



SPEX updates

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and the SPEX team

<https://www.sron.nl/astrophysics-spex/>

<https://spex-xray.github.io/spex-help/>

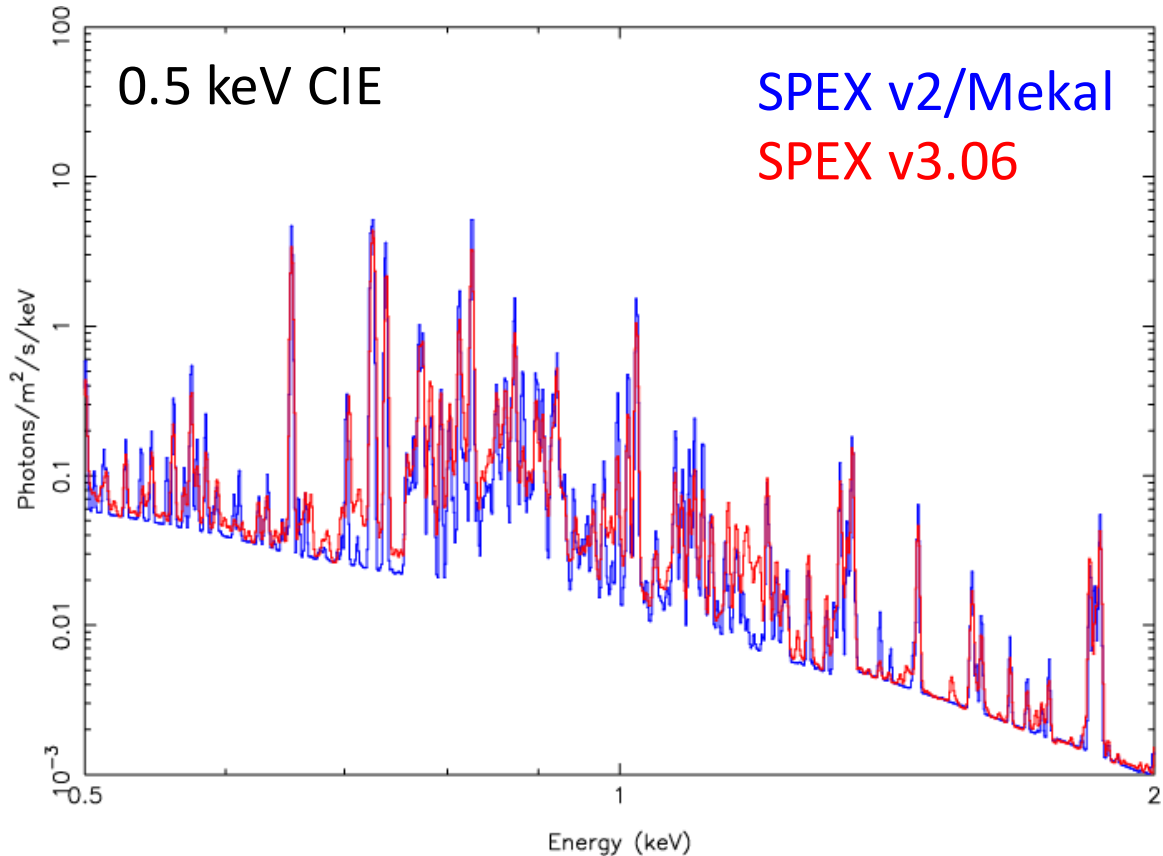
AtomDB 2020

SPEX: spectral modeling of various astrophysical conditions

- developed @ SRON since 1972
- handles X-ray spectrum for
 - collisional plasma (clusters, SNRs, stars, etc)
 - photoionized plasma (AGNs, etc)
 - molecular dust absorption (ISM, etc)
 - charge exchange (heliosphere, etc)
- backed by atomic database of 9 processes, ~400 ions, ~ 10^7 transitions
- run on-the-fly to solve multi-dimension (e.g., temperature- and density-) dependence

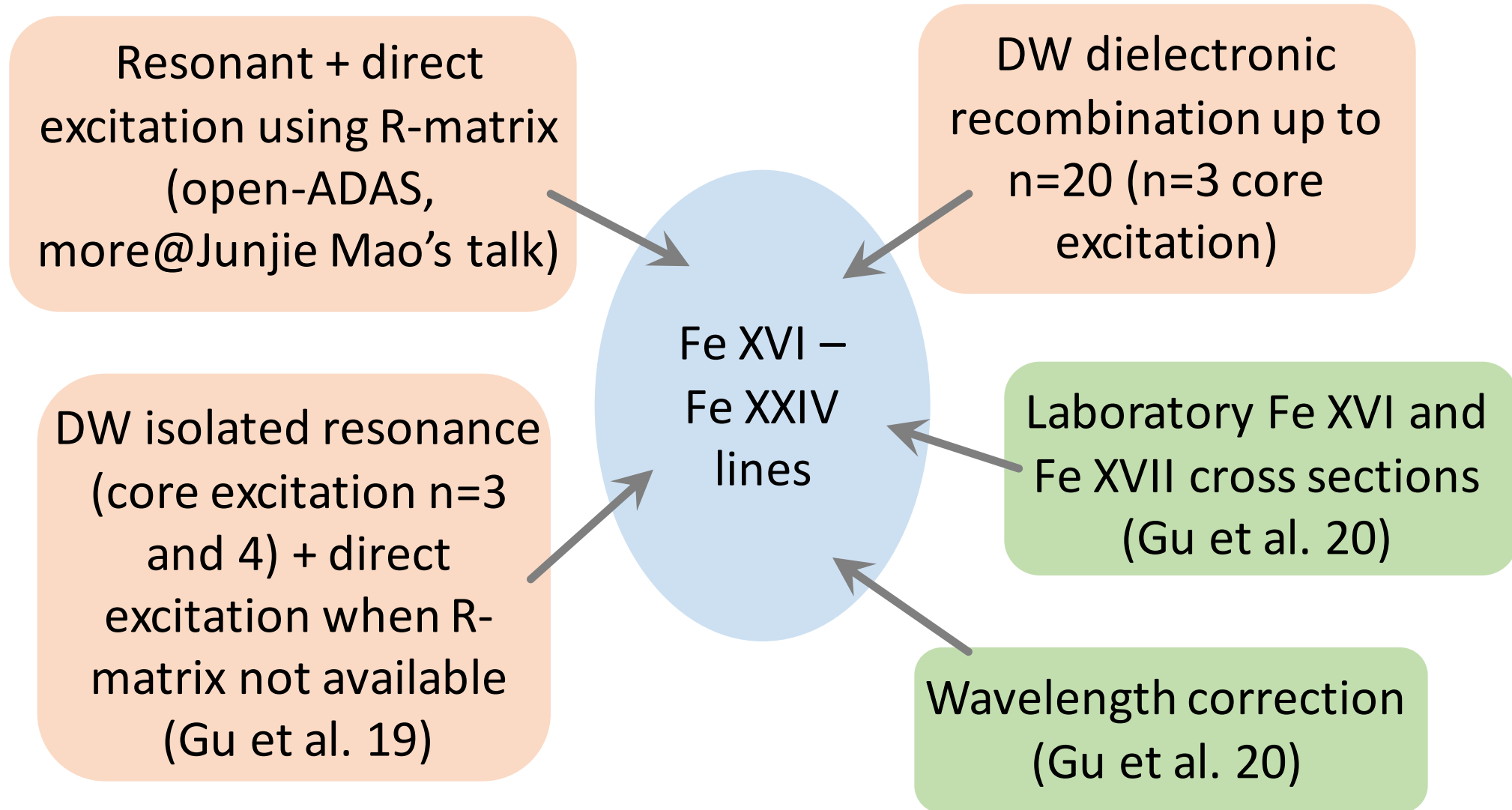
SPEX version 3.06 updates

- Fe-L complex atomic data update (Gu et al. 2019, 2020)

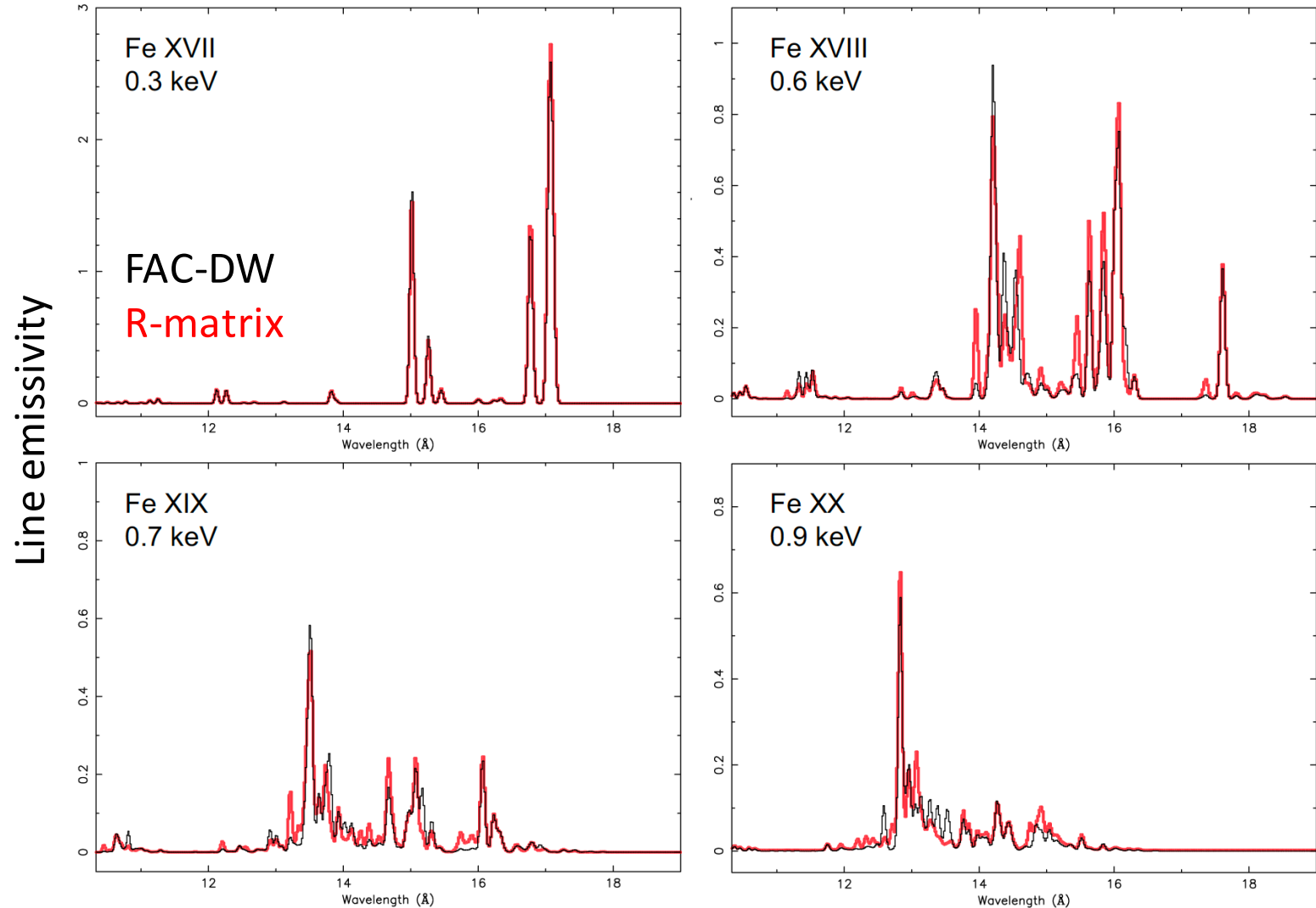


- New cooling function from updates in collisional excitation data (Stofanova et al. submitted)
- Python interface (pyspex)
- New dust extinction data from laboratory measurements (Zeegers et al. 17, 19; Rogantini et al. 19; Costantini et al. 19)

Fe-L atomic data updates

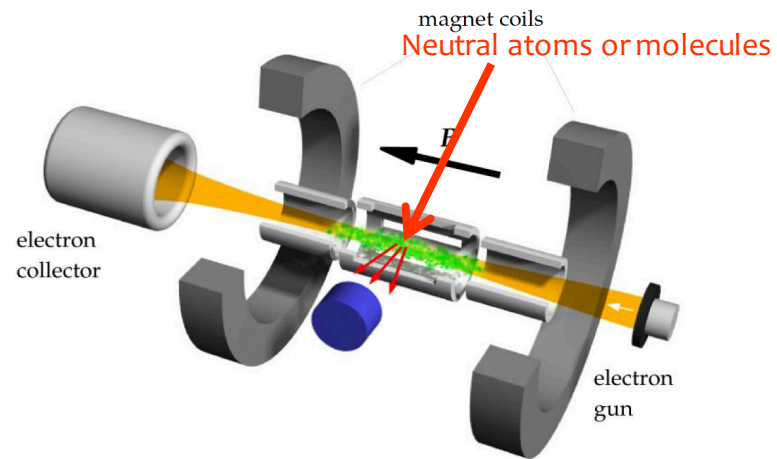
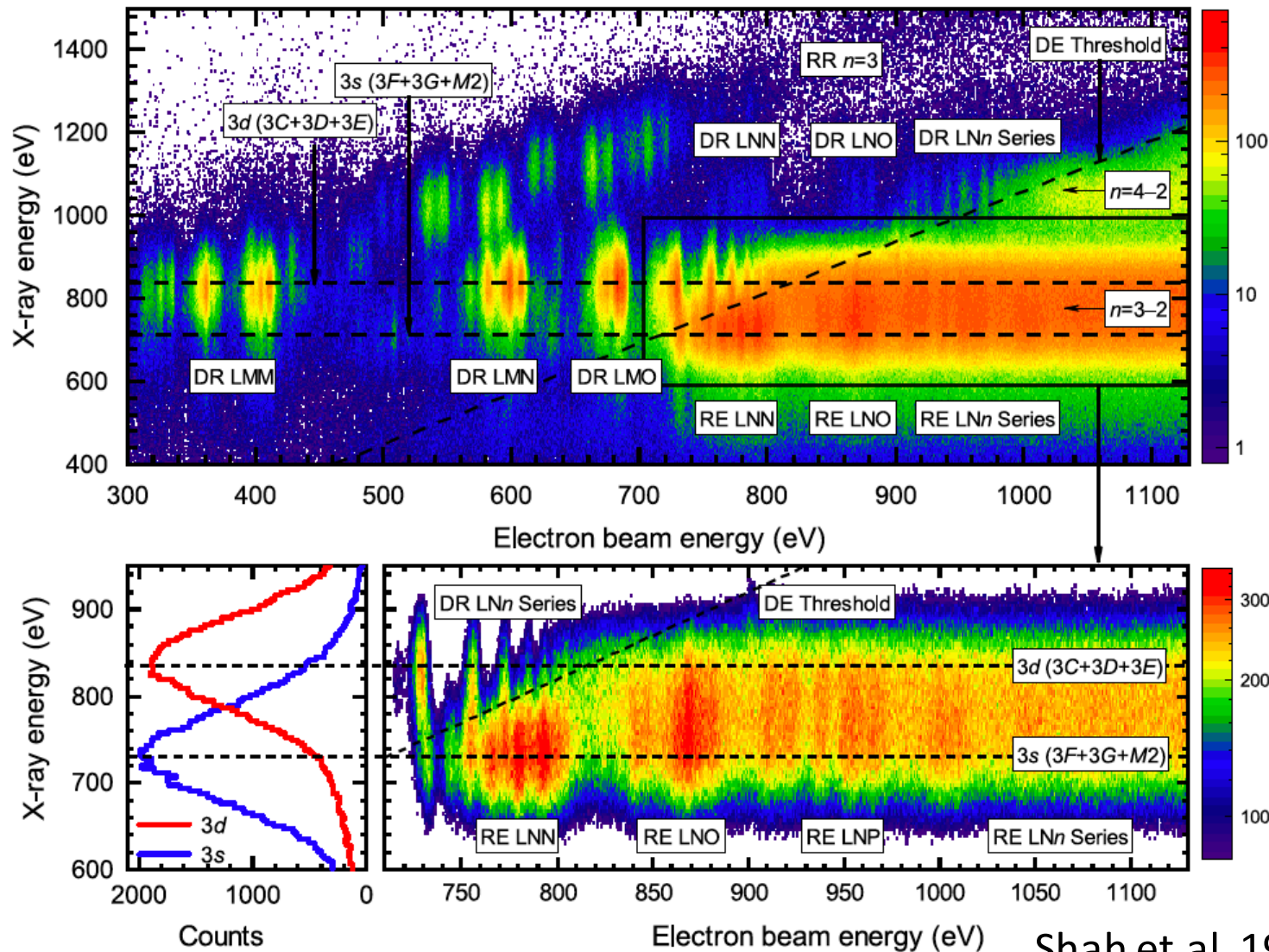


Theoretical excitation rates



- A systematic comparison between DW and R-matrix for Fe-L ions (Gu et al. 19)
- Full relativistic DW can reproduce R-matrix within 10-20% on the strong lines
- Larger differences on the weaker transitions

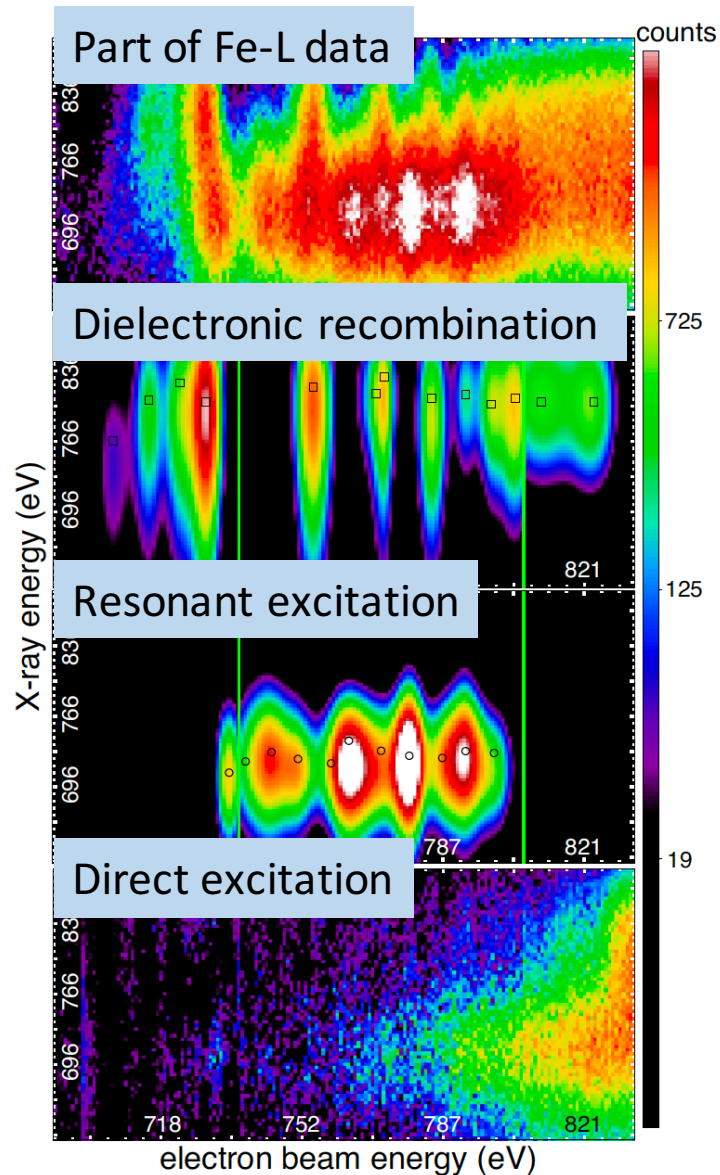
Laboratory measurement of Fe XVI and Fe XVII cross sections



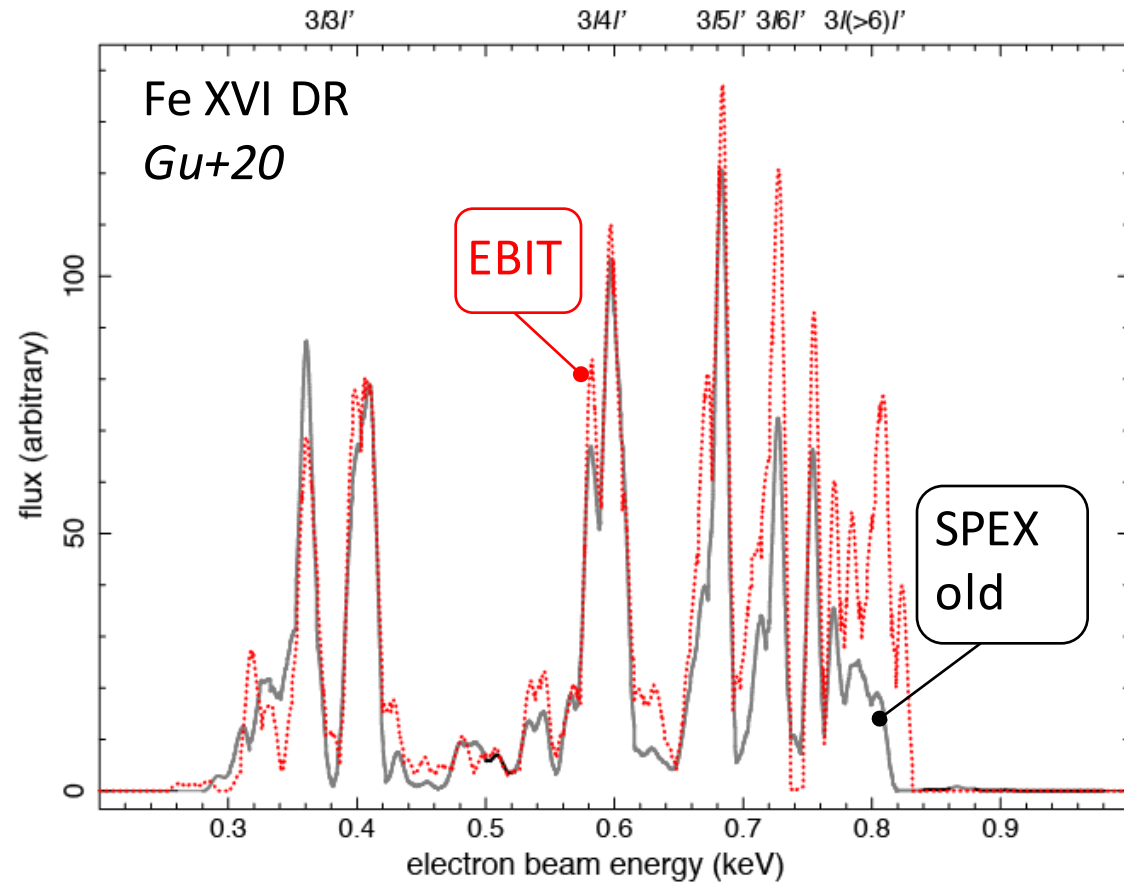
- Heidelberg Flash-EBIT measurement of Fe XVI DR and Fe XVII excitation (see Chintan Shah's talk)
- Resolve DR to $n \geq 10$
- Distinguish resonant excitation peaks from the direct excitation continuum

Shah et al. 19

EBIT cross sections incorporated in SPEX

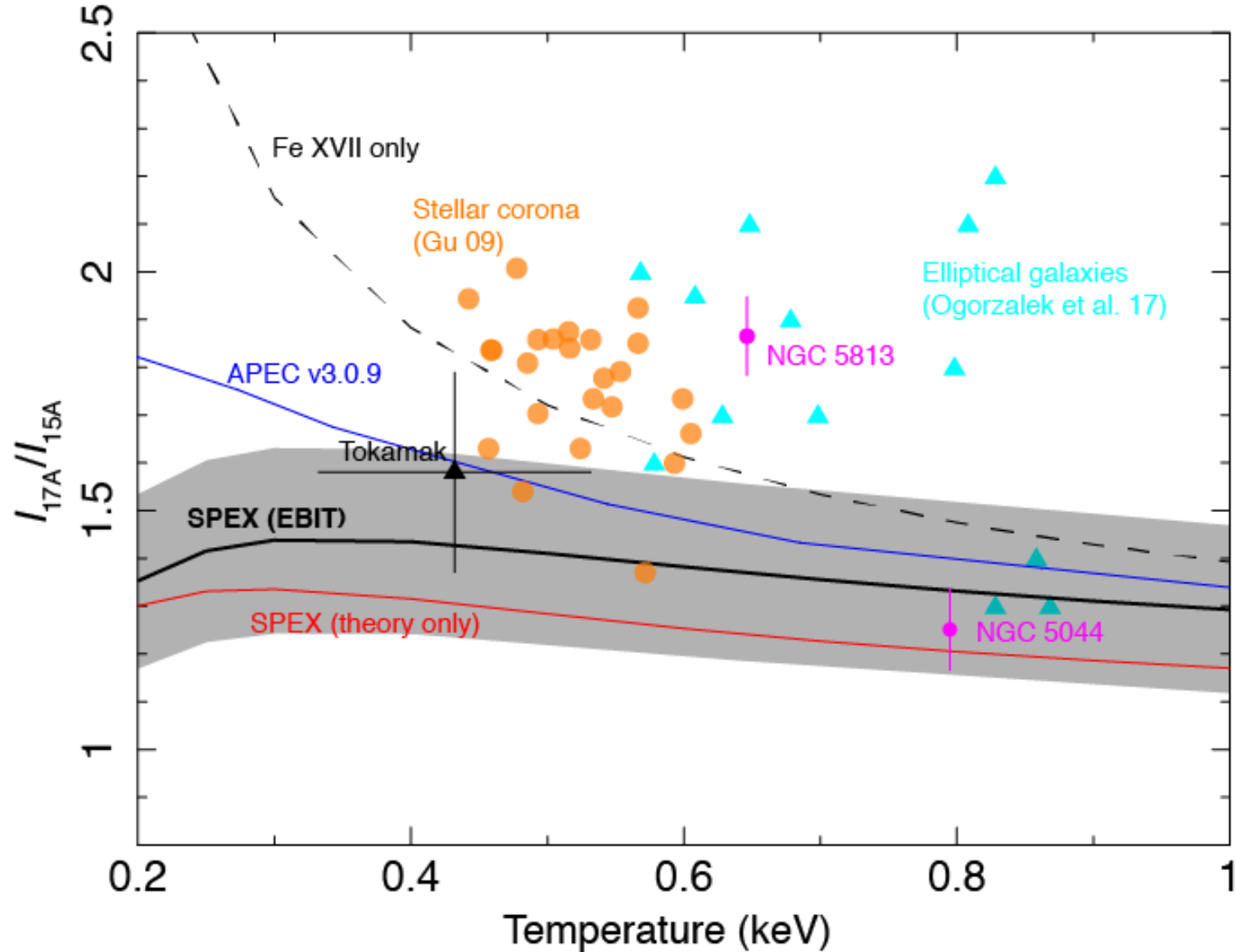


- analyzed in 2-D: decompose data into continuum and resonances; recover flux at detector response tail
- directly compare with SPEX



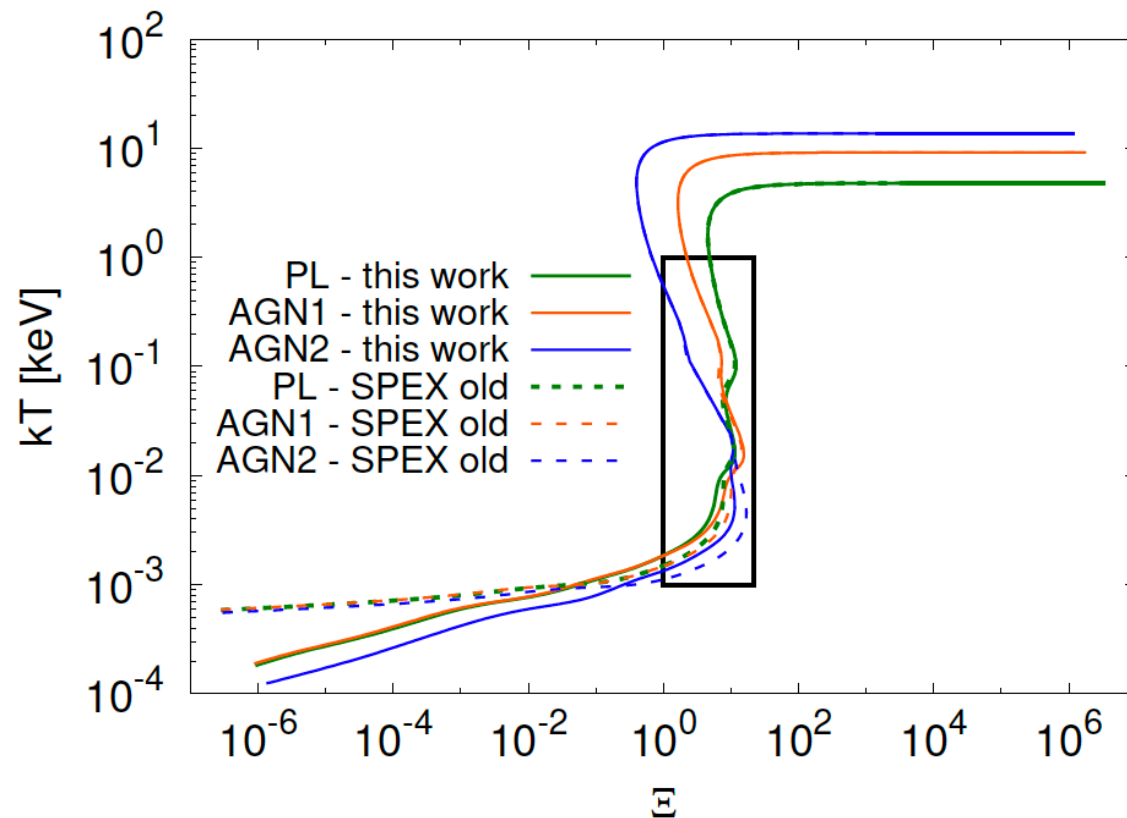
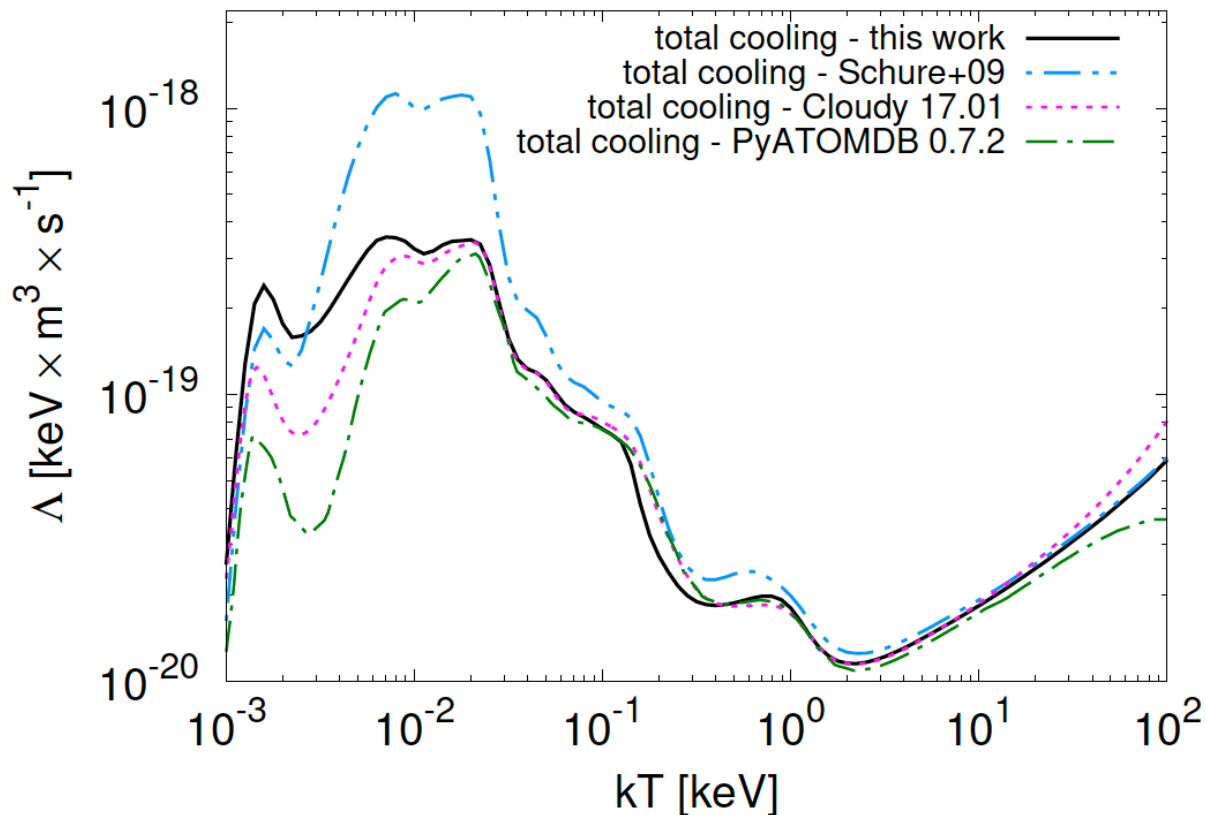
For the first time, Laboratory cross sections (error $\sim 10\%$) incorporated in SPEX (Gu et al. 20).

Fe XVI + Fe XVII 17A/15A ratio



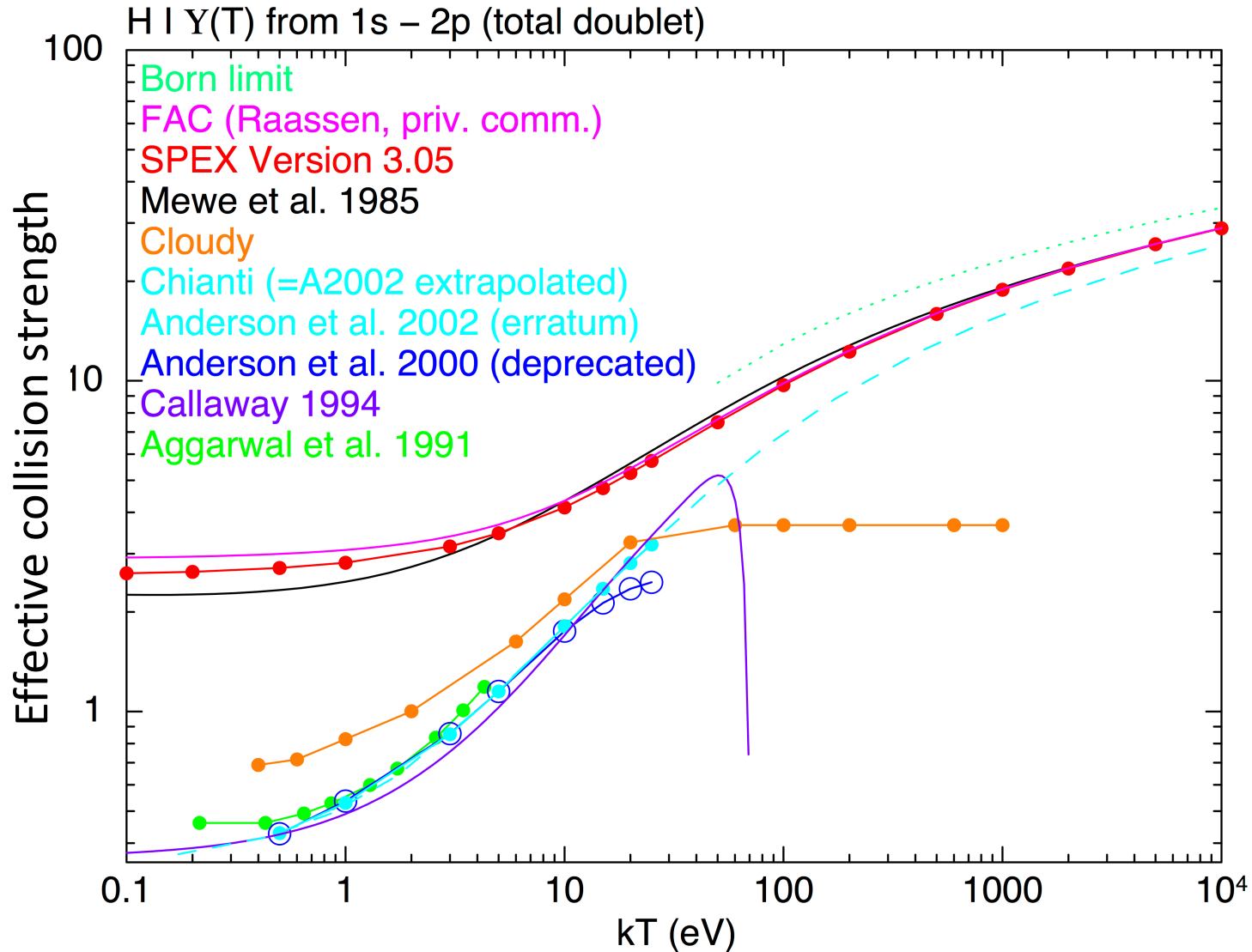
- Important for science such as resonant scattering
- 15 A flux contributed by both Fe XVII and Fe XVI DR (blended), 17 A flux dominated by Fe XVII
- Fe XVI DR is important for the line ratio at low temperature
- For the 15 A line, theory flux is lower than EBIT for Fe XVI, but higher for Fe XVII
- APEC-SPEX discrepancy at low temperature mainly from Fe XVI

Updates in cooling function



- Difference at 10 eV between SPEX old and new mainly caused by improved C, N, and O excitation data (Stofanova et al. submitted)
- Strongly affect the stability curve for the photoionized model (*pion*) and the cooling flow model (*cf*)

Collisional excitation of the simplest atom

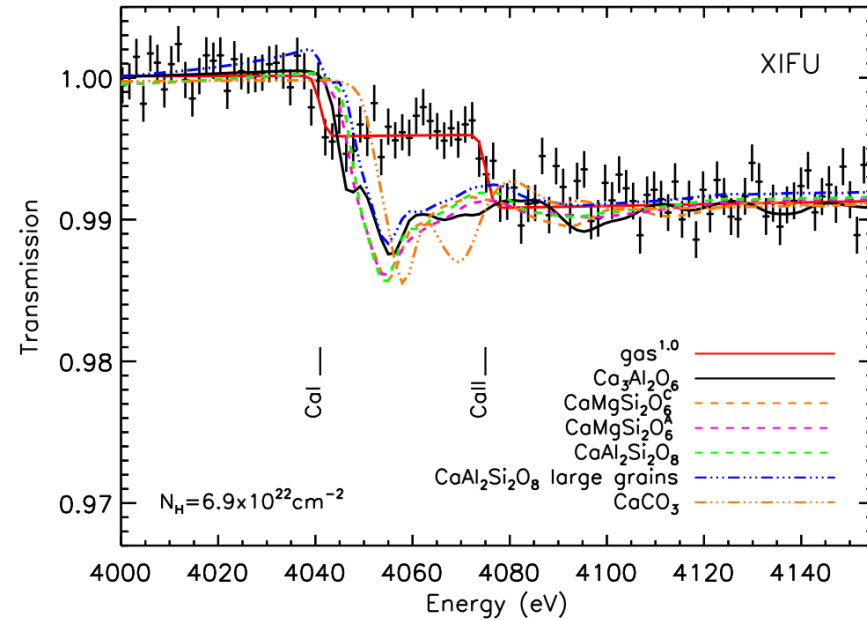


- H I 1s-2p is the dominant coolant at 2.5 eV
- R-matrix/close-coupling and other calculations differ near/below the threshold for this seemingly simplest transition
- Laboratory measurement (Williams et al. 1988) near the threshold in favor of the R-matrix curve
- Possible change in SPEX under discussion

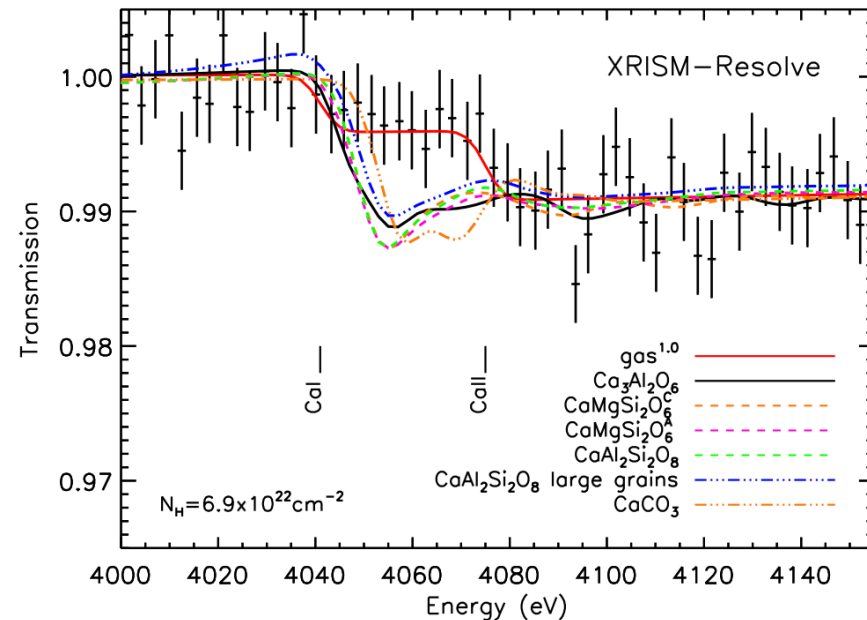
Improvements in the ISM dust absorption modeling

New dust extinction profiles measured at synchrotron beam line implemented in the *amol* model (Zeegers et al. 17, 19; Rogantini et al. 19; Costantini et al. 19)

- ~20 new dust candidates, amorphous/crystalline forms
- ~15 have multiple edges (Mg, Si, Fe, etc)
- needed for dust astrochemistry with future instruments (Arcus, Athena, XRISM, etc)



Costantini et al. 19



PYSPEX: the SPEX Python interface

SPEX 3.06 contains a Python interface.

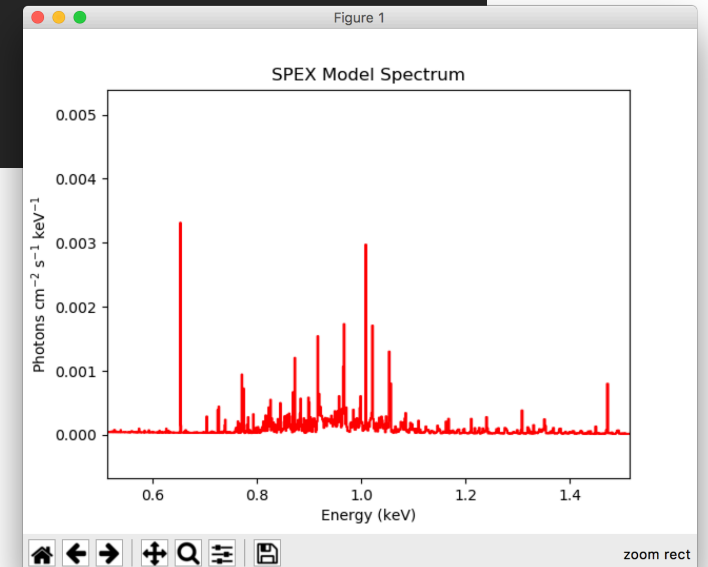
- Pass commands from Python to SPEX
- Get results and other data from SPEX back in Python.
- Plot in matplotlib
- This is a first version. More development on its way.

<https://spex-xray.github.io/spex-help/pyspex.html>

```
(spex) mac-204:~ jellep$ python
Python 3.5.6 [Anaconda, Inc.] (default, Aug 26 2018, 16:30:03)
[GCC 4.2.1 Compatible Clang 4.0.1 (tags/RELEASE_401/final)] on darwin
Type "help", "copyright", "credits" or "license" for more information.
>>> from pyspex.spex import Session
>>> s=Session()
Welcome jellep to SPEX version 3.06.00

NEW in this version of SPEX:
05-06-2019 Update of cooling processes
18-12-2019 Included new atomic data (Fe-L, Gu et al. 2019)
05-02-2020 Included Python interfaces for SPEX
24-03-2020 Included new molecular dust data
10-07-2020 SPEX manual now at: https://spex-xray.github.io/spex-help
10-07-2020 Report questions and issues to: https://github.com/spex-xray/spex-help/issues

Currently using SPEXACT version 2.07.00. Type `help var calc` for details.
>>> s.var_calc('new')
Now using SPEXACT version 3.06.00
>>> s.com('cie')
You have defined 1 component.
>>> s.calc()
>>> s.plot_model()
<pyspex.plot.PlotModel object at 0x1101b1860>
>>>
```



An example SPEX session in Jupyter Notebook

In this example, we show how to do a spectral fit with the Python interface to SPEX (pyspex). The first thing we need to do is to start a SPEX session in Python. We do that by importing the Session class from `pyspex.spex` and then we create a Session instance `s` which will be the pointer to our SPEX session:

```
In [1]: from pyspex.spex import Session
        s = Session()
        %matplotlib inline
```

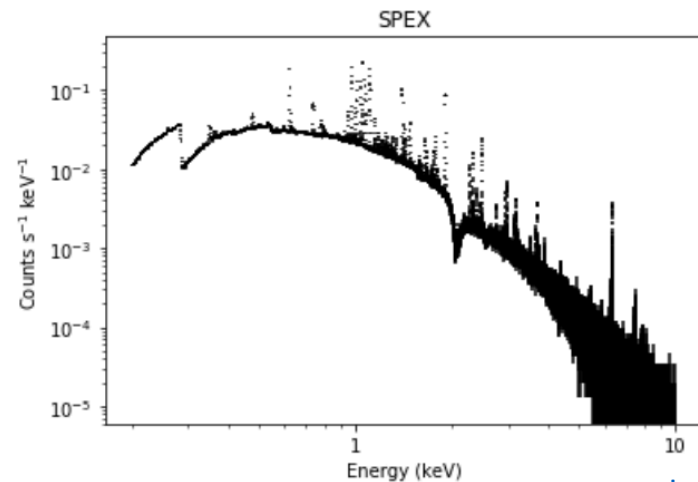
Reading a dataset

Let's first read in the example dataset, which is a spectrum and response for the future XIFU instrument aboard Athena. This is done by calling the session method `data` and provide the filename for the res and spo file:

```
In [2]: s.data('xifu.res', 'xifu.spo')
```

Using a plot, we can see what the data look like. So let's make a log-log plot to look at the spectrum:

```
In [3]: plt = s.plot_data(xlog=True, ylog=True, show=True)
```



<https://github.com/spex-xray/spex-help/blob/master/jupyter/Simple-Session.ipynb>

Achievements by now

- Fe L-shell complex atomic data improved → affect collisional and photoionized plasma models ([cie](#), [nei](#), [pion](#), etc)
- Cooling function re-calculated with updated collisional data → photoionized ([pion](#)) and cooling flow ([cf](#)) models
- New dust extinction profiles implemented in [amol](#)
- Python interface introduced

Future plan (by the launch of XRISM)

- L-shell atomic data of other abundant elements (Ni, Si, Mg, Ca)
- Revisit Fe K-shell with laboratory measurements
- Uncertainties on atomic data (my talk tomorrow)