



Atomic data for Astrophysics



Opacity and Radiative acceleration

Workshop PNPS - Astrophysique de laboratoire

Données atomiques pour la physique stellaire

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Atomic data for Astrophysics



Atomic data - Opacities - Radiative accelerations

Spectroscopy
Synthetic spectra

Atomic data

Experiments
Calibration, experimental path,
scaling (PALS, LULI, LMJ)

What are the uncertainties attached to atm. Data and derived products?

How do they propagate on application?

What are their limitation for experiments and applications?

What experiments are available / doable to help improve them?

Atmosphere modeling

Age of globular clusters

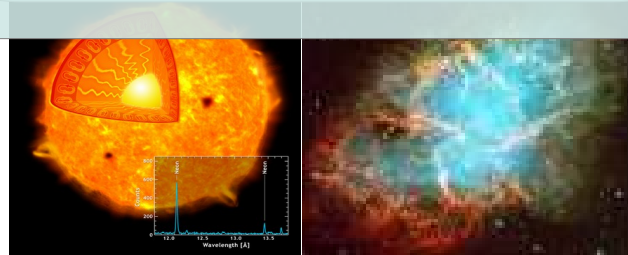
Opacities - Radiative accelerations

Stellar models

Characteristics: mass, radius,
composition
metallicity
turnoff, variability
Evolution:



Chemical evolution of
the ISM and Galaxies



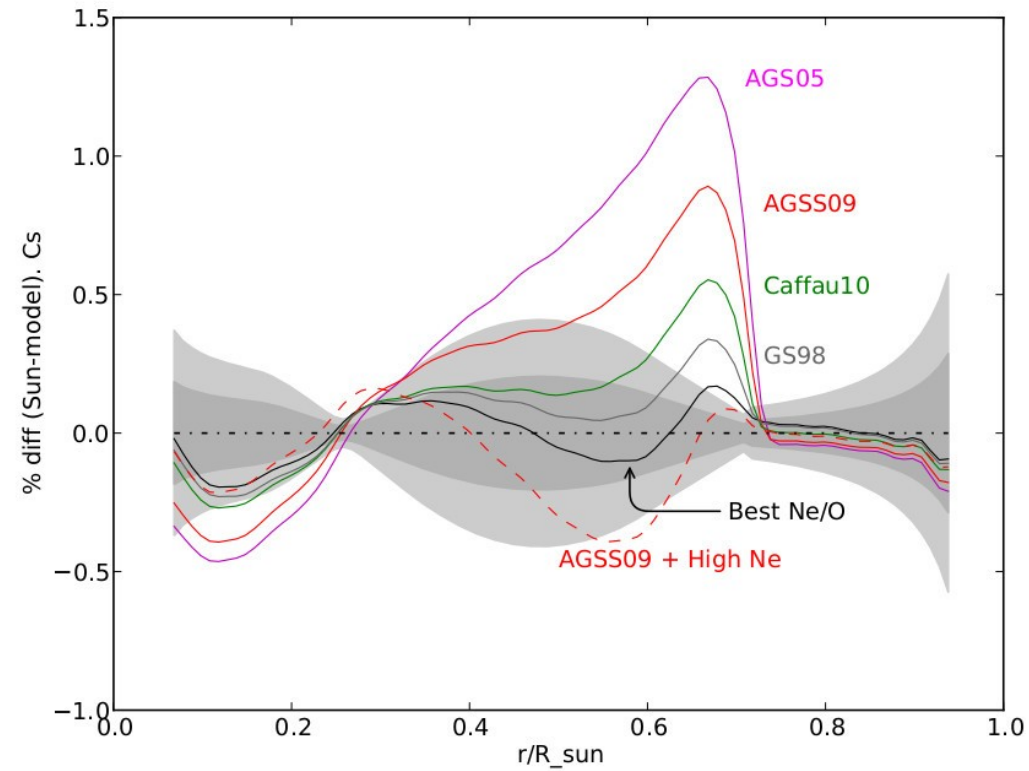
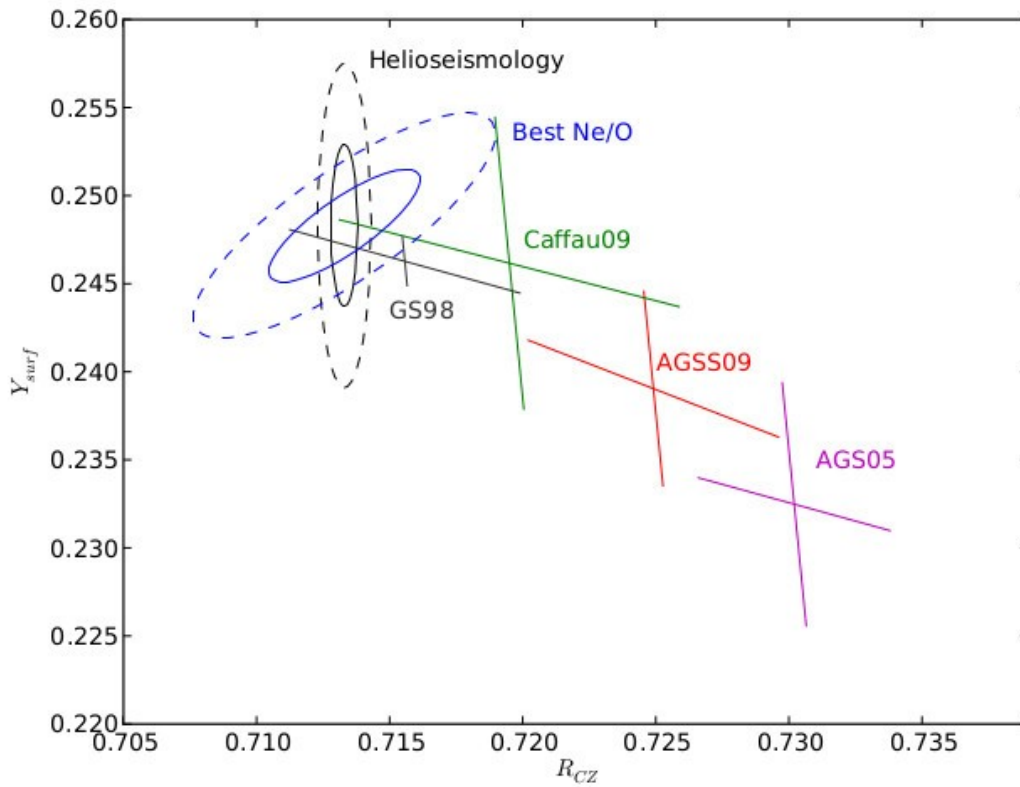
H																				He
Li	Be									B	C	N	O	F	Ne					
Na	Mg									Al	Si	P	S	Cl	Ar					
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr			
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe			
Cs	Ba		Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn			
Fr	Ra		Rf	Db	Sg	Bh	Hs	Mt	Uun	Uuu	Uub									
			La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu			
			Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr			



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Mean opacities and Solar composition

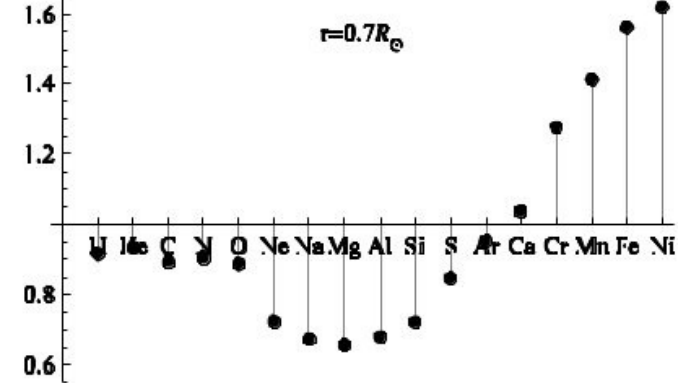
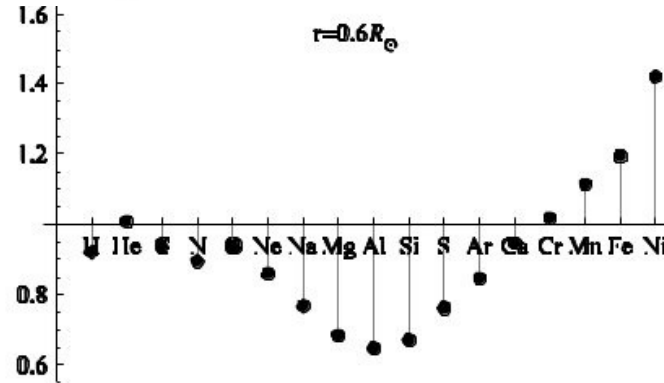
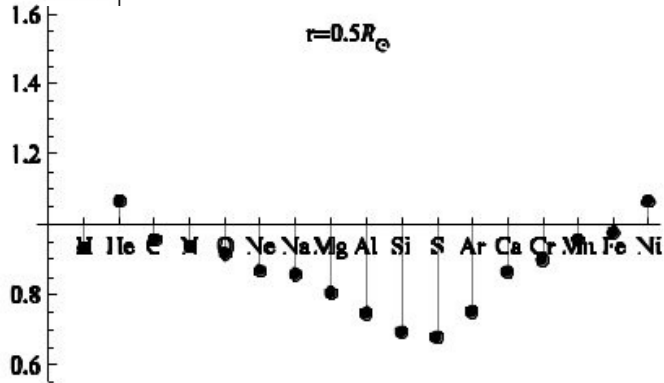
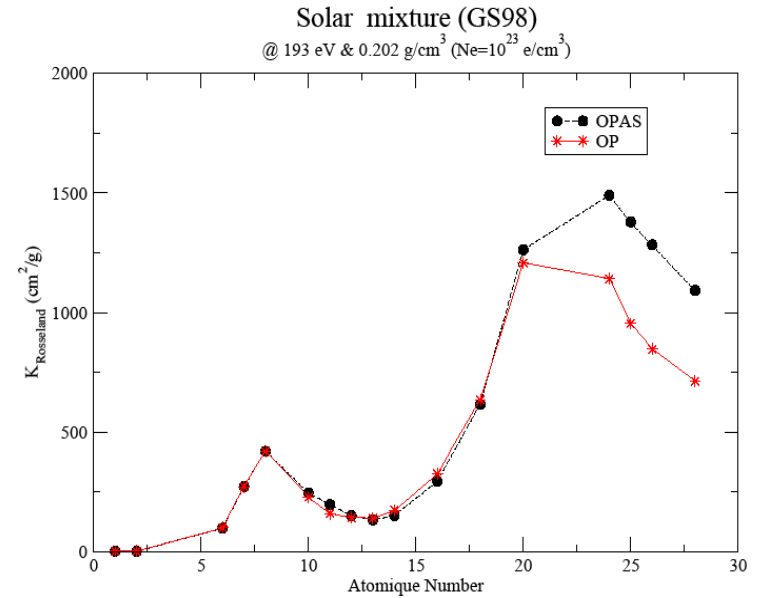
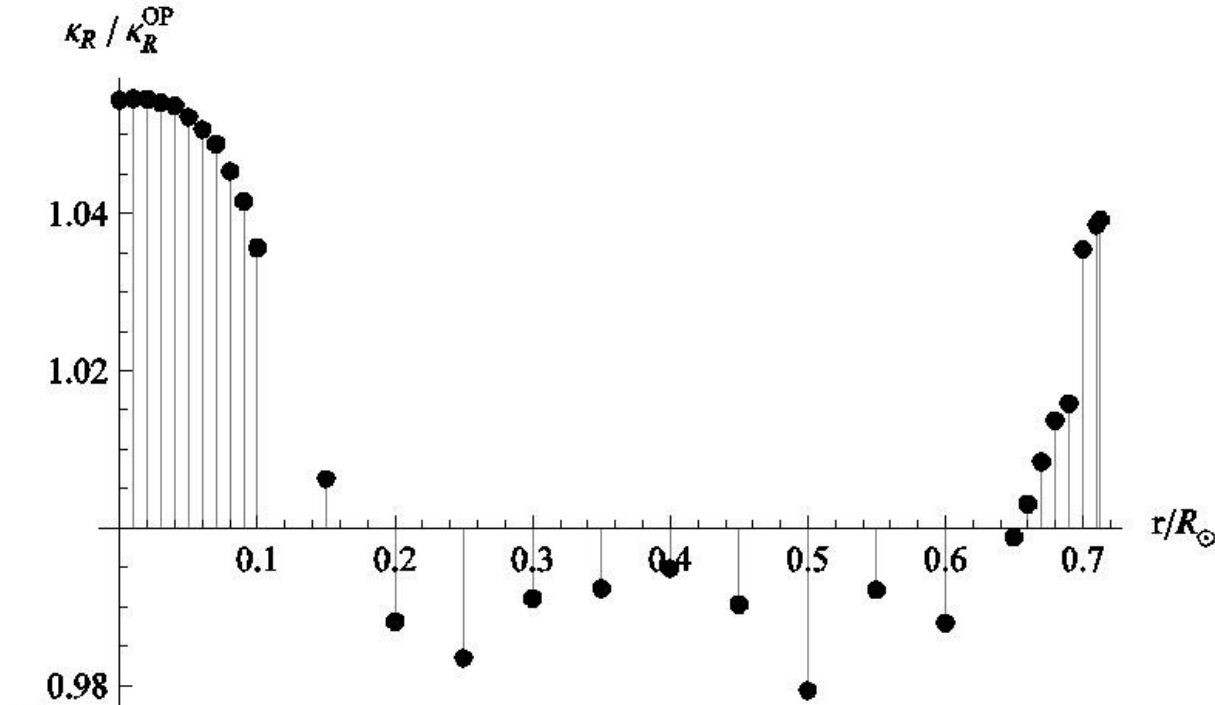




Atomic data for Astrophysics



Discrepancies for element specific mean



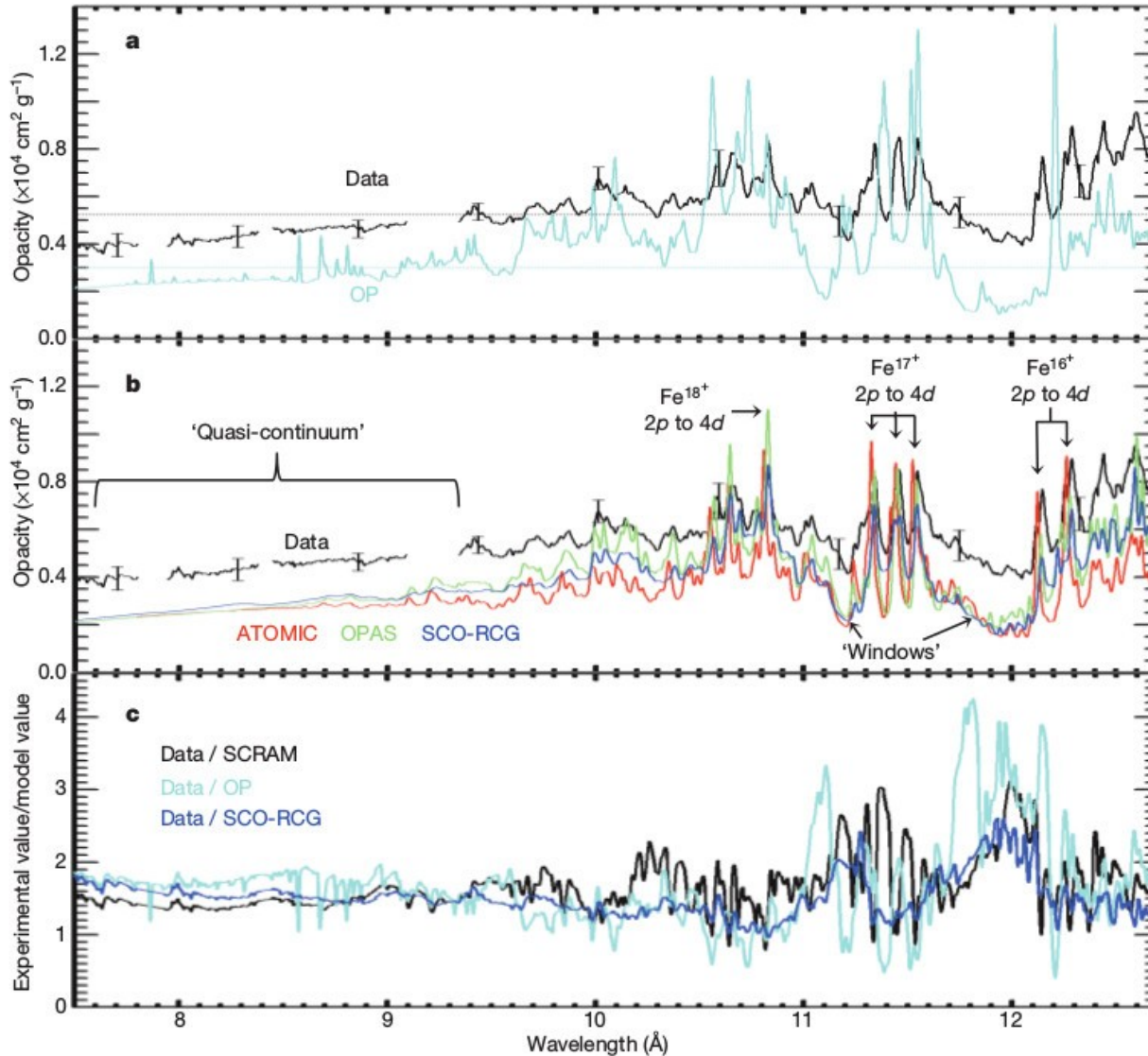
Blancard et al. 2012



Atomic data for Astrophysics



... and for the detailed monochromatic opacities .



J. Bailey et al. 2015,
Comparisons Experiment- Theory
Exp vs OP, ATOMIC, OPAS, SCO-RCG

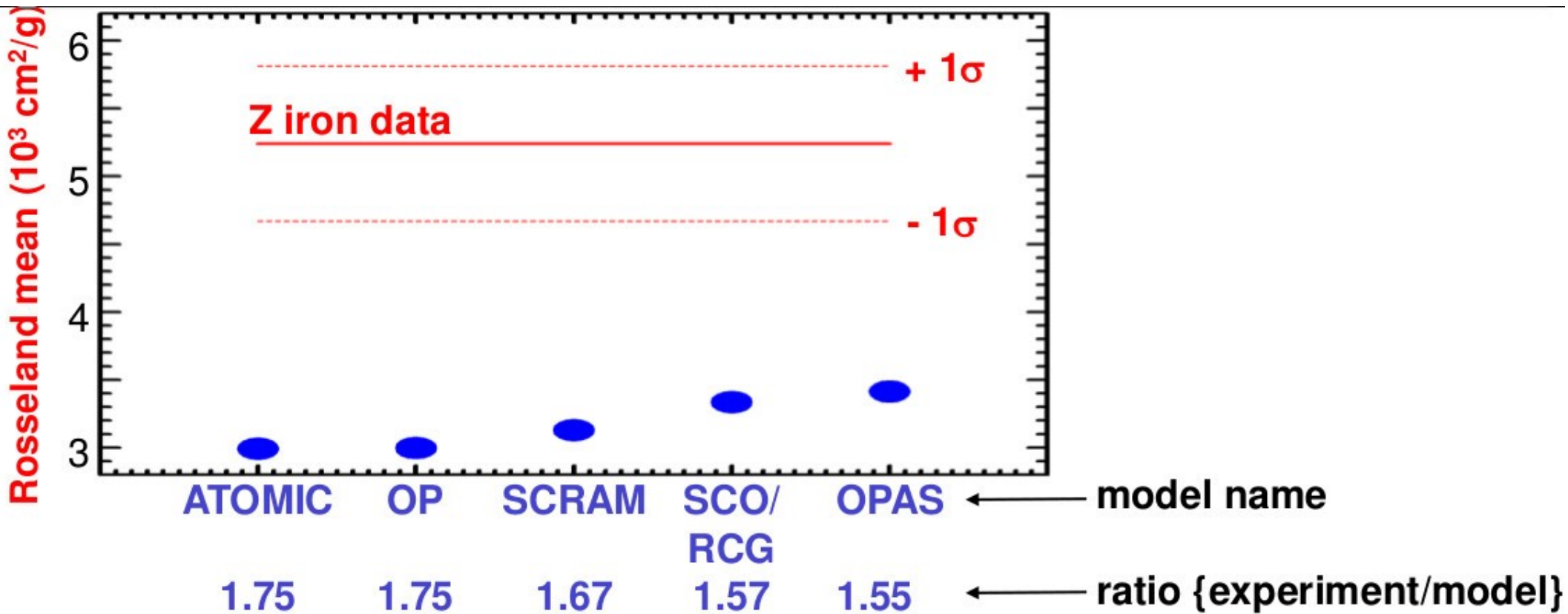
Theory vs Experiment: Fe at
 $T=150 \text{ eV}$ - $N_e = 8.6 \times 10^{21} \text{ cm}^{-3}$



Atomic data for Astrophysics



... and for the detailed monochromatic opacities .



J. Bailey et al. 2016, Experiment vs Theory



How about radiative acceleration?



First new atomic data and new monochromatic opacities

Comparison OP-OPAL

- Données OPAL extraites de travaux précédents par digitalisation des courbes.

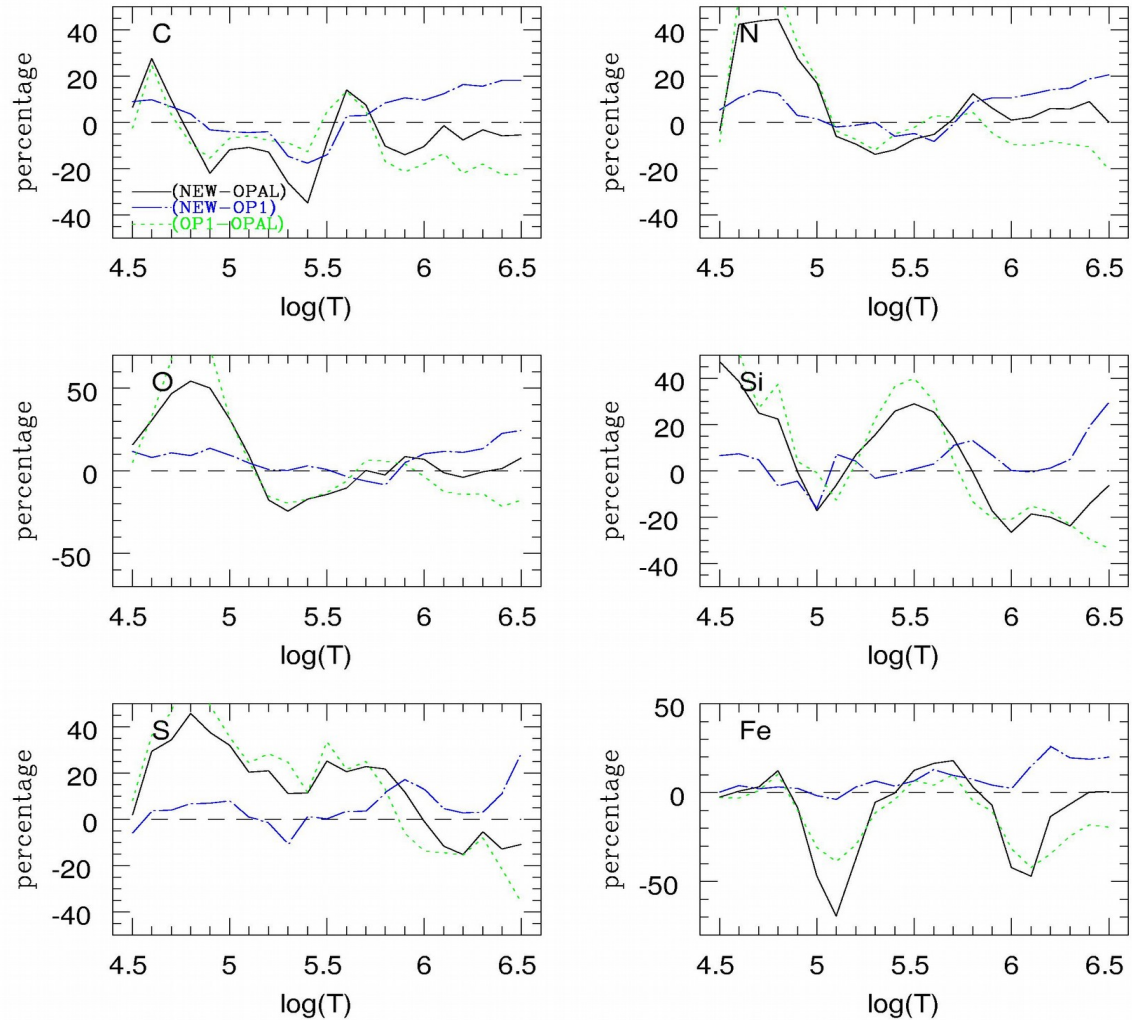
- Même Structure stellaire

 - Simulation d'étoiles HB ou de masse intermédiaire

- Trend: $Z \nearrow$ Diff. \nearrow

Delahaye & Pinsonneault (2005)

$T_{\text{eff}} = 10000 \text{ K}$ $\log(R) = -3$

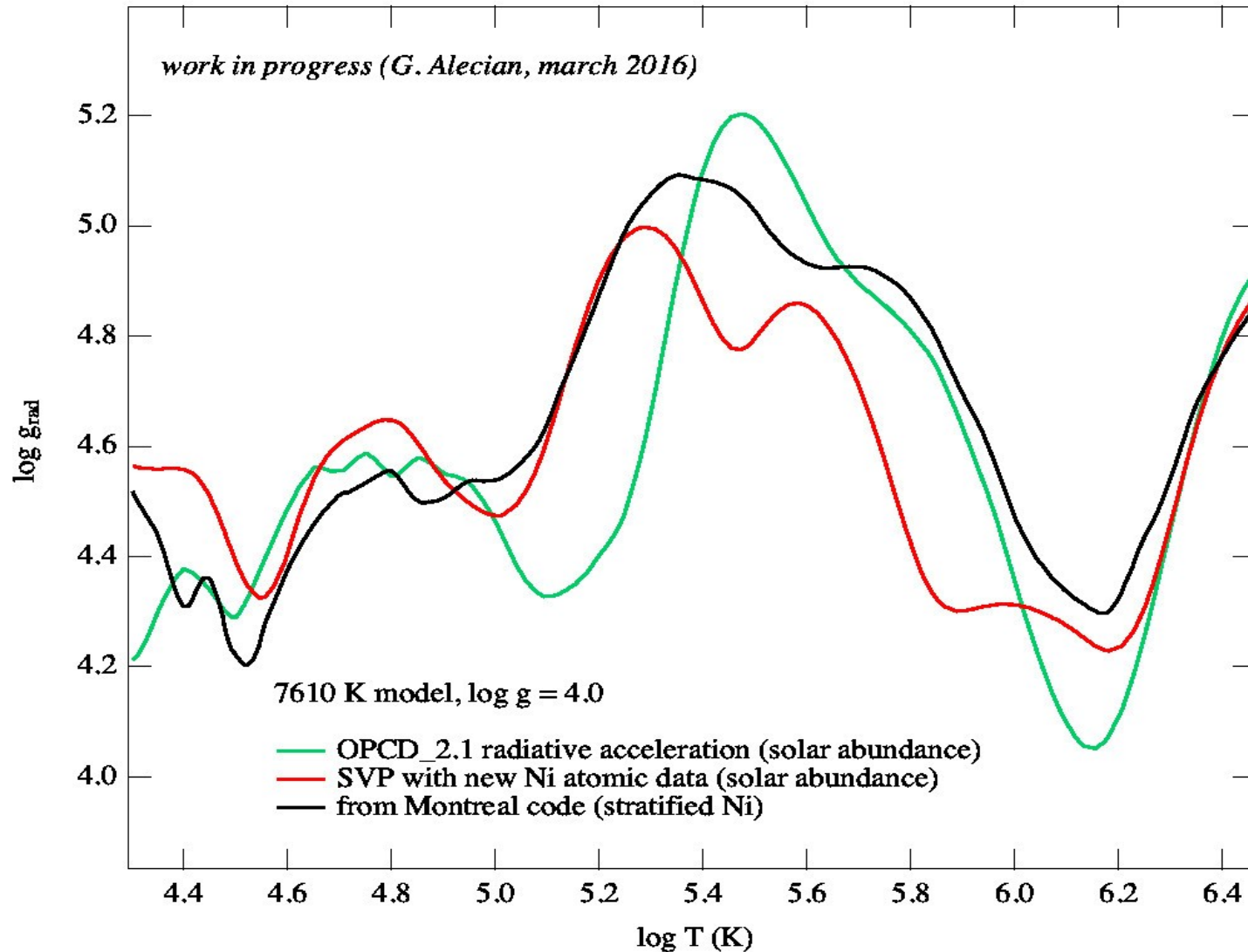




How about radiative acceleration?



First new atomic data and new monochromatic opacities





Atomic data for Astrophysics



Opacities

■ 3 Steps:

- Determination of levels populations and ionic fractions (Equation of State - EOS)
- Calculation of raw atomic data (Atm. Phys)
 - E-levels, radiative data (oscillator strengths , Photoionization cross sections)
- Derive Monochromatic and mean opacities
 - Broadening , near the hedge extrapolations for PI

■ Method:

Several approaches for different physical conditions and elements

Chemical approach

vs

Physical approach

The Opacity-Iron Project

CEA, LANL, LLNL

Free - isolated atoms/ions
 Density effect: Occupation probability approximations 'MHD eos'

Average atom + simplified atm. data
 No approximation for Plasma effects

■ Codes

- Autostructure/Superstructure
- BP-RMATRIX suite of codes

Hulac, Cowan, ATOMIC, FAC
 OPAS, OPAL, LEDCOP, SCO-RCG

■ Aims

High quality atomic data on db
 Monochromatic and mean opacities db + server
 Radiative accelerations on db

High quality eos on db
 Mean opacities



Atomic data for Astrophysics



Opacities: What could be wrong?

- Ionic Fractions and level populations = EOS
- Raw atomic data (Atm. Phys)
 - E-levels, radiative data (oscillator strengths , Photoionization cross sections)
- Monochromatic and mean opacities
 - Broadening , near the hedge extrapolations for PI
- Experiment

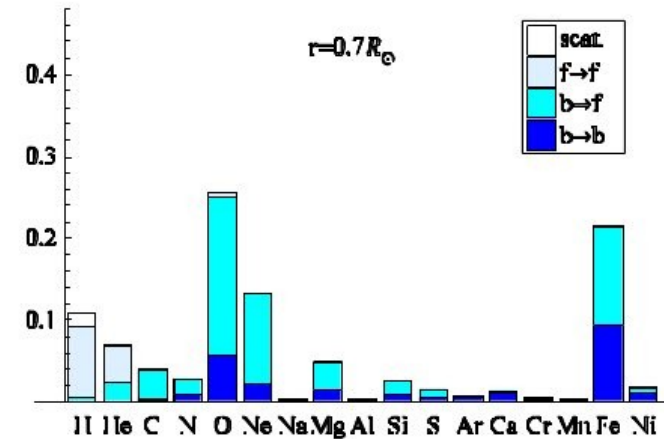
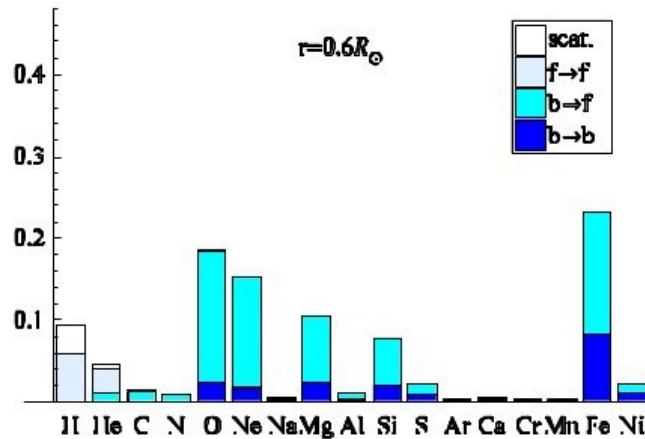
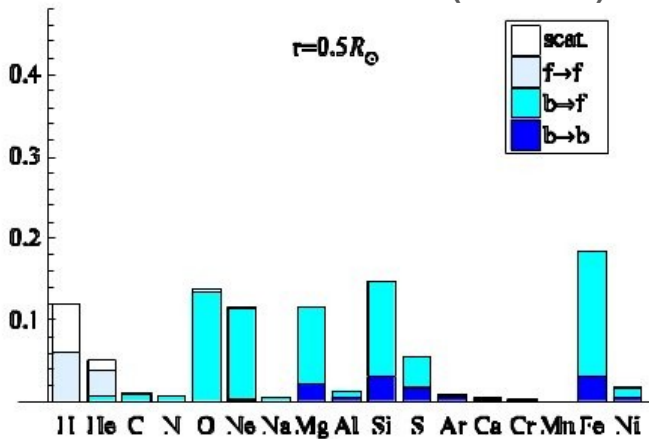
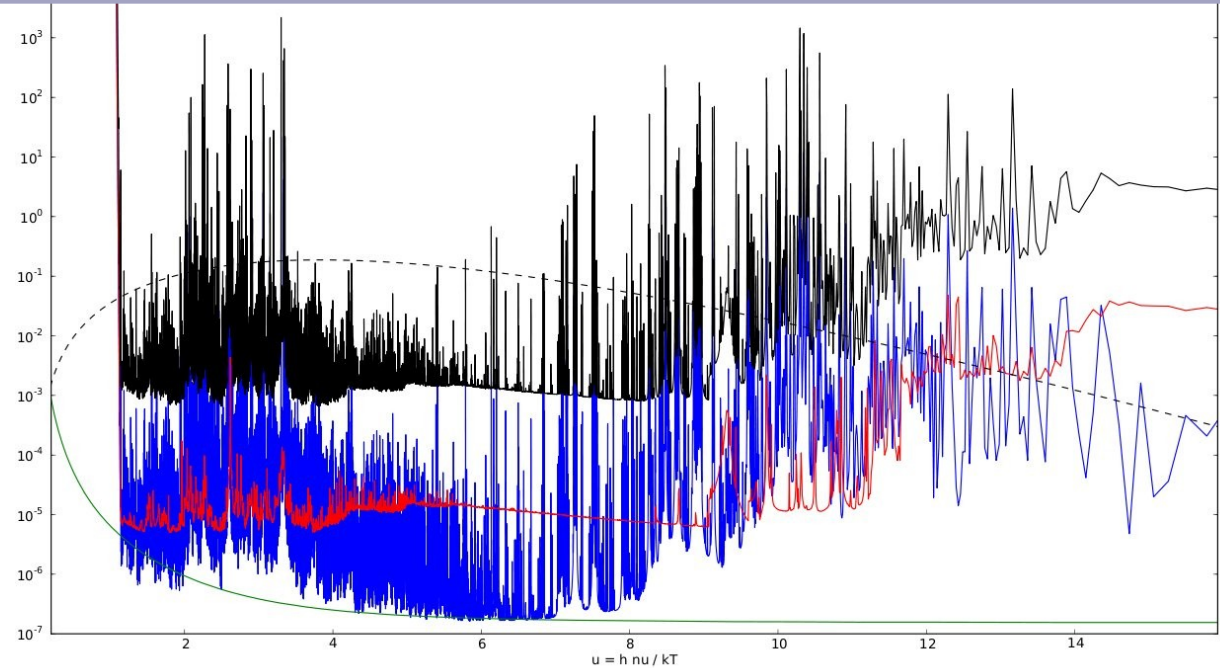


Different components of opacities



Bound-Bound vs Bound-Free vs Free-Free

- Depending on conditions, Bound-Free dominates opacity contribution in the total opacity
 - Bound-Bound (Blue)
 - Bound-Free (Red)
 - Free-Free (Green)
 - Total*100 (Black)





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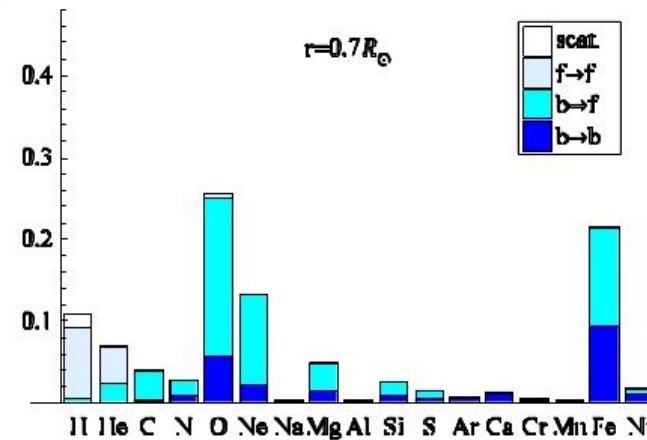
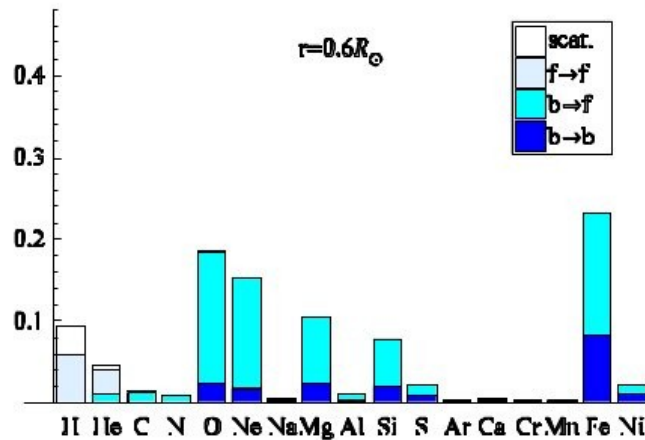
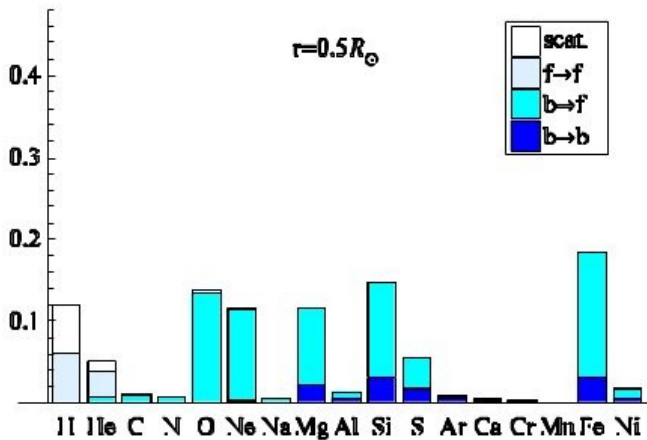
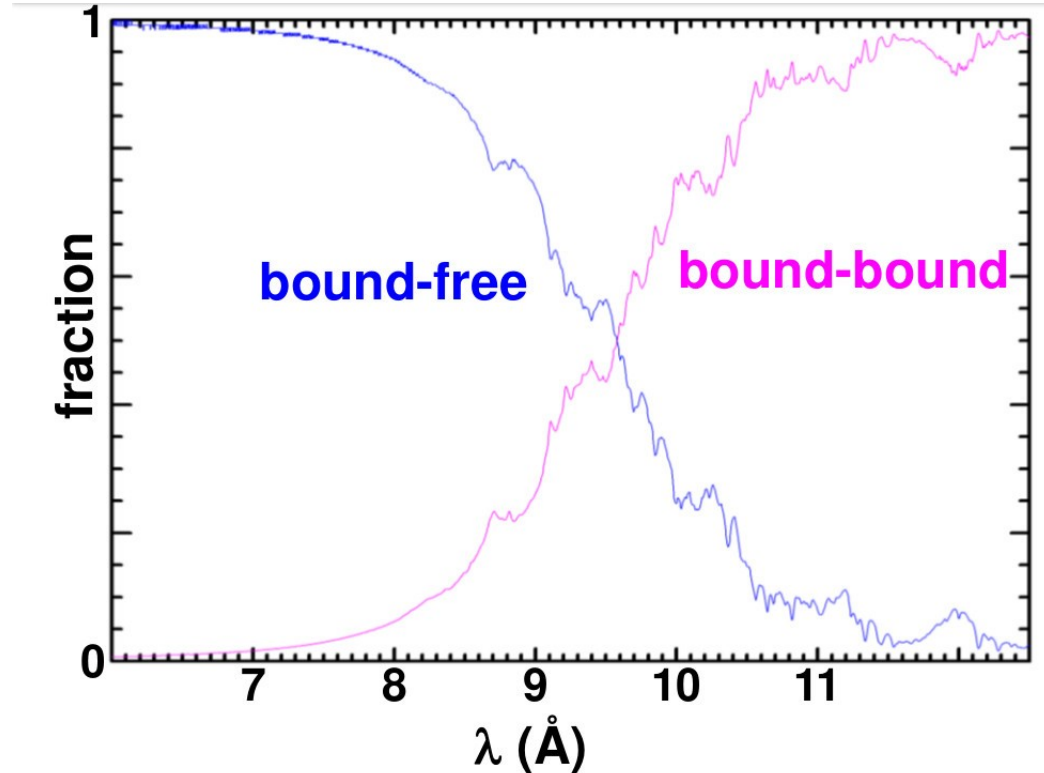


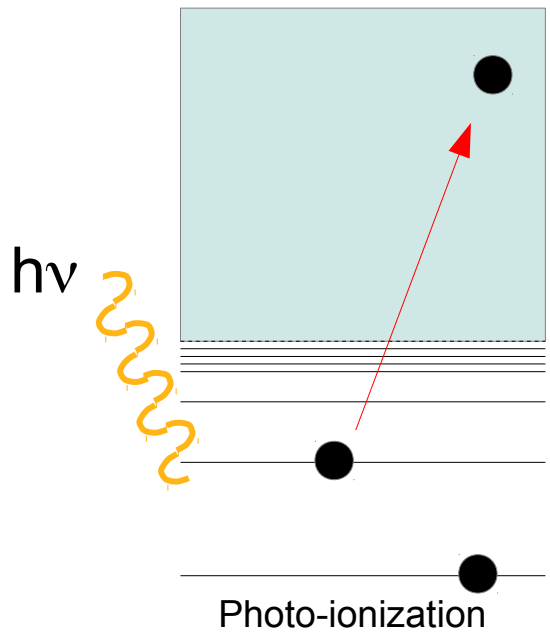
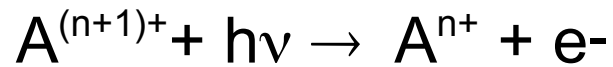


Photo-ionization - Bound-Free

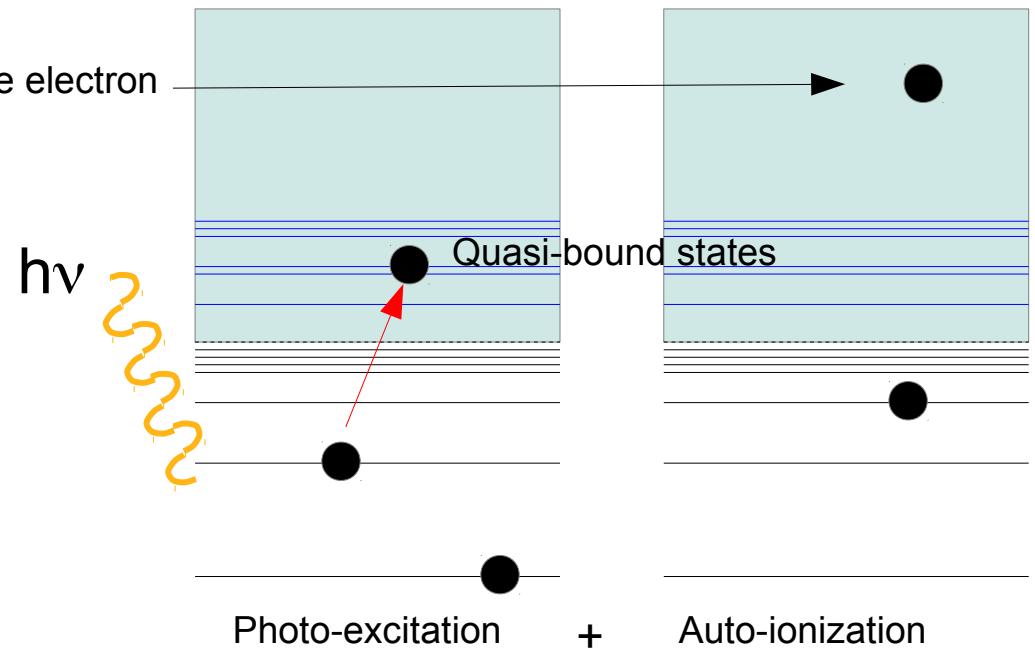
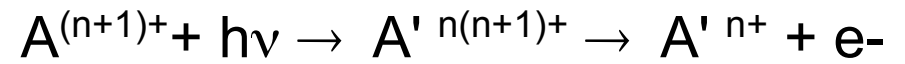


Two codes - Two approaches

Direct Process



Indirect Process



Autostructure: 2 distinct processes – 2 “independent” calculations

Rmatrix: One unique calculation – Resonances directly included.



Coupling of resonances



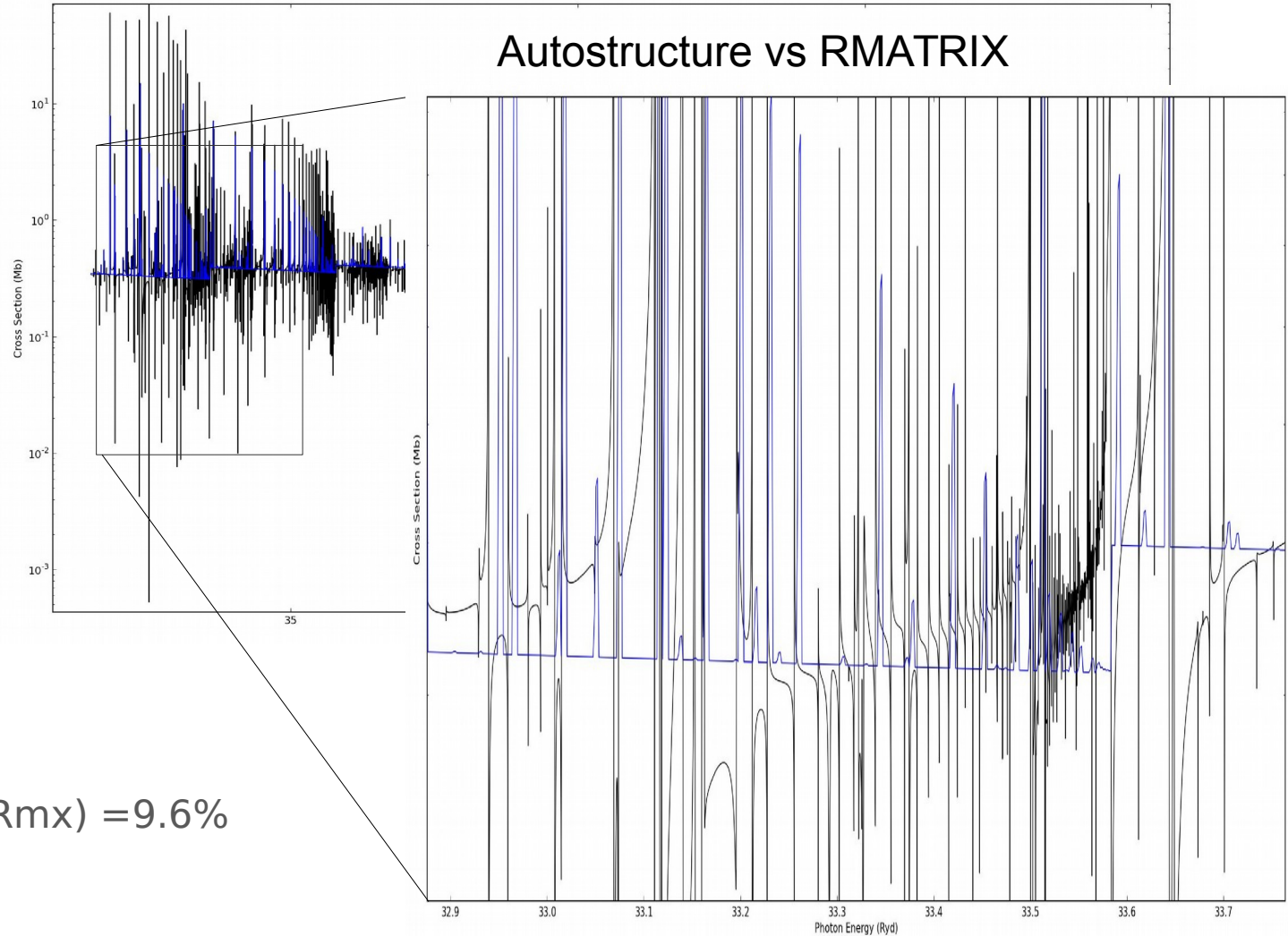
Ni XIV +hv → Ni XV+e⁻ - Ground state photoionization

- 2 methods:
Autostructure & BP-RMATRIX

- AS (Blue): Direct PI & Indirect PI - two distinct calculations
- BPRM (Black): interferences between resonances and background PI

- Results for GS:

- $(\kappa_R(\text{Rmx}) - \kappa_R(\text{AS})) / \kappa_R(\text{Rmx}) = 9.6\%$

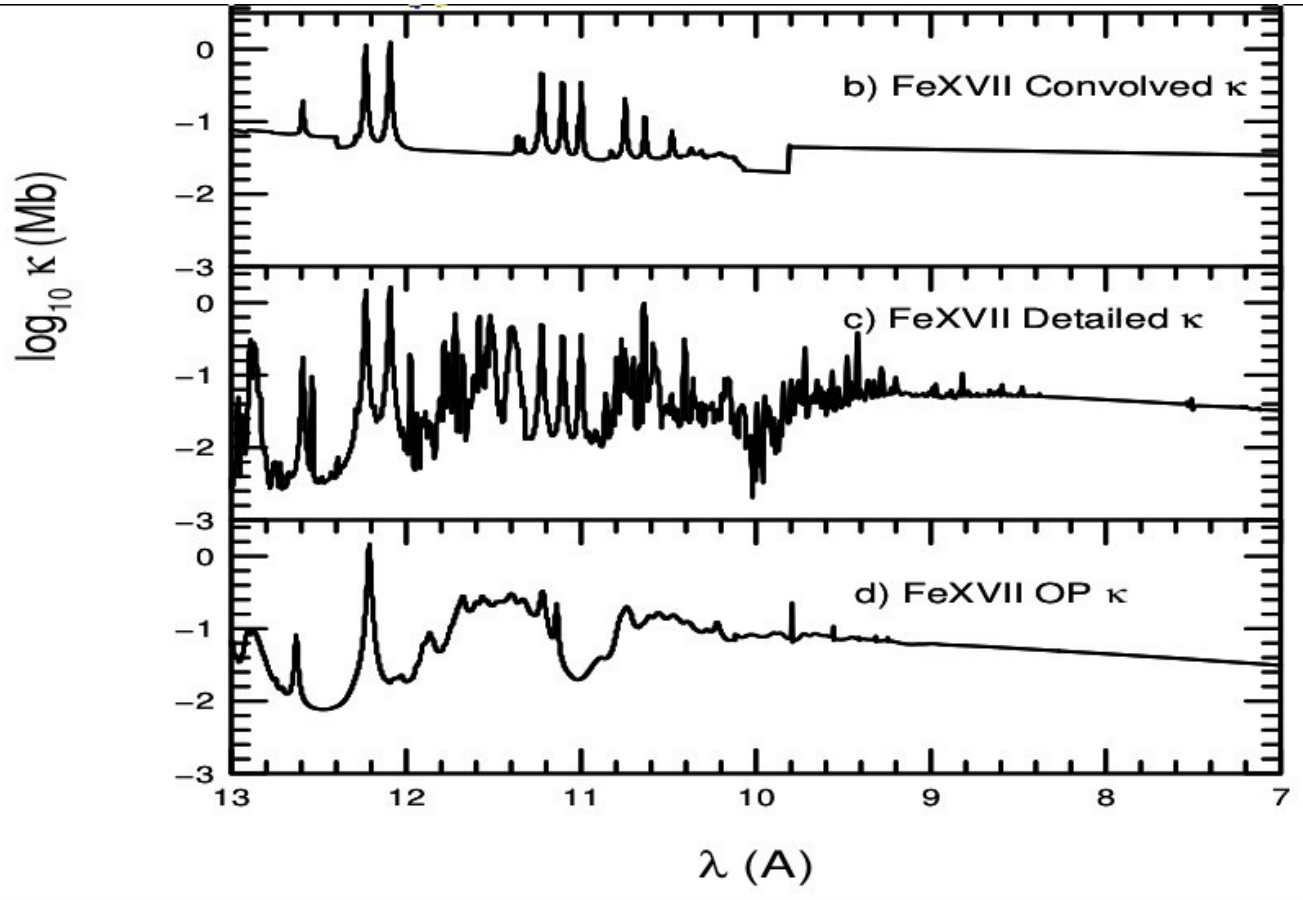
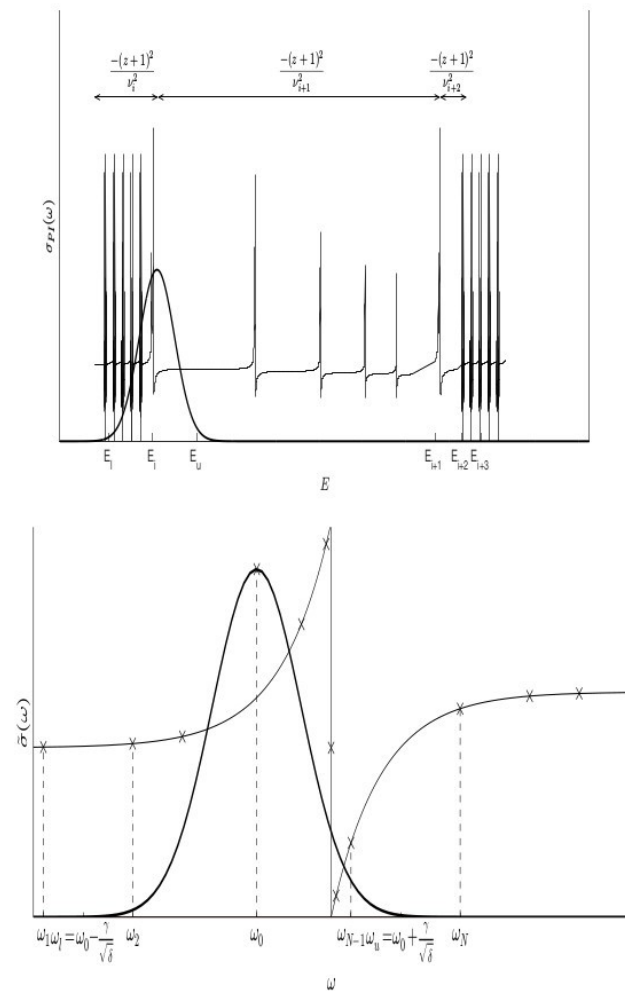




Broadening of resonances - Fe XVII test



Fe XVII + hv → Fe XVIII + e⁻ - Broadening



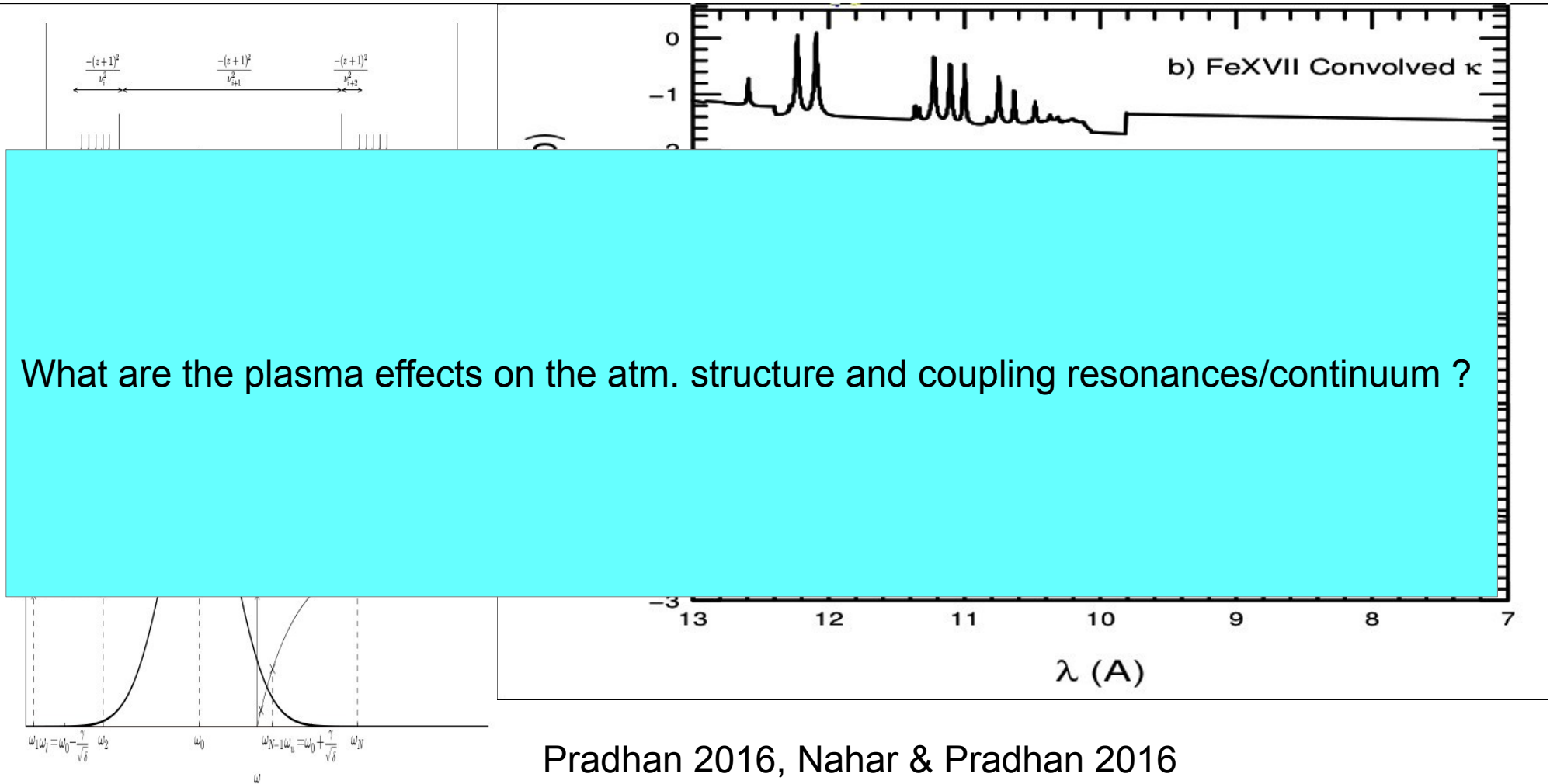
Pradhan 2016, Nahar & Pradhan 2016



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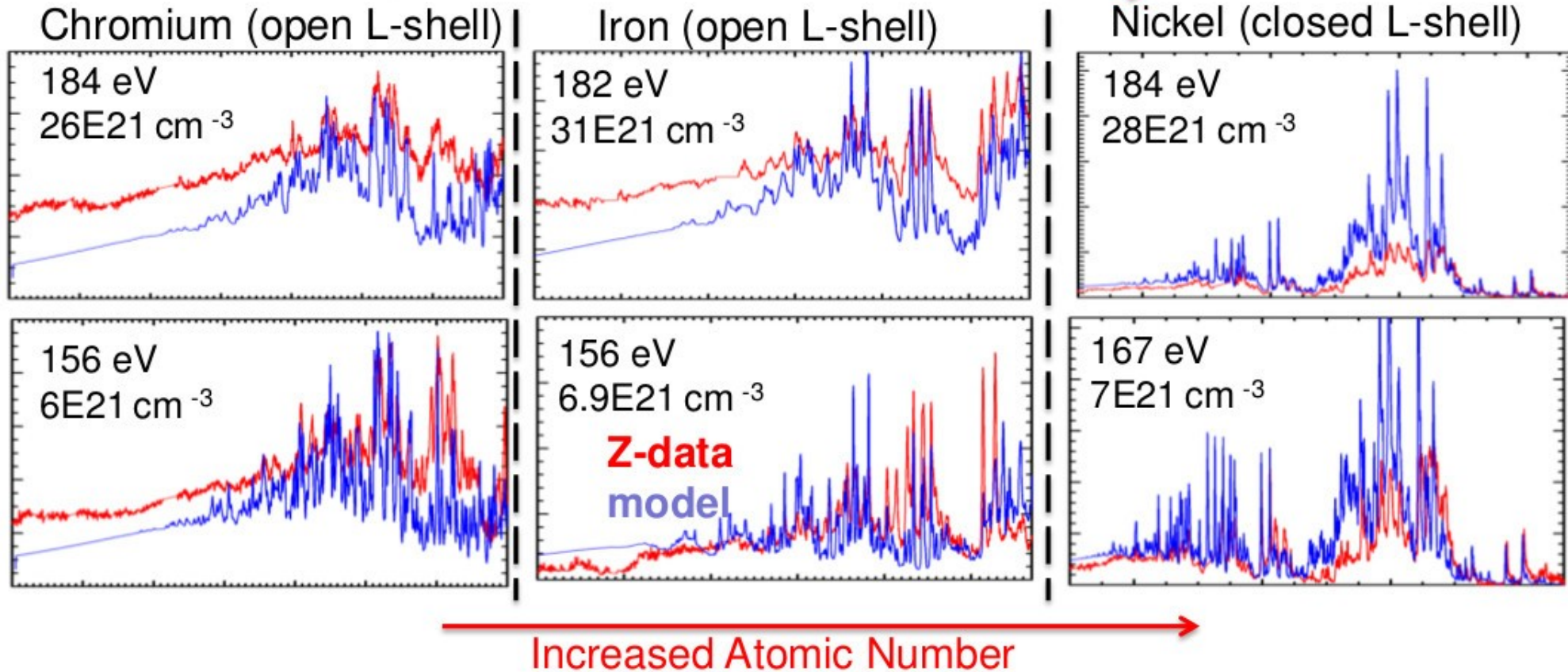
Any other ideas?



Cr, Fe and Ni

fewer L-shell vacancies, lower excited state populations

Increased Temp. and Density



Bailey et al. 2016



Lots of activities

Theory - Experiments - Applications cycle

Theoretical
Atomic Data

Applications
Modelisation/Simulation



Experiments

Stellar Structure & evolution:

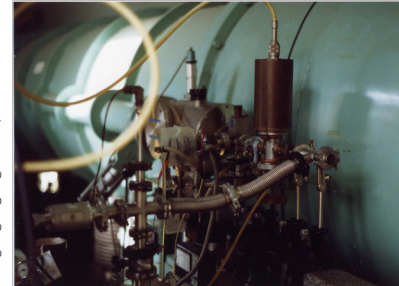
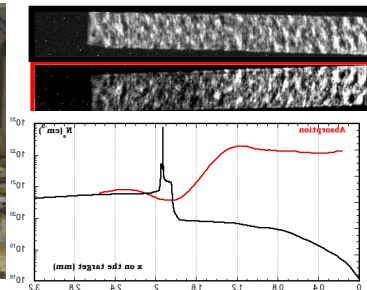
- New opacity tables with high density grid in T, Ne and compositions.
- Radiative acceleration - benchmarking

Code:

- Yale Rotational Evolution Code (YREC)

Prospective

- Experiments on intense laser (LMJ)?
 - Rejected!
- Photoionization experiment?
 - To be designed



Codes:

- The Iron Project & The Opacity Project (IPOPv2)
 - BPRM vs DARC vs Autostructure
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- Others:
 - LANL - DW code vs OP - DW AutoStructure
- Optimization of codes for heavy elements

Workshop in 2017:

Physical (OPAL-OPAS-LEDCOP ...) vs Chemical (IPOPv2)



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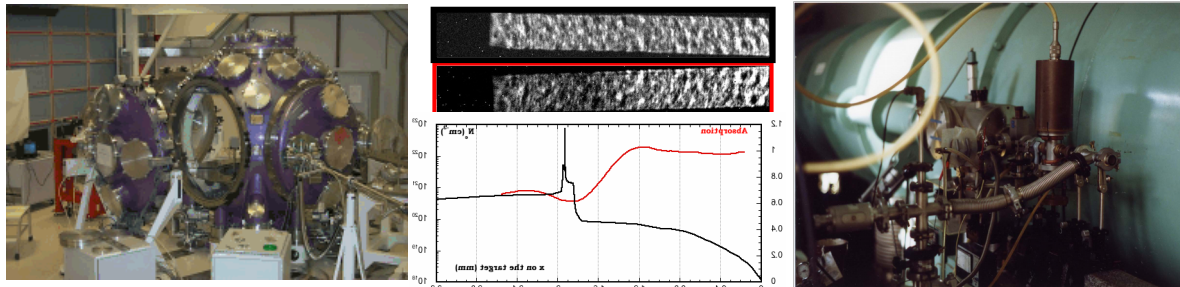
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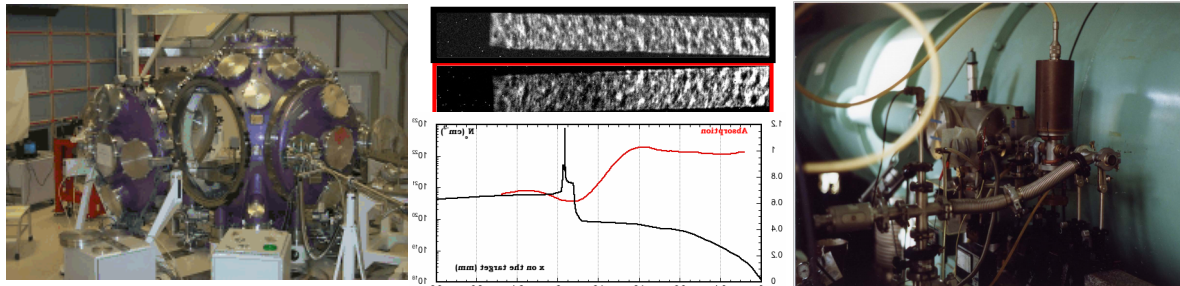
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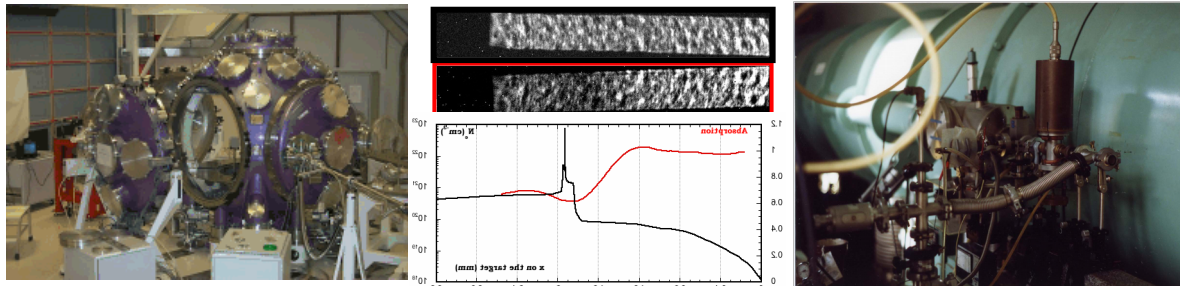
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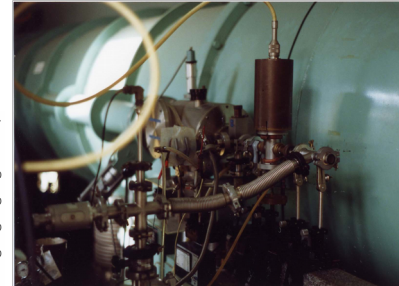
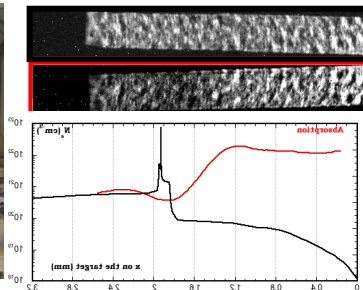
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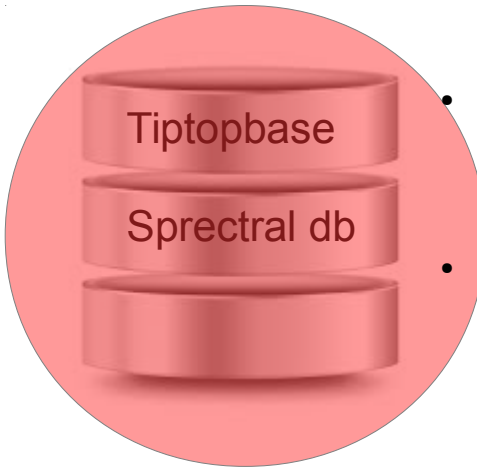


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- Tools for data analysis, comparison & visualization for users
- Data quality estimation

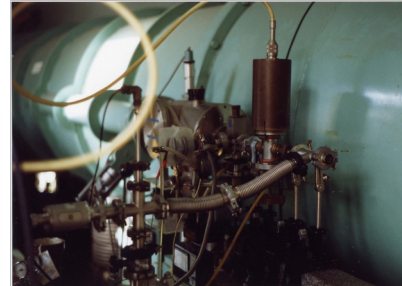
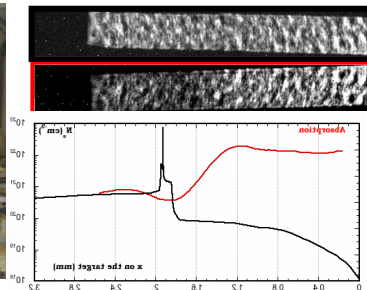
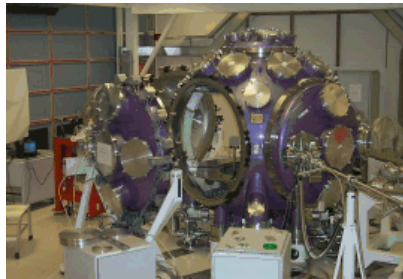
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