THE OHIO STATE UNIVERSITY

The Fourth Fundamental Science with Pulsed Power

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Progress Report:

Astrophysical Opacities and Abundances

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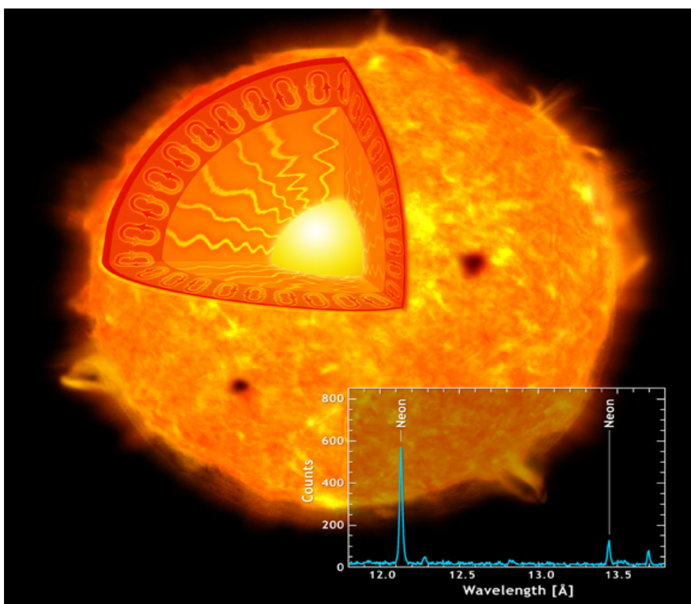
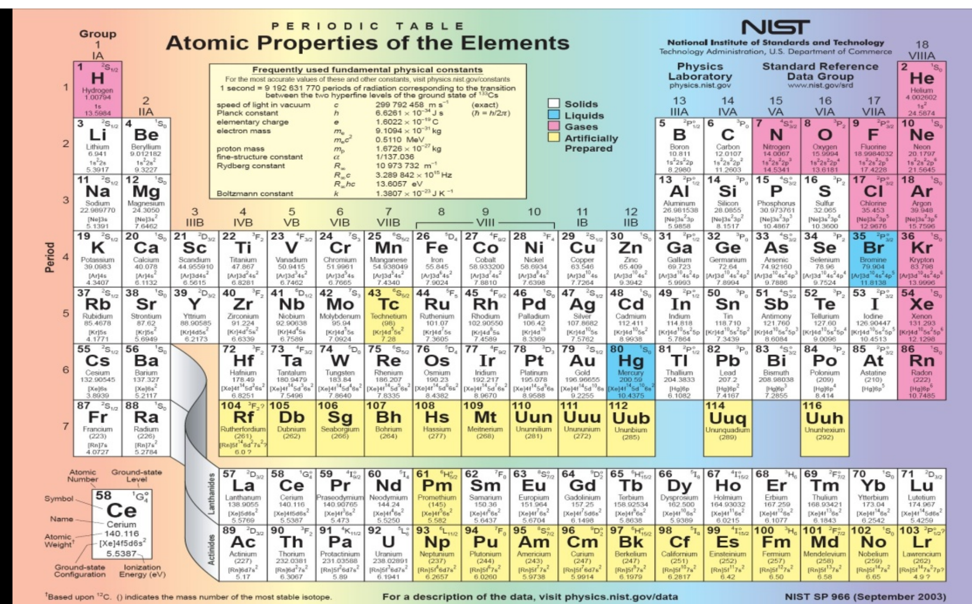




Why More Precise Opacities?

- **Fundamental Problems: Astro/Atomic/Plasma**

  → Solar Abundances: C, N, O, Ne lower by ~50%

  → Helioseismology: Solar oscillations, sound speed, boundary of conv/rad zones

  → Asteroseismology: Exo-planet host stars

  → Atomic/Plasma Physics → Resonances and lines

  - Missing physics of resonances (Nahar's talk)

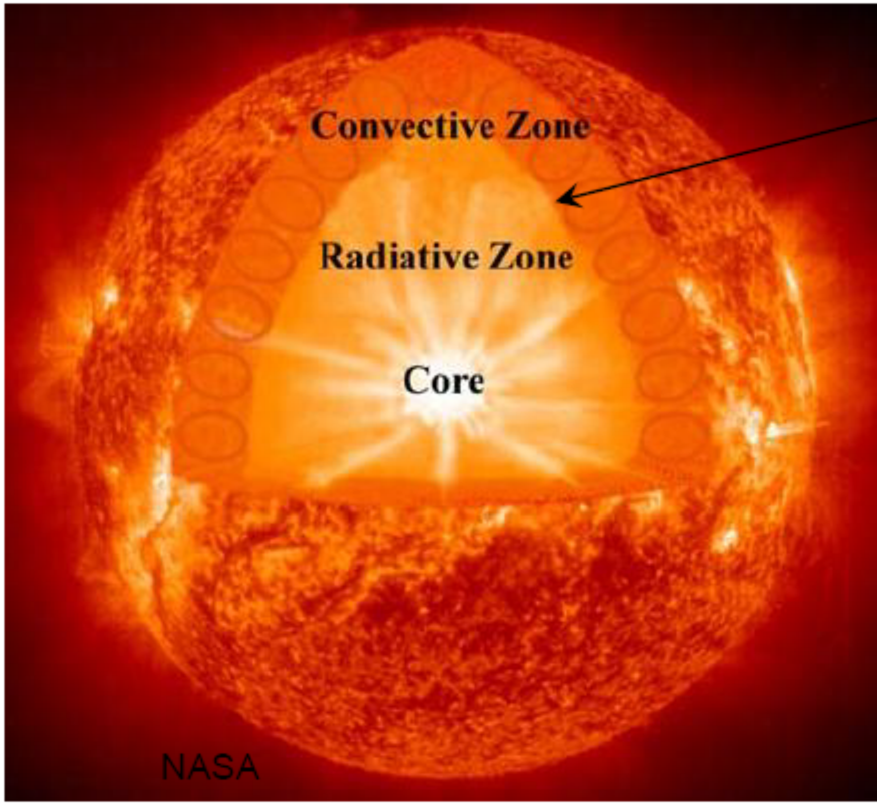
Quasi-Bound states treated as lines in opacities calculations:

Does that lead to "missing" opacity?

- Plasma broadening of autoioninzing resonances

- Equation-of-State (Regner Trampedach)

Stellar Radiation Transport and Opacities



- **Convection / Radiation Zones boundary R(BCZ) is highly sensitive to opacity:**
- **Measured → 0.713 +/- 0.001**
  Theory → 0.726 * R(Sun)
- **Helioseismology can reveal differences at < 1%**
- **KEPLER: Astroseismology solar-type stars' mass-radius (with earth-like planets)**

Opacities depend on

(i) Element abundances : Hydrogen to Nickel

(ii) Equation-of-state, (iii) Atomic physics: H – Ni

All elements, all ions, all transitions

Stellar Abudances, Opacity, and Seismology

- **What is the Sun made of ??**
- **Latest determination of solar abundances (Asplund et.al. 2009)**

→ **Spectroscopic measurements and 3D hydro NLTE models**

→ **30- 50% lower abundances of C, N, O, Ne,…..**

→ **Spectroscopy vs. stellar models (**Asplund, Pinsonneault)

- **Abundances and Helioseismology (sound speed, BCZ, etc.)**

→ **Need opacities higher ~30% (Christensen-Dalsgaard et al.2009)**

→ **Inverse relation between opacity and abundance**

From C Blancard, P. Cossé and
G. Faussurier, ApJ 745, 10, 201

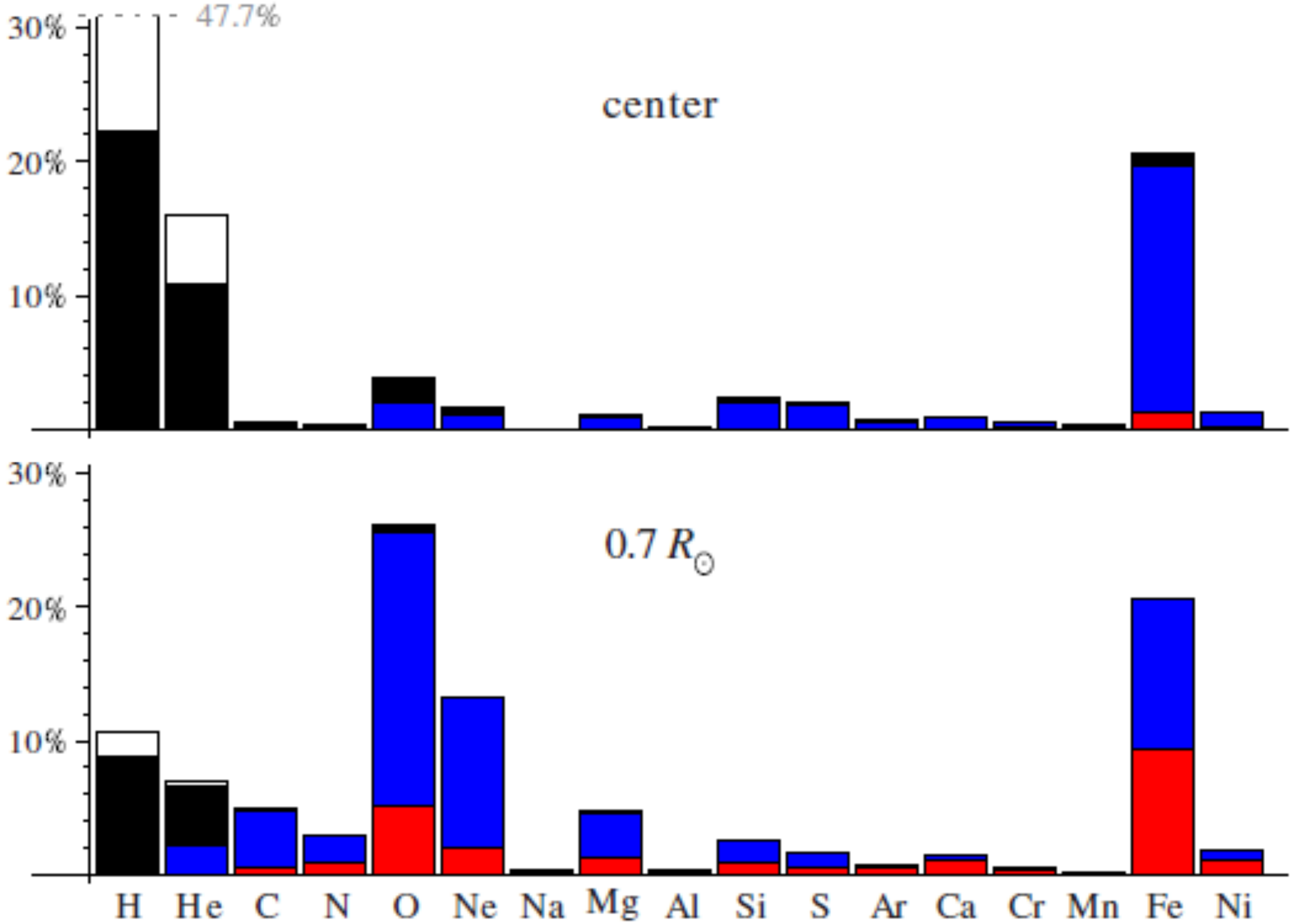


Figure 2. Relative contributions of each element to the OPAS Rosseland mean opacity of the mixture. Scattering (white), free–free (black), bound–free (blue), and bound–bound (red) contributions are indicated.

Opacity Problem

- Two independent opacity projects

-**The Opacity Project (OP)**

(**First paper**: Seaton, Yu, Mihalas, Pradhan 1994)

Electronic database Ohio Supercomputer Center: OPSERVER

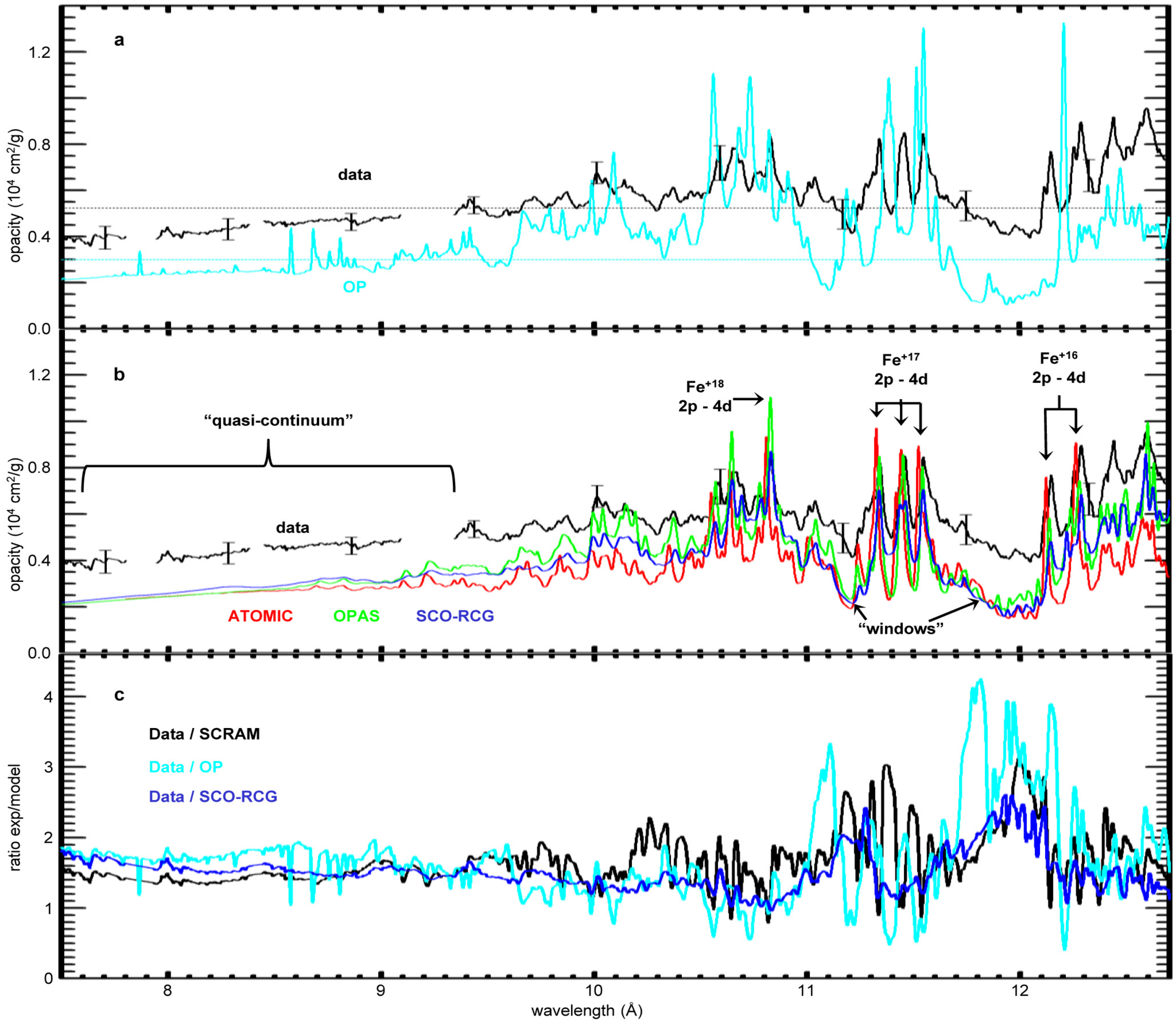
http://opacities.osc.edu (**Last paper**: Mendoza et al. 2007)

- The LLNL **OPAL Project** (Rogers and Iglesias 1994)

  - **Agree to <5% in Rosseland mean opacities**

- Other opacities codes (at **LULI, LANL, SNL** etc.) also largely agree with one another, but differences up to 25% or more
- Detailed theoretical opacity spectra differ greatly
- Main problem: Models disagree with experiment !!

Z-Opacity vs. Models (Bailey et al., Nature 2015)



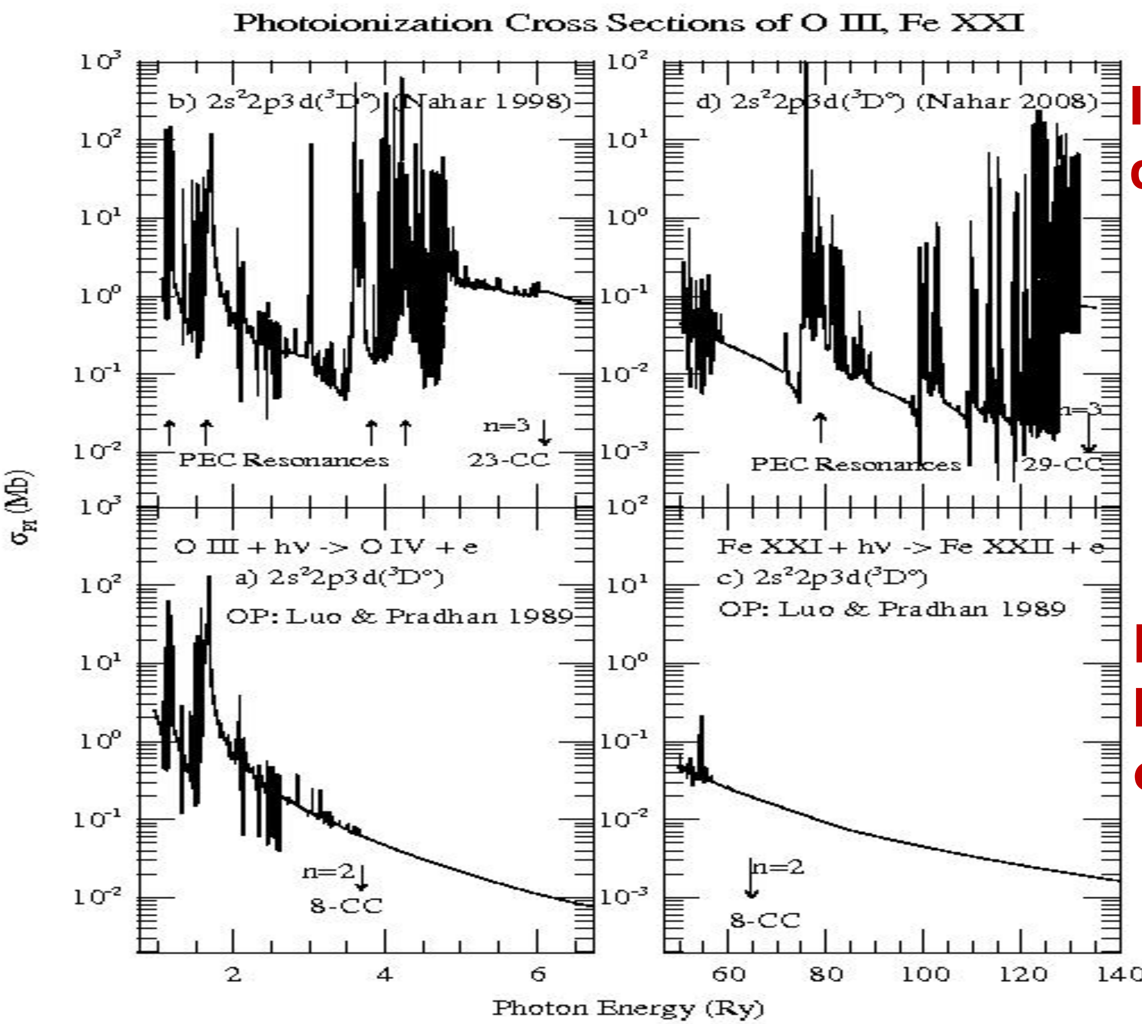
Are exisiting opacities accurate?

- Laboratory tests (Bailey et al.)
- Uncertainty in heavy element opacities

  What might be the problem ?
- All opacities codes employ the same basic atomic physics: similar atomic structure codes
- Most resonant excitations treated as lines
- Opacity Project (OP): Original Intent – Include resonances in the bound-free (Ergo: less bound-bound opacity)
- R-Matrix codes extended/modified
- But owing to computational constraints, OP calculations included only some outer-shell resonances,

  and no inner-shell excitation resonances !

Bound-free opacity:
Photoionization cross sections with Resonances



Inner-shell opacity dominated by resonances new Iron Project Relativistic R-Matrix

Earlier OP calculations Included limited outer-shell resonances

Atomic Physics of Opacities

- Much of the opacity is through **photoabsorption** by inner-shell electrons in heavy ions
- Inner-shell excitation leads to **resonances** in the **bound-free** continuum

BUT

- These excitations are currently treated as **bound-bound** transitions (lines)
- **Are the two equivalent?**

Resonances: Bound and continuum states (Coupled wavefunctions)

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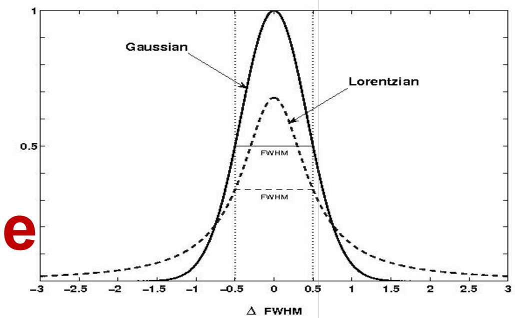
Uncoupled bound states

$$\Psi_i \rightarrow |< \Psi_j \| D \| \Psi_i >|^2 \rightarrow$$

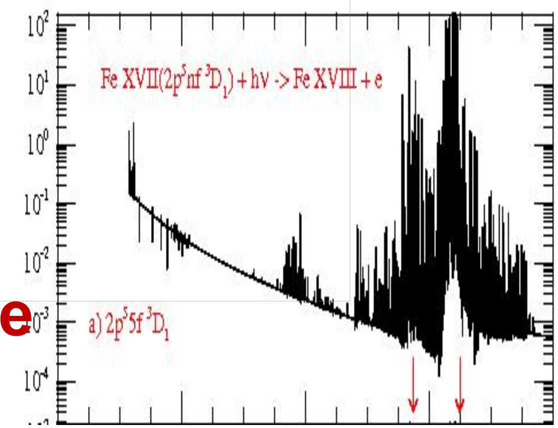


Symmetric line profile

Coupled bound and continuum states (channels)

Autoionization

$$\sum_i \Psi_i \rightarrow |< \sum_j \Psi_j \| D \| \sum_i \Psi_i >|^2 \rightarrow$$



Asymmetric resonance profile

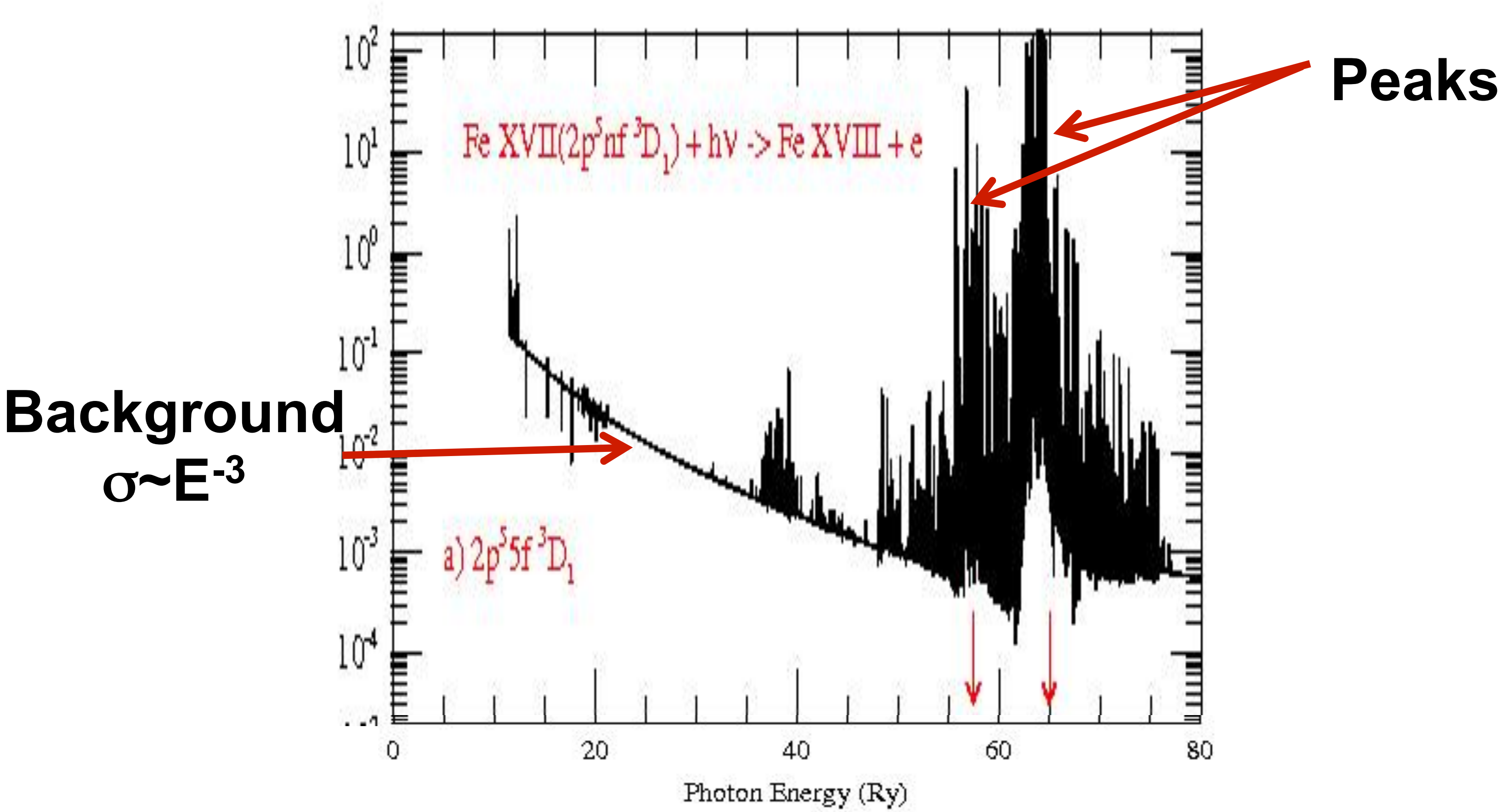
$$\sum\!\!\!\!\!\int$$

Coupled channel approximation

Consequences of Resonances in Opacities

- Owing to quantum interference in the bound-free: **channel coupling → autoionization**
- Intrinsically **asymmetric** resonance profiles
- **Giant PEC resonances** → Most of the opacity may lie in the bound-free
- Monochromatic opacities energy distribution fundamentally **different from lines**
- Resonances are broadened, smeared and wiped out **more rapidly** than lines
- **Continuum lowering** of opacity below all thresholds in each ion

Giant Photoexcitation-of-Core (PEC) Resonances In Photoionization Cross Sections



Distribution of absorption oscillator strength varies asymmetrically by orders of magnitude across the PEC resonance profile(s)

Plasma Broadening of Autoionizing Resonances

- No analytic theory or computational method
- R-matrix photoionization cross sections include autoionization broadening *ab initio*
- No treatment available for

  - Electron impact
  - Stark
  - Doppler (thermal)

  (Lorentzian and Gaussian profiles)
- New algorithm for electron impact broadening

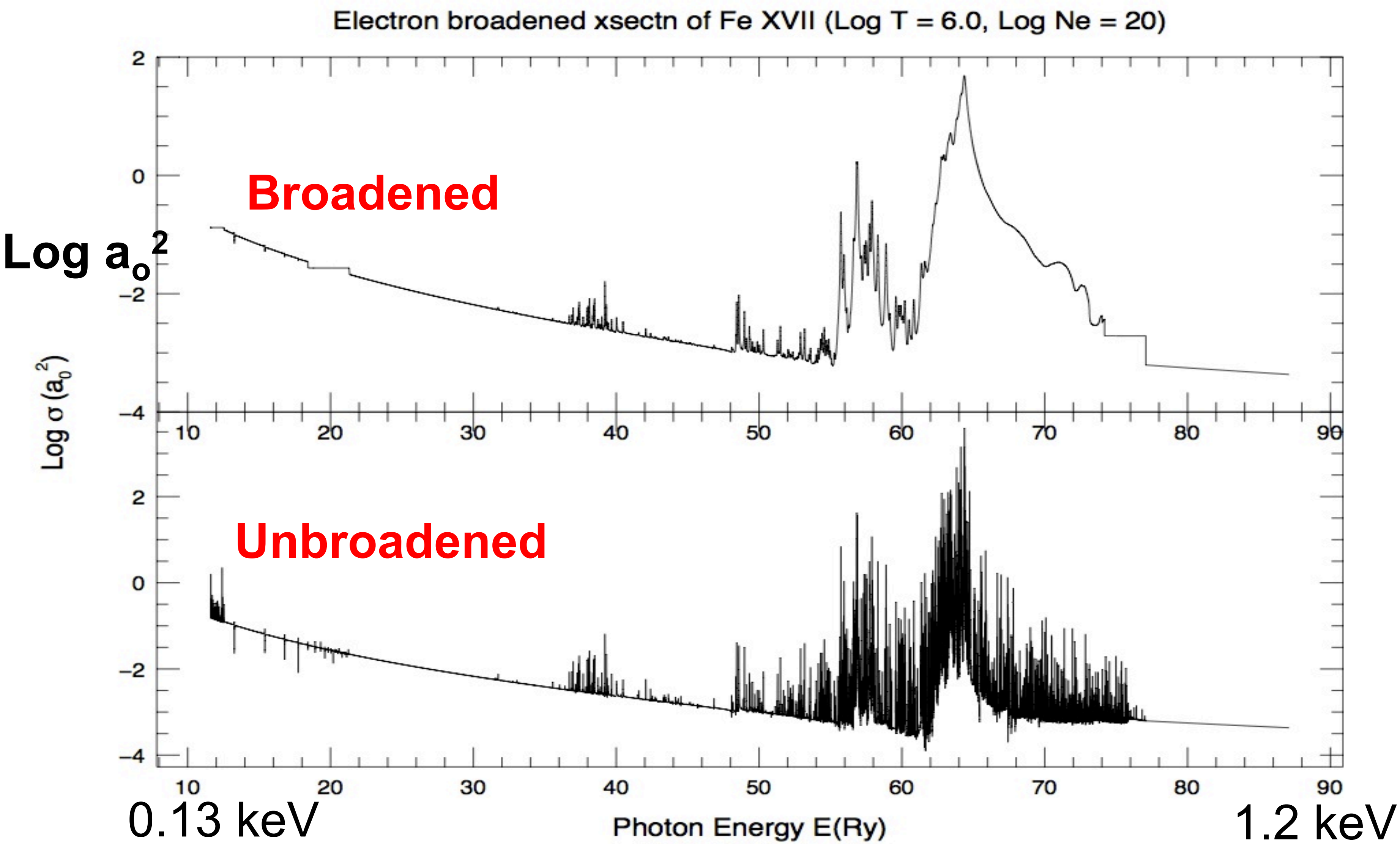
Resonance Broadening Processes

- **Autoionization → R-Matrix (*ab initio*)**
- **T, Ne dependent processes:**
- **Electron impact → Convolution (Lorentzian)**
- **Stark → Simplified (Dimitrijevic & Konjevic)**
- **Thermal → Doppler (Gaussian)**
- **Debye → Length vs. ν**

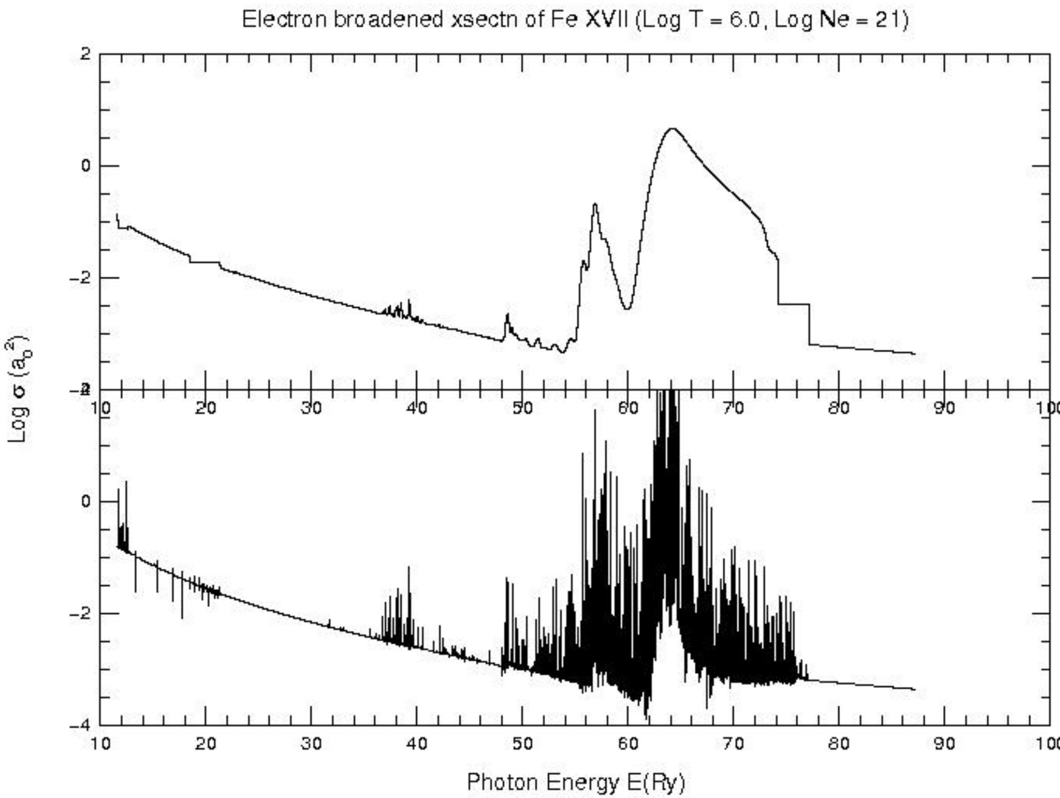
  - Inter-particle distance vs. effective q.n. of resonance

  - $T = 10^6$ K, $Ne = 10^{23}$ /cm^3 → $R_D = 4.13\ a_o$, $\nu = 8.6$

Electron Impact Broadening of Autoionizing Resonances
Log T = 6.0, Log Ne = 20.0



Electron Impact Resonance Broadening
Log T = 6.0, Log Ne = 21.0



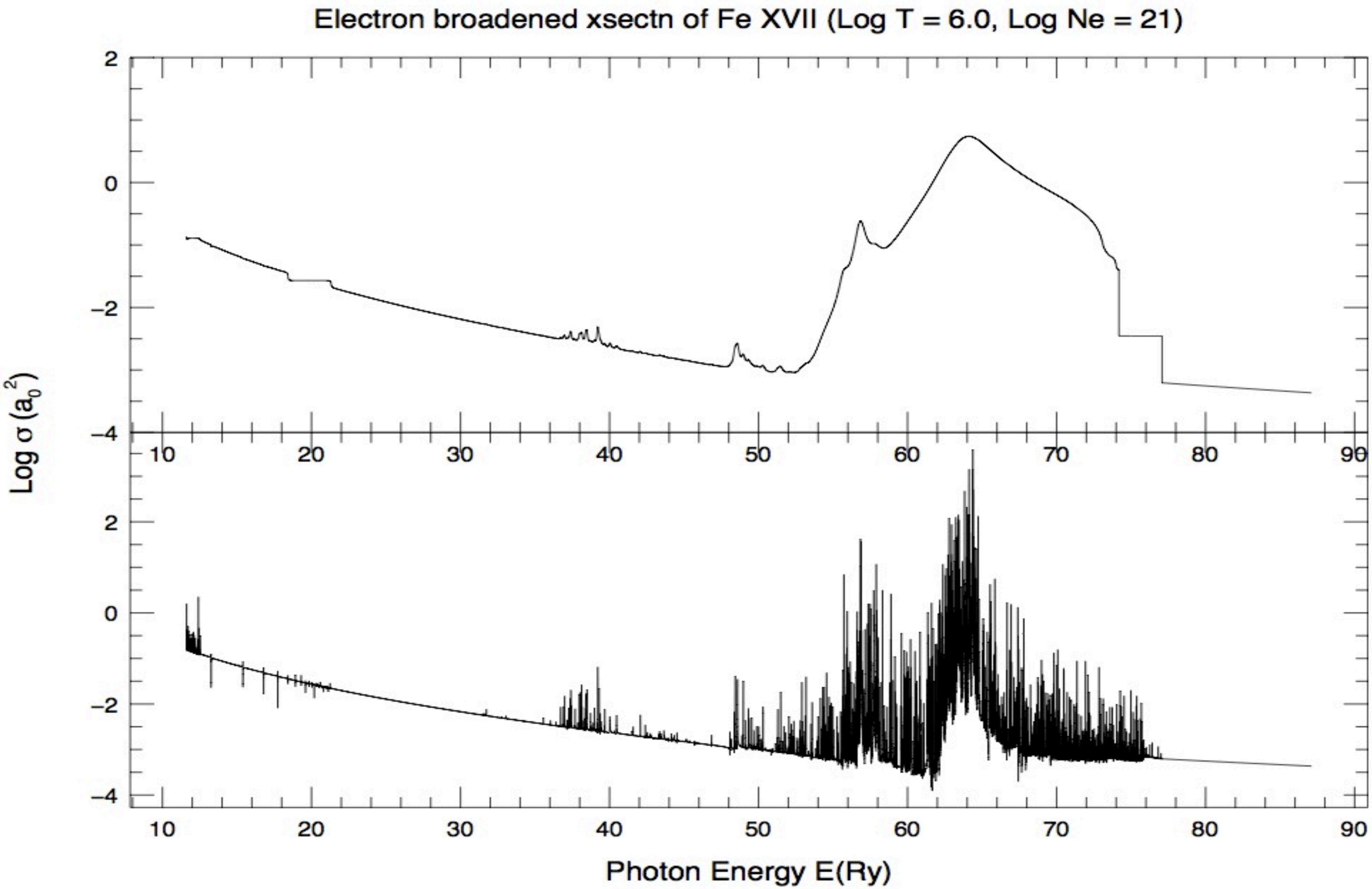
Broadened

Unbroadened

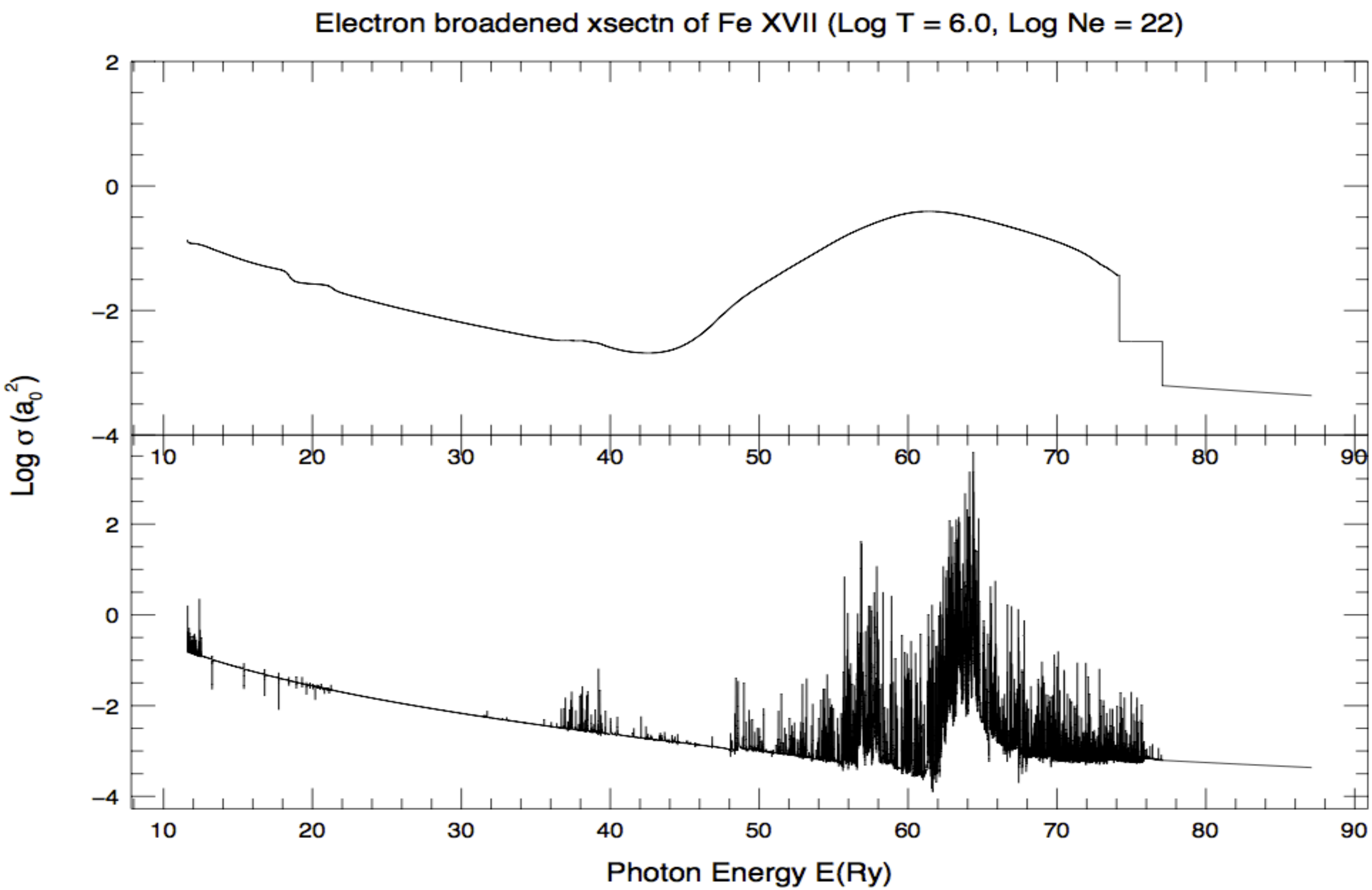
Log (a_o^2)

Photon Energy (keV)

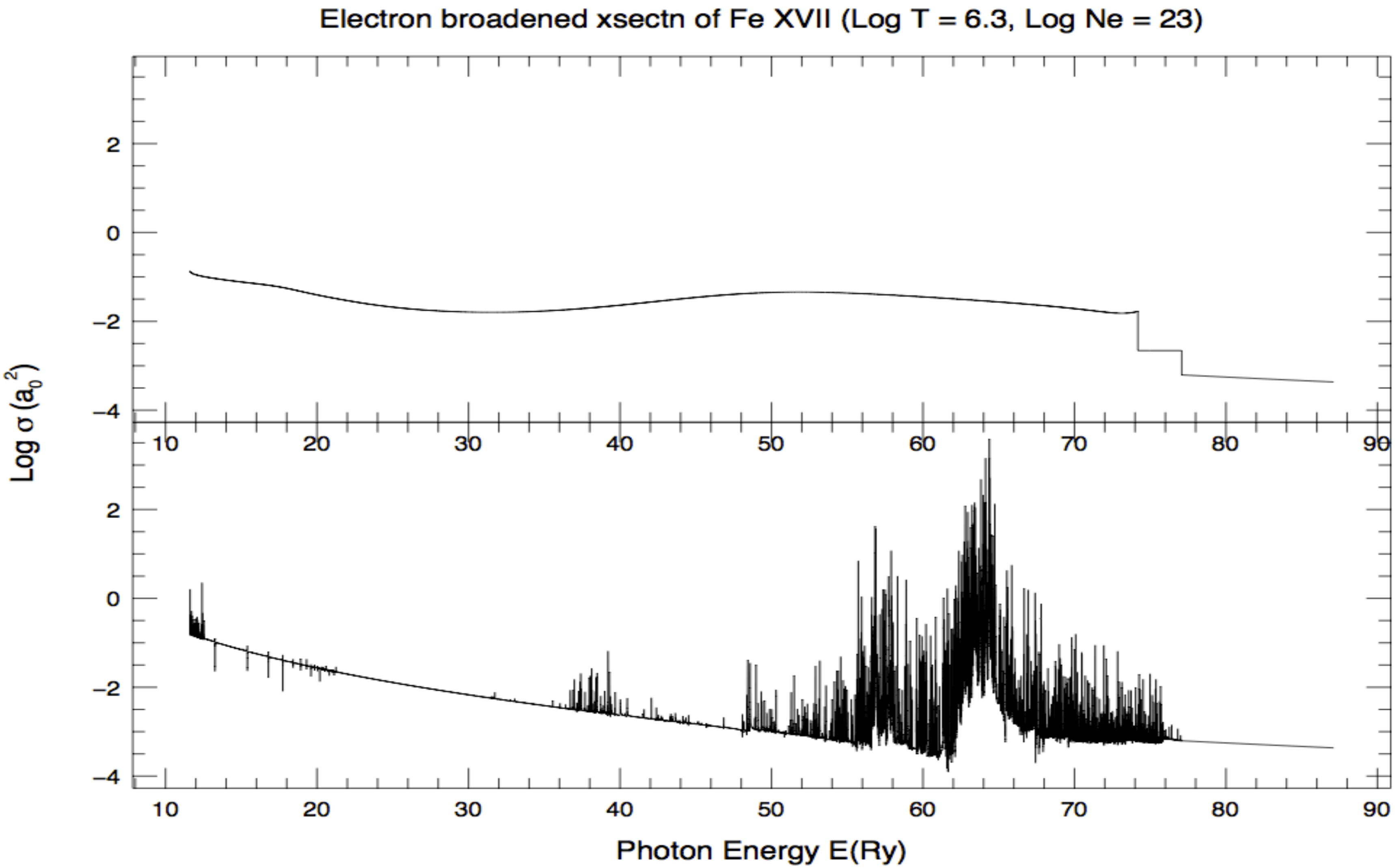
Electron Impact Broadening of Autoionizing Resonances
Log T = 6.3, Log Ne = 22.0



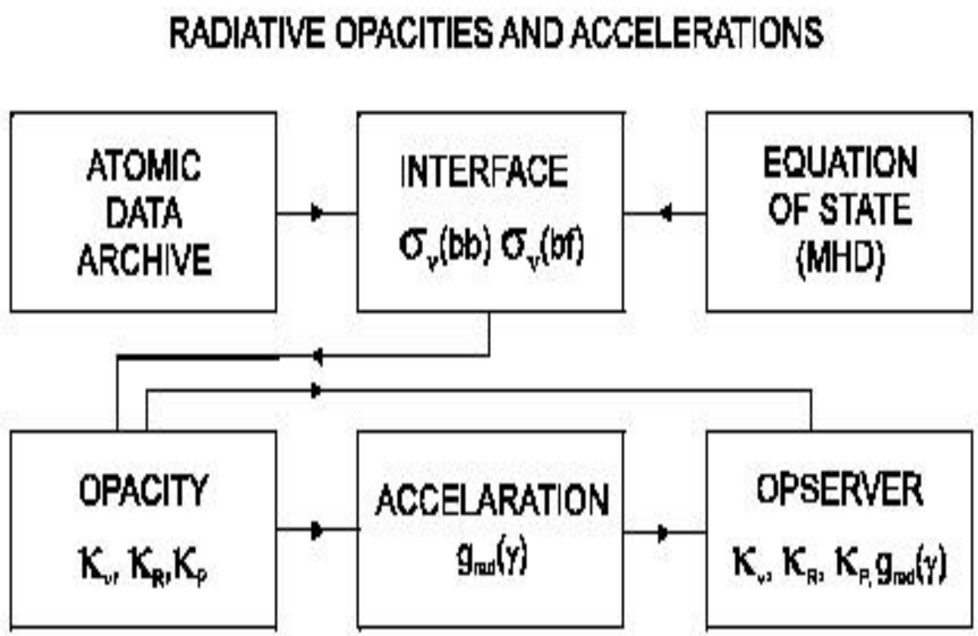
Electron Impact Broadening of Autoionizing Resonances
Log T = 6.0, Log Ne = 22.0



Electron Impact Broadening of Autoionizing Resonances
Log T = 6.3, Log Ne = 23.0



High-Precision Opacities (HIPOP) Codes and Atomic Data



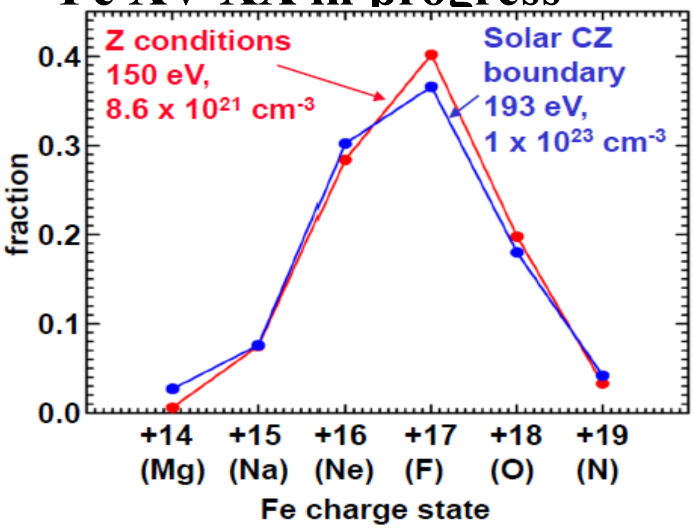
ISSUES

- **Lines and resonances**
- **Large-scale atomic computations**
- **Resonance broadening (vs. line broadening)**
- **Equation-of-state at high-temperature-density**

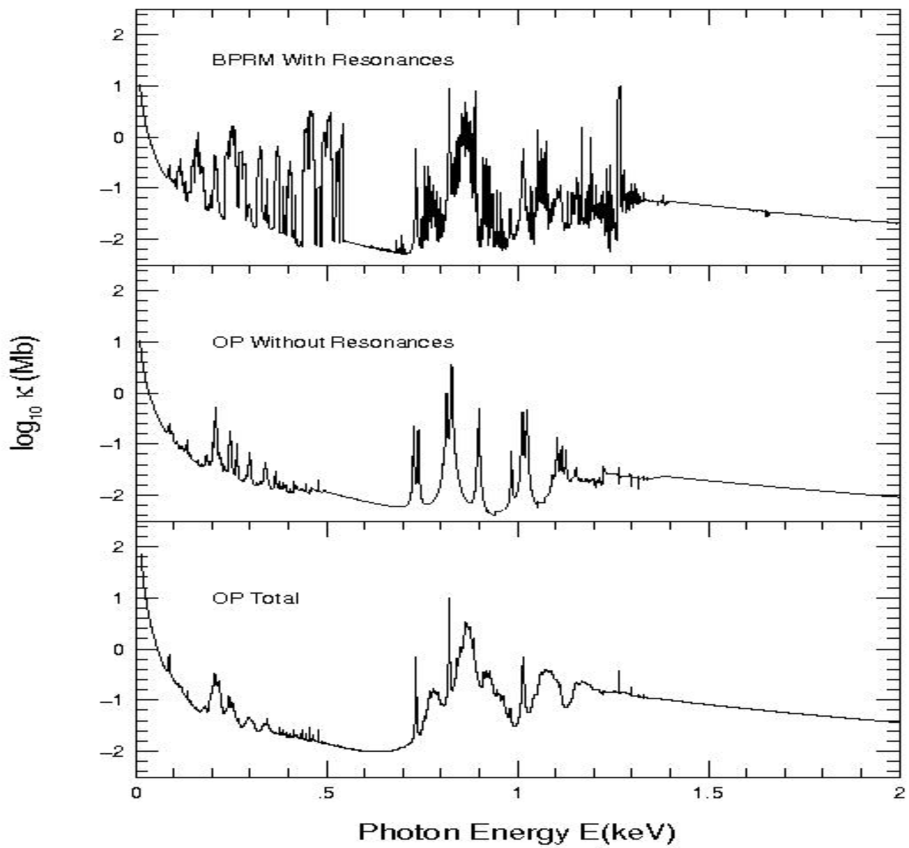
Breit-Pauli R-Matrix Opacities

(with fine structure resonances, Nahar et al. 2011)

- Monochromatic opacity
  Fe XVII, 2.25 MK, 10^{23} cc
- Rosseland Mean with more extensive resonances is 12% higher
- BCZ: Iron opacity
  Fe XV-XX in progress



Ion Fractions



Monochromatic Opacity

Opacities Work Status

- Extended OP opacity tables for astro elements
- New Opacity Project (OP) High-Precision codes (HIPOP)
- Iron Opacity Project: New Iron atomic data and

→ Relativistic Breit-Pauli R-Matrix (BPRM)

→ Ab initio treatment of fine structure

→ Autoionization resonance profiles delineated

→ Resonance broadening modeling (not Voigt line profiles)

→ Order of magnitude more computational effort than OP

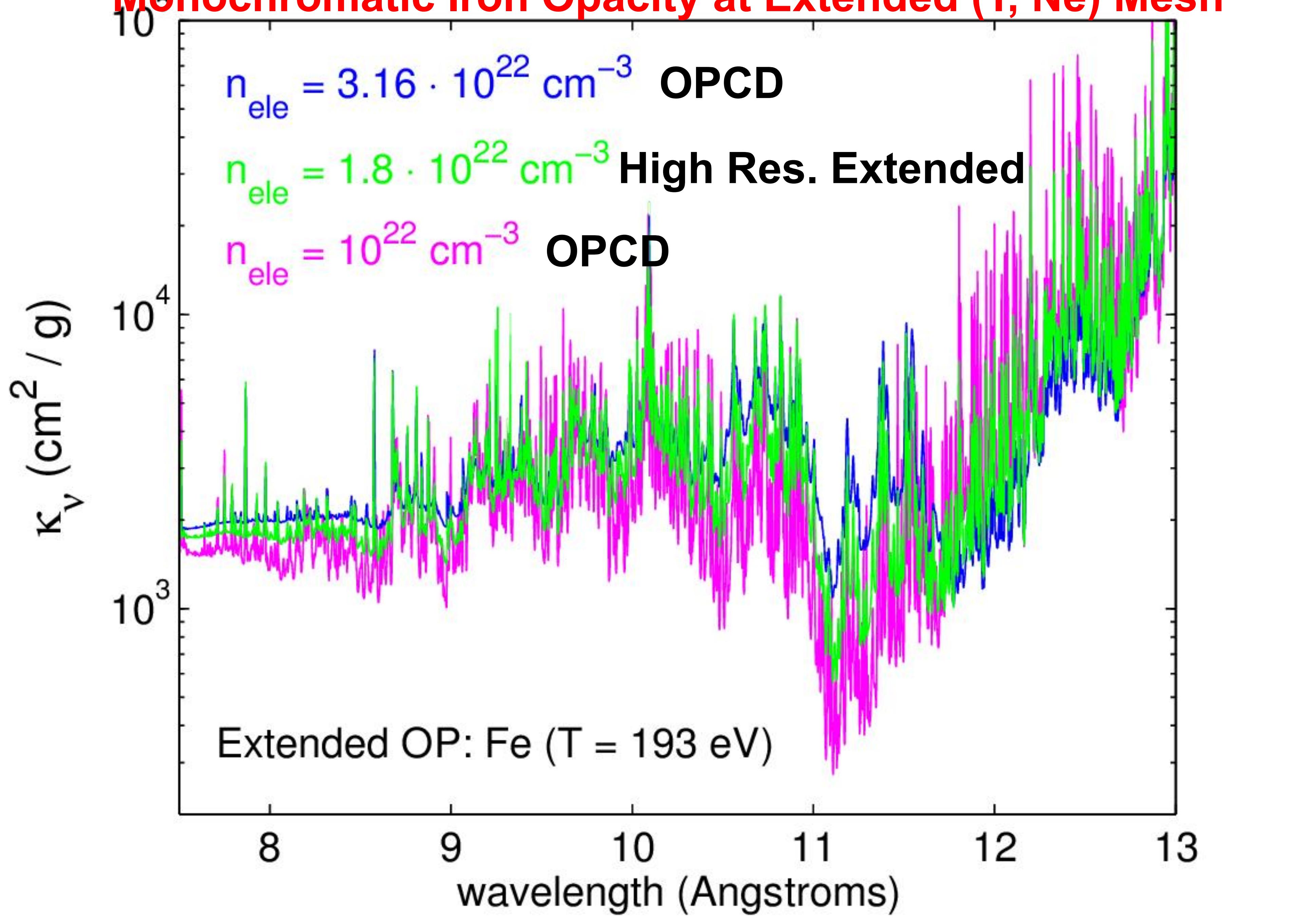
→ Finer (T,Ne) and 10^5 photon frequencies (OP, OPAL: 10^4)

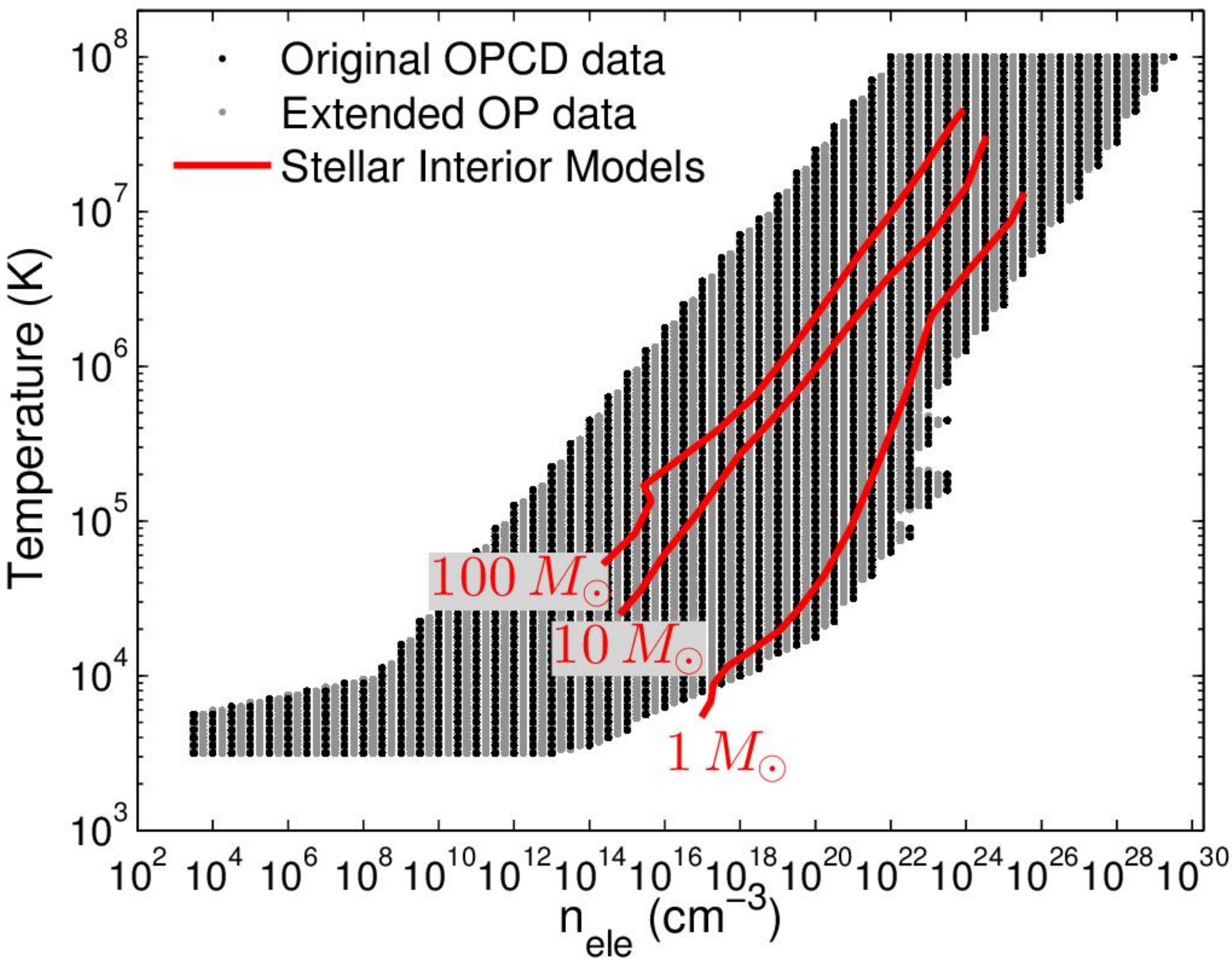
- Publications

Extended OP Tables: Astro Elements

1 H																	2 He
3	4											5	6 C	7 N	8 O	9	10 Ne
11 Na	12 Mg											13 Al	14 Si	15	16 S	17	18 Ar
19	20 Ca	21	22	23	24 Cr	25 Mn	26 Fe	27	28 Ni	29	30	31	32	33	34	35	36
37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54
55	56	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86
87	88	103	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118
		57	58	59	60	61	62	63	64	65	66	67	68	69	70		
		89	90	91	92	93	94	95	96	97	98	99	100	101	102		

Monochromatic Iron Opacity at Extended (T, Ne) Mesh





Original OPCD data
Extended OP data
Stellar Interior Models
100 $M_\odot$
10 $M_\odot$
1 $M_\odot$
Temperature (K)
n_{ele} (cm^{-3})
10^3
10^4
10^5
10^6
10^7
10^8
10^2
10^4
10^6
10^8
10^{10}
10^{12}
10^{14}
10^{16}
10^{18}
10^{20}
10^{22}
10^{24}
10^{26}
10^{28}
10^{30}

NIF – Implosion Plasma Opacity

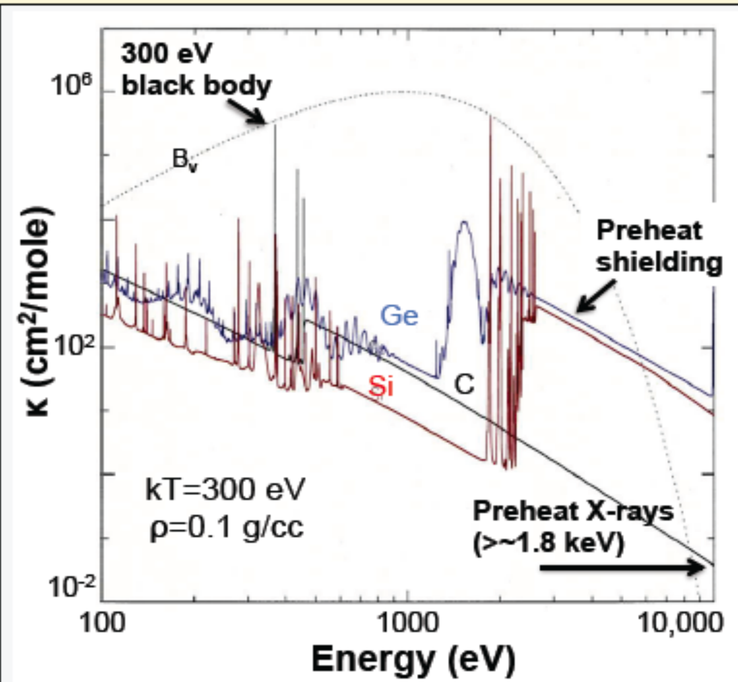
LLNL-PRES-557971

NIC

Optimizing implosion performance requires accurate opacities and emissivities (Si, C, Ge, Au, U)

- **Ablator opacity (C, Si, Ge) is important for tuning ablation performance, mix and preheat.**
- **Both NLTE and LTE opacities have been improved recently (**H. Scott, S. Hansen, HEDP 6, (2010). B.G. Wilson, et al *PRE* **76**, 032103 (2007).) **but still DCA differs from more sophisticated models and EOS and Opacity are not self consistent.**
- **Important to consider convergence effects in photon binning and material zoning while considering effects of Opacity** (Hill and Rose).

C, Ge and Si opacity at .1g/cc and 300 eV



Conclusion and Work in Progress

- **Iron Opacity Project: New *ab initio* calculations**

  -- Missing resonant opacity (Nahar's talk)

  -- Resonance broadening vs. line broadening

- **Compare with Z-pinch and other lab sources**
- **Higher-Z elements and future experiments**