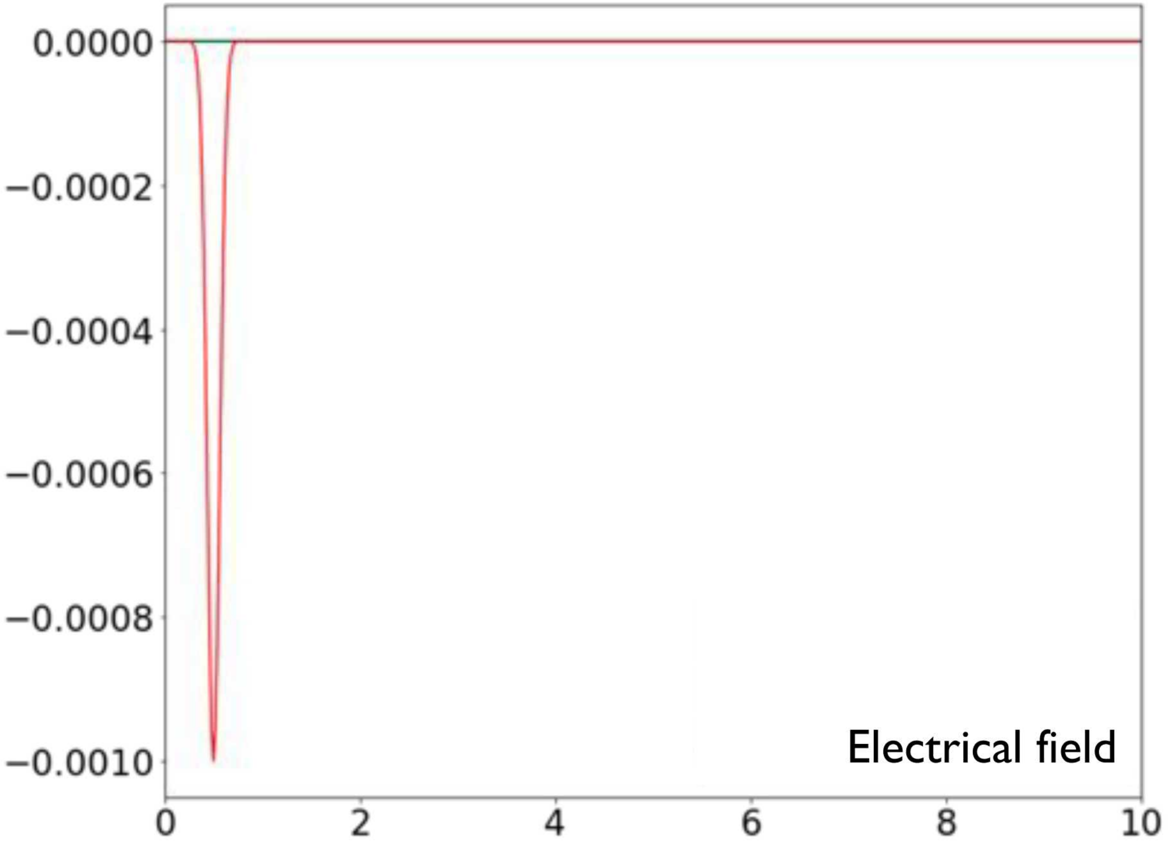
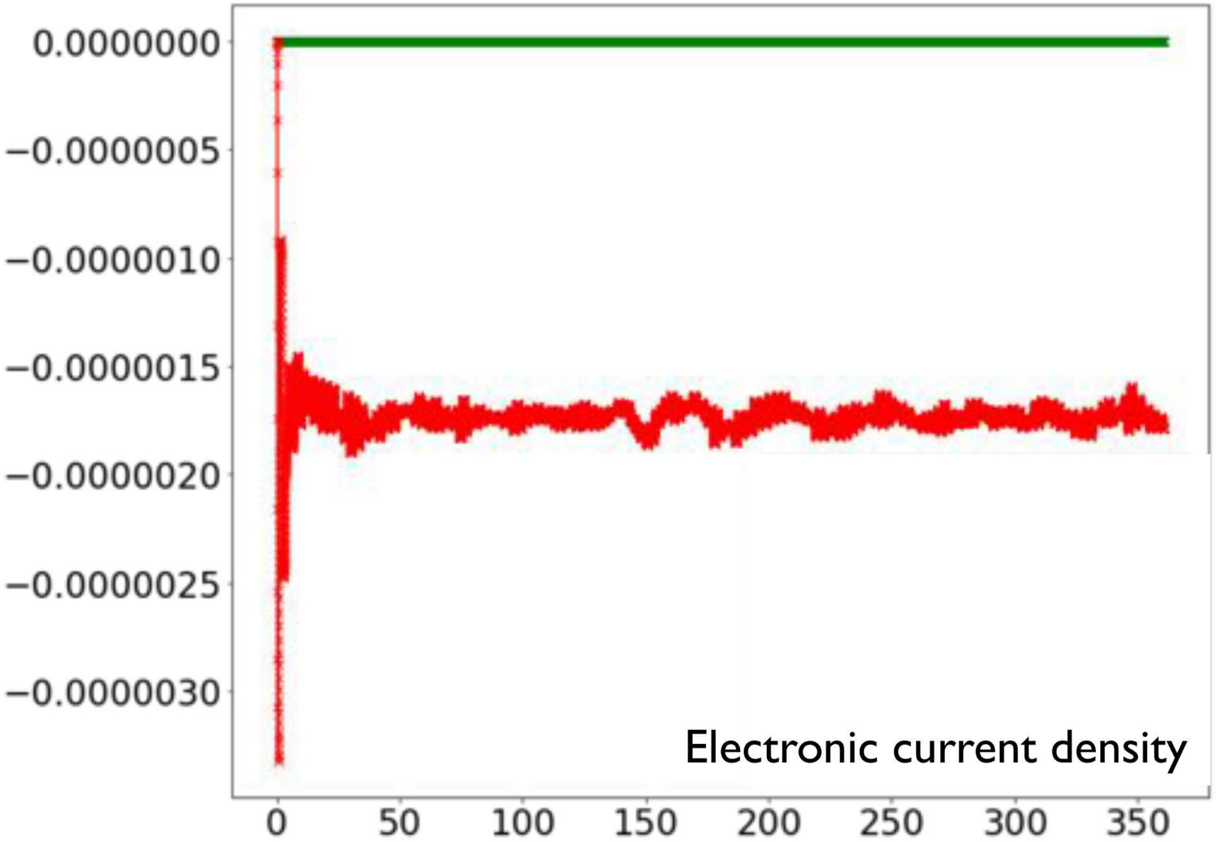
Electrical Conductivity from TDDFT

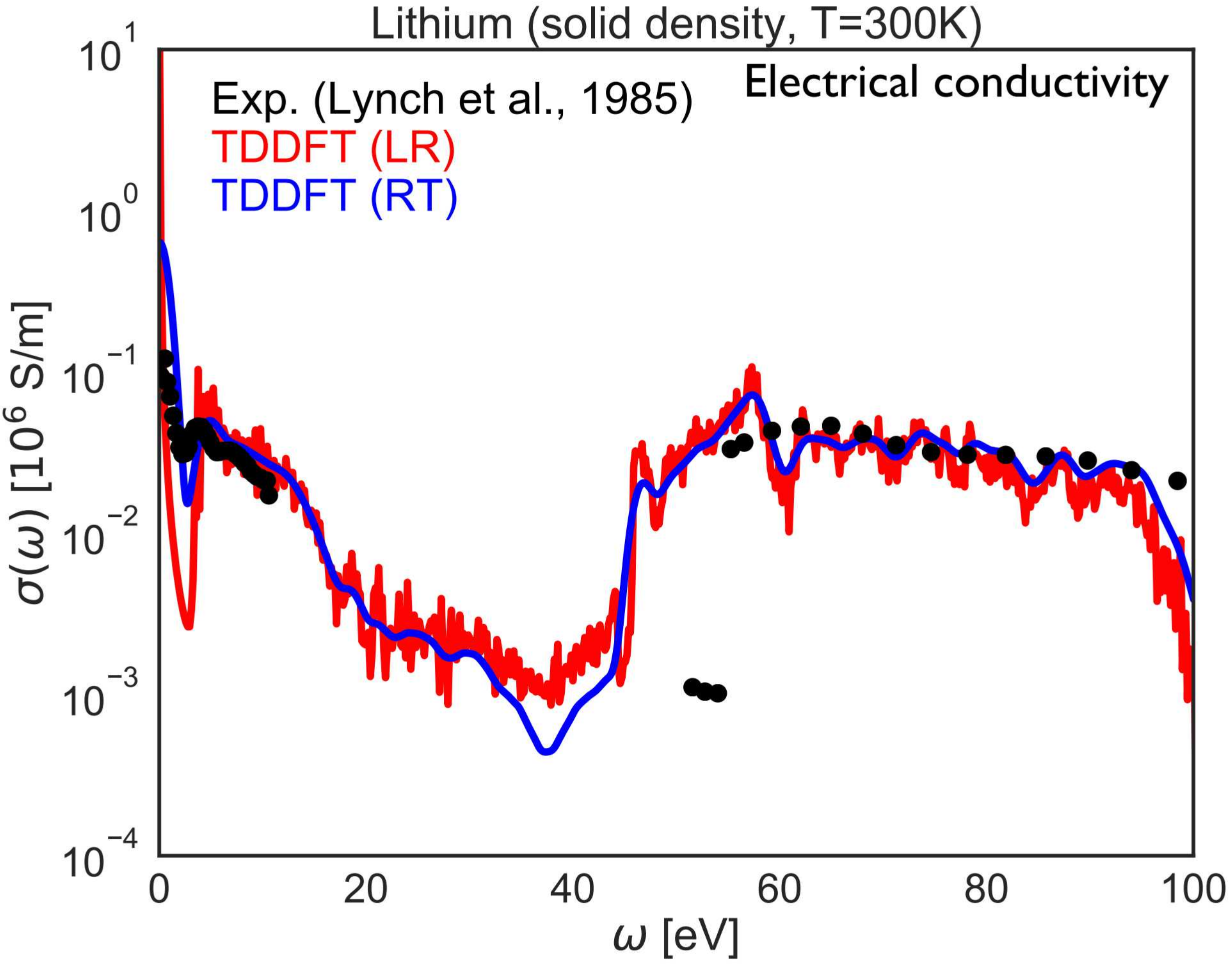
Linear response: $$\epsilon(\omega) = 1 + 4\pi i \frac{\sigma(\omega)}{\omega}$$

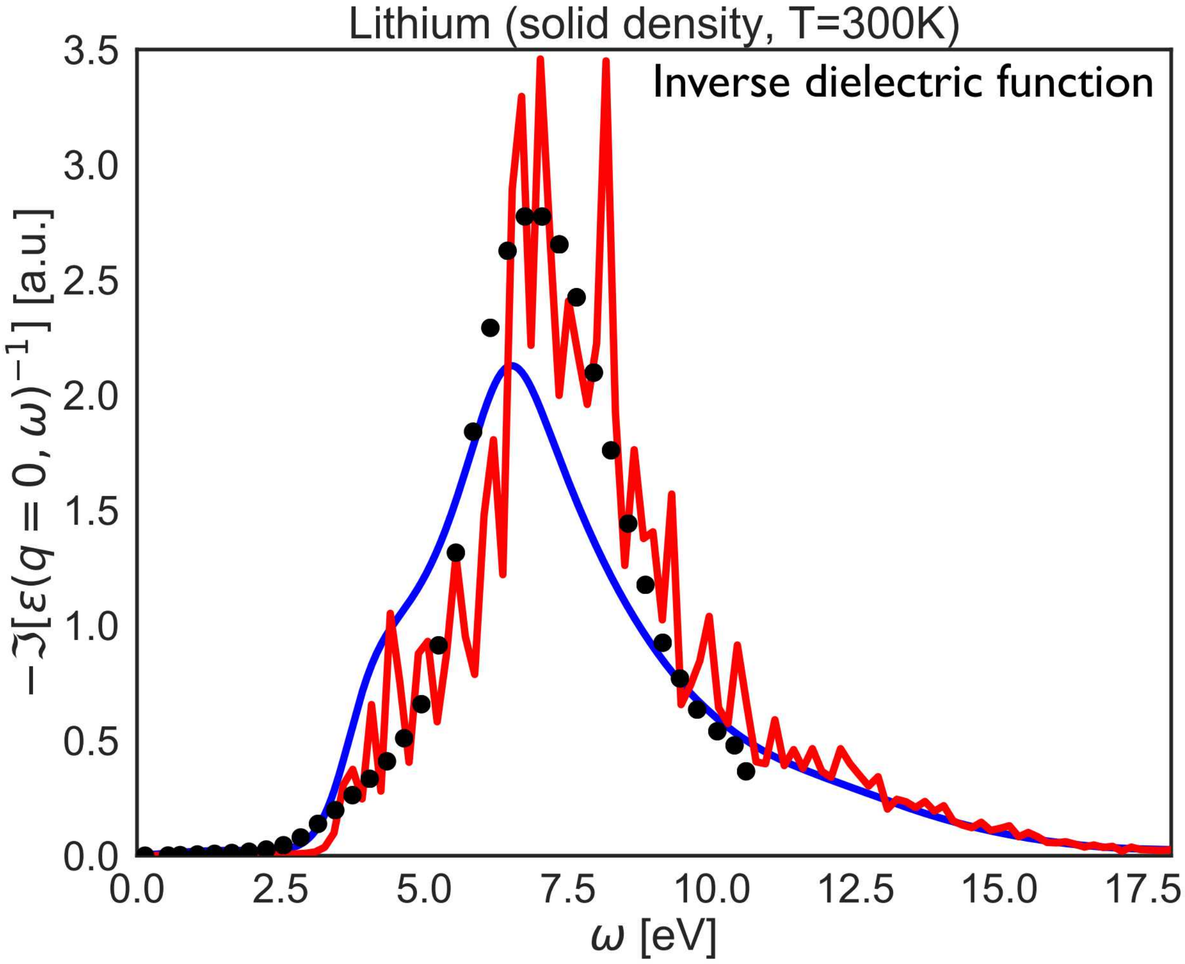
Real-time: $$\mathbf{E}(t) = -\frac{1}{c}\frac{\mathbf{A}(t)}{dt}\,, \qquad \mathbf{J}(t) = -\frac{i}{\Omega}\int d\mathbf{r} \sum_j \phi_j^*(\mathbf{r})[\hat{H}(t), \hat{\mathbf{r}}]\phi_j(\mathbf{r})\,, \qquad \mathbf{J}(\omega) = \sigma(\omega)\mathbf{E}(\omega)$$





Baseline (simple metal)





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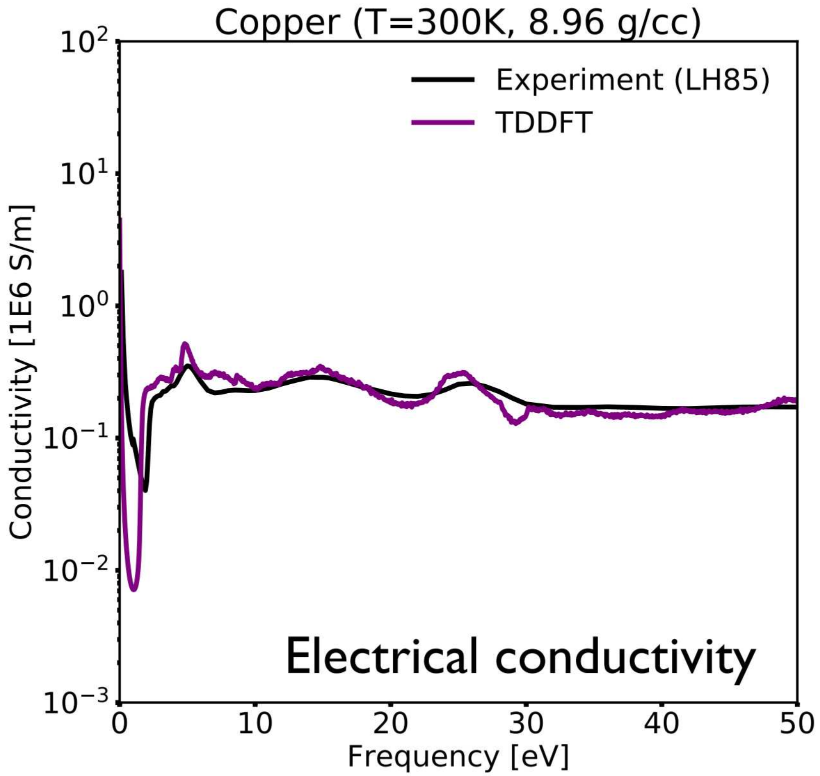
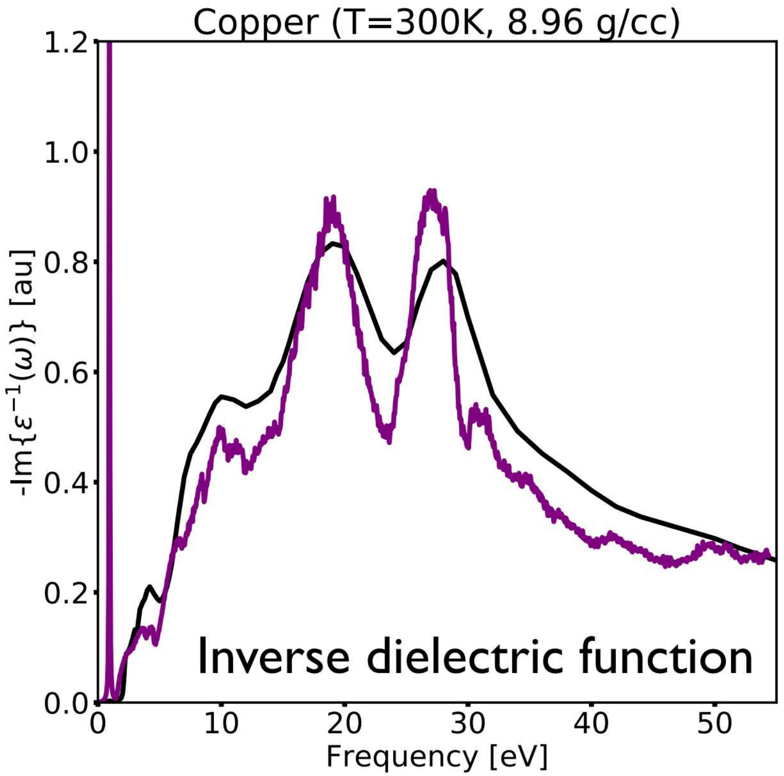
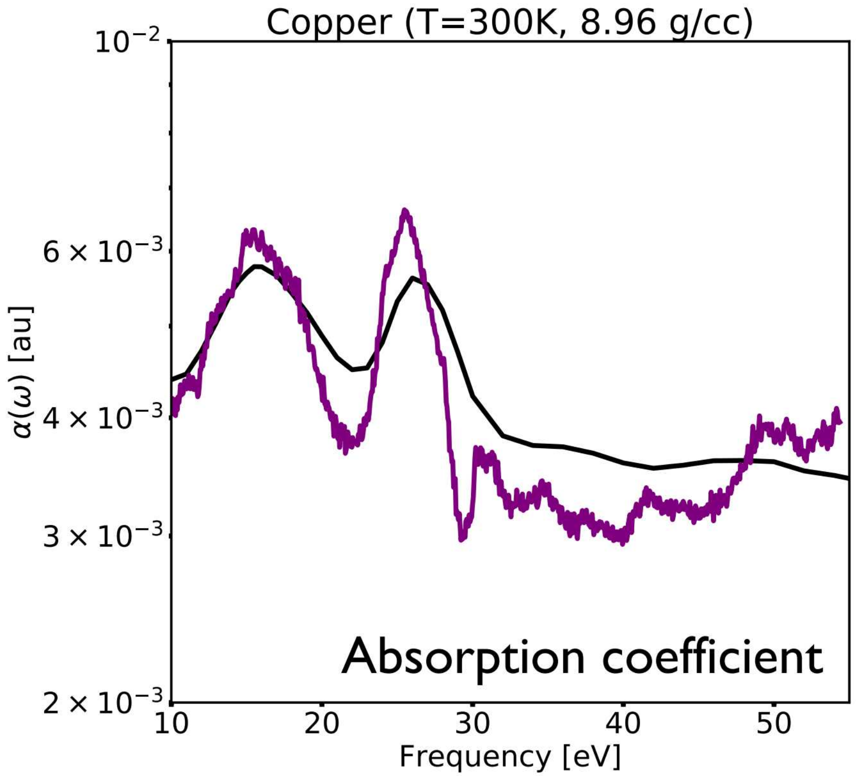
Copper under ambient conditions

Baseline (a somewhat more complex metal)







$$\lim_{q\to 0}\int_0^\infty d\omega\ \frac{1}{\omega}\Im\left[\frac{1}{\epsilon(q,\omega)}\right] = -\frac{\pi}{2}$$

	Sum rule	Error	Relative error
Experiment	-1.50	-0.07	0.04
TDDFT (1)	-1.41	-0.15	0.10

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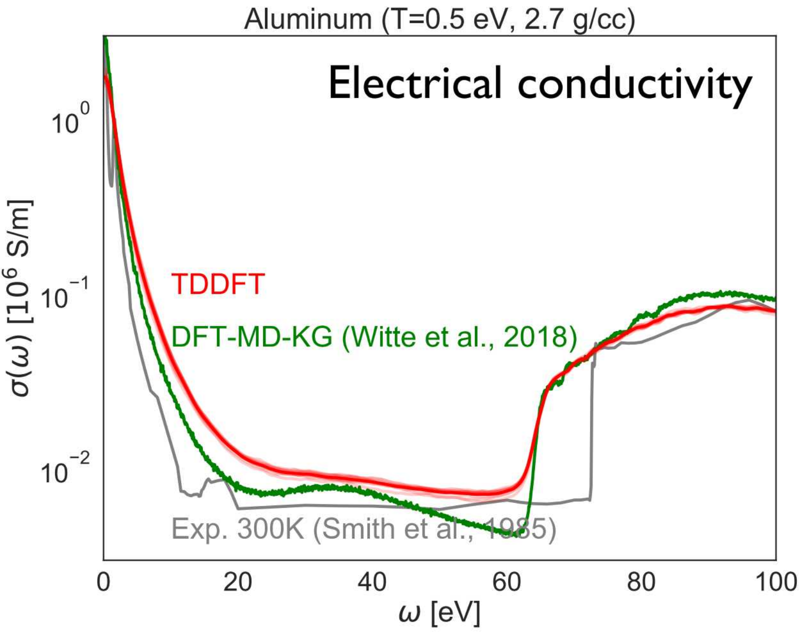
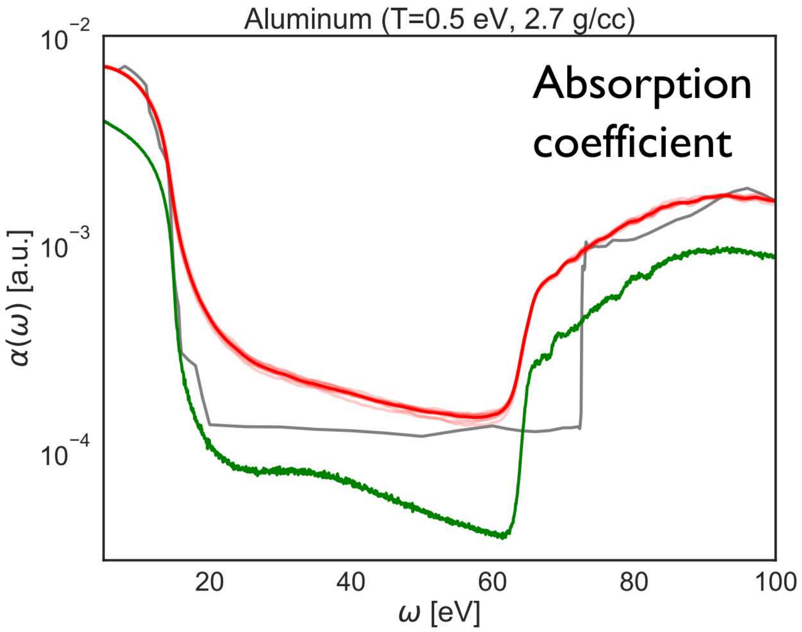
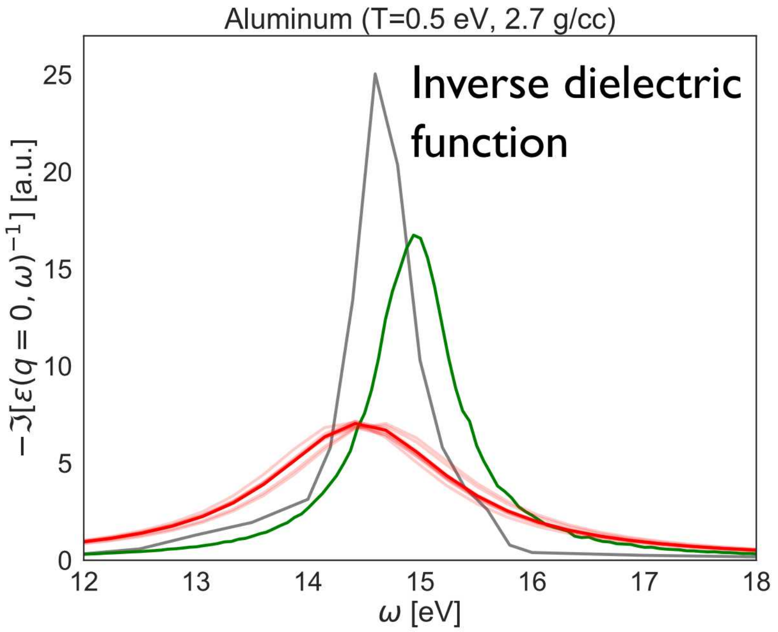
Isochorically heated Aluminum







$$\lim_{q\to 0}\int_0^\infty d\omega\ \frac{1}{\omega}\Im\left[\frac{1}{\epsilon(q,\omega)}\right] = -\frac{\pi}{2}$$

	Sum rule	Error	Relative error
Experiment	-1.577	0.007	-0.004
DFT-MD-KG	-1.568	-0.003	0.002
TDDFT	-1.563	-0.007	0.005

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Avoid Chihara decomposition:

$$S(\mathbf{q},\omega) = \underbrace{|f_I(\mathbf{q}) + \rho(\mathbf{q})|^2 S_{ii}(\mathbf{q},\omega)}_{\text{Bound electrons following ions}} + \underbrace{Z_f S_{ee}(\mathbf{q},\omega)}_{\text{Free electrons}} + \underbrace{S_{bf}(\mathbf{q},\omega)}_{\text{Photoionized electrons}}$$

Probe system with x-ray:

$$v(\mathbf{r},t) = v_0\, e^{i\mathbf{q}\cdot\mathbf{r}} f(t)$$

$$|\mathbf{q}| = \frac{4\pi \sin(\theta/2)}{\lambda_0}$$

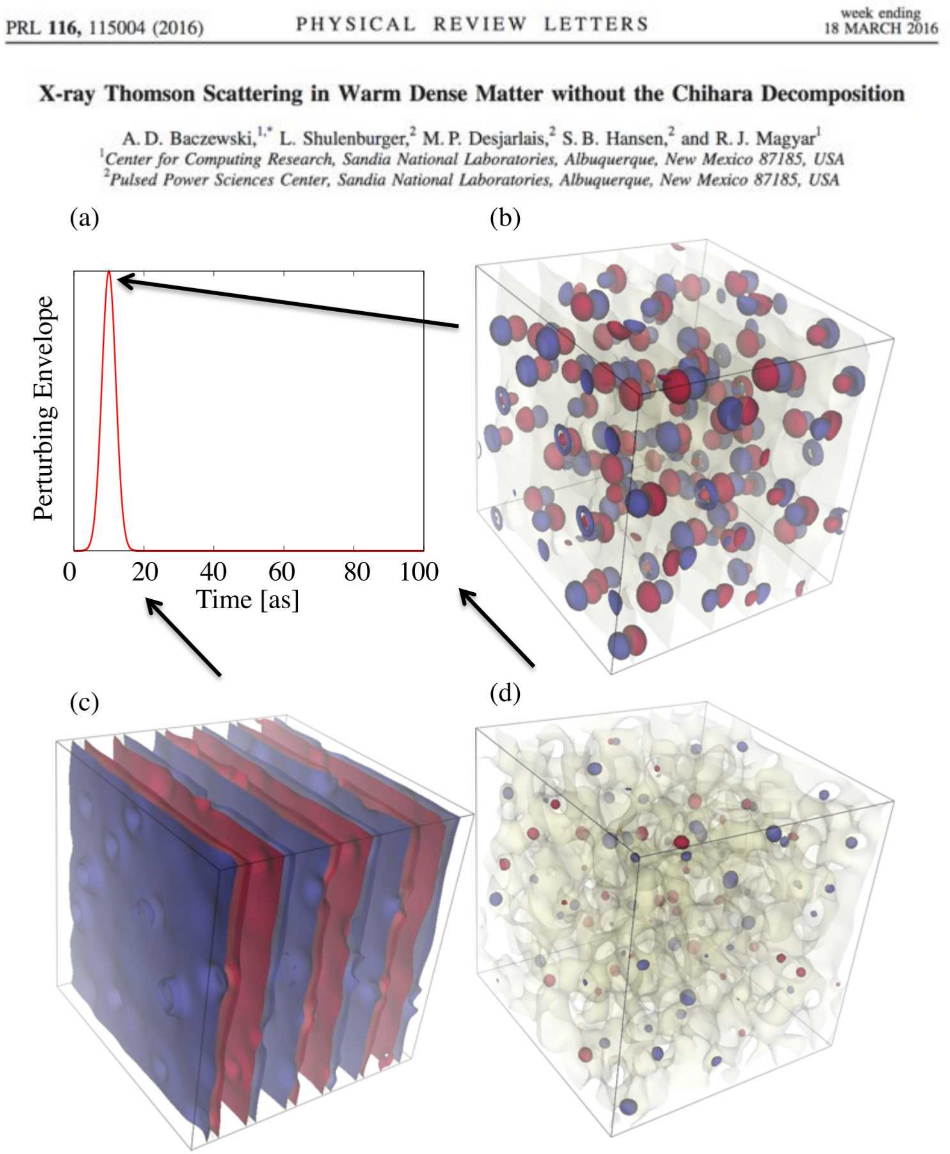
$$\lambda_0 : \text{probe wavelength } (2\text{Å})$$

Record density response:

$$\delta n(\mathbf{q},t) = \int_0^\infty d\tau\ \chi(\mathbf{q},-\mathbf{q},\tau)\, v_0\, f(t-\tau)$$

Apply dissipation-fluctuation theorem:

$$\chi(\mathbf{q},-\mathbf{q},\omega) = \frac{\delta n(\mathbf{q},\omega)}{v_0 f(\omega)} \qquad S(\mathbf{q},\omega) = -\frac{1}{\pi}\frac{\Im[\chi(\mathbf{q},-\mathbf{q},\omega)]}{1-e^{-\omega/T}}$$


PRL 116, 115004 (2016) PHYSICAL REVIEW LETTERS week ending 18 MARCH 2016

X-ray Thomson Scattering in Warm Dense Matter without the Chihara Decomposition

A. D. Baczewski,[1,*] L. Shulenburger,[2] M. P. Desjarlais,[2] S. B. Hansen,[2] and R. J. Magyar[1]
[1]Center for Computing Research, Sandia National Laboratories, Albuquerque, New Mexico 87185, USA
[2]Pulsed Power Sciences Center, Sandia National Laboratories, Albuquerque, New Mexico 87185, USA

Dynamical Structure Factor from Linear-response TDDFT

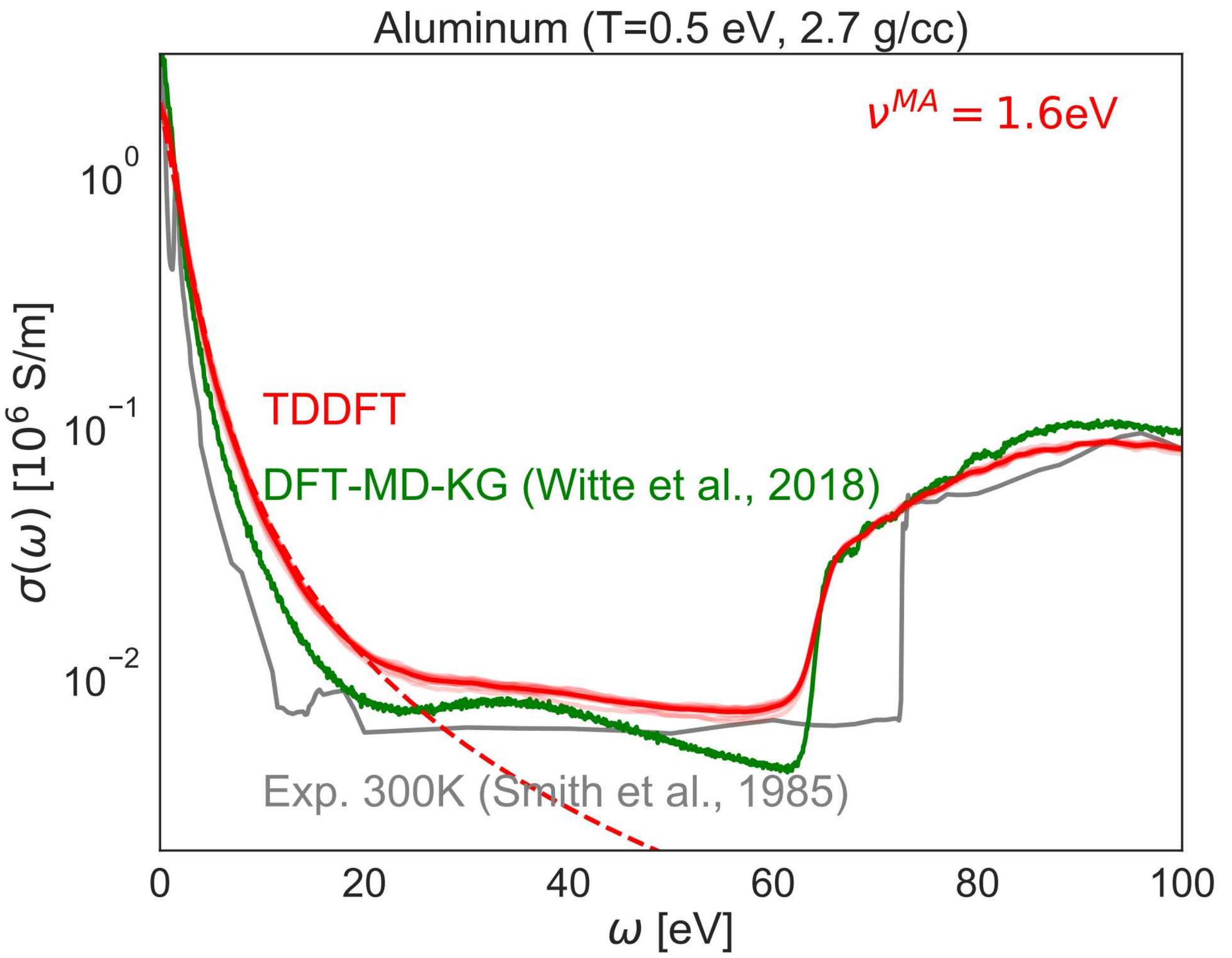
Mermin approximation to the dielectric function:

$$\epsilon^M(\mathbf{q},\omega) = 1 + \frac{\left(1 + i\frac{\nu(\omega)}{\omega}\right)\left[\epsilon^{RPA}(\mathbf{q},\omega + i\nu(\omega)) - 1\right]}{1 + \frac{\nu(\omega)}{\omega}\frac{\epsilon^{RPA}(\mathbf{q},\omega+i\nu(\omega))-1}{\epsilon^{RPA}(\mathbf{q},0)-1}}$$

Ab-initio collision frequencies from Drude-fit to TDDFT electrical conductivity.

$$\Re(\sigma^D) = \frac{\lim_{\omega\to 0}\sigma(\omega)}{1+\omega^2\tau^2}$$

Mermin approximation with ab-initio collision frequencies from TDDFT (**MA-AICF-TDDFT**).



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Comparison to Experiment

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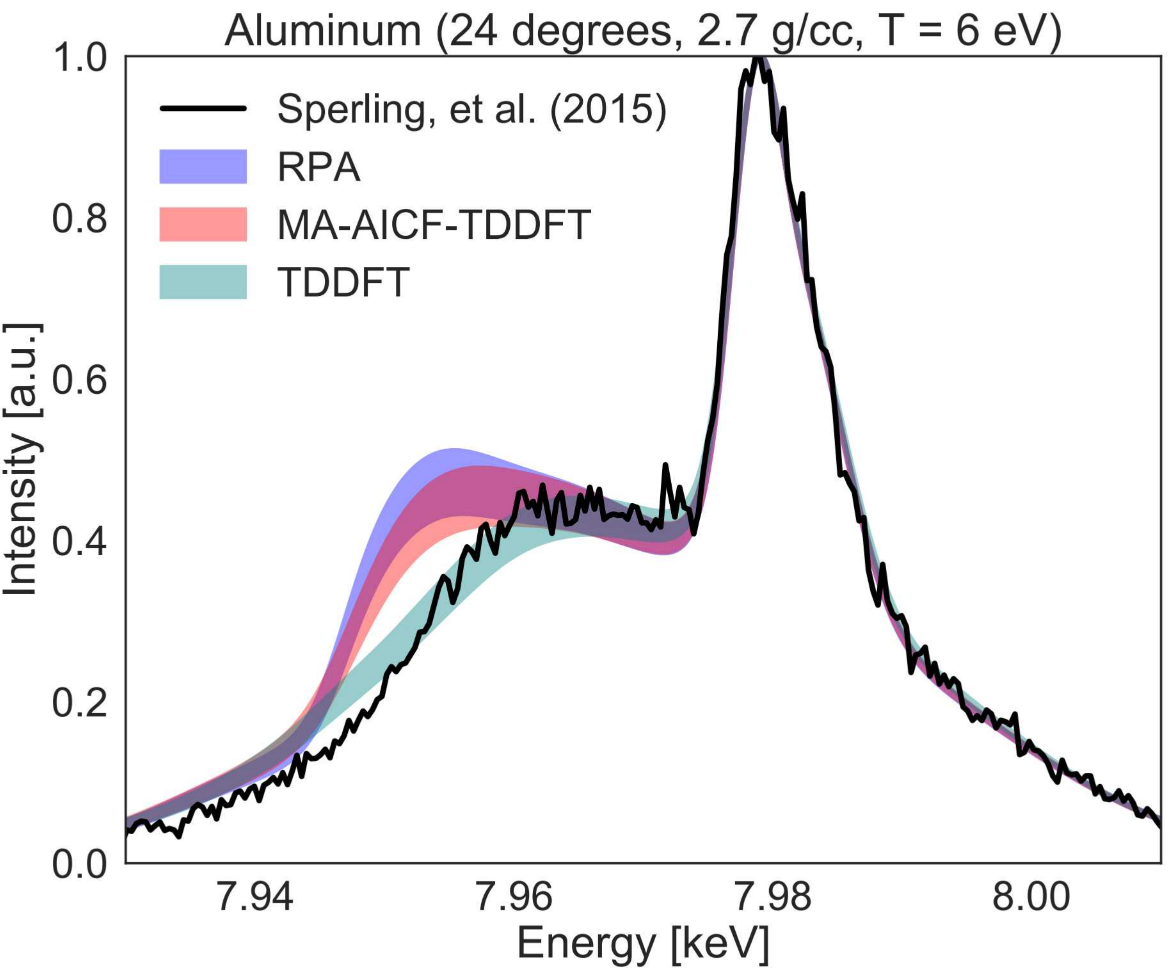
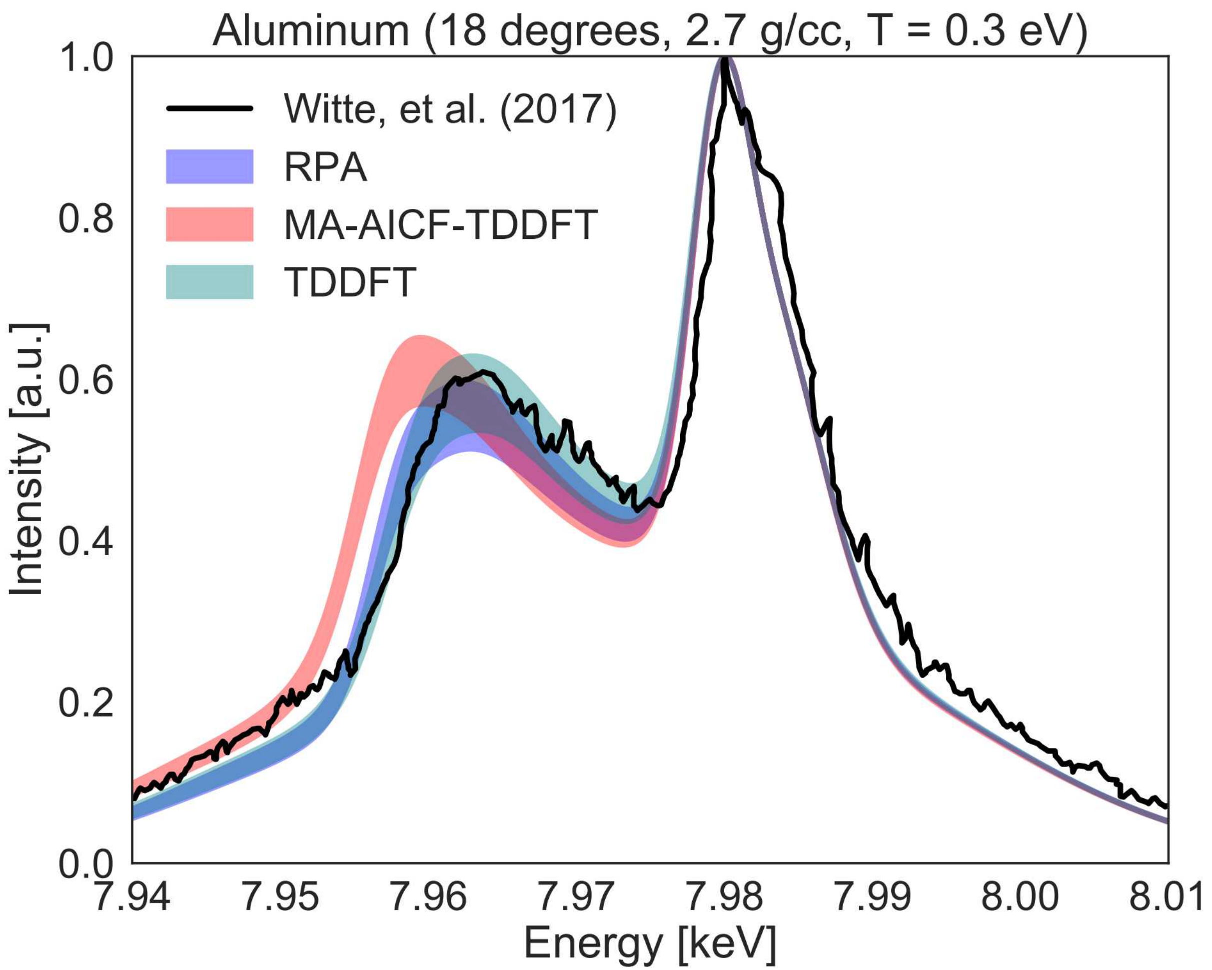




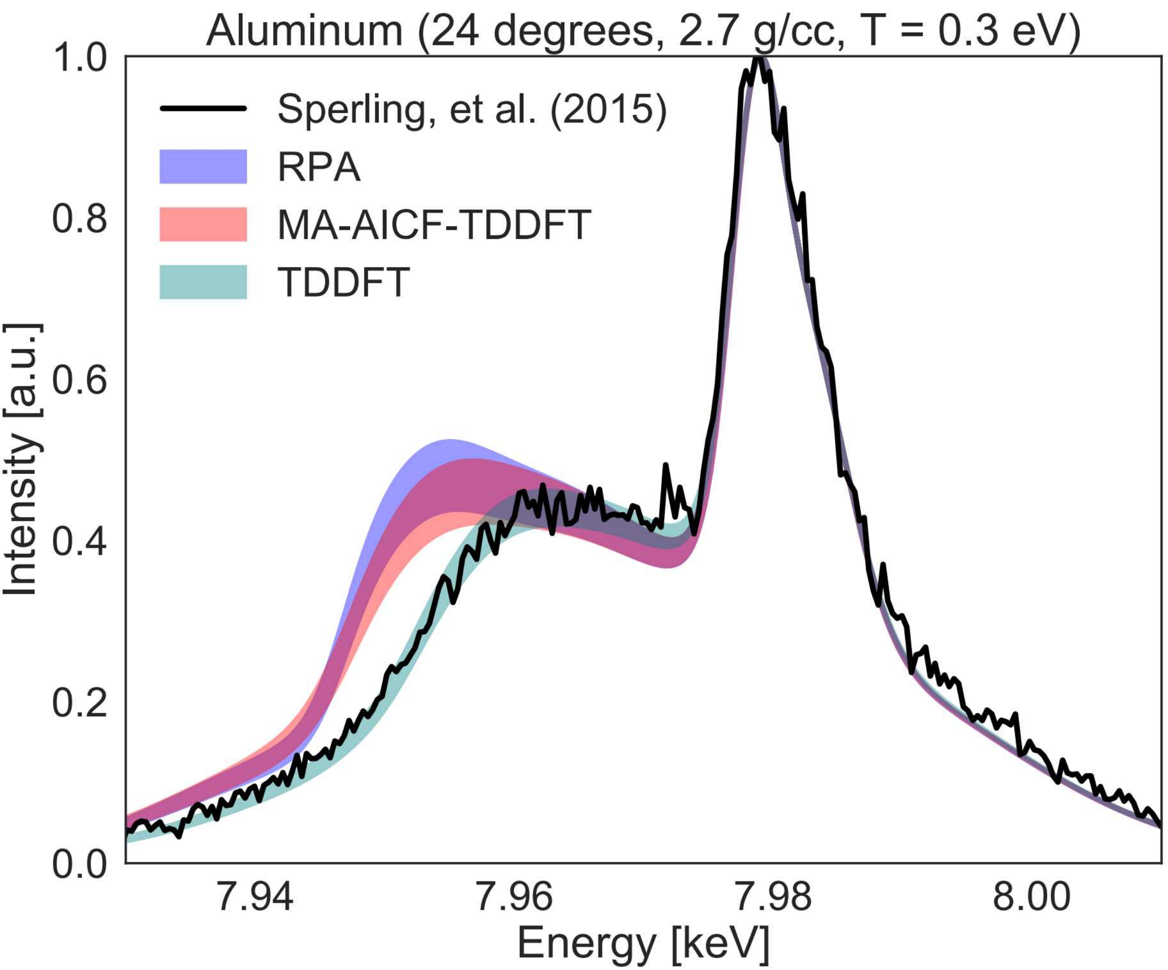
Free-Electron X-Ray Laser Measurements of Collisional-Damped Plasmons in Isochorically Heated Warm Dense Matter

P. Sperling, E. J. Gamboa, H. J. Lee, H. K. Chung, E. Galtier, Y. Omarbakiyeva, H. Reinholz, G. Röpke, U. Zastrau, J. Hastings, L. B. Fletcher, and S. H. Glenzer
Phys. Rev. Lett. **115**, 115001 – Published 9 September 2015

Warm Dense Matter Demonstrating Non-Drude Conductivity from Observations of Nonlinear Plasmon Damping

B. B. L. Witte, L. B. Fletcher, E. Galtier, E. Gamboa, H. J. Lee, U. Zastrau, R. Redmer, S. H. Glenzer, and P. Sperling
Phys. Rev. Lett. **118**, 225001 – Published 31 May 2017

Comparison to Experiment: Temperature in TDDFT



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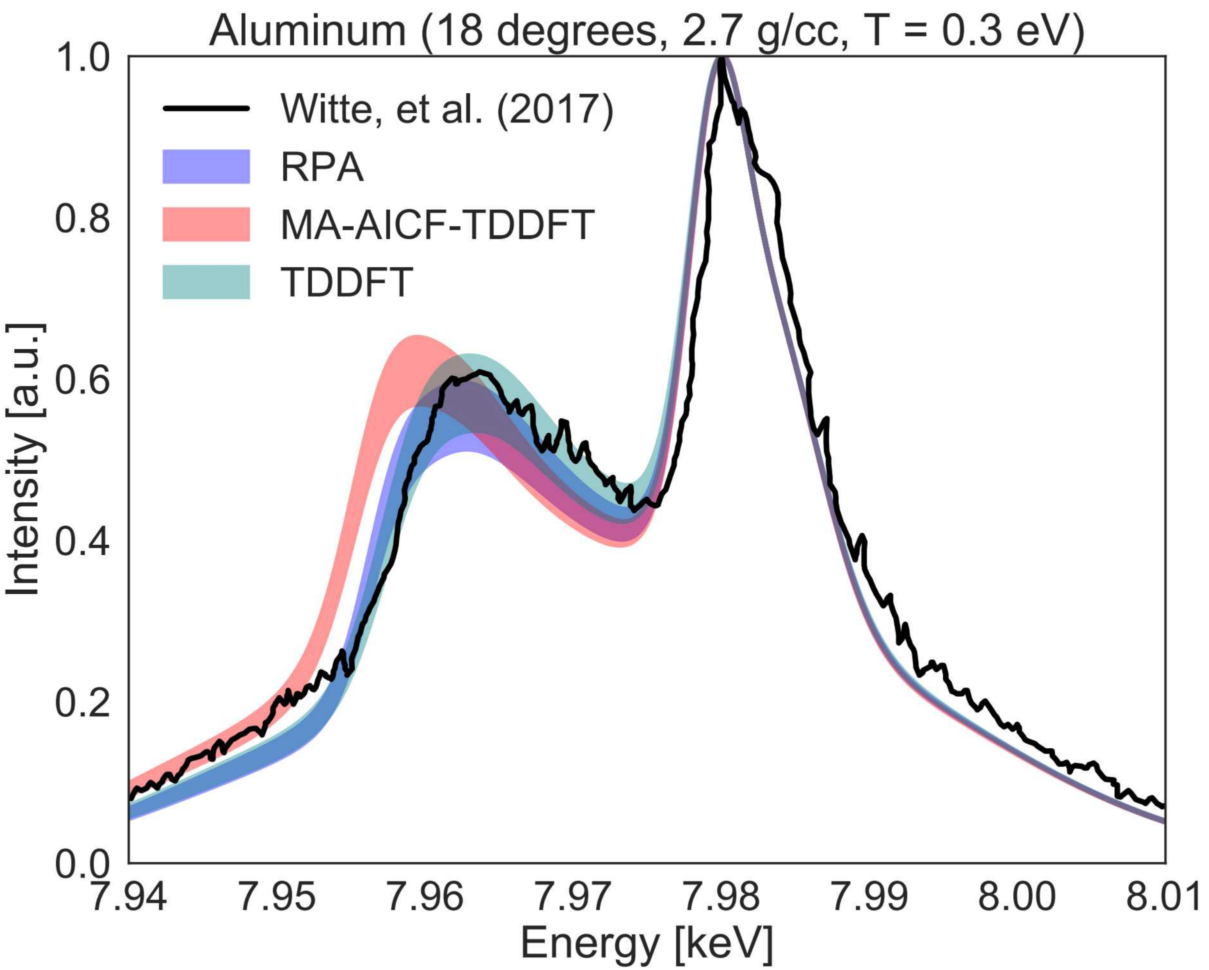

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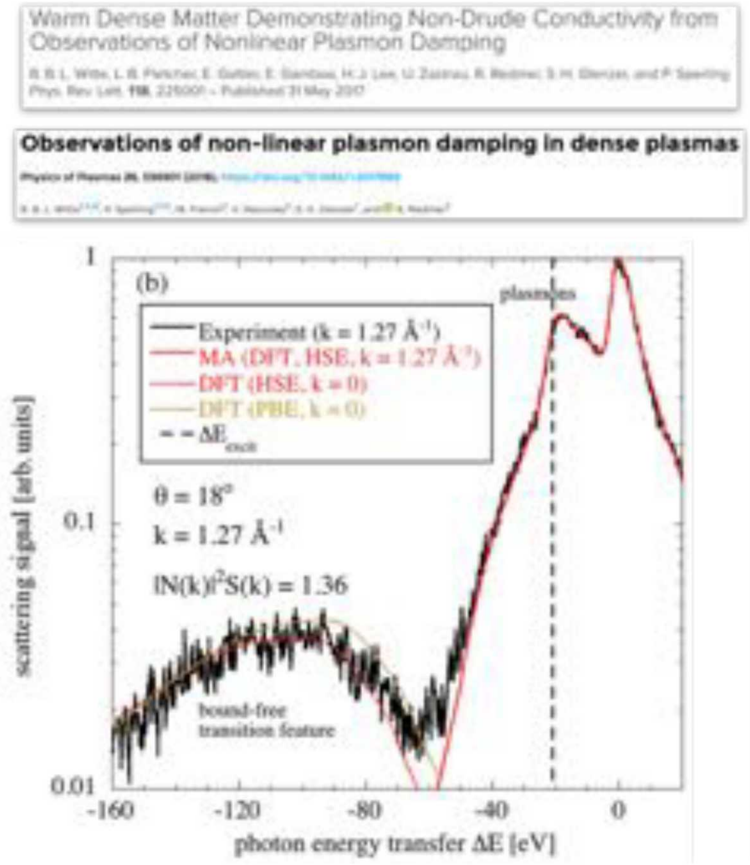
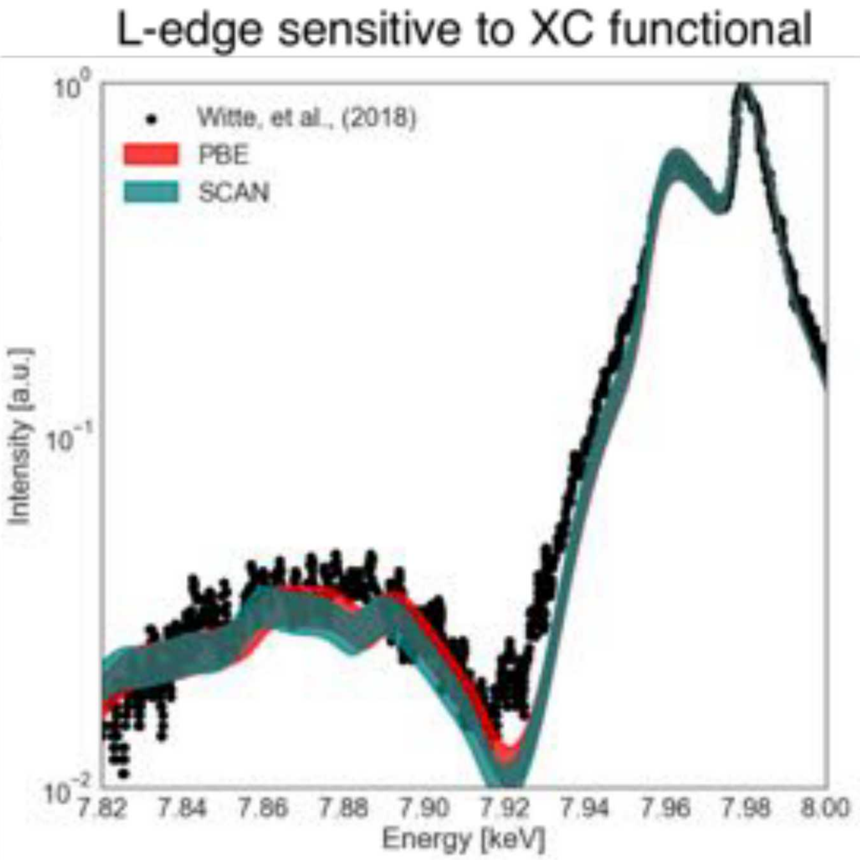
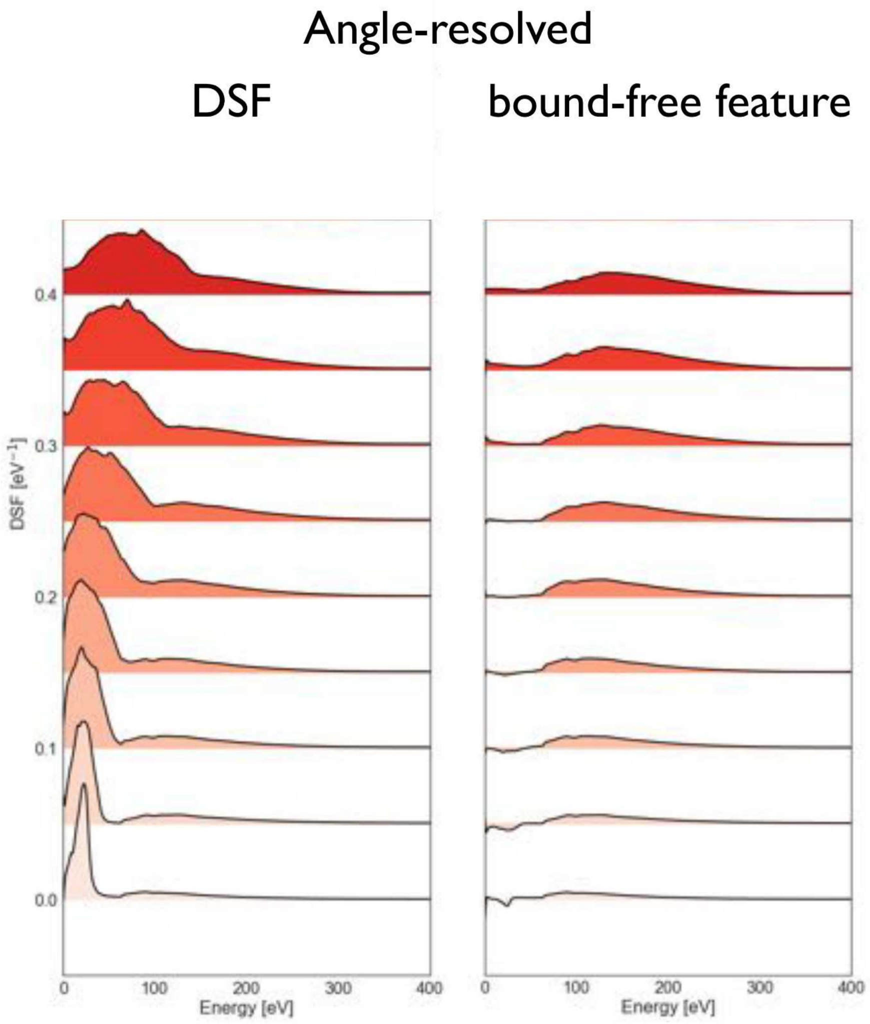
A Closer Look at the Bound-free Feature







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Summary

Capability to predict first-principles transport properties of HED from TDDFT

- Systematic approach with minimal need for post-processing
- Better scaling in real time than in energy domain
- Nonlinear effects

Support other simulation tools

- Constrain parameters in average-atom models
- Validate DFT-MD Kubo-Greenwood results
- Input for resistive magneto-hydrodynamics

Support interpretation of experiments

- Combine TDDFT tools to provide consistent predictions
- Recent experiments at LCLS
- Isochorically heated and shock-compressed materials (such as Al and Cu)

Collaborators

- Andrew D. Baczewski (Sandia National Laboratories)
- Stephanie B. Hansen (Sandia National Laboratories)

Advertisement

- Poster session: "Transport properties of magnetized warm dense matter using time-dependent density functional theory", Andrew Baczewski

Thank you for your attention!

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Supplemental Material

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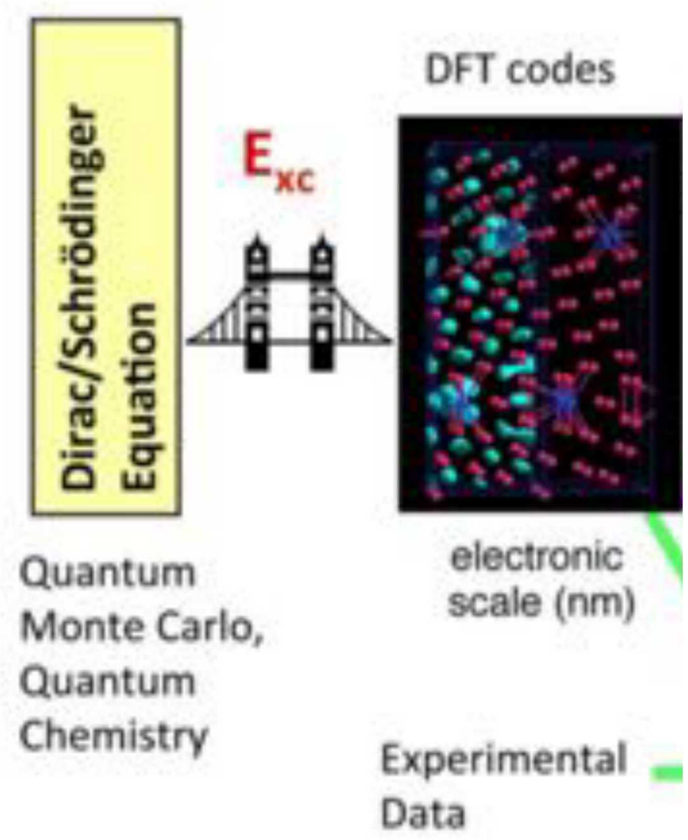
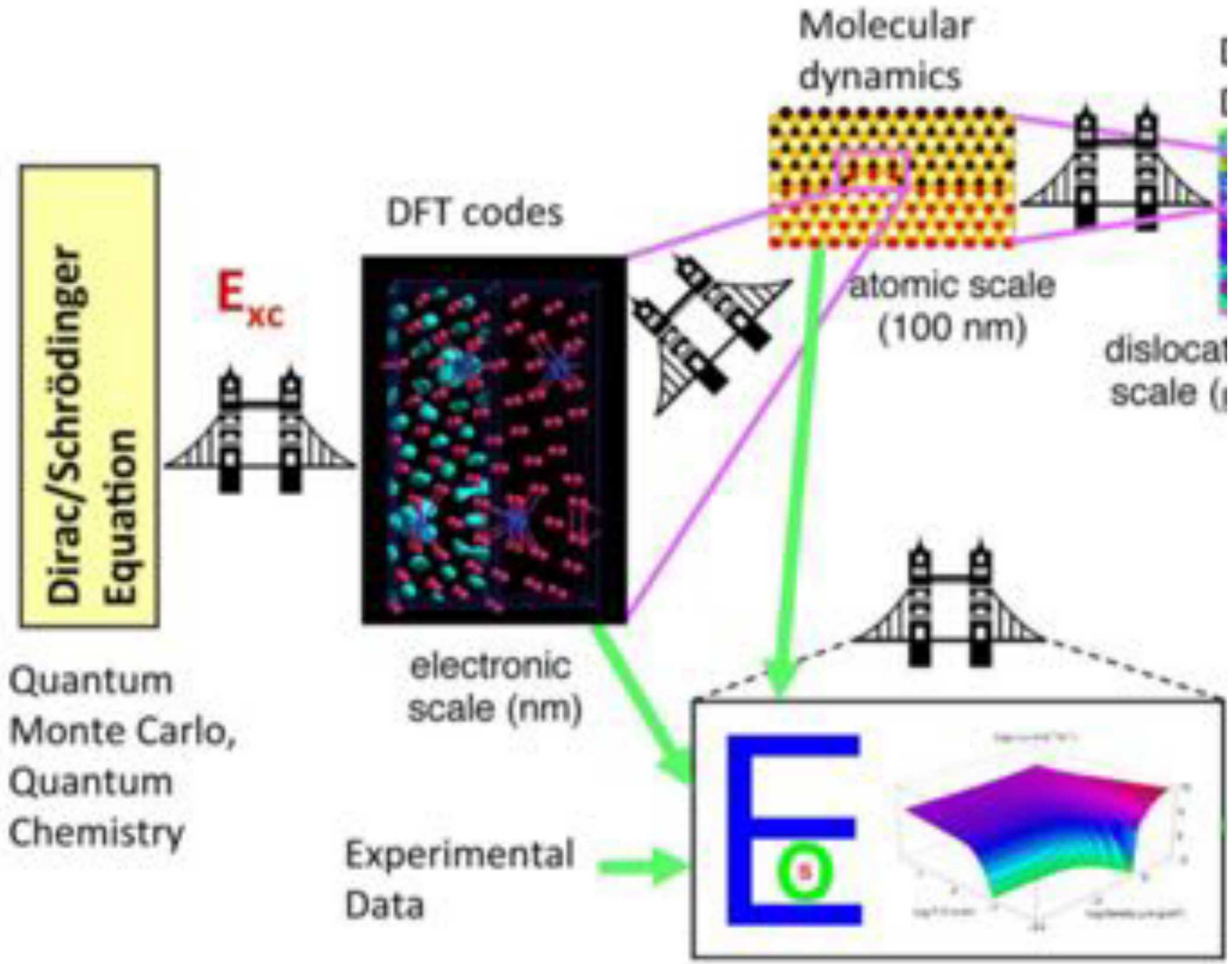
Multiscale Science



Multiscale Science



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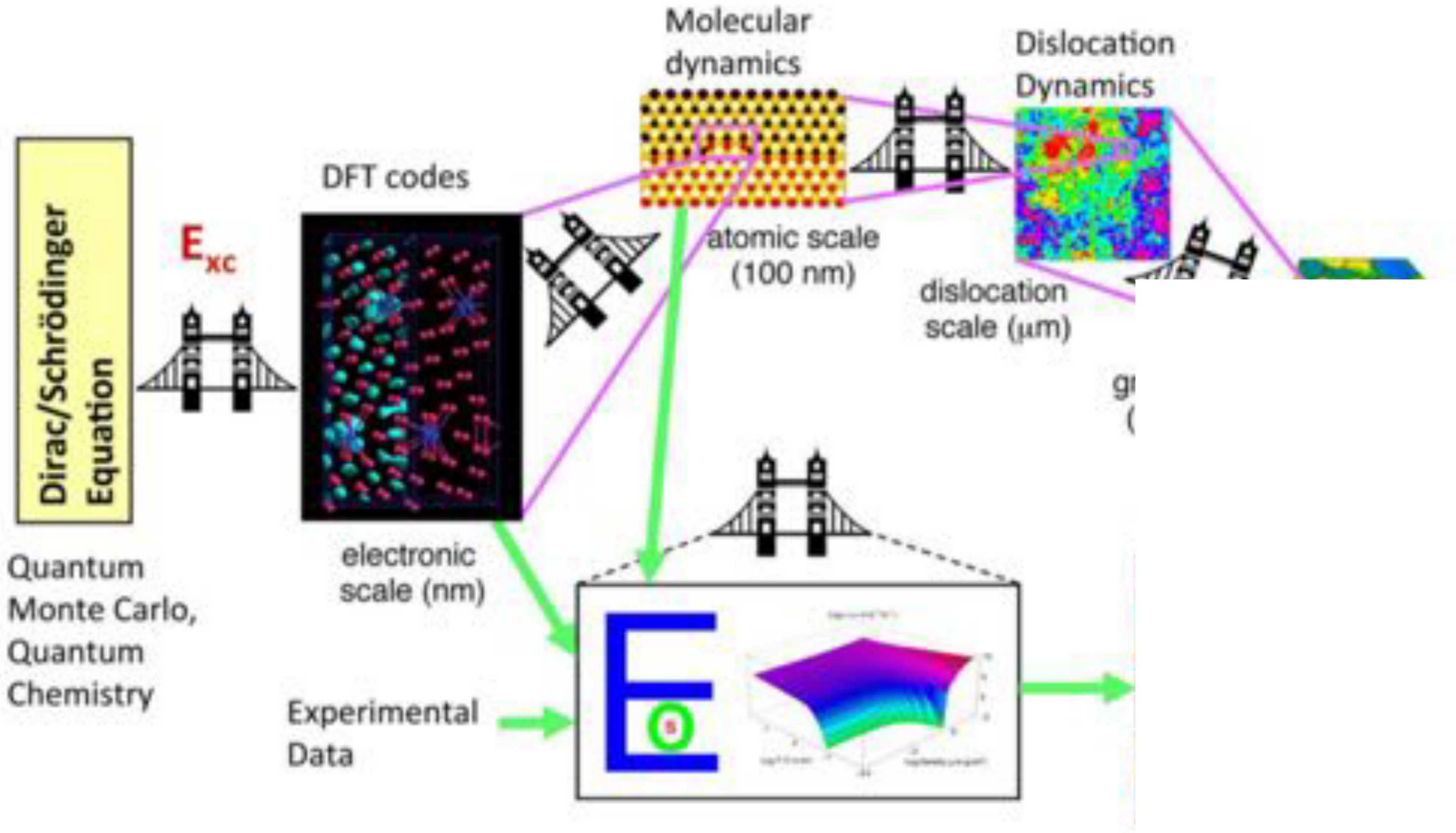

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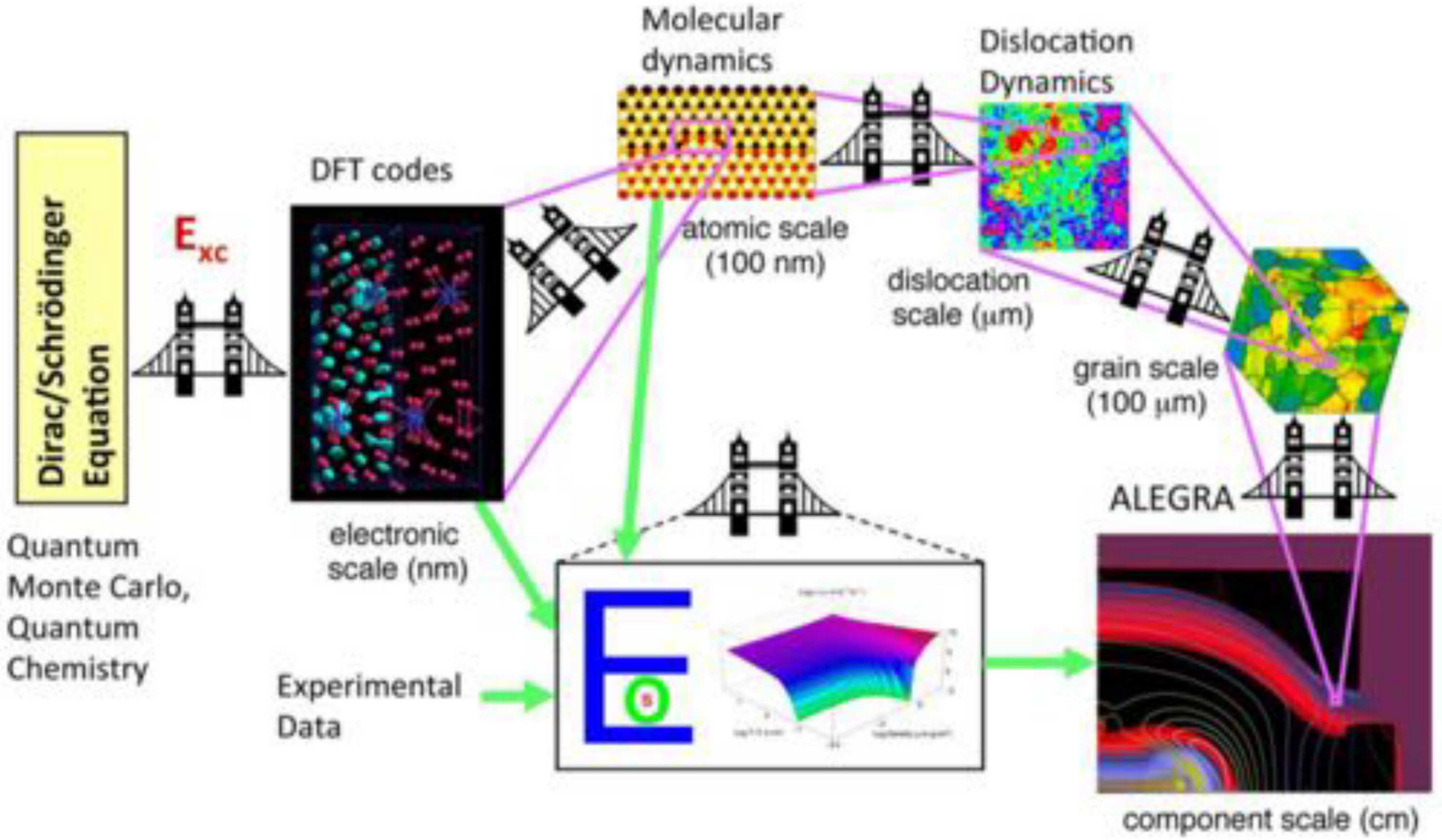
Multiscale Science



Ann E. Mattson *et al.*, International Journal of Quantum Chemistry (2016), DOI: 10.1002/qua.25097.

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Interplay between Theory, Simulations, and Experiment

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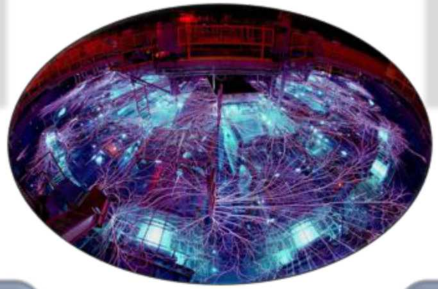
Electronic structure theory

Electronic structure theory provides input to magneto-hydrodynamics simulations.



HED experiments and diagnostics benchmark theory.

Computational fluid dynamics

HED experiments

Computational fluid dynamics simulations support design of HED experiments.

LCLS

Stopping power

Measurement of Charged-Particle Stopping in Warm Dense Plasma

A. B. Zylstra, J. A. Frenje, P. E. Grabowski, C. K. Li, G. W. Collins, P. Fitzsimmons, S. Glenzer, F. Graziani, S. B. Hansen, S. X. Hu, M. Gatu Johnson, P. Keiter, H. Reynolds, J. R. Rygg, F. H. Séguin, and R. D. Petrasso

Phys. Rev. Lett. **114**, 215002 – Published 27 May 2015

$$\frac{\partial E}{\partial x} = \frac{1}{v}\frac{\partial}{\partial t}\langle E\rangle$$

Electrical conductivity

Free-Electron X-Ray Laser Measurements of Collisional-Damped Plasmons in Isochorically Heated Warm Dense Matter

P. Sperling, E. J. Gamboa, H. J. Lee, H. K. Chung, E. Galtier, Y. Omarbakiyeva, H. Reinholz, G. Röpke, U. Zastrau, J. Hastings, L. B. Fletcher, and S. H. Glenzer

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$$\sigma(\omega) = \frac{\mathbf{J}(\omega)}{\mathbf{E}(\omega)}$$

Dynamic structure factor

LETTER

doi:10.1038/nature14048

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

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$$S(\mathbf{q},\omega) = -\frac{1}{\pi}\frac{\Im[\chi(\mathbf{q},-\mathbf{q},\omega)]}{1-e^{-\omega/k_{\mathrm{B}}T}}$$

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Coulomb coupling parameter

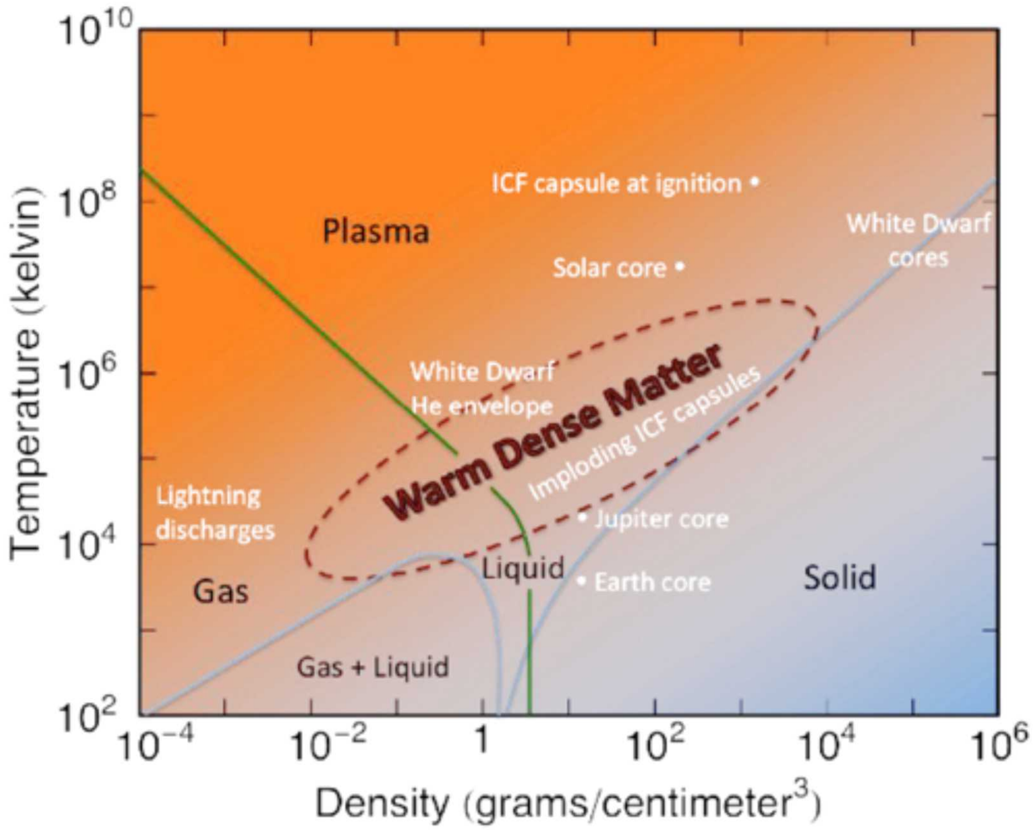
$$\Gamma = \frac{V}{T} = \frac{Ze^2}{r_\mathrm{S} k_\mathrm{B} \tau}$$

Electron degeneracy parameter

$$\Theta = \frac{k_\mathrm{B}\tau}{E_\mathrm{F}}$$

Warm dense matter regime

$$\Gamma \approx 1\,, \quad \Theta \approx 1$$



Basic Research Needs for HEDLP, Report of the Workshop on HEDLP Research Needs, DOE (2008).

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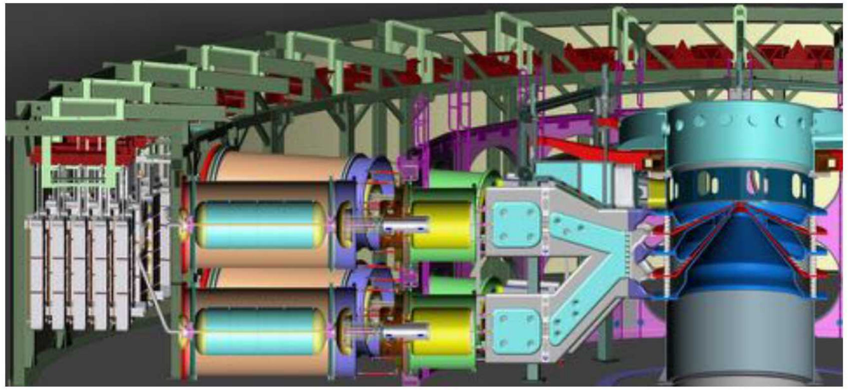
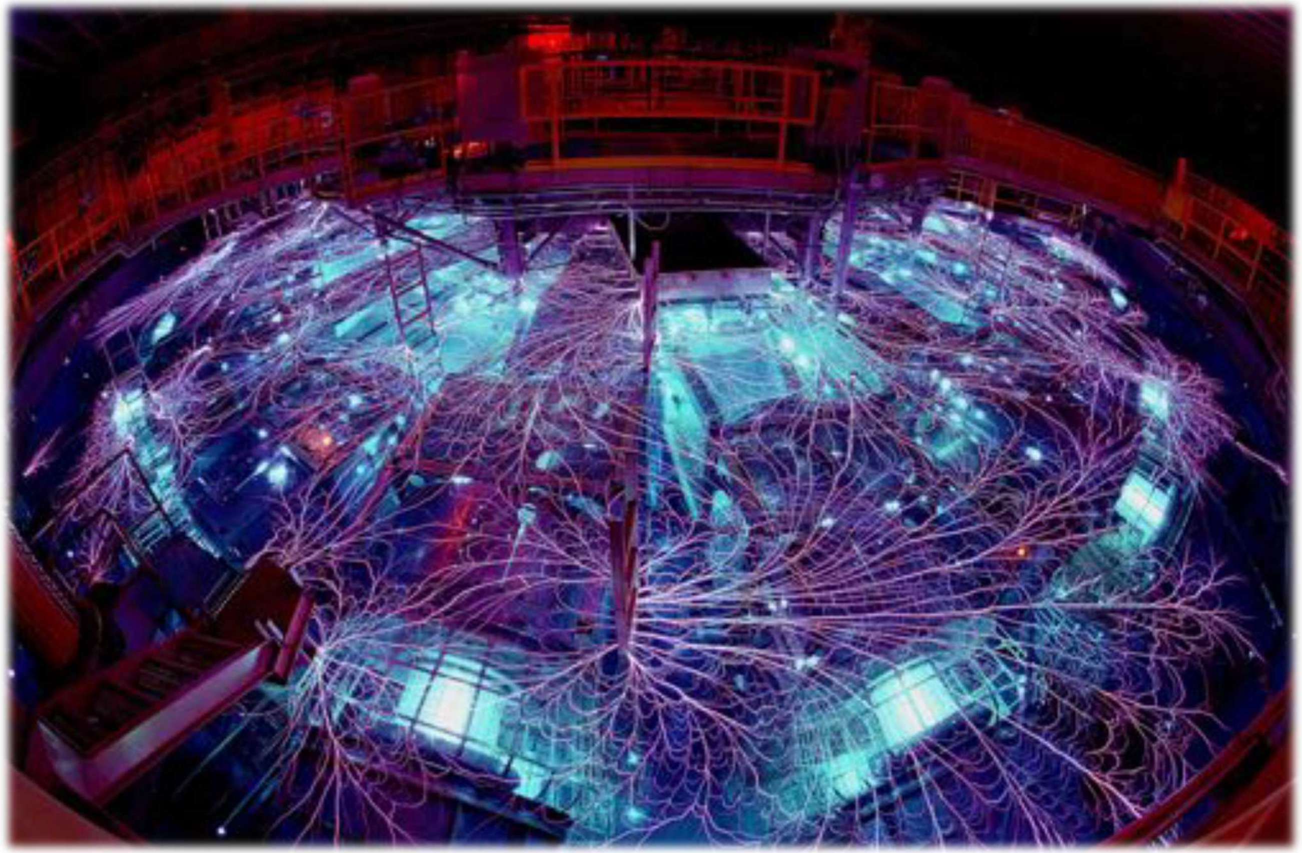
Generating Warm Dense Matter in the Lab

Creating HED conditions requires transferring an enormous amount of energy to a target in a very short period of time.



Z Machine, Sandia National Laboratories.
(https://www.sandia.gov/z-machine/about_z/how-z-works.html)



Z Machine, Sandia National Laboratories.

Compression of energy in time and space in pulsed power facilities (Z machine) enables exciting science (astrophysics, planetary science, inertial confinement fusion).

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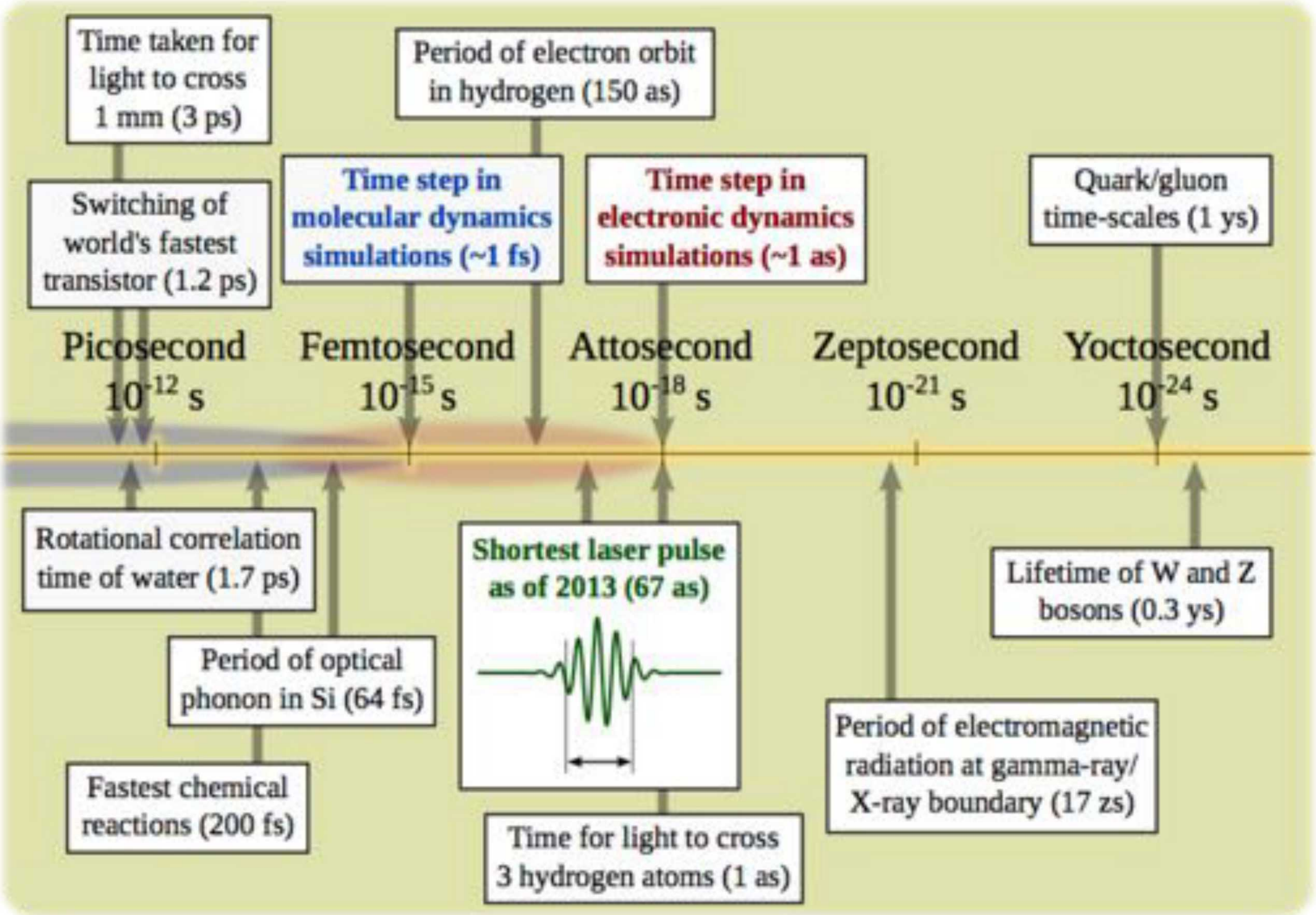
Time Scales



Courtesy of K. Dewhurst, Max Planck Institute of Microstructure Physics (2015).

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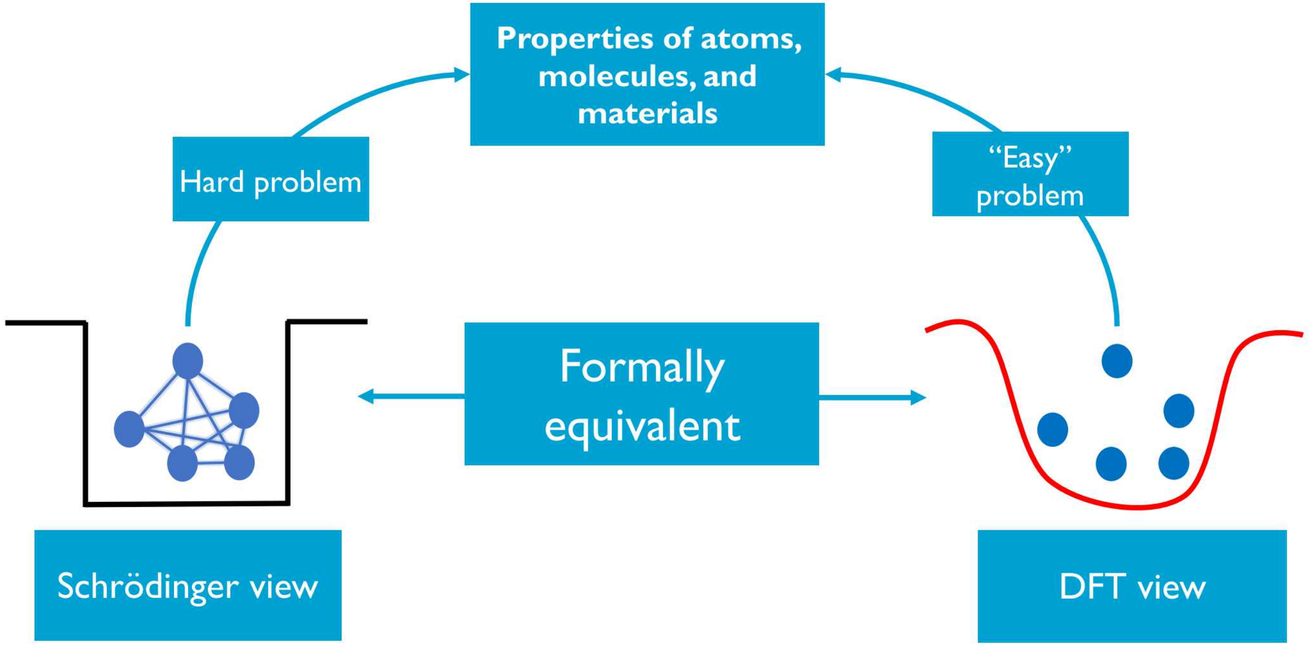
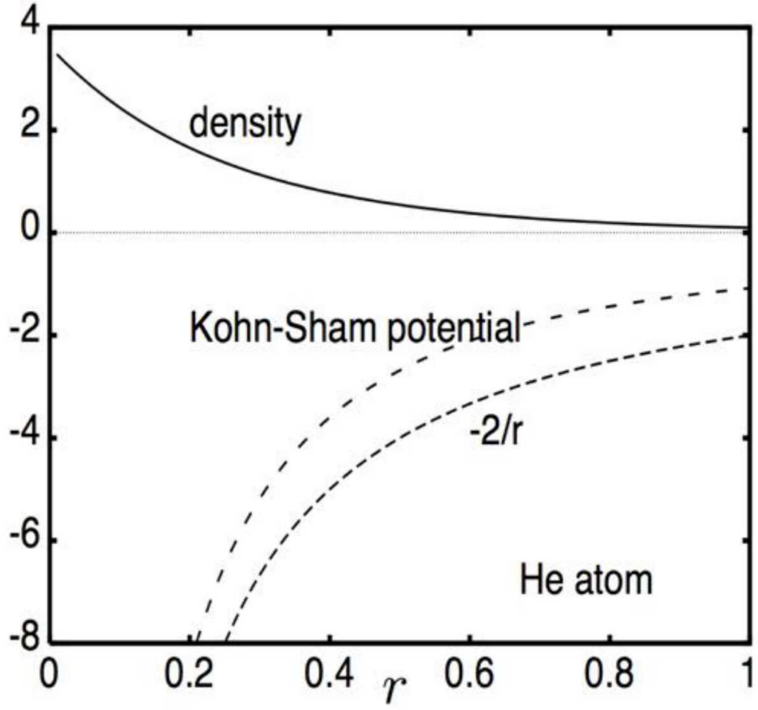
Introduction to Density Functional Theory (DFT)





The ABC of DFT (dft.uci.edu/doc/g1.pdf).

$$\left[-\frac{\nabla^2}{2} + \boxed{v_{\mathrm{S}}(\mathbf{r})}\right] \phi_j(\mathbf{r}) = \epsilon_j \phi_j(\mathbf{r}) \qquad \text{(Kohn-Sham equations)}$$

$$v_{\mathrm{S}}(\mathbf{r}) = v(\mathbf{r}) + \frac{\delta U}{\delta n(\mathbf{r})} + \frac{\delta E_{\mathrm{XC}}}{\delta n(\mathbf{r})} \qquad \text{(Kohn-Sham potential)}$$

$$n(\mathbf{r}) = \sum_i \phi_i^*(\mathbf{r}) \phi_i(\mathbf{r}) \qquad \text{(Electronic density)}$$

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Definitions of Transport Properties

$$\chi(\omega) = \chi_1(\omega) + \mathrm{i}\,\chi_2(\omega)$$

$$\chi_1(\omega) = \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} d\omega' \ \frac{\chi_2(\omega')}{\omega' - \omega}$$

$$\chi_2(\omega) = \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} d\omega' \ \frac{\chi_1(\omega')}{\omega' - \omega}$$

$$\epsilon(\omega) = 1 + 4\pi\, i\,\frac{\sigma}{\omega}$$

$$\alpha(\omega) = \frac{2}{c}\omega\,\Im\left[\sqrt{\epsilon(\omega)}\right]$$

$$\mathbf{E}(t) = -\frac{1}{c}\frac{d\mathbf{A}(t)}{dt}$$

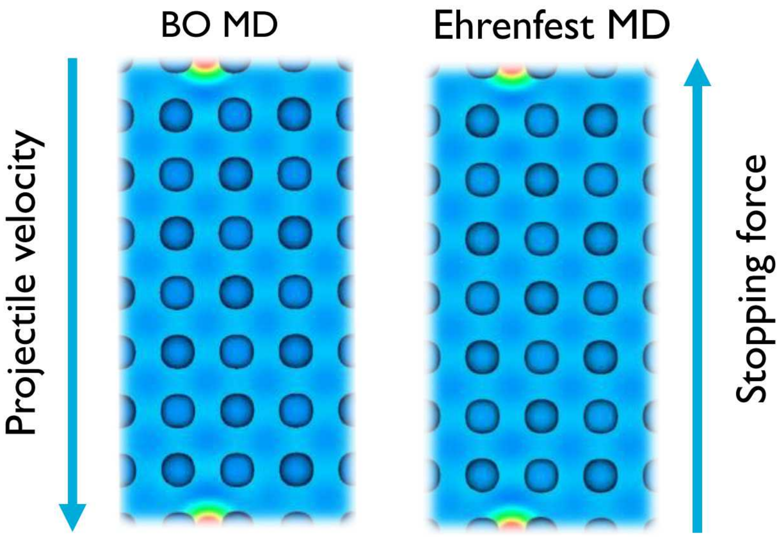
$$\mathbf{J}(t) = -\frac{i}{\Omega}\int d\mathbf{r}\ \sum_j \phi_j^*(\mathbf{r})[\hat{H}(t), \hat{\mathbf{r}}]\phi_j(\mathbf{r})$$

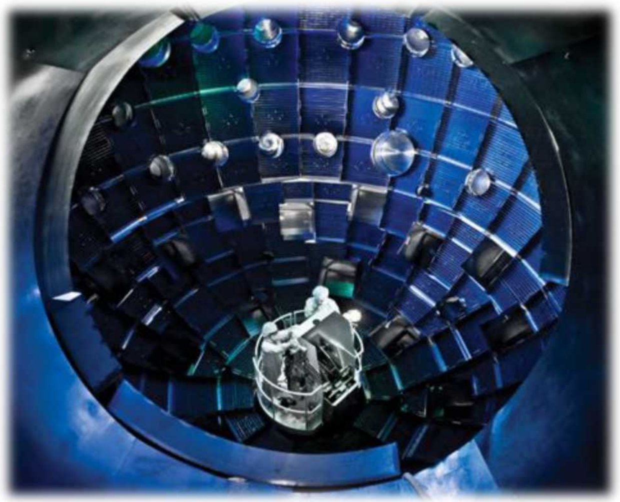
$$\mathbf{J}(\omega) = \sigma(\omega)\,\mathbf{E}(\omega)$$

$$\sigma_{\mathbf{k}}(\omega) = \frac{2\pi}{3\omega\Omega}\sum_{i,j}[f(\epsilon_{i,\mathbf{k}}) - f(\epsilon_{j,\mathbf{k}})]$$
$$\times|\langle\phi_{j,\mathbf{k}}|\nabla|\phi_{j,\mathbf{k}}\rangle|^2\delta(\epsilon_{j,\mathbf{k}} - \epsilon_{i,\mathbf{k}} - \omega)$$

Example: Hydrogen moving through cold, bulk aluminum in a channeling trajectory

$$\frac{\partial E}{\partial x} = \frac{1}{v}\frac{\partial}{\partial t}\langle E\rangle$$

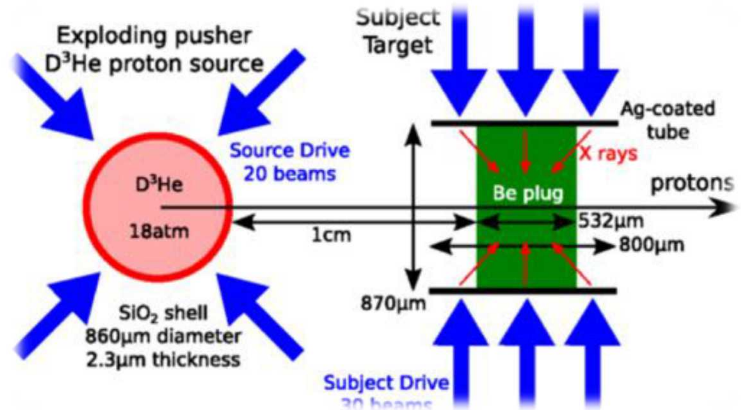




Target chamber, National Ignition Facility, Lawrence Livermore National Laboratories.

Stopping mechanisms

- Nuclear stopping (lattice vibrations)
- Electronic stopping (electronic excitations)

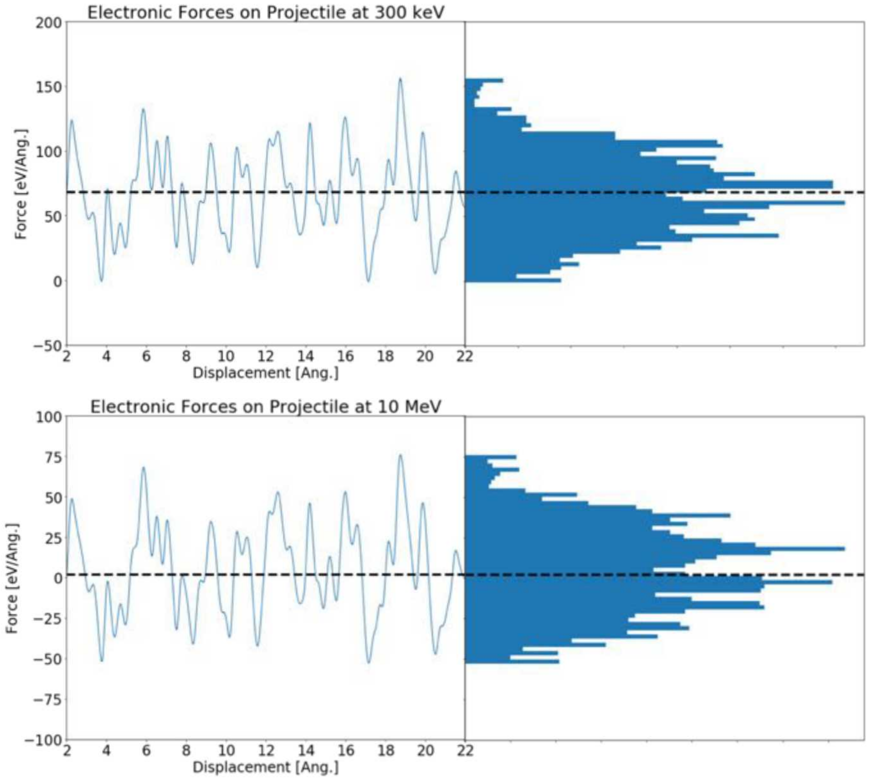


Zylstra et al., Phys. Rev. Lett. 114, 215002 (2015).

Large body of literature for cold targets

- Empirical approximations (Rutherford, Thomson, Bohr, Bethe)
- Parameter-free atomistic simulations
- Electronic structure coupled to molecular dynamics
- Cold stopping power (Echenique, Correa, Artacho, Schleife)

Distribution of microscopic forces in warm dense beryllium



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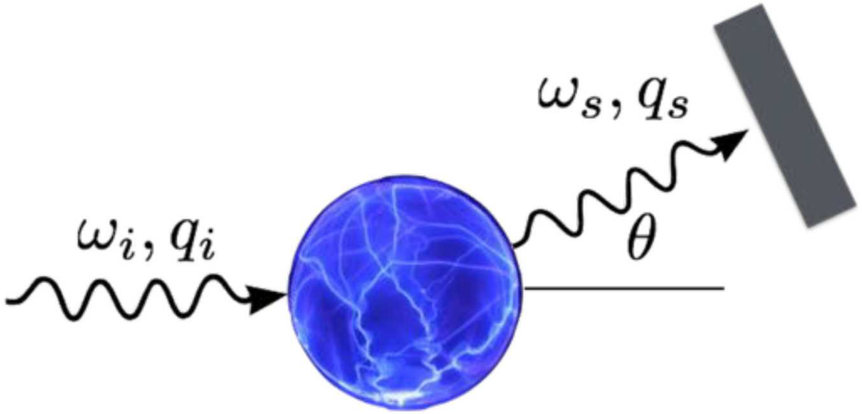
X-Ray Thomson Scattering

Sandia National Laboratories

Hard x-rays



Measure inelastically scattered x-rays

Sample of WDM (opaque to optical probes)

$$\omega = \omega_i - \omega_s$$
$$q = q_i - q_s$$
$$q_s = 2q_i \sin(\theta/2)$$

- X-ray Thompson scattering probes density, ionization state, structure, temperature, etc.

X-ray Thomson scattering in high energy density plasmas
Siegfried H. Glenzer and Ronald Redmer
Rev. Mod. Phys. **81**, 1625 – Published 1 December 2009

- Cross section is proportional to dynamic structure factor

$$\frac{d^2\sigma}{d\Omega d\omega} = \sigma_T \frac{q_s}{q_i} S(q,\omega)$$

Dynamic Structure Factor from real-time TDDFT

Probe system with x-ray:

$$v(\mathbf{r},t) = v_0\, e^{i\mathbf{q}\cdot\mathbf{r}} f(t)$$

$$|\mathbf{q}| = \frac{4\pi \sin(\theta/2)}{\lambda_0}$$

λ_0 : probe wavelength (2Å)

Record density response:

$$\delta n(\mathbf{q},t) = \int_0^\infty d\tau\ \chi(\mathbf{q},-\mathbf{q},\tau)\, v_0\, f(t-\tau)$$

Apply dissipation-fluctuation theorem:

$$\chi(\mathbf{q},-\mathbf{q},\omega) = \frac{\delta n(\mathbf{q},\omega)}{v_0\, f(\omega)}$$

$$S(\mathbf{q},\omega) = -\frac{1}{\pi}\frac{\Im\left[\chi(\mathbf{q},-\mathbf{q},\omega)\right]}{1-e^{-\omega/k_\mathrm{B} T}}$$

X-ray Thomson scattering in high energy density plasmas

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