

The Fourth Fundamental Science with Pulsed Power

Albuquerque NM, July 20-22, 2015

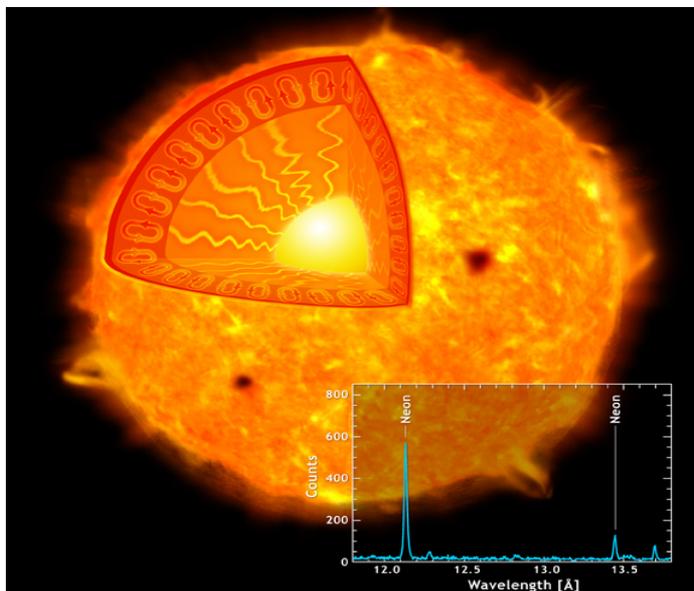
Progress Report:

Astrophysical Opacities and Abundances

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Franck Delahaye (Meudon), Jim Bailey (SNL)



PERIODIC TABLE
Atomic Properties of the Elements

NIST
National Institute of Standards and Technology
Technology Administration, U.S. Department of Commerce

Frequently used fundamental physical constants
For the most accurate values of these and other constants, visit physics.nist.gov/constants
1 second = 9 192 631 770 periods of radiation corresponding to the transition between the two hyperfine levels of the ground state of ¹³³Cs
speed of light in vacuum $c = 299\,792\,458\text{ m s}^{-1}$ (exact)
Planck constant $h = 6.626\,070\,15 \times 10^{-34}\text{ J s}$ (exact)
elementary charge $e = 1.602\,176\,634 \times 10^{-19}\text{ C}$ (exact) ($h = h/2\pi$)
electron mass $m_e = 9.109\,383\,56 \times 10^{-31}\text{ kg}$
proton mass $m_p = 1.672\,621\,923 \times 10^{-27}\text{ kg}$
fine-structure constant $\alpha = 1/137.035\,999\,074$
Rydberg constant $R_\infty = 10\,973\,731.762\text{ m}^{-1}$
Boltzmann constant $k_B = 1.380\,658\,367 \times 10^{-23}\text{ J K}^{-1}$

Physics Laboratory
Standard Reference Data Group
physics.nist.gov
www.nist.gov/srd

Legend:
Solids (blue)
Liquids (red)
Gases (green)
Artificially Prepared (yellow)

1 1 H Hydrogen (1.00784)	2 4 He Helium (4.00260)	Frequently used fundamental physical constants																18 4 He Helium (4.00260)																																																																																		
3 3 Li Lithium (6.941)	4 9 Be Beryllium (9.01218)	5 10 B Boron (10.811)	6 12 C Carbon (12.011)	7 14 N Nitrogen (14.006)	8 16 O Oxygen (15.999)	9 18 F Fluorine (18.998)	10 19 Ne Neon (19.992)	11 23 Na Sodium (22.98977)	12 24 Mg Magnesium (24.304)	13 27 Al Aluminum (26.981538)	14 28 Si Silicon (28.08558)	15 29 P Phosphorus (30.973762)	16 32 S Sulfur (32.06)	17 35.5 Cl Chlorine (35.453)	18 39.9 Ar Argon (39.948)	19 39 K Potassium (39.0983)	20 40 Ca Calcium (40.078)	21 44 Sc Scandium (44.95591)	22 48 Ti Titanium (47.88)	23 51 V Vanadium (50.9415)	24 52 Cr Chromium (51.9961)	25 55 Mn Manganese (54.93804)	26 56 Fe Iron (55.845)	27 58.9 Co Cobalt (58.9332)	28 58.9 Ni Nickel (58.9332)	29 63.5 Cu Copper (63.546)	30 65.4 Zn Zinc (65.38)	31 69.7 Ga Gallium (69.723)	32 72.6 Ge Germanium (72.64)	33 74.9 As Arsenic (74.9216)	34 78.9 Se Selenium (78.96)	35 79 Br Bromine (79.904)	36 83.8 Kr Krypton (83.80)	37 85.4 Rb Rubidium (85.468)	38 87.6 Sr Strontium (87.62)	39 88.9 Y Yttrium (88.9058)	40 91.2 Zr Zirconium (91.224)	41 92.9 Nb Niobium (92.906)	42 95.9 Mo Molybdenum (95.94)	43 95.9 Tc Technetium (95.908)	44 101.1 Ru Ruthenium (101.07)	45 101.1 Rh Rhodium (101.07)	46 106.4 Pd Palladium (106.42)	47 106.4 Ag Silver (107.8652)	48 107.8 Cd Cadmium (112.411)	49 112.4 In Indium (114.818)	50 114.8 Sn Tin (117.90)	51 118.7 Sb Antimony (121.757)	52 127.6 Te Tellurium (127.60)	53 127.6 I Iodine (126.905)	54 131.3 Xe Xenon (131.29)	55 132.9 Ba Barium (137.327)	56 137.3 La Lanthanum (138.905)	57 138.9 Ce Cerium (140.118)	58 140.1 Pr Praseodymium (140.907)	59 140.9 Nd Neodymium (144.24)	60 144.2 Pm Promethium (144.9126)	61 144.9 Sm Samarium (150.36)	62 150.4 Eu Europium (151.964)	63 151.9 Gd Gadolinium (157.25)	64 157.2 Tb Terbium (158.92534)	65 158.9 Dy Dysprosium (162.50085)	66 162.5 Ho Holmium (164.93032)	67 164.9 Er Erbium (167.259)	68 167.3 Tm Thulium (168.93421)	69 168.9 Yb Ytterbium (173.054)	70 173.1 Lu Lutetium (174.967)	71 174.9 Hf Hafnium (178.49)	72 178.5 Ta Tantalum (180.94788)	73 180.9 W Tungsten (183.84)	74 183.8 Re Rhenium (186.207)	75 186.2 Os Osmium (192.227)	76 192.2 Ir Iridium (192.222)	77 197.0 Pt Platinum (195.084)	78 197.0 Au Gold (196.966569)	79 197.0 Hg Mercury (200.59)	80 200.6 Tl Thallium (204.3833)	81 204.4 Pb Lead (207.2)	82 207.2 Bi Bismuth (208.9804)	83 208.9 Po Polonium (209)	84 209 At Astatine (210)	85 210 Rn Radon (222)	86 222 Uuq Ununquadium (223)	87 223 Fr Francium (223)	88 226 Ra Radium (226)	89 227 Ac Actinium (227)	90 232 Th Thorium (232.0377)	91 232.0 Pa Protactinium (231.03626)	92 238 U Uranium (238.02891)	93 238 U Np Neptunium (237.048173)	94 237.0 Pu Plutonium (239.0521634)	95 239.0 Am Americium (241.063288)	96 241.0 Cm Curium (247)	97 247 Bk Berkelium (247)	98 247 Cf Californium (251)	99 251 Es Einsteinium (252)	100 252 Fm Fermium (257)	101 257 Md Mendelevium (258)	102 258 No Nobelium (259)	103 259 Lr Lawrencium (260)

Atomic Number

Ground-state Level

Symbol

Name

Atomic Weight

Ground-state Configuration

Transition Energy (eV)

Antineutrinos

Antineutrinos

Based upon ¹²C. () indicates the mass number of the most stable isotope.

For a description of the data, visit physics.nist.gov/data

NIST SP 986 (September 2003)

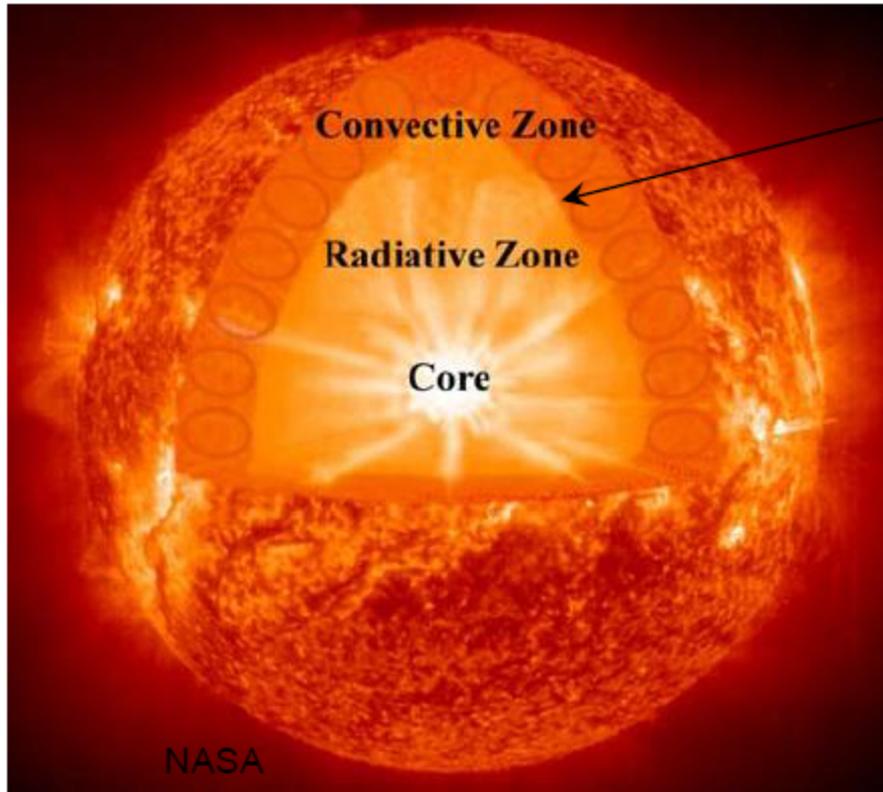
Why More Precise Opacities?

- **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 autoionizing resonances**
- **Equation-of-State (Regner Trampedach)**

Stellar Radiation Transport and Opacities



- **Convection / Radiation Zones** boundary $R(\text{BCZ})$ is highly sensitive to opacity:
- Measured $\rightarrow 0.713 \pm 0.001$
Theory $\rightarrow 0.726 * R(\text{Sun})$
- **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 Abundances, 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*

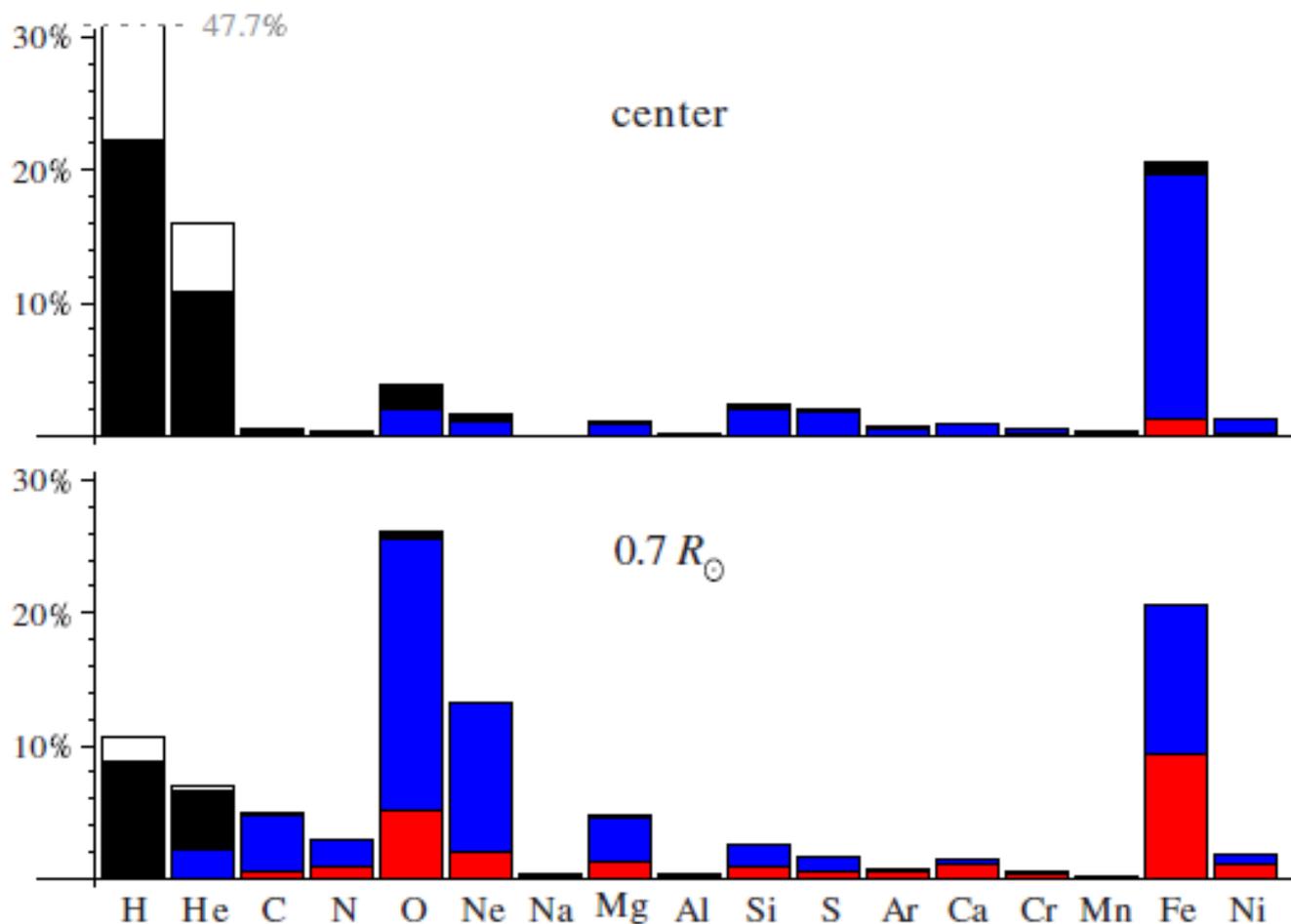


Figure 2. Relative contributions of each element to the OPAS Rosseland mean opacity of the mixture. Scattering (white), free–free (black), bound–free (blue), and bound–bound (red) contributions are indicated.

Opacity Problem

- Two independent opacity projects

-The Opacity Project (OP)

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

Electronic database Ohio Supercomputer Center: OPSERVER

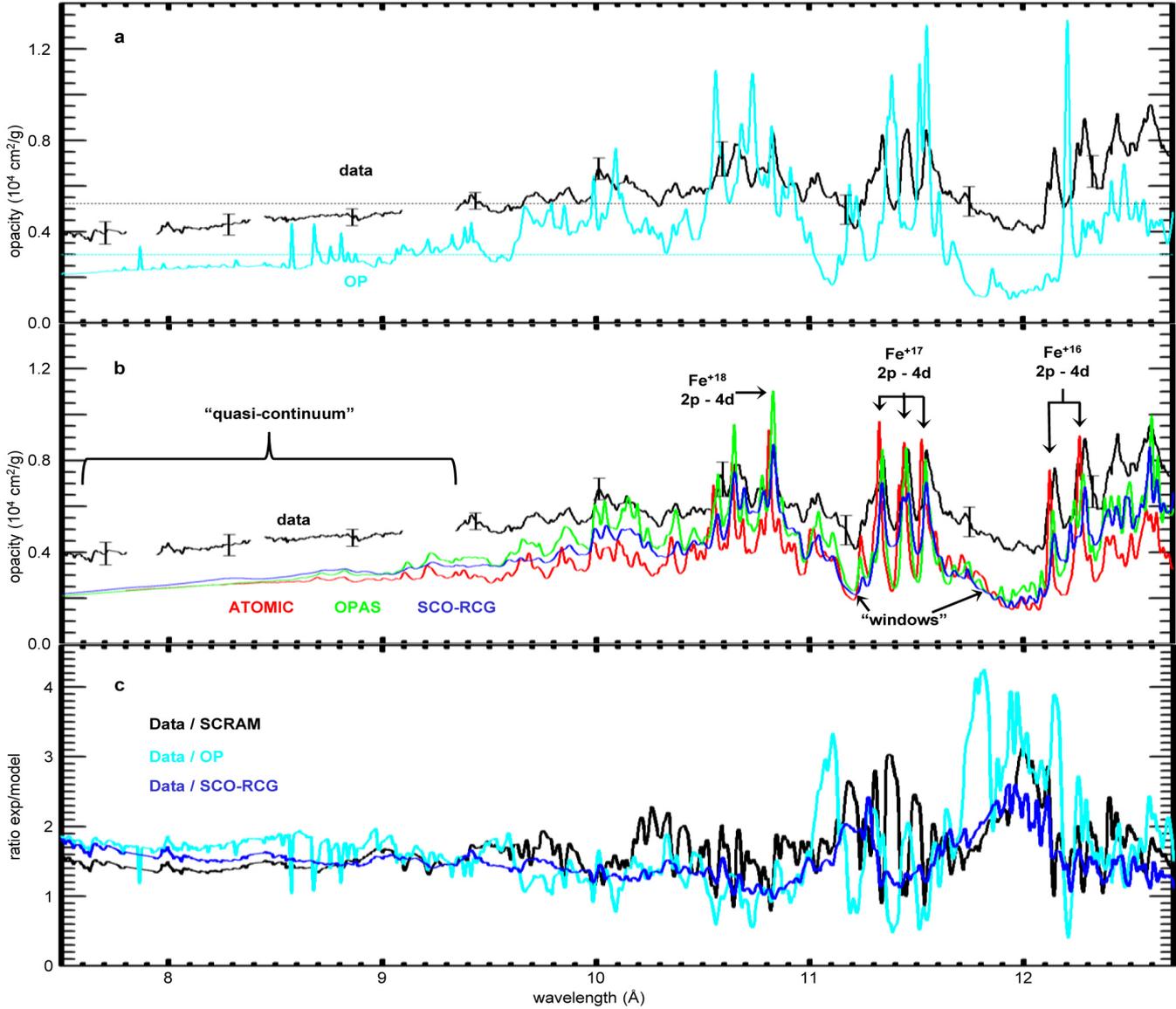
<http://opacities.osc.edu> (Last paper: Mendoza et al. 2007)

- 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 !!

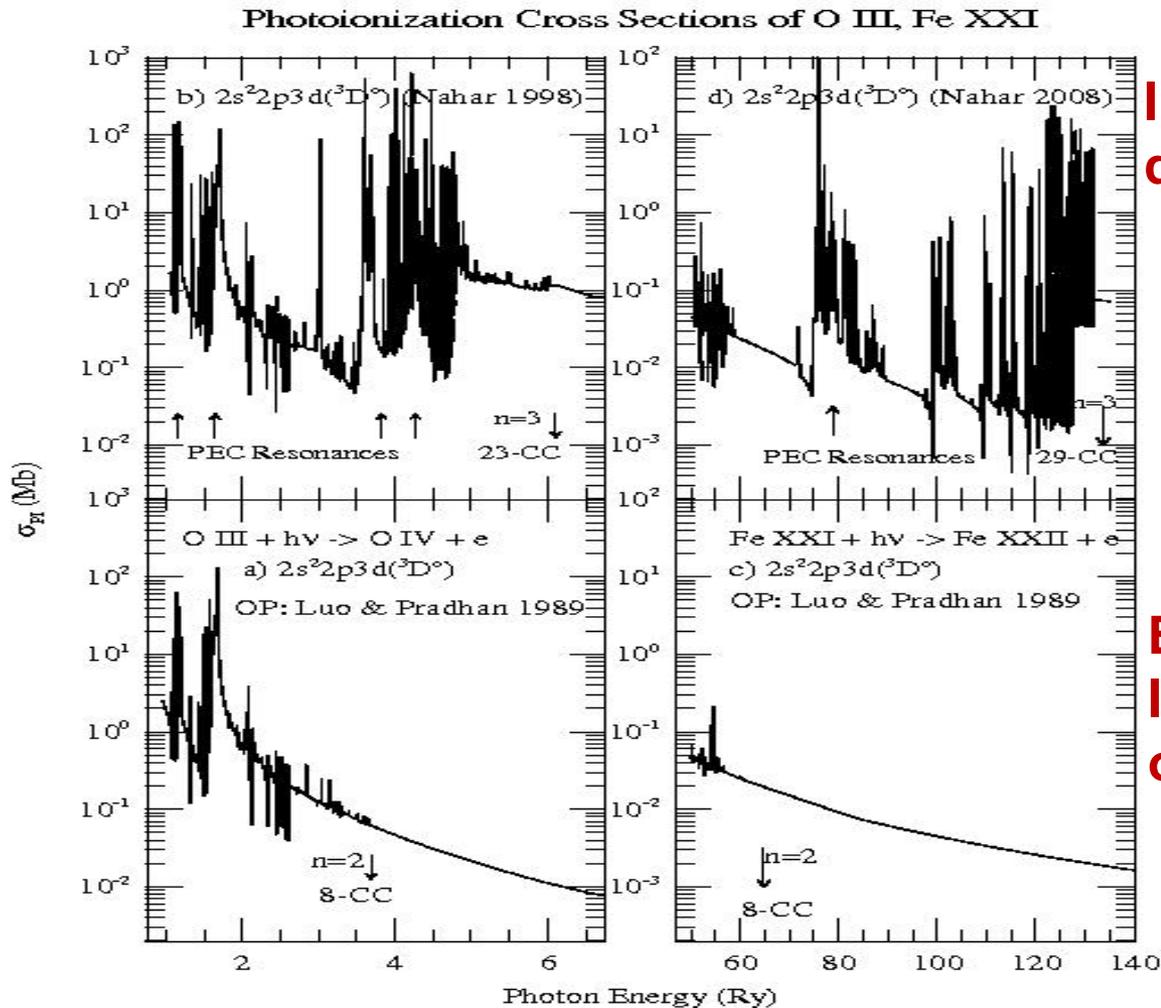
Z-Opacity vs. Models (Bailey et al., Nature 2015)



Are existing 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

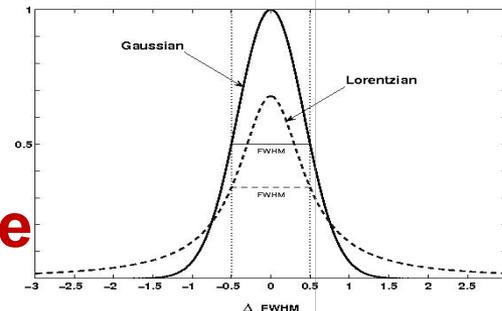
- These excitations are currently treated as **bound-bound** transitions (lines)
- **Are the two equivalent?**

Resonances: Bound and continuum states (Coupled wavefunctions)

Uncoupled bound states

$$\Psi_i \rightarrow \left| \langle \Psi_j \parallel D \parallel \Psi_i \rangle \right|^2 \rightarrow$$

Symmetric line profile



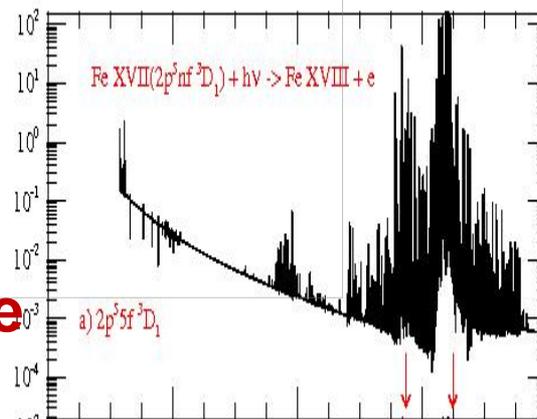
Coupled bound and continuum states (channels)

Autoionization

$$\sum_i \Psi_i \rightarrow \left| \langle \sum_j \Psi_j \parallel D \parallel \sum_i \Psi_i \rangle \right|^2 \rightarrow$$

Asymmetric resonance profile

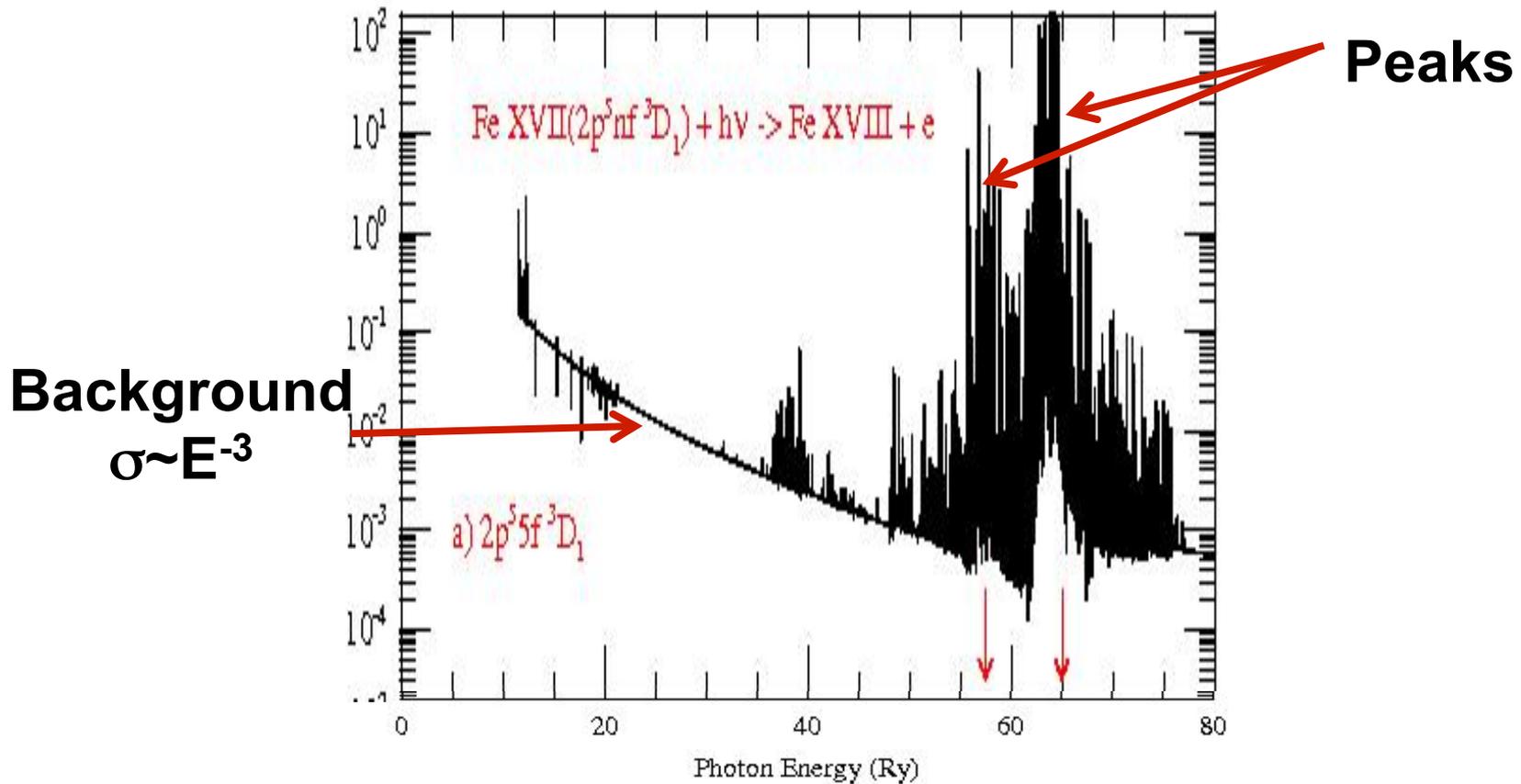
Coupled channel approximation



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

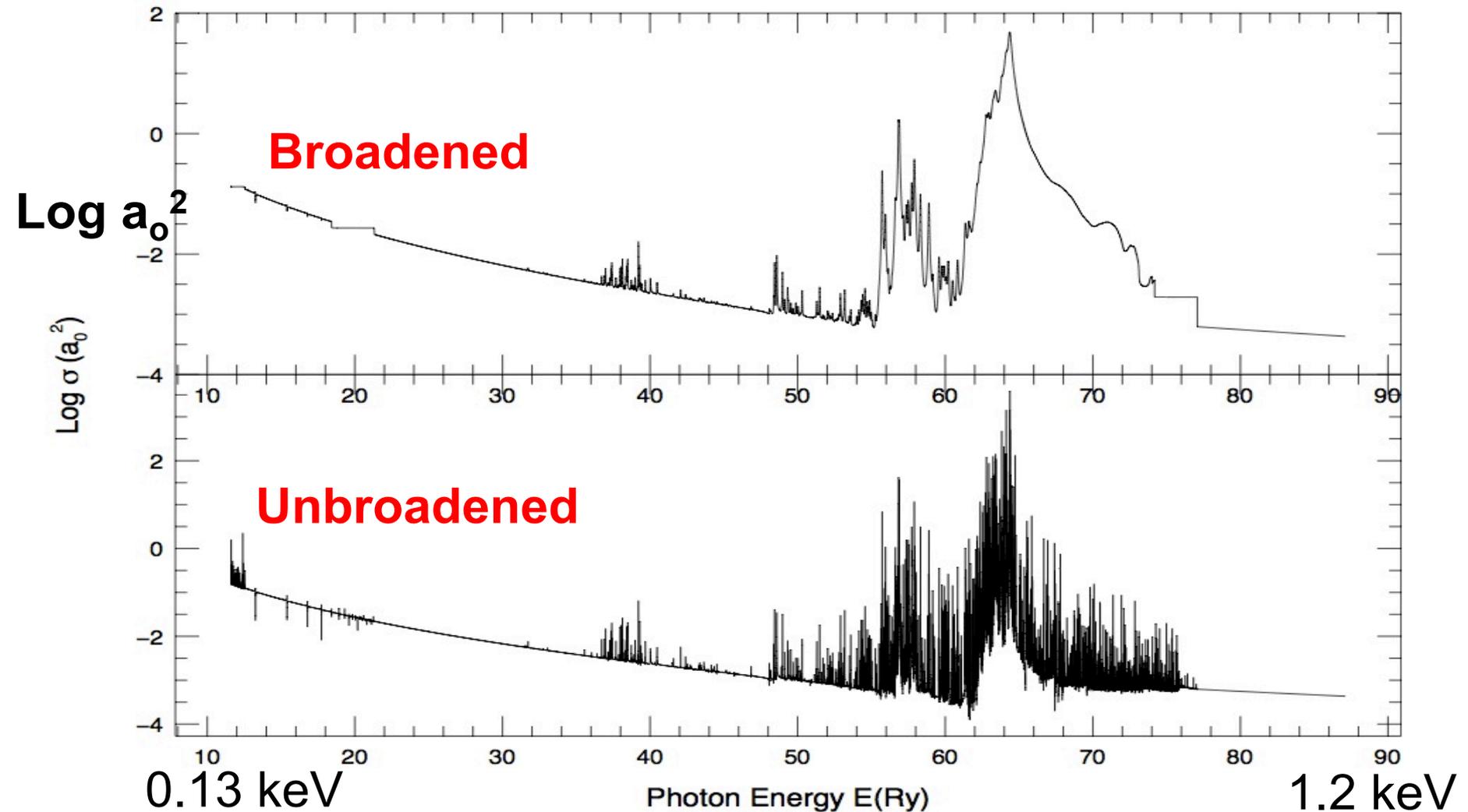
Resonance Broadening Processes

- 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, $Ne = 10^{23}$ /cm³ → $R_D = 4.13 a_0$, $\nu = 8.6$

Electron Impact Broadening of Autoionizing Resonances

Log T = 6.0, Log Ne = 20.0

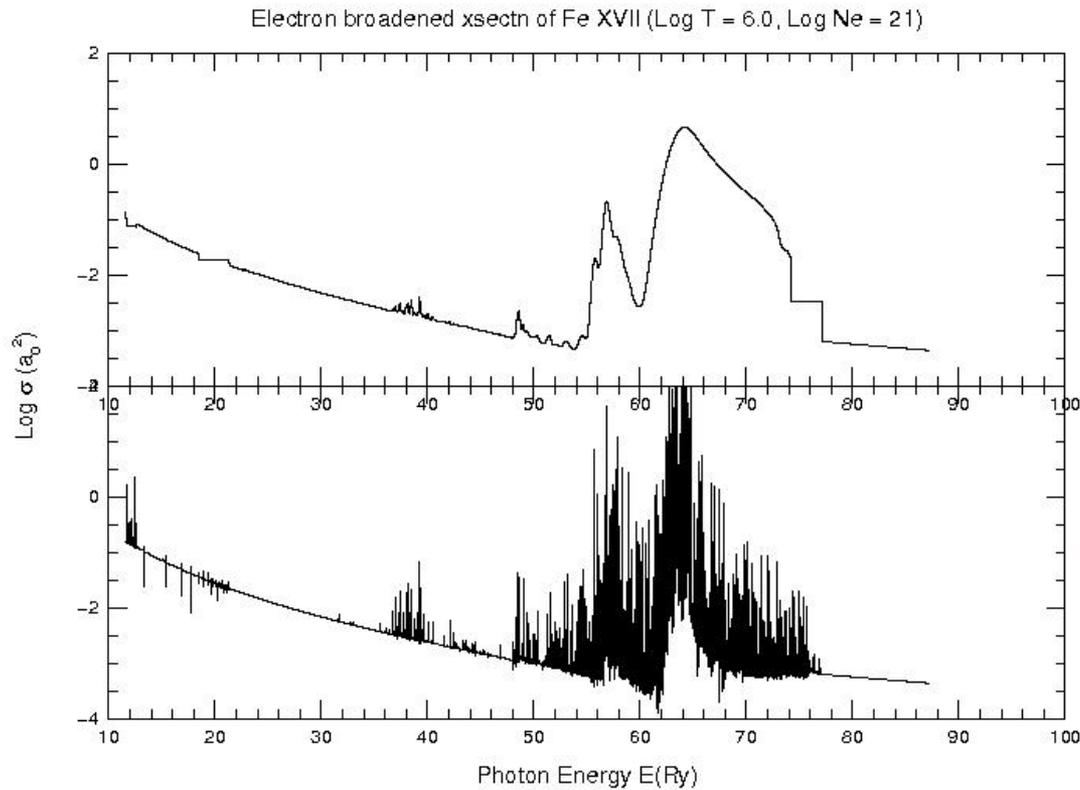
Electron broadened xsectn of Fe XVII (Log T = 6.0, Log Ne = 20)



Electron Impact Resonance Broadening

Log T = 6.0, Log Ne = 21.0

Log (a_0^2)



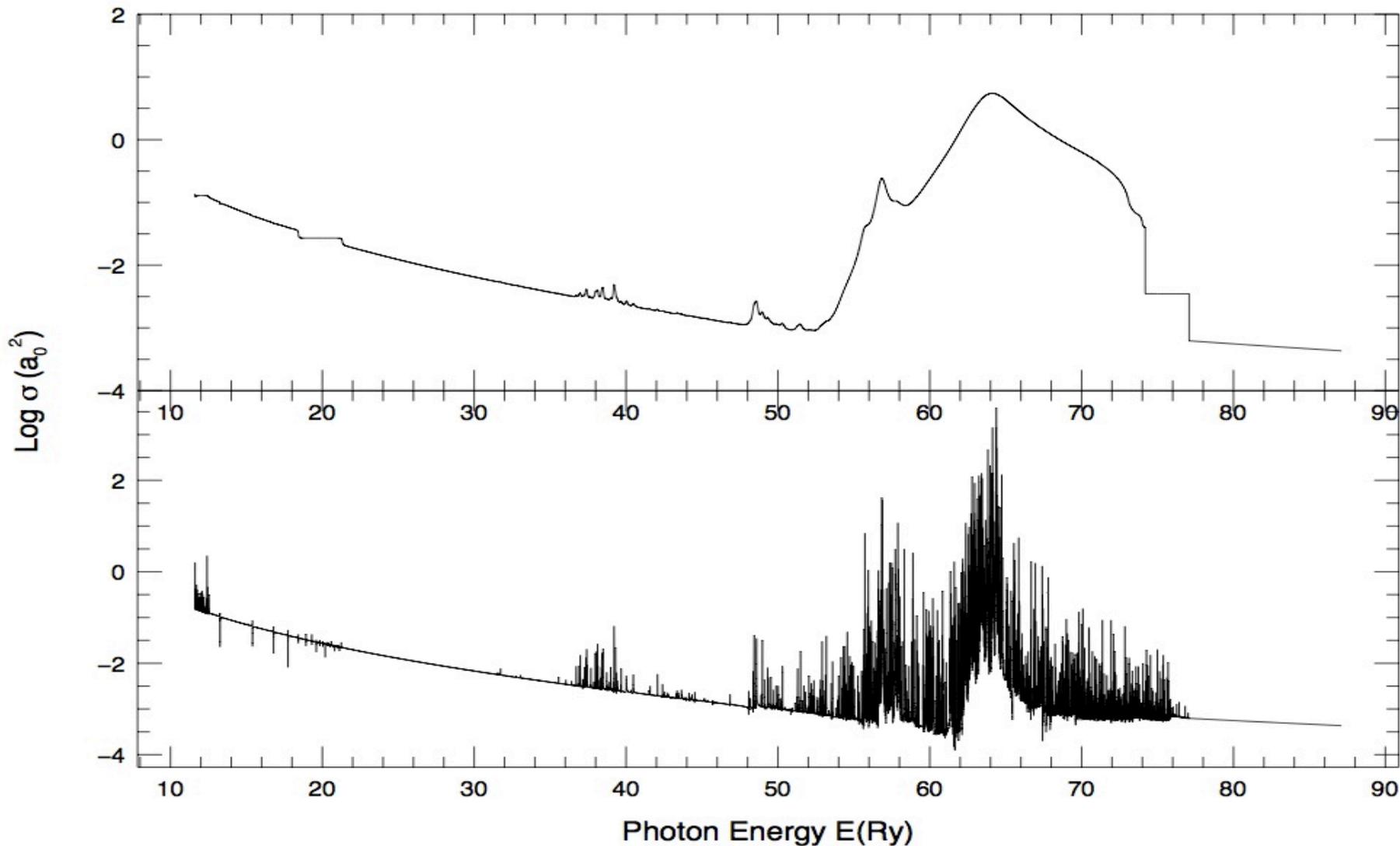
Broadened

Unbroadened

Electron Impact Broadening of Autoionizing Resonances

Log T = 6.3, Log Ne = 22.0

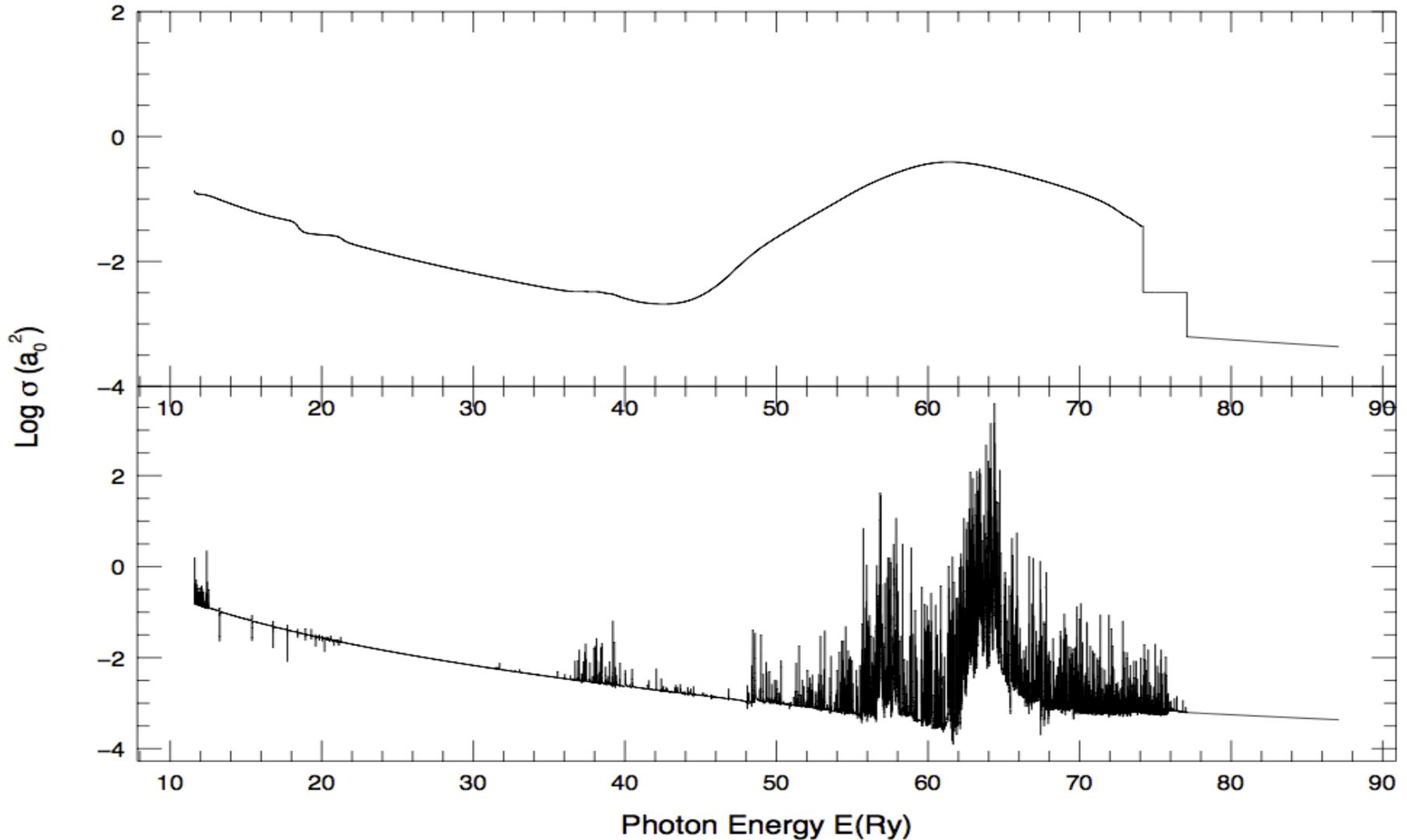
Electron broadened xsectn of Fe XVII (Log T = 6.0, Log Ne = 21)



Electron Impact Broadening of Autoionizing Resonances

Log T = 6.0, Log Ne = 22.0

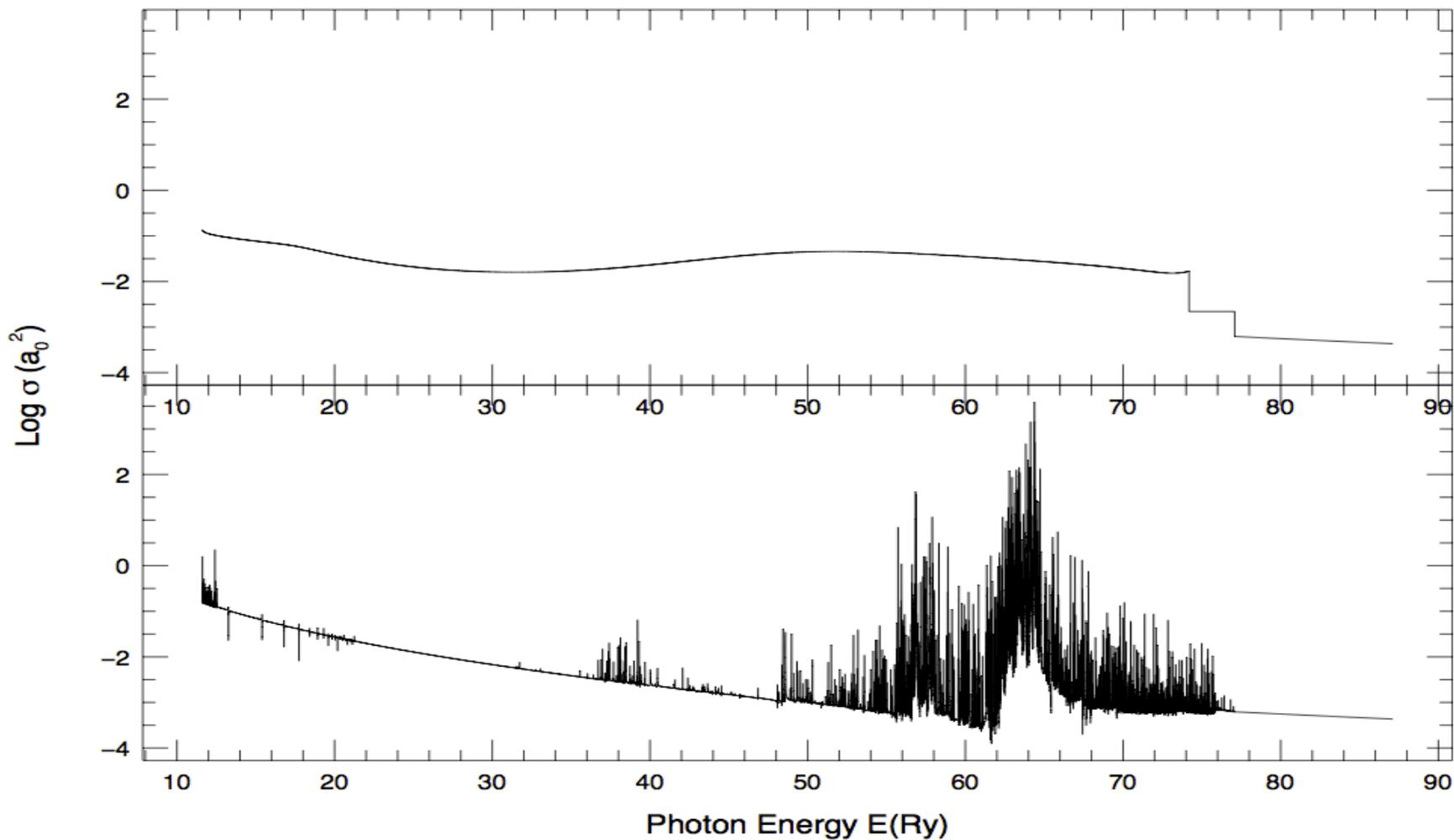
Electron broadened xsectn of Fe XVII (Log T = 6.0, Log Ne = 22)



Electron Impact Broadening of Autoionizing Resonances

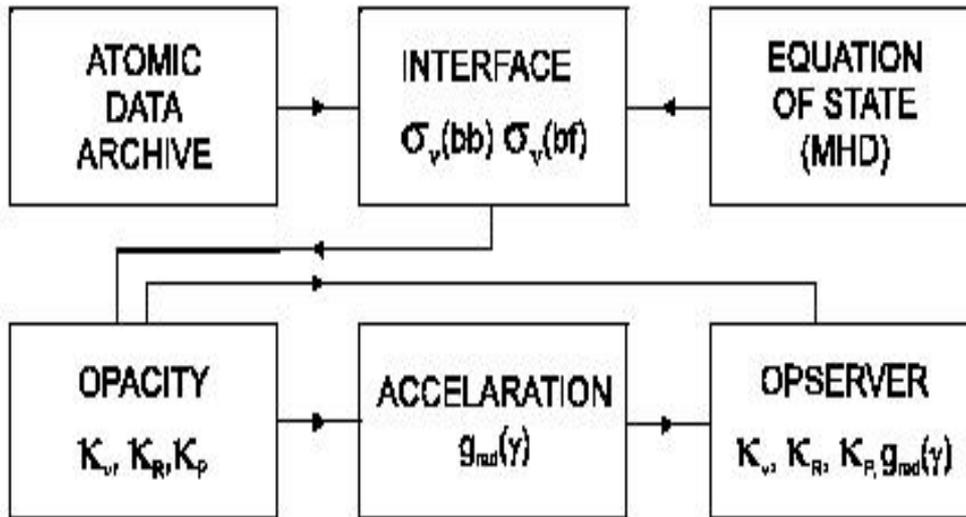
Log T = 6.3, Log Ne = 23.0

Electron broadened xsectn of Fe XVII (Log T = 6.3, Log Ne = 23)



High-Precision Opacities (HIPOP) Codes and Atomic Data

RADIATIVE OPACITIES AND ACCELERATIONS



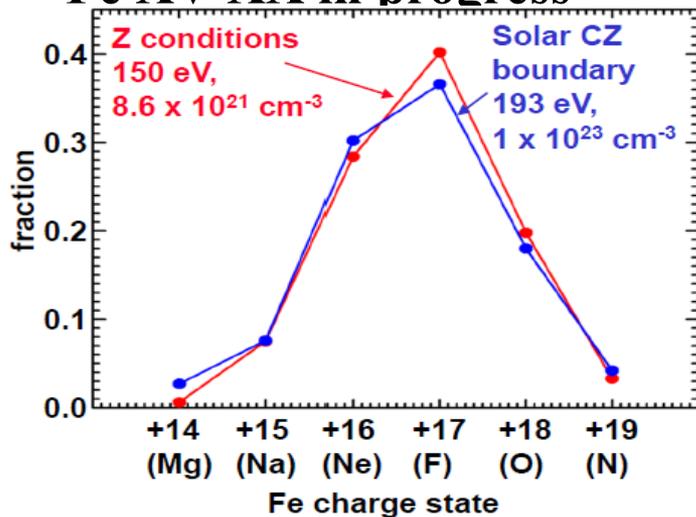
ISSUES

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

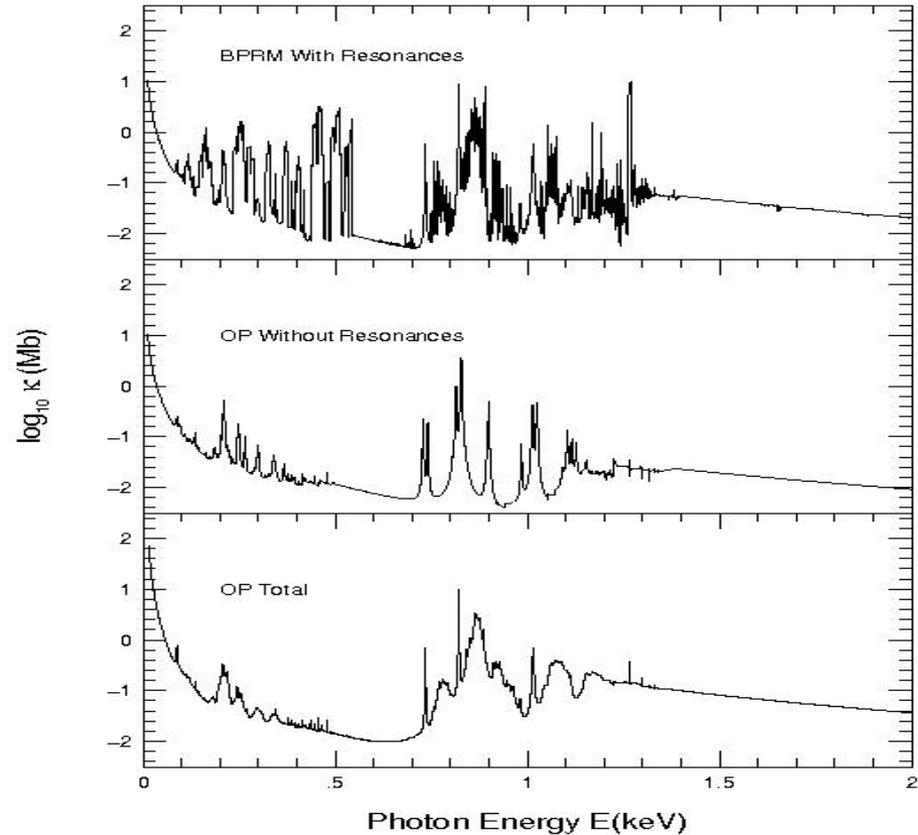
Breit-Pauli R-Matrix Opacities

(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

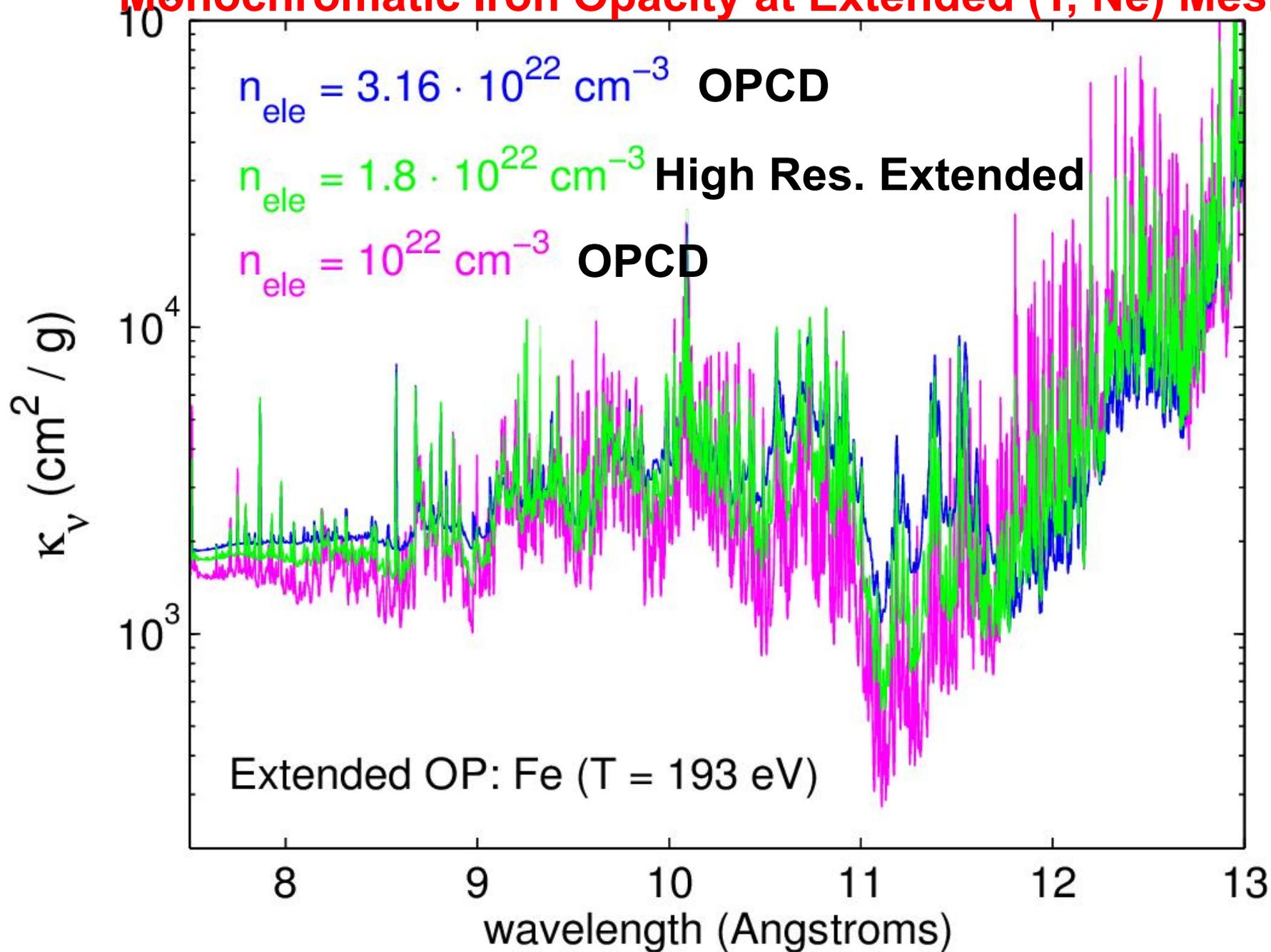


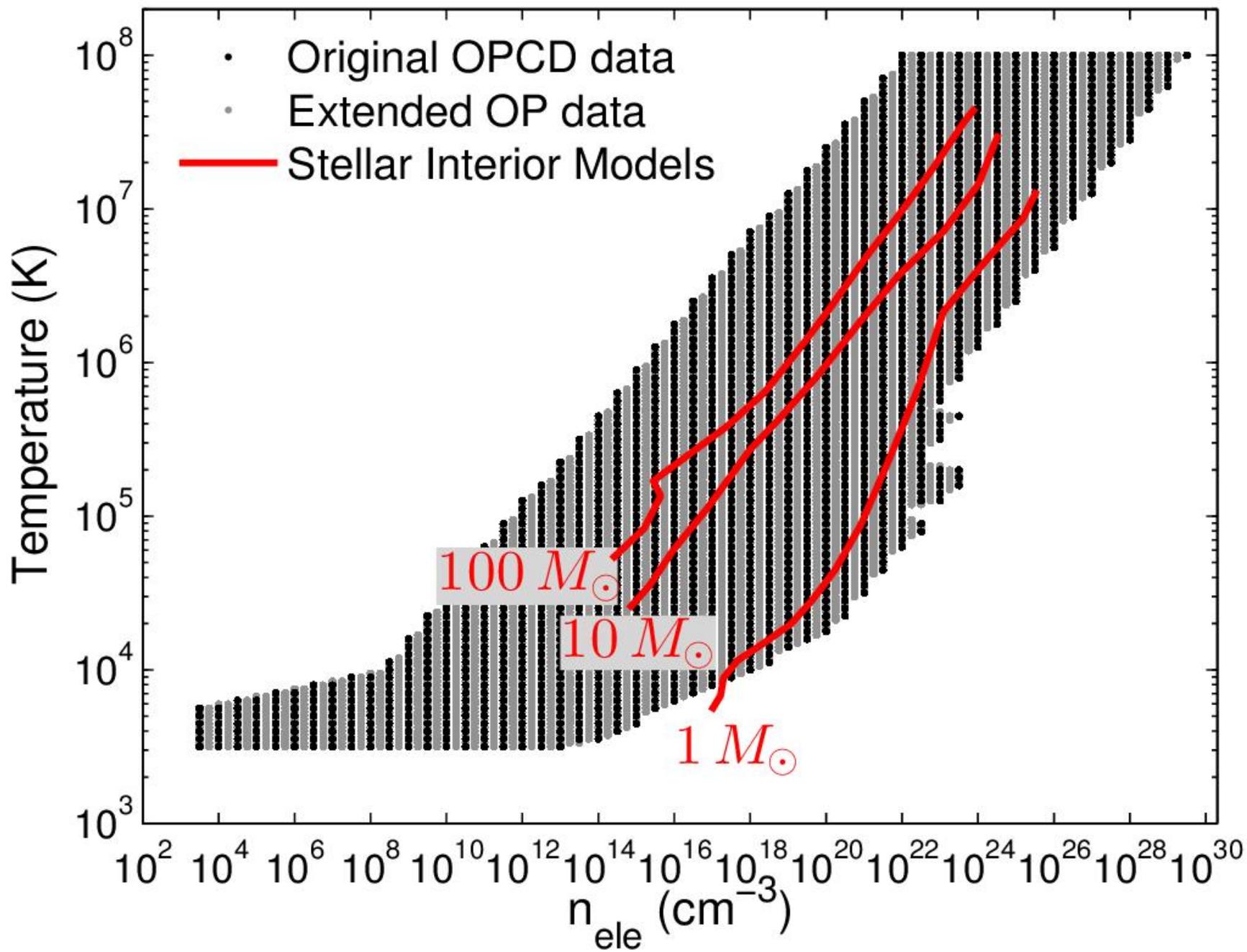
Monochromatic Opacity

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

Monochromatic Iron Opacity at Extended (T, Ne) Mesh





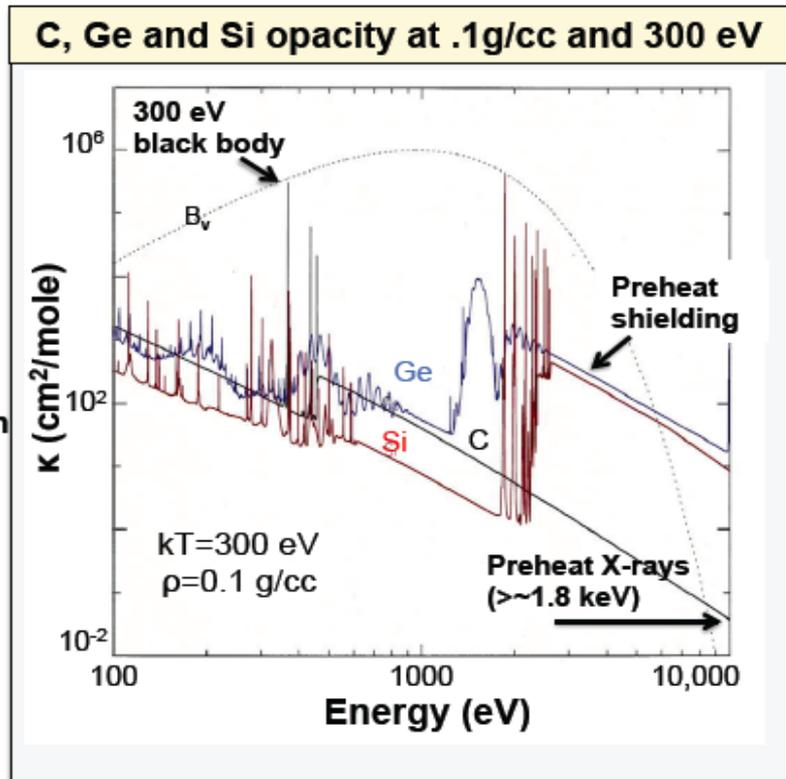
NIF – Implosion Plasma Opacity

LLNL-PRES-557971



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).



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**