Light element opacities of astrophysical interest from ATOMIC

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Outline of talk

- Introduction to opacities
  - What is an opacity? Why are opacities important?
  - LTE Opacity efforts worldwide
  - Astrophysical applications
- The LANL suite of atomic physics codes
  - Structure codes
  - ATOMIC: collisional-radiative modeling and opacities
- New tables for Z=1-10
  - What is improved in new set of tables?
  - Comparisons of new LANL opacities with OP & OPAL databases
  - Comparisons of new LANL opacities with measurement and other efforts for Fe

What is an opacity?

- Opacity, κ_ν, gives a measure of how much radiation a certain material will absorb/scatter (i.e. how “opaque” is the material)
- An opacity can be thought of as a macroscopic quantity that is built up from fundamental atomic cross sections
- In local thermodynamic equilibrium (LTE), we can compute the populations using: $$N_{il} \propto (N_i)e^{-E_{il}/kT}$$
- Opacity=(atomic population)(cross section)/(mass density)
NB: For LTE conditions, we only require *photo* cross sections

$$\kappa_\nu(\rho,T) = \frac{1}{\rho}\sum_{i,l} N_{il}(\rho,T)\sigma_{il}(\nu) +$$

mass density

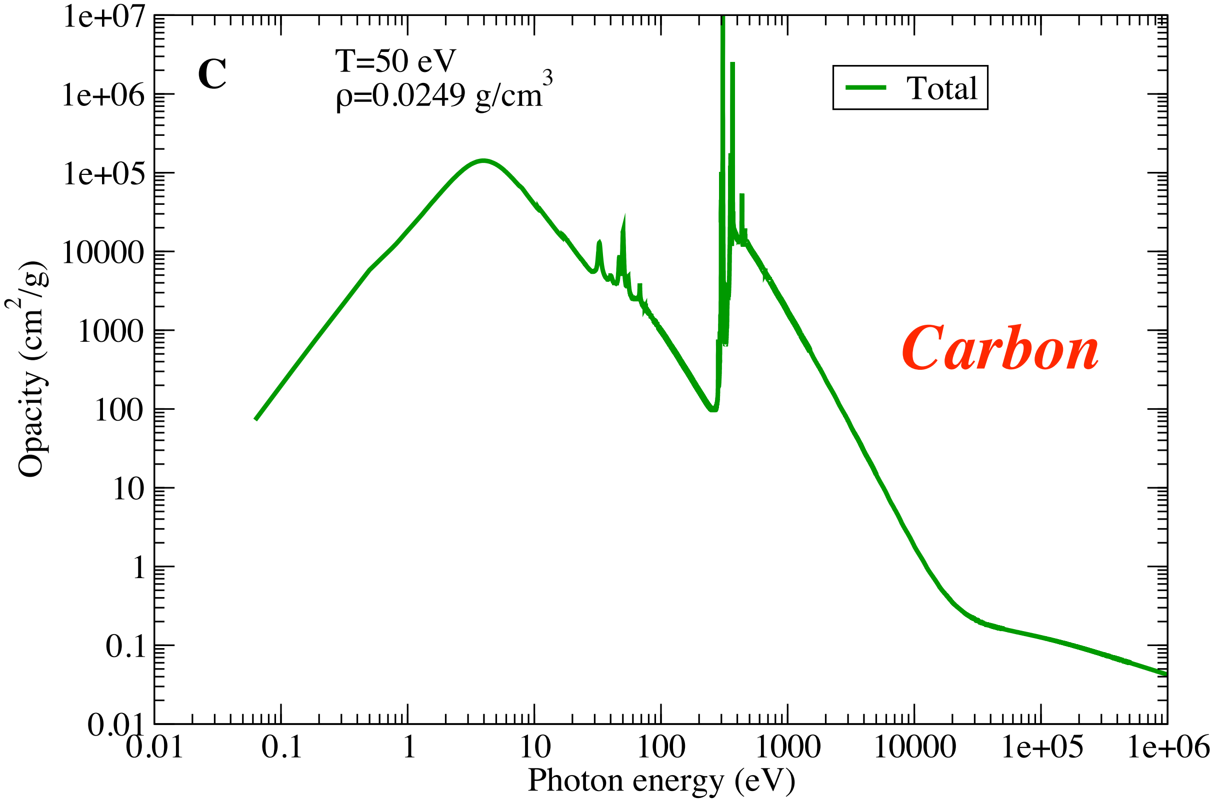
atomic level populations

photoexcitation cross sections

What constitutes an opacity?

- Opacities usually have four main contributions:

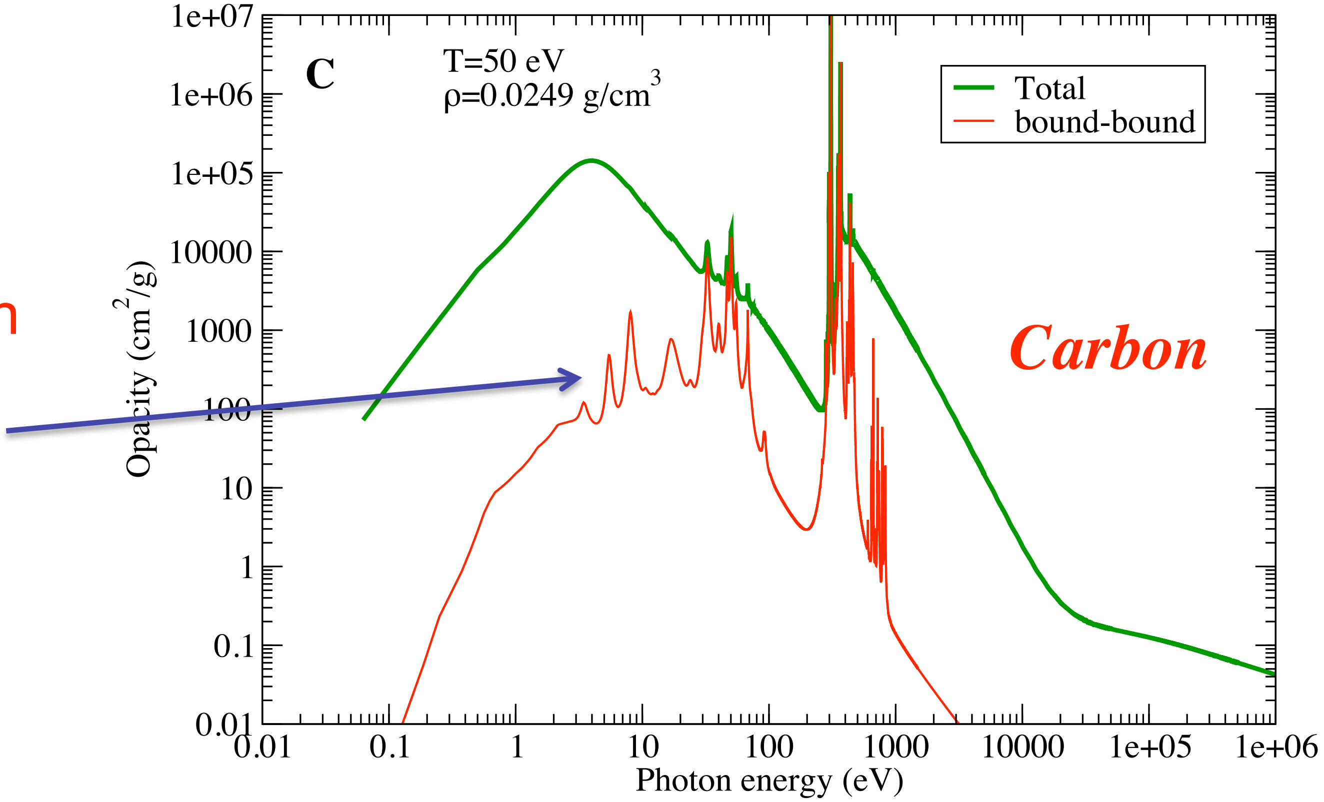
T=50 eV and ρ=0.0249 gcm^{-3}



What constitutes an opacity?

- Opacities usually have four main contributions:
- Bound-bound: a bound electron absorbs a photon and moves to an excited state

T=50 eV and ρ=0.0249 gcm^{-3}

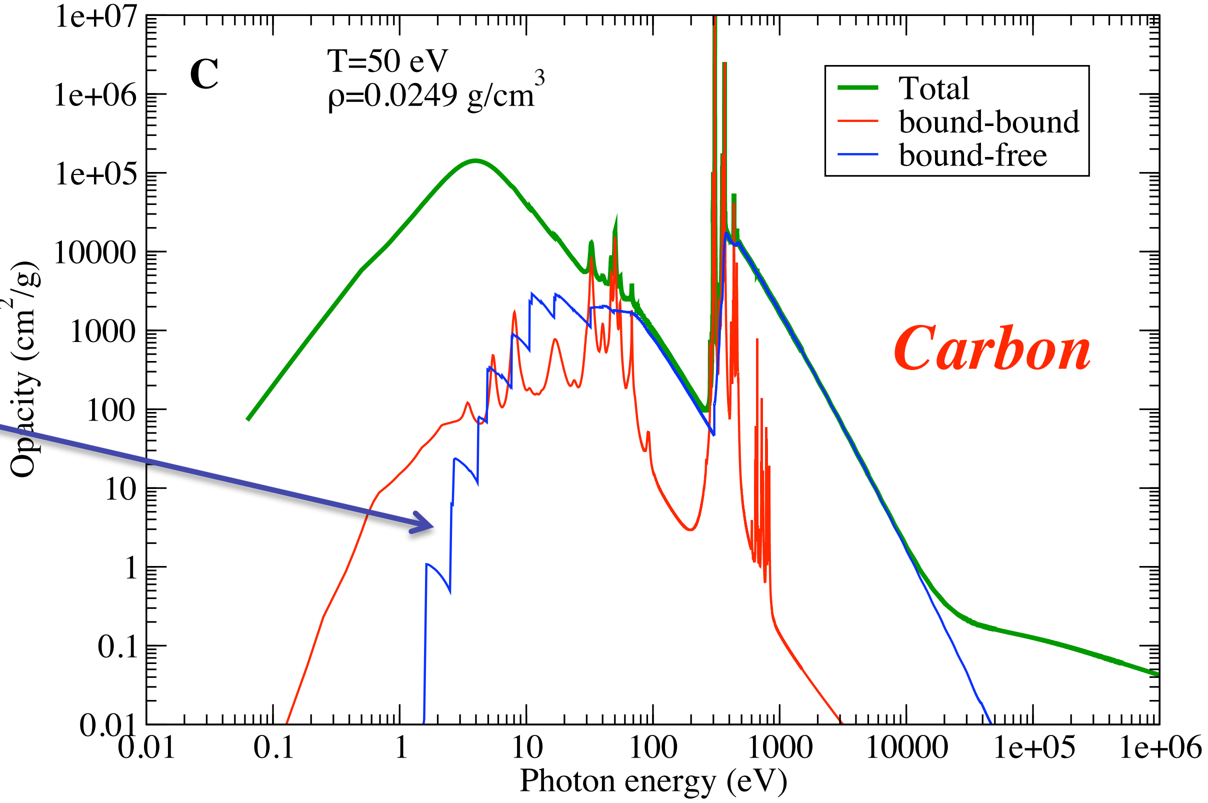


What constitutes an opacity?

- Opacities usually have four main contributions

- Bound-free: an electron absorbs a photon and is ionized: photoionization

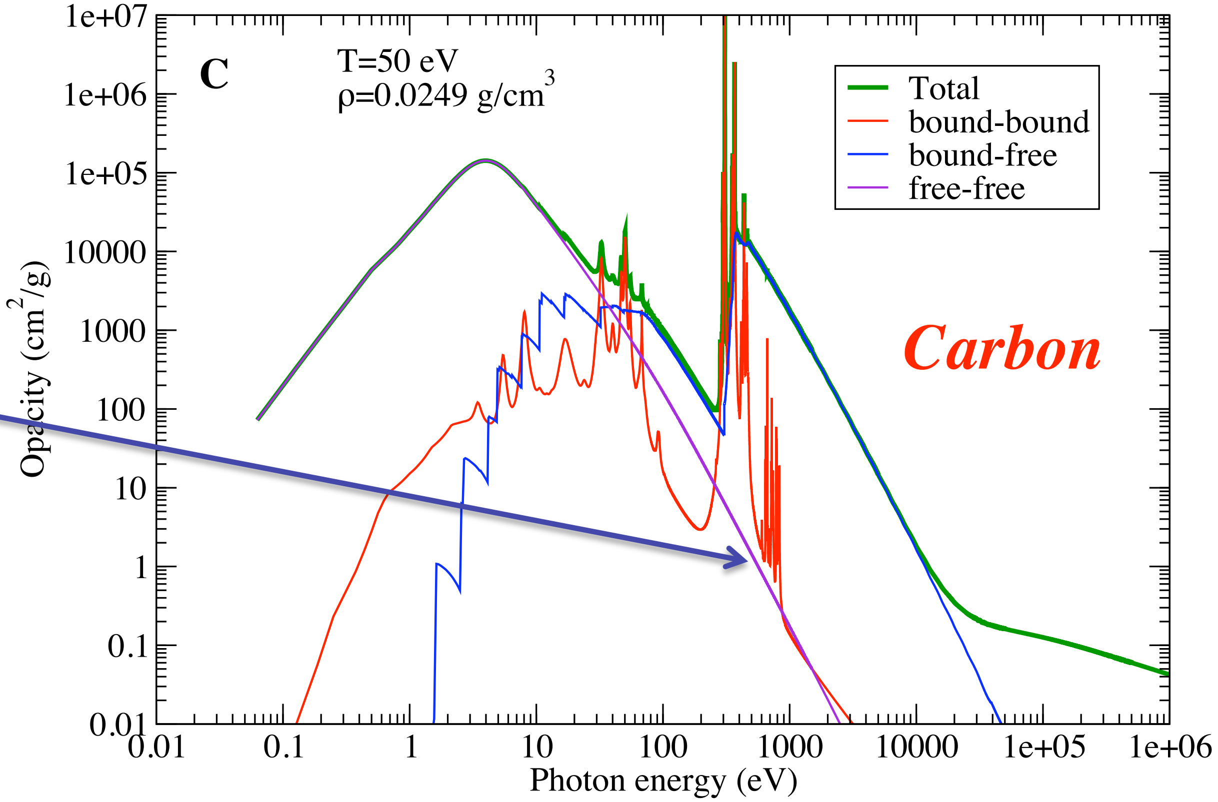
$T=50$ eV and $\rho=0.0249$ gcm^{-3}



What constitutes an opacity?

- Opacities usually have four main contributions
- Free-free: a free electron absorbs a photon and changes its energy
  - Also known as inverse Bremsstrahlung

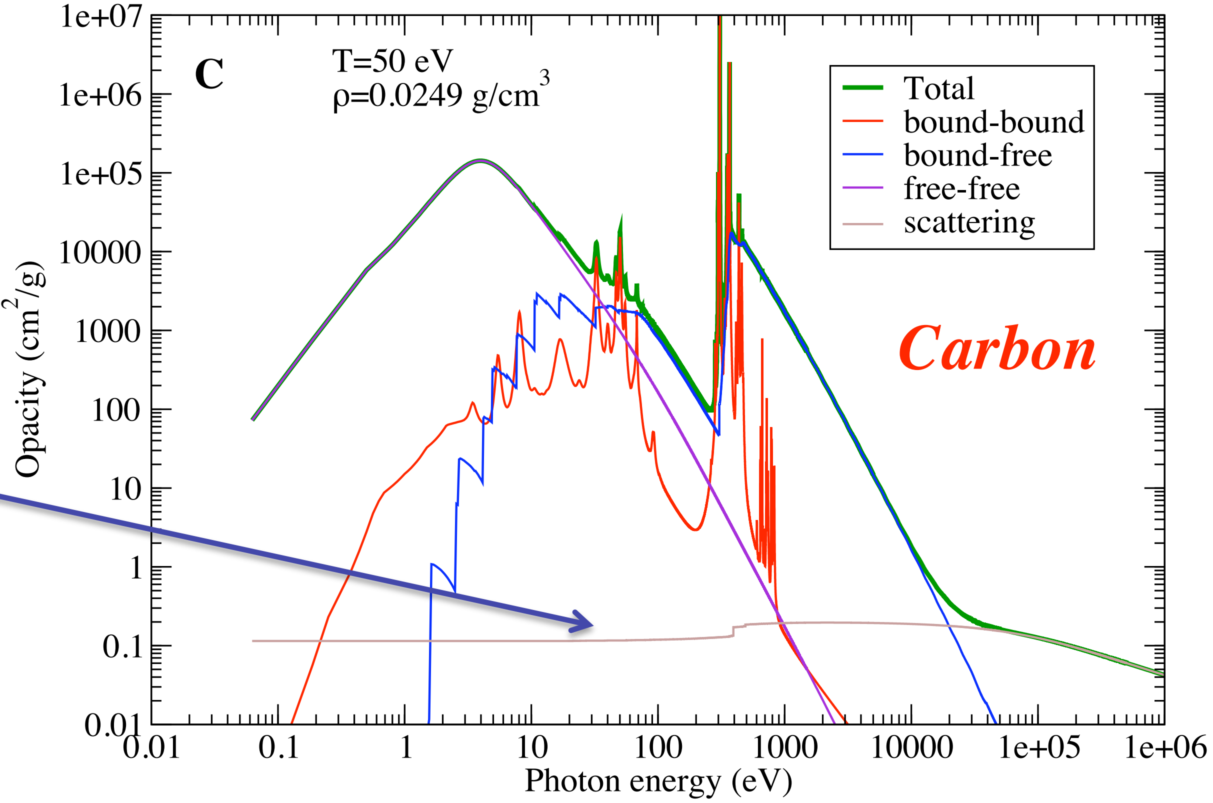
T=50 eV and ρ=0.0249 gcm^{-3}



What constitutes an opacity?

- Opacities usually have four main contributions:
- **Scattering**: scattering of a photon by an electron, resulting in a change of energy of the photon through an elastic or inelastic process
  - Thomson scattering (or known as Compton scattering for high energies)

T=50 eV and ρ=0.0249 gcm^{-3}

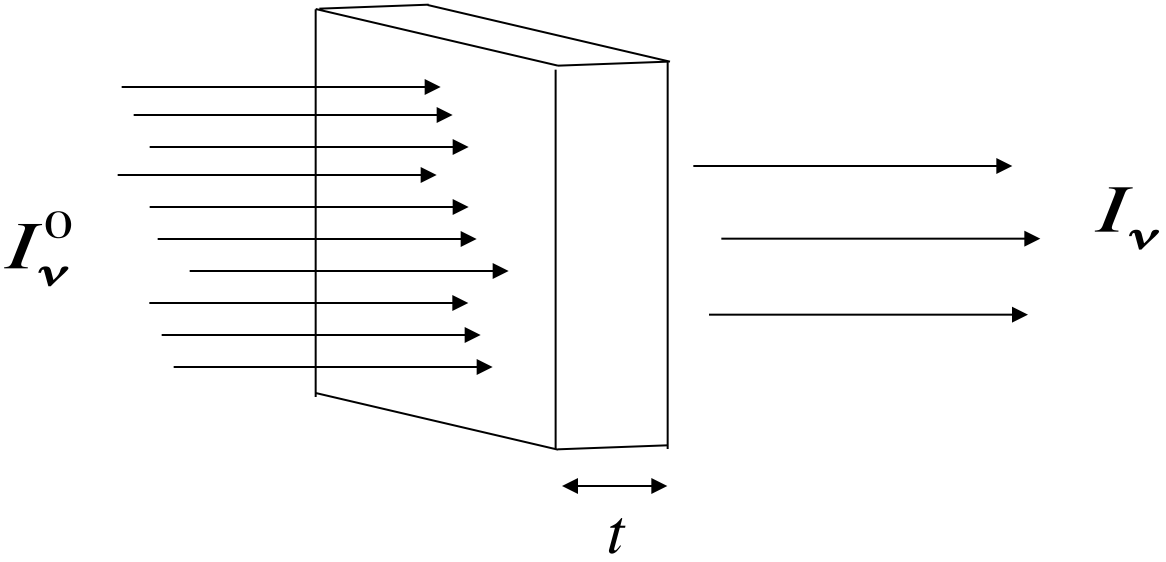


The classic opacity (transmission) experiment

- Prepare a very thin sample (so that plasma is ‘optically thin’) of thickness *t* and shine incident radiation with intensity I_ν^0

$$I_\nu = I_\nu^0 e^{-(\rho \kappa_\nu t)}$$

- The transmitted intensity will be attenuated:



Opacities are used in astrophysics

- 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
  - 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
- Opacities are also important in attempting to model the light curves arising from supernovae
  - One requires monochromatic opacities to calculate the light curves
  - Non-LTE data may also be required (beyond the scope of this talk)

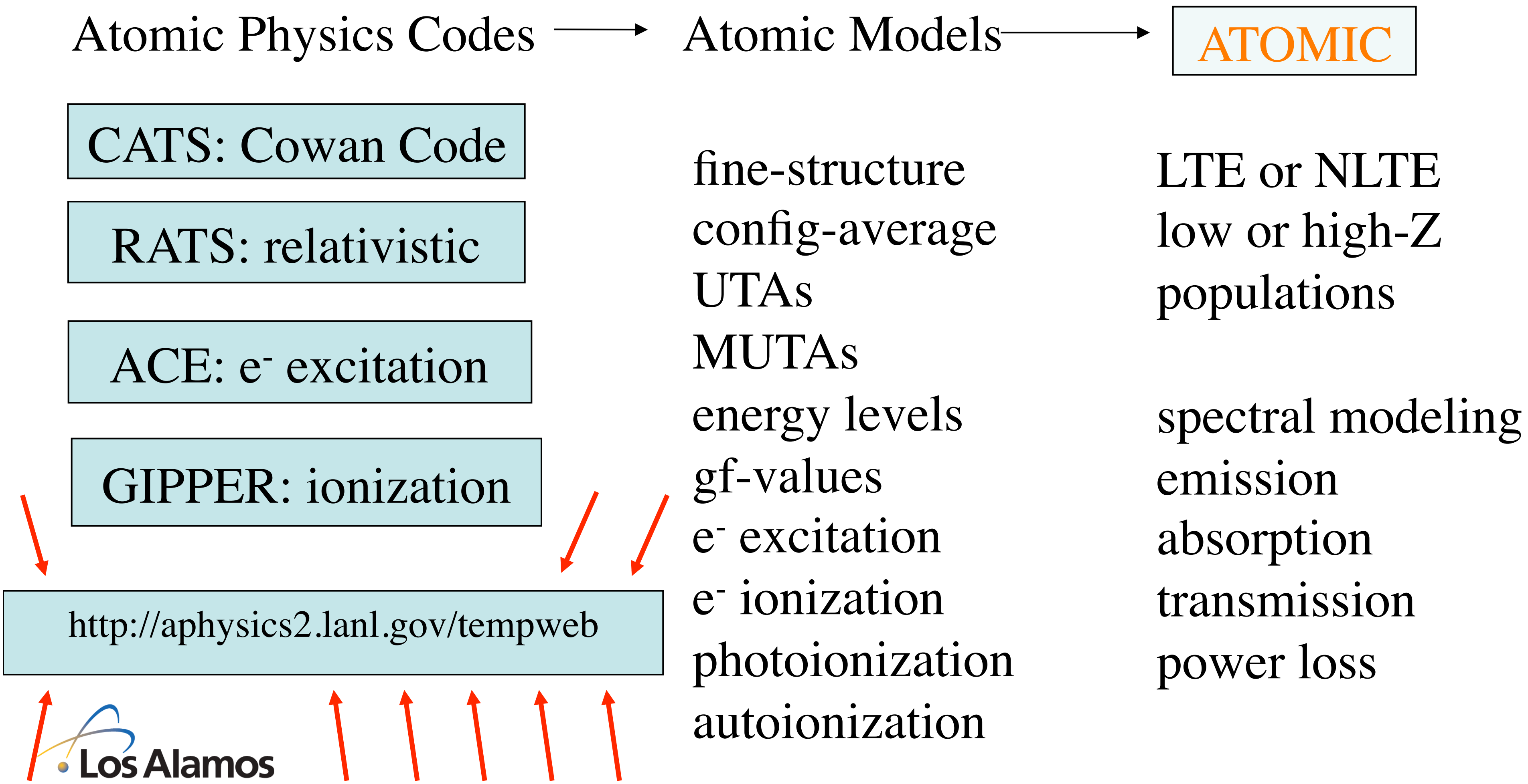
Worldwide opacity efforts:

- The Opacity Project (OP)
  - Started in the UK by Mike Seaton & collaborators and aimed to provide LTE opacities for elements of astrophysical interest
- OPAL
  - Lawrence Livermore National Laboratory has an independent LTE opacity code, which has been used extensively in the astrophysics community
- OPLIB
  - Los Alamos has developed and maintained an LTE opacity database for many years, most recently populated with data generated from the LEDCOP code written by N. Magee
- *Of course, other opacity databases exist, but these are the 3 that I will discuss today*

Los Alamos National Laboratory opacity efforts:

- Our long-term goal is to upgrade the legacy LEDCOP opacity data in the OPLIB database by performing new opacity calculations for all astrophysically important elements
  - We use the atomic physics capabilities at LANL to perform large-scale data calculations
  - The ATOMIC code will be used to perform the opacity calculations

The LANL suite of atomic modeling codes



Atomic Physics Codes → Atomic Models → **ATOMIC**

- CATS: Cowan Code
- RATS: relativistic
- ACE: e^- excitation
- GIPPER: ionization

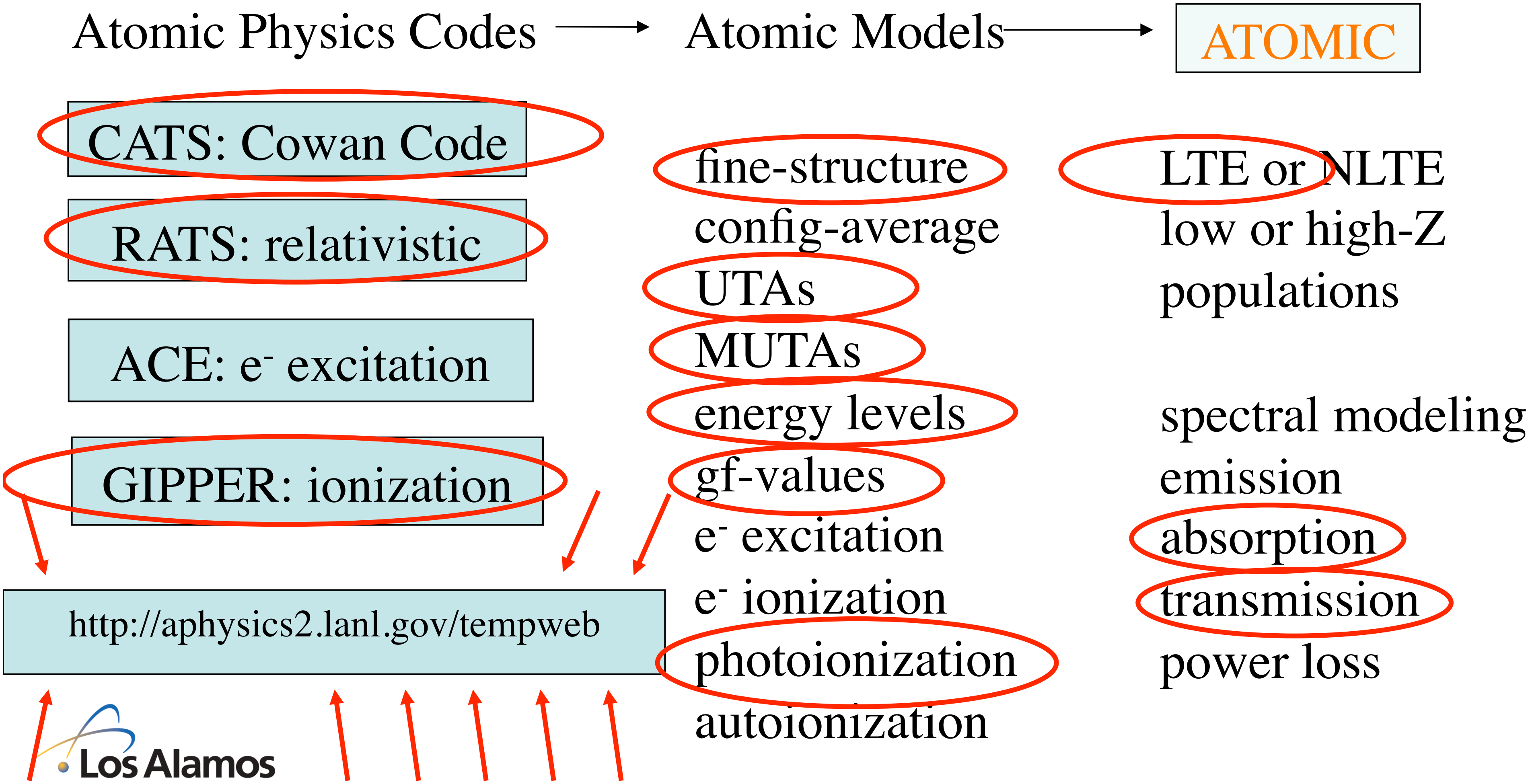
http://aphysics2.lanl.gov/tempweb

fine-structure
config-average
UTAs
MUTAs
energy levels
gf-values
e^- excitation
e^- ionization
photoionization
autoionization

LTE or NLTE
low or high-Z
populations

spectral modeling
emission
absorption
transmission
power loss

The LANL suite of atomic modeling codes: LTE opacity needs



Atomic Physics Codes → Atomic Models → ATOMIC

CATS: Cowan Code

RATS: relativistic

ACE: e⁻ excitation

GIPPER: ionization

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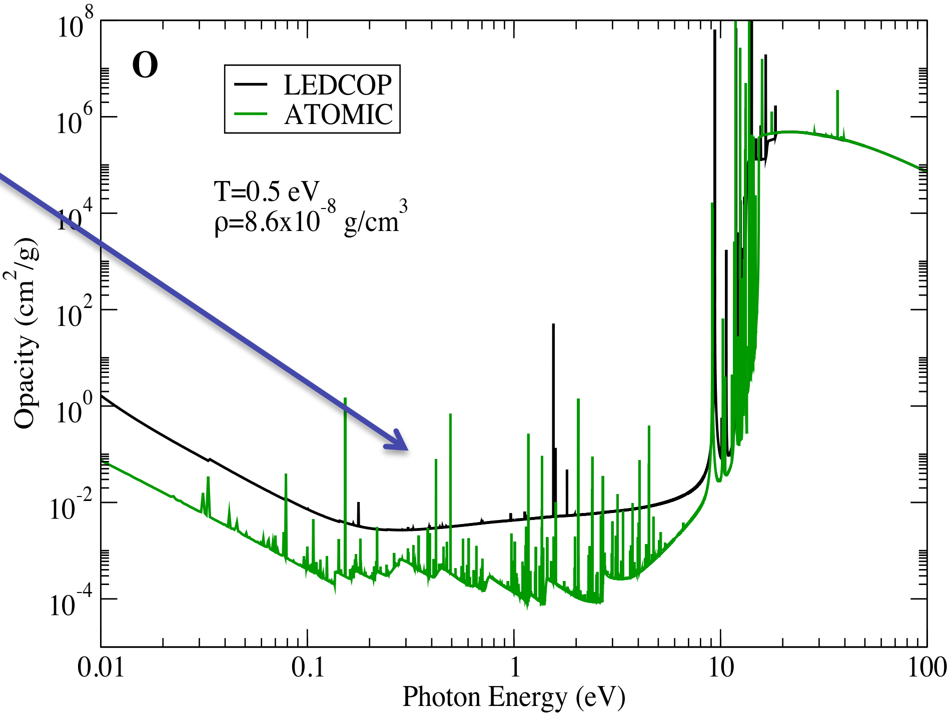
Improvements in new LANL opacity tables

- Atomic structure:
  - New opacity calculations for Z=1-10 (H-Ne) all use fine-structure (*LSJ*) resolved atomic structure sets
  - Results in many more b-b transitions in the new calculations
  - For example: Neon database includes > $2x10^7$ levels (all ion stages) and more than 6.5 billion transitions (totaling 200GB)
  - Calculations include intermediate-coupling within a configuration

$T=0.5$ eV and $\rho=8.6x10^{-8}$ g/cm^3

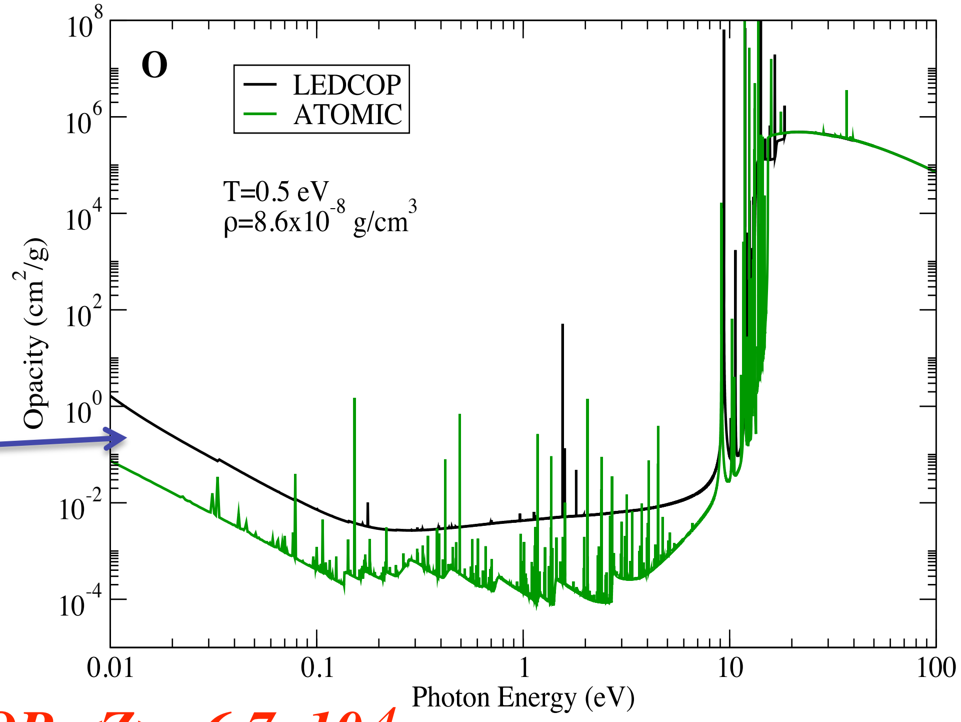


Oxygen

Improvements in new LANL opacity tables

- EOS:
  - New opacity calculations use ChemEOS package for all EOS calculations
  - Package based on the minimization of free energy in a chemical picture
  - Results in a more accurate average ionization (<Z>) of the plasma
  - Changes f-f contribution to the opacity

T=0.5 eV and ρ=$8.6x10^{-8}$ g/cm^3



P. Hakel & D. P. Kilcrease, 14^{th} Topical Conference on Atomic Processes in Plasmas), pp190-202 (2004).

LEDCOP <Z>=$6.7x10^{-4}$

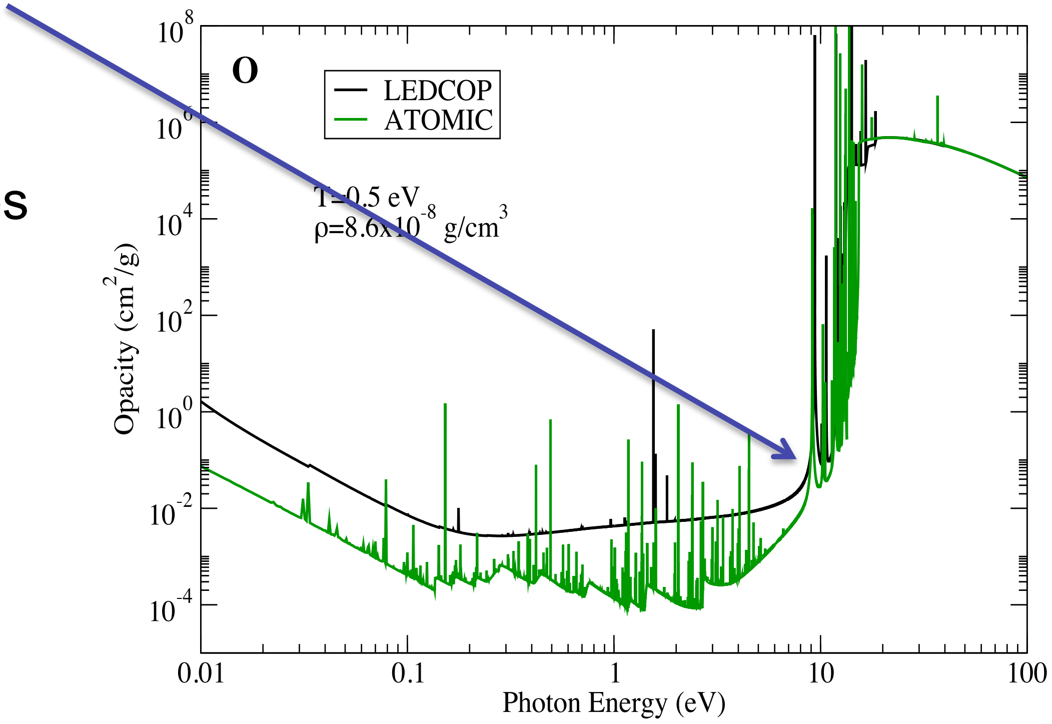
ATOMIC <Z>=$1.8x10^{-4}$

Oxygen

Improvements in new LANL opacity tables

- Line broadening:
  - Improvements made in our line shape package and line broadening, which are very important in opacity calculations
  - Improvements in line shapes far away from line center
  - Neutral resonance and neutral Van der Waals broadening included

T=0.5 eV and ρ=8.6x10^{-8} g/cm^3

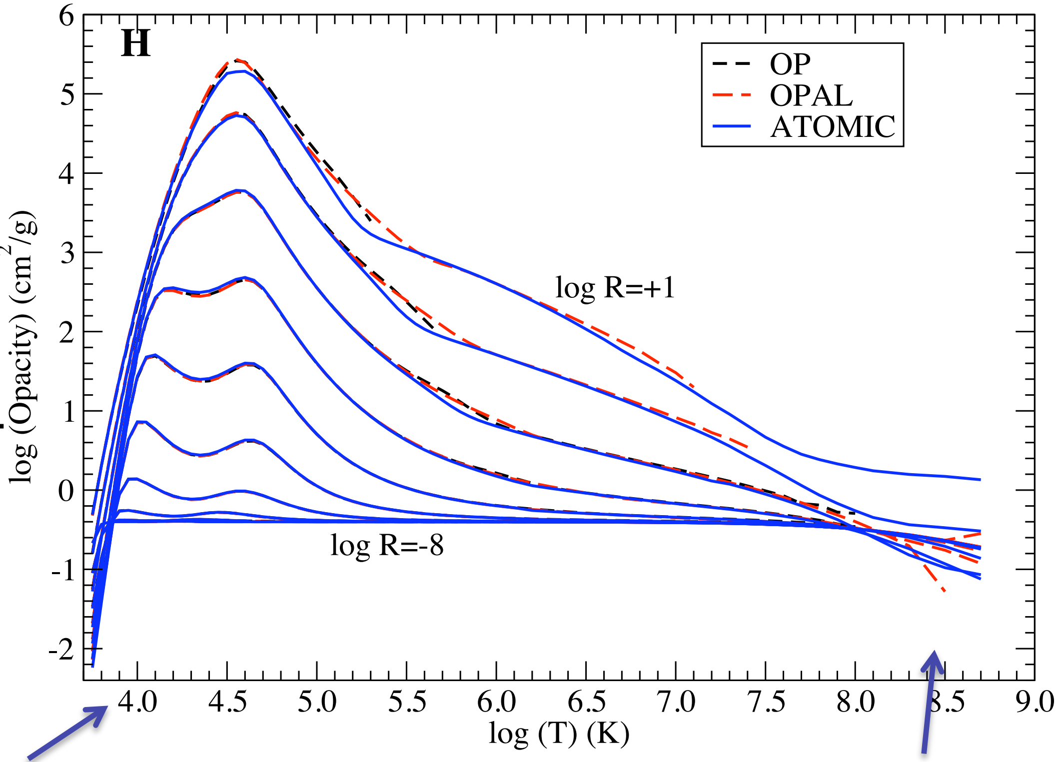


Oxygen

Comparisons with other opacity table efforts: H

- OP & OPAL website data are tabulated for constant log R values
  - R commonly used in astrophysical modeling
- We compare *Rosseland mean* opacity – integrated over all photon energies
- Agreement with OP and OPAL data is generally excellent
- Major feature [‘bump’ at log(T)~4.6] due to b-b contributions

$$R = \rho / T_6^3 \qquad T_6 = 10^{-6} T(K)$$



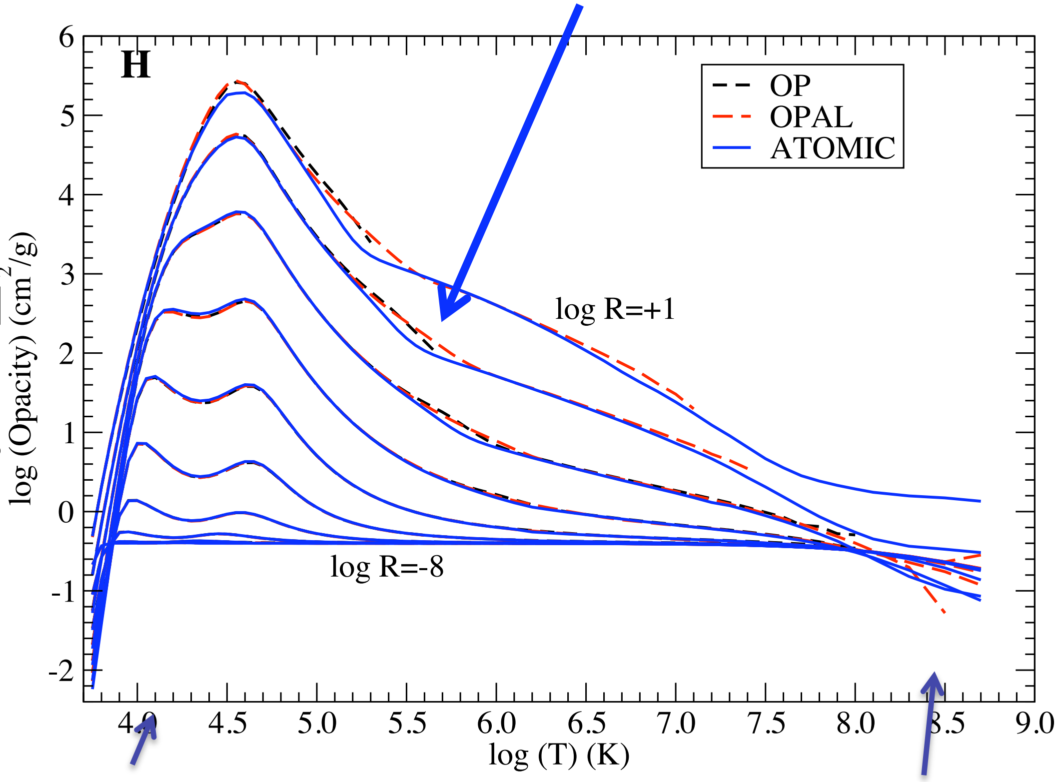
~0.5 eV

~45 keV

Comparisons with other opacity table efforts: H

- Focus on a lower temperature region (log T~ 5.2; 15-30 eV)
  - All three calculations differ from each other
  - Opacity sensitive to EOS, and specifically to H excited state populations
  - This occurs when plasma is almost fully ionized, i.e. <Z>~0.98
  - This sensitivity already noted by Seaton & Badnell [MNRAS 354, 457 (2004)]

Opacity sensitive to populations of excited states of H



~0.5 eV

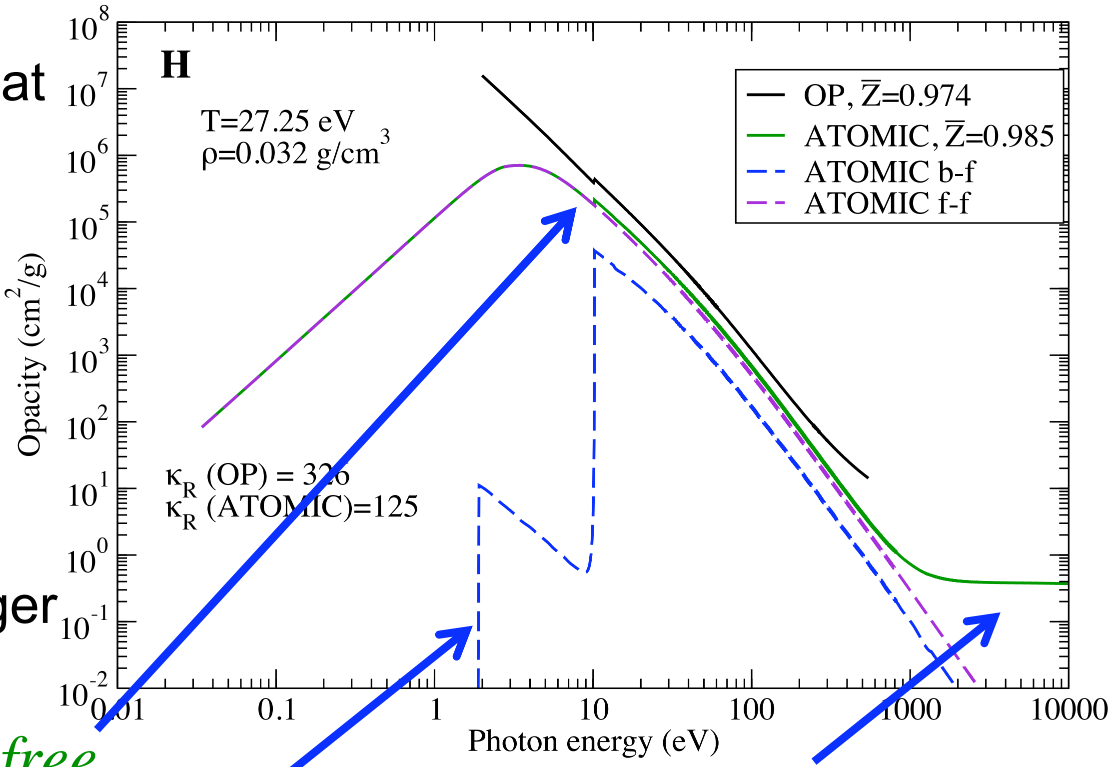
~45 keV

Comparisons with other opacity table efforts: H

Lower temperature region (log T~ 5.2; 15-30 eV)

- ATOMIC <Z> (measure of ionization) is greater than that of OP by only 1% but κ_R differs by ~50%
- This small <Z> difference implies more bound state occupation probability of neutral H in OP calculation
- This results in more bound-free opacity, resulting in larger total opacities and so larger mean opacity

H at 27.25 eV and ρ=0.032 g/cm³



Free-free

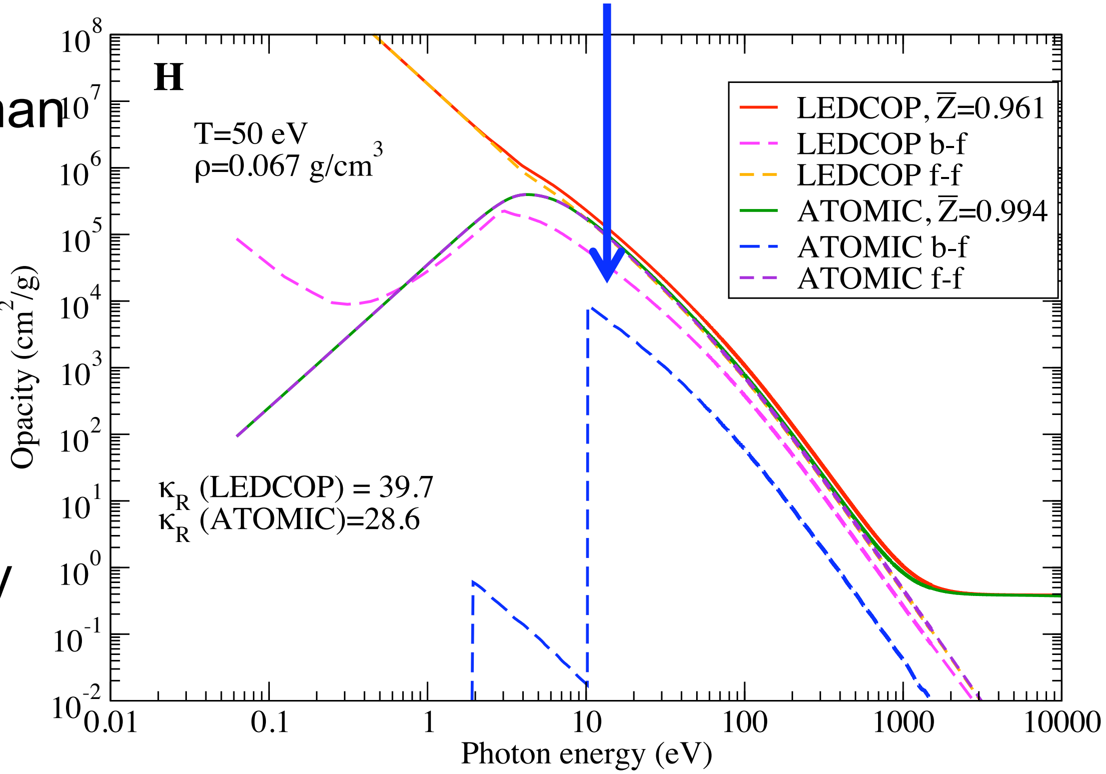
Bound-free

Scattering

Comparisons with other opacity table efforts: H

- We observe similar trends in comparing ATOMIC with LEDCOP data
  - ATOMIC <Z> is greater than that of LEDCOP by ~3%
  - LEDCOP calculation has more neutral H present
  - Excited-state populations can differ by an order of magnitude
  - This results in significantly more bound-free opacity

H at 50 eV and ρ=0.067 g/cm³; differences are due to b-f contribution



Fe opacity

- Fe is one of the most important astrophysical elements, as it is the heaviest stable element produced through nucleosynthesis, and because its many ion stages and huge number of energy levels provide many absorption possibilities
- Atomic structure calculations for Fe are significantly more complicated than for lighter elements
  - The 3d subshell is open for a range of ion stages, resulting in very large numbers of possible levels
  - Mixing between these levels is also significant, requiring complex atomic structure calculations to obtain acceptable accuracy

Fe opacity and the Sun

- Fe opacity also under renewed interest due to the recent "solar abundance" problem
- The solar abundance issue arose when new analyses of the solar photosphere (in early 2000s) produced new (smaller) abundances for many of the elements (mostly 'metals') within the Sun
- The new abundances resulted in discrepancies with helioseismology data for solar quantities such as the sound-speed and density profile
  - Previously accepted solar abundances were in excellent agreement with helioseismology data
  - Helioseismology predictions are generally thought to be very accurate

Fe opacity and the Sun

- One potential resolution would be if the "standard" opacities for the elements in solar conditions were to be changed
  - For example, an increased Fe mean opacity of ~20% (along with more modest changes in other elemental opacities) could resolve this discrepancy
- However, for the conditions of relevance, most large-scale opacity databases agreed to within ~5%
- More recent abundance revisions have slightly shifted downwards the change needed in the opacities; but a discrepancy still remains
- Worldwide efforts underway to *measure* opacities for these conditions, in case *all* calculations are inaccurate

Fe LANL opacity

- Our opacity calculation is based on the MUTA (mixed-UTA) capabilities within ATOMIC
  - Such a calculation uses EOS populations for configurations only, but includes the important bound-bound contributions in a detailed (fine-structure) manner
  - This is accomplished through the use of fine-structure calculations when the number of lines within a transition array is below some threshold (in this case 10^5)
  - Contributions from weak lines included within a statistical manner (see reference)
  - For large number (> 10^6) of lines within a transition array, the standard UTA approximations are used

S. Mazevet & J. Abdallah, J. Phys. B ***39****, 3419 (2006).*

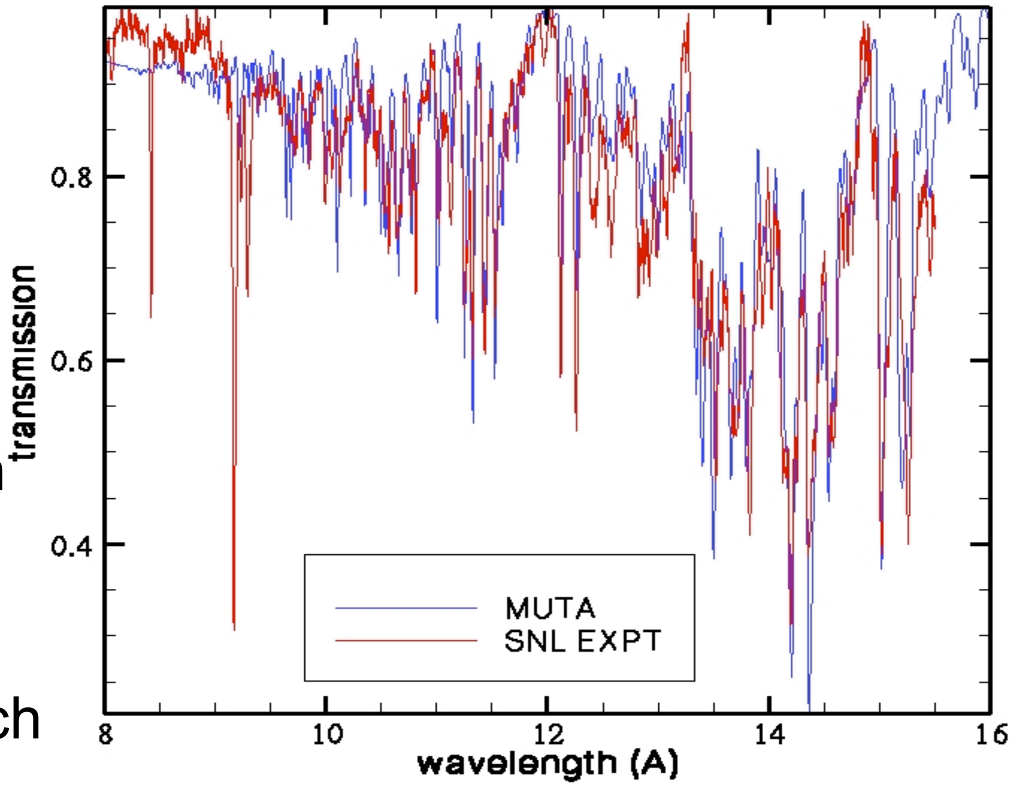
Fe LANL opacity

- Structure calculations with these settings results in large number of transitions, especially for the open n=3 subshells
- Calculations of opacities can include > 10^{11} lines
- Atomic database for Fe requires ~1.0 TB of disk space
- Complete opacity table (> 3000 temperature/density points) can take some weeks to run

Fe opacity – comparison with measurement

- A few transmission measurements are available for Fe using the Sandia Z-pinch facility
- Conditions near, but not quite, at solar convection zone conditions
- ATOMIC MUTA calculations in good agreement with the Z-pinch measurement
- Shows that the MUTA approach is valid at such conditions

T_e=160 eV and N_e~1.5x10^{22} cm^{-3}

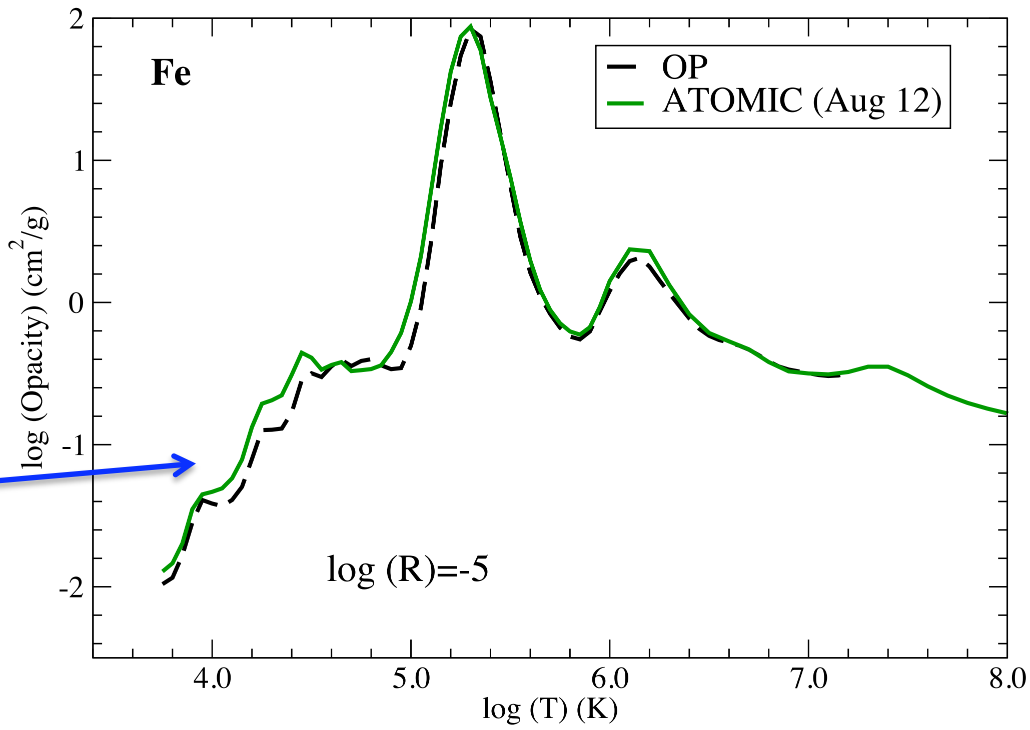


Bailey et al, Phys. Rev. Lett. ***99****, 26502 (2007)*

Fe opacity – comparison with OP calculations

- We compare with OP data for various log R values (no OPAL data available for pure Fe)
- Overall agreement between ATOMIC & OP is good for these relatively low density conditions
- Some differences at low temperature where near-neutral Fe is dominant
- This is where atomic structure is most complex and difficult to calculate

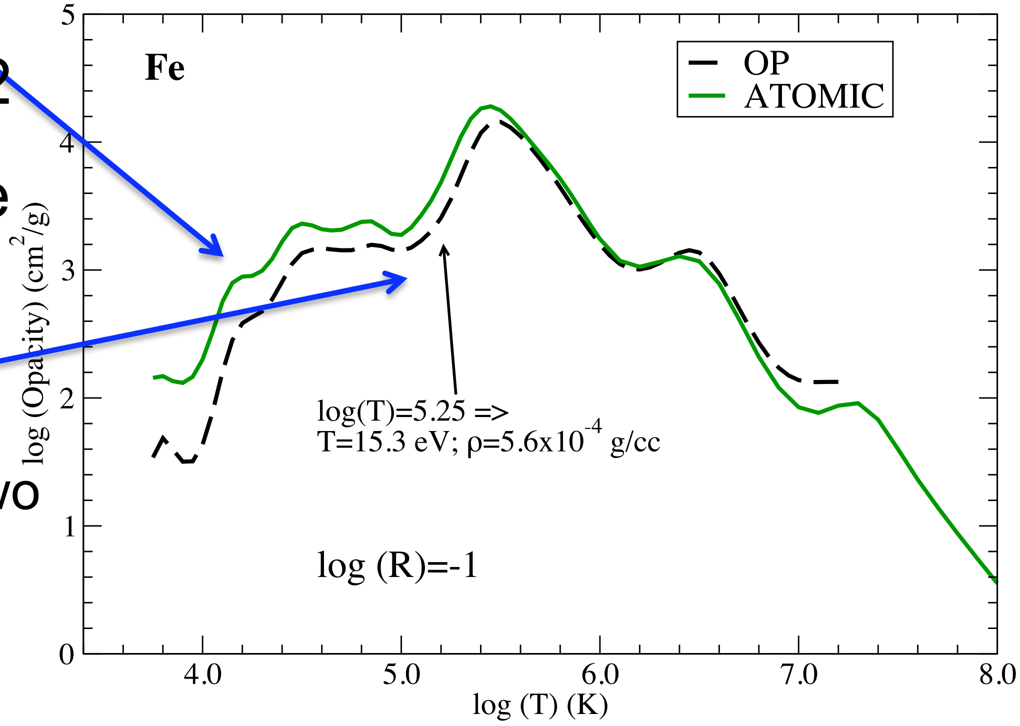
Log (R)=-5



Fe opacity – comparison with OP calculations

- Now examine log (R) of -1
- Larger differences at low temperatures of ~factor of 2
- Also a noticeable difference at moderate temperatures around 15-20 eV;
  - OP data are lower than ATOMIC data by ~factor of two
- This is similar to region explored in recent French study

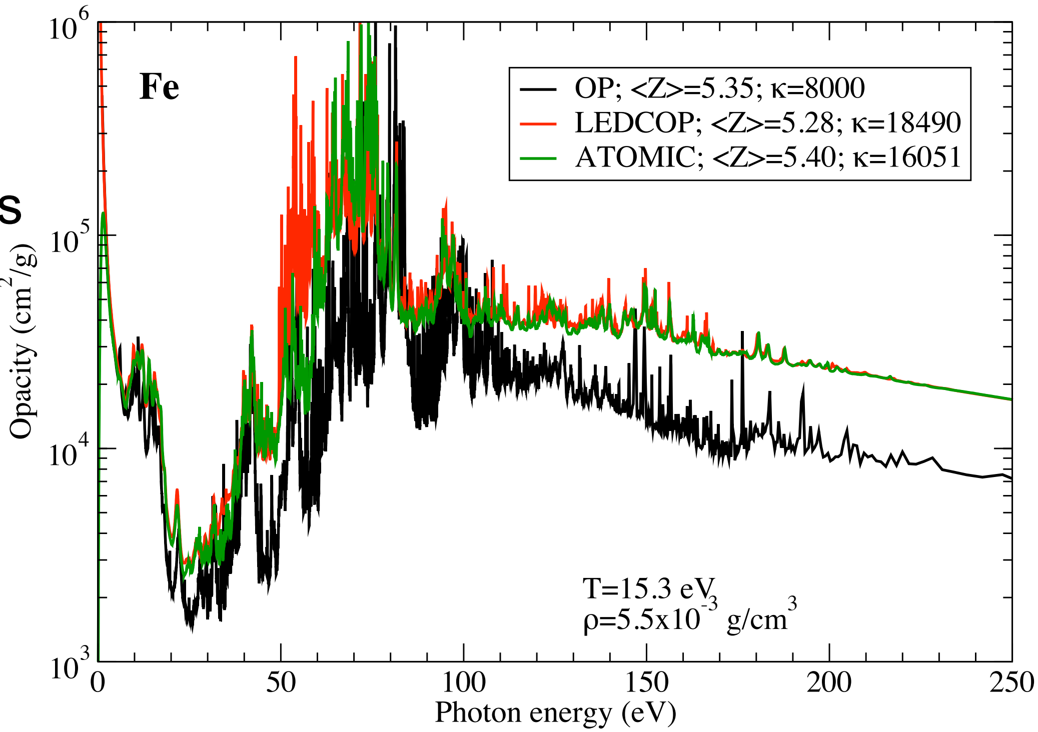
Log (R)=-1



Fe opacity – comparison with OP calculations

- OP calculation significantly lower than ATOMIC & LEDCOP calculations
  - Differences appear to be in both b-b and b-f contributions
- OP lower than SCO-RCG calculations (not shown) presented in a recent publication
- ATOMIC is in good agreement with SCO-RCG

Fe at 15.3 eV and **ρ** *=5.5 mg/cm³*

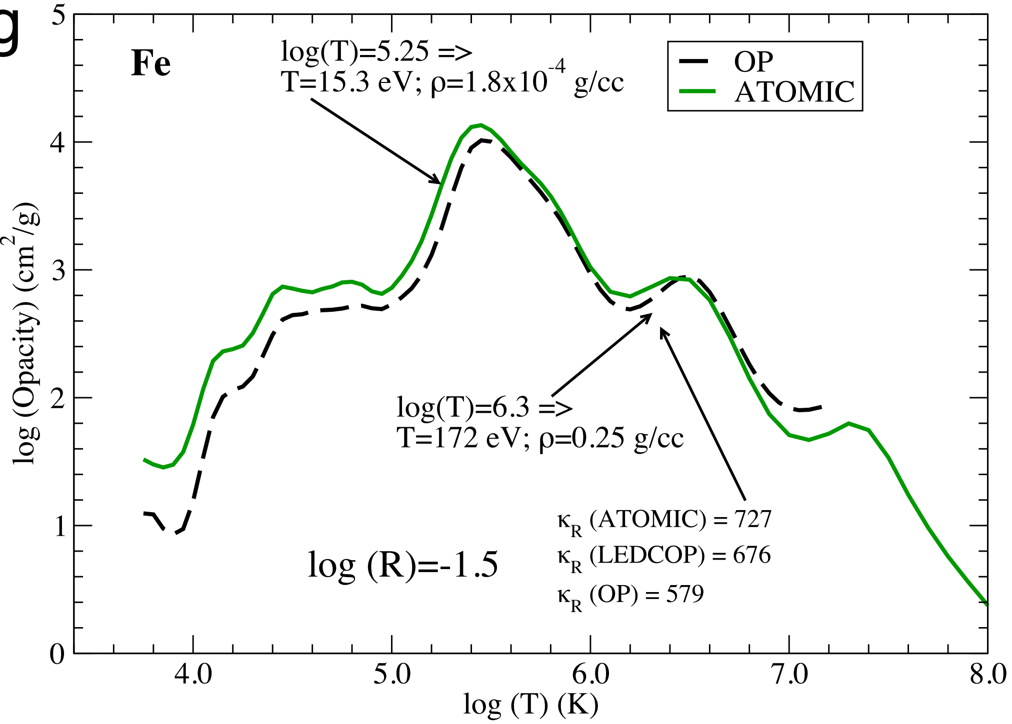


Gilles et al, High Energy Density Physics 7, 312 (2011)

Fe opacity – comparison with OP calculations

- Now examine log (R) of -1.5
- These cases are interesting as they are close to conditions at base of solar convection zone
  - T=188.5 eV; ρ=0.19 g/cm^3
  - Relevant to solar abundance problem
- We note OP again lower (~30%) at temperatures around 170 eV

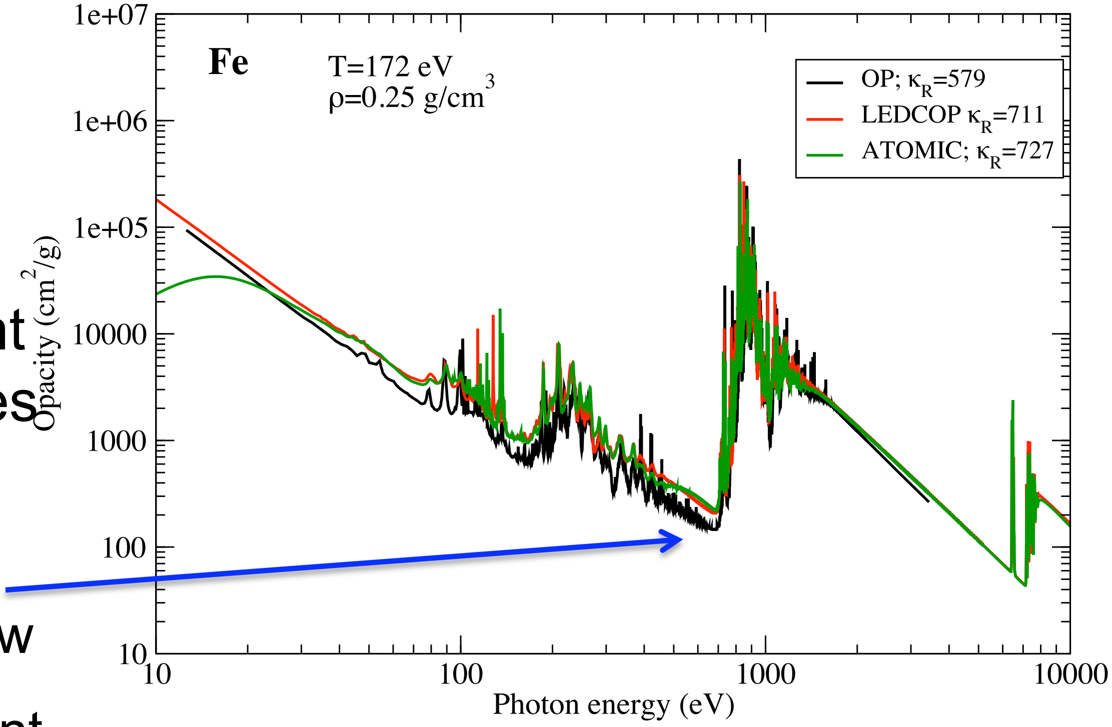
Log (R)=-1.5



Fe opacity – comparison with OP calculations

- OP calculation significantly lower than ATOMIC & LEDCOP calculations
  - Differences appear to be in both b-b and b-f contributions
- Opacities in good agreement above 700 eV but differences at lower energies
  - Most relevant region is 500-700 eV where OP is low
  - Bound-free opacity important in this range

Fe at 172 eV and ρ =0.25 g/cm^3



Conclusions & Future Work

- We have presented opacity comparisons for a selection of astrophysically important elements
- Our ATOMIC calculations will be extended over the next few years to include all elements up to Zn
  - Priority at present to complete an Fe opacity table over a wide range of temperatures and densities
- We continue to improve the physics approximations used in our opacity-generating capabilities
  - For example, we are currently testing a new free-free opacity package which should be incorporated into ATOMIC soon

Conclusions & Future Work

- We are always interested in comparisons of our opacities with independent codes or measurements
  - Please contact us!

- Finally, we plan to make our new opacity data publicly available through our website, which should be online soon

- ***http://aphysics2.lanl.gov/opacity/lanl***