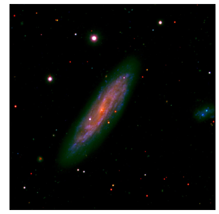

"HIGH ACCURACY RADIATIVE DATA FOR PLASMA OPACITIES"

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PLASMA OPACITY

- **Opacity determines radiation transport in plasmas**
- **Opacity is the resultant effect of repeated absorption and emission of the propagating radiation by the constituent plasma elements.**
- **Radiation energy created in the core (gamma rays) of the sun takes over a million years to travel to the surface: Reason - OPACITY**
- **Microscopically opacity depends on two radiative processes: i) photo-excitation (bound-bound transition) & ii) photoionization (bound-free transition)**
- **These determine monochromatic opacity $\kappa(\nu)$ at a single photon frequency ν.**
- **The mean opacity, Rosseland mean opacity, depends also on the physical conditions, such as, temperature, density, elemental abundances and equation of state**
- **The total $\kappa(\nu)$ is obtained from summed contributions of all possible transitions from all ionization stages of all elements in the source. Calculation of accurate parameters for such a large number of transitions has been the main problem for obtaining accurate opacities.**

THE OPACITY PROJECT and THE IRON PROJECT: Accurate Study of Atoms & Ions, Applications to Astronomy

- **International Collaborations: France, Germany, U.K., U.S., Venezuela, Canada, Belgium**

- **Earlier opacities were incorrect by factors of 2 to 5 resulting in inaccurate stellar models leading to - initiation of the Opacity Project in 1981**

- **THE OPACITY PROJECT - OP (1981 - 2006): study radiative atomic processes (E, f, σ_{PI}) of all elements from H to Fe and calculate opacities in astrophysical plasmas**

- **THE IRON PROJECT - IP (1993 -): collisional & radiative processes of Fe & Fe peak elements**

- **RMAX: Under IP, study X-ray atomic astrophysics**

- **Atomic & Opacity Databases (from OP & IP)**

- **TOPbase (OP) at CDS:**
http://vizier.u-strasbg.fr/topbase/topbase.html
- **TIPbase (IP) at CDS:**
http://cdsweb.u-strasbg.fr/tipbase/home.html
- **OPserver for opacities at the Ohio Supercomputer Center:**
http://opacities.osc.edu/
- **Latest radiative data at NORAD-Atomic-Data at OSU:**
http://www.astronomy.ohio-state.edu/~nahar/nahar_radiativeatomicdata/index.html

OUTCOME OF THE OP & THE IP

• Results from the OP and IP correspond to the first detailed study for most of the atoms and ions

• New features in photoionization cross sections are revealed

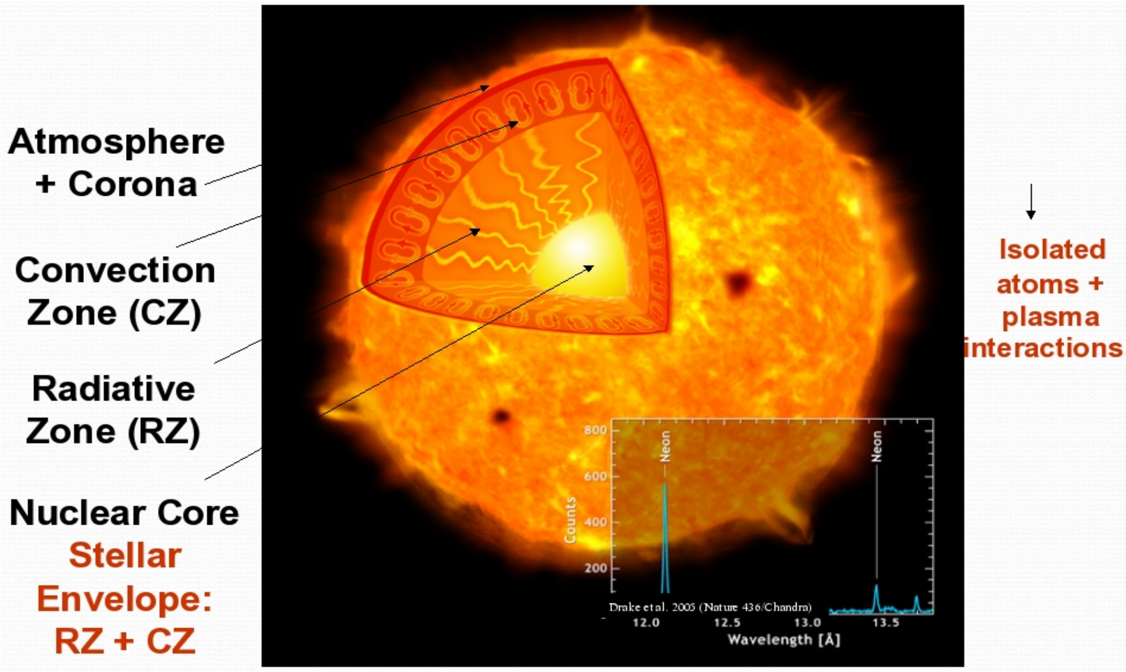
• OP opacities agreed with those computed under the OPAL, and both solved the outstanding problem on pulsations of cepheids

• Results from the OP and the IP continue to solve many outstanding problems, e.g., spectral analysis of blackhole environment, abundances of elements, opacities in astrophysical plasmas, dark matter

• HOWEVER, these are not complete and sufficiently accurate enough to solve all astrophysical problems

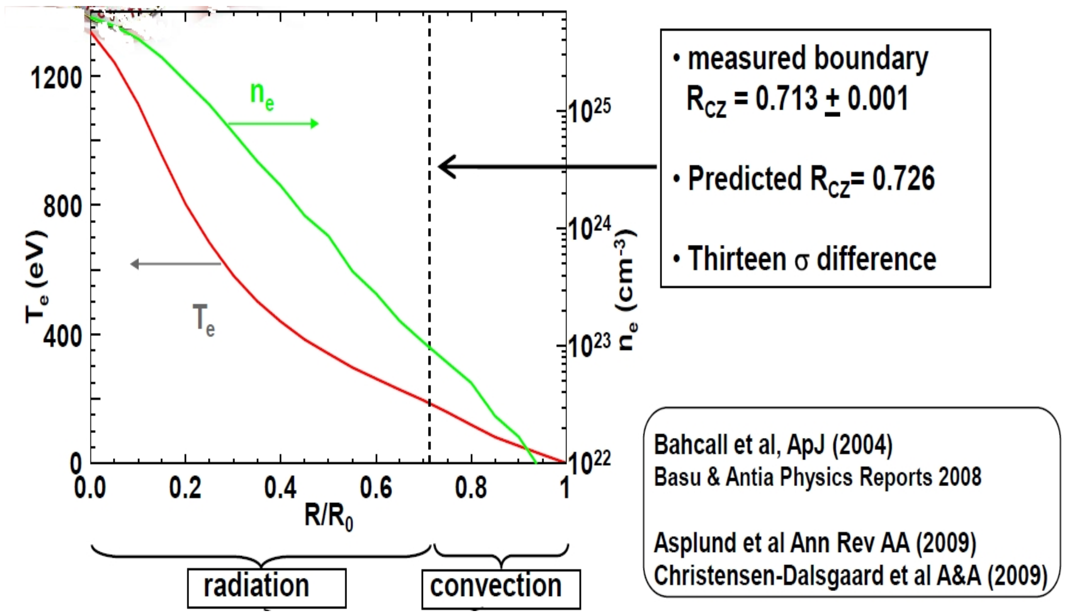
• Recent developments under the IP:
i) Able to calculate more accurate oscillator strengths for large number of transitions in relativistic Breit-Pauli R-matrix method
ii) finding existence of extensive and dominant resonant features in the high energy photoionization cross sections
iii) finding important fine structure effects in σ_{PI}

SOLAR OPACITY & ABUNDANCES



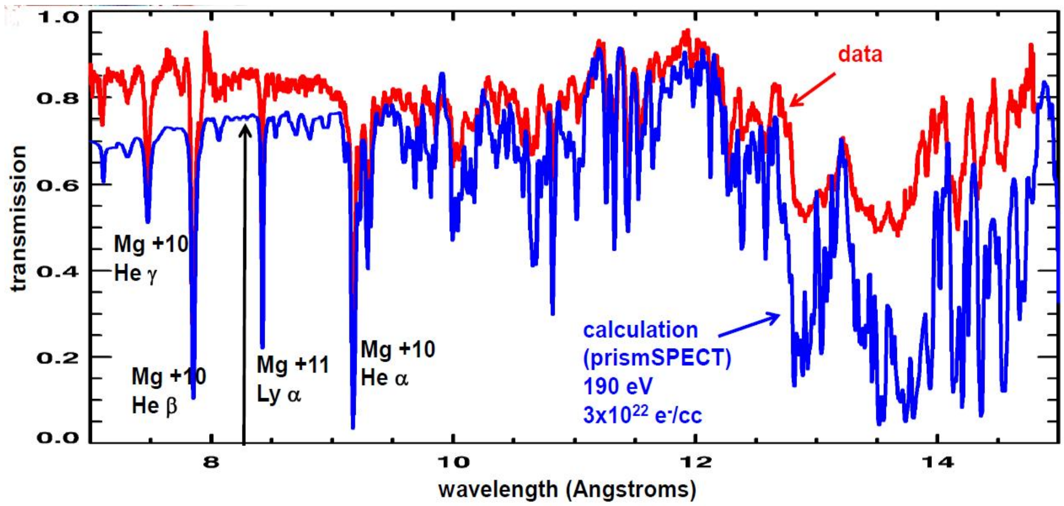
- Although the most studied star, we can not explain all observations.
- Sun's interior - nuclear core to the end of convection zone beyond which the radiation escapes
- At the convection zone boundary, R_{RZ}, the temperature $T_e \sim$193 eV, density $n_e \sim 10^{23}/cm^3$ (HED condition - NIF, Z-pinch)
- HED condition → important elements: O, Ne, especially Fe (Fe XVII-XIX)
- Radiation transport in the sun depends on the interior opacity (κ) through elemental abundances
- The opacity can determine R_{RZ}

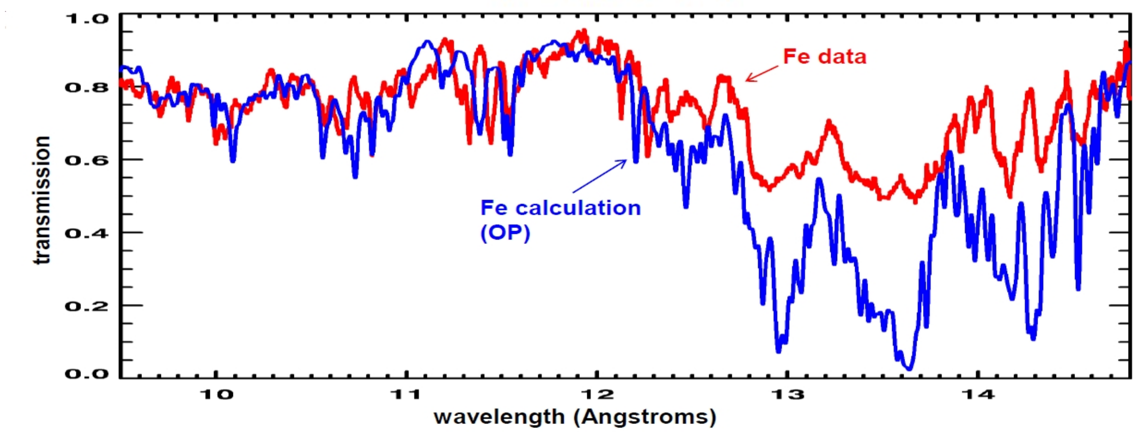
DISCREPANCY IN SOLAR RADIAIVE AND CONVECTION ZONES BOUNDARY (R_{CZ})



- The measured boundary, from helioseismology, of R_{RZ} is 0.713
- The calculated R_{CZ} is 0.726 - large
- A 1% opacity change leads to observable R_{CZ} changes
- Recent determination of abundances of light elements in the sun, C, N and O, are up to 30-40% lower than the standard values, long supported by astrophysical models, helioseismology, and meteoritic measurements
- This is a challenge in accuracy

DISCREPANCY BETWEEN EXPERIMENTAL & THEORETICAL OPACITIES (Bailey, Sandia lab)

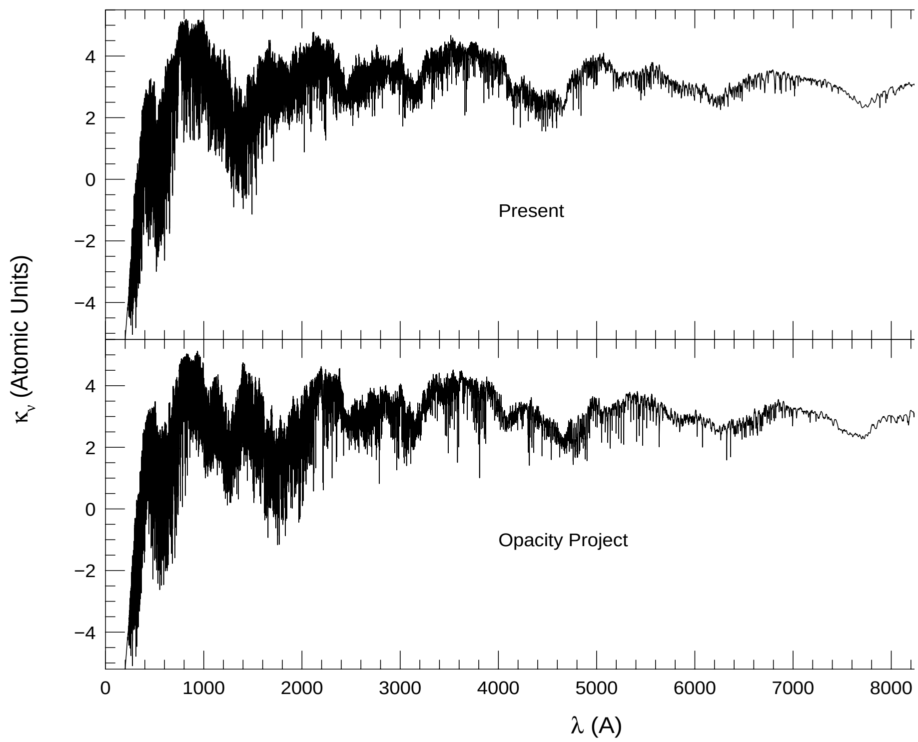




- Z PINCH spectra at Sandia lab: plasma temperature T_e ~193 eV & density $n_e \sim 10^{23}/cm^3$, similar to those at solar R_{CZ}
- Observed (red) and calculated (blue). Top: Diagnostic lines, Bottom: Iron - Large differences Reason: OPACITY
- Serious discrepancies for iron opacity using OP data (widely used) & observation
- Experimental n_e is wrong OR bound- free absorption (photoionization) is inaccurate

Monochromatic Opacities κ_ν of Fe IV

(Nahar & Pradhan 2006)



- logT=4.5, logN_e(cm^{-3}) = 17.0: condition when Fe IV dominates iron opacity
- κ_ν depends primarily on oscillator strengths (over 710,000 transitions)
- κ_ν(Fe IV) varies over orders of magnitude between 500 - 4000 $\AA$
- Comparison indicates systematic shift in groups of OP energies

DETERMINATION OF OPACITY:

1. Photoexcitation - Photon absorption for a bound-bound transition

$$\mathbf{X^{+Z} + h\nu \rightarrow X^{+Z*}}$$

- **Oscillator Strength (f_{ij})**

Monochromatic opacity (κ_ν) depends on f_{ij}

$$\kappa_\nu(\mathbf{i \rightarrow j}) = \frac{\pi \mathbf{e^2}}{\mathbf{mc}} \mathbf{N_i f_{ij}} \phi_\nu \quad (1)$$

N_i **= ion density in state i,** ϕ_ν **= profile factor**

- κ **inclues ~100M transitions of mid-Z elements**

2. Photoionization - Photon absorption for a bound-free transition: Direct -

$$\mathbf{X^{+Z} + h\nu \rightarrow X^{+Z+1} + \ e}$$

3. Autoionization (AI) in photoionization process :

$$\mathbf{e + X^{+Z} \rightleftharpoons (X^{+Z-1})^{**} \rightleftharpoons} \begin{cases} e + X^{+Z} & \text{AI} \\ X^{+Z-1} + h\nu & \text{DR} \end{cases}$$

Doubly excited "autoionizing state" → resonance

- **Photoionization Cross Sections (σ_{PI})**

κ_ν **depends on** σ_{PI}

$$\kappa_\nu = \mathbf{N_i} \sigma_{\mathbf{PI}}(\nu) \quad (2)$$

κ_ν **depends also on processes**

- **Inverse Bremstrahlung free-free Scattering:**

$$\mathbf{h}\nu + [\mathbf{X_1^+} + \mathbf{e}(\epsilon)] \rightarrow \mathbf{X_2^+} + \mathbf{e}(\epsilon'), \quad (3)$$

Cross section - from the elastic scattering matrix elements for electron impact excitation. An approximate expression for the free-free opacity is

$$\kappa_\nu^{\mathbf{ff}}(\mathbf{1},\mathbf{2}) = \mathbf{3.7} \times \mathbf{10^8 N_e N_i g_{ff}} \frac{\mathbf{Z^2}}{\mathbf{T^{1/2}}\nu^{\mathbf{3}}} \quad (4)$$

where g_{ff} **is a Gaunt factor**

- **Photon-Electron scattering:**

a) Thomson scattering when the electron is free

$$\kappa(\mathbf{sc}) = \mathbf{N_e}\sigma_{\mathbf{Th}} = \mathbf{N_e}\frac{\mathbf{8}\pi\mathbf{e^4}}{\mathbf{3m^2c^4}} = \mathbf{6.65} \times \mathbf{10^{-25}\ cm^2/g} \quad (5)$$

b) Rayleigh scattering when the electron is bound

$$\kappa_\nu^{\mathbf{R}} = \mathbf{n_i}\sigma_\nu^{\mathbf{R}} \approx \mathbf{n_i f_t}\ \sigma^{\mathbf{Th}} \left(\frac{\nu}{\nu_{\mathbf{I}}}\right)^{\mathbf{4}} \quad (6)$$

$h\nu_I$ **= binding energy,** f_t **= total oscillator strength associated with the bound electron.**

The equation of state (EOS)

• Ionization fractions and level populations of each ion of an element in levels with non-negligible occupation probability.

Rosseland mean $\kappa_R(T, \rho)$:

Harmonic mean opacity averaged over the Planck function, ρ is the mass density (g/cc),

$$\frac{1}{\kappa_R} = \frac{\int_0^\infty \frac{1}{\kappa_\nu} g(u) du}{\int_0^\infty g(u) du},$$

where $g(u)$ is the Planck weighting function

$$g(u) = \frac{15}{4\pi^4} \frac{u^4 e^{-u}}{(1 - e^{-u})^2}, \quad u = \frac{h\nu}{kT}$$

$g(u)$, for an astrophysical state is calculated with different chemical compositions H (X), He (Y) and metals (Z), such that

$$X + Y + Z = 1$$

THEORY: Relativistic Breit-Pauli Approximation

For a multi-electron system,

$$\mathbf{H^{BP}\Psi_E = E\Psi_E} \tag{7}$$

the relativistic Breit-Pauli Hamiltonian is:

$$\mathbf{H^{BP} = H^{NR} + H^{mass} + H^{Dar} + H^{so} +}$$

$$\frac{1}{2}\sum_{i\neq j}^{N}[g_{ij}(so+so') + g_{ij}(ss') + g_{ij}(css') + g_{ij}(d) + g_{ij}(oo')]. \tag{8}$$

where H_{NR} is the nonrelativistic Hamiltonian:

$$\mathbf{H^{NR}} = \sum_{i=1}^{N}\left\{-\nabla_i^2 - \frac{2Z}{r_i} + \sum_{j>i}^{N}\frac{2}{r_{ij}}\right\} \tag{9}$$

Relativistic Breit-Pauli R-matrix (BPRM) method

includes the three one-body correction terms:

$$\mathbf{H^{BP}_{N+1} = H^{NR}_{N+1} + H^{mass}_{N+1} + H^{Dar}_{N+1} + H^{so}_{N+1},} \tag{10}$$

$$\mathbf{H^{mass}} = -\frac{\alpha^2}{4}\sum_i p_i^4,\ \mathbf{H^{Dar}} = \frac{\alpha^2}{4}\sum_i \nabla^2\left(\frac{Z}{r_i}\right),\ \mathbf{H^{so}} = \left[\frac{Ze^2\hbar^2}{2m^2c^2r^3}\right]\mathbf{L.S}$$

H^{so} **splits LS energy in to fine structure levels.**

The latest BPRM codes include the two-body Breit interaction term:

$$\mathbf{H^{B}} = \sum_{i>j}[g_{ij}(so+so') + g_{ij}(ss')] \tag{11}$$

Close-coupling Approximation & R-matrix method

- **In close coupling (CC) approximation, the ion is treated as a system of (N+1) electrons: a target or the ion core of N electrons with the additional interating (N+1)th electron:**
- **Total wavefunction expansion is expressed as:**

$$\mathbf{\Psi_E(e+ion) = A\sum_i^N \chi_i(ion)\theta_i + \sum_j c_j\Phi_j(e+ion)}$$

$\chi_i \rightarrow$ **target ion or core wavefunction**
$\theta_i \rightarrow$ **interacting electron wavefunction (continuum or bound)**
$\Phi_j \rightarrow$ **correlation functions of (e+ion)**

- **The complex resonant structures in the atomic processes are included through channel couplings.**

- **Substitution of $\mathbf{\Psi_E(e+ion)}$ in $\mathbf{H\Psi_E = E\Psi_E}$ results in a set of coupled euqations**

- **Coupled equations are solved by R-matrix method**

- **E $<$ 0 $\rightarrow$ Bound (e+ion) states Ψ_B**
- **E $\geq$ 0 $\rightarrow$ Continuum states Ψ_F**

ATOMIC PROCESSES:
Quantity of Interest - S (Line Strength)

Transition Matrix elements:

$< \Psi_B||\mathbf{D}||\Psi_{B'} >$ → **Radiative Excitation**
$< \Psi_B||\mathbf{D}||\Psi_F >$ → **Photoionization**

$\mathbf{D} = \sum_i \mathbf{r}_i$ → **Dipole Operator**

The matrix element reduces to generalized line strength,

$$\mathbf{S} = \left| \left\langle \Psi_\mathbf{f} \right| \sum_{\mathbf{j}=1}^{\mathbf{N}+1} \mathbf{r_j} \left| \Psi_\mathbf{i} \right\rangle \right|^\mathbf{2} \tag{12}$$

PHOTO-EXCITATION AND DE-EXCITATION:
The oscillator strength (f_{ij}) and radiative decay rate (A_{ji}) for the bound-bound transition are

$$\mathbf{f_{ij}} = \left[\frac{\mathbf{E_{ji}}}{\mathbf{3g_i}}\right] \mathbf{S}, \quad \mathbf{A_{ji}}(\mathbf{sec}^{-1}) = \left[\mathbf{0.8032} \times \mathbf{10^{10}} \frac{\mathbf{E_{ji}^3}}{\mathbf{3g_j}}\right] \mathbf{S} \tag{13}$$

PHOTOIONIZATION:
The photoionization cross section, σ_{PI},

$$\sigma_\mathbf{PI} = \left[\frac{\mathbf{4}\pi}{\mathbf{3c}} \frac{\mathbf{1}}{\mathbf{g_i}}\right] \omega \mathbf{S}, \tag{14}$$

ω → **incident photon energy in Rydberg unit**

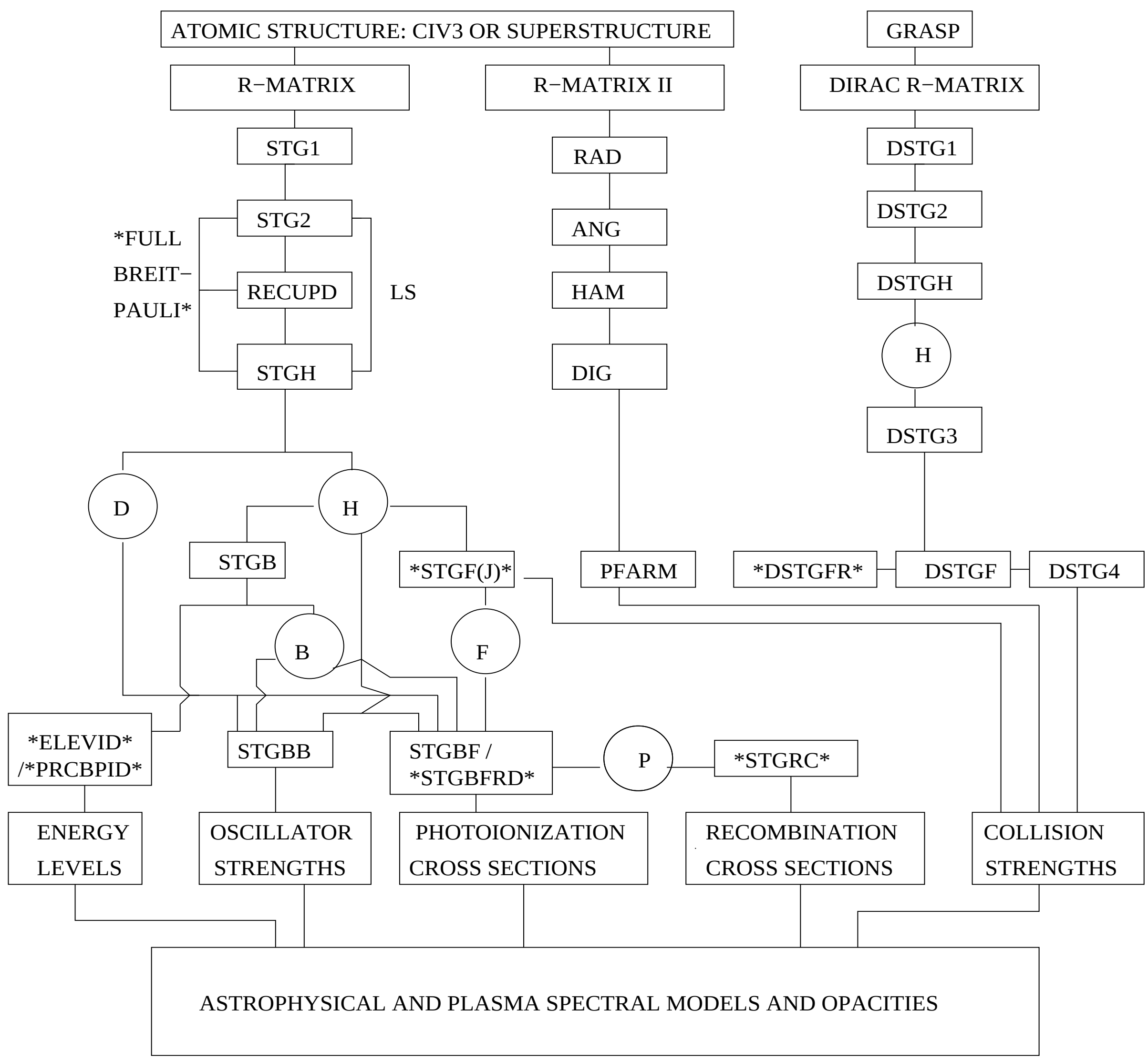
R-Matrix Codes For Large-Scale Atomic Calculations at the Ohio Supercomputer Center

VARIOUS COMPUTATIONAL STAGES

• R-matrix calculations cen proceed in 3 branches - 1) LS coupling & relativistic Breit-Pauli, 2) LS coupling R-matrix II for Large configuration interaction, 3) DARC for Full Dirac relativistic

• Results - 1) Energy Levels, 2) Oscillator Strengths, 3) Photoionization Cross sections, 4) Recombination Rate Coefficients, 5) Collision Strengths; - Astrophysical Models

THE R−MATRIX CODES AT OSU



RADIATIVE EXCITATIONS & DECAY RATES
(f-, S, A-values for various transitions)

Allowed electric dipole (E1) transtitions (BPRM)

i) Same spin multipliciy dipole allowed (Δ j=0,$\pm$1, ΔL = 0, $\pm$1, $\pm$2, ΔS = 0, parity π changes)

ii) Intercombination (Δ j=0,$\pm$1, ΔL = 0, $\pm$1, $\pm$2, ΔS $\neq$ 0, π changes)

$$\mathbf{A_{ji}(sec^{-1}) = 0.8032 \times 10^{10} \frac{E_{ji}^3}{3g_j} S^{E1}}, \quad \mathbf{f_{ij} = \frac{E_{ji}}{3g_i} S^{E1}(ij)} \tag{15}$$

• **Relativistic BPRM calculations include both types in contrast to LS coupling which includes same spin multiplicity dipole allowed only**

Forbidden transitions (Atomic Structure)

i) Electric quadrupole (E2) transitions (Δ J = 0,$\pm$1,$\pm$2, parity does not change)

$$\mathbf{A_{ji}^{E2} = 2.6733 \times 10^3 \frac{E_{ij}^5}{g_j} S^{E2}(i,j)}\ \mathrm{s}^{-1}, \tag{16}$$

ii) Magnetic dipole (M1) transitions (Δ J = 0,$\pm$1, parity does not change)

$$\mathbf{A_{ji}^{M1} = 3.5644 \times 10^4 \frac{E_{ij}^3}{g_j} S^{M1}(i,j)}\ \mathrm{s}^{-1}, \tag{17}$$

iii) Electric octupole (E3) transitions (Δ J= $\pm$2, $\pm$3, parity changes)

$$A_{ji}^{E3} = 1.2050 \times 10^{-3} \frac{E_{ij}^{7}}{g_j} S^{E3}(i,j)\ \mathrm{s}^{-1}, \tag{18}$$

iv) Magnetic quadrupole (M2) transitions (Δ J = $\pm$2, parity changes)

$$A_{ji}^{M2} = 2.3727 \times 10^{-2} \mathrm{s}^{-1} \frac{E_{ij}^{5}}{g_j} S^{M2}(i,j)\,. \tag{19}$$

• **Under the Iron Project, the above transitions are being calculated in the relativistic Breit-Pauli approximation**

LIEFTIME:

The lifetime of a level can be obtained from the A-values,

$$\tau_k(s) = \frac{1}{\sum_i A_{ki}(s^{-1})}. \tag{20}$$

"All new calculations are resulting in larger number of accurate transitions for more accurate opacities"

ENERGIES & OSCILLATOR STRENGTHS:

hν + Fe XIX $\leftrightarrow$ Fe XIX*

Fe XIX Energies (Nahar 2010):

- **Calculated: (BPRM) 1626, Observed (NIST): 63**

Agreement < 4%

Level		$J : I_J$	E_o(Ry,NIST)	E_c(Ry,BPRM)
$2s22p4$	$^3P^e$	2.0 : 1	107.90000	107.24300
$2s22p4$	$^3P^e$	1.0 : 1	107.08500	106.43000
$2s22p4$	$^3P^e$	0.0 : 1	107.21400	106.56300
$2s22p4$	$^1D^e$	2.0 : 2	106.36100	105.66900
$2s22p4$	$^1S^e$	0.0 : 2	104.93700	104.21700
$2s2p5$	$^3P^o$	2.0 : 1	99.49000	98.77570
$2s2p5$	$^3P^o$	1.0 : 1	98.92640	98.20250
$2s2p5$	$^3P^o$	0.0 : 1	98.51380	97.78800
$2s2p5$	$^1P^o$	1.0 : 2	96.34880	95.59100
$2p6$	$^1S^e$	0.0 : 3	88.45190	87.65300
$2s22p34So3s$	$^3S^o$	1.0 : 3	47.02740	46.32100
$2s22p32Do3s$	$^3D^o$	3.0 : 1	45.76980	45.00950
$2s22p32Do3s$	$^3D^o$	2.0 : 3	46.05230	45.34050
$2s22p32Do3s$	$^3D^o$	1.0 : 4	46.04320	45.32430
$2s22p32Do3s$	$^1D^o$	2.0 : 4	45.62400	44.83330
$2s22p32Po3s$	$^3P^o$	2.0 : 5	44.38470	43.65750
$2s22p32Po3s$	$^3P^o$	1.0 : 5	44.81300	44.19400
$2s22p32Po3s$	$^3P^o$	0.0 : 2	44.95880	44.26550
$2s22p32Po3s$	$^1P^o$	1.0 : 6	44.24800	43.51780
$2s22p34So3d$	$^3D^o$	3.0*: 3	41.84220	41.10710
$2s22p32Do3d3/2$	$^3P^o$	2.0*: 8	40.73960	40.48040
$2s22p32Do3d5/2$	$^3D^o$	3.0*: 7	40.50270	39.23750
$2s22p32Do3d5/2$	$^3D^o$	2.0*: 9	40.42070	39.90600
$2s22p32Do3d5/2$	$^1F^o$	3.0 : 6	40.01970	39.71650
$2s22p32Po3d1/2$	$^3F^o$	3.0*: 8	40.01060	39.05150
$2s22p32Po3d1/2$	$^3F^o$	2.0*:11	39.84660	39.53240
$2s22p32Po3d3/2$	$^3D^o$	3.0 : 9	38.96260	38.34430
$2s22p32Po3d3/2$	$^3D^o$	2.0 :13	39.06290	38.91690

Fe XIX: f, S, A for allowed & forbidden transitions

- **289,291 E1 transitions among 1626 levels**
- **66,619 forbidden (E2,E3,M1,M2) transitions**
- **Good agreement for most transitions**

E1 Transition Comparison: a-Shirai et al (2000), b- Fawcett (1986), c- Cheng et al (1979), d- Loulergue et al (1985), e- Jonauskas et al (2004), f- Buchet et al (1980), g- Safronova et al (1975), h- Feldman et al. (1975), i- Smith et al (1971)

λ(Å)	$A(s^{-1})$(NIST)	$A(s^{-1})$ (Present)	$C_i - C_j$	$SL\pi : i-j$	$g : i-j$
108.355	3.9e+10[a]: C,3.57e+10[e]	3.35e+10,3.54+10	$2s^22p^4 - 2s2p^5$	$^3P -^3 P^o$	5-5
109.952	1.6e+10[c]: C	1.40e+10,1.46+10	$2s^22p^4 - 2s^2p^5$	$^3P -^3 P^o$	1-3
111.695	1.26e+10[c]: C	1.09e+10,1.15+10	$2s^22p^4 - 2s2p^5$	$^3P -^3 P^o$	3- 3
119.983	1.04e+10[a]: C	9.02e+9,8.54+9	$2s^22p^4 - 2s2p^5$	$^3P -^3 P^o$	3- 5
101.55	3.17+10[c]:E,2.91e+10[e]	2.77e+10	$2s22p4 - 2s2p5$	$3P - 3P$	5-3
78.888	1.3e+10[c]:E	1.12+10 ,1.14+10	$2s22p4 - 2s2p5$	$3P - 1P$	5-3
83.87	1.6e+09[c]:E	1.19E+09,1.26+9	$2s22p4 - 2s2p5$	$3P - 1P$	1-3
84.874	9.3e+08[c]:E	8.75e+08,8.32+8,	$2s^22p^4 - 2s^2p^5$	$^3P -^1 P^o$	3-3
132.63	2.2e+09[a]: E	1.96e+9,2.01+9	$2s^22p^4 - 2s2p^5$	$^1D -^3 P^o$	5-5
91.012	1.49e+11[c]:C	1.32e+11,1.38e+11	$2s^22p^4 - 2s^2p^5$	$^1D -^1 P^o$	5-3
151.607	7.9e+08[c]:E	5.86e+8,6,65+8s	$2s^22p^4 - 2s2p^5$	$^1S -^3 P^o$	1-3
14.966	2.5e+12[a]:C	2.24e+12,2.09e+12	$2s22p4 - 2s22p3(4S)3s$	$3P - 3S$	5-3
14.929	2.5e+11[b]:D	2.45e+11,2.77e+11	$2s22p4 - 2s22p3(2D)3s$	$3P - 3D$	3-5
14.668	1.1e+12[b]:C	1.06e+12,1.12+12	$2s^22p^4 - 2s^22p^3(^2P^o)3s$	$^3P -^3 P^o$	3-1
14.735	9.8e+11[b]:D,9.53e+11[e]	9.29e+11 ,8.52+11	$2s22p4 - 2s22p3(2D)3s$	$3P - 3D$	5-5
14.929	1.2e+12[b]:D	1.16e+12 ,1.04e+12	$2s22p4 - 2s22p3(2D)3s$	$3P - 3D$	3-3
14.633	1.4e+11[b]:E,1.27e+11[e]	1.18E+11	$2s22p4 - 2s22p3(2D)3s$	$3P - 1D$	5-5
14.995	2.2e+12[b]:D	2.05e+12,2.0e+12	$2s22p4 - 2s22p3(2D)3s$	$1D - 1D$	5-5
14.534	6.8e+11[b]:D	6.36e+11,6.05+11	$2s22p4 - 2s22p3(2P)3s$	$3P - 3P$	3-5
14.603	7.5e+11[b]:D	6.94e+11,6,53+11	$2s22p4 - 2s22p3(2P)3s$	$3P - 3P$	1- 3
14.668	1.1e+12[b]:C	1.07e+12,9.74+11	$2s^22p^4 - 2s^22p^3(^2D^o)3s$	$^3P -^3 D^o$	5-7
14.70	6.8e+11[a]:E,6.49e+11[e]	5.05e+11,5.22+11	$2s^22p^4 - 2s^22p^3(^2P^o)3s$	$^1D -^3 P^o$	5-5
14.806	5.6e+11[b]: E	5.05e+11 ,4.88+11	$2s22p4 - 2s22p3(2P)3s$	$1D - 3P$	5-3
14.671	1.1e+12[b]:D,1.11e+12e	9.36e+11,1.03+12	$2s^22p^4 - 2s^22p^3(^2P^o)3s$	$^1D -^1 P^o$	5-3
13.424	4.8e+12[a]:E	4.02e+12	$2s^22p^4 - 2s^22p^3(^2P^o_{5/2})3d$	$^3P -^3 F^o$	5-7
13.52	2.0e+13[b]: D	1.90e+13	$2s^22p^4 - 2s^22p^3(^2D^o_{5/2})3d$	$^3P -^3 D^o$	5-7
13.735	1.0e+13[a]:D,2.06e+12[e]	8.10e+12	$2s^22p^4 - 2s^22p^3(^2P^o_{5/2})3d$	$^1D -^3 F^o$	5-7
86.999	1.2e+10[c]: E	1.09e+10,1.05e+10	$2s2p^5 - 2p^6$	$^3P^o -^1 S$	3-1
115.396	1.61e+11[c]: C	1.35e+11,1.51e+11	$2s2p^5 - 2p^6$	$^1P^o -^1 S$	3-1

Lifetime ($10^{-12}s$)

λ	Expt	Present	Others	$Conf$	Level
108.4	23.5±2.[f]	22.48	22.5[g],22.1[h],17.6[i]	$2s2p^5$	$^3P^o_2$

Fe XIX: Comparison of forbidden transitions

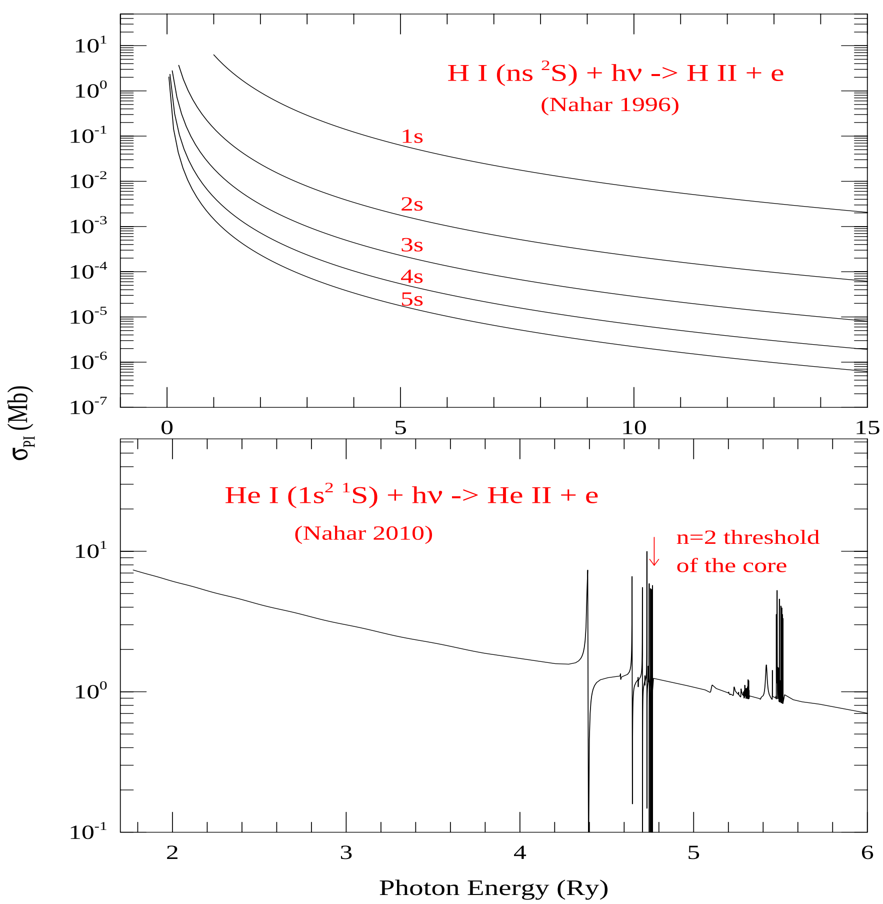
- **Good agreement with existing results**

E2, E3, M1, M2 transitions: a- Cheng et al (1979), b- Loulergue et al (1985), c- Jonauskas et al (2004).

λ ($\AA$)	$A(\mathrm{s}^{-1})$ (Others)	$A(\mathrm{s}^{-1})$ (present)	$C_i - C_j$	$SL\pi$ i-j	g i-j
424.26	1.50e+05[a]:C,1.39e+05[c]	1.41e+5	$2s^22p^4 - 2s^22p^4 : M1$	$^3P -^1 S$	3- 1
592.234	6.00[a]:E,6.18[c]	6.0	$2s^22p^4 - 2s^22p^4 : E2$	$^3P -^1 D$	5- 5
592.234	1.73e+04[a]:C,1.69e+04[c]	1.67e+4	$2s^22p^4 - 2s^22p^4 : M1$	$^3P -^1 D$	5-5
639.84	4.9e+01[a]:E,4.83e+01[c]	4.92e+1	$2s^22p^4 - 2s^22p^4 : E2$	$^1D -^1 S$	5-1
1118.06	0.611[a]:E,0.614[c]	0.635	$2s^22p^4 - 2s^22p^4 : E2$	$^3P -^3 P$	5-3
1118.06	1.45e+04[a]:C,1.42e+04[c]	1.46e+4	$2s^22p^4 - 2s^22p^4 : M1$	$^3P -^3 P$	5-3
1259.27	6.70e+02[a]:D,6.99e+02[c]	6.51e+2	$2s^22p^4 - 2s^22p^4 : M1$	$^3P -^1 D$	3- 5
1328.90	0.491[a]:E,0.509[c]	0.502	$2s^22p^4 - 2s^22p^4 : E2$	$^3P -^3 P$	5- 1
2207.8	4.820e+03[b]:C	4.96e+03	$2s2p^5 - 2s2p^5 : M1$	$^3P^o -^3 P^o$	3- 1
7045	4.0e+01[a]: C	41.0	$2s^22p^4 - 2s^22p^4 : M1$	$^3P -^3 P$	1- 3
353.532	9.4e+03[b]: D	8.79e+03	$2s2p^5 - 2s2p^5 : M1$	$^3P^o -^1 P^o$	3-3
420.911	7.7e+03[b]:D,8.06e+03[c]	7.31e+03	$2s2p^5 - 2s2p^5 : M1$	$^3P^o -^1 P^o$	1-3

PHOTOIONIZATION

- Atomic system with more than 1 electron - resonances in photoionization
- Earlier calculations for $\sigma_{\rm PI}$ under the OP considered low-lying resonances
- Core excitations to higher states - assumed weaker and hydrogenic
- Fine structure introduce new features
- New calculations under the IP $\rightarrow$ new and dominating features not studied before - these should change the current calculated opacities and resolve the gap



PHOTOIONIZATION OF Fe XVII (Nahar et al. 2010):

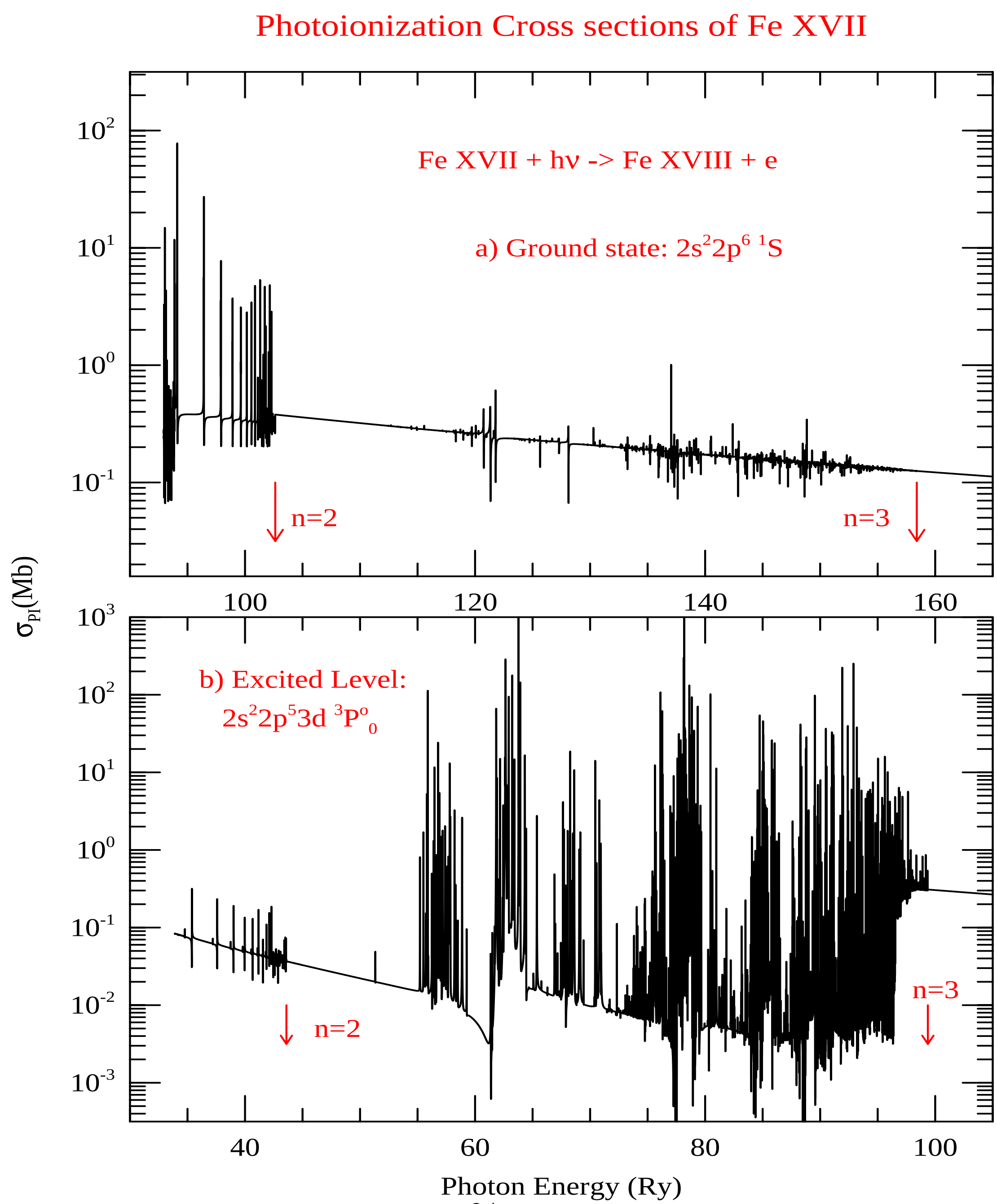
- **Bound levels ($n \leq 10$, $l \leq 9$, $J \leq 8$): N_b= 454**
- **Photoionization Cross Sections σ_{PI} for all levels**
- **Wavefunction expansion includes 60 core levels**
- **Note: Large energy gap ~47 Ry (n=2 & 3 levels)**

i	Configuration	Term	$2J$	E(Ry) Present	i	Configuration	Term	$2J$	E(Ry) Present
	n=2 states				30	$2s^22p^43p$	$^2P^o$	1	61.899
1	$2s^22p^5$	$^2P^o$	3	0.00000	31	$2s^22p^43d$	^4D	5	62.299
2	$2s^22p^5$	$^2P^o$	1	0.93477	32	$2s^22p^43d$	^4D	7	62.311
3	$2s2p^6$	^2S	1	9.70228	33	$2s^22p^43d$	^4D	1	62.906
	n=3 states				34	$2s^22p^43d$	^4D	3	63.050
4	$2s^22p^43s$	^4P	5	56.690	35	$2s^22p^43p$	$^2P^o$	3	62.461
5	$2s^22p^43s$	^2P	3	56.936	36	$2s^22p^43d$	^4F	9	62.535
6	$2s^22p^43s$	^4P	1	57.502	37	$2s^22p^43d$	^2F	7	62.629
7	$2s^22p^43s$	^4P	3	57.572	38	$2s^22p^43p$	$^2P^o$	1	62.686
8	$2s^22p^43s$	^2P	1	57.798	39	$2s^22p^43d$	^4P	1	62.496
9	$2s^22p^43s$	^2D	5	58.000	40	$2s^22p^43d$	^4P	3	62.625
10	$2s^22p^43s$	^2D	3	58.355	41	$2s^22p^43d$	^4F	5	62.985
11	$2s^22p^43p$	$^4P^o$	3	59.209	42	$2s^22p^43d$	^2P	1	63.123
12	$2s^22p^43p$	$^4P^o$	5	59.238	43	$2s^22p^43d$	^4F	3	63.156
13	$2s^22p^43p$	$^4P^o$	1	59.478	44	$2s^22p^43d$	^2F	5	62.698
14	$2s^22p^43p$	$^4D^o$	7	59.525	45	$2s^22p^43d$	^4F	7	63.271
15	$2s^22p^43p$	$^2D^o$	5	59.542	46	$2s^22p^43d$	^2D	3	63.302
16	$2s^22p^43s$	^2S	1	59.916	47	$2s^22p^43d$	^4P	5	62.911
17	$2s^22p^43p$	$^2P^o$	1	59.982	48	$2s^22p^43d$	^2P	3	63.308
18	$2s^22p^43p$	$^4D^o$	3	60.005	49	$2s^22p^43d$	^2D	5	63.390
19	$2s^22p^43p$	$^4D^o$	1	60.012	50	$2s^22p^43d$	^2G	7	63.945
20	$2s^22p^43p$	$^2D^o$	3	60.147	51	$2s^22p^43d$	^2G	9	63.981
21	$2s^22p^43p$	$^4D^o$	5	60.281	52	$2s^22p^43d$	^2S	1	63.919
22	$2s^22p^43p$	$^2P^o$	3	60.320	53	$2s^22p^43d$	^2F	5	64.200
23	$2s^22p^43p$	$^2S^o$	1	60.465	54	$2s^22p^43d$	^2F	7	64.301
24	$2s^22p^43p$	$^4S^o$	3	60.510	55	$2s^22p^43d$	^2P	3	64.138
25	$2s^22p^43p$	$^2F^o$	5	60.851	56	$2s^22p^43d$	^2D	5	64.160
26	$2s^22p^43p$	$^2F^o$	7	61.028	57	$2s^22p^43d$	^2D	3	64.391
27	$2s^22p^43p$	$^2D^o$	3	61.165	58	$2s^22p^43d$	^2P	1	64.464
28	$2s^22p^43p$	$^2D^o$	5	61.272	59	$2s^22p^43d$	^2D	5	65.305
29	$2s^22p^43p$	$^2P^o$	3	61.761	60	$2s^22p^43d$	^2D	3	65.468

PHOTOIONIZATION CROSS SECTION: Fe XVII

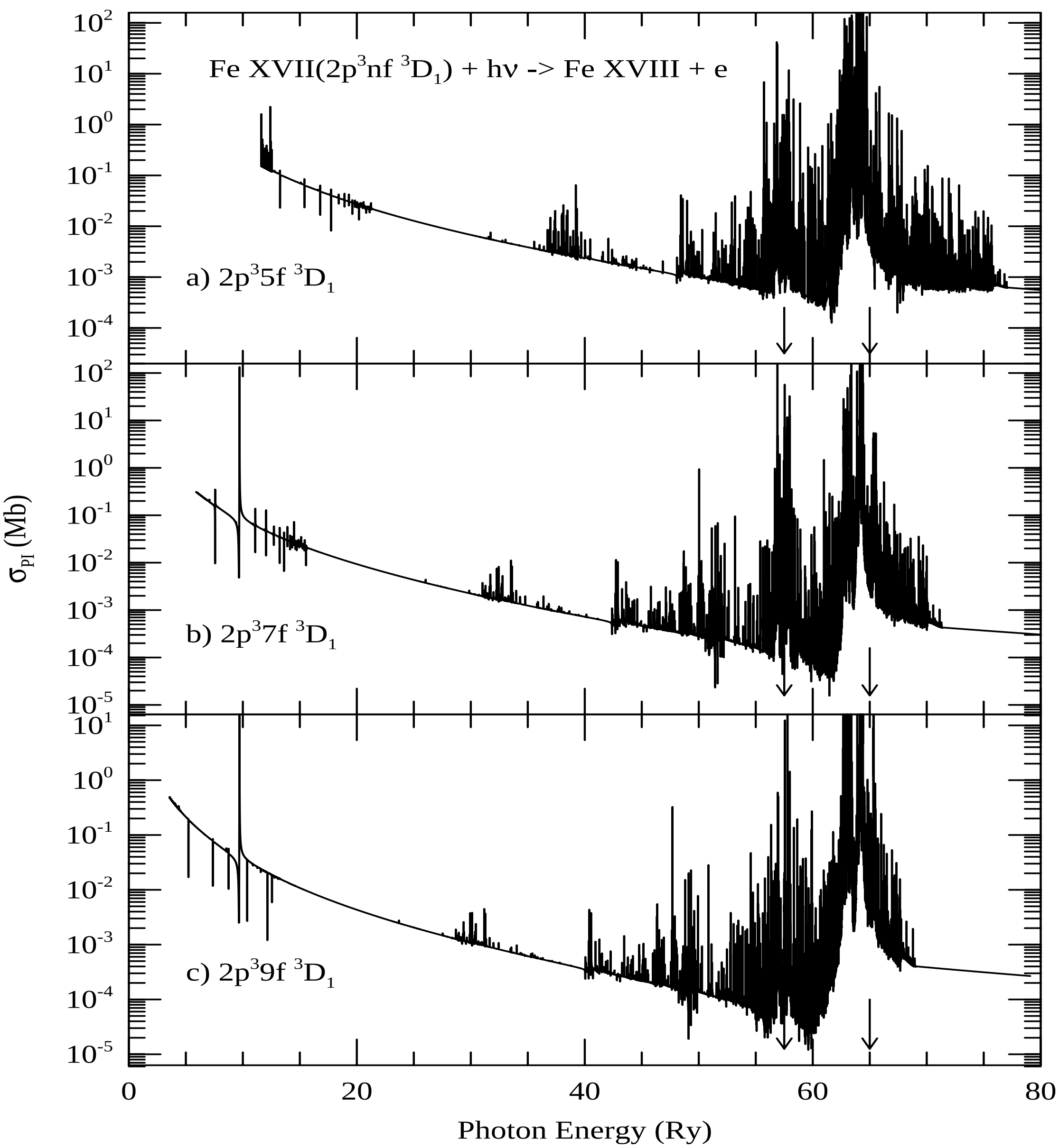
- Top: Ground level: n=2 resonances are important
- Bottom: Excited levels: n=3 resonances are important

Arrows point energy limits of n=2 & 3 core states



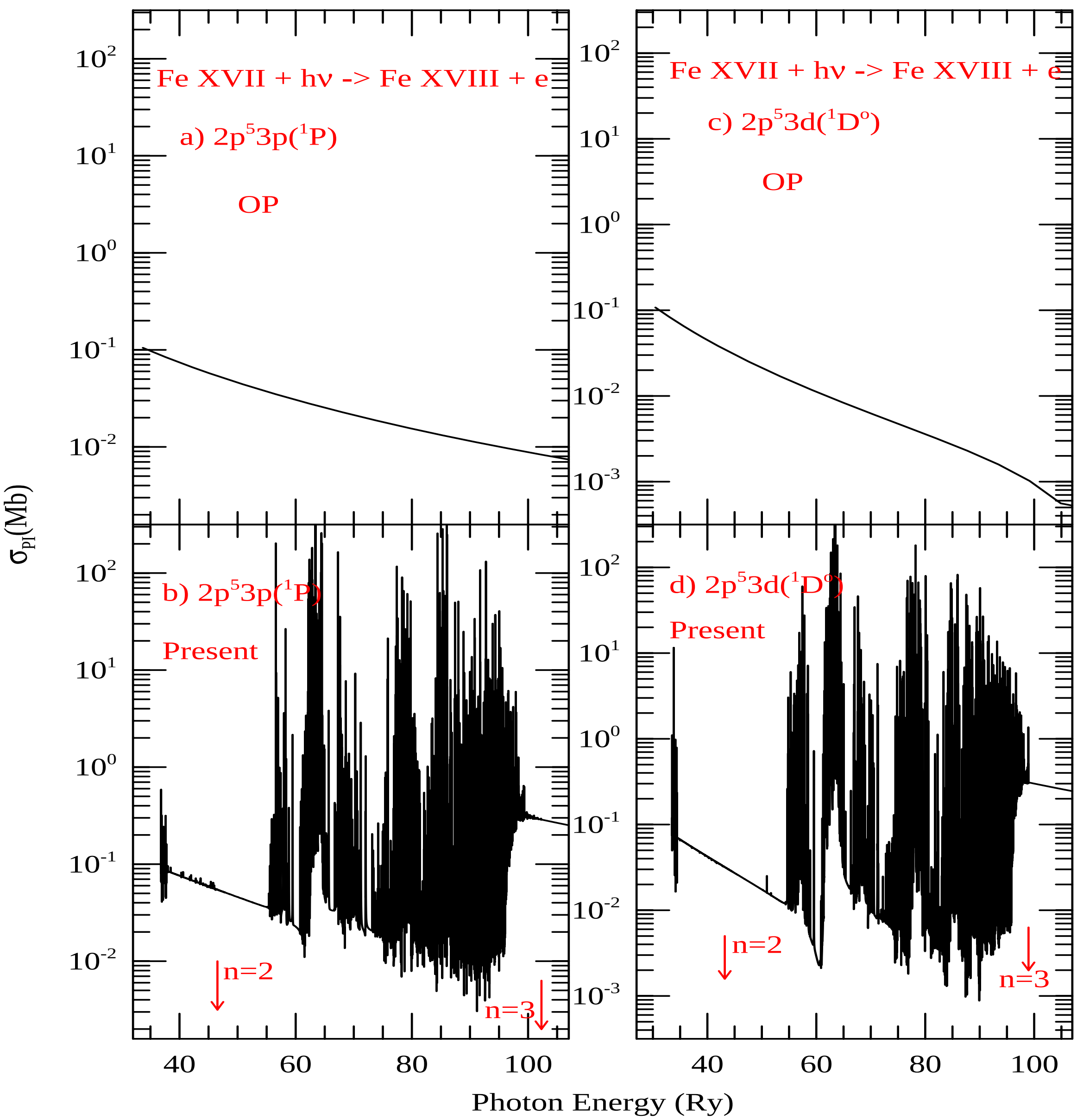
Fe XVII: PEC (Seaton) RESONANCES IN σ_{PI}:

- PEC (Photo-Excitation-of-Core) resonances appear for single valence-electron excited levels
- Appear at energies for core dipole transitions
- PEC resonances are strong and enhance the background cross sections by orders of magnitude
- PEC resonances will affect photoionization and recombination rates of high temperature plasmas



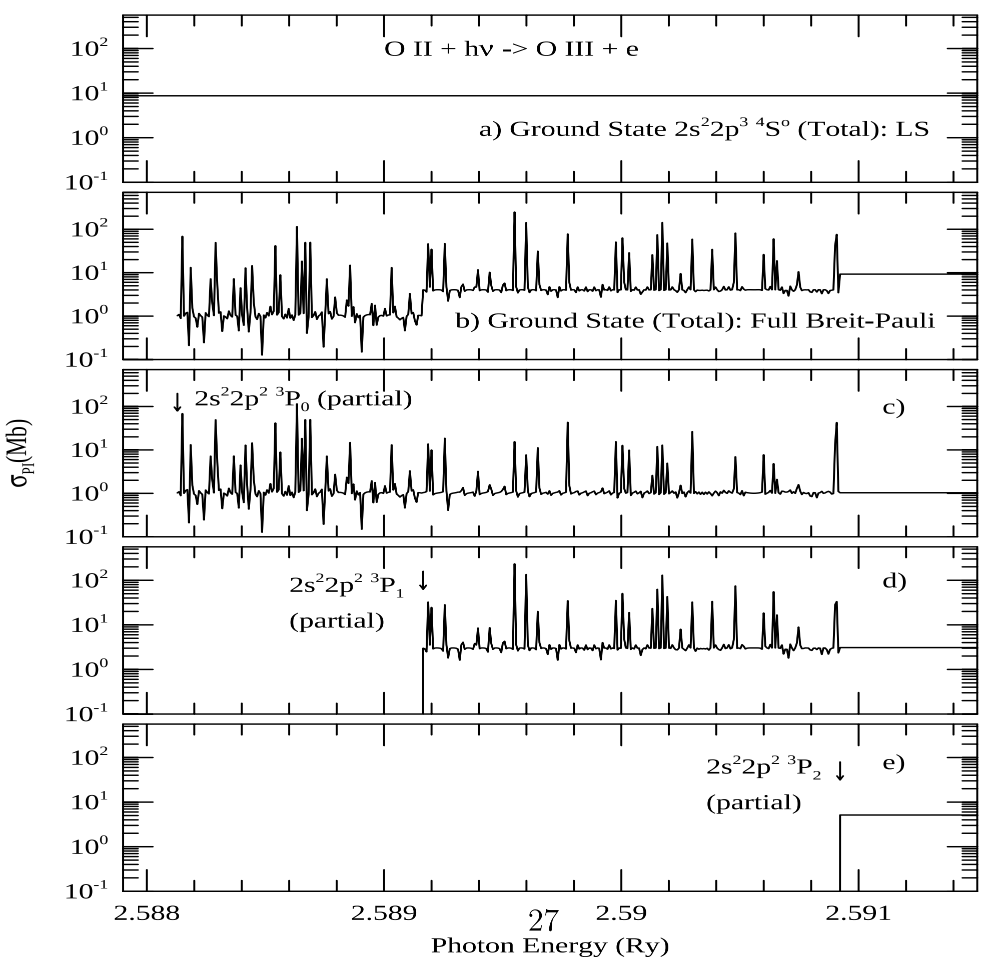
COMPARISON OF $\sigma_{\rm PI}$: Fe XVII

- **(a,b) level** $2p^53p^1P$ **& (c,d) level** $2p^53d(^1D^o)$
- **Present** σ_{PI} **(Nahar et al 2010) show importance of resonant effects compared to those from the Opacity Project (OP)**
- **Without n=3 core states,** σ_{PI} **is considerably underestimated**



Relativistic Fine Structure Effects on Low Energy Photoionization

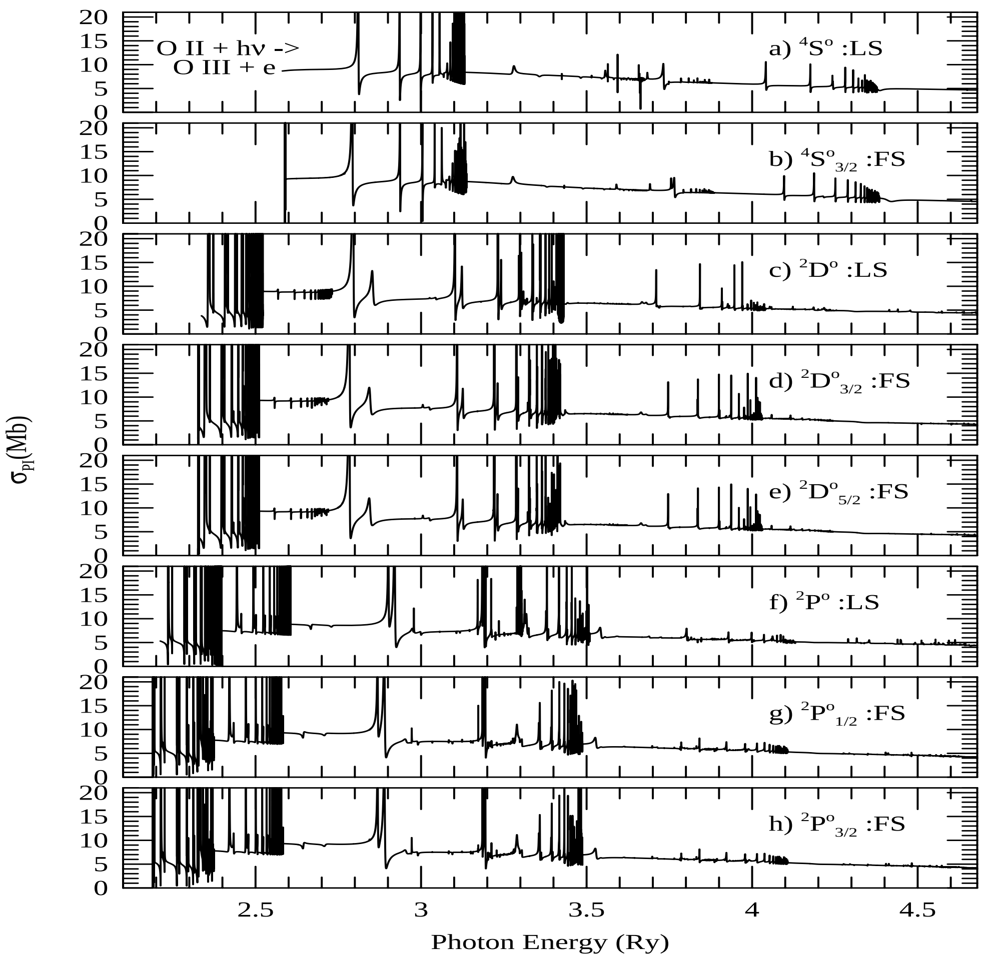
- More important in low energy region
- Introduce features not allowed in LS coupling; Ex. O II (Nahar et al. 2010)
- Figure: σ_{PI} of ground state $2s^22p^3(^4S^o_{3/2})$
- a) σ_{PI}(LS)- a smooth line (Nahar 1998)
- b) total σ_{PI} in full Breit-Pauli - background jump at each core ionization threshold $^3P_0$, $^3P_1$, & $^3P_2$ (latest BPRM)
- Resonances at $^3P_{0,1}$ ionization - due to couplings of fine structure channels



Fine Structure Effects on Low Z ion: O II

Nahar et al. 2010

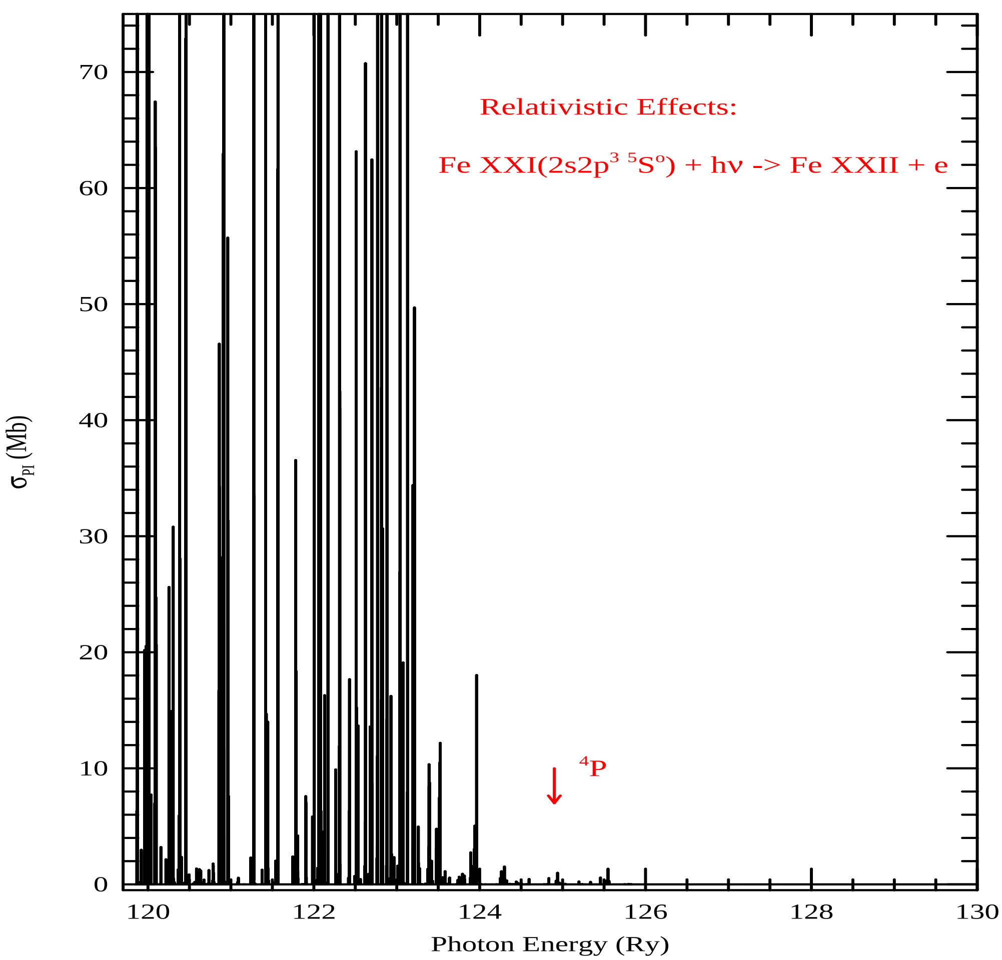
- σ_{PI}(LS) of O II states: LS coupling similar to fine structure except at thresholds
- σ_{PI}(LS) showed good agreement with experiment (ALS: Covington et al. 2001)
- However, problem with O II abundance at low T astrophysical plasmas remains
- Low energy structure in σ_{PI}(FS) is expected to narrow the difference gap



Observed Fine Structure Resonances in σ_{PI} of Fe XXI

- σ_{PI} of excited $2s2p^3(^5S^o_2)$ state (Nahar 2008)
- Strong resonant structures below the arrow - from relativistic fine structure couplings, not allowed in LS coupling
- Observed in recombination spectrum
- These will increase the elemental opacities, and decrease the abundances agreeing with the new findings

Total Photoionization Cross Sections of Fe XXI



CONCLUSION

1. **There is a lack of large amount of highly accurate atomic data**
2. **Solar elemental abundances are widely discordant**
3. **Z-pinch experiments reveal problems in existing models**
4. **High precision opacity is crucial to understand astrophysical conditions**
5. **Consideration of accurate radiative transitions and photoionization resonances due to highly excited core states are essential for more accurate opacity**

New **TEXTBOOK - Bridging Physics & Astronomy:**

"ATOMIC ASTROPHYSICS AND SPECTROSCOPY"

Anil K. Pradhan, Sultana N. Nahar

(Cambridge University Press, 2010)

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