Spectral simulations of a H-C-O-Si plasma

David Cohen
with V. Swisher, M. Brown

Swarthmore College

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For the Plasma Dynamics Laboratory, University of Washington

We present here some simple, preliminary spectral simulations using the *PrismSPECT* non-LTE modeling code (see http://www.prism-cs.com/Software/PrismSpect/PrismSPECT.htm) and the *ATBASE ab initio* atomic models (see http://www.prism-cs.com/Software/AtomicData/AtomicData.htm)

The assumptions for these calculations are:

Time-independent, non-LTE (“collisional radiative equilibrium”) ionization and level population calculation, with optically thin radiation transport

Predominantly hydrogen plasma, but with the following impurities, % atomic:

C: 0.25%

O: 0.50%

Si: 0.10%

$n_{ion} = 3 \times 10^{15}$ cm^{-3}

$T_e = T_i = 15, 50$ eV (two separate calculations)

Atomic Model
ATBASE v. 5.1

Detailed Configuration Accounting (L-S coupling):

H: 12 levels

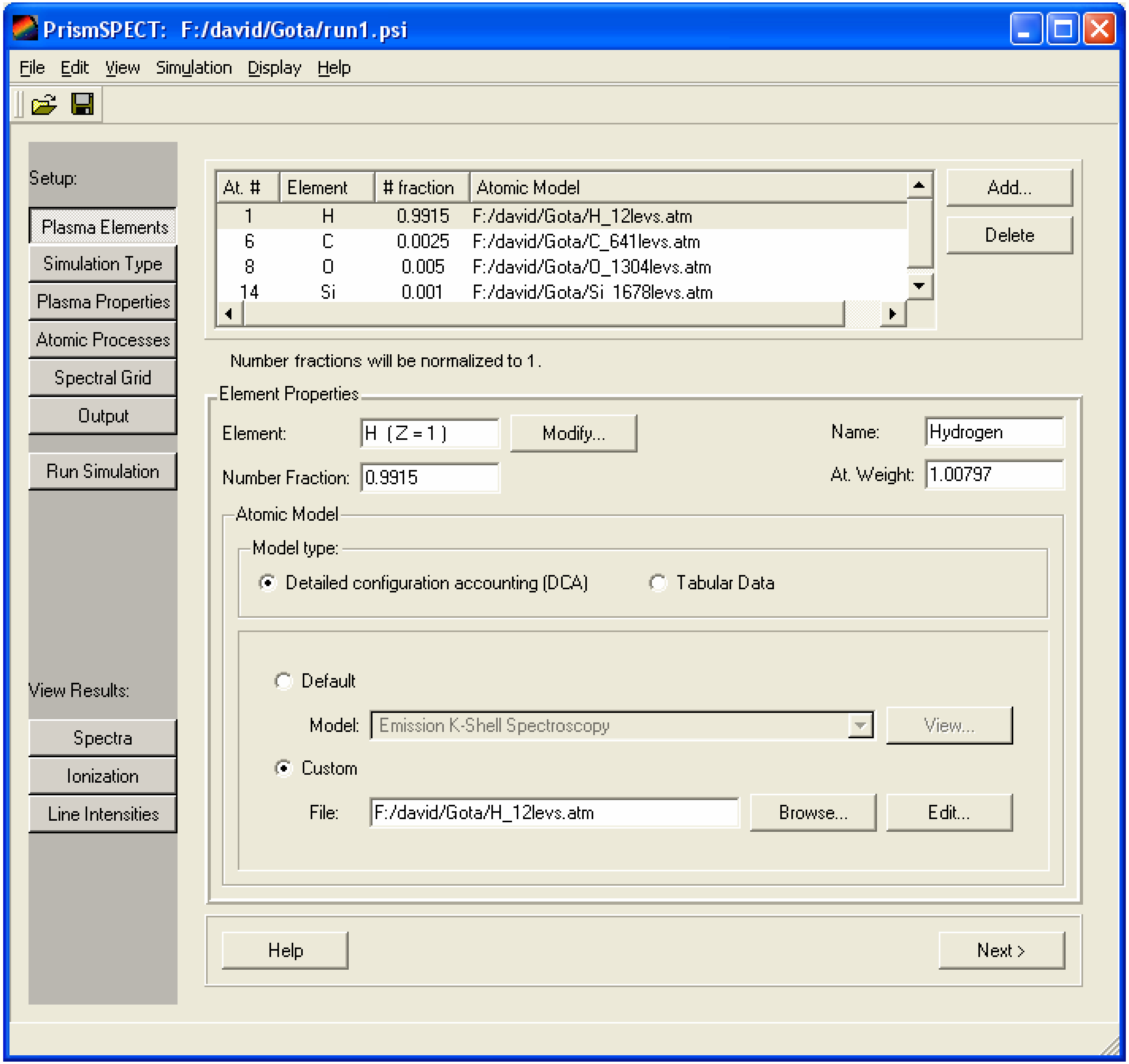
C: 641 levels

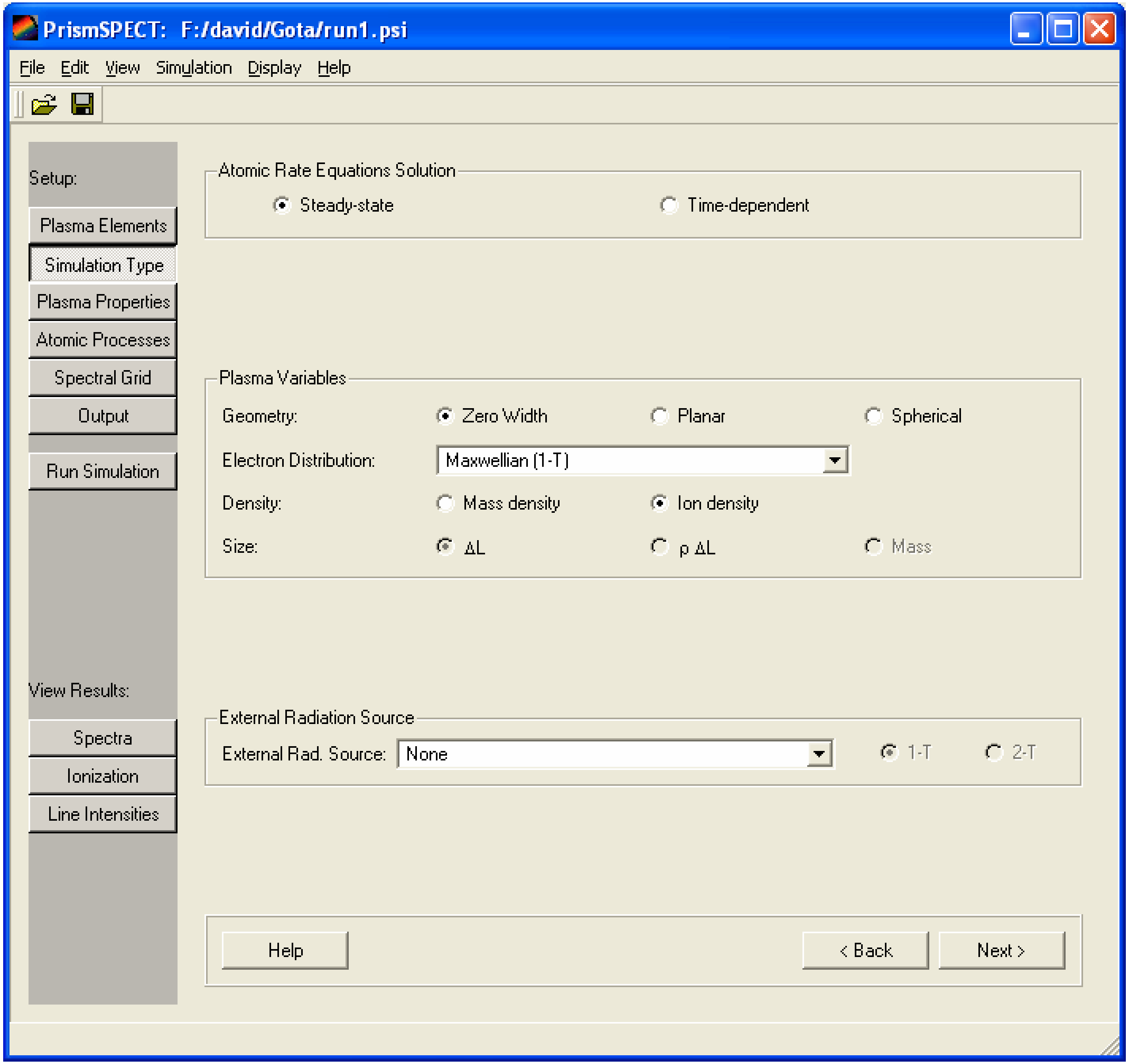
O: 1304 levels

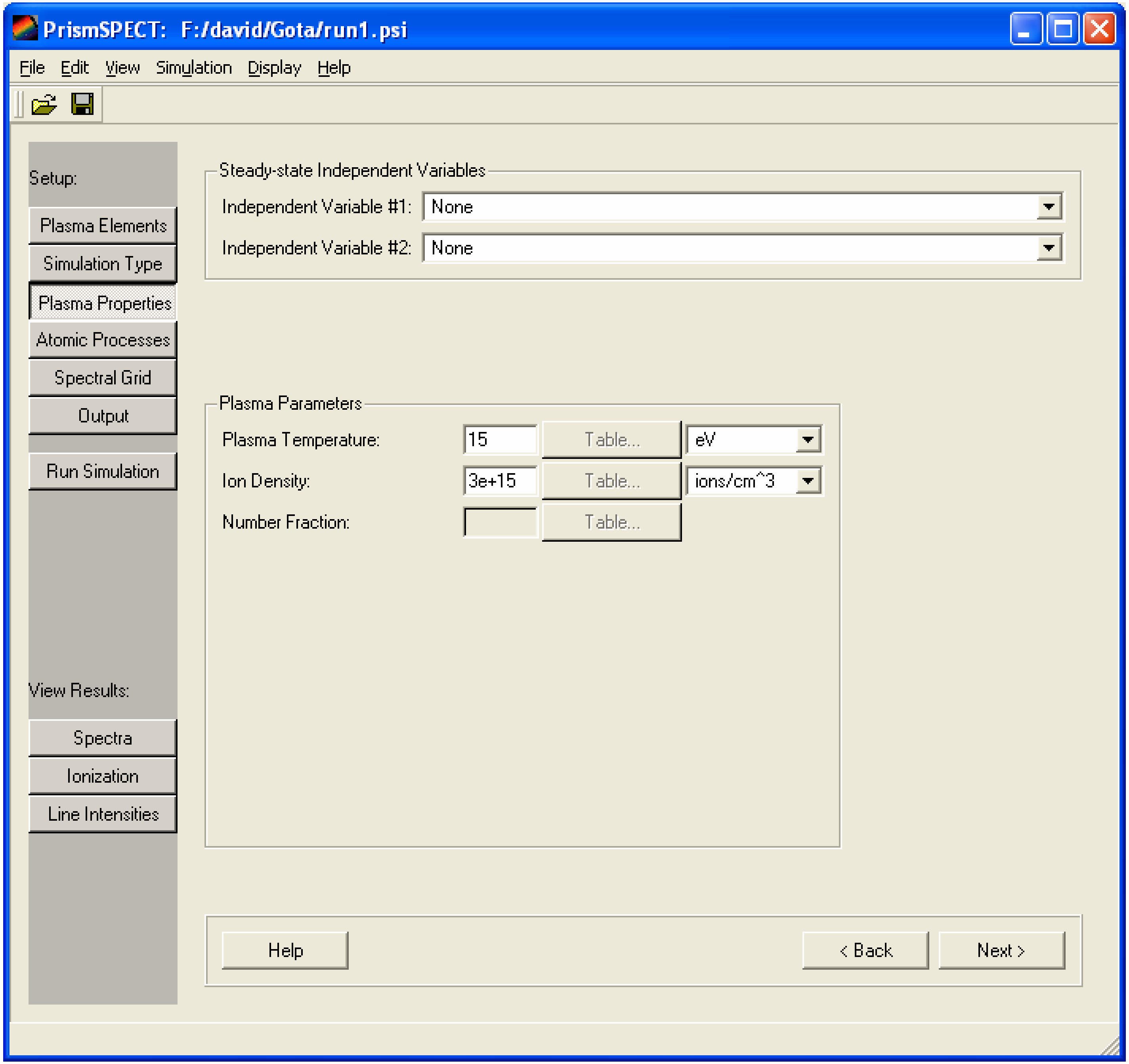
Si: 1678 levels

For C, O, and Si, we use all non-autoinizing levels of each ion stage (for Si, only up through Si^{+7}, above which we use only ground states)

The following five slides show the *PrismSPECT* GUI for setting up the calculations.


PrismSPECT: F:/david/Gota/run1.psi
File Edit View Simulation Display Help
Setup:
Plasma Elements
Simulation Type
Plasma Properties
Atomic Processes
Spectral Grid
Output
Run Simulation
View Results:
Spectra
Ionization
Line Intensities
At. # | Element | # fraction | Atomic Model
1 H 0.9915 F:/david/Gota/H_12levs.atm
6 C 0.0025 F:/david/Gota/C_641levs.atm
8 O 0.005 F:/david/Gota/O_1304levs.atm
14 Si 0.001 F:/david/Gota/Si_1678levs.atm
Add...
Delete
Number fractions will be normalized to 1.
Element Properties
Element: H (Z = 1)
Modify...
Name: Hydrogen
Number Fraction: 0.9915
At. Weight: 1.00797
Atomic Model
Model type:
Detailed configuration accounting (DCA)
Tabular Data
Default
Model: Emission K-Shell Spectroscopy
View...
Custom
File: F:/david/Gota/H_12levs.atm
Browse...
Edit...
Help
Next >


PrismSPECT: F:/david/Gota/run1.psi
File Edit View Simulation Display Help
Setup:
Plasma Elements
Simulation Type
Plasma Properties
Atomic Processes
Spectral Grid
Output
Run Simulation
View Results:
Spectra
Ionization
Line Intensities
Atomic Rate Equations Solution
Steady-state
Time-dependent
Plasma Variables
Geometry:
Zero Width
Planar
Spherical
Electron Distribution:
Maxwellian (1-T)
Density:
Mass density
Ion density
Size:
ΔL
ρ ΔL
Mass
External Radiation Source
External Rad. Source:
None
1-T
2-T
Help
< Back
Next >


PrismSPECT: F:/david/Gota/run1.psi
File Edit View Simulation Display Help
Setup:
Plasma Elements
Simulation Type
Plasma Properties
Atomic Processes
Spectral Grid
Output
Run Simulation
View Results:
Spectra
Ionization
Line Intensities
Steady-state Independent Variables
Independent Variable #1: None
Independent Variable #2: None
Plasma Parameters
Plasma Temperature: 15 Table... eV
Ion Density: 3e+15 Table... ions/cm^3
Number Fraction: Table...
Help
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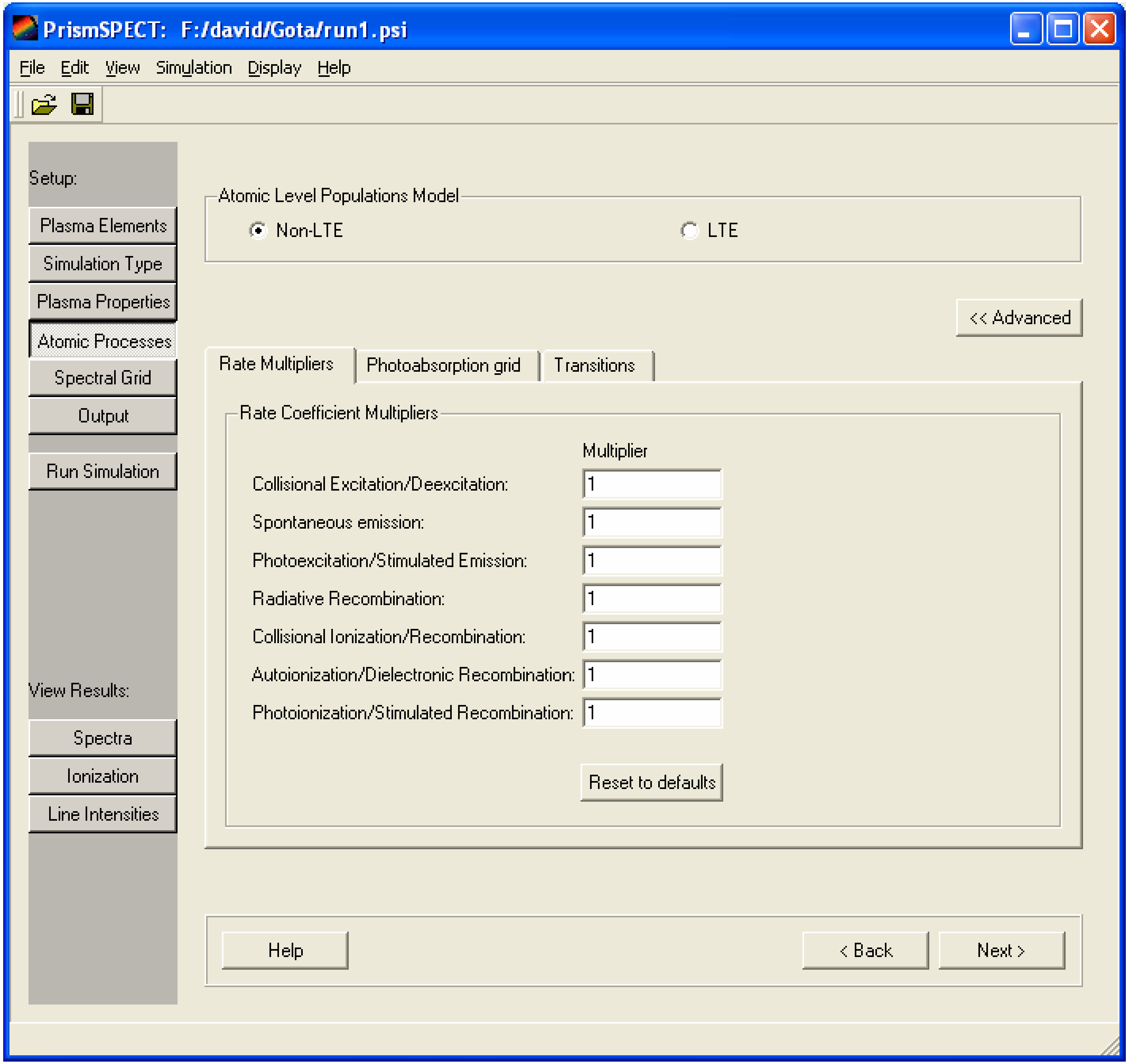
PrismSPECT: F:/david/Gota/run1.psi
File Edit View Simulation Display Help
Setup:
Plasma Elements
Simulation Type
Plasma Properties
Atomic Processes
Spectral Grid
Output
Run Simulation
View Results:
Spectra
Ionization
Line Intensities
Atomic Level Populations Model
Non-LTE
LTE
<< Advanced
Rate Multipliers
Photoabsorption grid
Transitions
Rate Coefficient Multipliers
Multiplier
Collisional Excitation/Deexcitation: 1
Spontaneous emission: 1
Photoexcitation/Stimulated Emission: 1
Radiative Recombination: 1
Collisional Ionization/Recombination: 1
Autoionization/Dielectronic Recombination: 1
Photoionization/Stimulated Recombination: 1
Reset to defaults
Help
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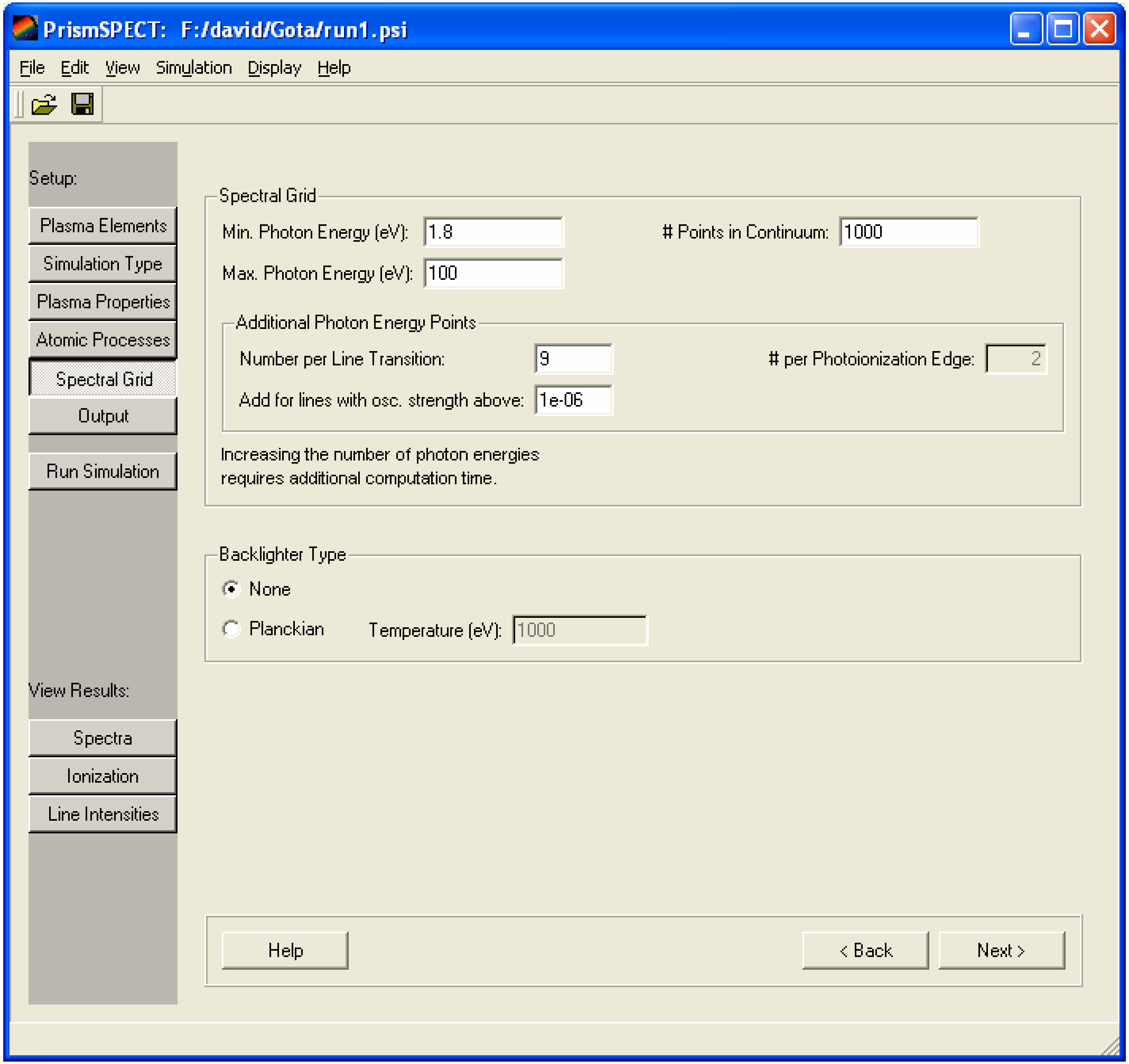
PrismSPECT: F:/david/Gota/run1.psi
File Edit View Simulation Display Help
Setup:
Plasma Elements
Simulation Type
Plasma Properties
Atomic Processes
Spectral Grid
Output
Run Simulation
View Results:
Spectra
Ionization
Line Intensities
Spectral Grid
Min. Photon Energy (eV): 1.8
Points in Continuum: 1000
Max. Photon Energy (eV): 100
Additional Photon Energy Points
Number per Line Transition: 9
per Photoionization Edge: 2
Add for lines with osc. strength above: 1e-06
Increasing the number of photon energies requires additional computation time.
Backlighter Type
None
Planckian
Temperature (eV): 1000
Help
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Low temperature (15 eV) results

Ionization balance – mean charge states:

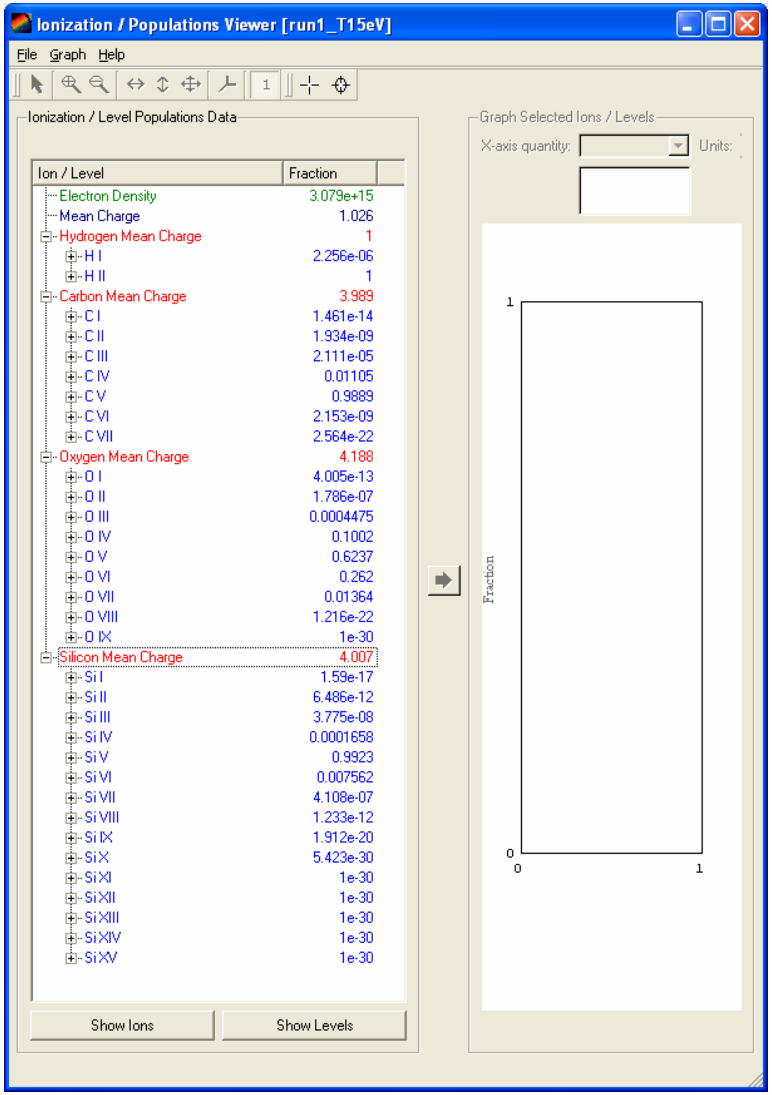
Z_H:1 (2.3 X 10^{-6} H^o)

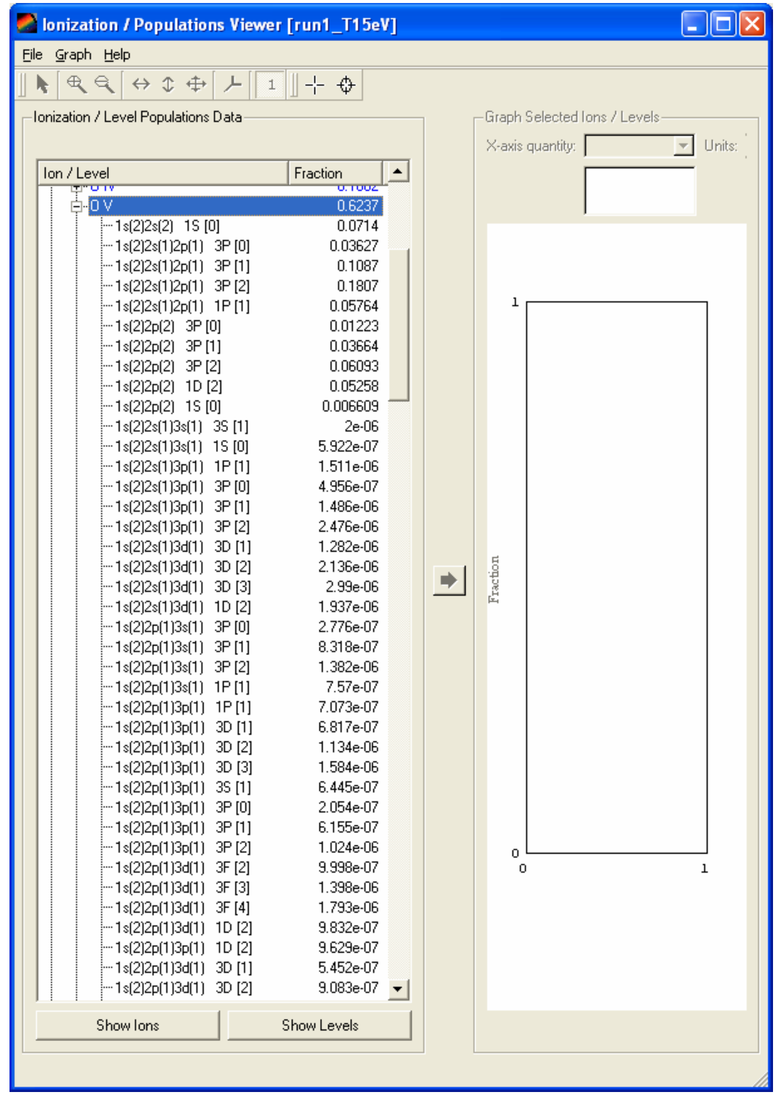
Z_C:3.99 (~1% C^{+3})

Z_O:4.19 (62% O^{+4}, 26% O^{+5}, 10% O^{+3}, 1% O^{+6})

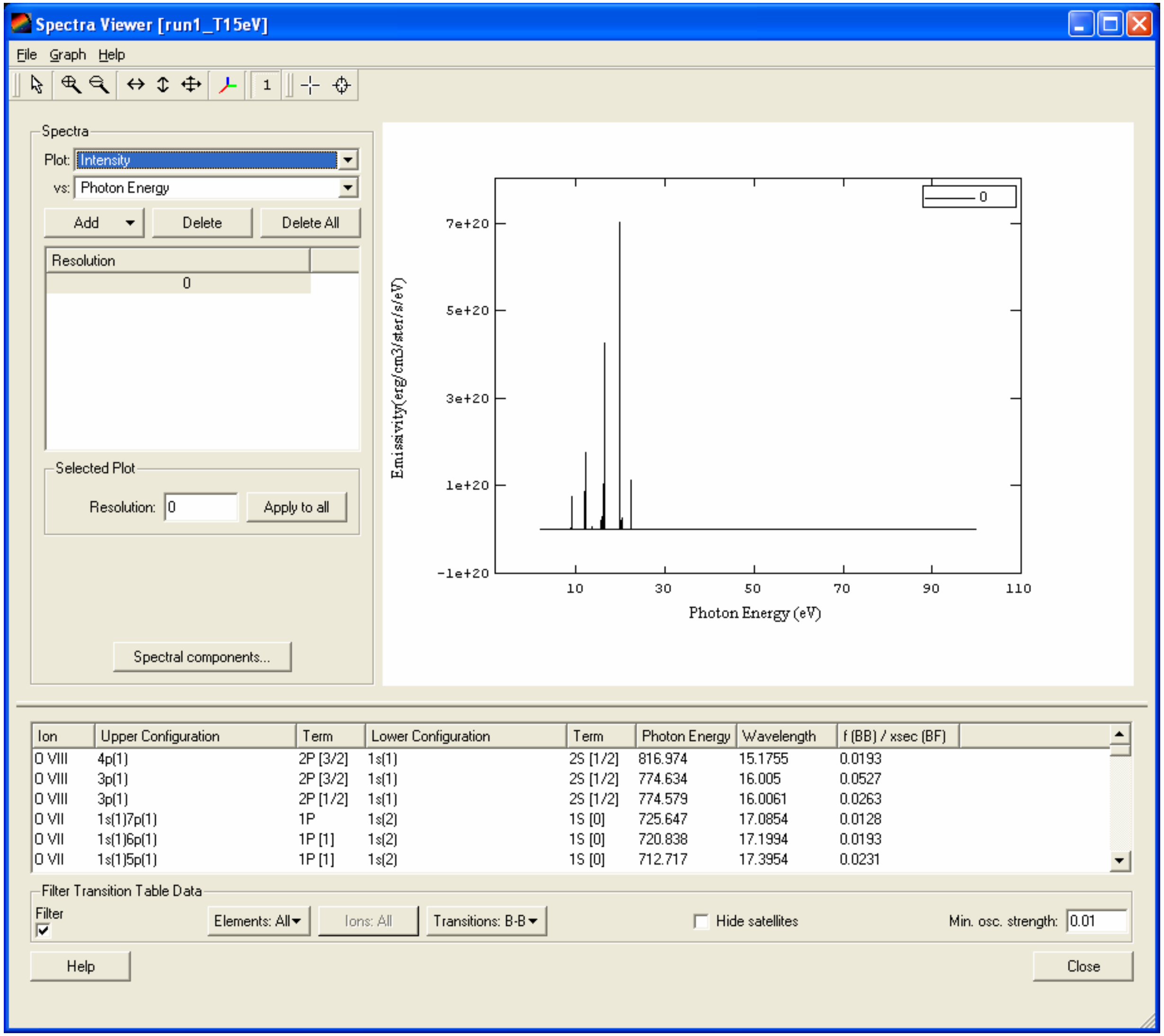
Z_{Si}:4.01 (>99% Si^{+4})

PrismSPECT ionization and excitation output

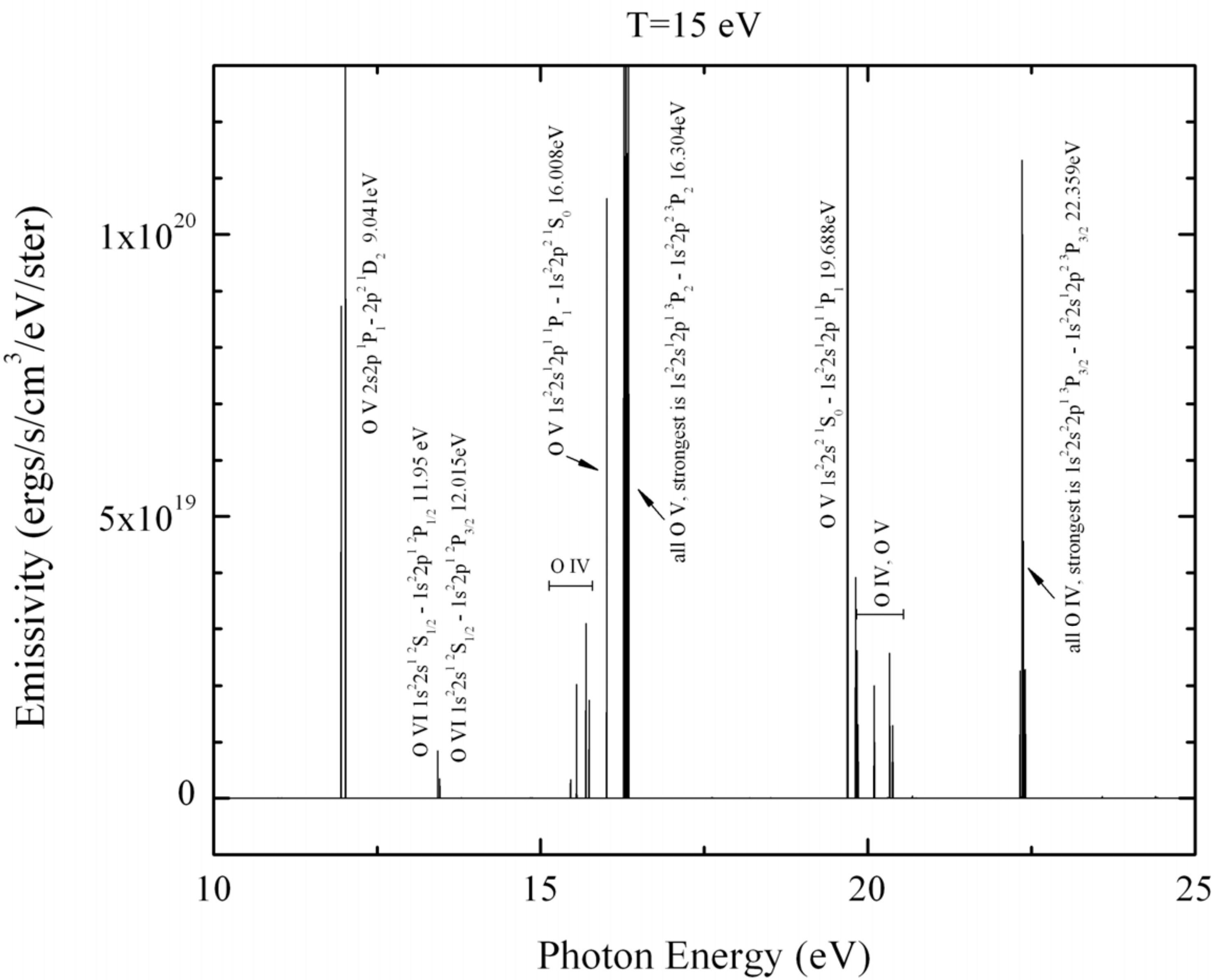




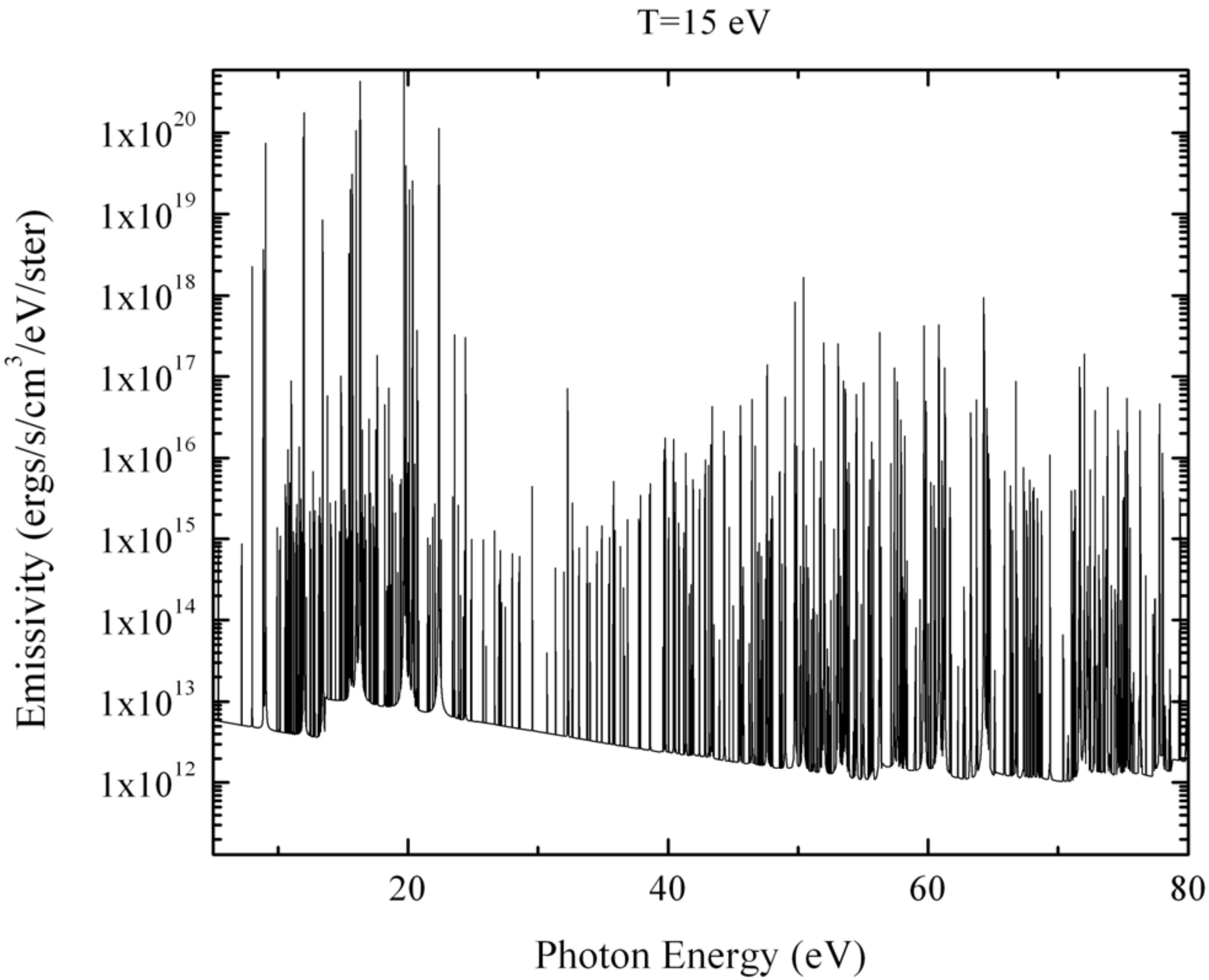
The GUI for the *PrismSPECT* spectrum viewer



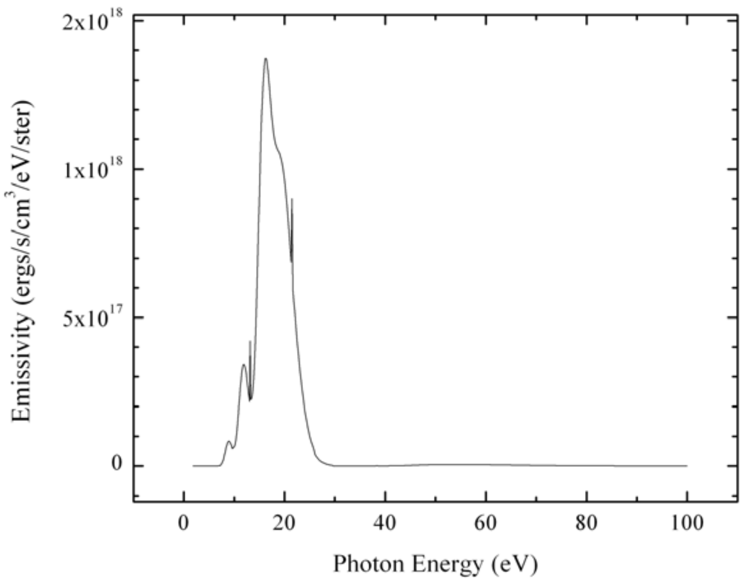
PrismSPECT simulated spectrum, with strong lines labeled…note: every line is from oxygen

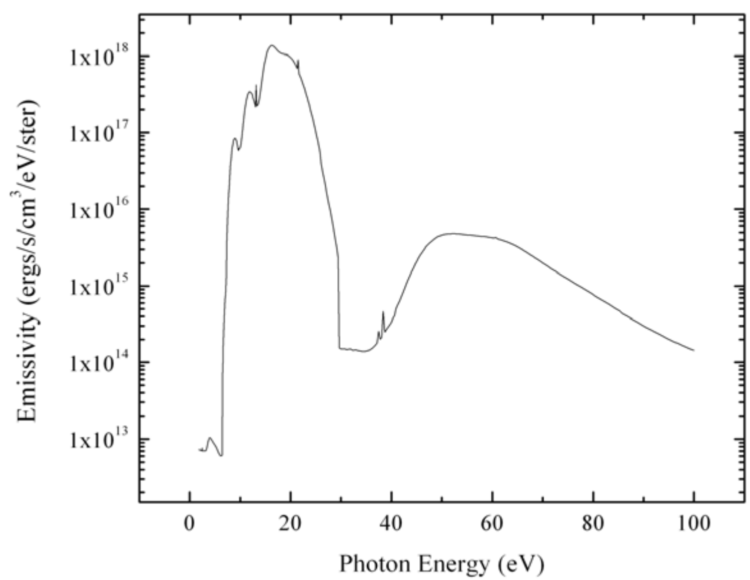


Same simulated spectrum as previous slide, but with a logarithmic y-axis: note domination of lines over continuum, and also note that the continuum is dominated by recombination, rather than free-free emission.



Again, the same simulated spectrum, but here it is degraded down to a very low resolution. This should enable us to better estimate what signal would be expected in a broad-band EUV/soft-x-ray detector.





The only difference between these two figures are the y-axes – linear (left) vs. log (right).

We next did a second calculation, identical in every way, except that the plasma temperature was increased to 50eV.

High temperature (50 eV) results

Ionization balance – mean charge states:

Z_H:1 (3.3 X 10^{-7} H^o)

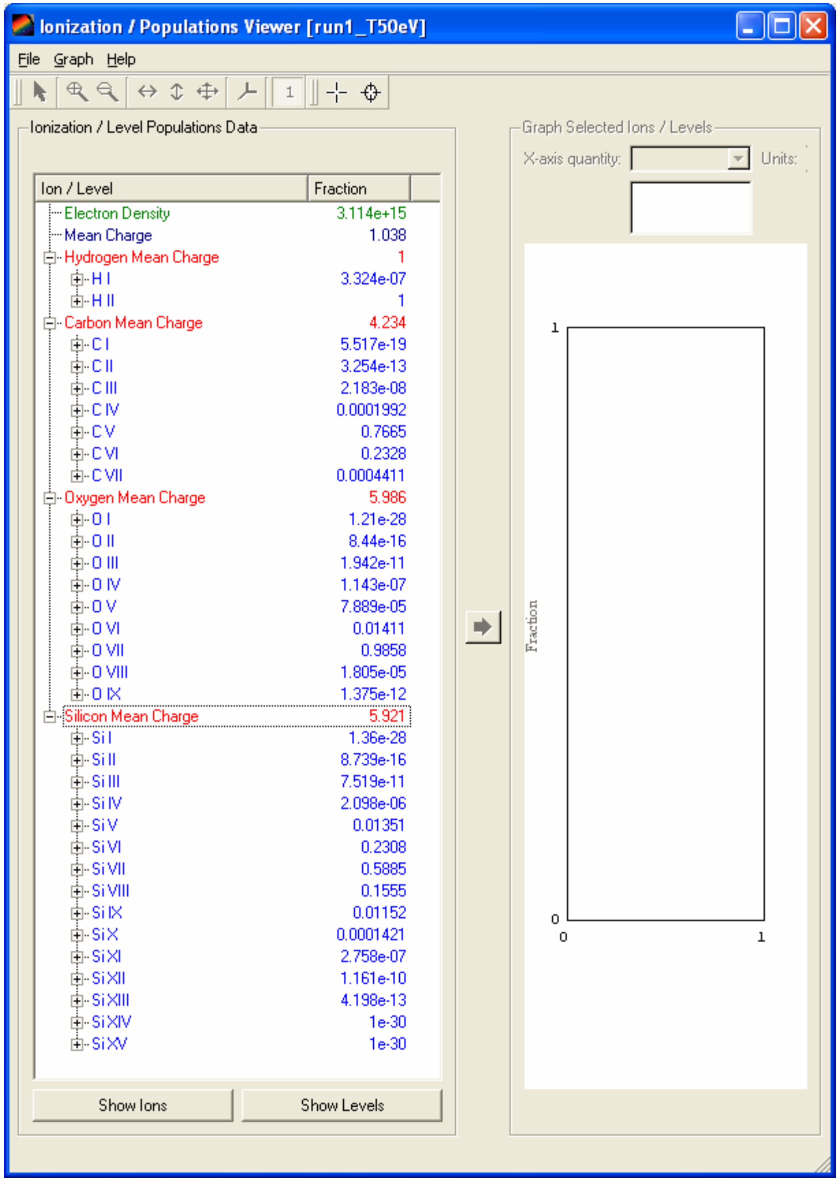
Z_C:4.23 (77% C^{+4}, 23% C^{+5})

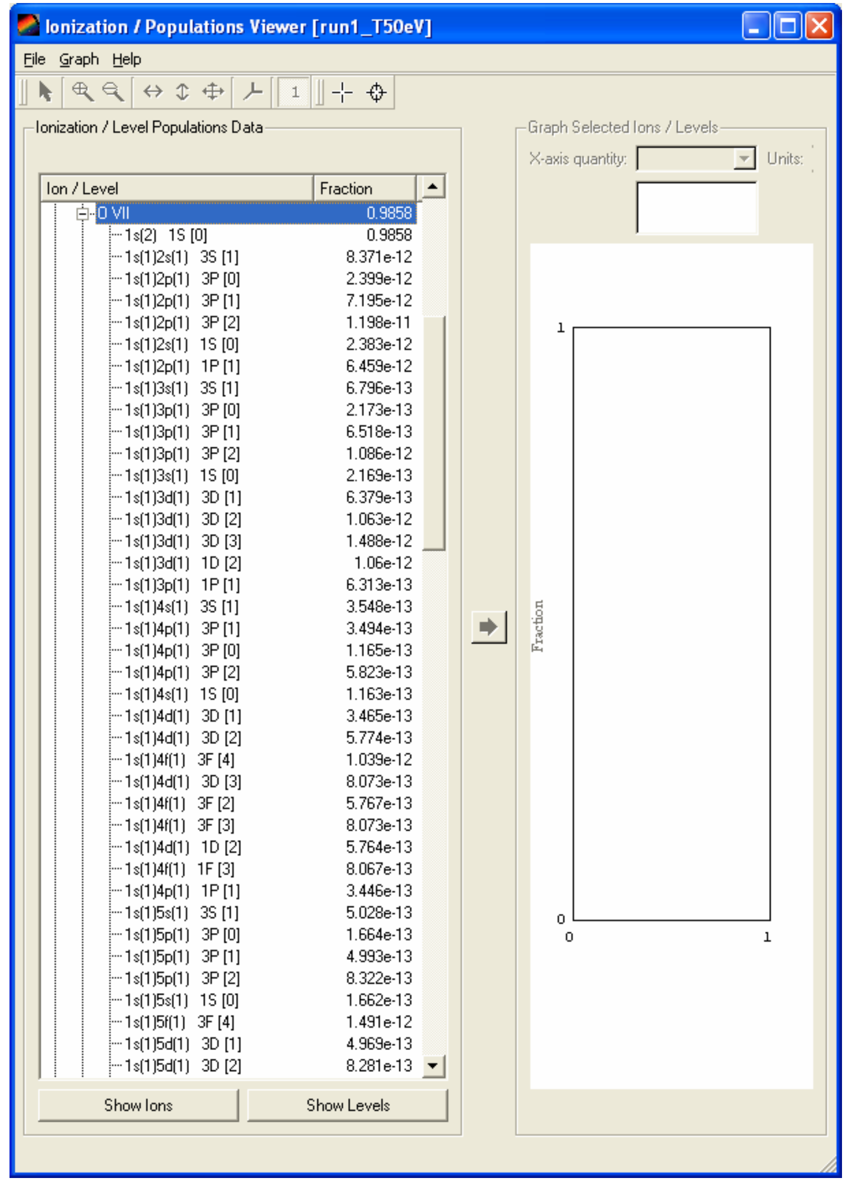
Z_O:5.99 (1% O^{+5}, 99% O^{+6})

Z_{Si}:5.92 (1% Si^{+4}, 23% Si^{+5}, 59% Si^{+6}, 16% Si^{+7})

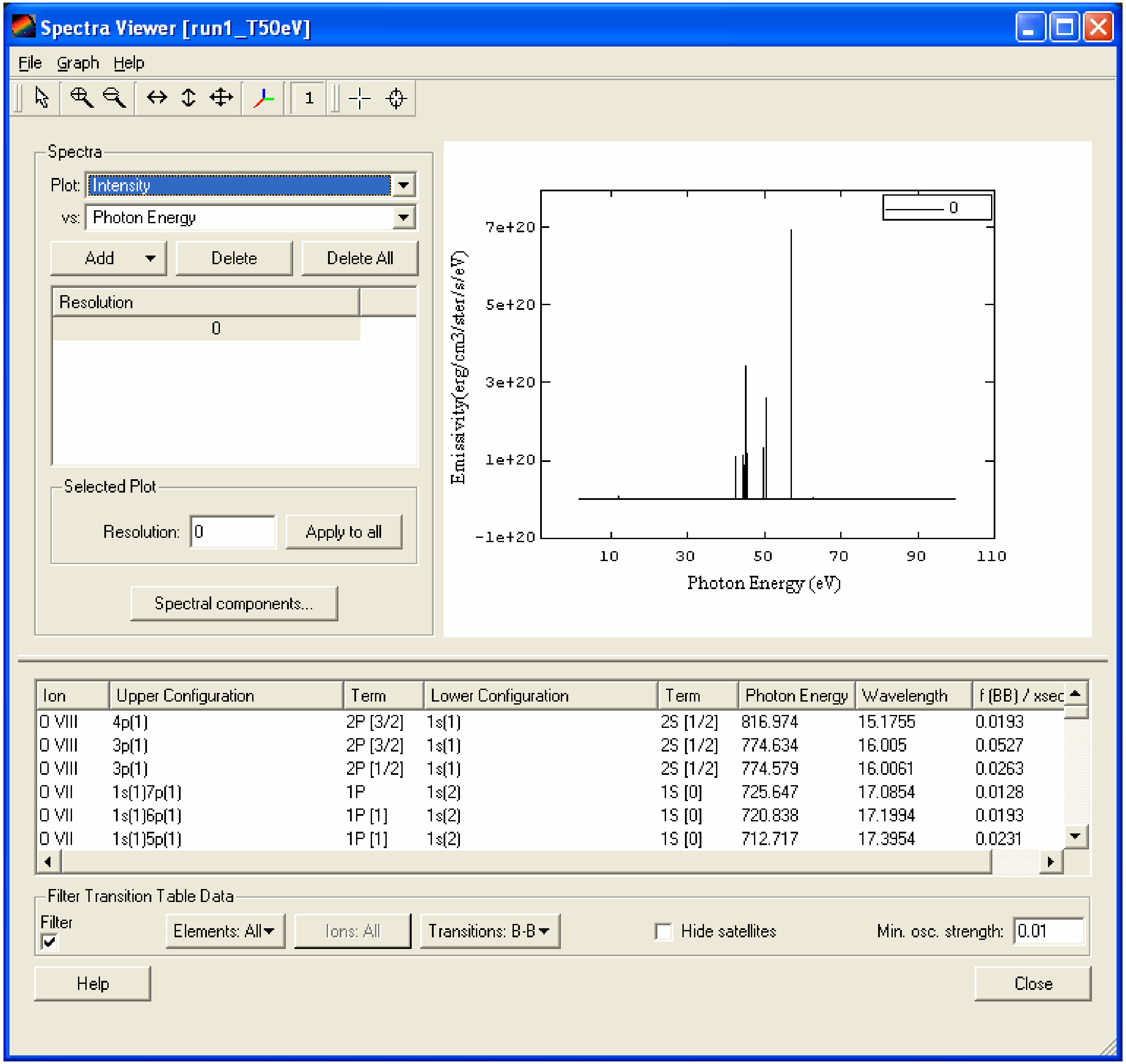
Note: increase by >1 charge state, compared to 15 eV calculation

PrismSPECT ionization and excitation output

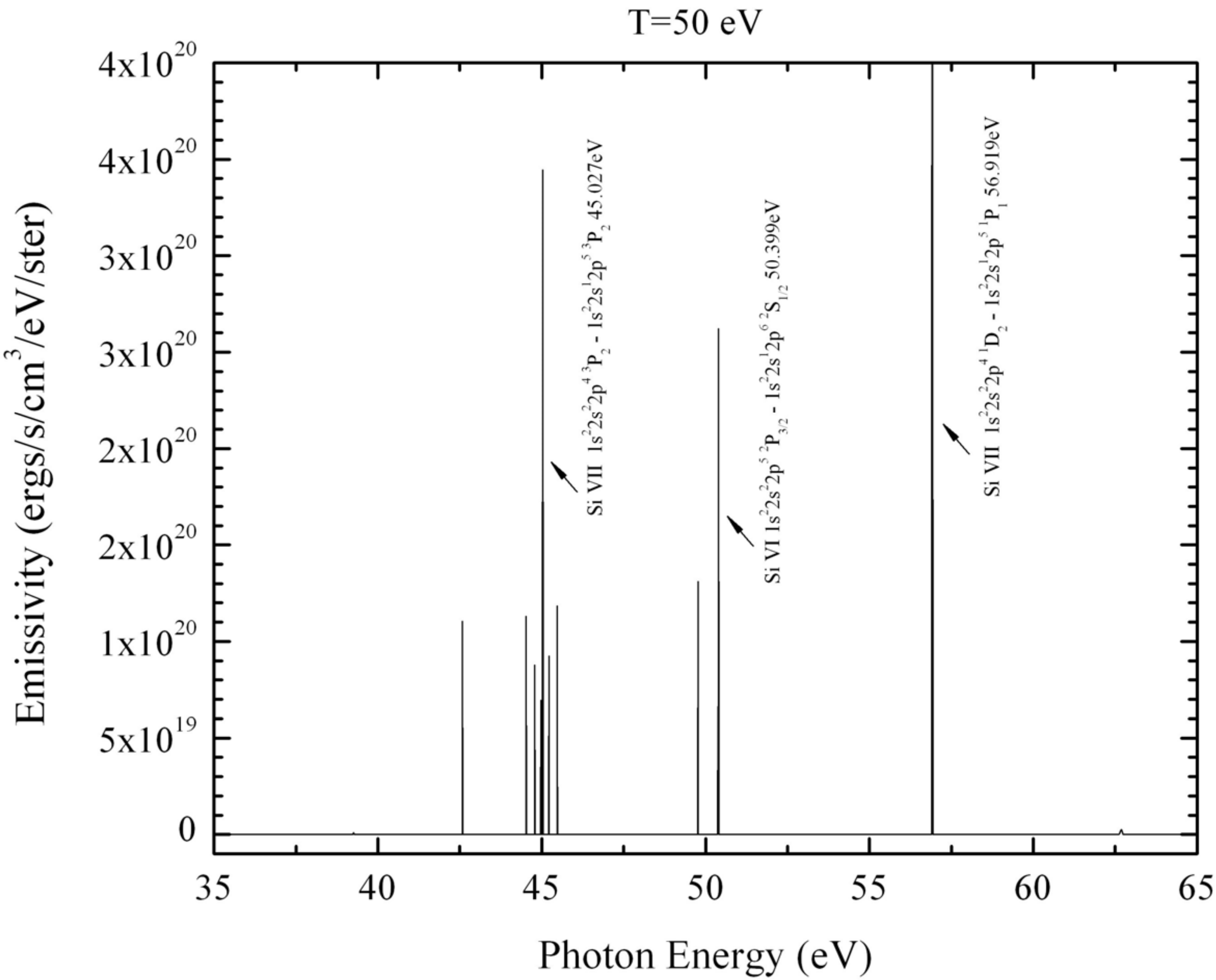




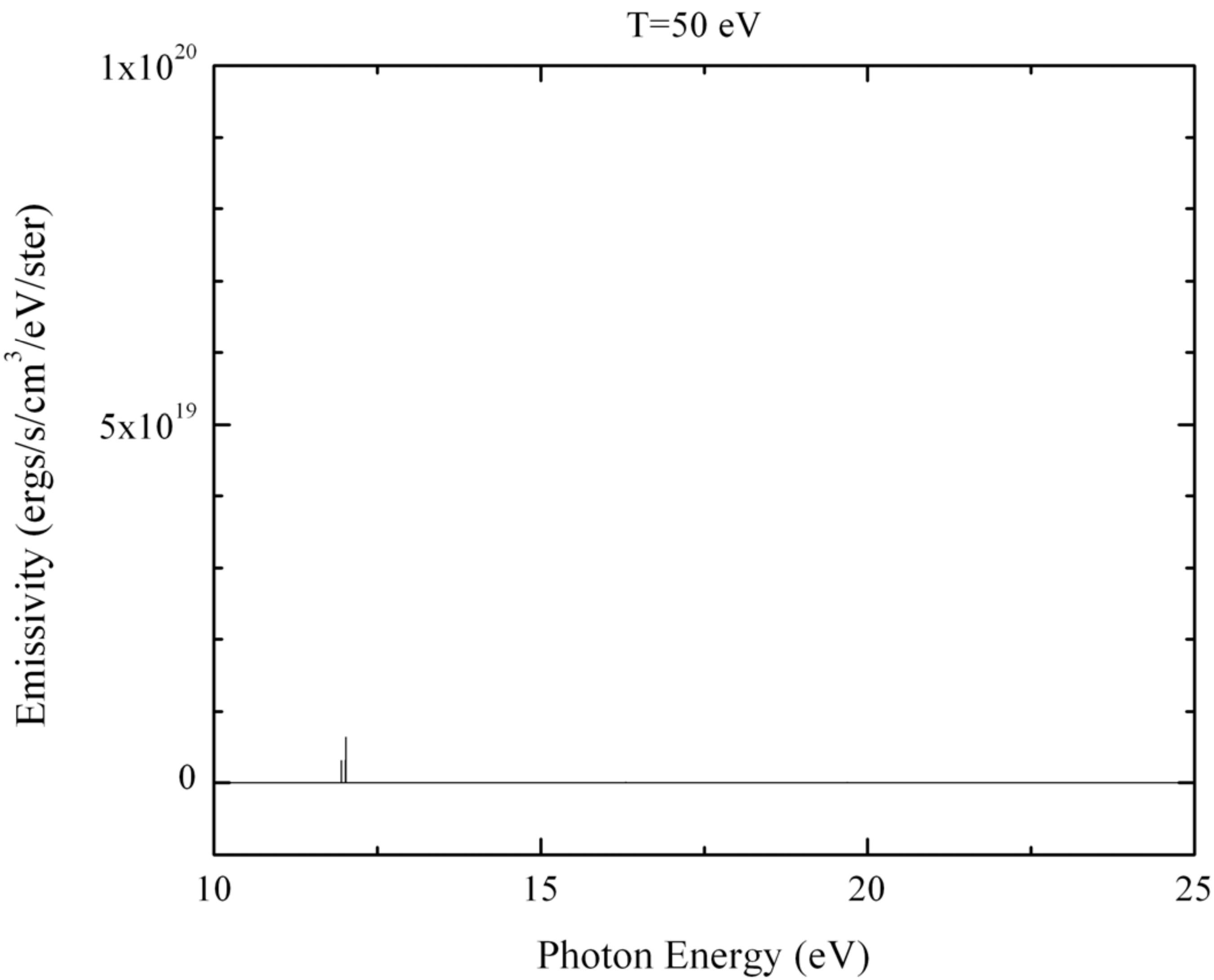
The GUI for the *PrismSPECT* spectrum viewer



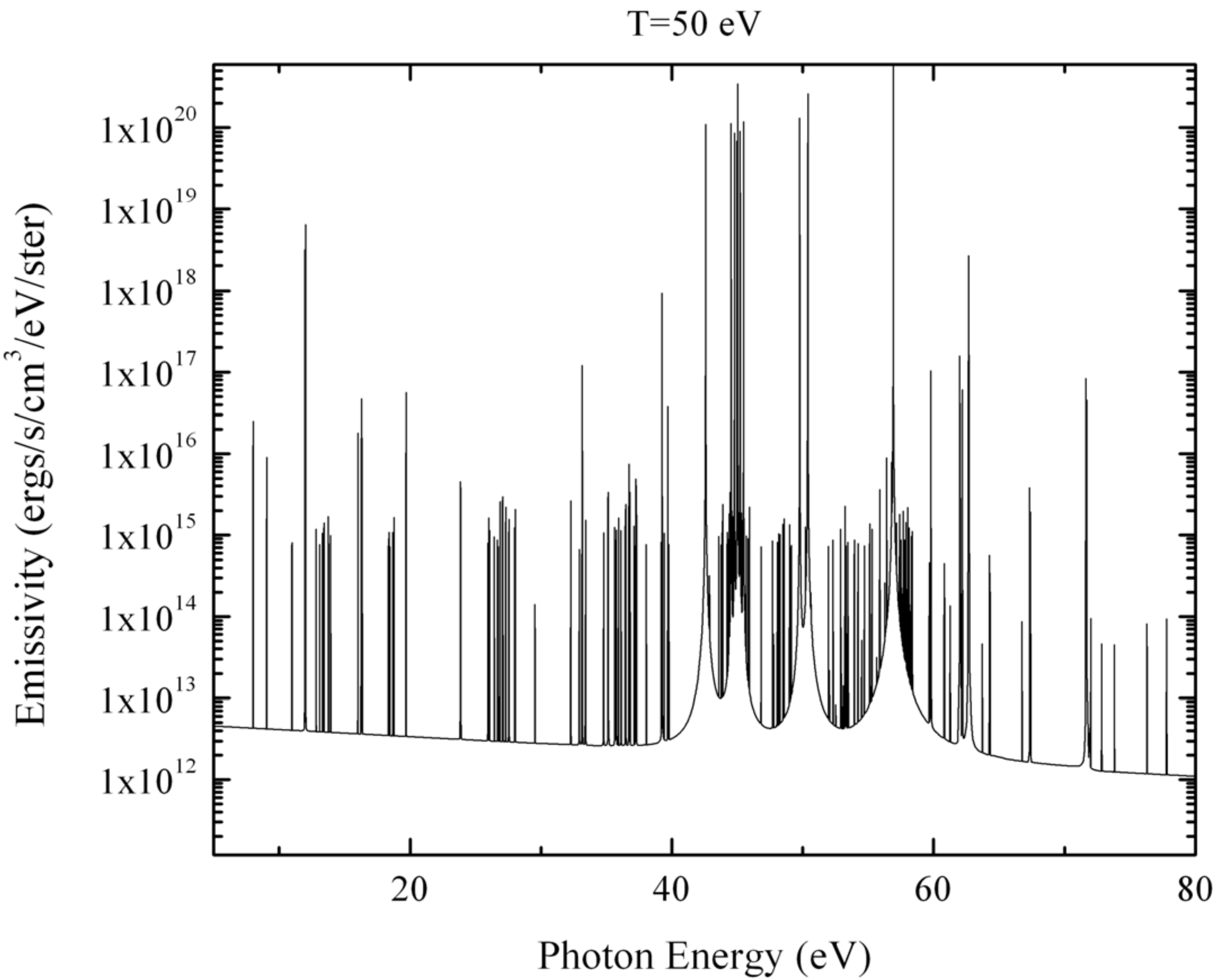
PrismSPECT simulated spectrum. Note the different wavelength coverage. Also, only the three strongest lines are identified (and they are all from silicon).



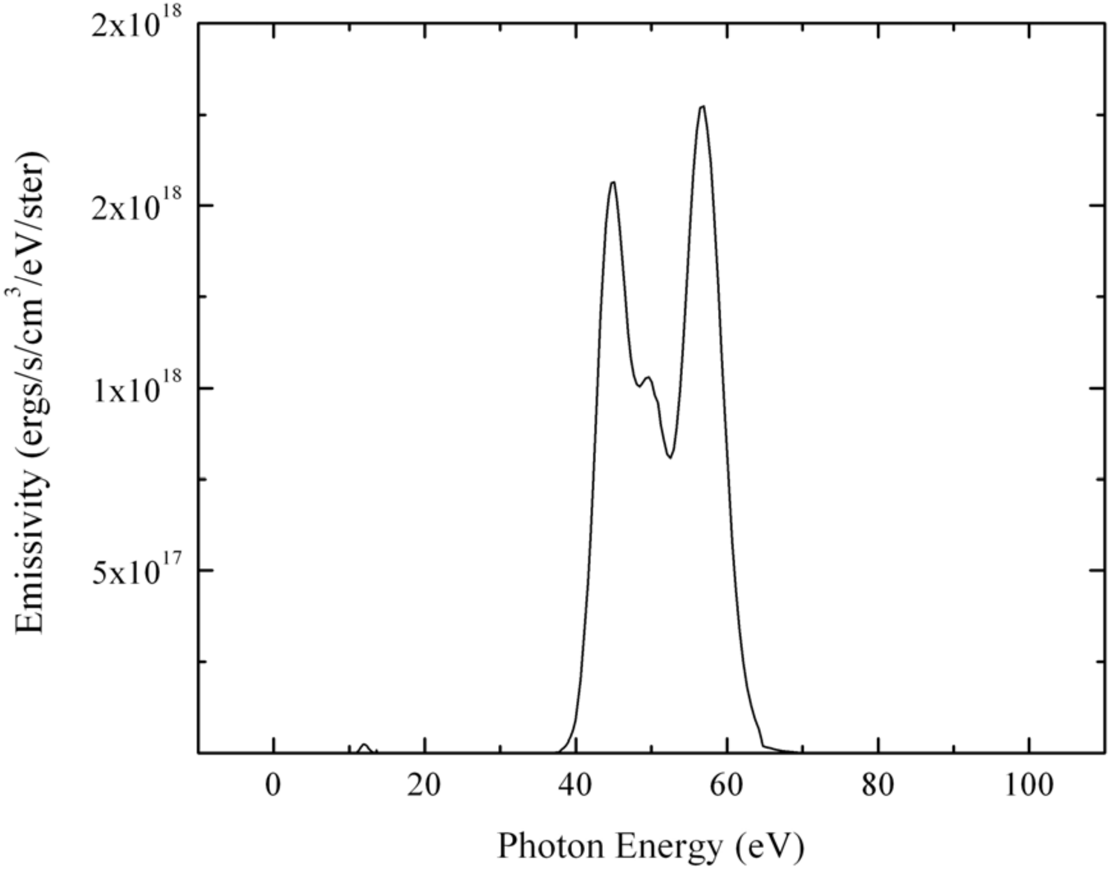
This is what the 50 eV spectrum looks like in the same photon energy range we showed for the 15 eV spectrum.



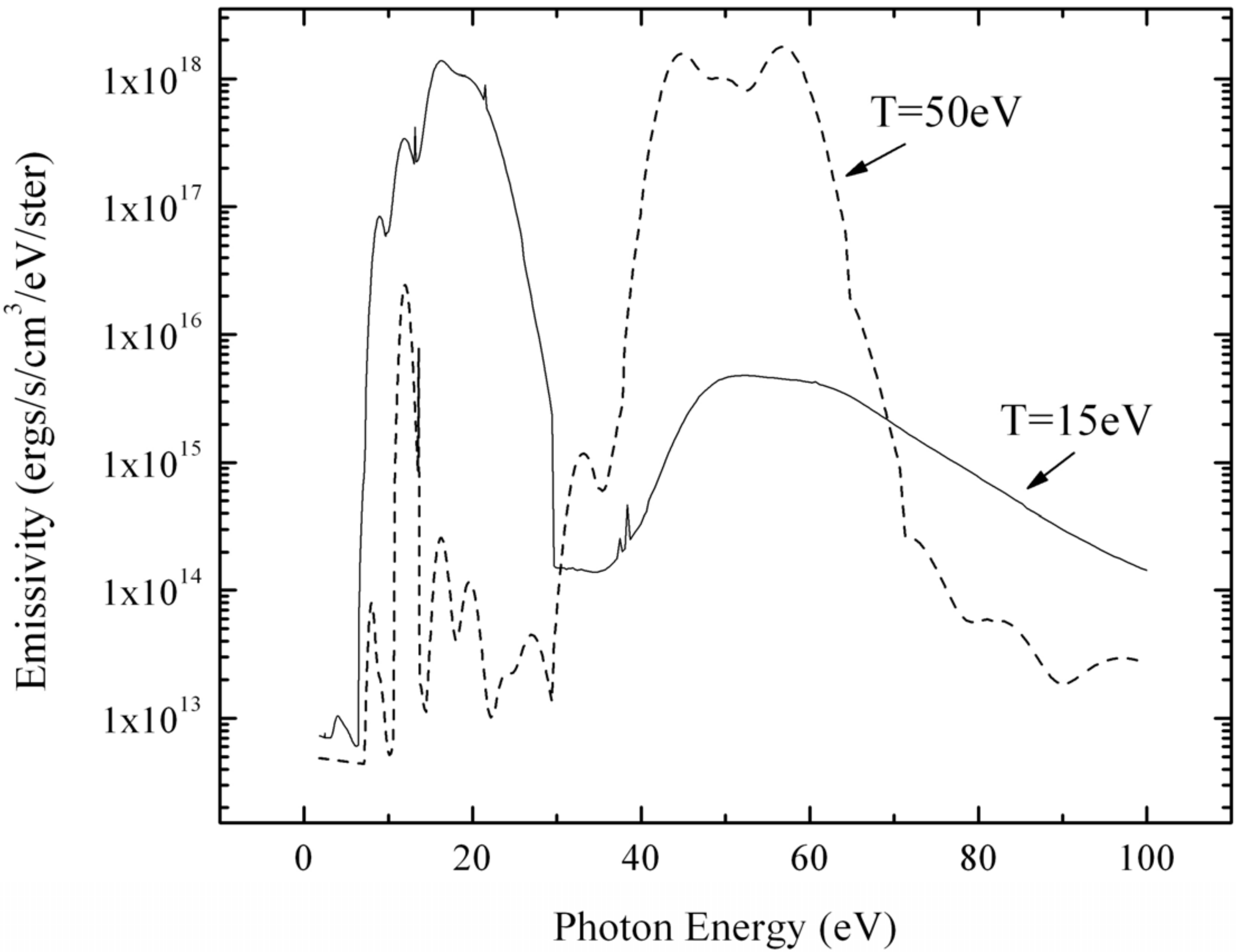
Spectrum plotted with logarithmic y-axis. Note the even weaker continuum than in the 15 eV spectrum, as well as the damping wings of the strongest lines.



And the 50 eV spectrum degraded to low resolution
(note linear y-axis)



Logarithmic representation of the low-resolution spectrum, compared to the 15 low-resolution spectrum.



Conclusions

- The spectrum is line dominated (and seems that it would be for significantly lower impurity levels)
- A small number of strong lines dominate
- In a given spectrum (at a specific temperature) a single element can completely dominate the emission
- At low resolution, the spectrum is moderately peaked, at $h\nu \sim kT$
- Over this range – a few 10s of eV – the emissivity is of order 10^{18} ergs/s/cm^3/ster/eV

Future Work

- More of the strong lines should be identified in the 50 eV case
- Lower (or different) impurity levels could be explored
- Given a time-history of temperature and density, we could perform a time-dependent calculation – there’s a very good chance that the plasma is far from equilibrium