SAND2018-10868C

Developing Consistent Models for Matter in Extreme Conditions

S. Hansen, T. Nagayama, T. Gomez, A. Baczewski, and A. Cangi

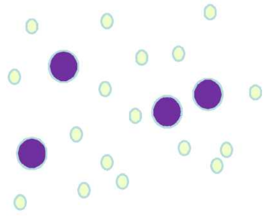
Sandia National Laboratories

APS-DPP/GEC Meeting
Portland, OR
November 4 – 9, 2018

SAND2018-ZZ

What's so difficult about modeling extreme conditions?

- HED plasmas are (usually) not well described by classical plasma models
  - Partial ionization / complex screening
  - Degeneracy effects
  - Density effects on electronic structure
  - Strongly coupled ions



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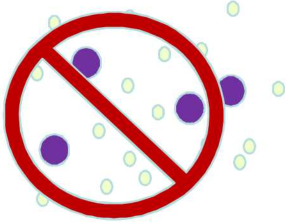
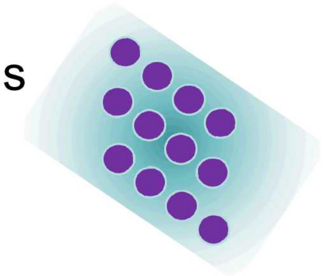


- HED plasmas are (almost) never well described by solid-state models
  - Enormous state space for excited electrons
  - Standard simplifications are suspect



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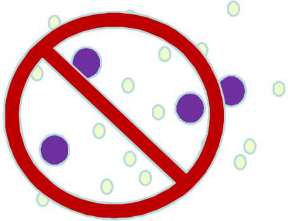

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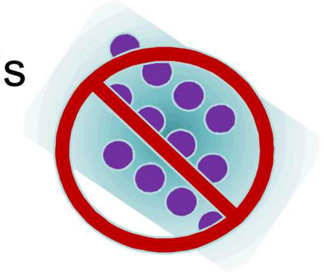
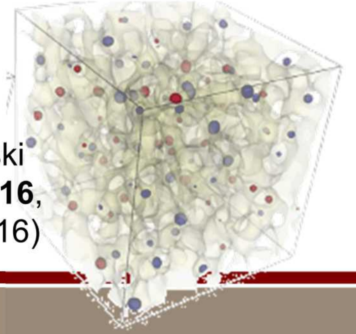


- Rigorous and reliable models exist:
  - Quantum Molecular Dynamics (QMD)
  - Time-dependent Density Functional Theory (TD-DFT)
  - But these are expensive and can be difficult to extend to high temperatures, low densities, and complex ions



A. Baczewski *et al*, PRL **116**, 115004 (2016)

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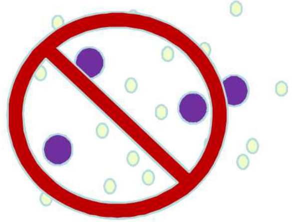

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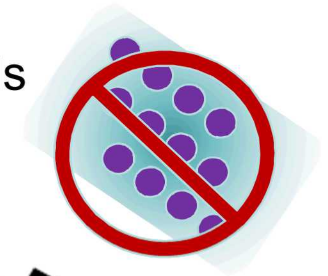

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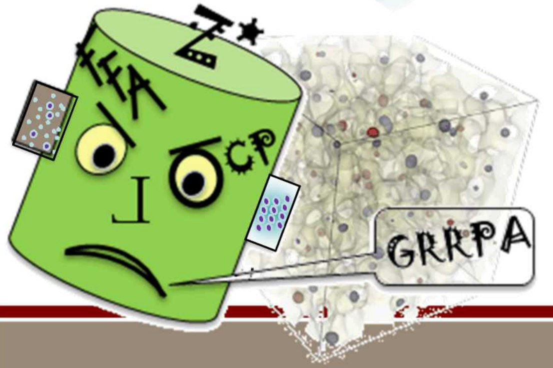

Central question: What happens to material when you squish it very hard and/or heat it quite a lot?

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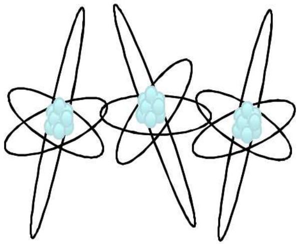
Experiments/Observables

Measurements from small, short-lived lab plasmas and large, distant astrophysical objects are inherently challenging

Observables (yields, images, spectra) can be difficult to interpret; may require both models and simulations



Simulations

Simulations help to design experiments and interpret data from laboratory and astrophysical plasmas

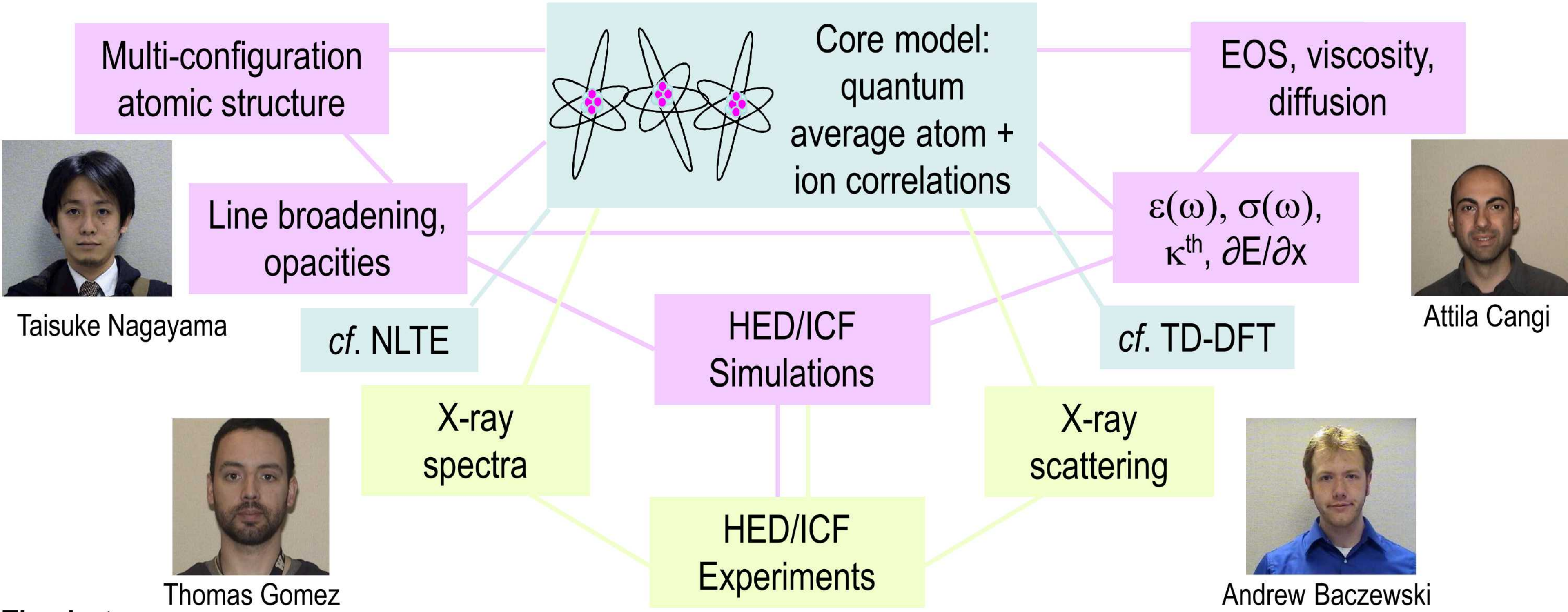
Rad-hydro simulations themselves require extensive input from adequate material models (EOS, transport, opacity)

Additional questions:

How can we tell if our models are right?

How important is model consistency?

Our central goal: Develop a unified, tractable, and consistent model for matter in extreme conditions



Thanks to:

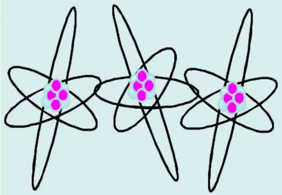
Charles Starrett, David Kilcrease (LANL), Carlos Iglesias, Brian Wilson, Phil Sterne, Paul Grabowski (LLNL), Richard More

Primary funding: U.S. DOE, Office of Science Early Career Research Program, OFES FWP-14-017426

Fully self-consistent core model: Quantum average-atom + ion correlations

v_{XC}

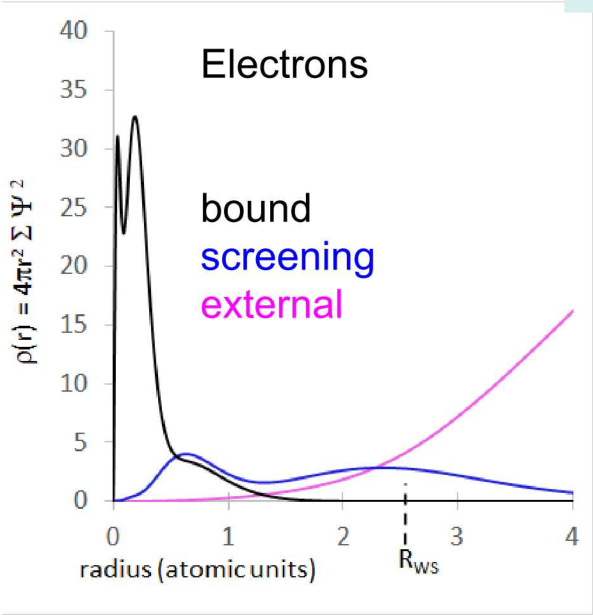
ρ_{scr}

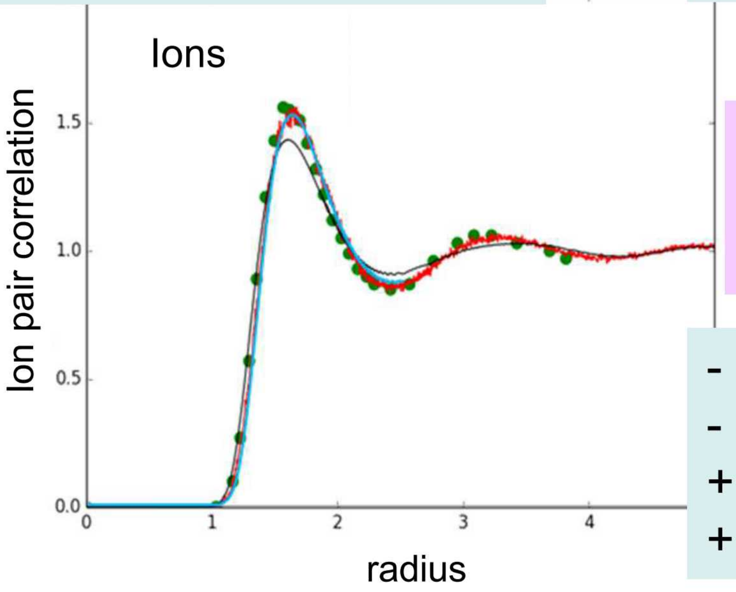


Core model: quantum average atom + ion correlations

Self-consistent $V_{ei}(r)$, $\Psi(r)$, $\rho(r)$, $V_{ext}(r)$. $\rho_{ext}(r)$, $V_{ii}(r)$, $\rho_{ion}(r)$

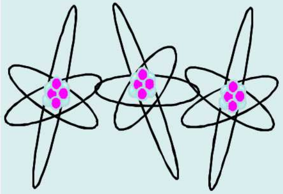
Observable and constitutive properties





- Spherical
- semi-relativistic
+ orthonormal $\Psi(r)$
+ runtime ~ 3 minutes

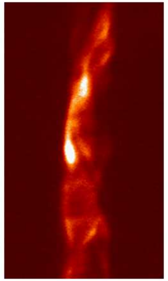
The model yields highly constrained Equations of State and ionic transport coefficients

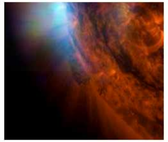


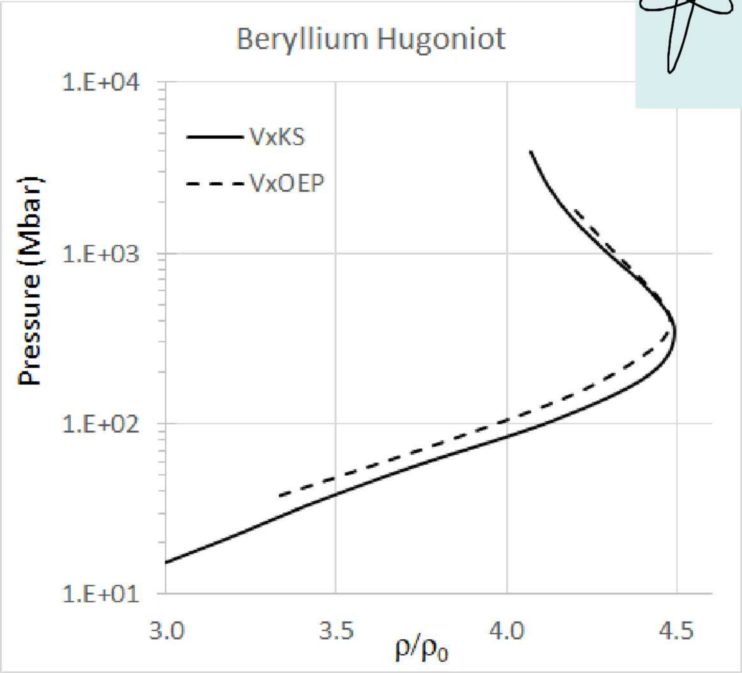
Core model: quantum average atom + ion correlations

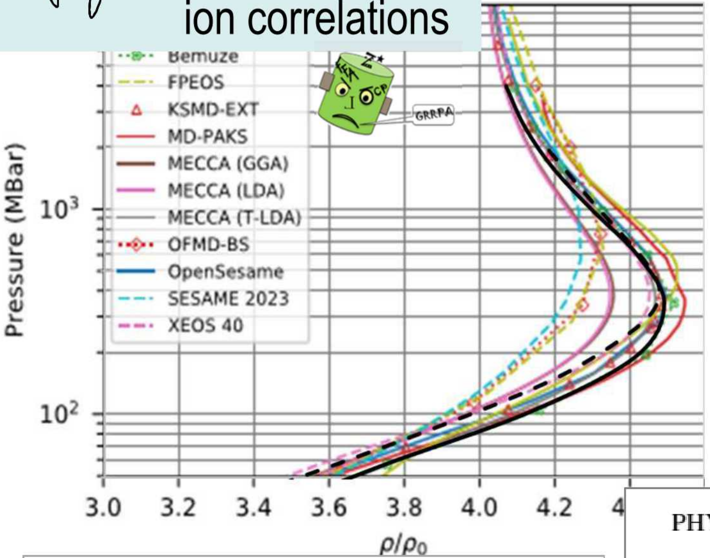
EOS, viscosity, diffusion

Astrophysics & ICF









A Review of Equation-of-State Models for Inertial Confinement Fusion Materials

J.A. Gaffney, S.X. Hu, P. Arnault, A. Becker, ... E. Zurek

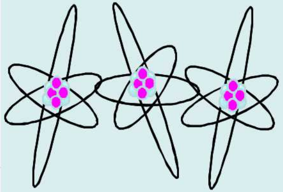
In Press, Accepted Manuscript, Available online 18 August 2018

PHYSICAL REVIEW E **91**, 013104 (2015)

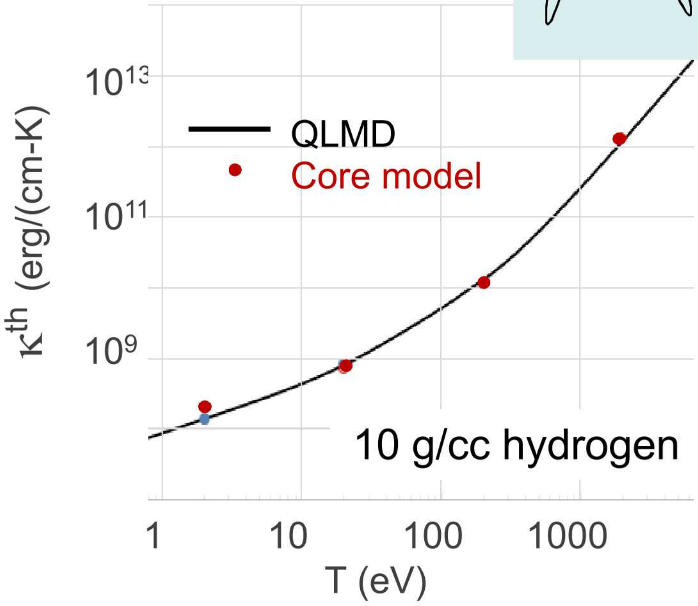
Pseudoatom molecular dynamics

C. E. Starrett,* J. Daligault, and D. Saumon

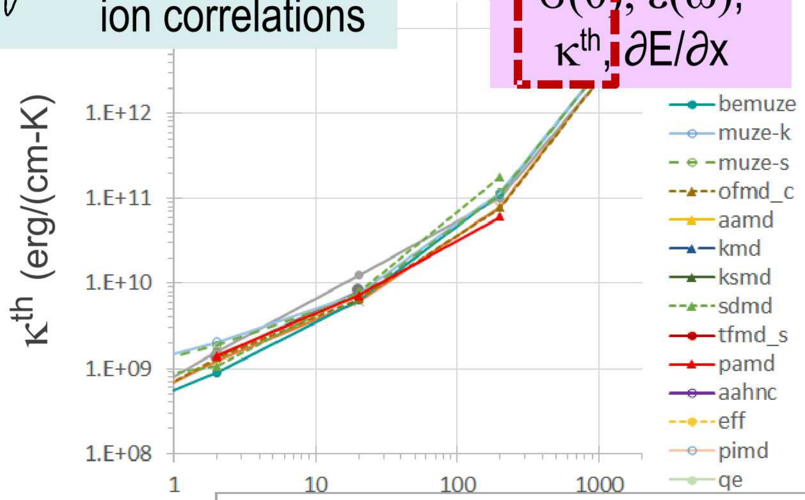
The electronic response from self-consistent wavefunctions yields electrical & thermal conductivities…



$\sigma(0)$, $\varepsilon(\omega)$, κ^{th}, $\partial E/\partial x$



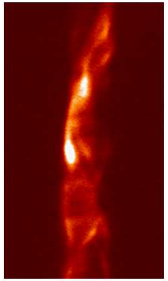
M. Desjarlais *et al.* 2018

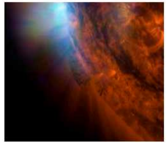


Review of the First Charged-Particle Transport Coefficient Comparison Workshop

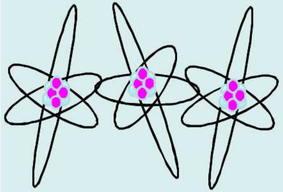
P. Grabowski, S. Hansen, M. Murillo, F. Graziani, A. Zlystra, S. Baalrud, A. Baczewski, L. Benedict, O. Certik, J. Clerouin, S. Copeland, J. Dai, J. Daligault, M. Desjarlais, C. Dharma-wardana, G. Faussurier, J. Haack, S. Haan, T. Haxhimali, A. Hayes-Sterbenz, Y. Hou, S. Hu, D. Jensen, D. Kang, J. Kress, Q. Ma, M. Marciante, E. Meyer, R. Rudd, D. Saumon, R. Singleton, L. Shulenburger, T. Sjostrom, L. Stanton, C. Starrett, C. Ticknor

Astrophysics & ICF





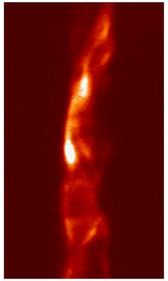
… and stopping powers

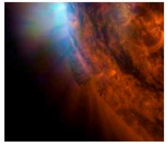


Core model: quantum average atom + ion correlations

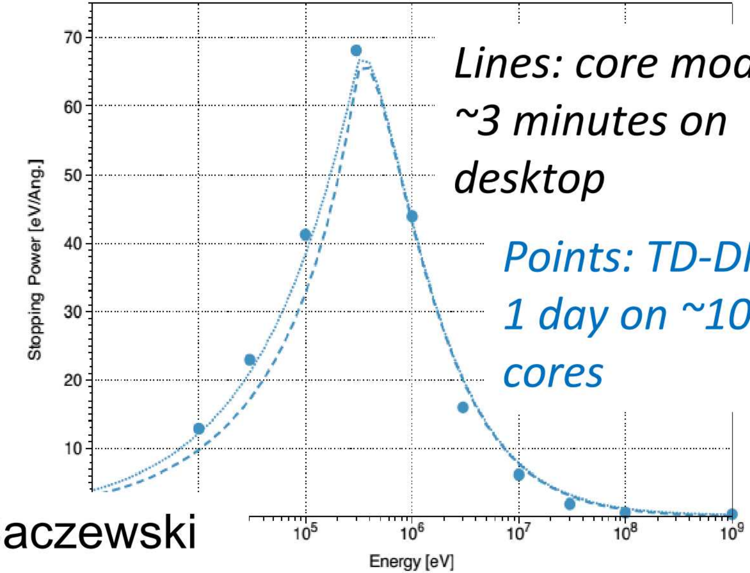
$\sigma(\omega)$, $\varepsilon(\omega)$, κ^{th}, $\partial E/\partial x$

Astrophysics & ICF





Protons stopping in 10 g/cc deuterium



Lines: core model ~3 minutes on desktop

Points: TD-DFT 1 day on ~1000 cores

A. Cangi, A. Baczewski

Measurement of Charged-Particle Stopping in Warm Dense Plasma

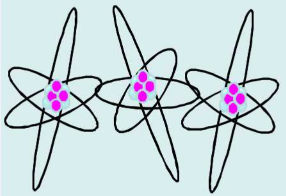
A. B. Zylstra, J. A. Frenje, P. E. Grabowski, C. K. Li, G. W. Collins, P. Fitzsimmons, S. Glenzer, F. Graziani, S. B. Hansen, S. X. Hu, M. Gatu Johnson, P. Keiter, H. Reynolds, J. R. Rygg, F. H. Séguin, and R. D. Petrasso
Phys. Rev. Lett. **114**, 215002 – Published 27 May 2015

Stopping of Deuterium in Warm Dense Deuterium from Ehrenfest Time-Dependent Density Functional Theory

R. J. Magyar*, L. Shulenburger, and A. D. Baczewski

Wang *et al.*, *Phys Plas* **5**, 2977 (1998); Magyar *et al.*, *C. Plas Phys*. 56 459 (2016)

… and x-ray scattering signals



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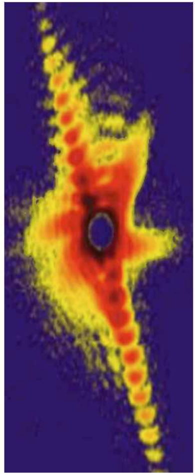
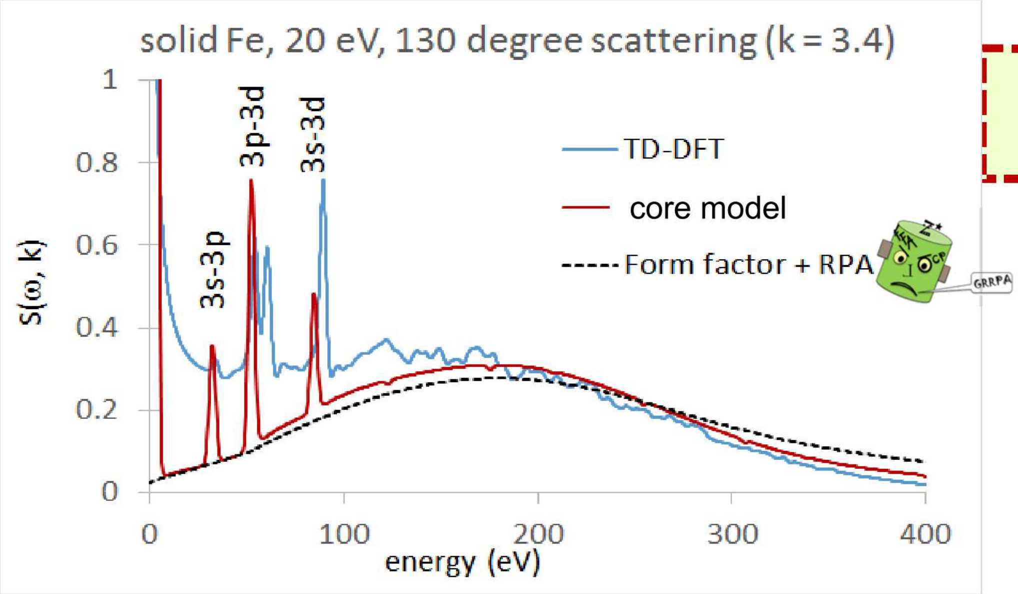
$\sigma(\omega)$, $\varepsilon(\omega)$, κ^{th}, $\partial E/\partial x$

X-ray scattering

XFEL & ICF





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

A. D. Baczewski, L. Shulenburger, M. P. Desjarlais, S. B. Hansen, and R. J. Magyar
Phys. Rev. Lett. **116**, 115004 – Published 18 March 2016

Johnson *et al*, *PRE* **86**, 036410 (2012); Chihara, J. Phys. Cond. Matt. **12**, 231 (2000)

… and detailed opacities

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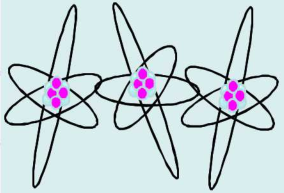
Multi-configuration atomic structure

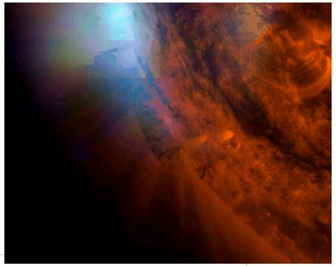
Line broadening, opacities $\alpha(\omega)$

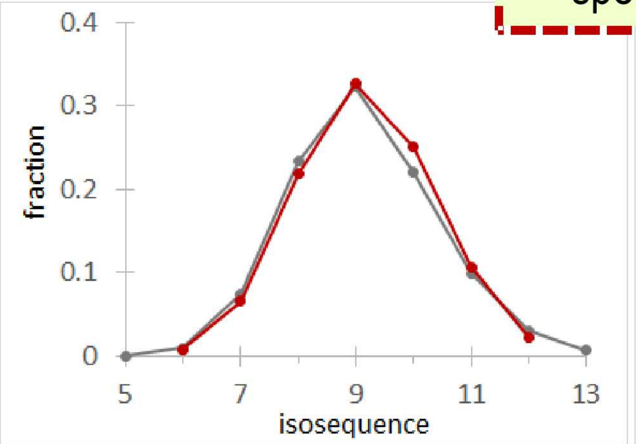


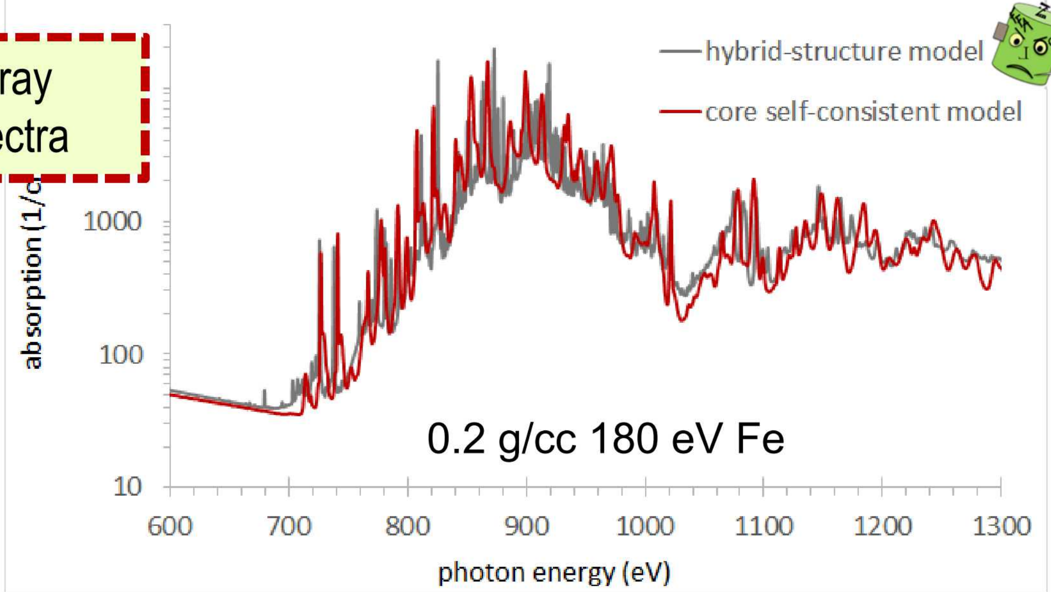
Core model: quantum average atom + ion correlations

X-ray spectra

Solar physics







Cowan, Theory of Atomic Structure and Spectra (1981); Lao, *Astron & Astro* **281**, 460 (1994)

… with self-consistent line broadening

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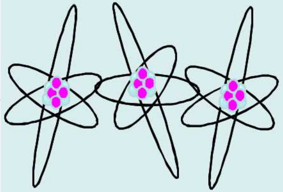
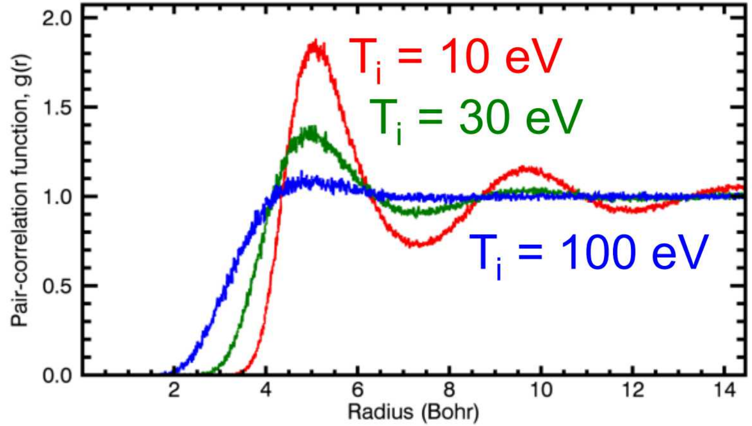
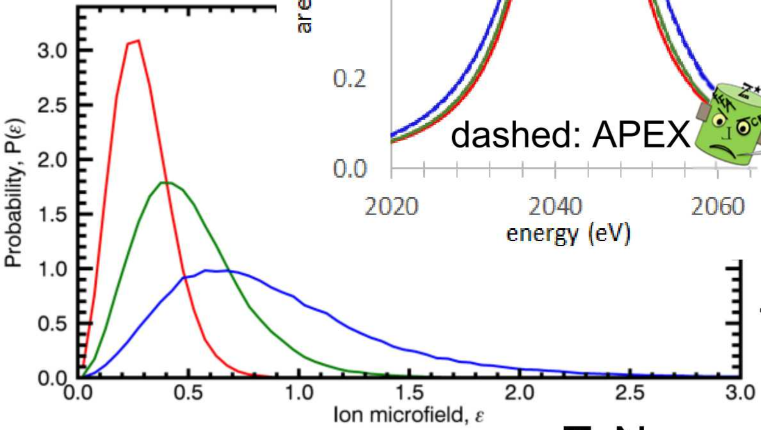
Line broadening, opacities

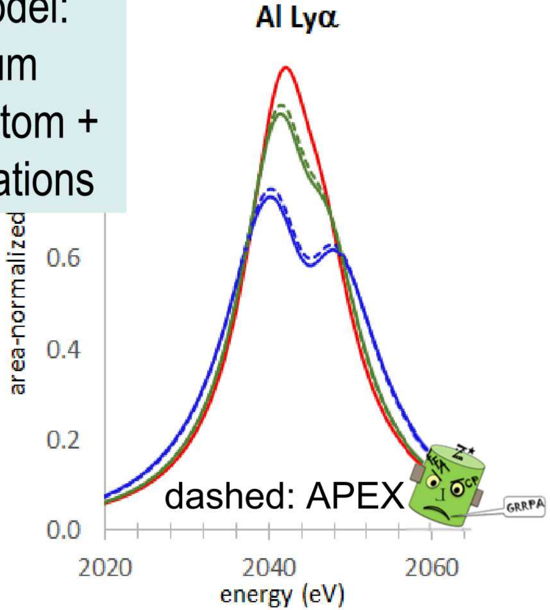


Core model: quantum average atom + ion correlations

Solid-density Al, T_e = 250 eV







T. Gomez

T. Nagayama

Cosmology, Astrophysics & ICF

APEX: Iglesias *et al.*, *Phys Rev A* **31**, 1698 (1985)

Conclusions

We are working to build a self-consistent model of material at extreme conditions with:

- Constitutive properties adequate for use in simulations
  → Enforced consistency can improve sensitivity studies & increase constraints

- Observable predictions adequate for comparison with experiment
  → Enforced consistency means that if part of this model is wrong, the whole thing is wrong – and its wrongness should be detectable

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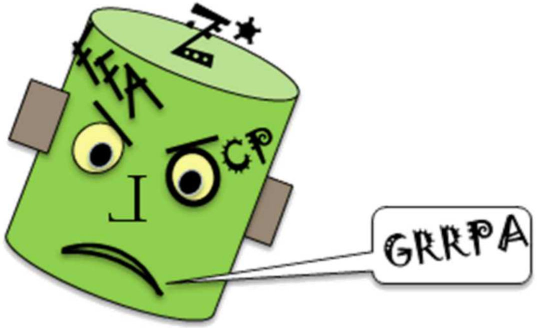
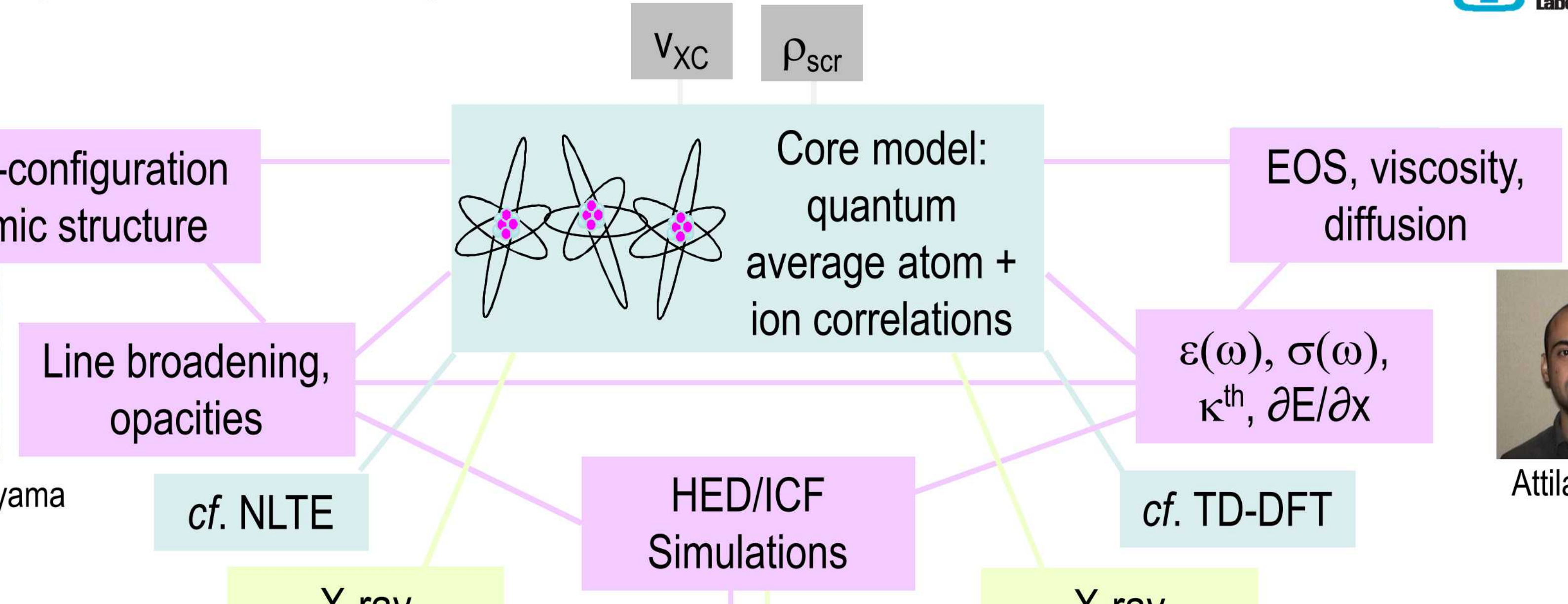
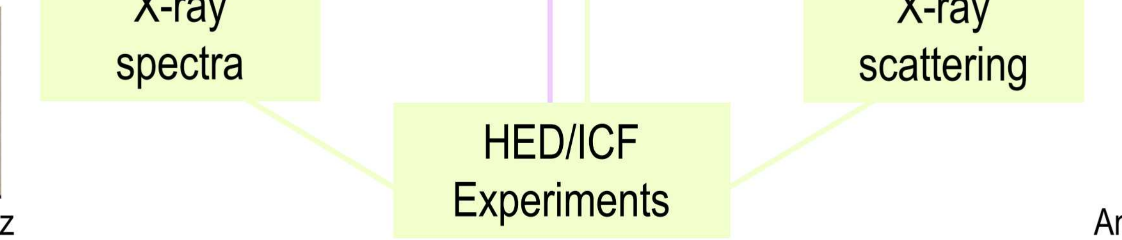
> For complex systems, internally consistent models that can be falsified by comparison to detailed data have more epistemic value than tunable models made to fit integrated data



Thank you!

Summary & acknowledgements





Taisuke Nagayama

Attila Cangi

Thomas Gomez

Andrew Baczewski

Thanks to:

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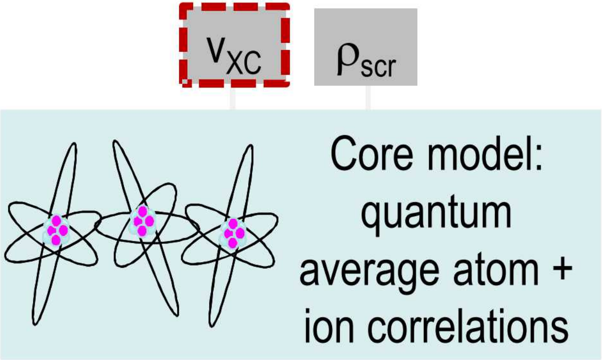
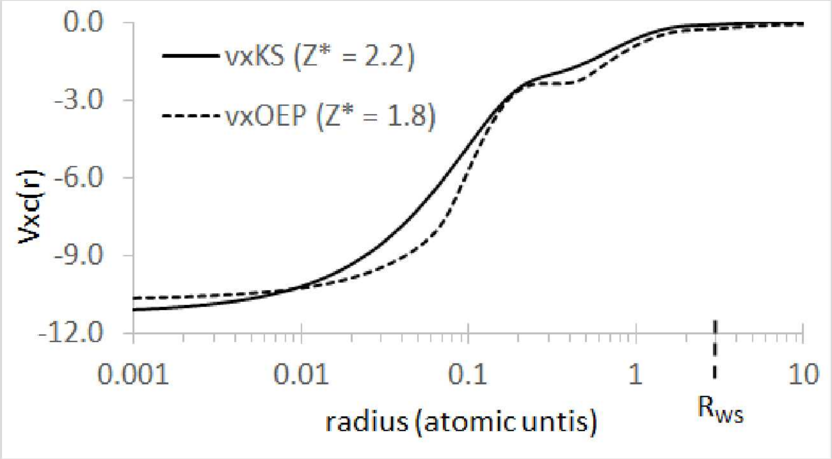
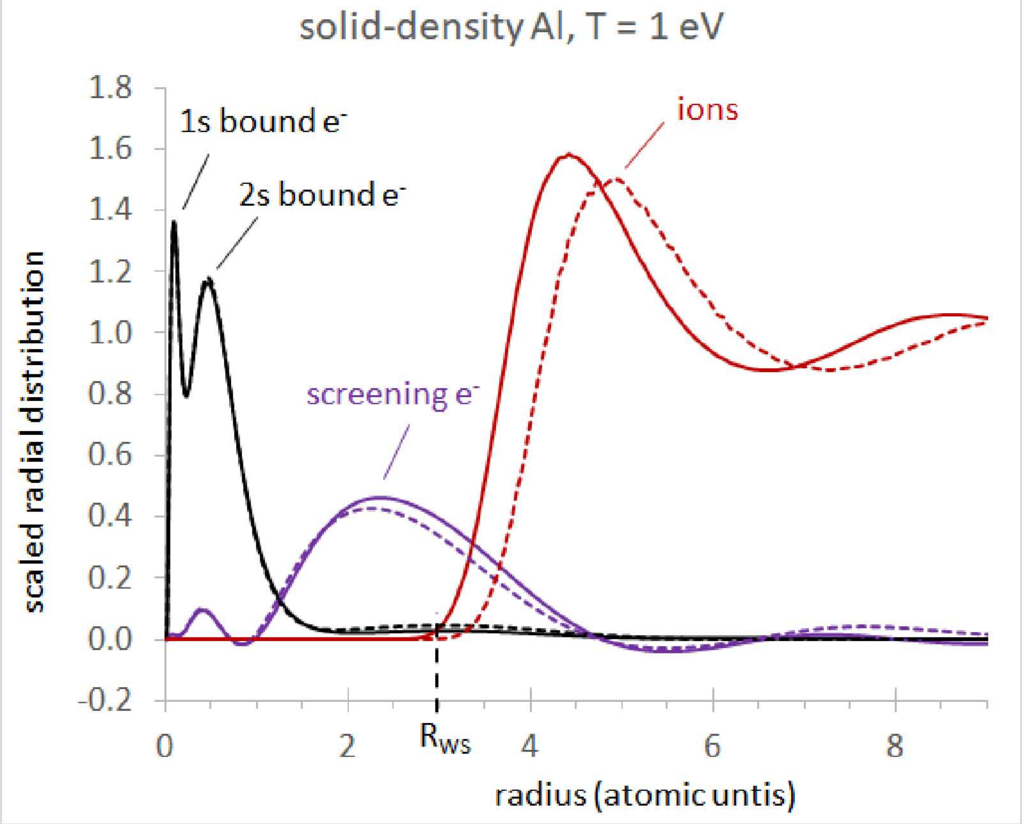
Primary funding: U.S. DOE, Office of Science Early Career Research Program, OFES FWP-14-017426

The core model is sensitive to the choice of exchange potential

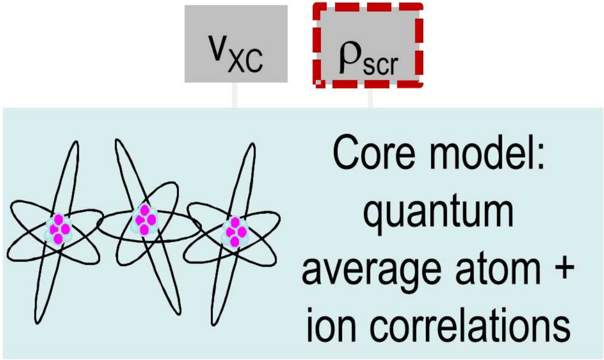


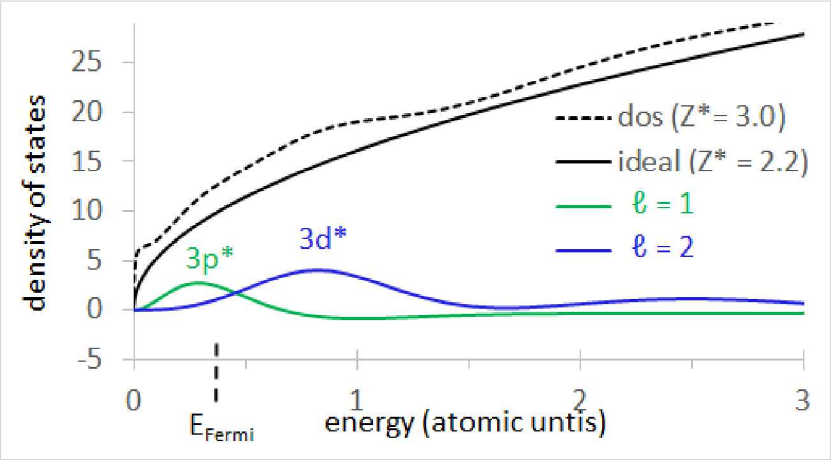


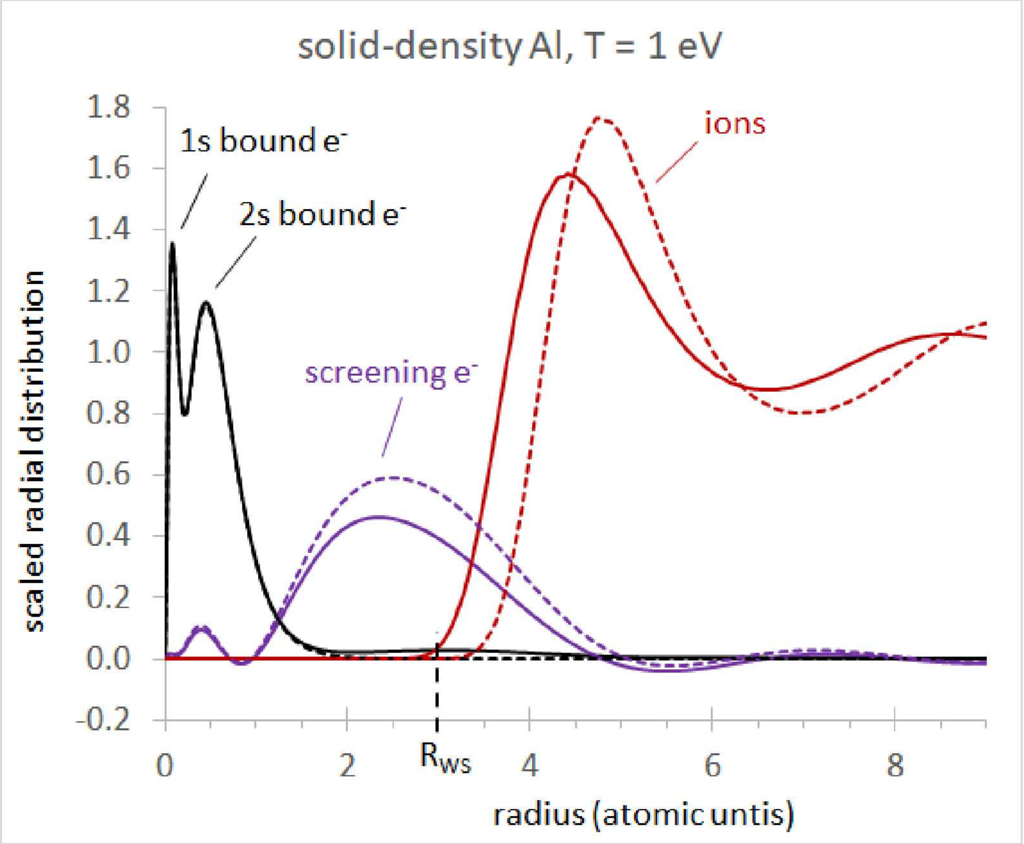


Becke & Johnson J Chem Phys **124**, 221101 (2006); Wilson & Liberman, JQSRT **54**, 427 (1995)

The core model is sensitive to whether the screening density includes the pressure-ionized “scars” of bound states



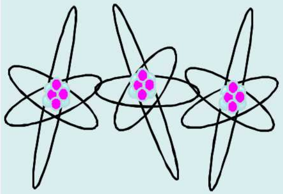




Examining the full dielectric function indicates a missing piece in the standard Chihara decomposition

Chihara decomposition:

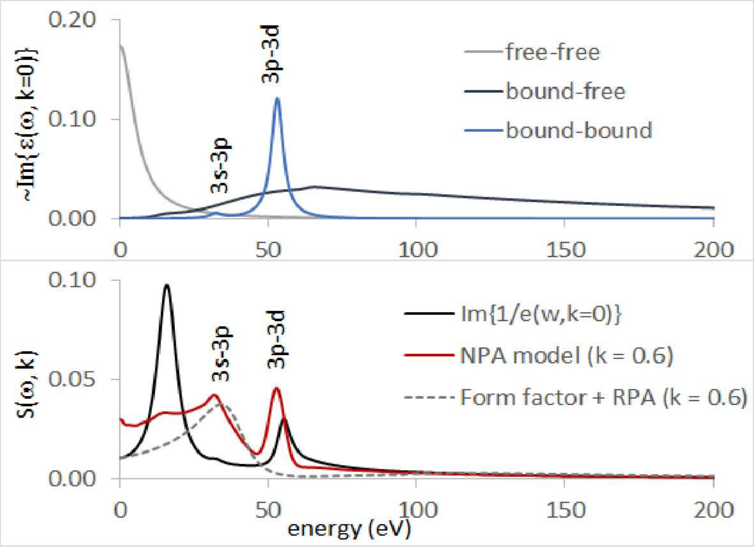
$$S(k,\omega) = \underbrace{|f_I(k) + q(k)|^2 S_{ii}(k,\omega)}_{\text{elastic}} + \underbrace{\bar{Z} S_{ee}(k,\omega)}_{\text{free-free}} + \underbrace{S_{bf}(k,\omega)}_{\text{bound-free}} + \underbrace{S_{bb}(k,\omega)}_{\text{bound-bound}}$$



Core model: quantum average atom + ion correlations

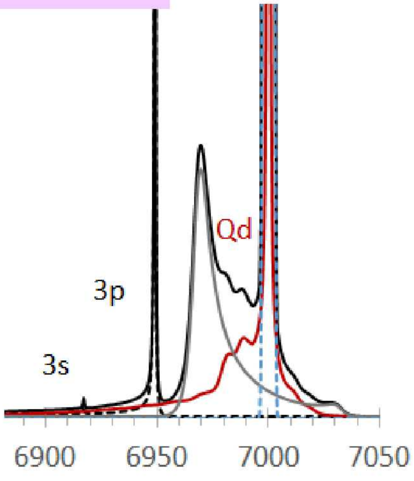
$\sigma(\omega)$, $\varepsilon(\omega)$, κ^{th}, $\partial E/\partial x$

X-ray scattering



The bound-bound features in Im{$1/\varepsilon_{bb}(\omega)$} are reminiscent of sharp bound-free features previously noted by Johnson *et al.* and Souza *et al.**

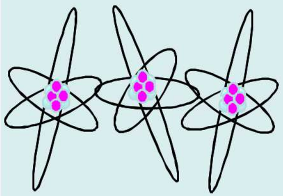
5 g/cc Fe, 10 eV



8 g/cc Fe, 1 eV

*Johnson *et al*, *PRE* **86**, 036410 (2012); Souza, Starrett *et al.*, PRE **89**, 023108 (2015)

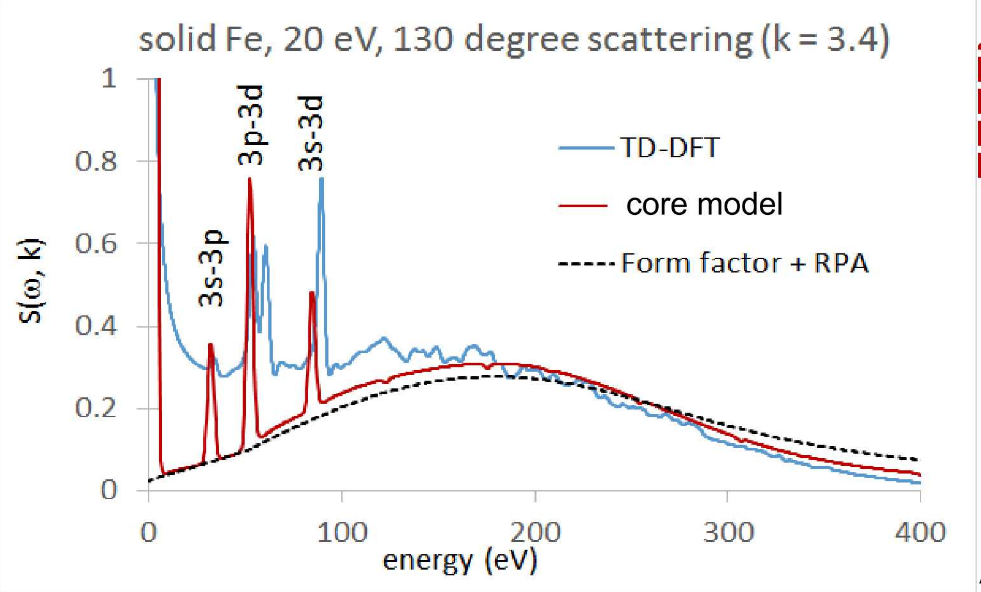
Both the core model and TD-DFT capture bound-bound scattering features in S(ω, k)



Core model: quantum average atom + ion correlations

X-ray scattering

While S(ω,0) ~ Im{1/ε(ω,0)} roughly describes edges and line, a more general S(ω,k) can be obtained directly from core-model wavefunctions



Experimental diagnostics benefit from consistent and complete atomic-scale models

A. Baczewski