WG9: Opacity, screening

How opacities are computed

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Outline

- Background. What is an opacity and why do we care?
- How do we compute wide-ranging opacity tables?
- How do we compare to opacity measurements?
- Fe opacity
- New physics?

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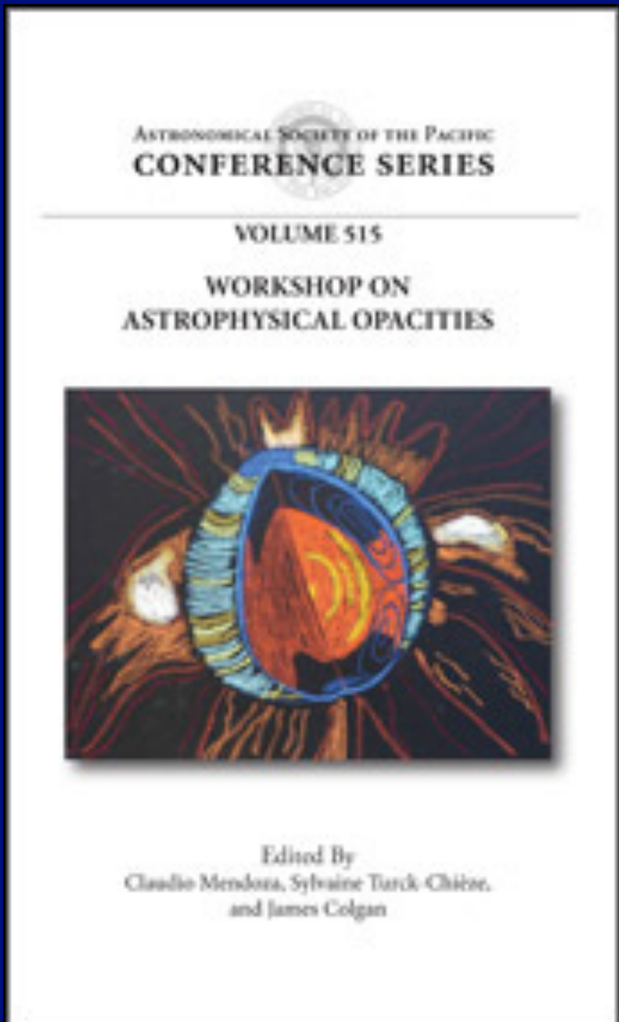

Title: ***Workshop on Astrophysical Opacities***

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Editors: **Claudio Mendoza, Sylvaine Turck-Chièze, James Colgan**

Synopsis: Workshop on Astrophysical Opacities
Western Michigan University,
Kalamazoo, Michigan
1-4 August 2017

Reliable atomic and molecular opacity tables are essential to a wide variety of

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Current State of Astrophysical Opacities: A White Paper

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Opacities are crucial for understanding radiative energy transfer in plasmas

- The coefficients for absorption & emission of radiation are necessary to solve the radiation transport equation
  - Important in modeling plasmas of all types, eg stellar evolution, supernova core-collapse, laser-produced plasmas, industrial plasmas,…
- Assuming problem is time-independent and one-dimensional with isotropic radiation, the transport equation can be written:

$$\frac{1}{\rho}\frac{dI_\nu}{dx} = \frac{\varepsilon_\nu}{4\pi} - \kappa_\nu I_\nu$$

radiation intensity

radiation frequency

material density

emissivity

opacity

- So, to properly compute the radiation & energy moving through or from a material, one needs to know the opacity.

But…Opacities are by far the most bothersome factor!

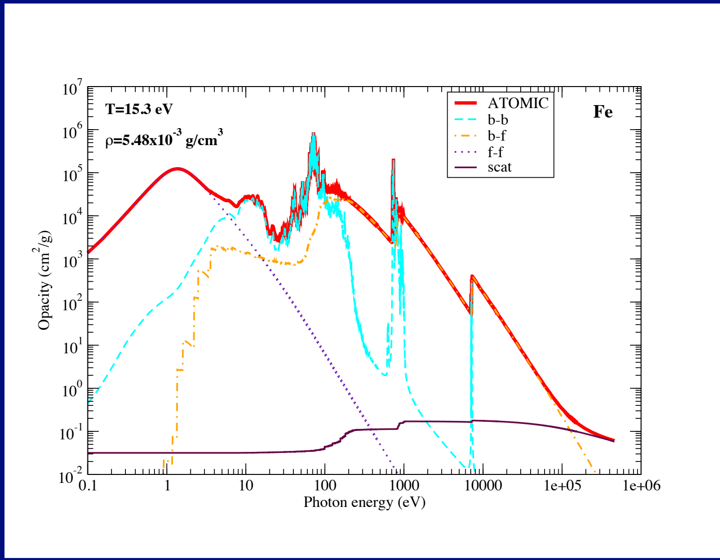
- Opacities are crucial in determining the structure and evolution of stars
  - As commented by Seaton, the fundamental physics has been known for a long time, but the complexity of the problem makes accurate calculations very daunting.
  - Why? Because a proper account has to (in principle) keep track of all radiative transitions between any possible populated state of the material in question (atom, molecule, ion,…)
  - For warm/hot plasmas that contain ionized matter, the number of possible excited states is in principle, infinite, and so the computational challenge is significant. Approximations are needed to make the problem tractable.

  - Schwarzschild comments that the determination of opacities to be "***by far the most bothersome factor in the entire theory***" (of stellar evolution)

  - However, intensive work over the last 30 years has vastly improved the LTE opacity databases available. Opacity tables are now available from LANL, LLNL, the Opacity Project (UK), and several French groups:

  - ***http://aphysics2.lanl.gov/opacity/lanl;*** *J. Colgan et al, ApJ* ***817****, 116 (2016) [OPLIB]*
  - https://opalopacity.llnl.gov [OPAL]
  - *Blancard C., Cossé P. and Faussurier G. 2012 ApJ* ***745*** *10 [OPAS]*
  - https://opserver.obspm.fr [OP]

How do we compute opacities: A 3-legged approach



Atomic Data
(Structure, Transitions, cross sections)

Equations of State (EOS)

Line broadening

Monochromatic Opacity

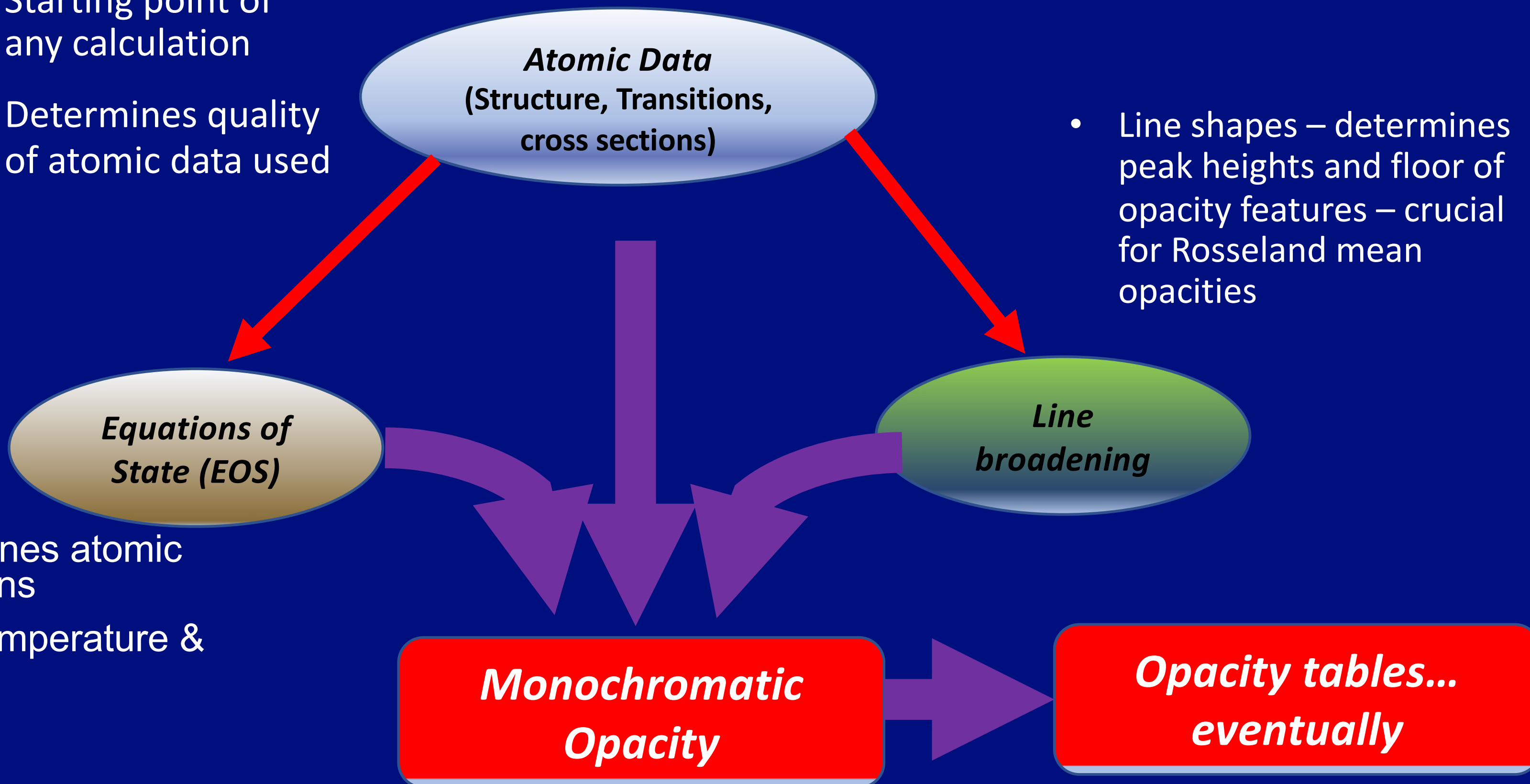
Opacity tables… eventually

$$\sigma_{tot} = \sigma_{b\text{-}b} + \sigma_{b\text{-}f} + \sigma_{f\text{-}f} + \sigma_{scat}$$

- *Other variants on this approach are used; in particular methods that start by explicitly treating the atom-plasma interaction within the Schrödinger equation. These are often “average-atom” approaches*

How do we compute opacities: A 3-legged approach

- Starting point of any calculation
- Determines quality of atomic data used

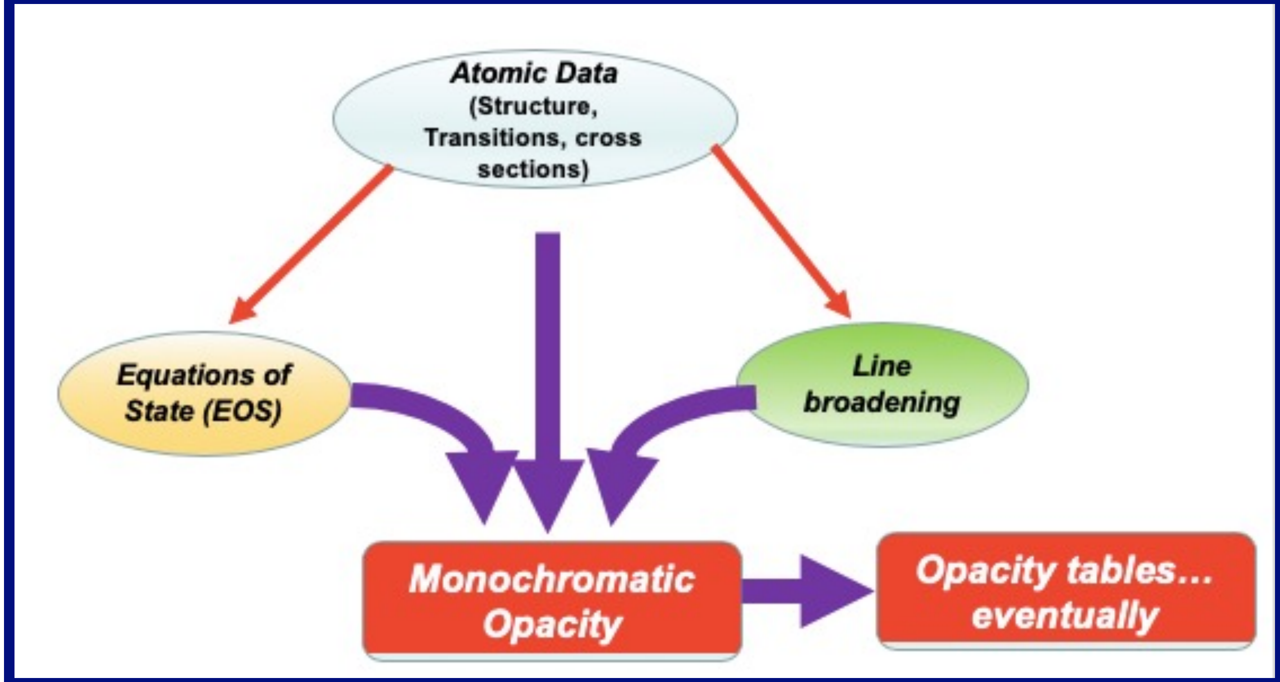


- Line shapes – determines peak heights and floor of opacity features – crucial for Rosseland mean opacities

- EOS – determines atomic state populations
- Depends on temperature & density

- Tables contain opacities from 1000s of temperature & density points

Leg 1: Atomic data



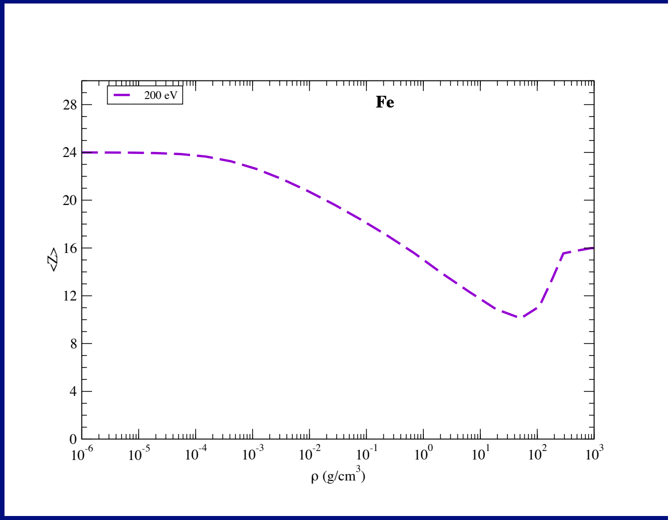
- *Atomic structure usually from an ab-initio code (eg Cowan, FAC, HULLAC)*
- *Can be non-, semi-, fully-relativistic*
- *Super-configurations; configuration-average; terms; fine-structure levels*
- *Close-coupling, configuration-interaction models can be considered*
- *Often requires data for many (> 10^6 states)*
- ***Accuracy** important but also must be able to compute data for **all** ion stages – neutral atom to bare ion*
- *Need energy levels and transition probabilities between all levels of relevance*
- *Photoionization cross sections from all populated states needed for bound-free cross sections*
- *Free-free cross sections also needed – usually small contribution but vital to fill in all photon energy ranges*
- *Scattering also has to be included for completeness*

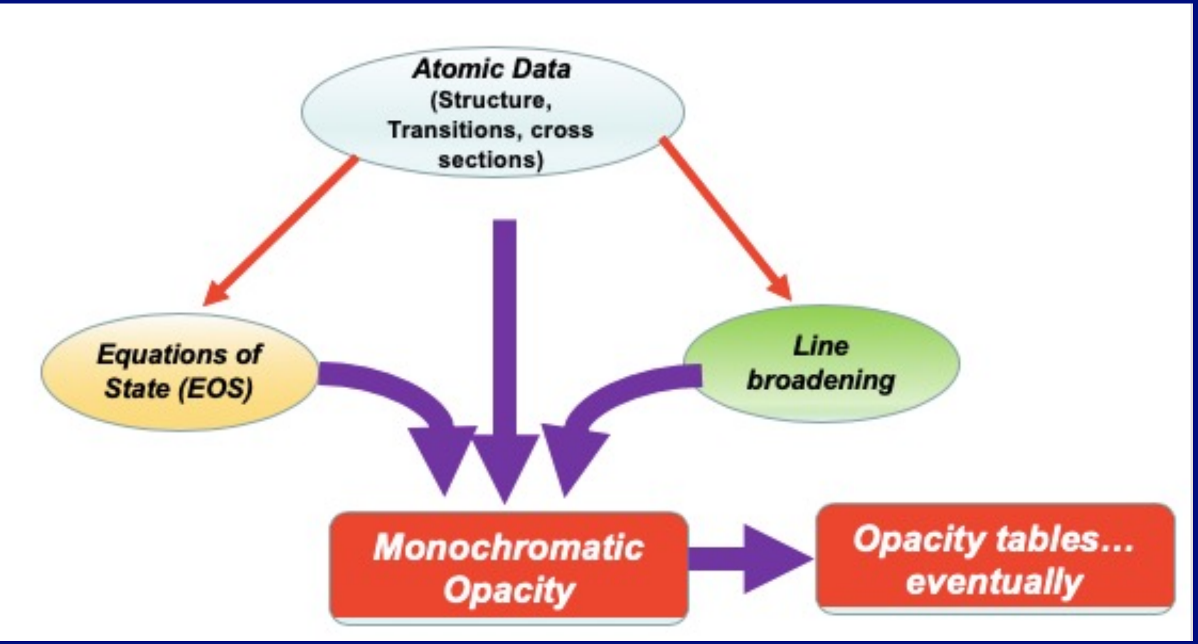
Note: Ab-inito atomic physics theory – we start from the Schrodinger equation and proceed from there – although (of course) we have to approximate some terms in our Hamiltonian

Leg 2: Equation-of-state (EOS)

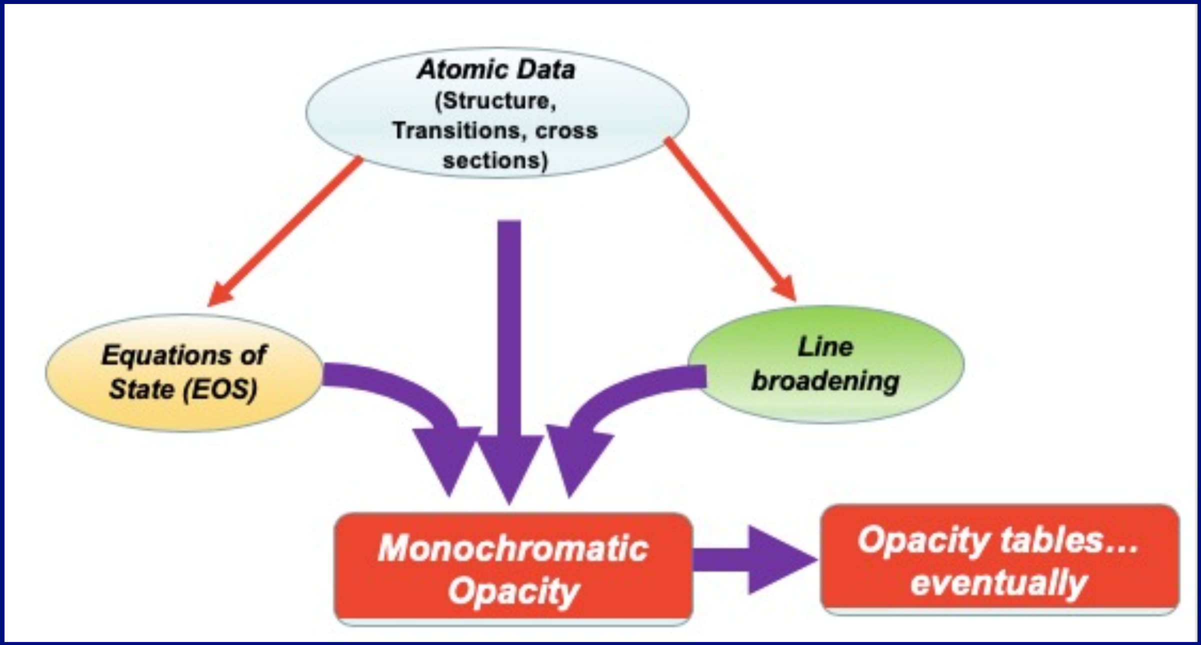
- *EOS **models** control the thermodynamics of the plasma*
- *Has to be able to treat ideal gas (Saha-Boltzmann) conditions through high density conditions plus **critical** intermediate areas of phase space which are often of most interest*
- ***Consistency** very important as density increases*
- *EOS often approached from a chemical or physical picture*
- *A number of choices for EOS model available in the literature*
- *Atomic energy levels used to assemble partition function. **Completeness** is always something to monitor*
- *Rate of convergence of this function depends greatly on plasma conditions.*

"zbar" (average ionization) of the plasma as a function of mass density for Fe at T=200 eV





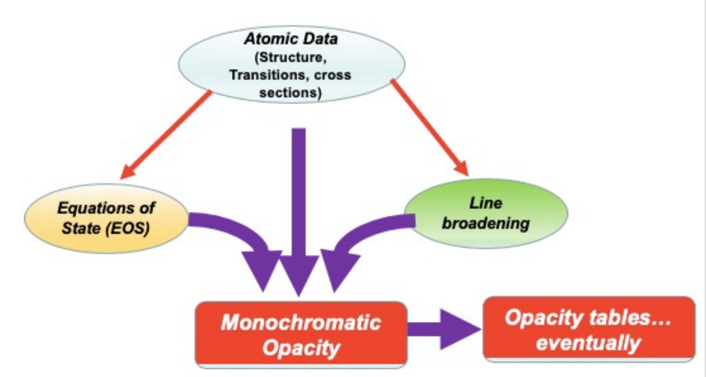
Leg 3: Line broadening



- *Broadening due to Doppler effects, natural broadening and collisions; all should be included*
- *Line broadening is due to plasma microfields caused by motion of electrons and ions in plasma*
- *Collisional broadening often most important – increases linearly with electron density*
- *Many line shape models available in the literature that contain lots of important physics – but often only tractable for one or few electron systems*
- *Opacity tables require line shape models that can handle broadening of transitions involving complex states and in a computationally feasible manner – billions of transitions have to be considered*

Combining all 3 legs

- Once all these legs have been considered, they are combined in a code that will produce opacities over a wide photon energy range
- Accuracy versus computational cost is **always** an ongoing consideration
- Then one is at the point of starting convergence checks – convergence rates (and with respect to what quantity) will vary depending on plasma conditions
- Comparisons can & should also be made to experiment where available
- If you are satisfied with all these outcomes you can then begin to build an opacity table
- Opacities normally produced on a given grid of temperatures & densities from cold (< 1 eV) to high temperatures (~ 100 keV), and encompassing 15 or more orders in density
- In the LANL case each opacity table contains 3000+ temperature density points, each with a photon energy spectrum with 10,000+ grid points.



Using opacities in solar modeling

Sound speed vs solar radius for the AGSS09 solar abundance

- The new LANL OPLIB opacities have been used in solar modeling – calculations performed at LANL by Katie Mussack and Joyce Guzik
- The new opacities **marginally** improve the difference in sound speeds compared to the use of OPAL opacities
- However the sound speed discrepancy is still quite statistically significant

COLGAN ET AL.

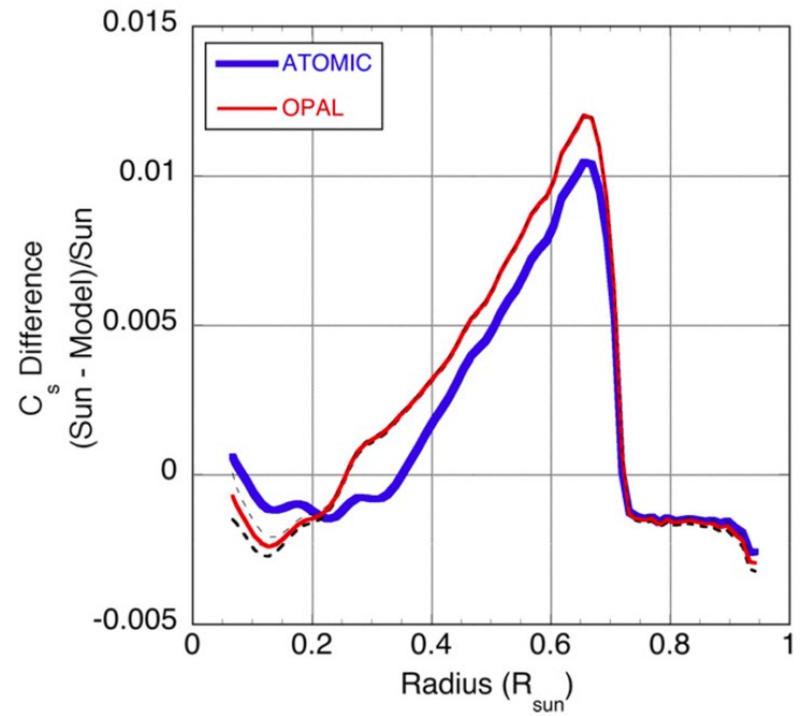


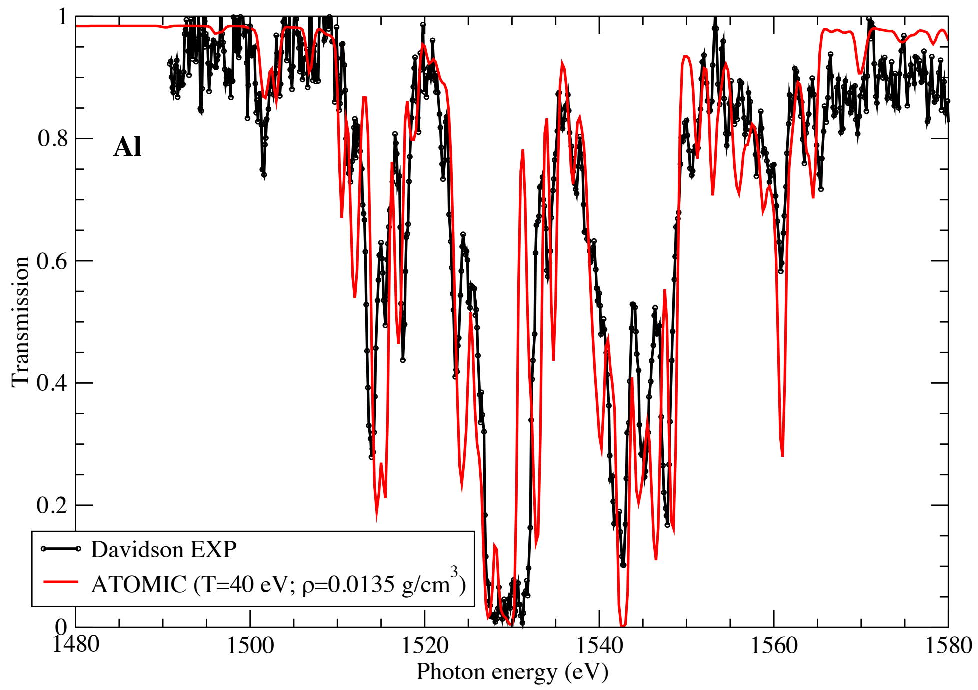
Figure 4. Helioseismically inferred (Basu et al. 2000) minus calculated sound speed differences vs. radius for solar models using the ATOMIC and OPAL opacities with the AGSS09 abundance mixture. The black dashed curves on either side of the OPAL profile show the magnitude of the uncertainty in the inferred sound-speed profile. The convection zone base radius is at $\sim 0.725\ R_{\odot}$.

Colgan et al, Ap J 817, 116 2016

Comparing opacity calculations with measurements: Al

- Al transmission measured using the laser at RAL (UK) in late 1980s
  - Agreement is very good over all photon energy range
  - Some differences of order 1% in line position
- Such differences can be reduced by using full configuration-interaction (CI) in atomic structure calculations
- Our atomic structure includes intermediate-coupling but not full CI due to large number of configurations required for opacity table calculations at all conditions
- Similar agreement found in comparison to NOVA measurements in the 1990s

Al at 40 eV and ρ=0.0135 g/cm³

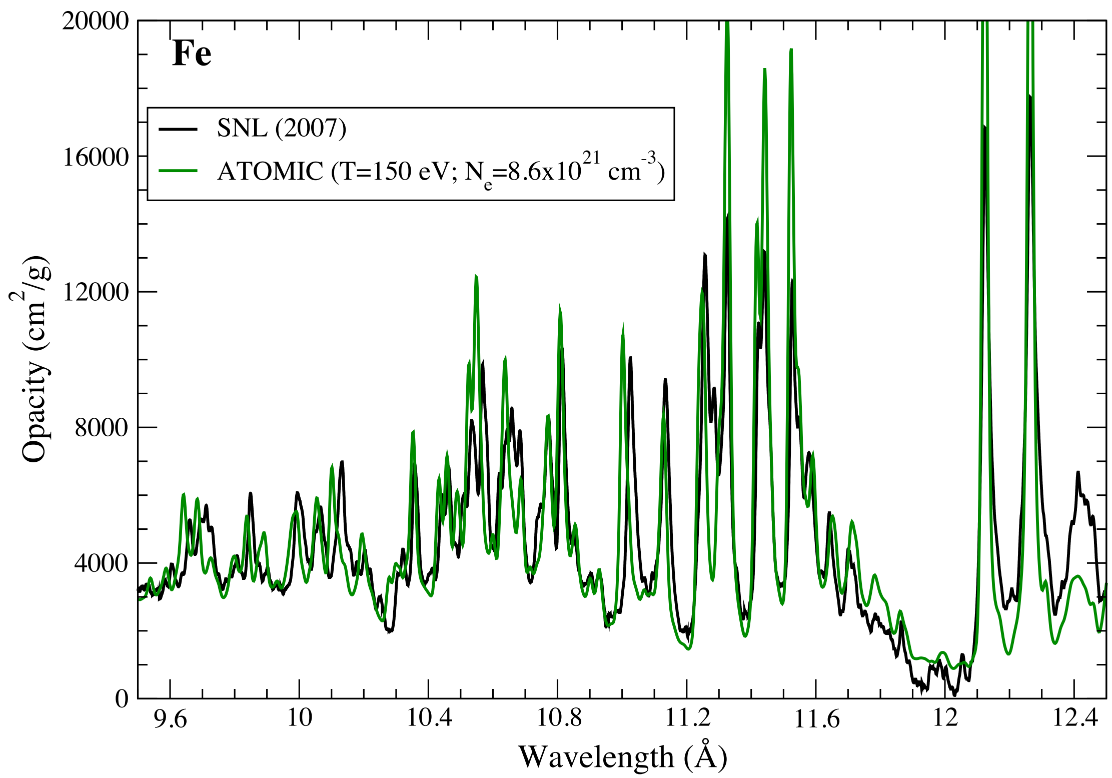


Davidson et al, Appl. Phys. Letts. ***52****, 847 (1988);*
Abdallah & Clark, J. Appl. Phys. ***69****, 23 (1991).*

Comparing opacity calculations with measurements: Fe

- A long-standing effort to measure opacities has also been underway closer to home in New Mexico at Sandia using the Z-pinch machine
- The imploding wire nature of the Z-pinch allows higher temperatures and densities to be explored than had previously been accessible
- The first major Fe SNL measurement was published in 2007; the agreement between the ATOMIC calculations used for our new Fe opacity table and this measurement is excellent

Fe at 156±6 eV and N_e=8.6x10^{21}/cm^3

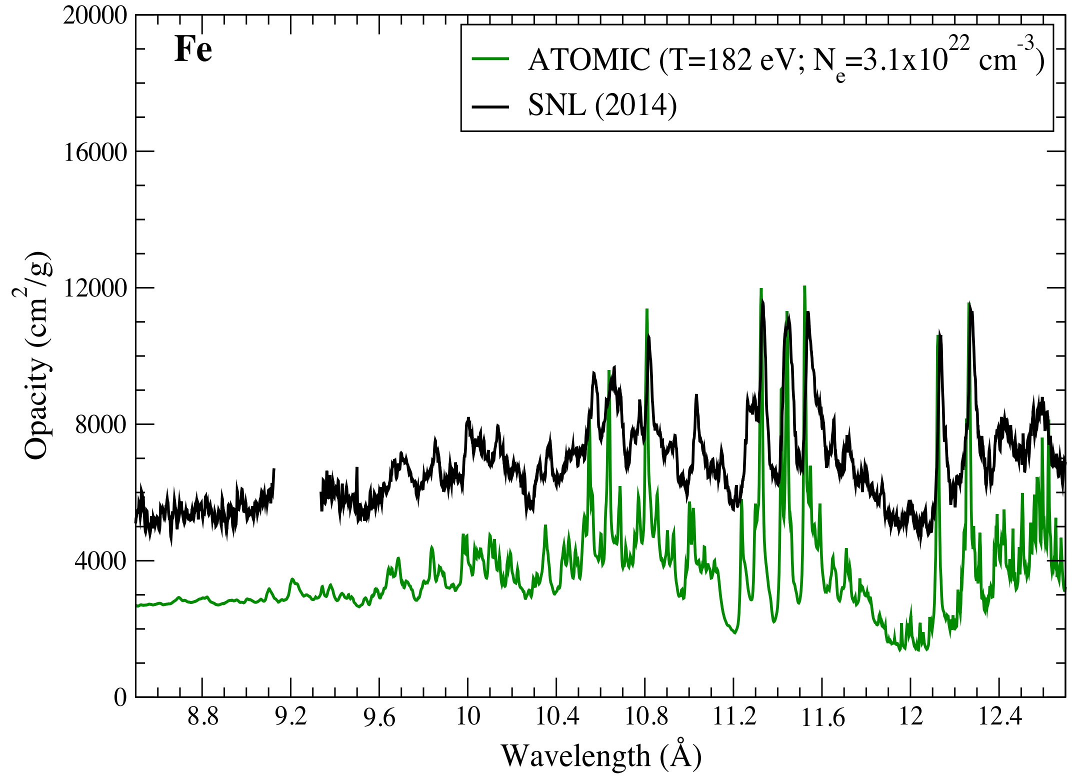


*Bailey et al, Phys. Rev. Letts **99**, 265002 (2006)*

Comparing opacity calculations with measurements: Fe

- The refurbished Z-pinch machine (completed several years ago) provides even more power than used in the 2006 measurements
- This increased power, plus targets that were more thickly tamped, allowed measurements of Fe opacity at temperatures/densities approaching those needed to explore solar physics problems
- However, all calculations are in quite **poor** agreement with these new measurements
- In particular, the underlying (bound-free) opacity differs by close to 50%

Fe at 182±3 eV and N_e=3.1x10^{22}/cm^3

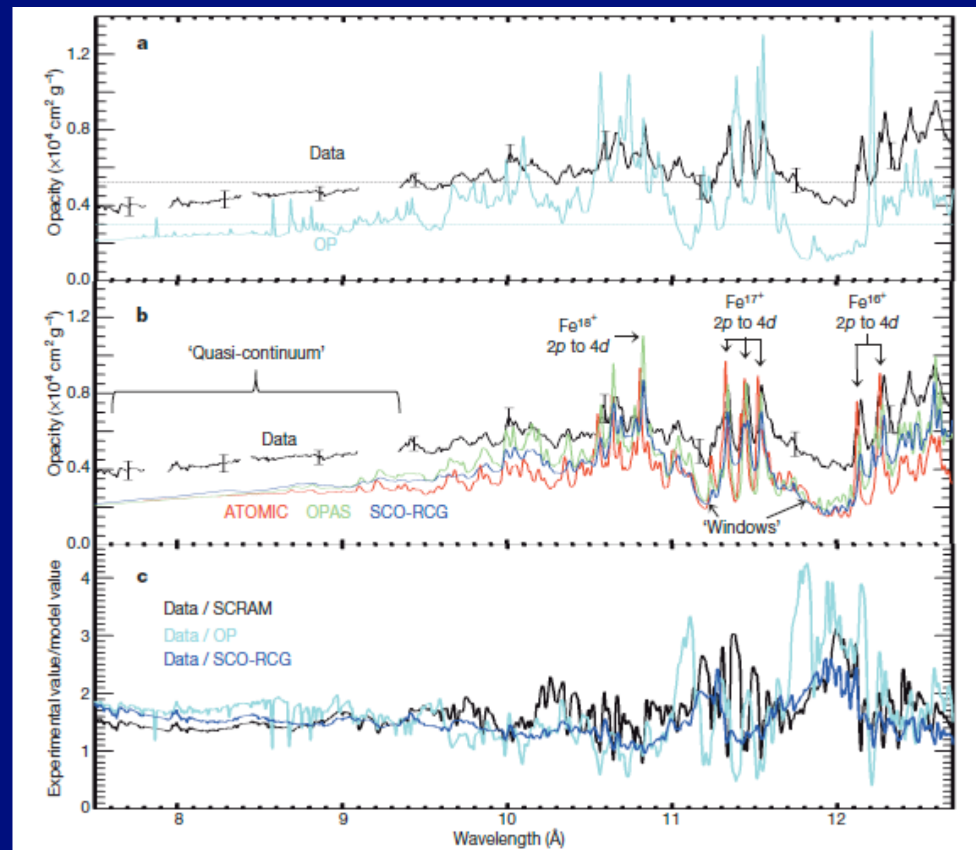


*Bailey et al, Nature **57**, 516 (2015)*

Comparing opacity calculations with measurements: Fe

- Why is this measurement and theory comparison so poor when other comparisons were quite reasonable?
- It is not just ATOMIC: several other opacity codes (OPAS/SCO-RCG/SCRAM, etc) are also in disagreement with this measurement
- This discrepancy is quite unexpected and potentially very important – solar models disagree with helioseismology measurements and differences in opacities of solar elements such as Fe, Ne, O, could potentially resolve the discrepancy
- One important difference with previous measurements is the high electron density in this Fe measurement – at least a factor of 10 larger than any previous measurement

Fe at 182 eV and N_e=3.1x10^{22} /cm^3

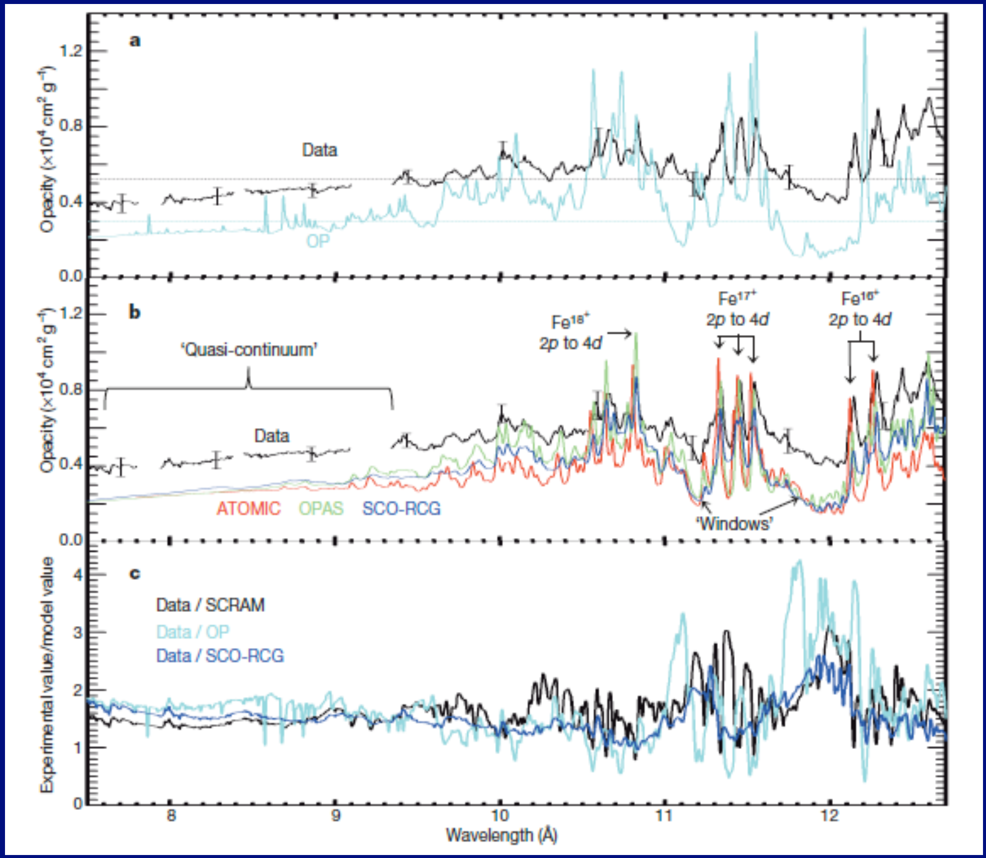


*Bailey et al, Nature **57**, 516 (2015)*

Comparing opacity calculations with measurements: Fe

- This higher density may imply that the atomic populations of the relevant Fe ions change and that populations in excited states is more important. Perhaps the calculations do not retain enough atomic configurations?
- We have tested this by systematically increasing (by ~ 1 order of magnitude) the number of excited configurations retained in our calculations
- However this made little difference to the resulting opacity
- One other possibility is that the most recent measurements are more sensitive to the hydrodynamics of the plasma that is formed
  - Simulations of this have hinted at some effects but firm conclusions are difficult to draw
  - A new Opacity-on-NIF campaign was launched some years ago to provide an independent measurement of the Fe opacity. Good agreement with theory is observed for lower density and the higher density measurements are still ongoing
  - Stay tuned for eventual publications on this work!

Fe at 182 eV and N_e=3.1x10^{22} /cm^3



*Bailey et al, Nature **57**, 516 (2015);*

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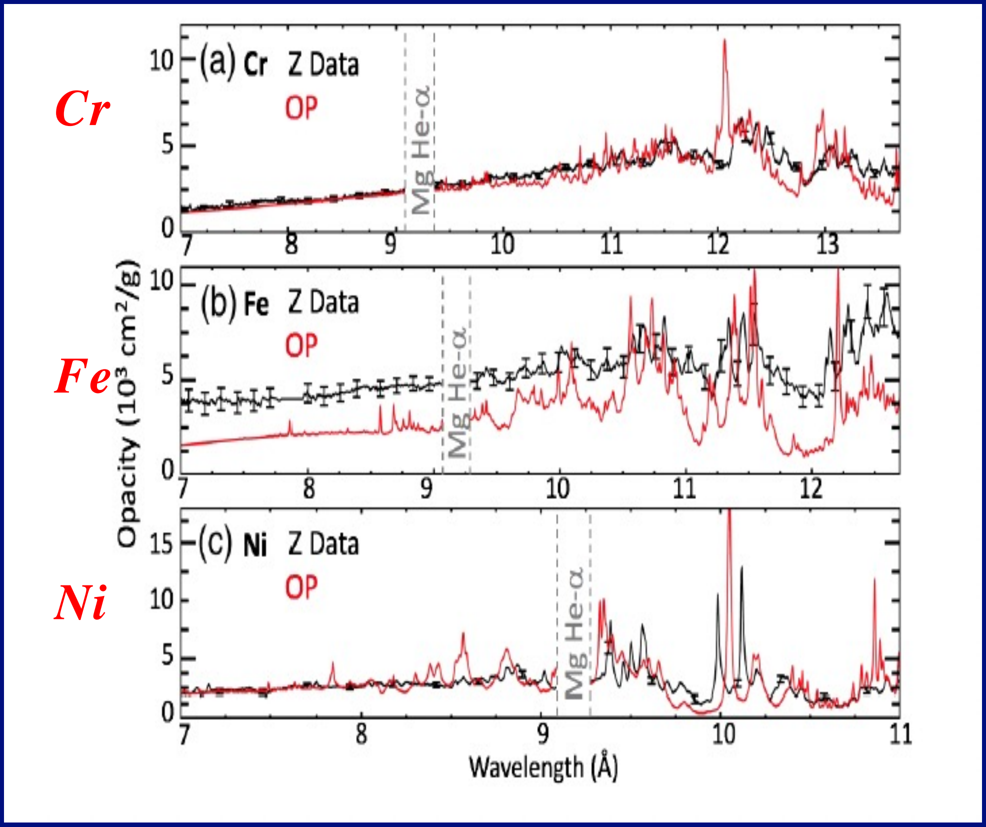
Comparing opacity calculations with measurements: Cr, Ni

- Studies of neighboring elements to Fe were made by the Sandia group to see if the puzzling differences for Fe persisted for similar species
- Recent (2019) measurements on Ni and Cr showed quite good (but not perfect) agreement between measurement and theory.
  - Is Fe a special case somehow?!
- In particular, theory & measurement are in excellent agreement for the bound-free opacity, which dominates at lower wavelengths.
- This nagging issue of the Fe opacity continues and we hope that the new NIF measurements will help our understanding of this.

Cr, Ni at similar conditions



Nagayama et al, PRL 122, 235001 (2019).

Are we missing physics in our opacity models? Maybe…

Several recent papers have proposed new opacity contributions or missing physics in an effort to address the Fe opacity controversy

- For example, Dick More has proposed that two-photon absorption might be important in the SNL measurements and perhaps should be included in opacity tables
  - Two-photon processes are normally considered unimportant since the probability of a state simultaneously absorbing two photons is thought to be low. It's usually only considered in intense (coherent) laser atom interactions.
  - These works note that absorption of two photons of different energies is larger than the probability of absorption of two photons of equal energy
  - The new calculations are considered preliminary since full calculations including 2-photon processes have not been completed.

Opacity from two-photon processes[☆]

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[b] Sandia National Laboratories, Albuquerque NM, USA

A B S T R A C T

The recent iron opacity measurements performed at Sandia National Laboratory by Bailey and collaborators have raised questions about the completeness of the physical models normally used to understand partially ionized hot dense plasmas. We describe calculations of two-photon absorption, which is a candidate for the observed extra opacity. Our calculations do not yet match the experiments but show that the two-photon absorption process is strong enough to require careful consideration.

Free-free matrix-elements for two-photon opacity

R. More[a,1], J.-C. Pain[b], S.B. Hansen[c,*], T. Nagayama[c], J.E. Bailey[c]

[a] Retired from National Institute for Fusion Science, Toki, Gifu, Japan
[b] CEA, DAM, DIF, F-91297 Arpajon, France
[c] Sandia National Laboratories, Albuquerque, NM, USA

Are we missing physics in our opacity models? Maybe not..

Several recent papers have proposed new opacity contributions or missing physics in an effort to address the Fe opacity controversy

- However, recent calculations by the LLNL group find that the two-photon contributions are negligible.
- The two-photon opacity contribution is still at least 2 orders of magnitude lower than one-photon opacity contributions

Two-photon ionization in solar opacity experiments

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Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, CA 94550, United States of America

A B S T R A C T

The discrepancies between theoretical and experimental opacities reported by experiments performed at the Sandia National Laboratory Z-pinch relevant to the solar interior remain unexplained. The suggestion that two-photon ionization could help resolve the discrepancies was recently examined and found not to account for the higher than predicted measured opacities. That test, however, was limited in scope and is now extended to include excited configurations and different charge states of several elements. Comparisons of one- and two-photon ionization cross-sections show that the latter fail to resolve the aforementioned discrepancies.

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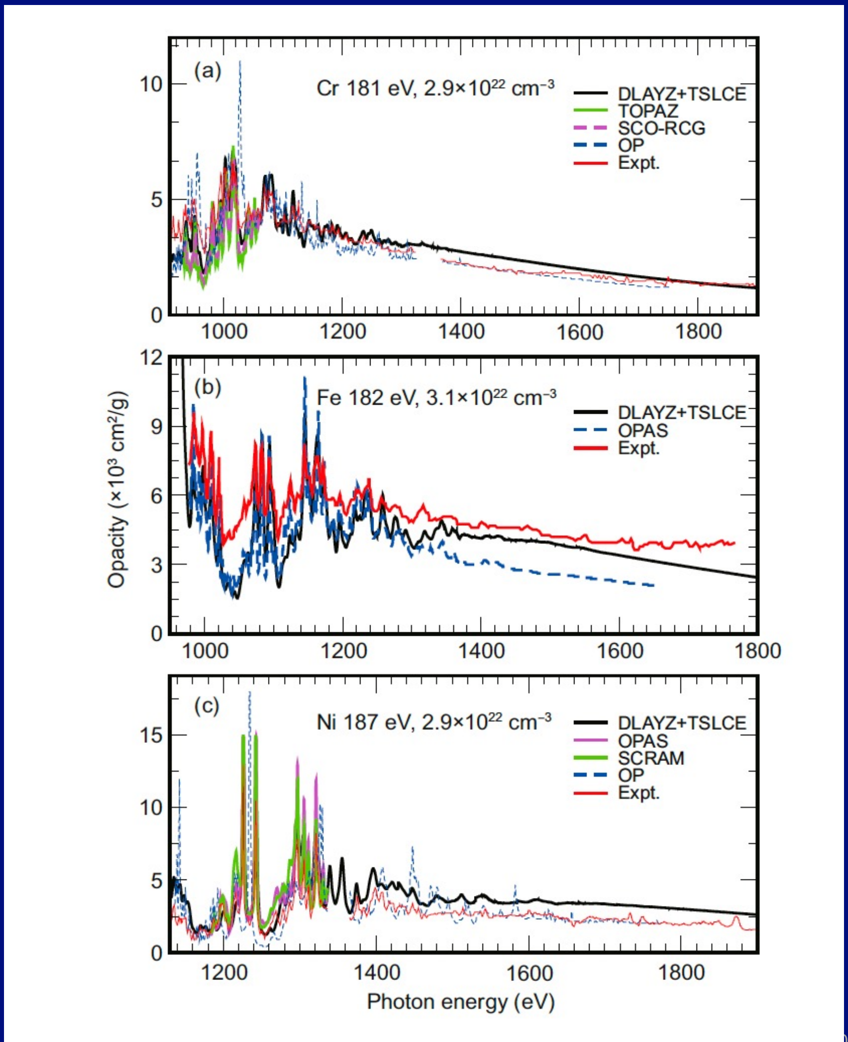
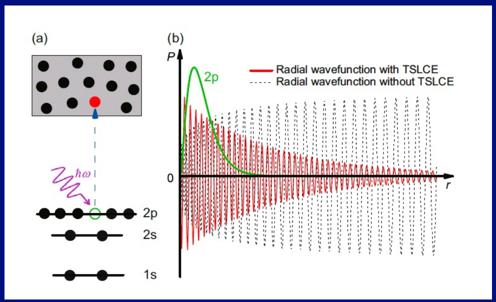
Are we missing physics in our opacity models?

- A recent study by a Chinese group has proposed that **transient spatial localization** might be important at the densities of the SNL measurements, and should be included in opacity calculations.
- This effect is found in solid-state physics and can be thought of as a distortion of the continuum electron wavefunction by other plasma electrons, which can be significant near the atom under consideration.
- However the details of this approach are still unclear (at least to me!)
- It also seems that the proposed increase in opacities would help the theory/expt agreement for Fe, but would likely worsen it for Ni and Cr.
- So it is something that deserves more study but a long way from being completely understood

Electron localization enhanced photon absorption for the missing opacity in solar interior

JiaoLong Zeng[1,3*], Cheng Gao[3], PengFei Liu[3], YongJun Li[3], CongSen Meng[3], Yong Hou[3], DongDong Kang[3], and JianMin Yuan[2,3*]





Discussion

- Topics we plan to expand on in the discussion groups:

- Experimental progress in measuring opacities (presentation to be made by Taisuke Nagayama)
- Assessing the **uncertainty** associated with opacities, particularly in models, is not well developed, and something that needs attention – this is a key topic for WG9
  - Uncertainty should be associated with each step in the process, and we have to recognize that uncertainties will certainly be a function of photon energy, Z, temperature, density, ….
  - Also we note that averaging opacities from fine-grid frequency-resolved opacities to grey or band-averaged opacities will introduce yet more uncertainty.
- Implications of the new solar abundances discussed yesterday by Aldo
- We look forward to good discussions this afternoon!