FLYCHK *@ NIST*

http://nlte.nist.gov/FLY/

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2017 Joint ICTP-IAEA School on Atomic Processes in Plasmas

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International Atomic Energy Agency

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ictp01	787960	ABDELTAWWAB MOHAMED	ictp18	723518	DIFALLAH MOSBAH
ictp02	654332	ABRANTES RICHARD JUNE	ictp19	531947	DOBRODEY STEPAN
ictp03	792548	AGGARWAL SUNNY	ictp20	704461	DOU LI
ictp04	223002	ALBRECHT MARTIN	ictp21	456302	EKSAEVA ALINA
ictp05	785332	ANAND VENU	ictp22	885562	GOYAL ARUN
ictp06	015238	BEERWERTH RANDOLF	ictp23	322575	GALL AMY
ictp07	219075	BENTOTOCHE MOHAMED	ictp24	545845	GAO CHENG
		SADEK	ictp25	315419	GAO LAN
ictp08	089206	BISWAS SUBIR	ictp26	018550	GARTEN MARCO
ictp09	752765	CHO MIN SANG	ictp27	280801	GRUCA MARTA
ictp10	403691	CAO SHIQUAN	ictp28	544762	GU LIYI
ictp11	336321	CARIATORE NELSON	ictp29	598412	GUPTA DHANOJ
ictp12	496889	CHANNPRIT KAUR	ictp30	181375	HALA
ictp13	401827	CHEN ZHAN-BIN	ictp31	655797	HOSSAIN MOHAMMAD
ictp14	938990	CLAUSER CESAR			AFAQUE
ictp15	918970	CONDAMINE FLORIAN	ictp32	015021	HUEBL AXEL
ictp16	895373	CUMBEE RENATA	ictp33	080588	IORGA CRISTIAN
ictp17	035430	DOHL LEONARD	ictp34	424946	JOURDAIN NOEMIE

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ictp35	725423	KELLA VARA
ictp36	119429	KHIAR BENJAMIN
ictp37	847007	KNOTT SEAN
ictp38	089150	KOSTIC ANA
ictp39	381771	KRUSIC SPELA
ictp40	783330	LOPEZ SEBASTIAN
ictp41	924662	LANE THEODORE
ictp42	513660	LIU LIPING
ictp43	456011	LIU PENGFEI
ictp44	099669	MELSHEIMER FLORIAN
ictp45	839230	MIN QI
ictp46	982656	ONGALA-EDOUMOU SAMUEL GWLANOLD
ictp47	496533	PEHLIVAN ASLI
ictp48	208381	PRITI PRITI
ictp49	447035	SAHA JAYANTA
ictp50	600432	SRIVASTAVA ANAND KUMAR
ictp51	926923	SAXENA VIKRANT
ictp52	560508	SEREDA STEPAN
ictp53	739888	SHAH CHINTAN
ictp54	810463	SHARMA PRASHANT
ictp55	438455	SHEIL JOHN
ictp56	128232	SILWAL ROSHANI
ictp57	840757	TORRETTI FRANCESCO
ictp58	629008	VAZQUEZ FERNADEZ TELLO ELISA
ictp59	862626	WEI YANLING
ictp60	426683	WAN YIER
ictp61	043910	WU DONG
ictp62	585323	WU YUANBIN
ictp63	073033	ZAMMIT MARK
ictp64	743175	BHATTACHARYYA SUKHAMOY
ictp65	275040	Kaur Jaspreet
ictp66	329493	SAXENA ANKITA
ictp67	085878	Della Picca Renata

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ABOUT FLYCHK

Population Kinetics Modeling

Rate equations are solved for level population distributions for a given plasma conditions

$$\frac{dn_i}{dt} = -n_i \sum_{j \neq i}^{N\max} W_{ij} + \sum_{j \neq i}^{N\max} n_j W_{ji}$$

$$W_{ij} = B_{ij}\overline{J_{ij}} + n_e C_{ij} + \beta_{ij} + n_e \gamma_{ij}$$

$$W_{ji} = A_{ij} + B_{ji}\overline{J_{ji}} + n_e D_{ji} + n_e(\alpha_{ji}^{RR} + \alpha_{ji}^{DR}) + n_e^2 \delta_{ij}$$

- B_{ij} Stimulated absorption
- C_{ij} Collisional excitation
- γ_{ij} Collisional ionization
- β_{ij} Photoionization (+st. recom)

- A_{ij} Spontaneous emission
- B_{ij} Stimulated emission
- D_{ij} Collisional deexcitation
- α_{ij}^{DR} Dielectronic recombination
- α_{ij}^{RR} Radiative recombination
- δ_{ij} Collisional recombination

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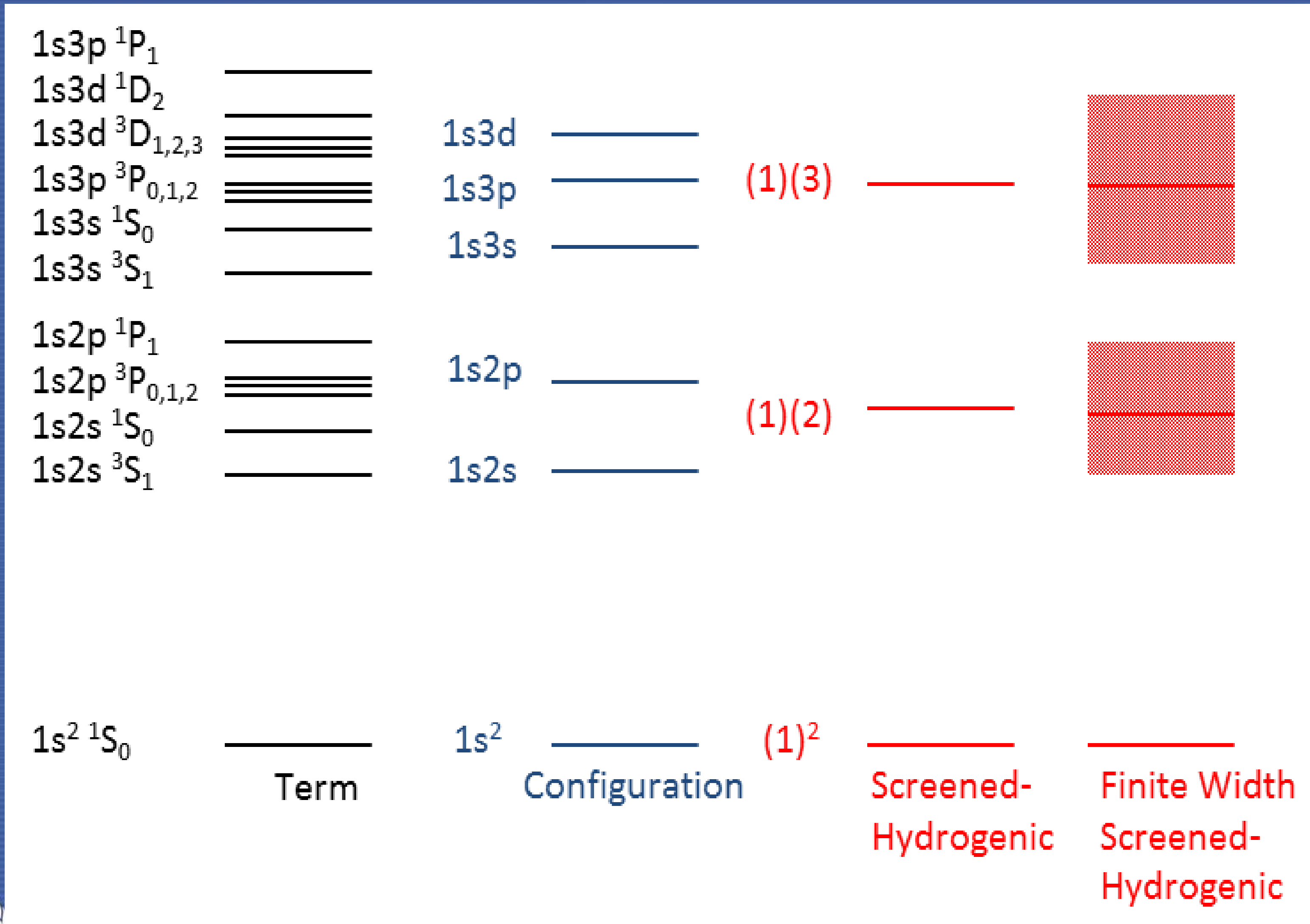
FLYCHK uses screened hydrogenic levels (super configurations)



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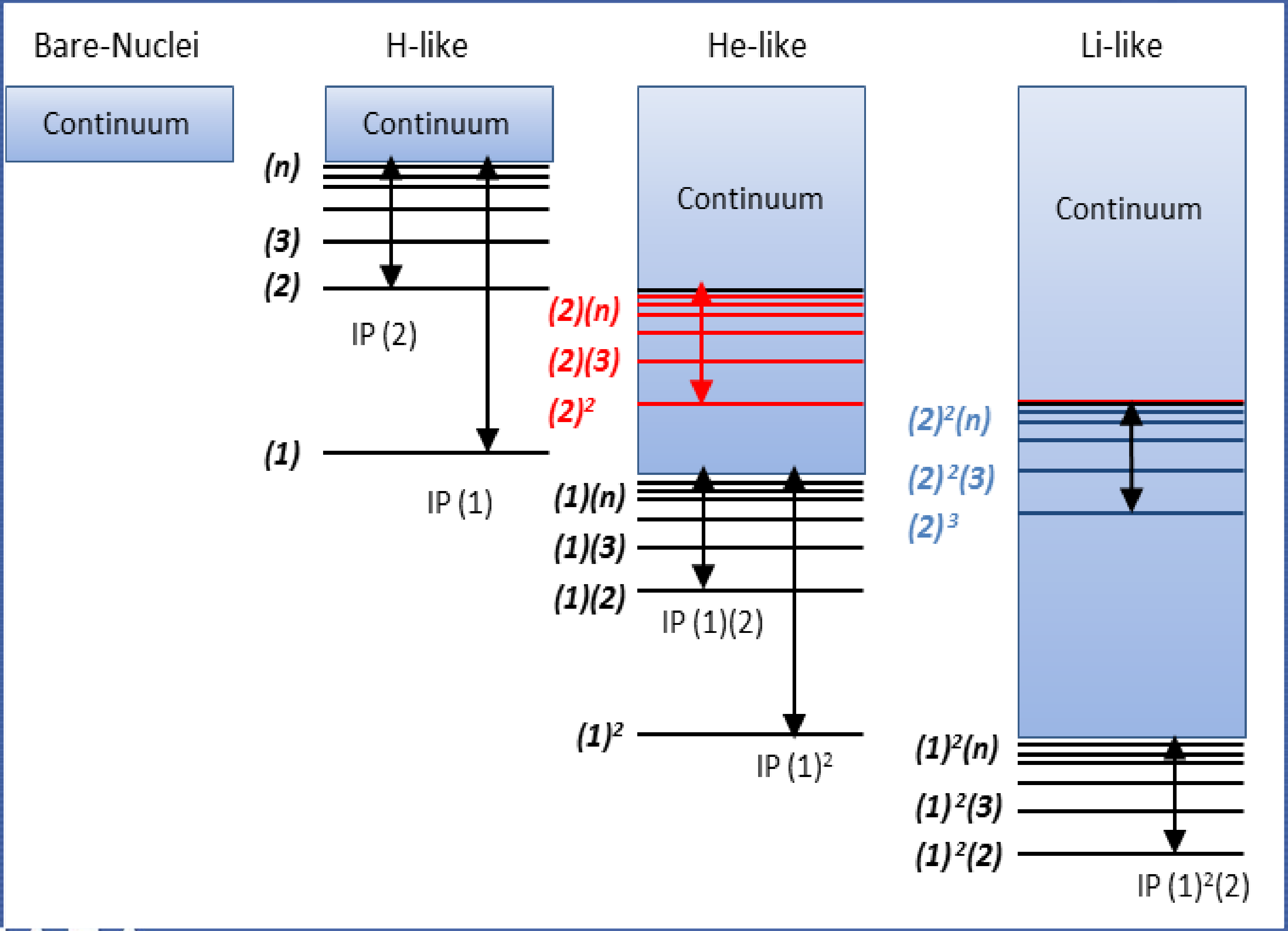
Level energy obtained with ionization potential from its 1st continuum level



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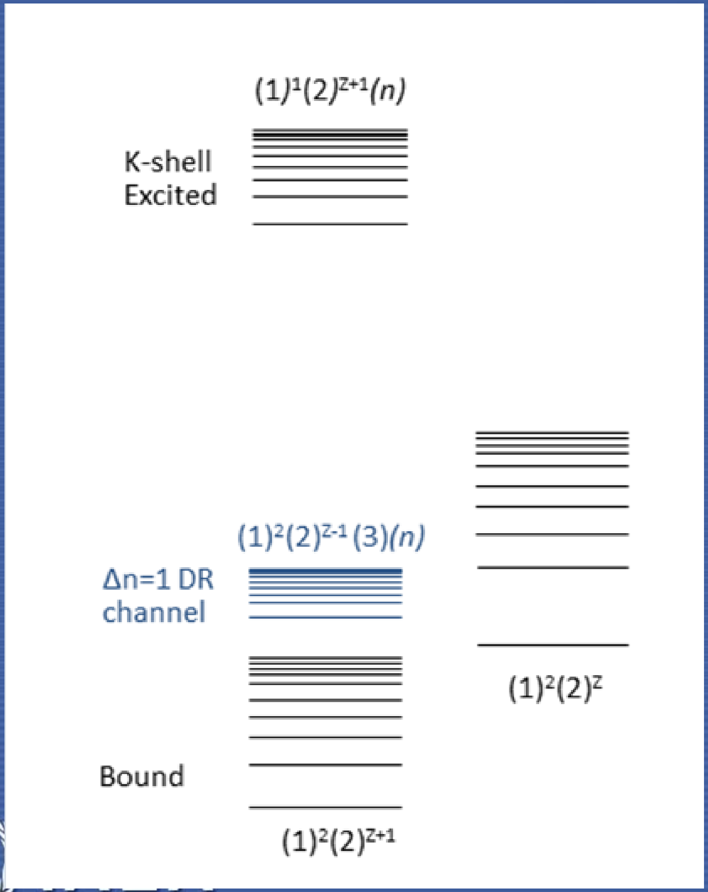
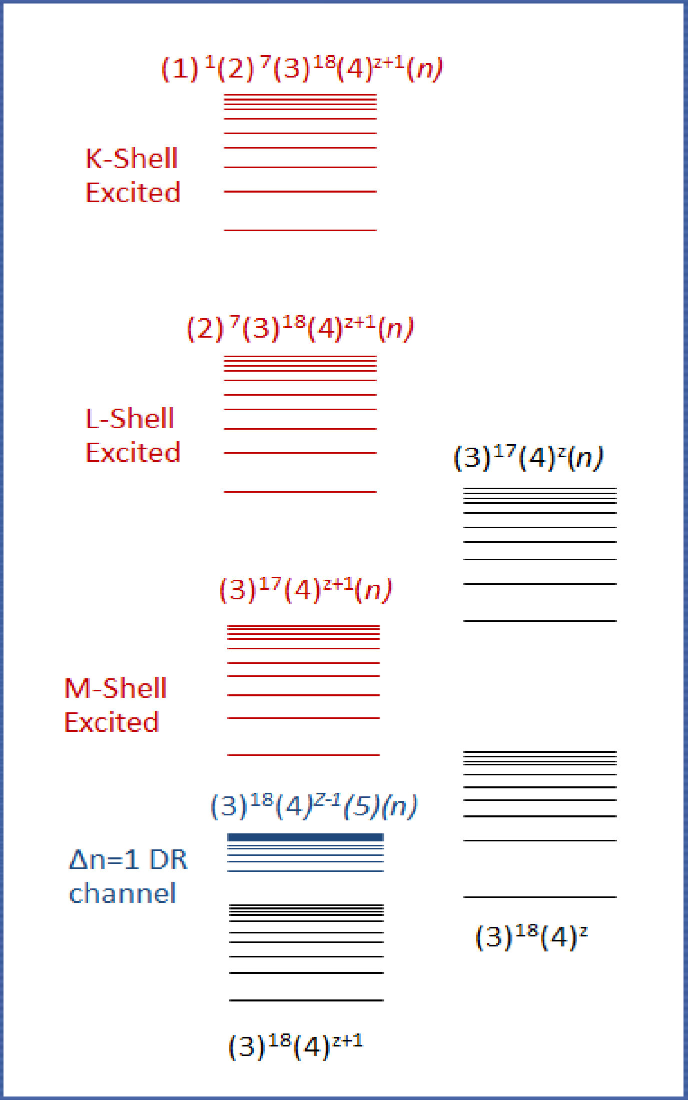
Configurations included in FLYCHK

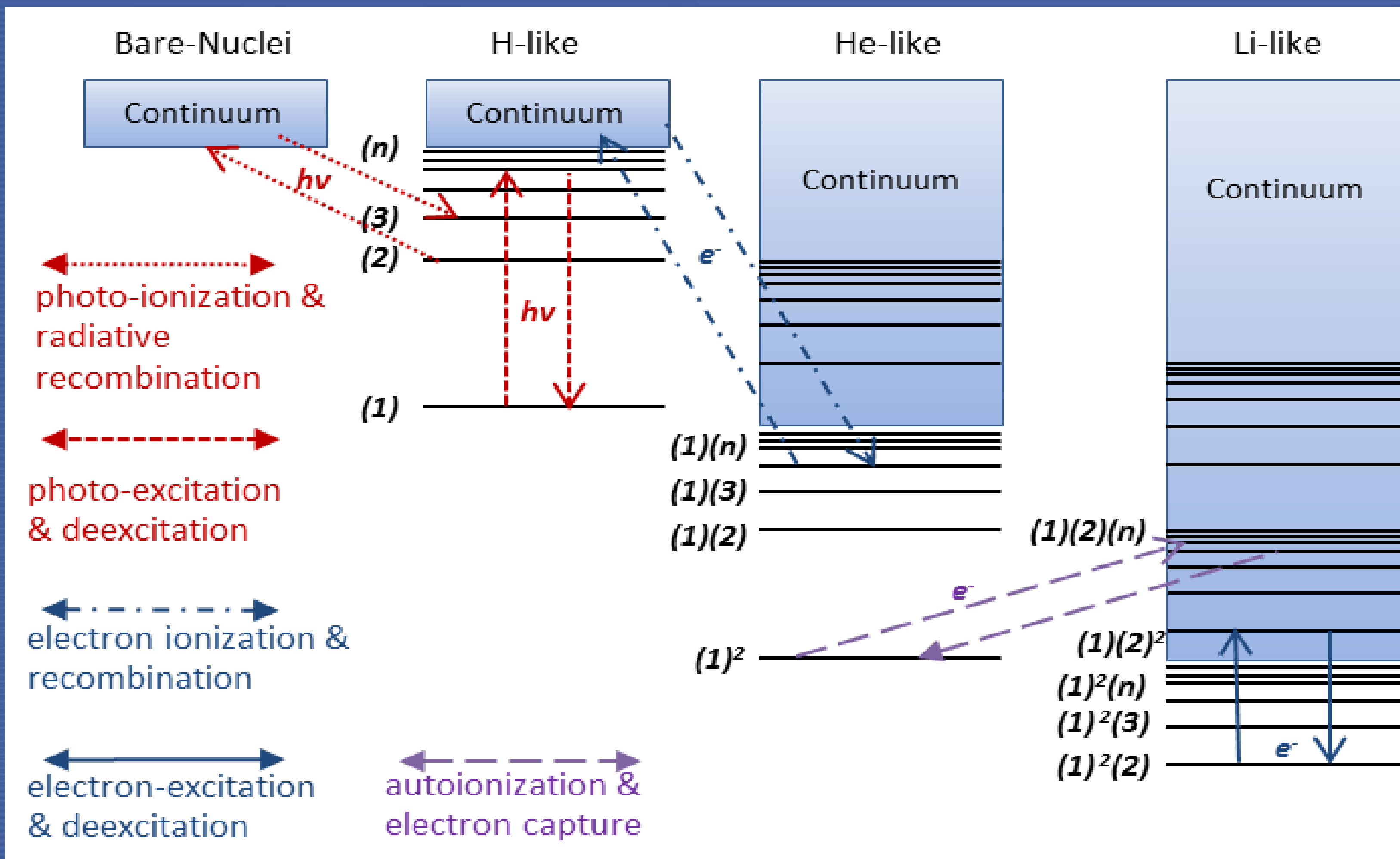
L-shell Ions



N-shell Ions



Atomic processes included in FLYCHK



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FLYCHK Model : *simple, but complete*

- Screened hydrogenic energy levels with relativistic corrections
- Relativistic Hartree-Slater oscillator strengths (M. Chen) and photoionization cross-sections (J. Scofield,+ Kramer)
- Fitted collisional cross-section to PWB approximation (M. Chen)
- Semi-empirical cross-sections for collisional ionization (A. Burgess)
- Detailed counting of autoionization and electron capture (M. Chen)
- Continuum lowering (Stewart-Pyatt, Ecker-Kroll)

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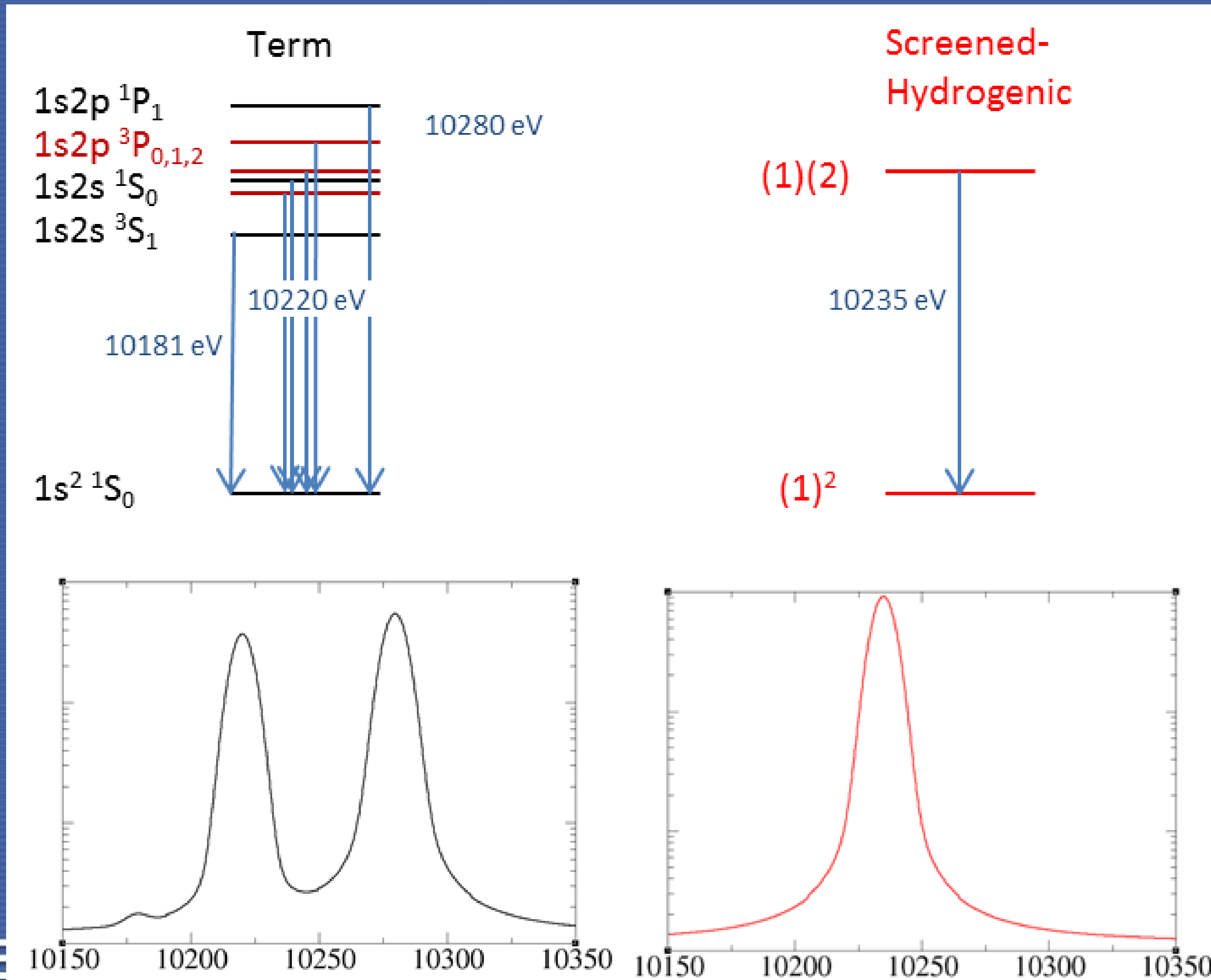
ABOUT FLYSPEC

FLYSPEC uses detailed (H, He, Li-like) and Super Transition Array for spectra



Spectral Types

Z < 27 H, He and Li	FLY model
Z > 27 H, He and Li	HULLAC data (term levels up to n=4)
Be-like and lower charge states	Super Transition Array (STA) made with Configurations (jj) 1s, 2s, $2p^-$, $2p^+$, 3s, $3p^-$, $3p^+$, $3d^-$, $3d^+$, Up to n=6

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Energy-dependent spectral intensity in the STA formalism

Spectra for specific E/ ranges: STA formalism

Spectra using configuration-average atomic data generated by the DHS (Dirac-Hartree-Slater) code (M.Chen)

$$\eta(\nu) = n_A A_{AB} E_{AB} \phi(\nu) = \frac{n_A \sum\limits_{i \in A: j \in B} g_i \exp(-E_i / kT_e) A_{ij} E_{ij} \phi(\nu)}{\sum\limits_{i \in A: j \in B} g_i \exp(-E_i / kT_e)}$$

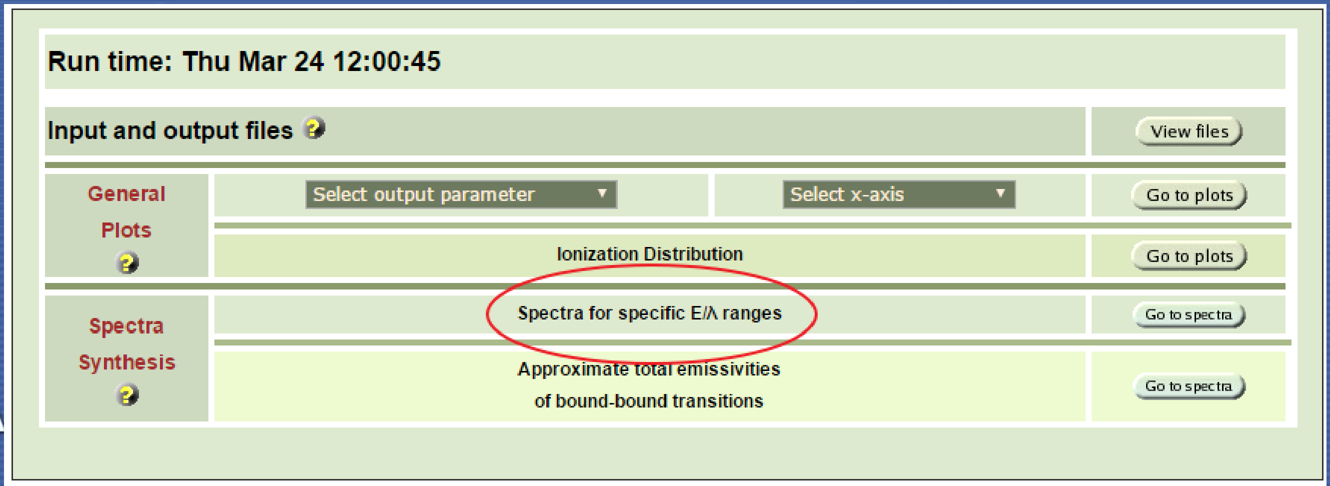
[ergs/s/Hz/cm^3/ster]

$$A_{AB} = \frac{\sum\limits_{i \in A: j \in B} g_i \exp(-E_i / kT_e) A_{ij}}{\sum\limits_{i \in A: j \in B} g_i \exp(-E_i / kT_e)}$$

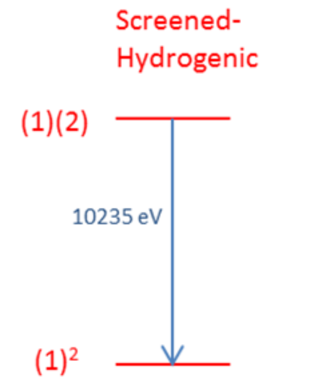
$$E_{AB} = \frac{\sum\limits_{i \in A: j \in B} g_i \exp(-E_i / kT_e) A_{ij} E_{ij}}{\sum\limits_{i \in A: j \in B} g_i \exp(-E_i / kT_e) A_{ij}}$$

STA width

$$\mu_{AB}^2 = \left[\frac{\sum\limits_{i \in A: j \in B} g_i \exp(-E_i / kT_e) A_{ij} E_{ij}^2}{\sum\limits_{i \in A: j \in B} g_i \exp(-E_i / kT_e) A_{ij}} \right]^2 - E_{AB}^2$$



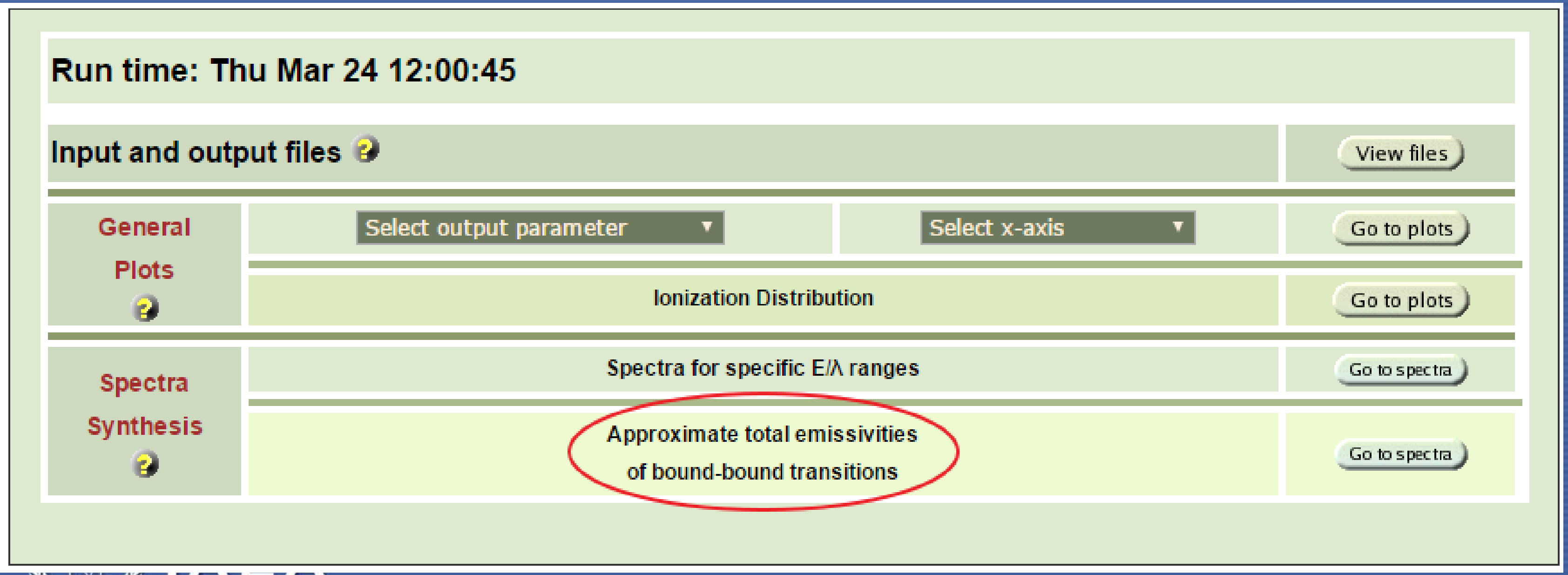
Total line emissivity in the STA formalism



Approximate total line emissivity:

A plot show approximate line emission spectra and provides information on energy range of dominant emission

$$S = n_u A_{ul} E_{ul} / N_e \qquad [\mathrm{eVcm^3/s/atom}]$$



APPLICATIONS

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FLYCHK Help Pages

- http://nlte.nist.gov/FLY/Doc/Manual_FLYCHK_Nov08.pdf
- http://nlte.nist.gov/FLY/README.html
- http://nlte.nist.gov/FLY/EXAMPLE.html
- Click on the Question Marks
  - http://nlte.nist.gov/FLY/Help/runfile.html
  - http://nlte.nist.gov/FLY/Help/opacity.html

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Available to the community at password-protected NIST website: http://nlte.nist.gov/FLY

Advantages: simplicity and versatility→ applicability

- <Z> for fixed any densities: electron, ion or mass
- Mixture-supplied electrons (eg: Argon-doped hydrogen plasmas)
- External ionizing sources : a radiation field or an electron beam.
- Multiple electron temperatures or arbitrary electron energy distributions
- Optical depth effects

Outputs: population kinetics code and spectral synthesis

- <Z> and charge state distribution
- Radiative Power Loss rates under optically thin assumption
- Energy-dependent spectral intensity of uniform plasma with a size

Caveats: simple atomic structures and uniform plasma approximation

- Less accurate spectral intensities for non-K-shell lines
- Less accurate for low electron densities and for LTE plasmas
- When spatial gradients and the radiation transport affect population significantly

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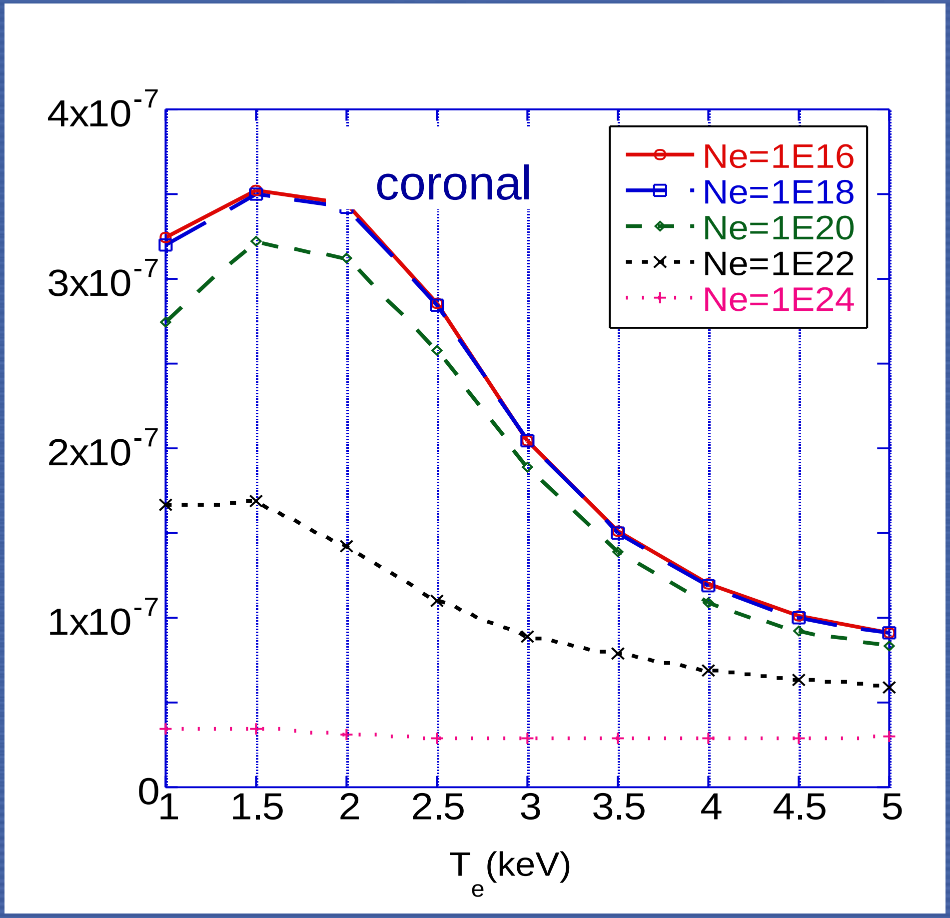
Example: Radiative loss rates are important as an energy loss mechanism of high-Z plasmas

Calculated Kr radiative cooling rates per N_e [eV/s/atom/cm^{-3}]



# of radiative transitions using HULK code

Ion	HULLAC+DHS
1	3049
2	27095
3	30078
4	404328
5	3058002
6	5882192
7	7808014
8	6202123
9	5544814
10	1050919
11	841094
Sum	30,851,708

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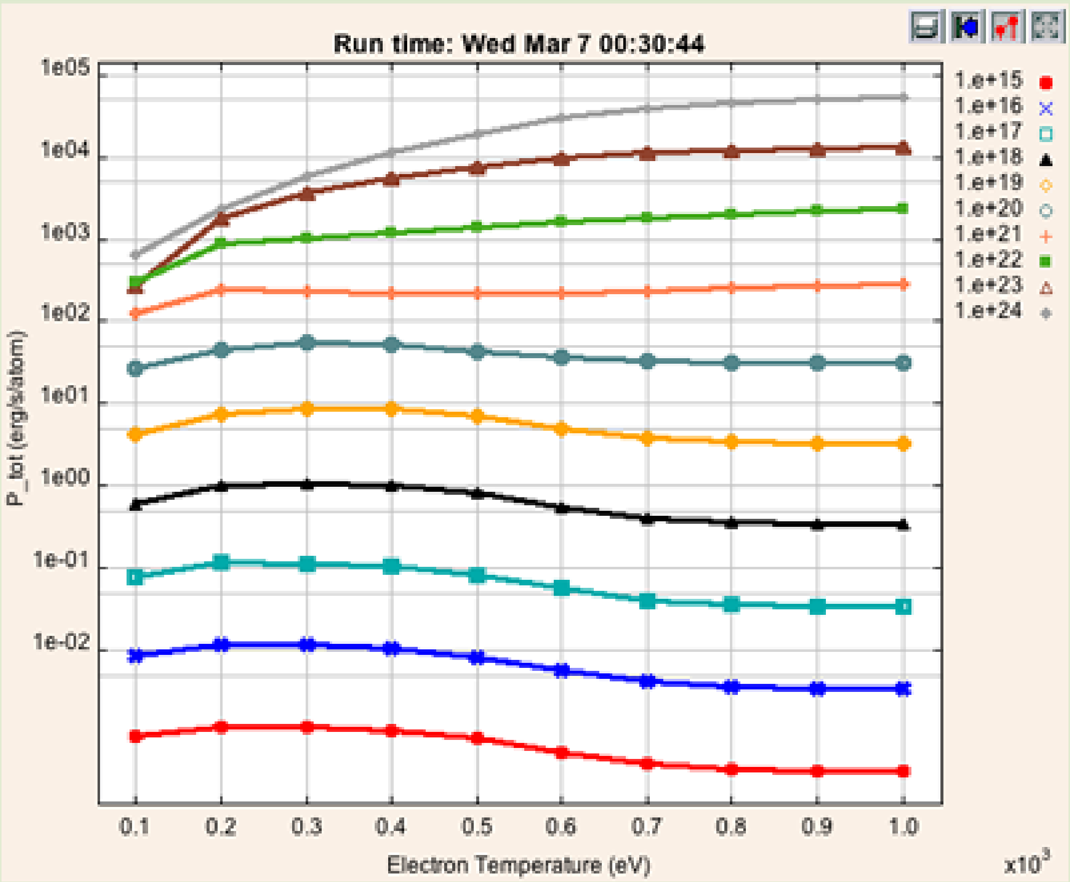
Data for Radiation Hydrodynamics: Kr Radiative loss rates over (Ne, Te)

Element: Kr

Comments: Radiative loss rates of Kr ions

The Java applet (PtPlot v.5.5) requires Java Runtime Environment installed.



Static plots: PDF | PS

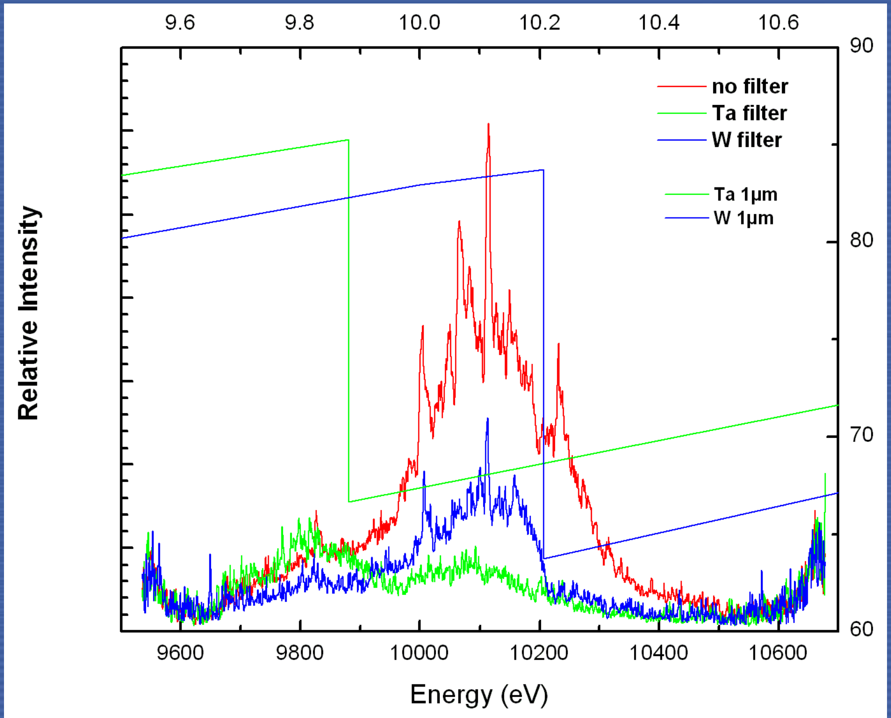
List of Selected Cases	
Dens	Data
1.e+15	file
1.e+16	file
1.e+17	file
1.e+18	file
1.e+19	file
1.e+20	file
1.e+21	file
1.e+22	file
1.e+23	file
1.e+24	file

The radiative loss rates show the similar coronal behavior up to $N_e=10^{17}$ and the rate/N_e stays constant.
As N_e increases, the rate/N_e decreases from the coronal value

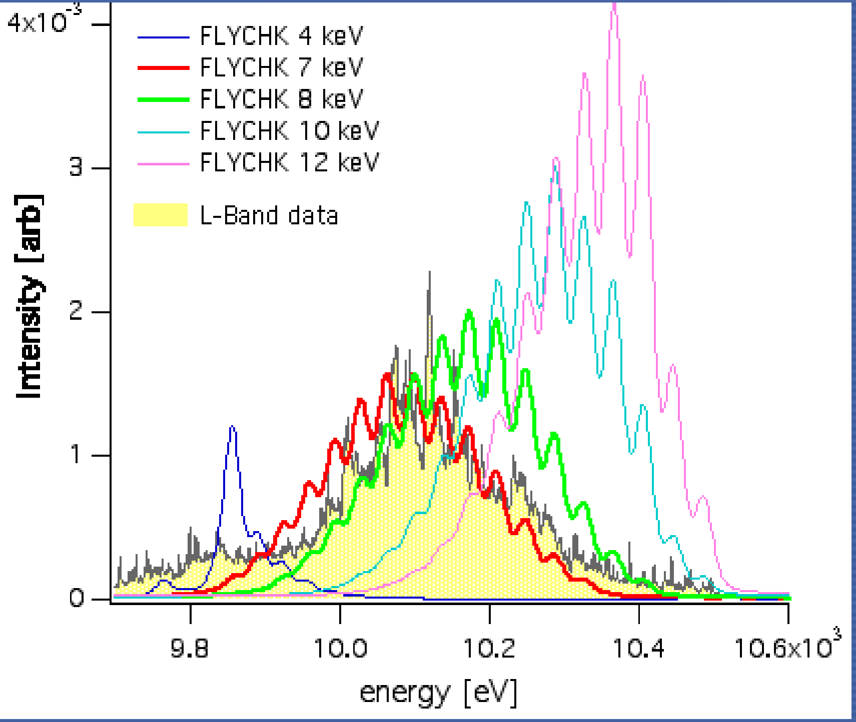
Example: Gold ionization balance in high temperature hohlraum (HTH) experiments

- High-T hohlraum reach temperatures: ~ 10 keV
- Spectrum from n_e ~ 4×10^{21} cm^{-3}, T_e ~ 7-10 keV measured for first time

L-shell gold spectra (K. Widmann)



Spectroscopic data and calculation



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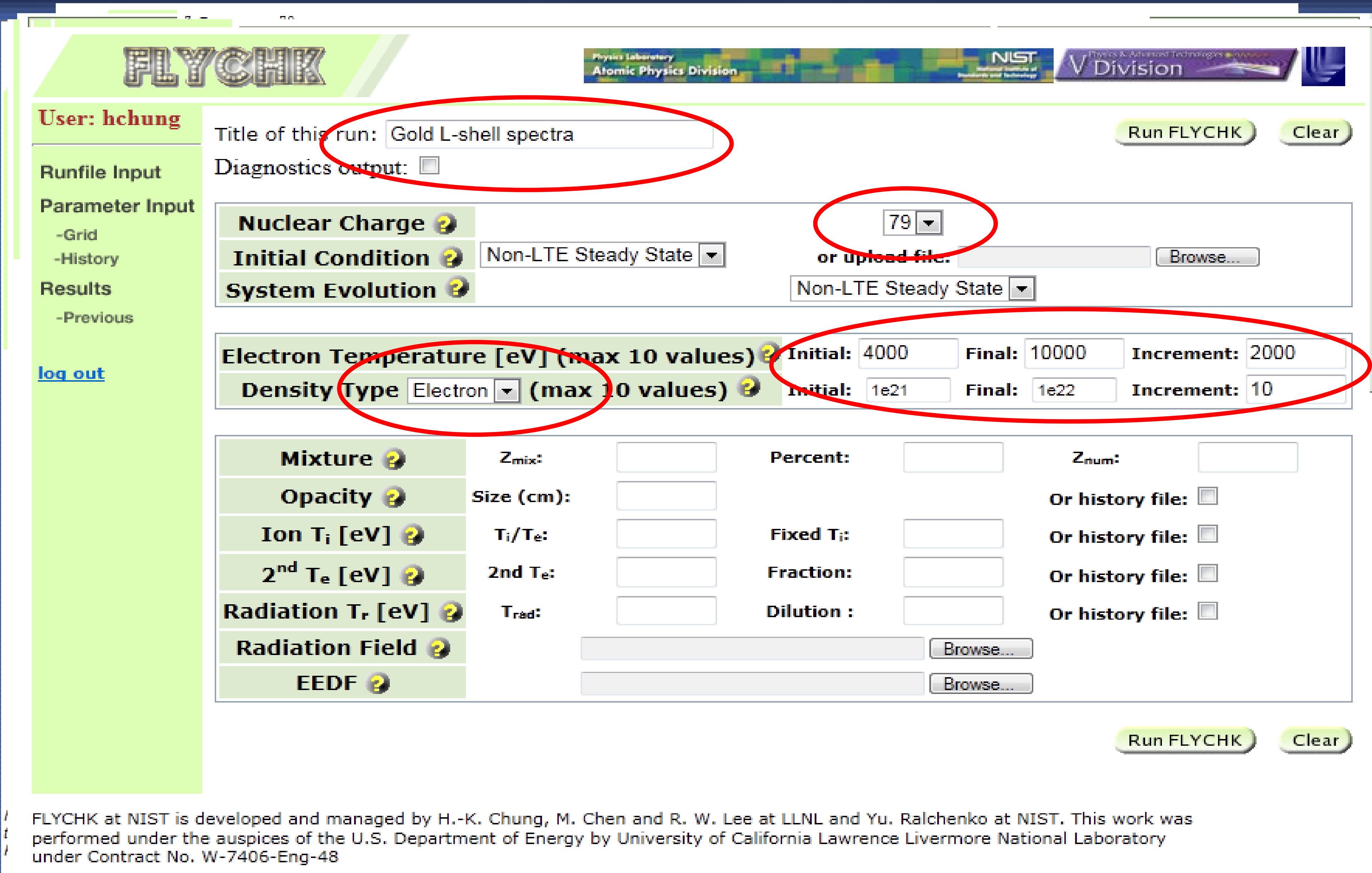
FLYCHK gives an estimate of Gold L-shell spectra

Long pulse laser plasmas: Gold L-shell spectroscopy

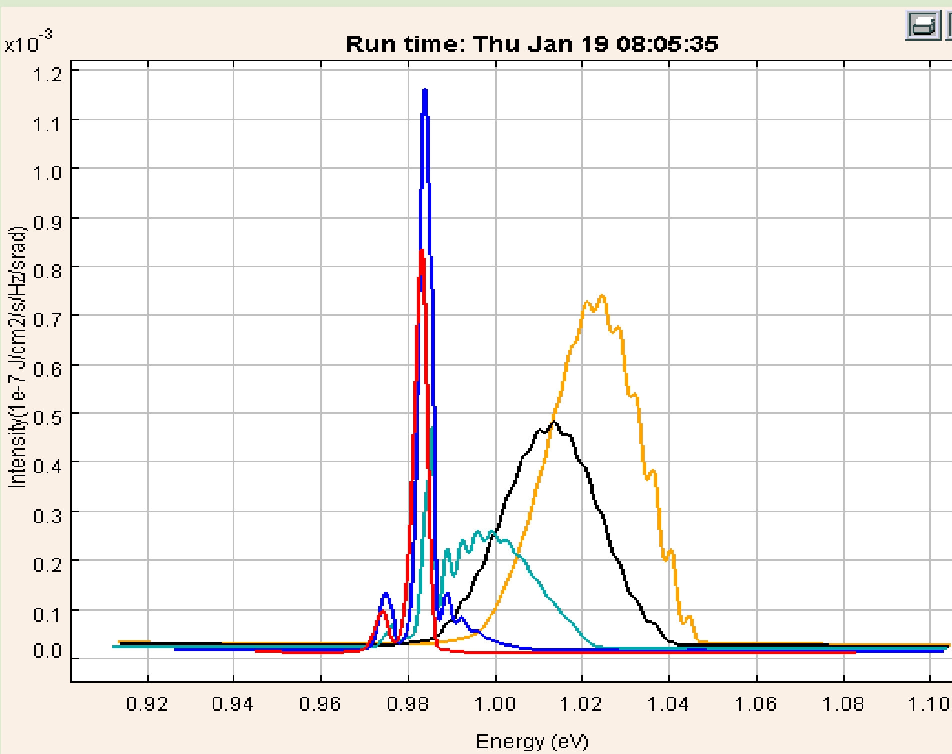


STA spectra compared with configuration-average spectra

FLYSPEC is running...

Log file

The Java applet (PtPlot v.5.5) requires Java installed.



List of Selected Cases				
Case #	Temp	Dens	Spectrum	Lines
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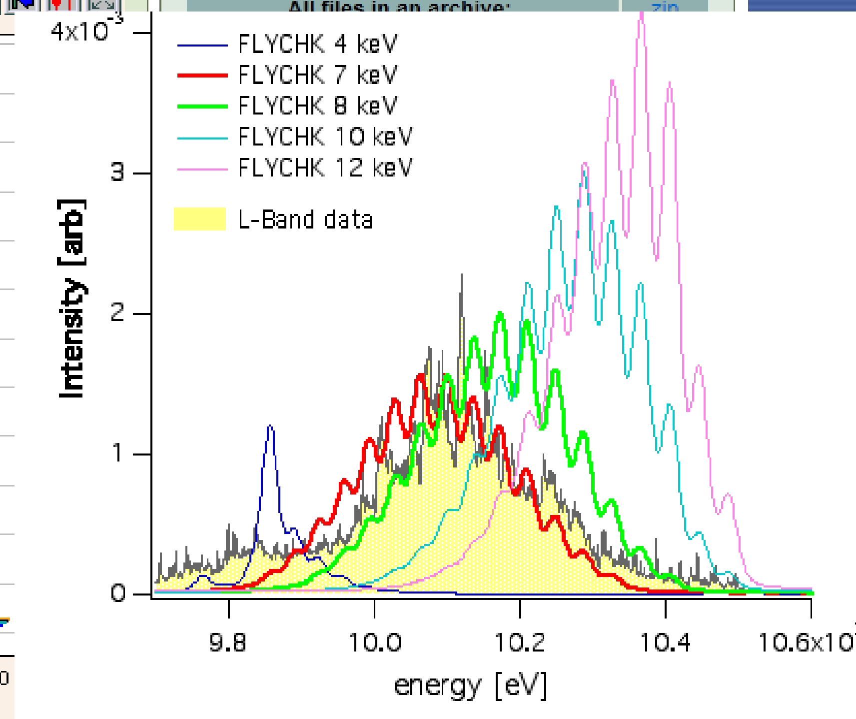
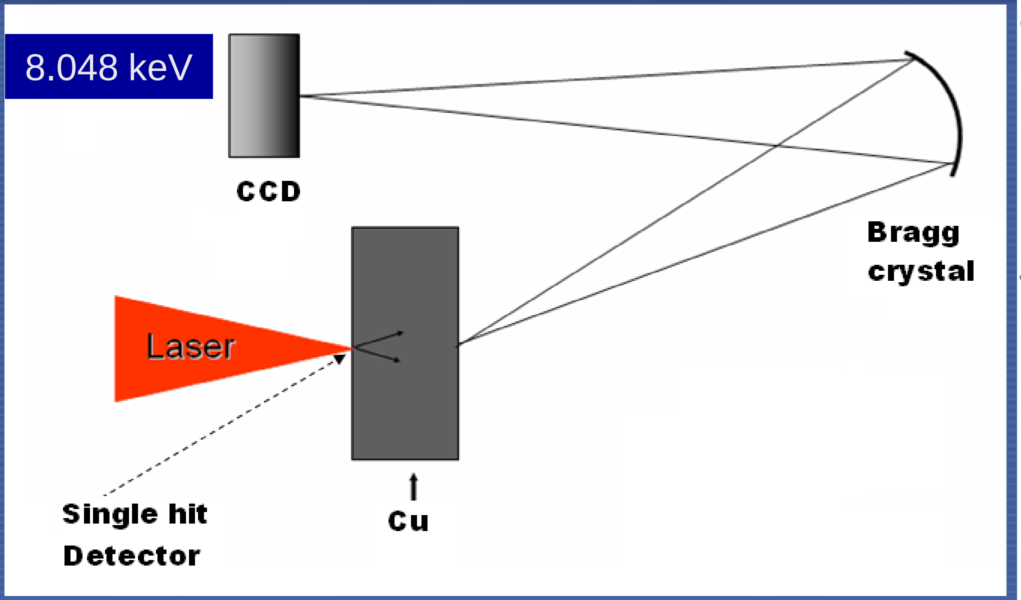
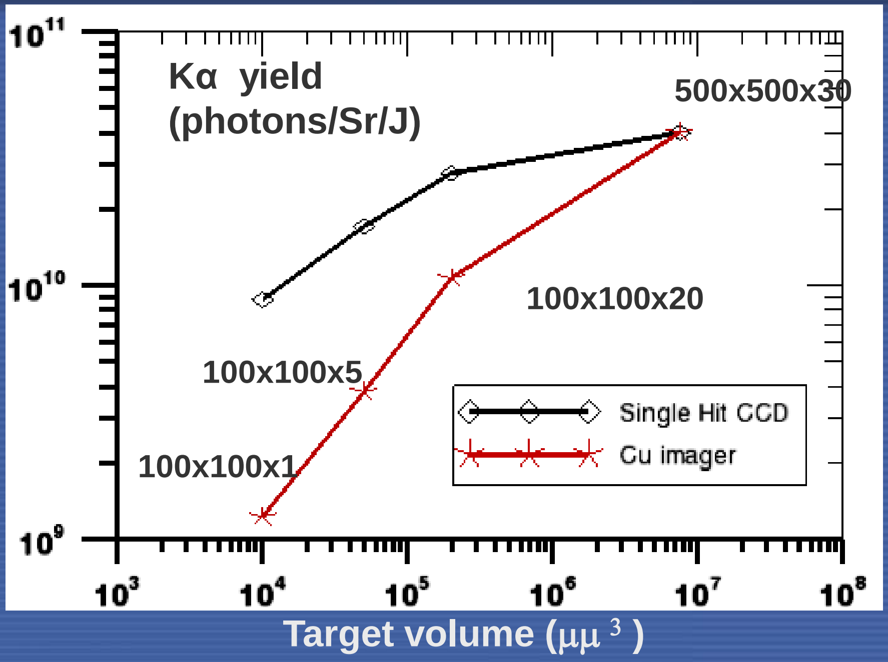
3	6000.0	1.e+21	file	lines
5	8000.0	1.e+21	file	lines
7	10000.0	1.e+21	file	lines
9	12000.0	1.e+21	file	lines
Opacities etc.			Spectra etc.	
All files in an archive:				zip



Example: Cu Kα radiation measured by single hit CCD spectrometer and 2-D imager for T_e diagnostics





Single Hit CCD Kα yield is higher than that of 2-D imager for smaller target volumes :

An experimental evidence of shifting and broadening of Kα emission lines in small targets with high temperatures

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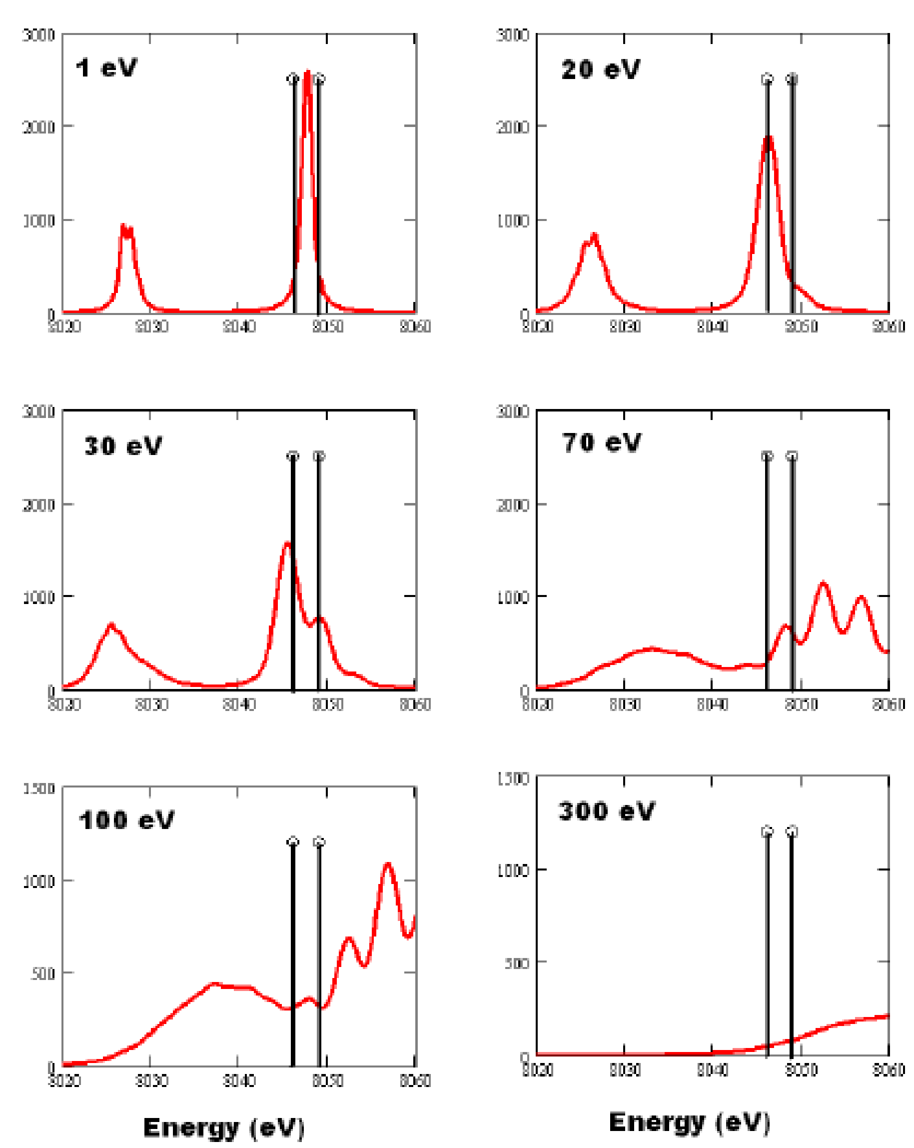
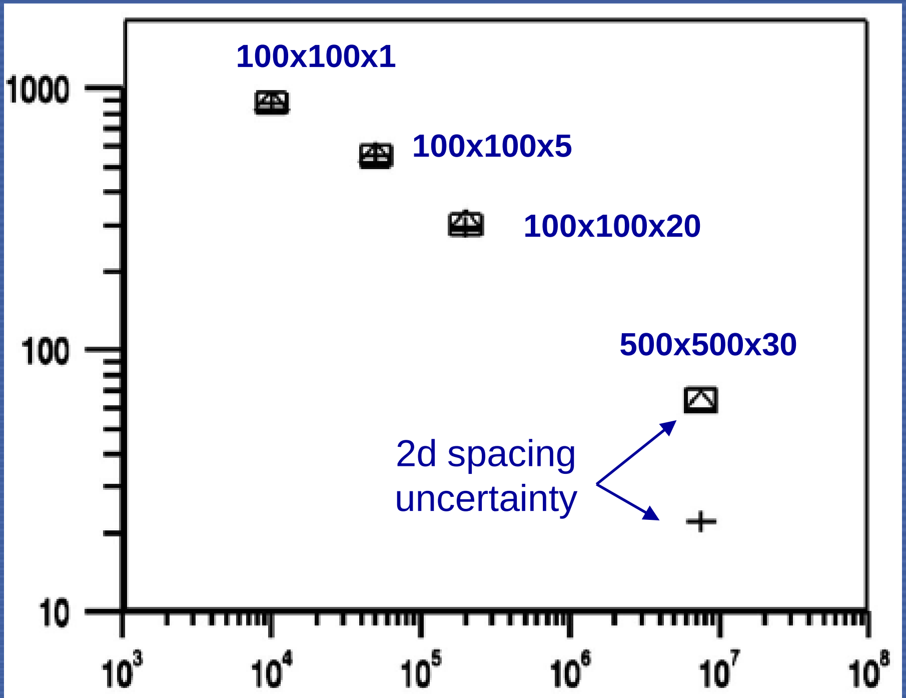
Shifts and Broadening of Kα emission as a function of electron thermal temperature

FLYCHK simulations



Average T_e(eV) of targets



Target volume (μμ ^{3})

Short pulse laser plasmas: Cu Kα Spectroscopy

User: hchung

Runfile Input

Parameter Input
- -Grid
- -History

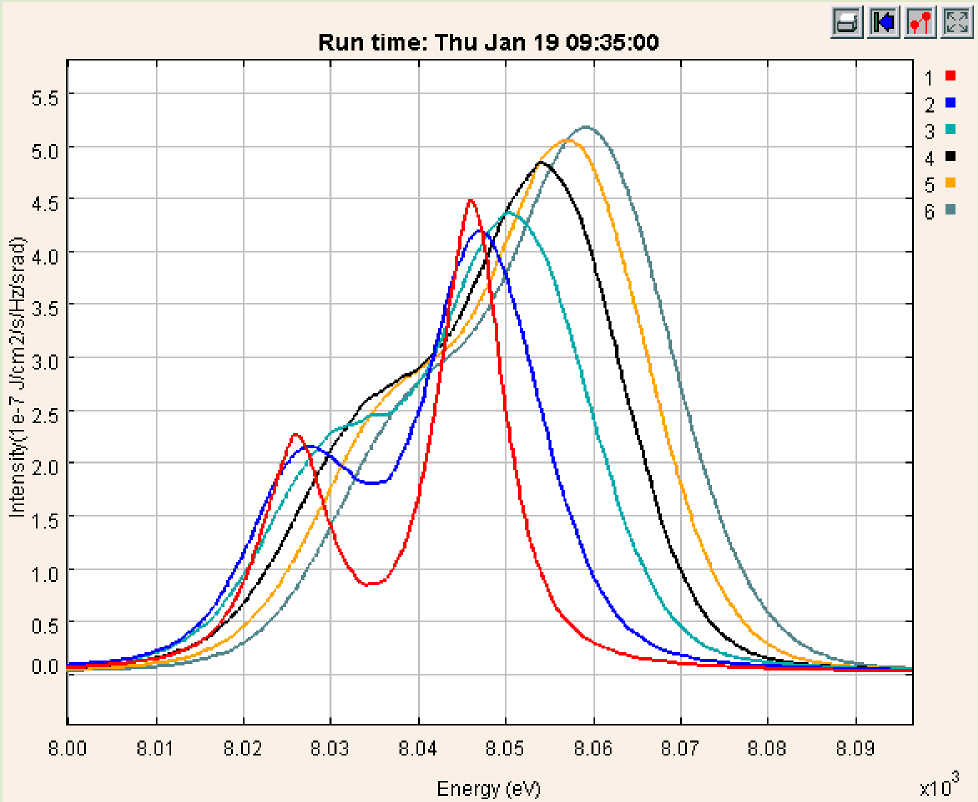
Results
- -Current
- -Previous

log out

FLYSPEC is running...

Log file

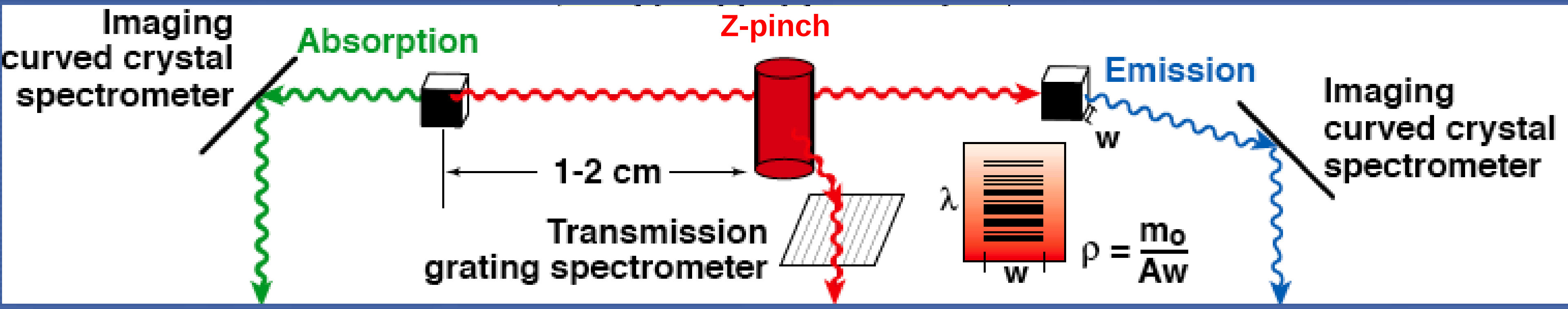
The Java applet (PtPlot v.5.5) requires Java installed.

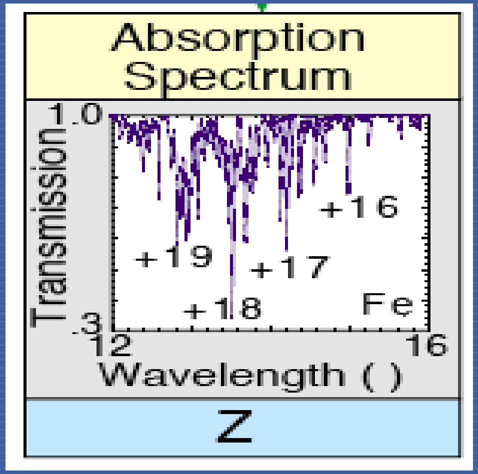


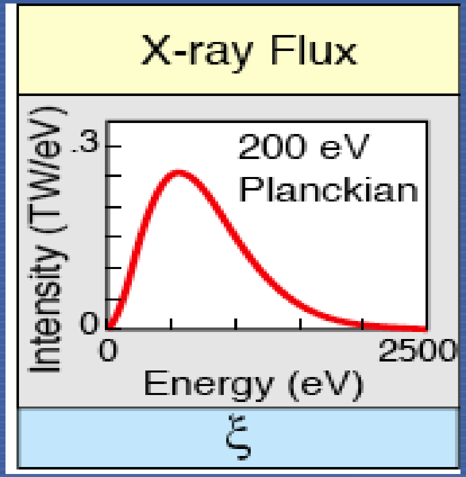
Help on spectra

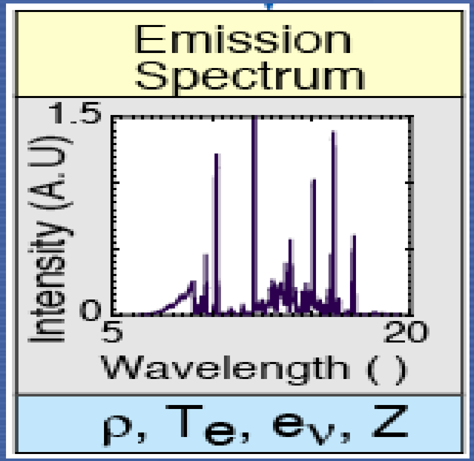
List of Selected Cases				
Case #	Temp	Dens	Spectrum	Lines
1	20.0	8.9e+00	file	lines
2	40.0	8.9e+00	file	lines
3	60.0	8.9e+00	file	lines
4	80.0	8.9e+00	file	lines
5	100.0	8.9e+00	file	lines
6	120.0	8.9e+00	file	lines
Opacities etc.		Spectra etc.		
All files in an archive:				zip

Example: Photoionized plasmas produced by Z-Machines – Astrophysical model benchmark







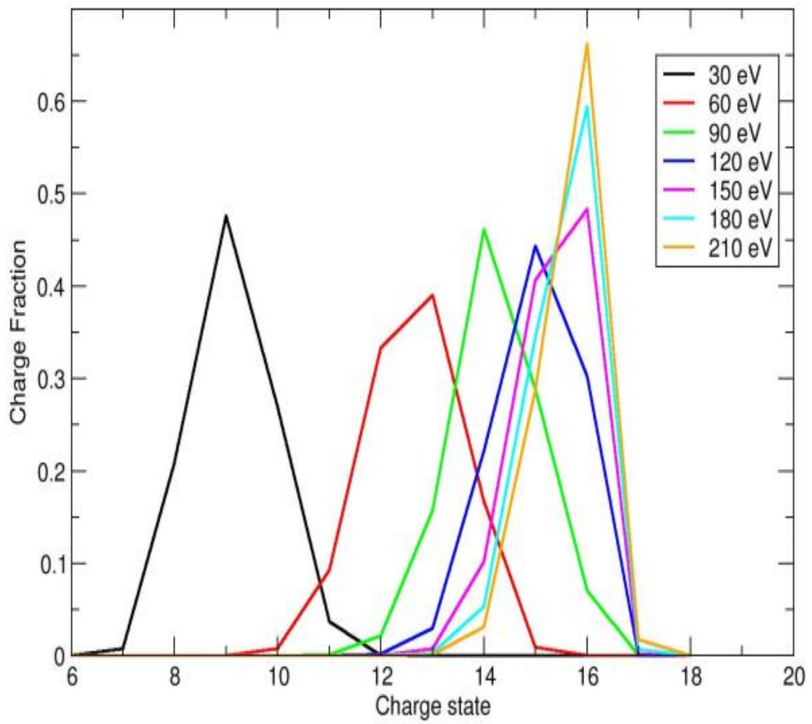


ξ=20-25 ergs-cm/s

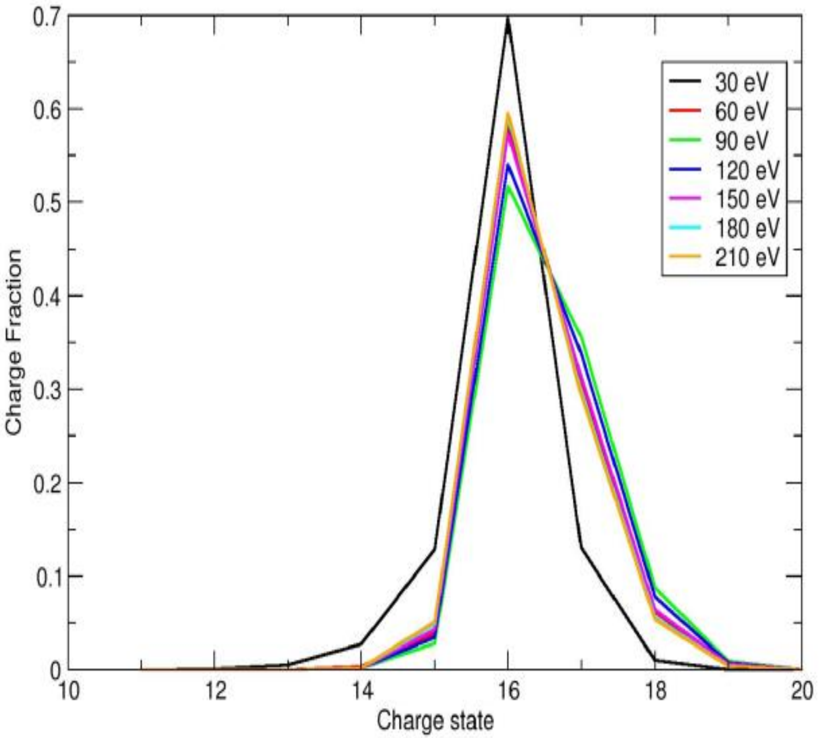
Charge state distribution is a function of N_e and Radiation field strength

N_e =1.95E19cm^{-3}
Radiation field of 165 eV and 0.01 dilution

Without Radiation Field



With Radiation Field



Photoionization equilibrium plasmas: Fe Z-Pinch Plasma

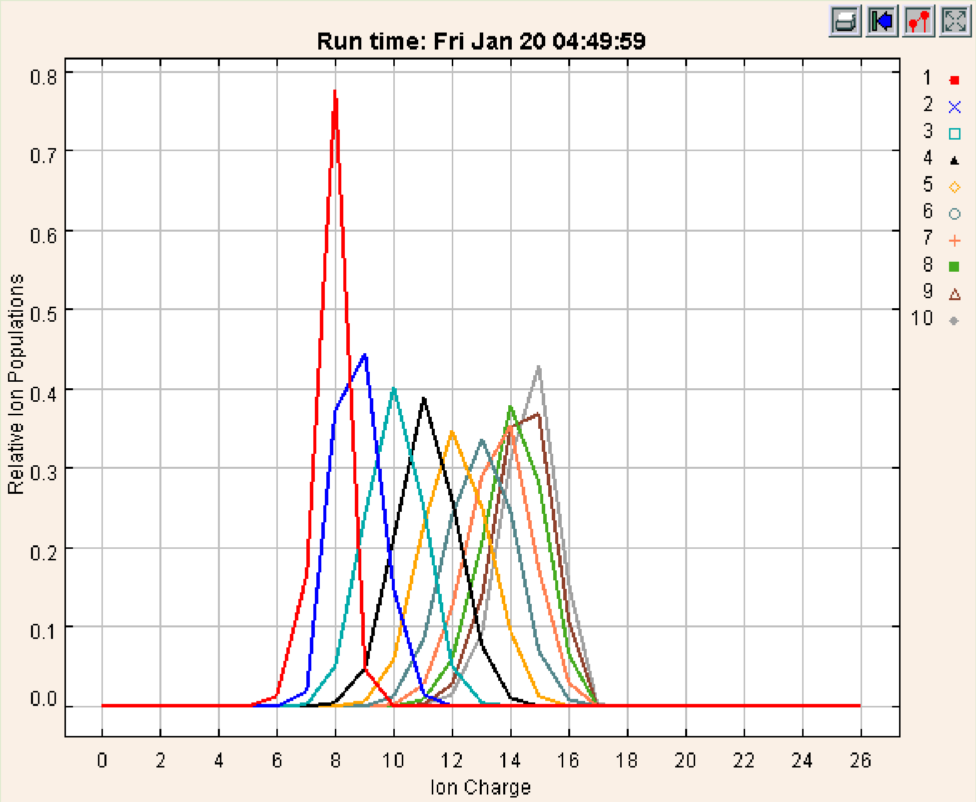
User: hchung

- Runfile Input
- Parameter Input
  - -Grid
  - -History
- Results
  - -Current
  - -Previous
- log out

Element: Fe

Comments: Iron steady state

The Java applet (PtPlot v.5.5) requires Java installed.

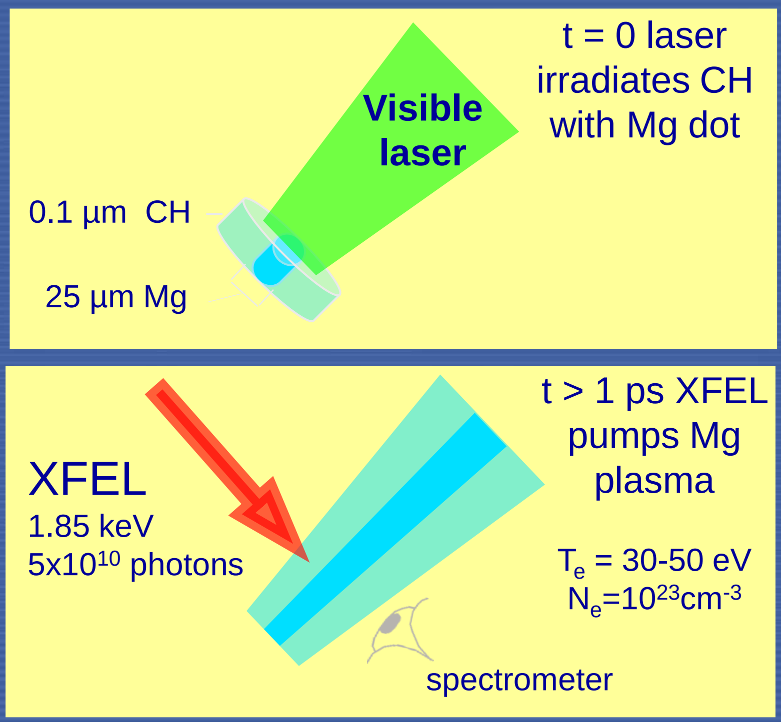


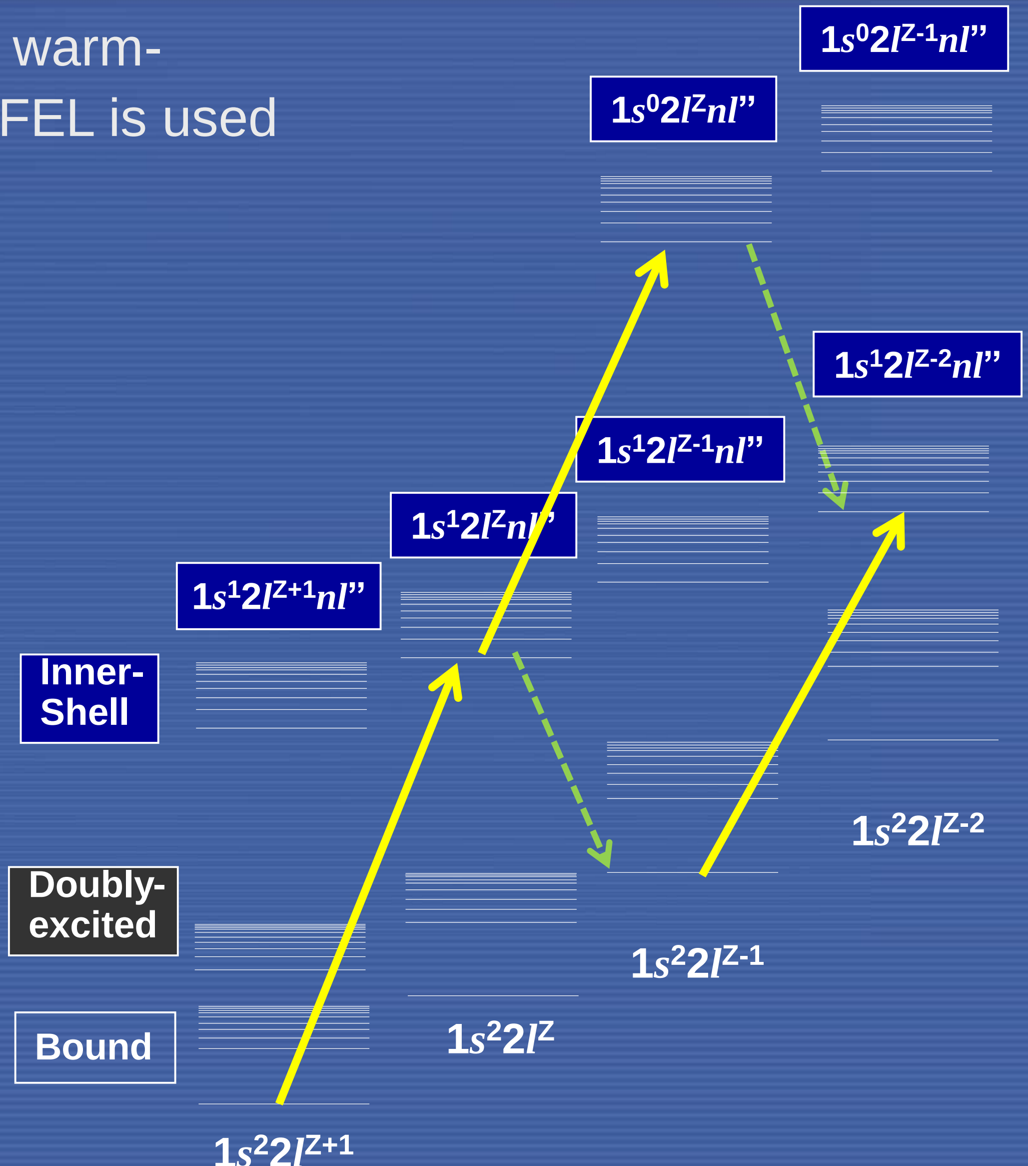
Static plots: PDF | PS

List of Selected Cases			
Case #	Temperature	Density	Data
1	30.0	1.95e+19	file
2	50.0	1.95e+19	file
3	70.0	1.95e+19	file
4	90.0	1.95e+19	file
5	110.0	1.95e+19	file
6	130.0	1.95e+19	file
7	150.0	1.95e+19	file
8	170.0	1.95e+19	file
9	190.0	1.95e+19	file
10	210.0	1.95e+19	file

Example: XFEL provides an opportunity for HEDS plasma spectroscopy

Long-pulse laser is used to create warm-dense-matter plasmas and then XFEL is used to probe the internal state.





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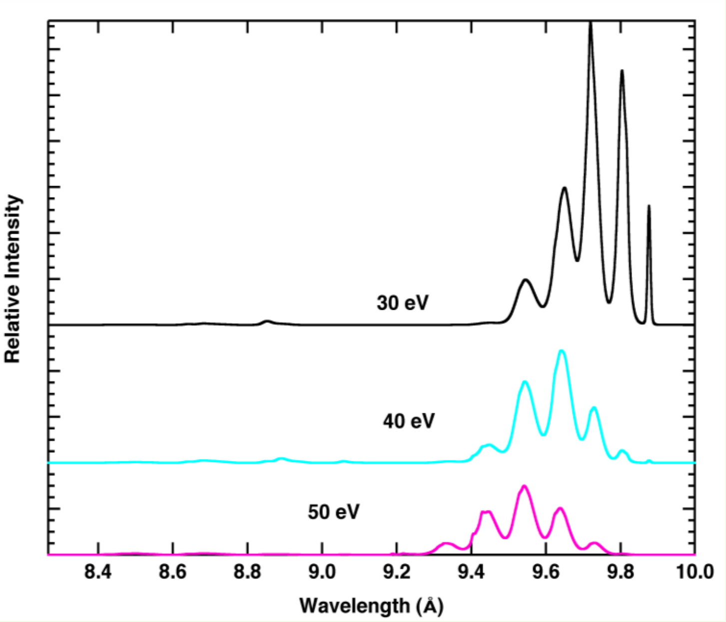
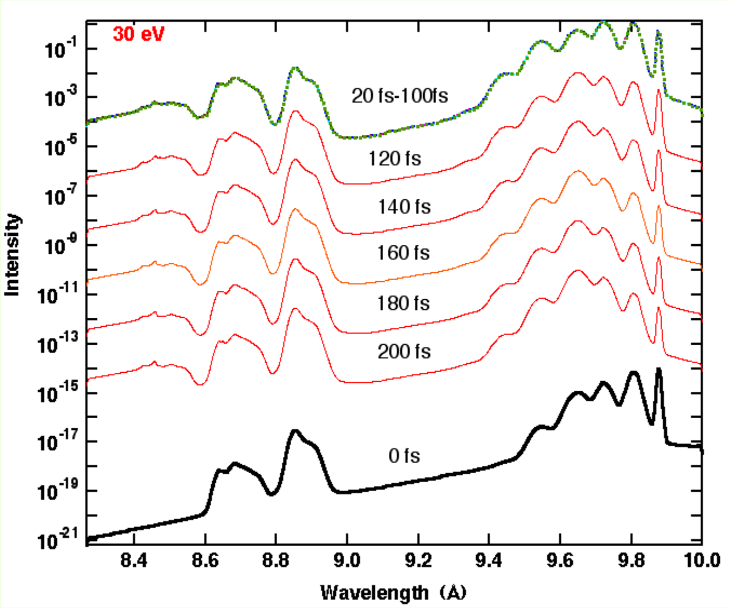
In Warm Dense Matter regime the hollow ions provide time-resolved diagnostic information

- XFEL forms unique states ***and*** provides *in situ* diagnostics with ~100 fs res.
  - 5×10^{10} 1.85 keV photons in 30 μm spot into a **$n_e=10^{23}$ cm^{-2}** plasma
  - Strong coupling parameter, Γ_{ii} = Potential/Kinetic Energy ~ 10



• Steady-state Spectra at various T_e



• At high n_e emisson lasts ~100 fs

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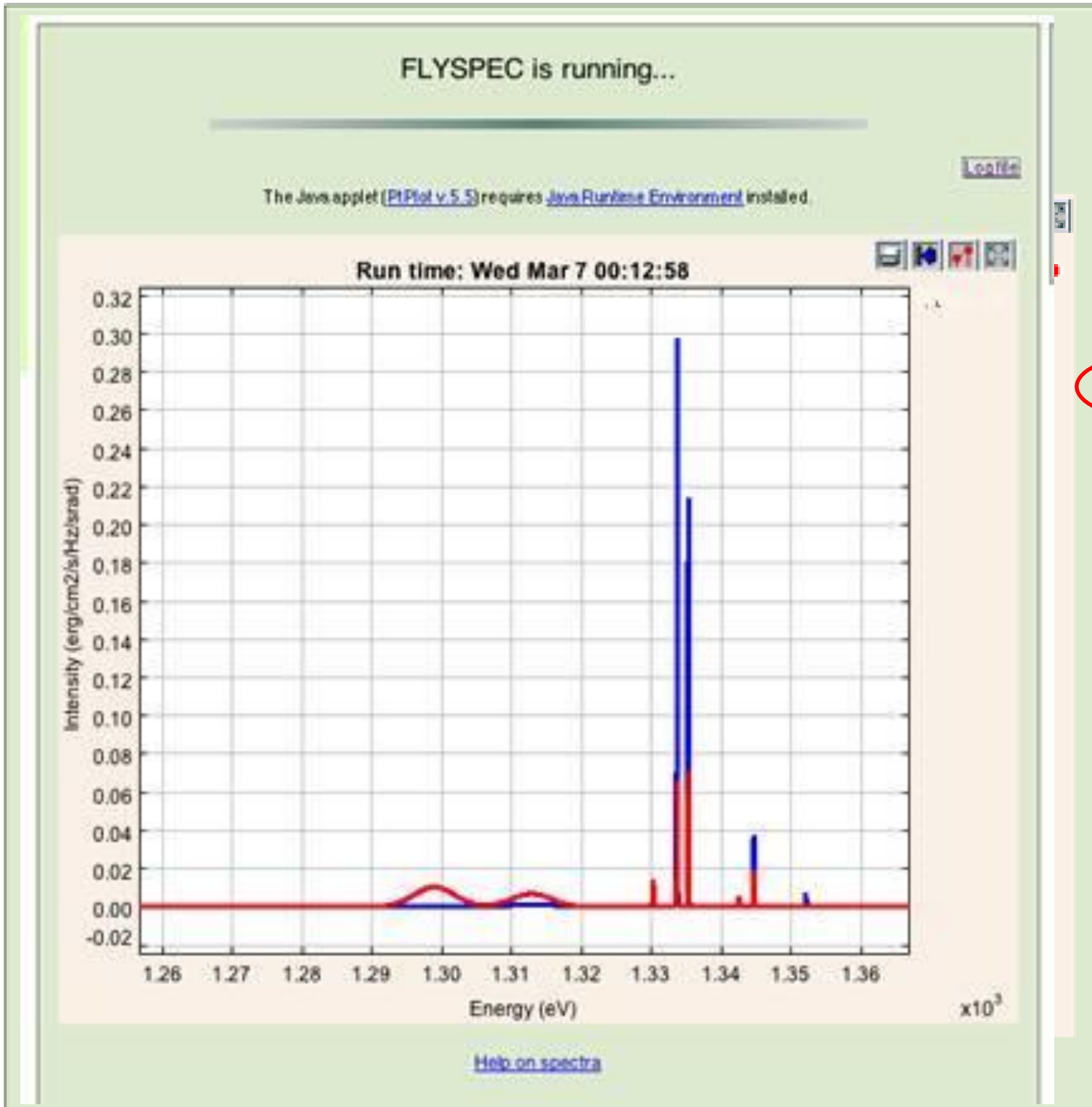
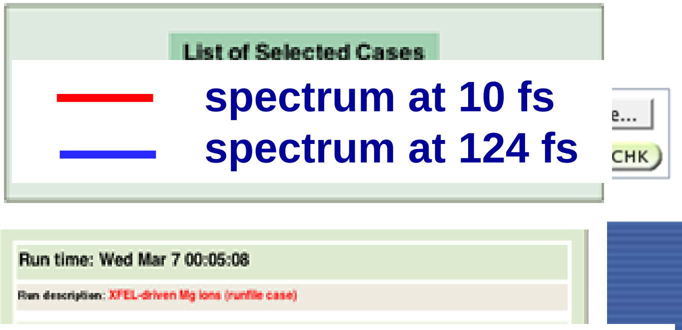
XFEL ionized plasma:
Mg time-dependent K-shell spectroscopy



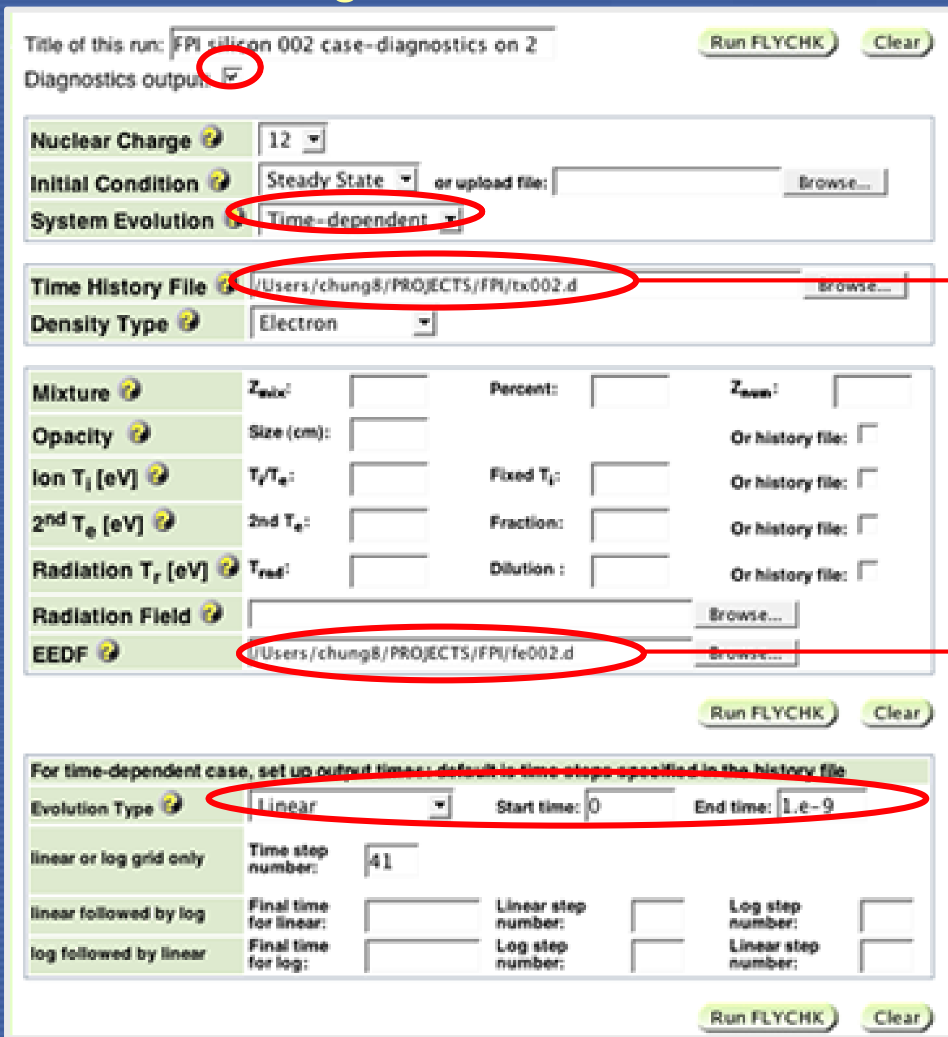


Even with 3.1 keV photons, the <Z> and hence the ionization distribution do not change significantly in 1000 fs. However, the details in the K-shell spectrum can change to reflect the change in K-hole state population.
This can lead to a pump diagnostics

depression) removes a highly excited states.
Unless the fluctuation is not an order of a charge, it is not a serious concern.

Postprocessing electron kinetic simulation

- SiO_2 aerogel targets doped with Ge or Ti for X-ray backlighter development
- 1-D e- kinetic code FPI shows Non-maxwellian energy functions due to strong laser heating and nonlocal electron heat flow -- J-P. Matte & K.B. Fournier



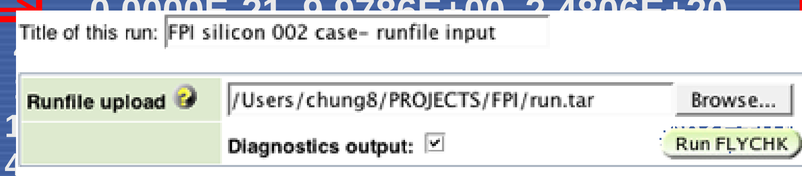
History input always includes thermal T_e

EEDF is added as additional e- source

Runfile input can specify

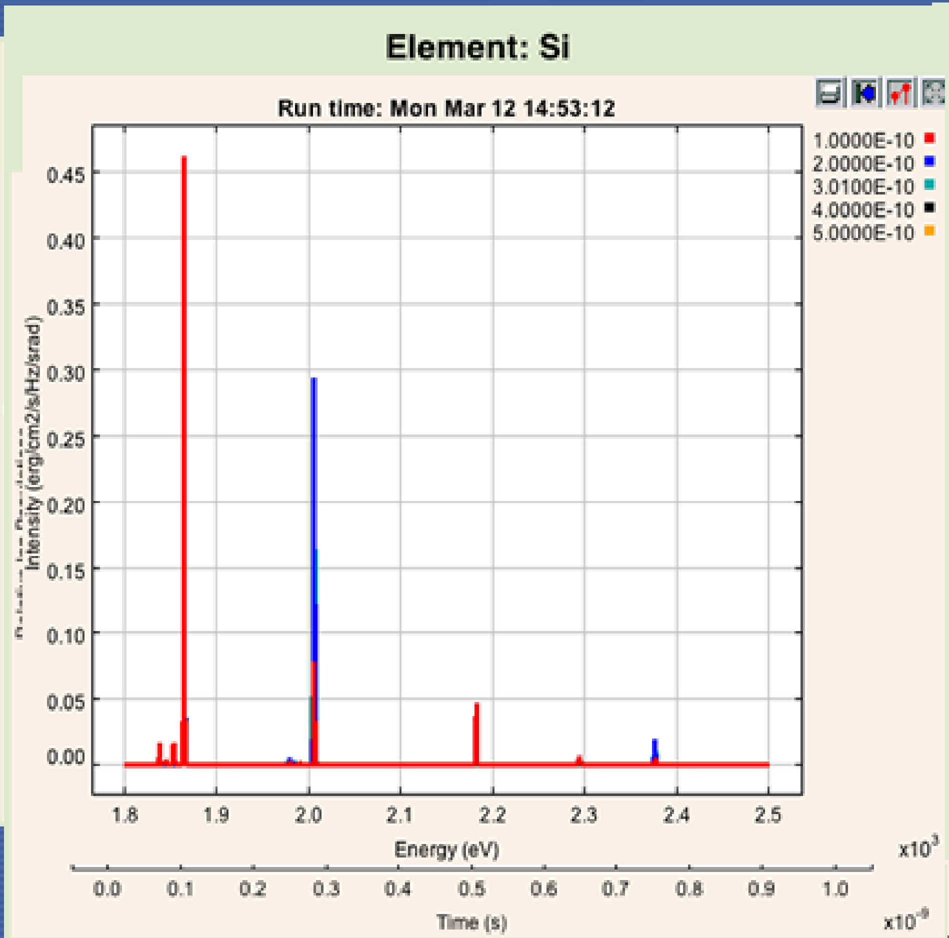
EEDF to be the only e- source

time te ne
0.0000E-21 9.9786E+00 2.4806E+20
2.5000E-10 1.8787E+03 8.3812E+20
6.89062E+01 8.26562E+01 9.76562E+01 1.13906E+02
c Te and Ne should be always included
1.31406E+02 1.50156E+02 1.70156E+02 1.91406E+02
c for continuum lowering model
2.13906E+02 ... 8.5216E+20
3.75156E+02 4.06406E+02 4.38906E+02 4.72656E+02
5.07656E+02 5.43906E+02
3.7600E-10 2.2745E+03 8.6984E+20
5.81406E+02 6.20156E+02 6.60156E+02 7.01406E+02
7.43906E+02 7.87656E+02 8.32656E+02 8.78906E+02
outfile outfile.dat
7.0000E-10 2.9818E+03 9.0895E+20
initial ss
evolve td
fe fe002.d only
1.47016E+03 1.53141E+03
history tx002.d ne
time 0. 1.e-9 41
end

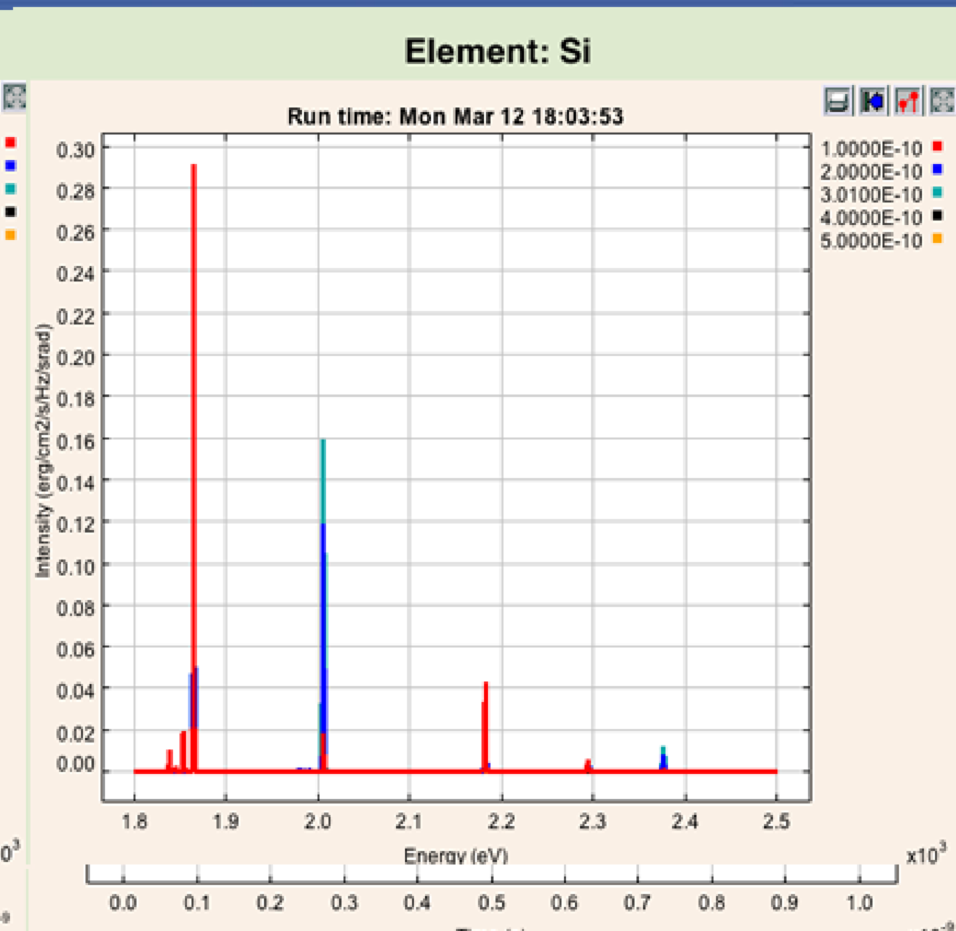


Output: <Z> is quite similar with/without thermal e-

Using fe(E) with thermal e-



Using fe(E) only without thermal e-



Useful Examples

http://nlte.nist.gov/FLY/EXAMPLE.html

Please check the Screen shot of each case