Identifying Dust Features

in high resolution X-ray spectra

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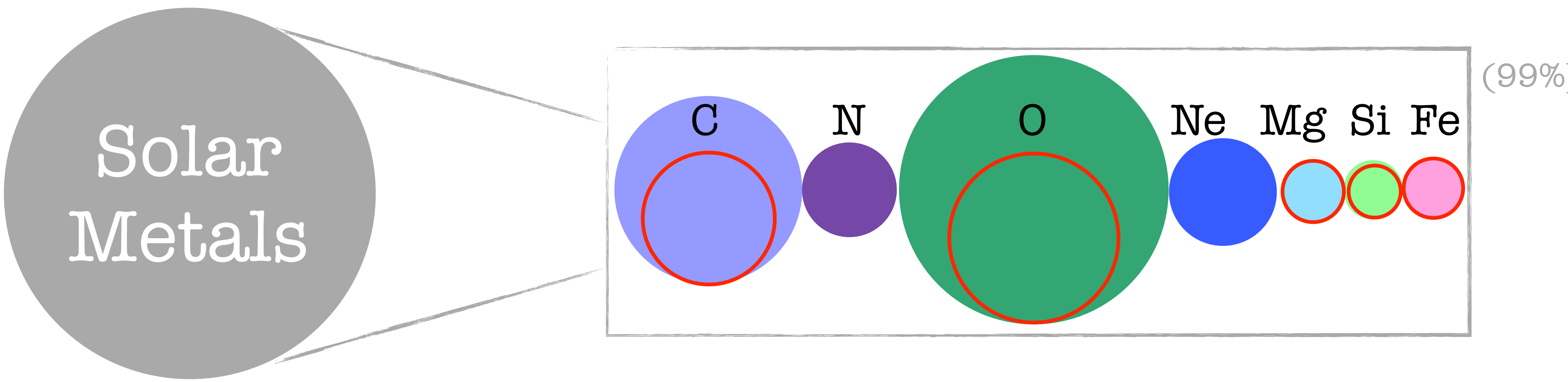
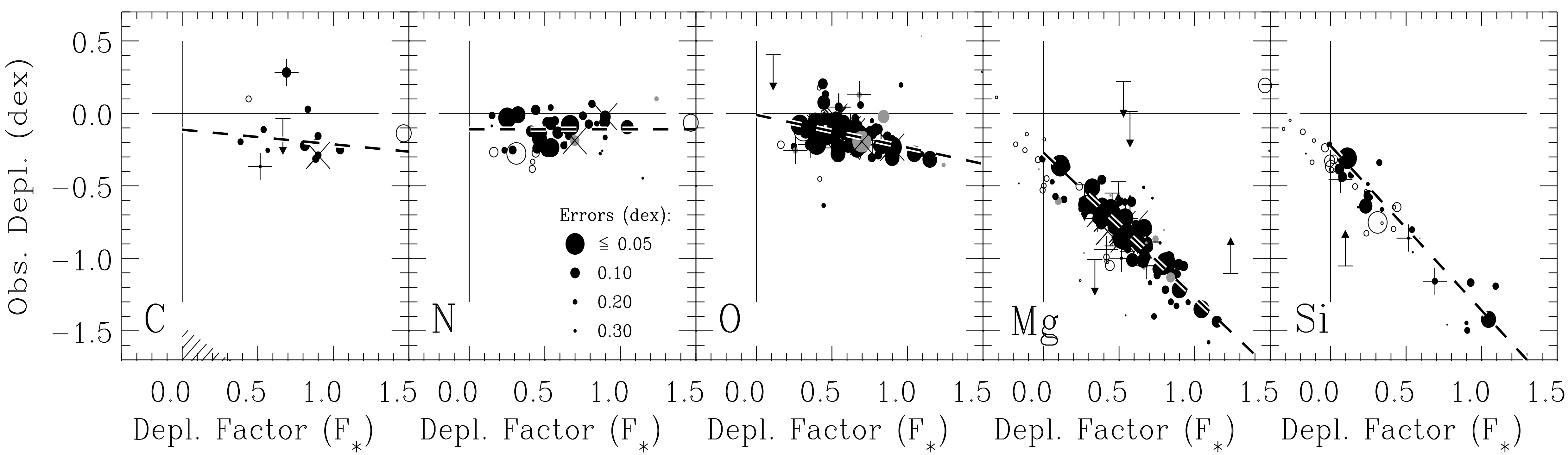
Crash course in ISM dust

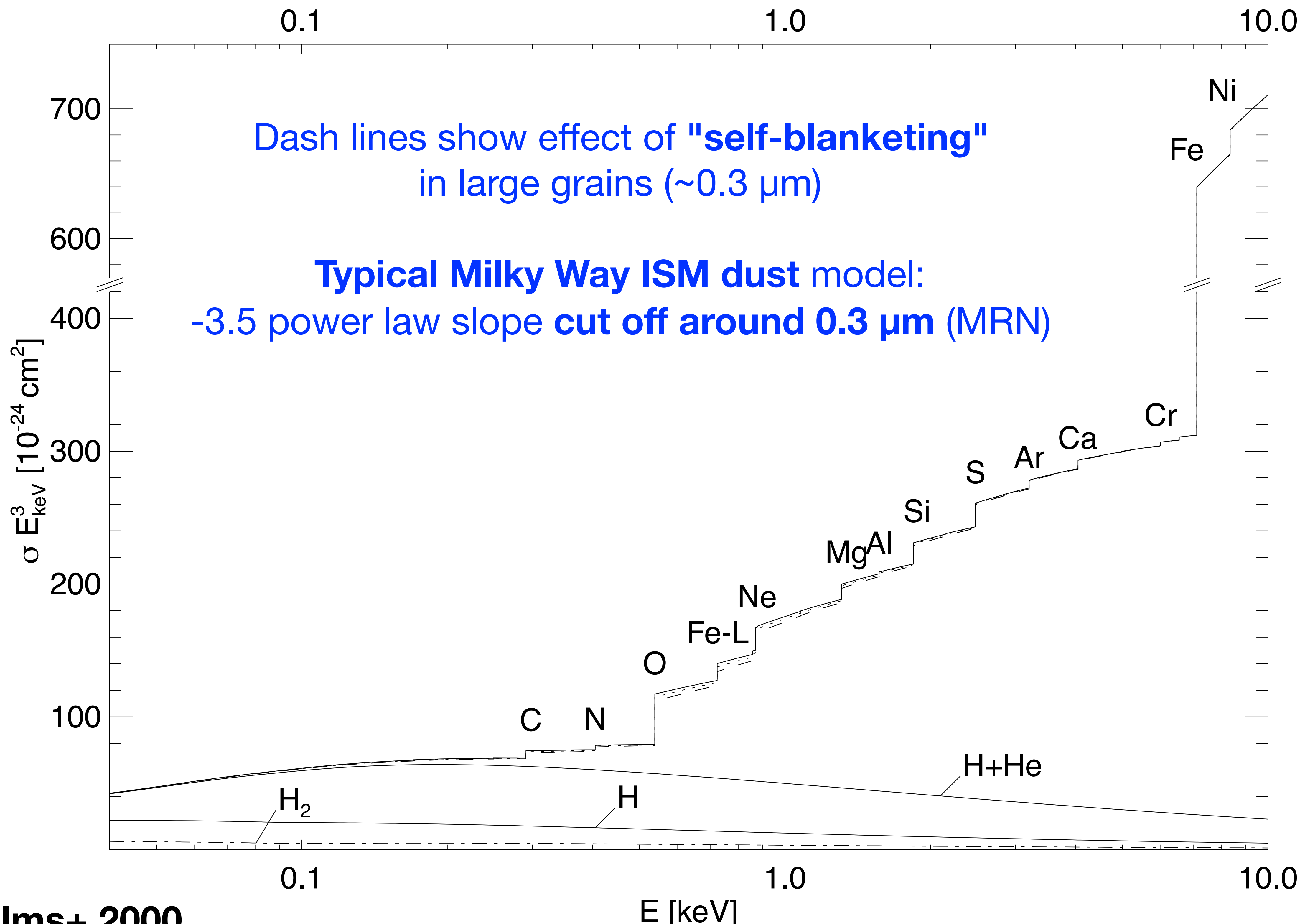
A large fraction of interstellar metals are locked up in dust grains





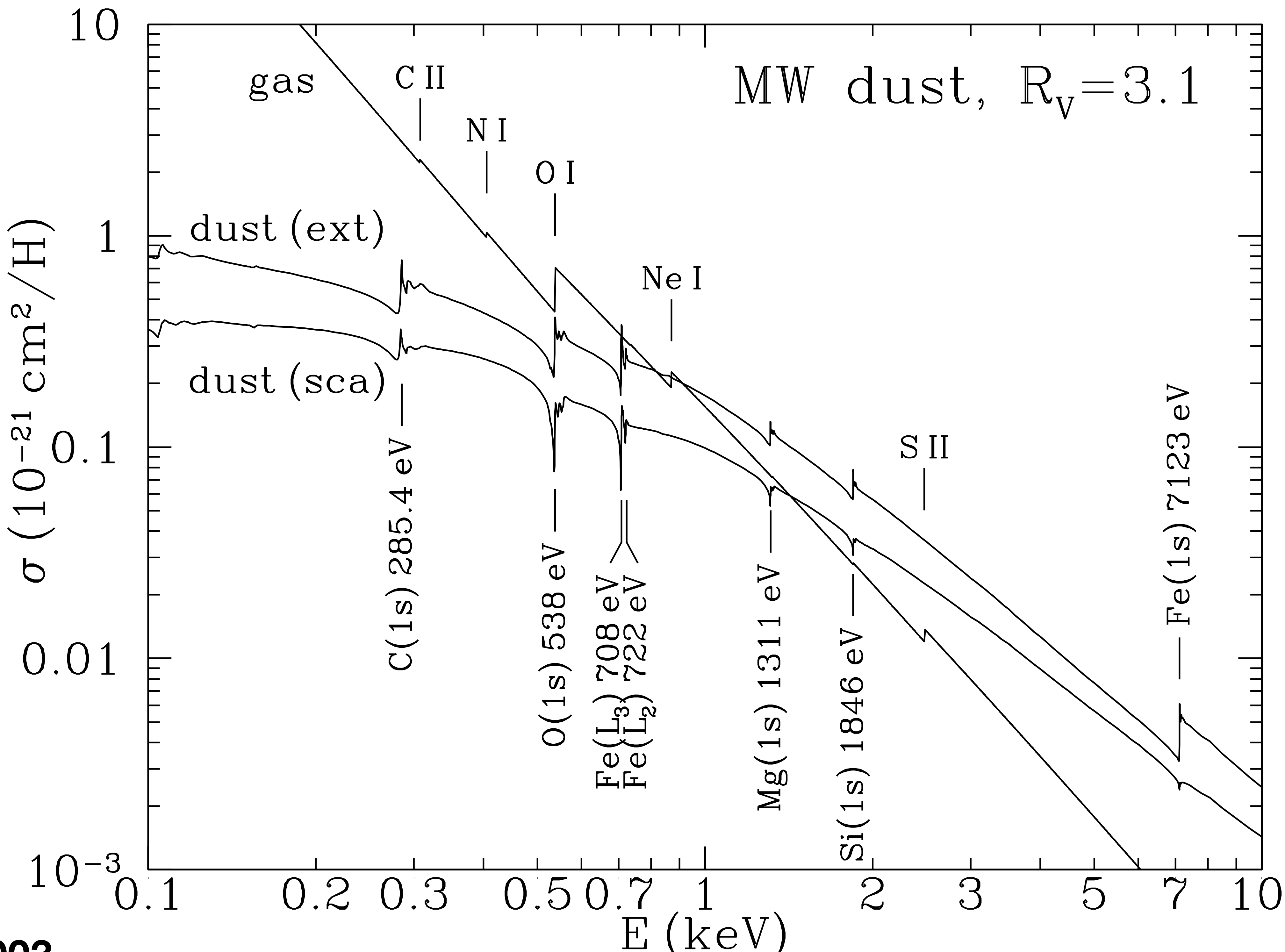
Jenkins 2009, see also Savage & Sembach 1996

Fortunately, interstellar **dust grains** are (mostly) **transparent** to X-rays



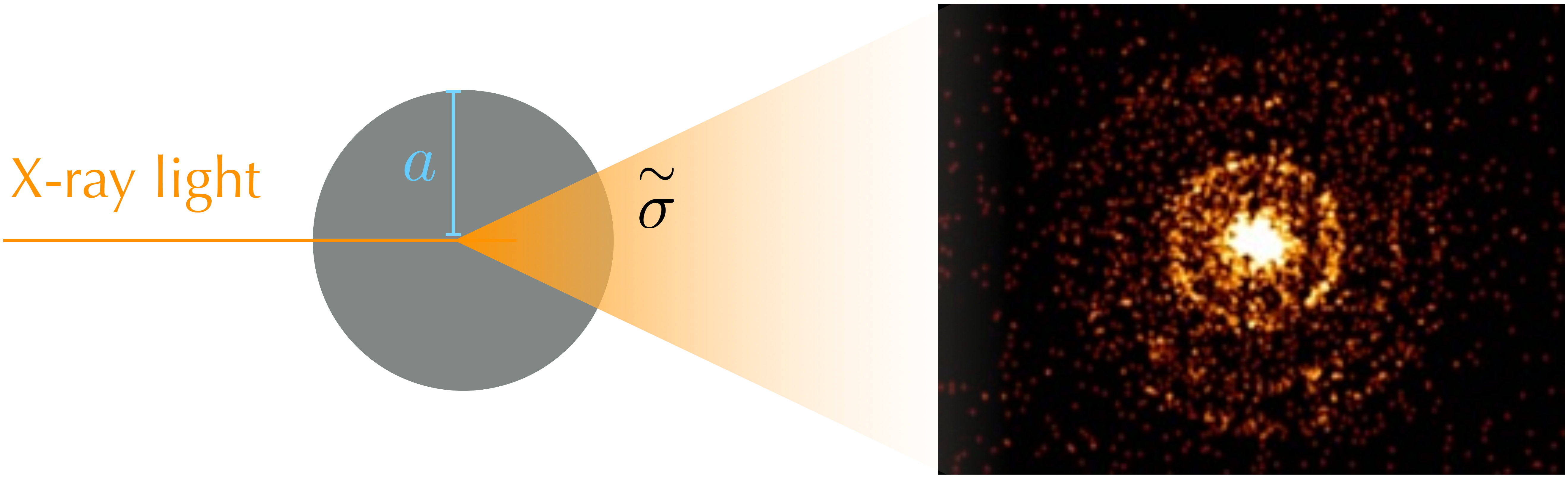
Wilms+ 2000

BUT dust scatters X-ray light, and
extinction = absorption + scattering



Draine 2003

Crash course in dust scattering

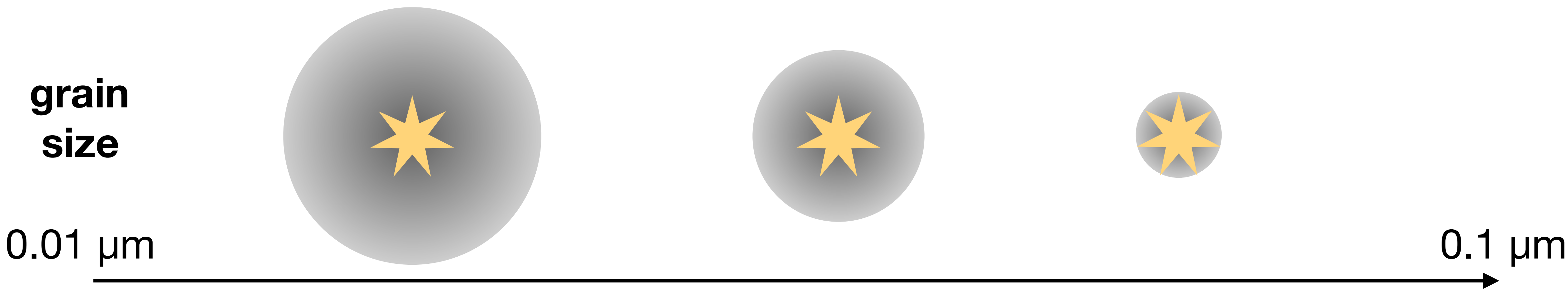


SGR J1550-5418 (NASA/Swift/Halpern)

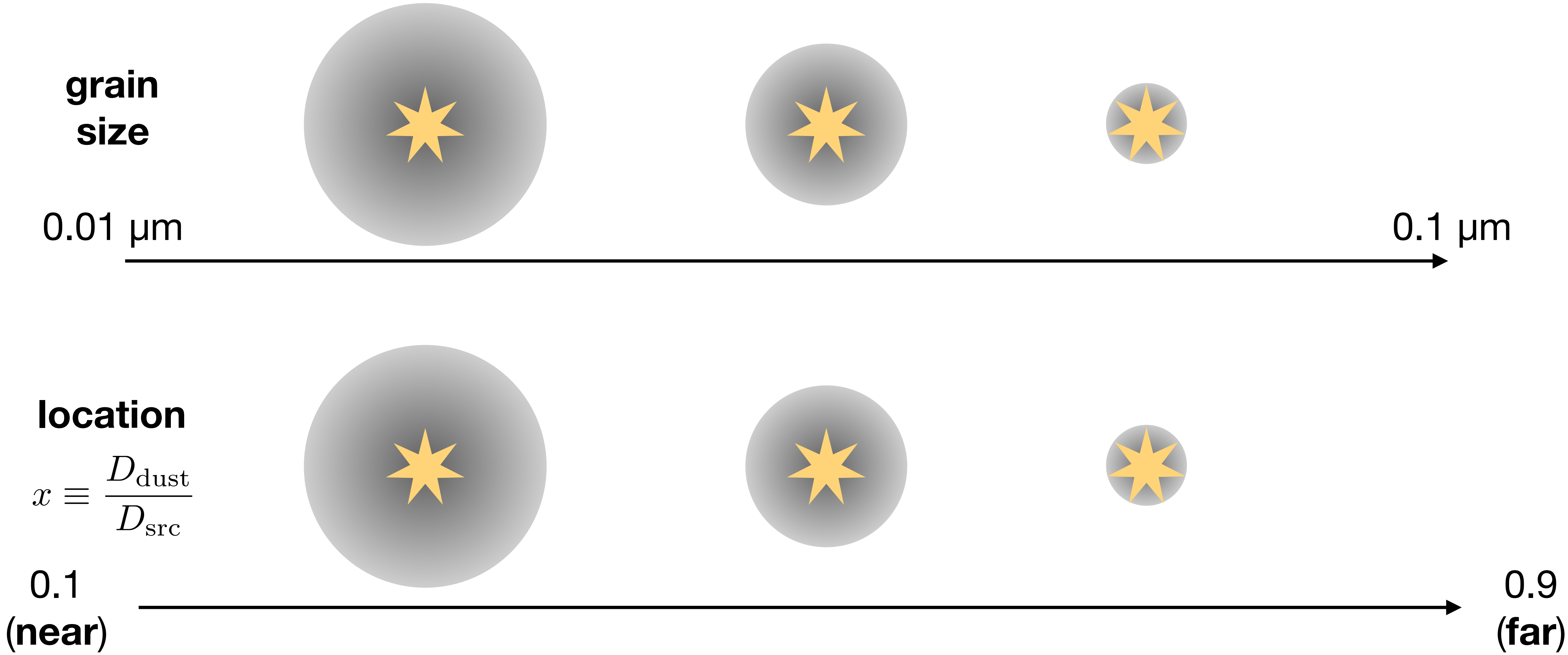
Strongly forward (small angle) scattering → $\tilde{\sigma} \approx \dfrac{10'}{a(0.1\ \mu\mathrm{m})\ E(\mathrm{keV})}$

Strongly sensitive to grain size → $\sigma_{\mathrm{sca}} \propto a^4 E^{-2}$

Dust scattering halo shapes depend on ...

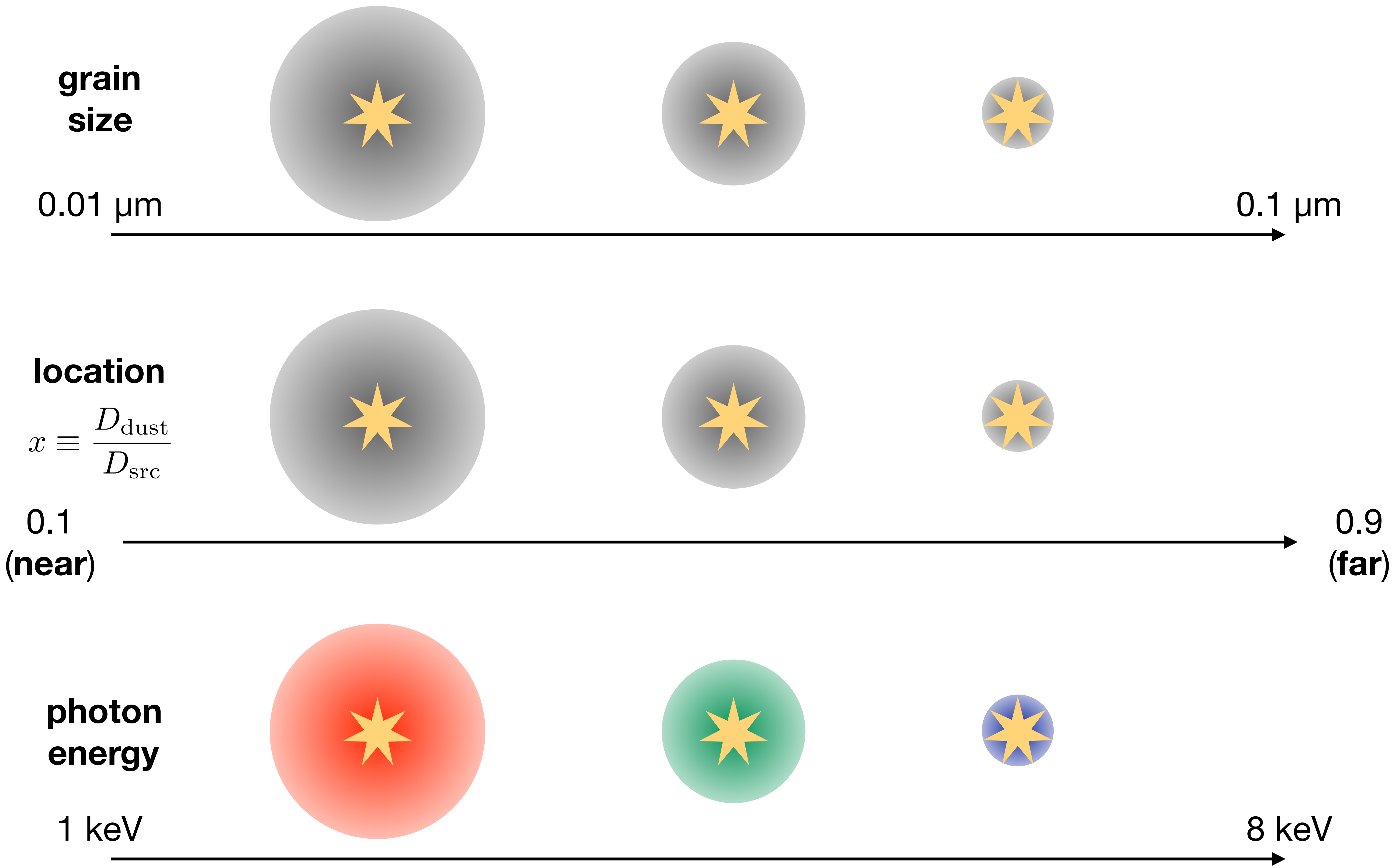


Dust scattering halo shapes depend on ...



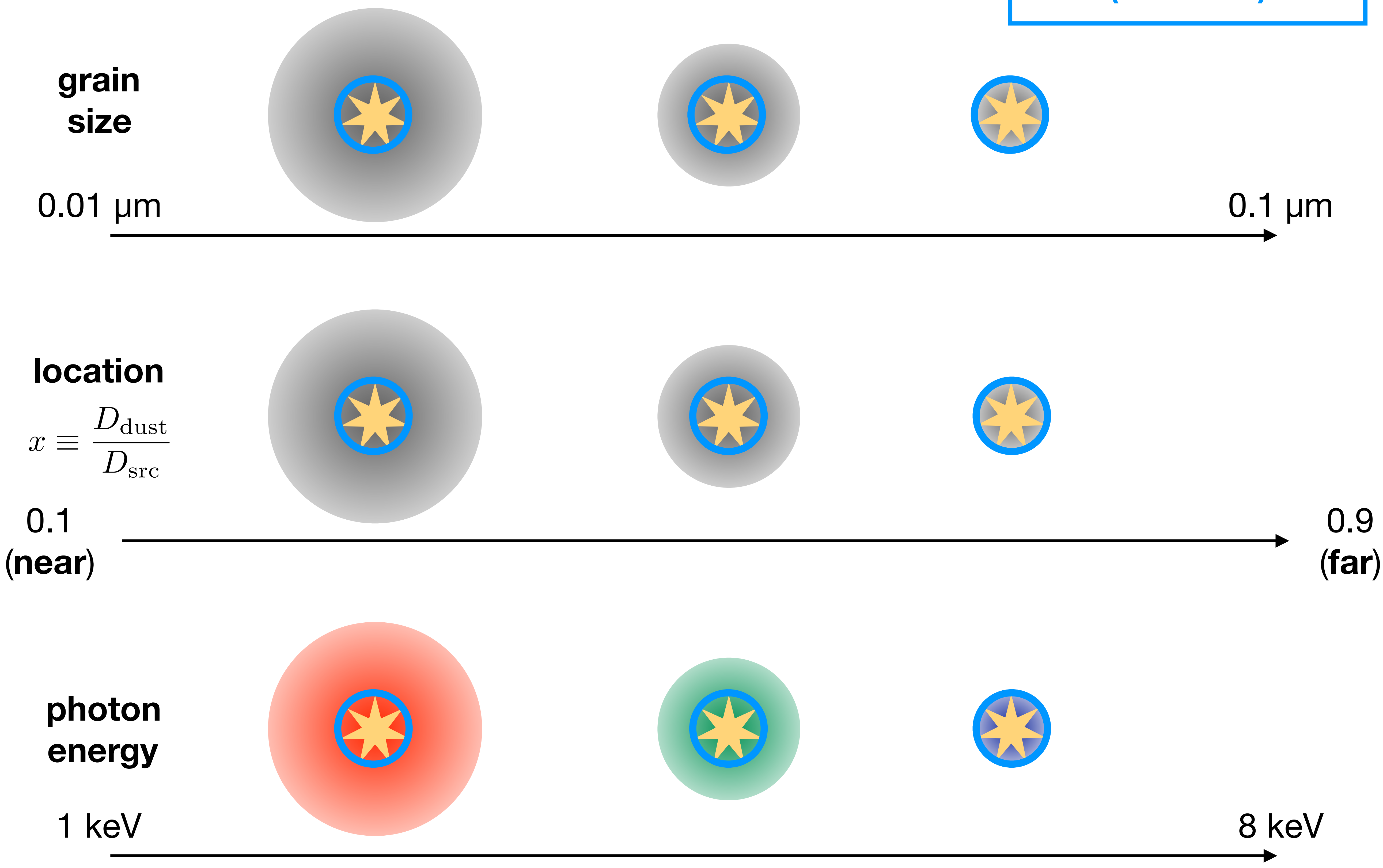
Crash course in dust scattering

Dust scattering halo shapes depend on ...

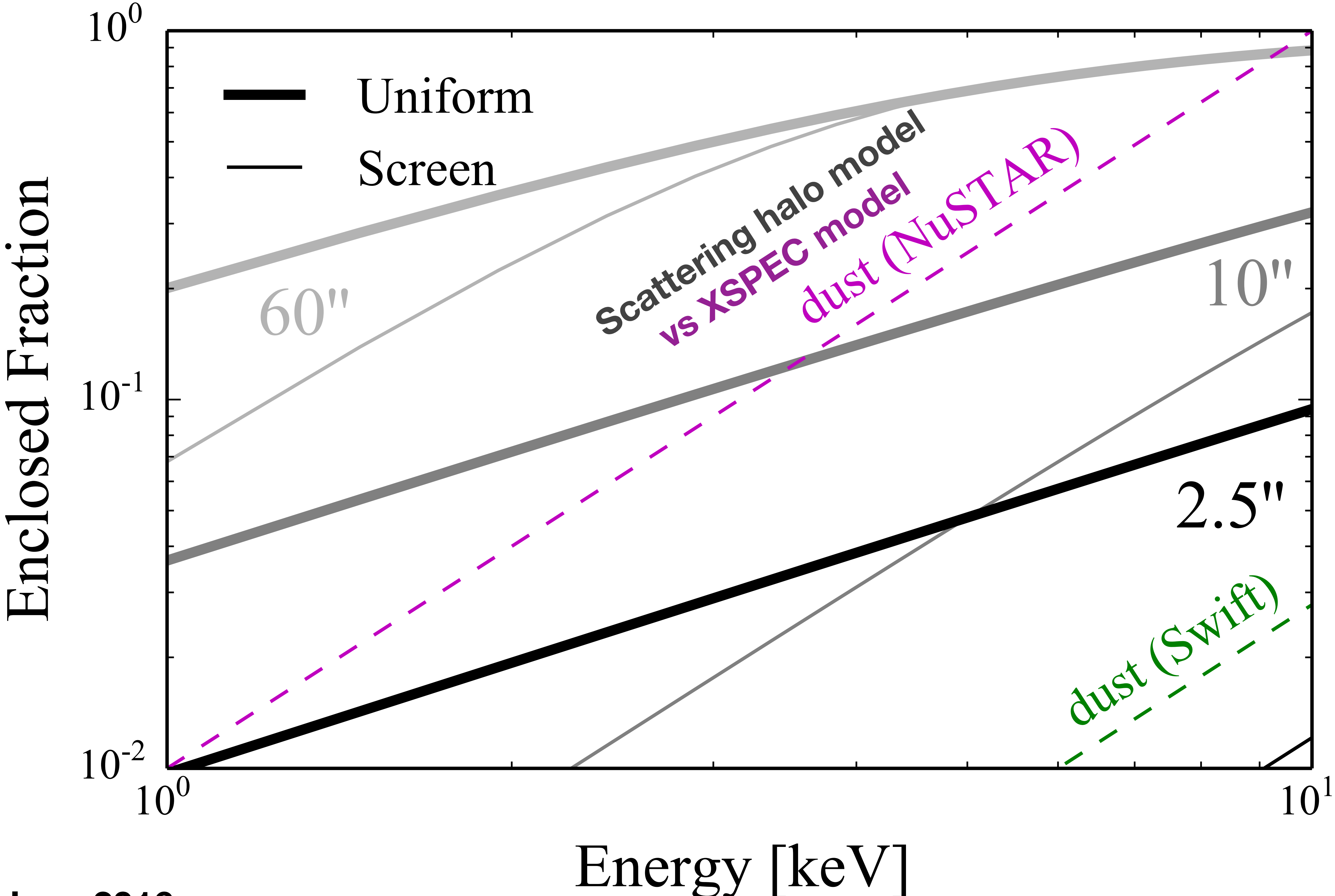


Dust scattering halo **effect** depends on ...

telescope aperture (PSF size)



Fraction of scattering halo captured within spectrum extraction aperture

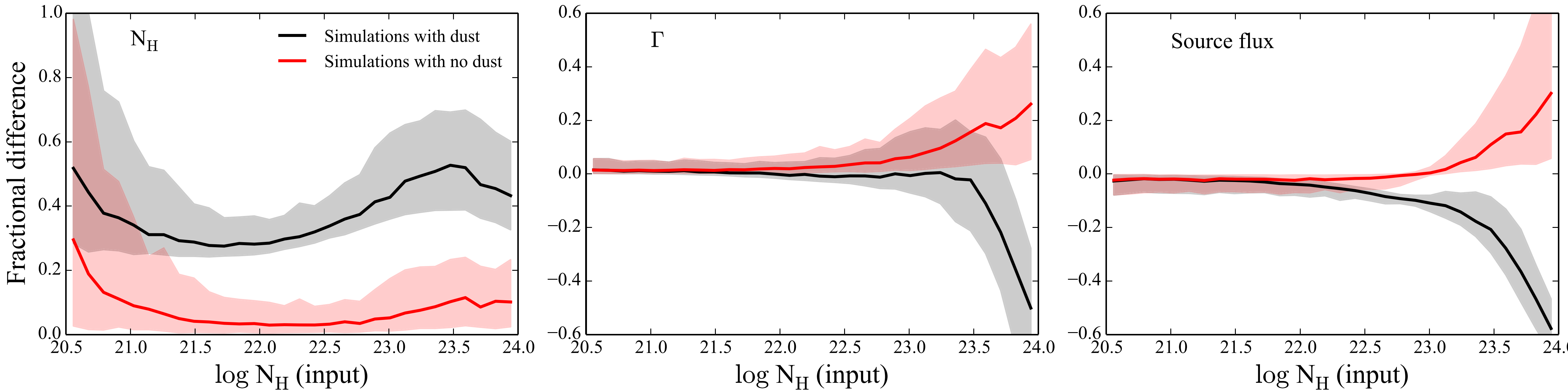


Corrales+ 2016

How does X-ray scattering affect my science?

How does dust scattering affect my science?

Experiment: Simulated datasets **with dust** and **without dust**, then **fit without dust**



Corrales+ 2016

Table 4

Best-fit Spectral Parameters for GRS 1758-258

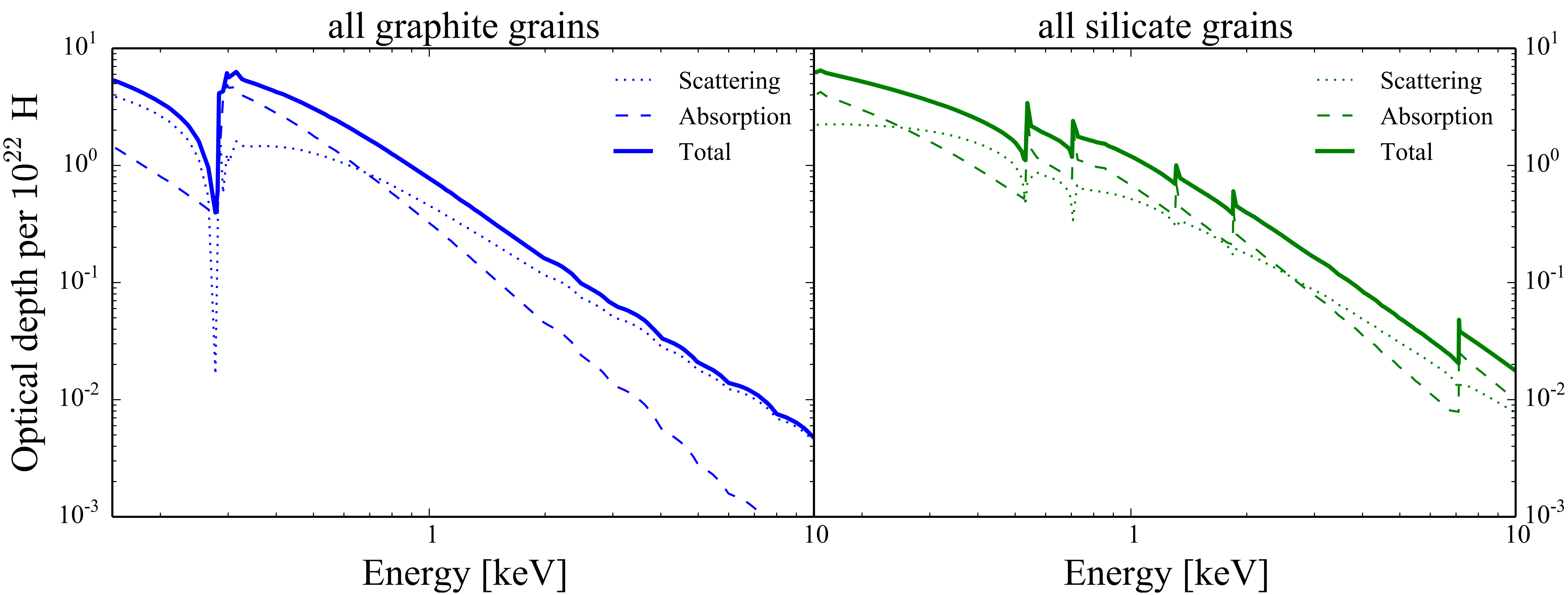
Parameter	Soria + (11)	This Paper	+xscat
N_H(gal, abs)[a]	0.75	0.75	0.75
N_H(gal, scat)[a]	…	…	0.75
N_H(int)[a]	$0.99^{+0.04}_{-0.02}$	1.02 ± 0.02	0.77 ± 0.02
kT_{dbb} (keV)	$0.45^{+0.01}_{-0.01}$	0.447 ± 0.004	0.429 ± 0.004
N_{dbb}	1668^{+112}_{-105}	1990^{+130}_{-120}	2628^{+170}_{-150}
Γ	$2.85^{+0.33}_{-0.32}$	2.85	2.85
N_{po}[b]	$0.54^{+0.43}_{-0.24}$	0.61 ± 0.03	0.64 ± 0.03

For **continuum** fitting, **mostly** ISM column (**NH**) is affected.

What level of precision are you seeking?

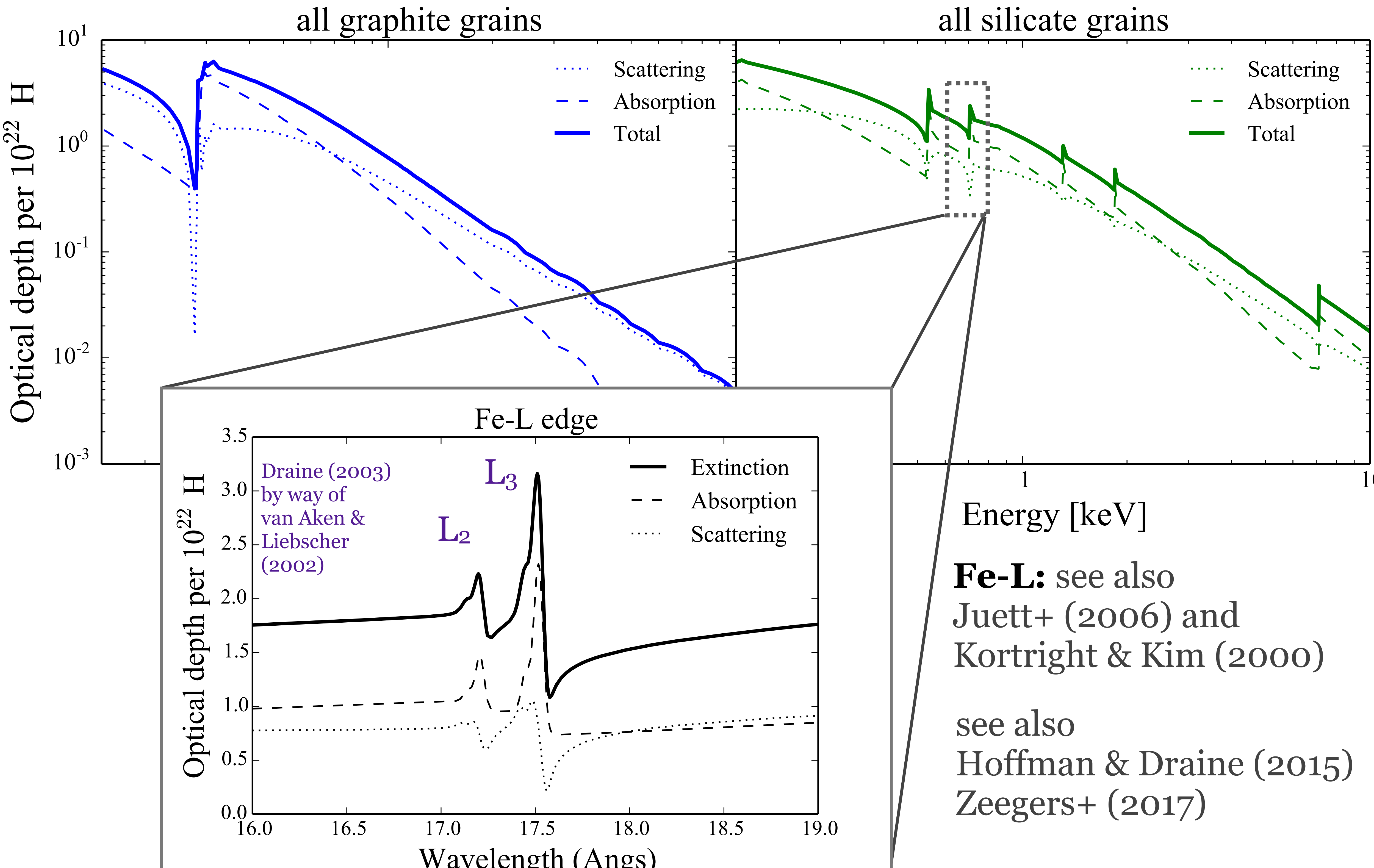
Smith+ 2016

High resolution spectra around **photoabsorption** features also affected



Corrales+ 2016

High resolution spectra around **photoabsorption** features also affected



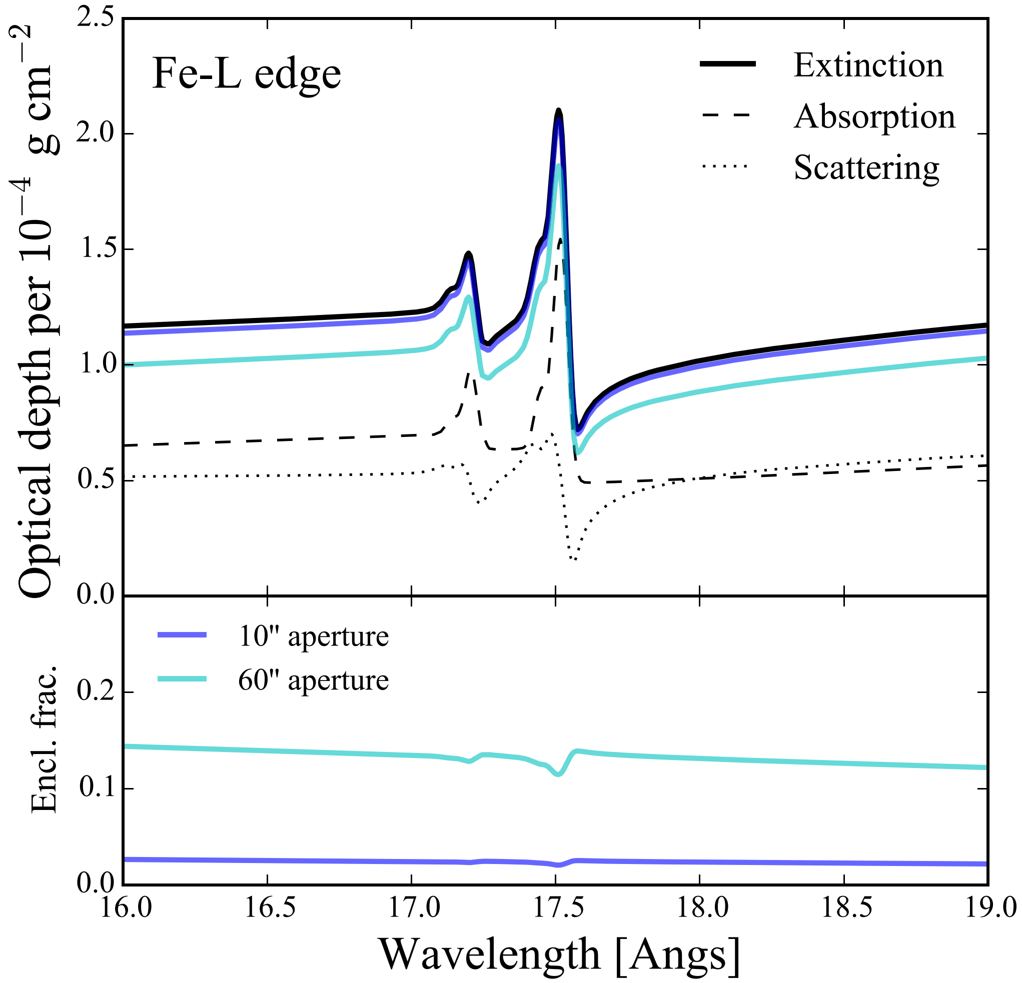
Fe-L: see also
Juett+ (2006) and
Kortright & Kim (2000)

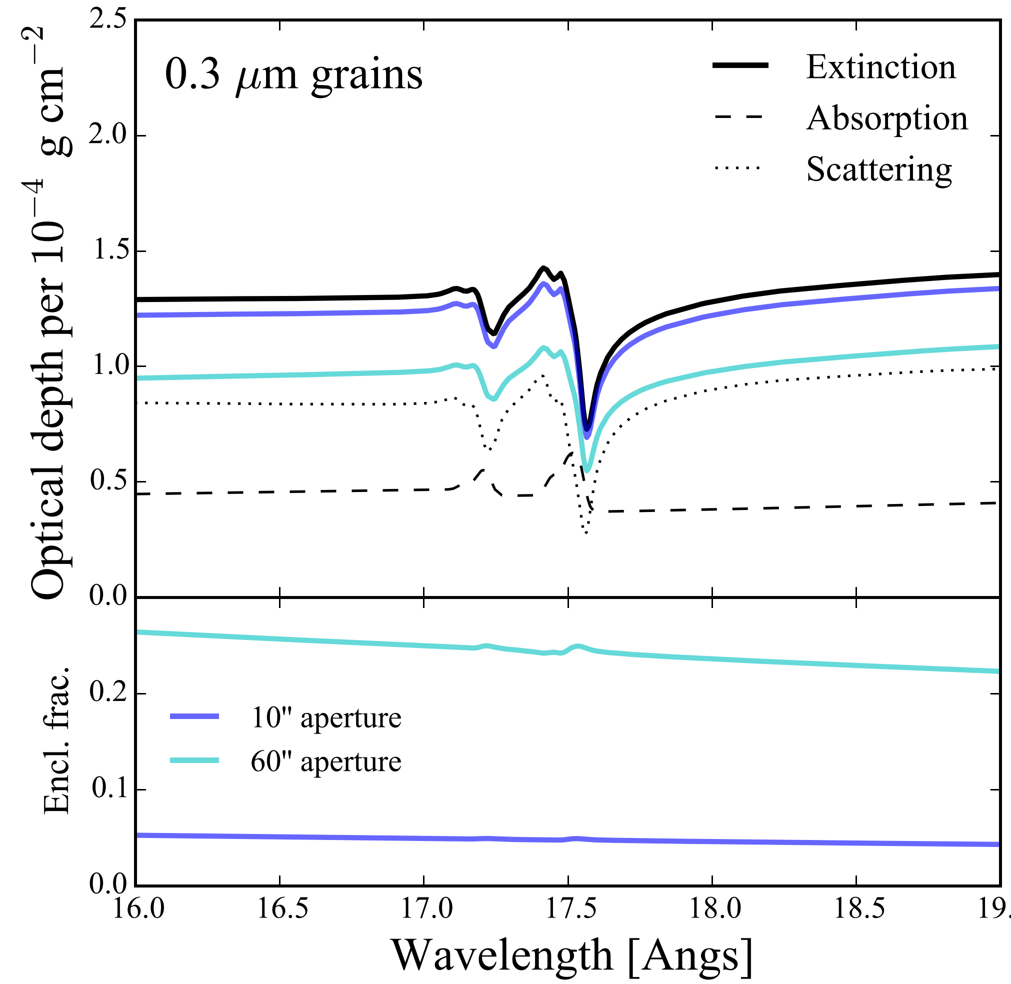
see also
Hoffman & Draine (2015)
Zeegers+ (2017)

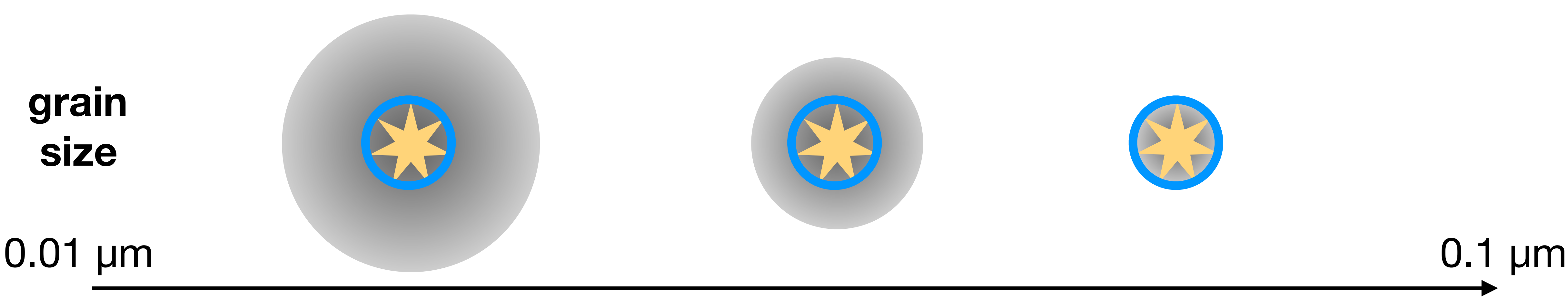
Corrales+ 2016

X-ray scattering fine structure (**XSFS**) **appearance** depends on **scattering halo shape** and telescope **imaging resolution**

Corrales+ 2016

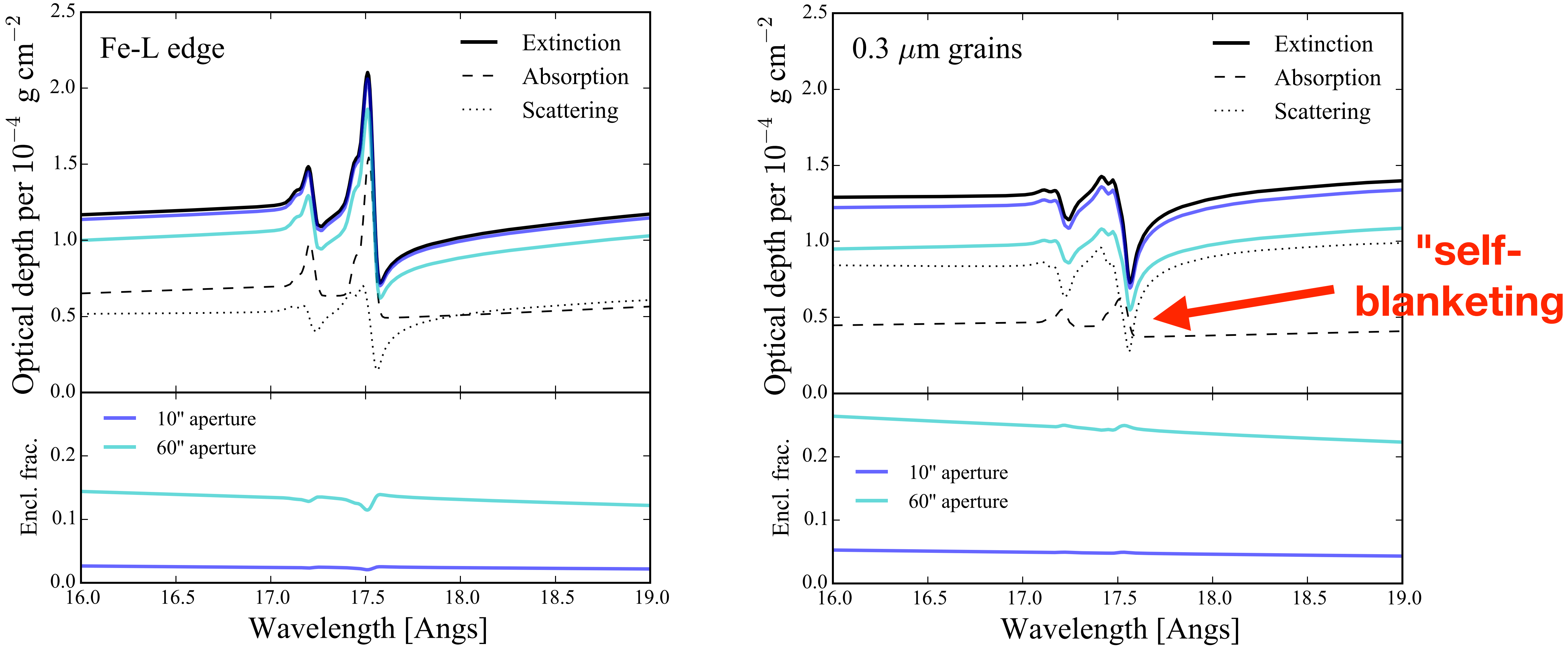




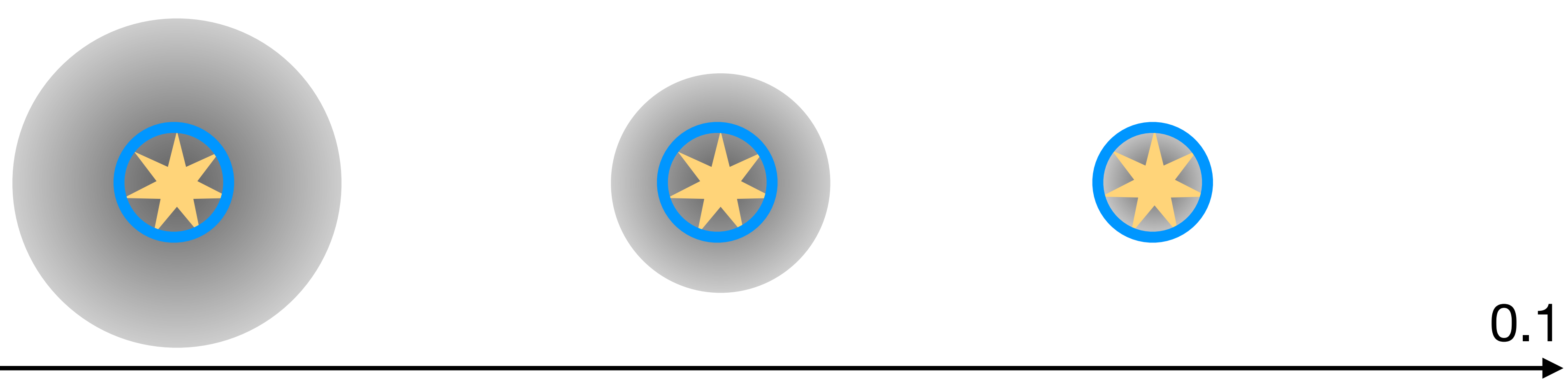


X-ray scattering fine structure (**XSFS**) **appearance** depends on **scattering halo shape** and telescope **imaging resolution**

Corrales+ 2016



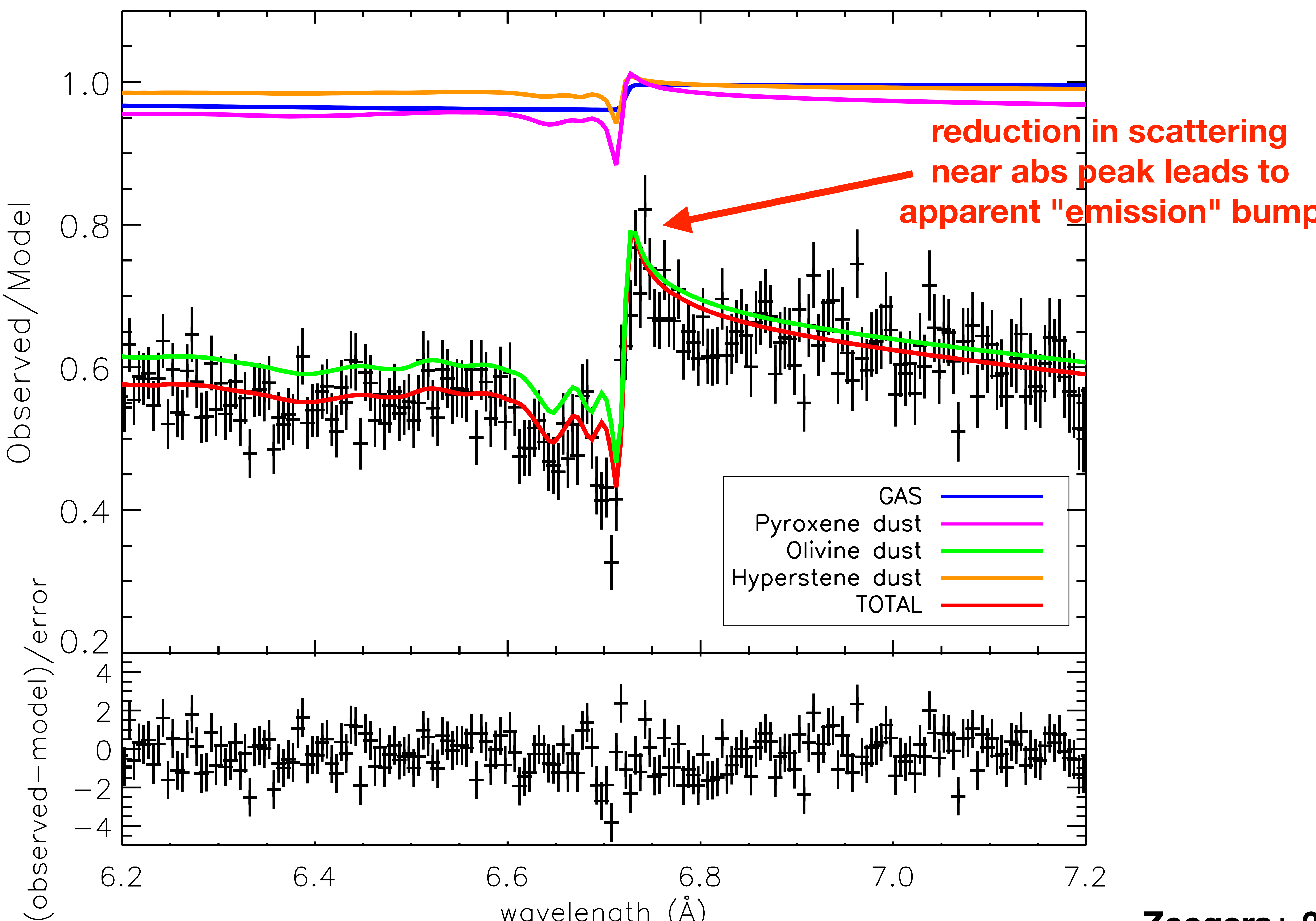
grain size



0.01 μm

0.1 μm

How does dust scattering affect my science?



Zeegers+ 2017

ISMdust: a simple interstellar dust model

- Utilizes **Draine (2003) optical constants** with **MRN** sizes
  – *dust properties for the continuum*

- **Absorption + Scattering**
  – intended for *Chandra* and XMM-Newton

- **XSFS included**

- **Good enough** if you care about **continuum science**

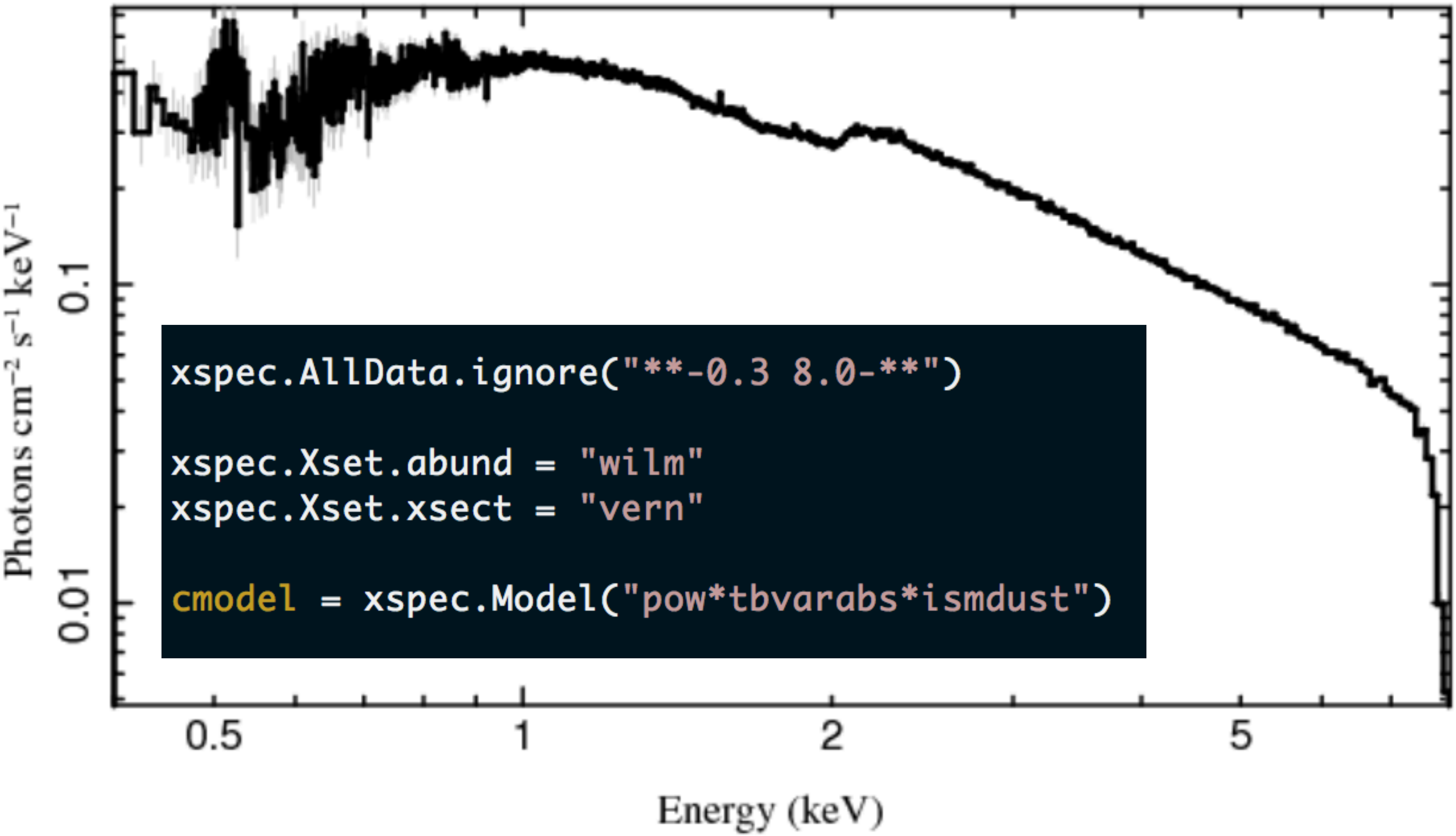
- If your **science goal is astromineralogy**, use
  SRON (Zeegers, Rogantini, Psadaraki, Costantini),
  J. Lee, or other **direct lab measurements**

For **low imaging resolution** telescopes (NuSTAR, Suzaku, NICER),
or if you want **more dust model settings**, use **xscat**

Exercise: Apply ISMdust to a continuum fit to GX 9+9

bit.ly/atomdb-2020-dust

LMXB GX 9+9 (Chandra ObsId 703) available in TGCat




```
xspec.AllData.ignore("**-0.3 8.0-**")

xspec.Xset.abund = "wilm"
xspec.Xset.xsect = "vern"

cmodel = xspec.Model("pow*tbvarabs*ismdust")
```

Exercise: Apply ISMdust to a continuum fit of GX 9+9

```
========================================================================
Model powerlaw<1>*TBvarabs<2>*ismdust<3> Source No.: 1   Active/On
Model Model Component  Parameter  Unit     Value
 par  comp
   1    1   powerlaw   PhoIndex            1.00000      +/-  0.0
   2    1   powerlaw   norm                1.00000      +/-  0.0
   3    2   TBvarabs   nH         10^22    1.00000      +/-  0.0
   4    2   TBvarabs   He                  1.00000      frozen
   5    2   TBvarabs   C                   1.00000      frozen
   6    2   TBvarabs   N                   1.00000      frozen
   7    2   TBvarabs   O                   1.00000      frozen
   8    2   TBvarabs   Ne                  1.00000      frozen
   9    2   TBvarabs   Na                  1.00000      frozen
  10    2   TBvarabs   Mg                  1.00000      frozen
  11    2   TBvarabs   Al                  1.00000      frozen
  12    2   TBvarabs   Si                  1.00000      frozen
  13    2   TBvarabs   S                   1.00000      frozen
  14    2   TBvarabs   Cl                  1.00000      frozen
  15    2   TBvarabs   Ar                  1.00000      frozen
  16    2   TBvarabs   Ca                  1.00000      frozen
  17    2   TBvarabs   Cr                  1.00000      frozen
  18    2   TBvarabs   Fe                  1.00000      frozen
  19    2   TBvarabs   Co                  1.00000      frozen
  20    2   TBvarabs   Ni                  1.00000      frozen
  21    2   TBvarabs   H2                  0.200000     frozen
  22    2   TBvarabs   rho        g/cm^3   1.00000      frozen
  23    2   TBvarabs   amin       mum      2.50000E-02  frozen
  24    2   TBvarabs   amax       mum      0.250000     frozen
  25    2   TBvarabs   PL                  3.50000      frozen
  26    2   TBvarabs   H_dep               1.00000      frozen
  27    2   TBvarabs   He_dep              1.00000      frozen
  28    2   TBvarabs   C_dep               1.00000      frozen
  29    2   TBvarabs   N_dep               1.00000      frozen
  30    2   TBvarabs   O_dep               1.00000      frozen
  31    2   TBvarabs   Ne_dep              1.00000      frozen
  32    2   TBvarabs   Na_dep              1.00000      frozen
  33    2   TBvarabs   Mg_dep              1.00000      frozen
  34    2   TBvarabs   Al_dep              1.00000      frozen
  35    2   TBvarabs   Si_dep              1.00000      frozen
  36    2   TBvarabs   S_dep               1.00000      frozen
  37    2   TBvarabs   Cl_dep              1.00000      frozen
  38    2   TBvarabs   Ar_dep              1.00000      frozen
  39    2   TBvarabs   Ca_dep              1.00000      frozen
  40    2   TBvarabs   Cr_dep              1.00000      frozen
  41    2   TBvarabs   Fe_dep              1.00000      frozen
  42    2   TBvarabs   Co_dep              1.00000      frozen
  43    2   TBvarabs   Ni_dep              1.00000      frozen
  44    2   TBvarabs   Redshift            0.0          frozen
  45    3   ismdust    msil       10^-4    1.00000      +/-  0.0
  46    3   ismdust    mgra       10^-4    1.00000      +/-  0.0
  47    3   ismdust    redshift            0.0          frozen
------------------------------------------------------------------------
```

powerlaw (2 parameters)

TBvarabs

NH: Hydrogen column density

Elemental abundance
with respect to abundance table
(17 parameters)

Dust model (4 parameters)

Gas fraction
(17 parameters)

Redshift

ismdust (3 parameters)

Exercise: Apply ISMdust to a continuum fit of GX 9+9

TABLE 2

MOLECULAR WEIGHT, K EDGE ENERGIES, ABUNDANCES, AND DEPLETION FACTORS $1 - \beta_Z$ FOR THE ABUNDANT ELEMENTS

Element	μ_Z (amu)	E_K[b] (keV)	$12 + \log A_Z$: Solar[c]	$12 + \log A_Z$: ISM[d]	$1 - \beta_Z$[e]: This Paper	$1 - \beta_Z$[e]: MM83	$1 - \beta_Z$[e]: Ride77
1 H	1	...	12.00	12.00	1.0	1.0	1.0
2 He	4	...	10.99	10.99	1.0	1.0	1.0
6 C	12	0.29	8.60	8.38	0.5	0.0	0.2
7 N	14	0.41	7.97	7.88	1.0	0.0	0.5
8 O	16	0.54	8.93	8.69	0.6	0.75	0.5
10 Ne	20	0.87	8.09	7.94	1.0	1.0	1.0
11 Na	23	1.08	6.31	6.16	0.25	0.0	...
12 Mg	24	1.31	7.59	7.40	0.2	0.0	0.2
13 Al	27	1.57	6.48	6.33	0.02	0.0	...
14 Si........	28	1.85	7.55	7.27	0.1	0.0	0.5
15 P	31	2.15	5.57	5.42	0.6	...	...
16 S	32	2.48	7.27	7.09	0.6	0.0	0.7
17 Cl	35	2.83	5.27	5.12	0.5	0.0	...
18 Ar	40	3.20	6.56	6.41	1.0	1.0	0.5
20 Ca	40	4.04	6.34	6.20	0.003	0.0	...
22 Ti	48	4.97	4.93	4.81	0.002	...	...
24 Cr	52	5.97	5.68	5.51	0.03	0.0	...
25 Mn......	55	6.55	5.53	5.34	0.07	...	...
26 Fe	56	7.12	7.50	7.43	0.3	0.0	0.2
27 Co	59	7.73	4.92	4.92	0.05	...	...
28 Ni	59	8.35	6.25	6.05	0.04	0.0	...

Wilms+ 2000

"wilm" abundance model

gas phase fraction

Exercise: Apply ISMdust to a continuum fit of GX 9+9

```
# Following Table 2 of Wilms et al. (2000),
# set the abundance values to the gas phase fraction
#
# 5  = C : 0.5
# 7  = O : 0.6
# 9  = Na : 0.25
# 10 = Mg : 0.2
# 11 = Al : 0.02
# 12 = Si : 0.1
# 13 = S : 0.6
# 14 = Cl : 0.5
# 16 = Ca : 0.003
# 17 = Cr : 0.03
# 18 = Fe : 0.3
# 19 = Co : 0.05
# 20 = Ni : 0.04
cmodel.setPars({5:0.5, 7:0.6, 9:0.25, 10:0.2, 11:0.02, 12:0.1, \
13:0.6, 14:0.5, 16:0.003, 17:0.03, 18:0.3, 19:0.05, 20:0.04})

# The ismdust parameters msil and mgra are the
# dust mass column in units of 10^-4 g cm^-2.
# We'll tie it to the TBvarabs NH parameter (par #3)
# using a typical dust-to-gas mass ration of 0.01
# and assuming a 60/40 mix of silicate/graphite grains
mdust = 1.0e22 * c.m_p.to('g').value * 0.01 / 1.e-4
msil  = 0.6 * mdust
mgra  = 0.4 * mdust
cmodel.ismdust.msil.link = "{:.6f} * 3".format(msil)
cmodel.ismdust.mgra.link = "{:.6f} * 3".format(mgra)
```

ISMdust parameters

msil: dust mass column of silicates

mgra: dust mass column of graphite

UNITS: $\mathbf{10^{-4}\ g\ cm^{-2}}$

Tie the dust mass column to NH by choosing a dust-to-gas mass ratio (typically 0.01)

Exercise: Apply ISMdust to a continuum fit of GX 9+9

```
========================================================================
Model powerlaw<1>*TBvarabs<2>*ismdust<3> Source No.: 1   Active/On
Model Model Component  Parameter  Unit     Value
 par  comp
   1    1   powerlaw   PhoIndex            1.00000      +/-  0.0
   2    1   powerlaw   norm                1.00000      +/-  0.0
   3    2   TBvarabs   nH         10^22    1.00000      +/-  0.0
   4    2   TBvarabs   He                  1.00000      frozen
   5    2   TBvarabs   C                   0.500000     frozen
   6    2   TBvarabs   N                   1.00000      frozen
   7    2   TBvarabs   O                   0.600000     frozen
   8    2   TBvarabs   Ne                  1.00000      frozen
   9    2   TBvarabs   Na                  0.250000     frozen
  10    2   TBvarabs   Mg                  0.200000     frozen
  11    2   TBvarabs   Al                  2.00000E-02  frozen
  12    2   TBvarabs   Si                  0.100000     frozen
  13    2   TBvarabs   S                   0.600000     frozen
  14    2   TBvarabs   Cl                  0.500000     frozen
  15    2   TBvarabs   Ar                  1.00000      frozen
  16    2   TBvarabs   Ca                  3.00000E-03  frozen
  17    2   TBvarabs   Cr                  3.00000E-02  frozen
  18    2   TBvarabs   Fe                  0.300000     frozen
  19    2   TBvarabs   Co                  5.00000E-02  frozen
  20    2   TBvarabs   Ni                  4.00000E-02  frozen
  21    2   TBvarabs   H2                  0.200000     frozen
  22    2   TBvarabs   rho        g/cm^3   1.00000      frozen
  23    2   TBvarabs   amin       mum      2.50000E-02  frozen
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  25    2   TBvarabs   PL                  3.50000      frozen
  26    2   TBvarabs   H_dep               1.00000      frozen
  27    2   TBvarabs   He_dep              1.00000      frozen
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  38    2   TBvarabs   Ar_dep              1.00000      frozen
  39    2   TBvarabs   Ca_dep              1.00000      frozen
  40    2   TBvarabs   Cr_dep              1.00000      frozen
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  42    2   TBvarabs   Co_dep              1.00000      frozen
  43    2   TBvarabs   Ni_dep              1.00000      frozen
  44    2   TBvarabs   Redshift            0.0          frozen
  45    3   ismdust    msil       10^-4    1.00357      = 1.003573*p3
  46    3   ismdust    mgra       10^-4    0.669049     = 0.669049*p3
  47    3   ismdust    redshift            0.0          frozen
________________________________________________________________________
```

powerlaw (2 parameters)

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Elemental abundance
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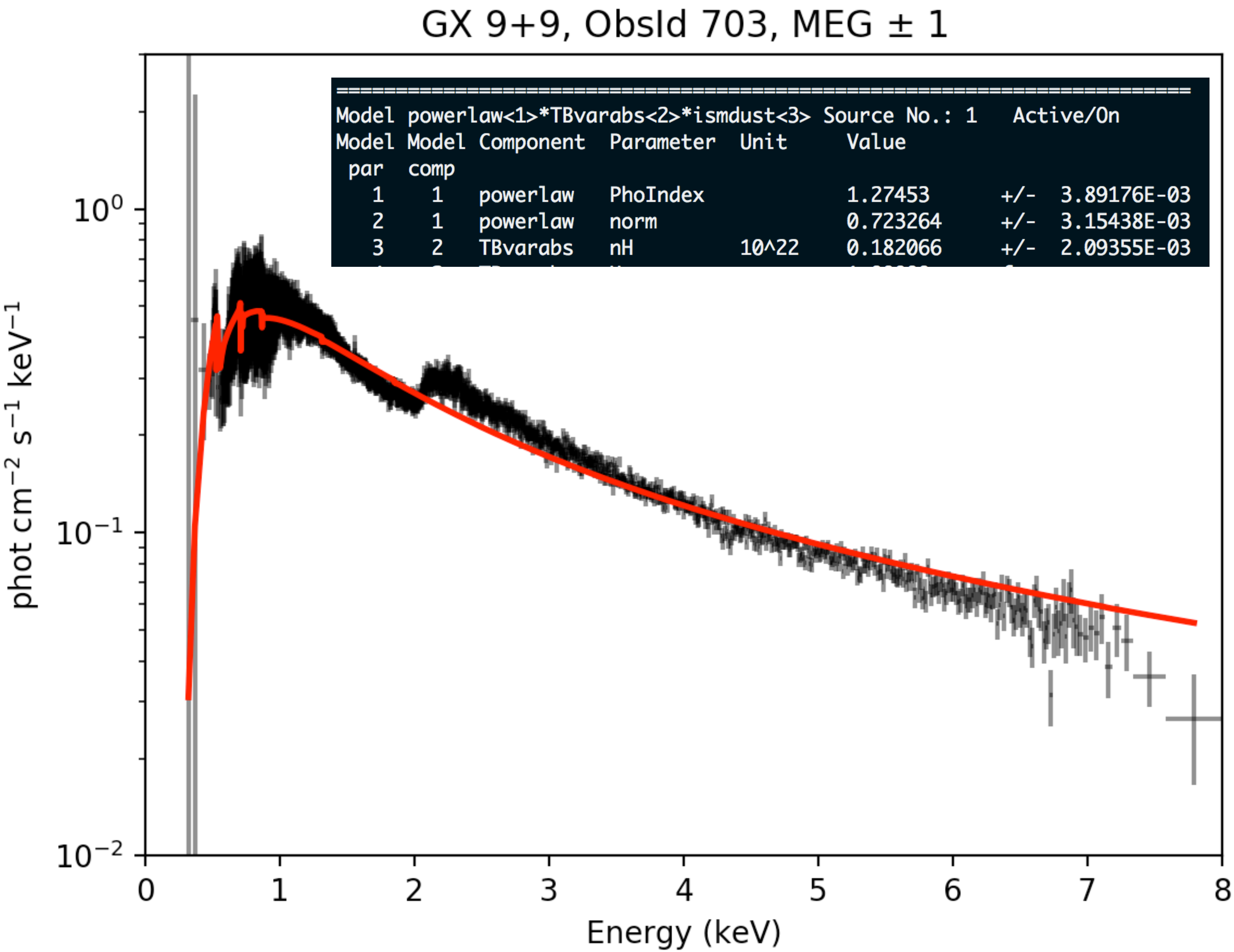
ismdust (3 parameters)

Exercise: Apply ISMdust to a continuum fit of GX 9+9



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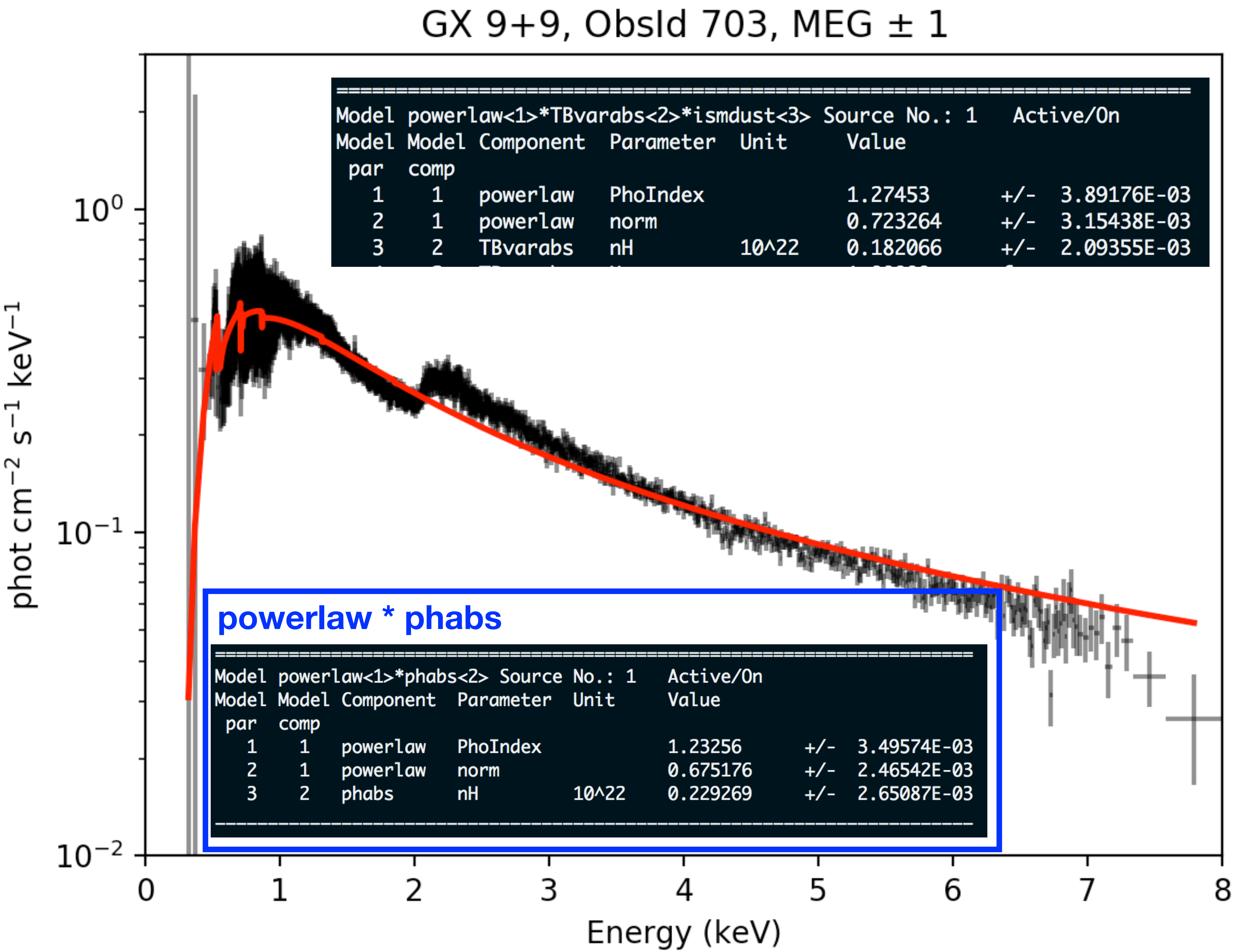
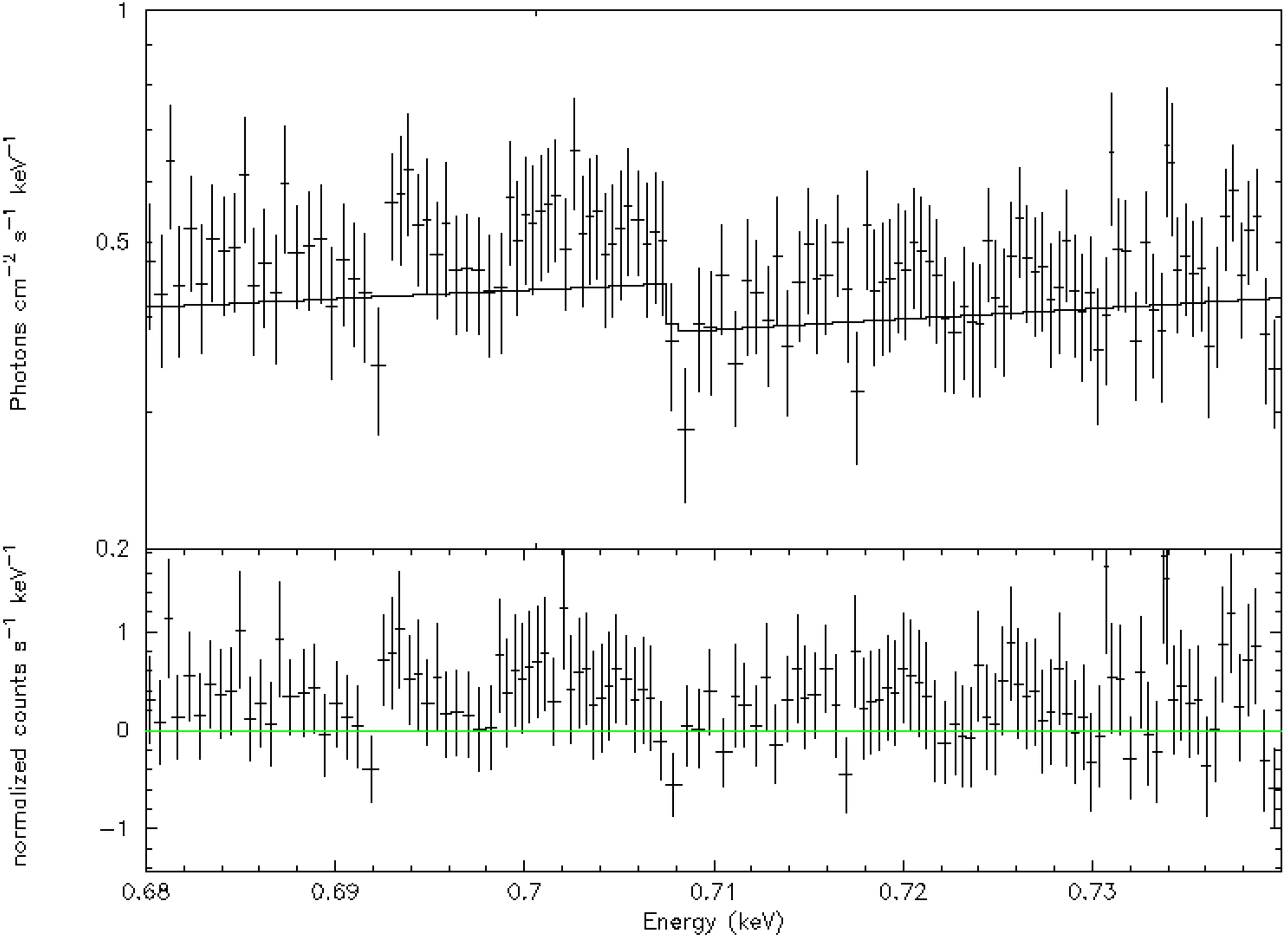


Exercise: Apply ISMdust to Fe L shell photoabsorption in GX 9+9

Exercise: Apply ISMdust to Fe L shell photoabsorption in GX 9+9

```
# 3.1: Local continuum fit with the XSPEC edge model
#-----------------------------------------------------

xspec.AllData.ignore("**-0.6 0.8-**")

# Set up the edge model and transfer parameters from the old fit
edge_model = xspec.Model("pow*edge")
edge_model.powerlaw.norm = norm
edge_model.powerlaw.PhoIndex = phind

# Set the initial parameter for the edge location and confine it to a
# reasonable range of 0.69 - 0.73 keV
edge_model.setPars({3:"0.7,,0.69,0.69,0.73,0.73"})

# Perform the fit
edge_model.show()
xspec.Fit.perform()

# Look at the new model and residuals
xspec.Plot("ufspec res")
```

Exercise: Apply ISMdust to Fe L shell photoabsorption in GX 9+9



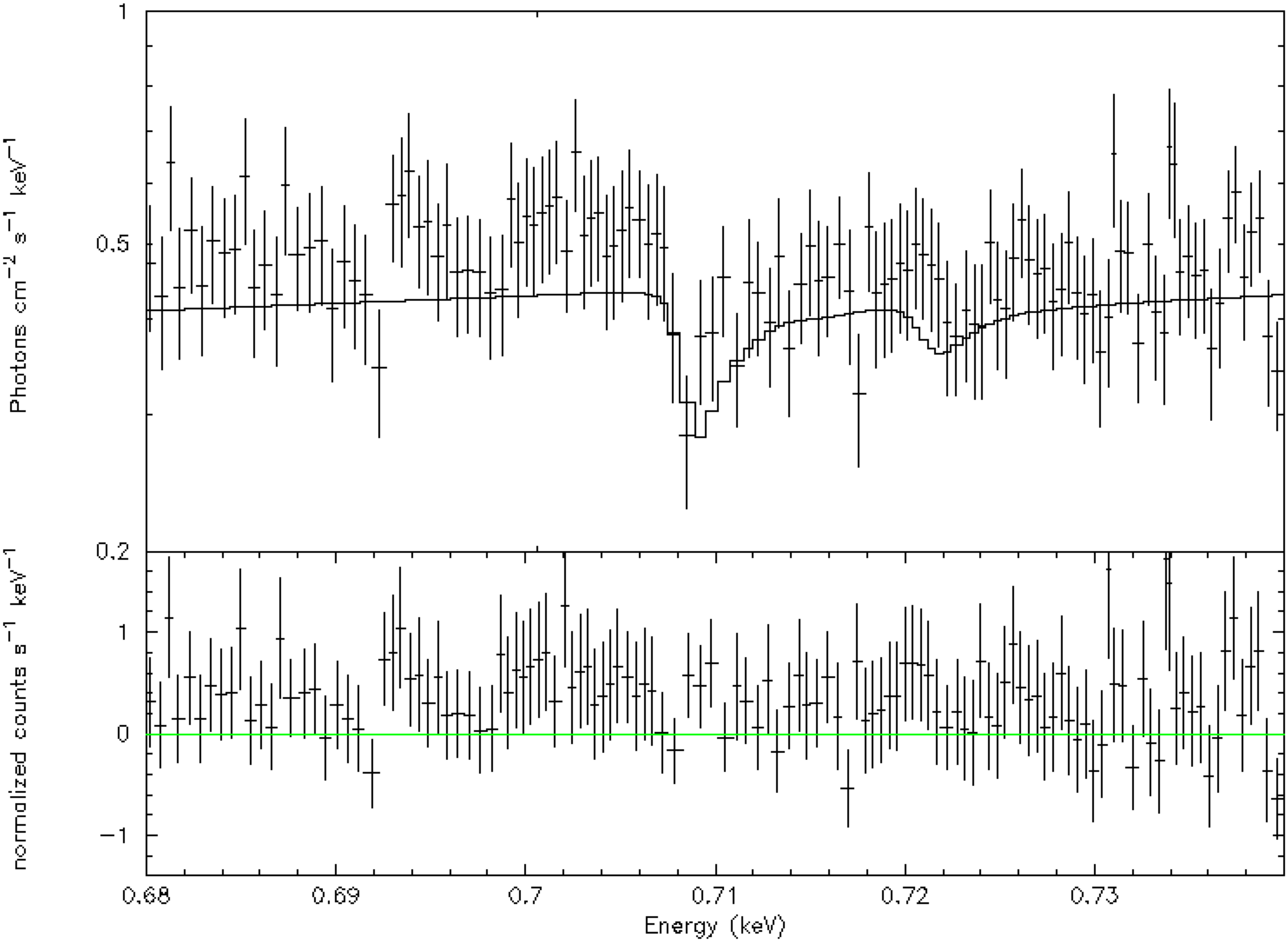
Exercise: Apply ISMdust to Fe L shell photoabsorption in GX 9+9

```
## Try a fit with ISMabs

ismabs_model = xspec.Model("pow*ismabs")
ismabs_model.powerlaw.norm = norm
ismabs_model.powerlaw.PhoIndex = phoind

# Set all abundances to 0, except Fe
ismabs_pars = dict(zip(range(3, 32), np.zeros(29)))
ismabs_model.setPars(ismabs_pars)

# Freeze non-relevant parameters to 0
ismabs_model.ismabs.H.frozen = True
ismabs_model.ismabs.CI.frozen = True
ismabs_model.ismabs.NI.frozen = True
ismabs_model.ismabs.OI.frozen = True
ismabs_model.ismabs.NeI.frozen = True
ismabs_model.ismabs.MgI.frozen = True
ismabs_model.ismabs.SiI.frozen = True
ismabs_model.ismabs.SI.frozen = True
ismabs_model.ismabs.ArI.frozen = True
ismabs_model.ismabs.CaI.frozen = True

xspec.Fit.perform()
xspec.Plot("ufspec res")
```

WARNING

ISMabs uses pure metallic Fe L shell absorption (not gas)

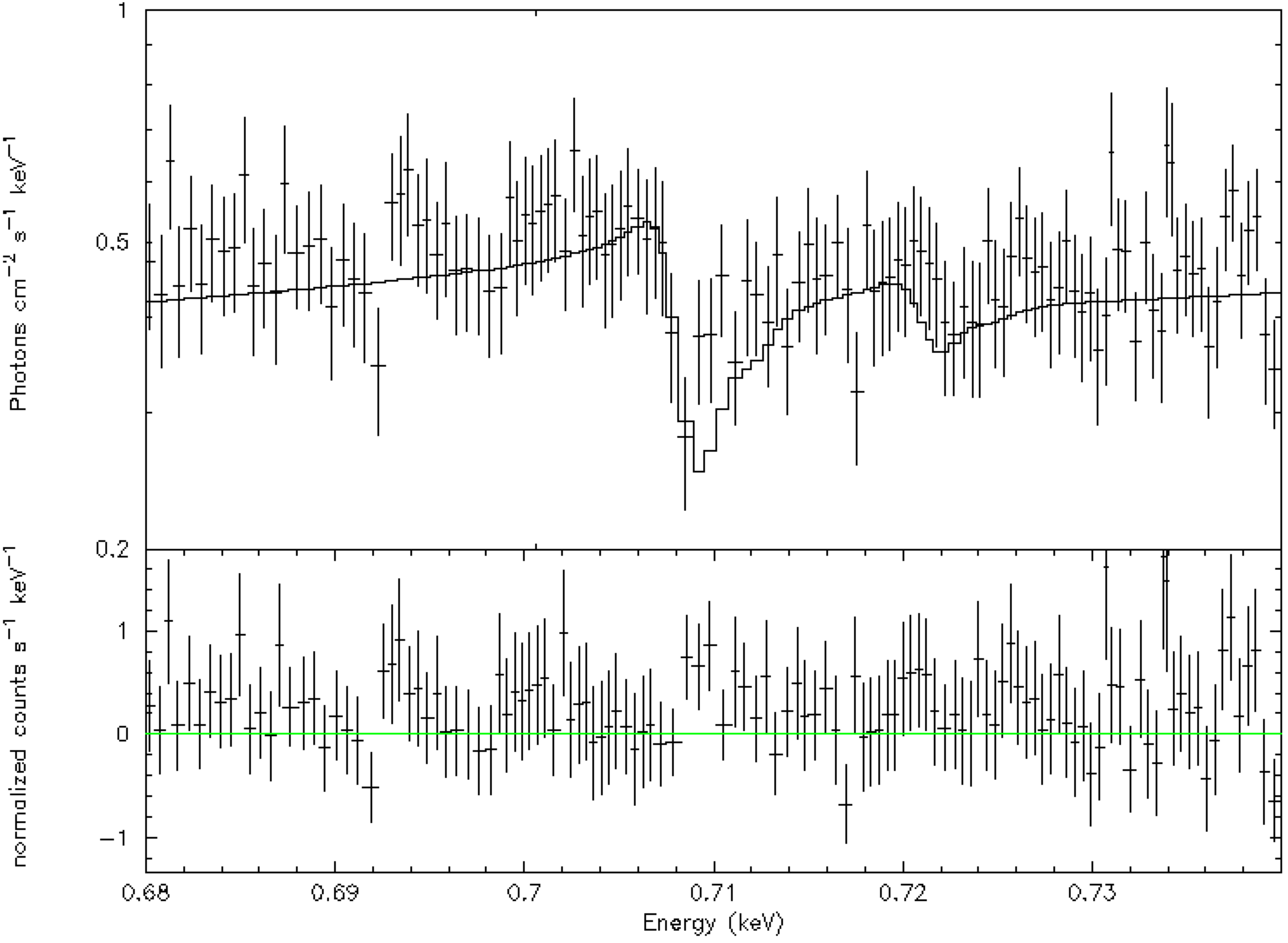
Exercise: Apply ISMdust to Fe L shell photoabsorption in GX 9+9



Exercise: Apply ISMdust to Fe L shell photoabsorption in GX 9+9

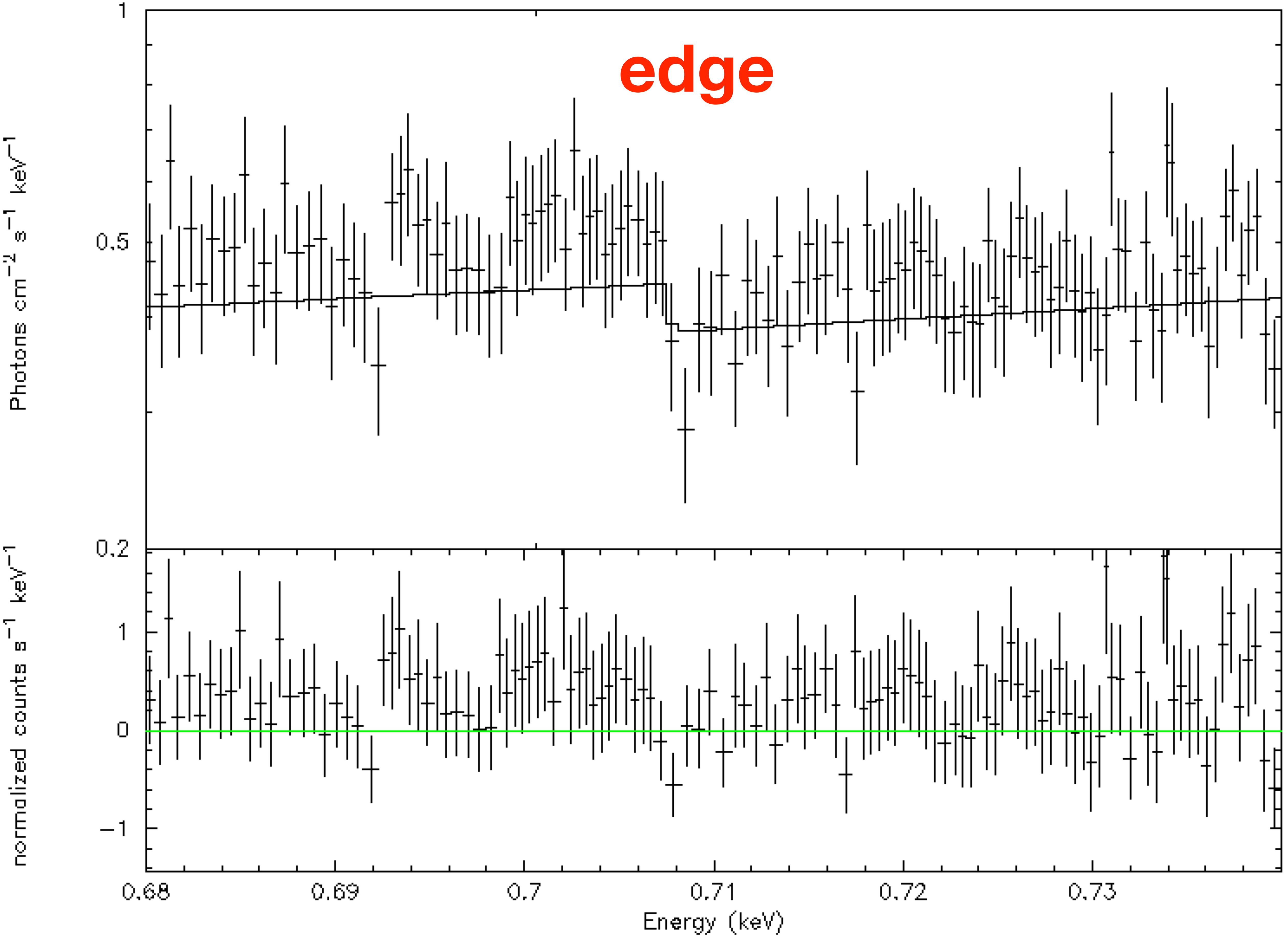
```
# 3.2: Local continuum fit with ISMdust model only
#----------------------------------------------

# Set up the ismdust model and transfer parameters from the old fit
ismdust_model = xspec.Model("pow*ismdust")
ismdust_model.powerlaw.norm = norm
ismdust_model.powerlaw.PhoIndex = phind

# Only the silicate grains have iron in them, so remove graphite
# grains from consideration
ismdust_model.ismdust.mgra = 0
ismdust_model.ismdust.mgra.frozen = True

ismdust_model.show()
xspec.Fit.perform()

# msil = 0.555256 g cm^-2

# Plot the results!
xspec.Plot("ufspec res")
```

Exercise: Apply ISMdust to Fe L shell photoabsorption in GX 9+9

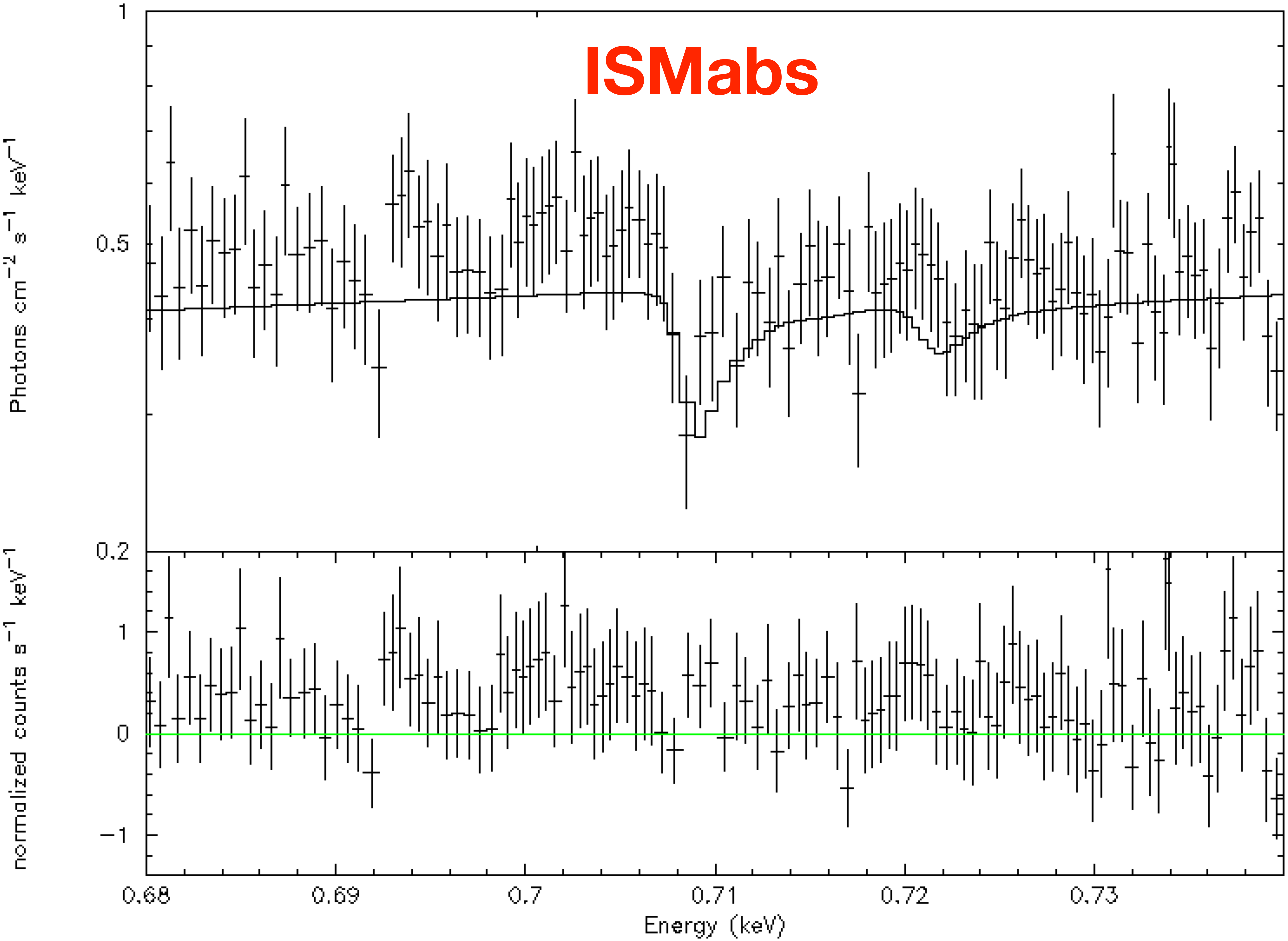


Quick Fe L shell model comparisons

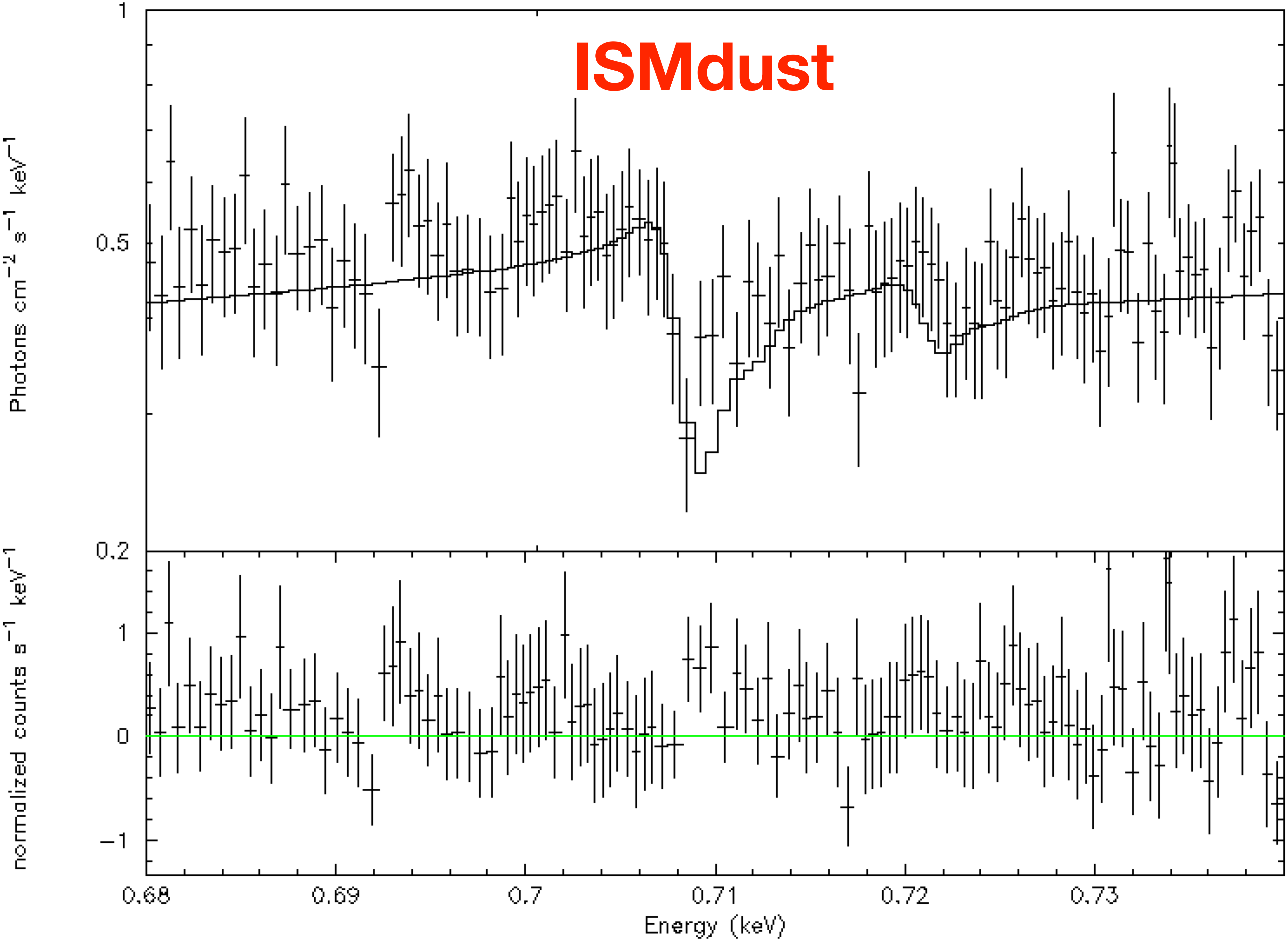
Fe L shell model comparisons



Fe L shell model comparisons



Fe L shell model comparisons

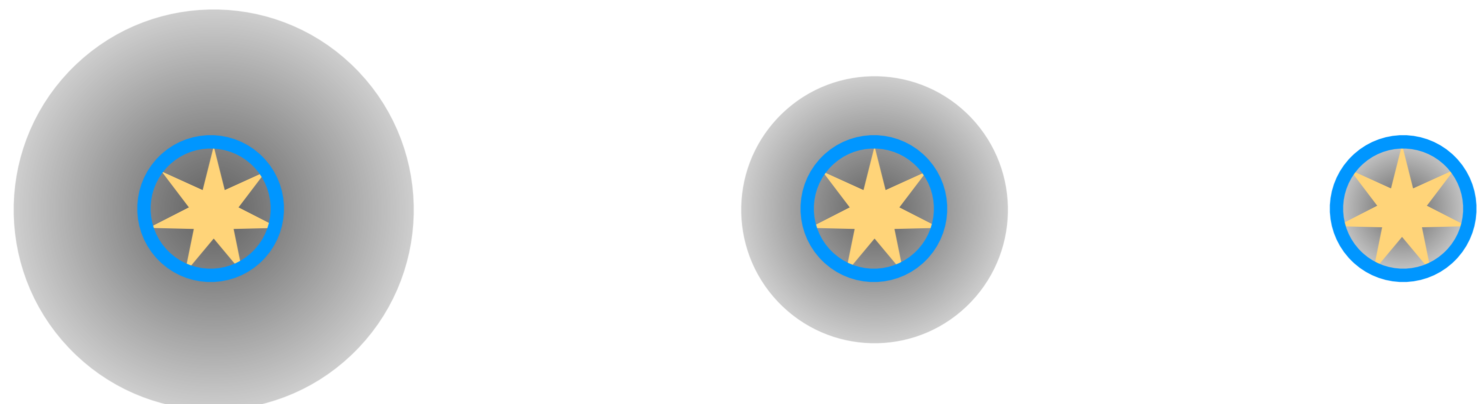


When to worry about dust and dust scattering

Rule of thumb: Where is your dust?

location

$$x \equiv \frac{D_{\rm dust}}{D_{\rm src}}$$



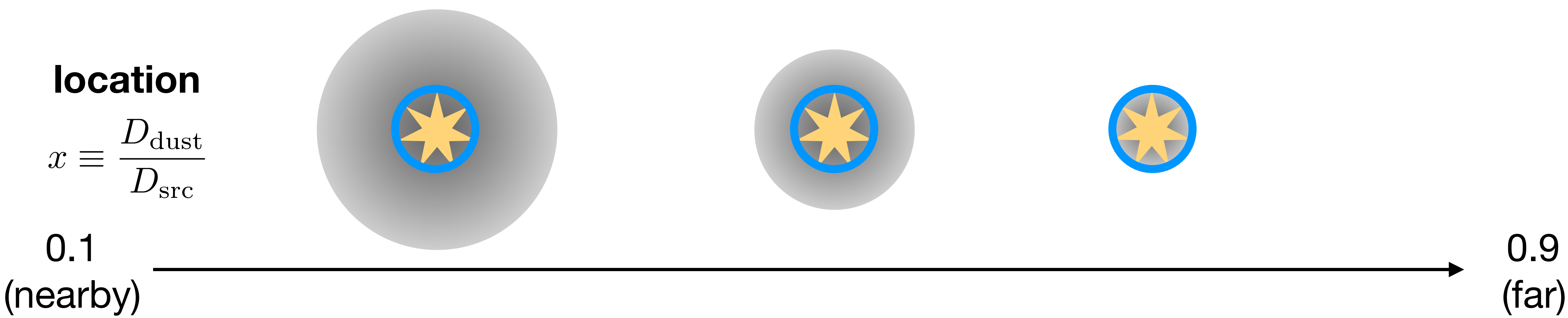
0.1 (nearby) → 0.9 (far)

Intrinsic to source?

Rule of thumb: Where is your dust?

location

$$x \equiv \frac{D_{\rm dust}}{D_{\rm src}}$$



Intrinsic to source?

yes

Ignorance is bliss!
Use tbabs or ISMabs

except

partial covering / dust clumps
like perhaps in AGN
– use **ISMdust**

When to worry about dust and dust scattering

Rule of thumb: Where is your dust?

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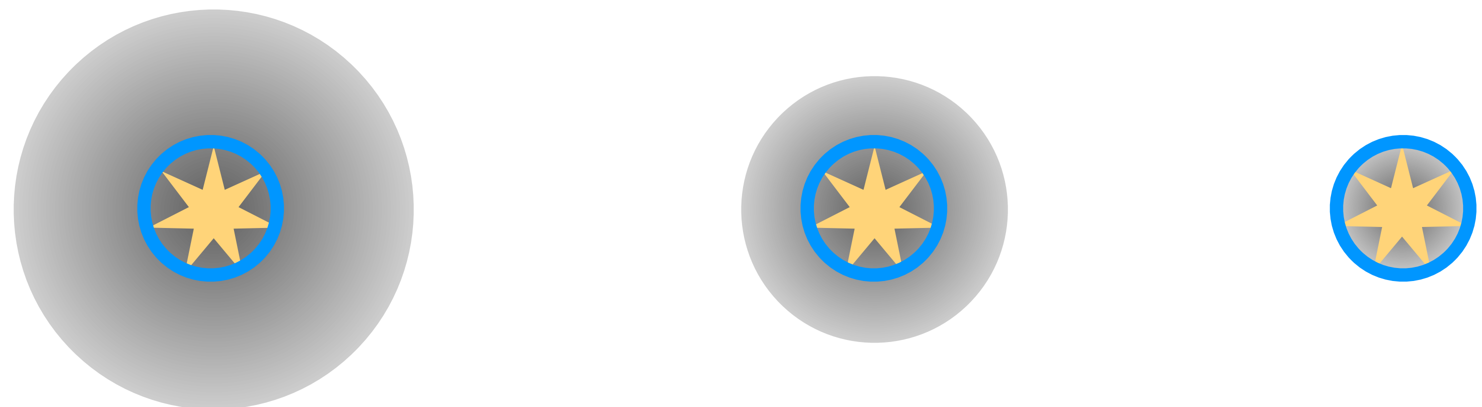
$$x \equiv \frac{D_{\rm dust}}{D_{\rm src}}$$



0.1 (nearby) → 0.9 (far)

Intrinsic to source?

yes

Ignorance is bliss!
Use tbabs or ISMabs

except

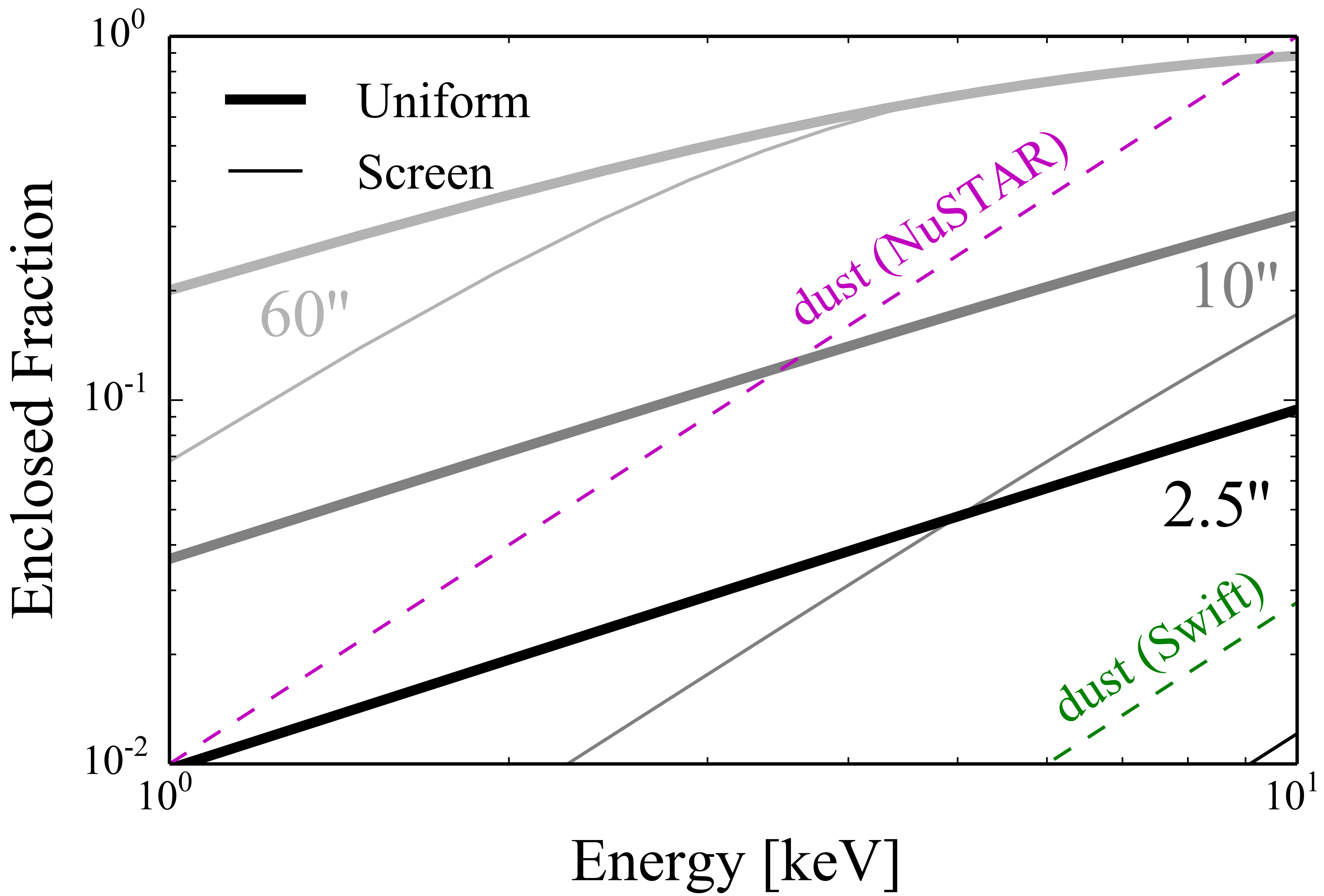
partial covering / dust clumps
like perhaps in AGN
– use **ISMdust**

no

Use dust scattering
rule of thumb in
the next slide

Rule of thumb: **Is** $\tau_{\rm sca}\ (1 - f_{\rm encl}) \geq$ **desired accuracy?**

$$\tau_{\rm sca} \sim 5\% \left(\frac{\rm NH}{10^{21}\ {\rm cm}^{-2}} \right) \left(\frac{E}{\rm keV} \right)^{-2}$$

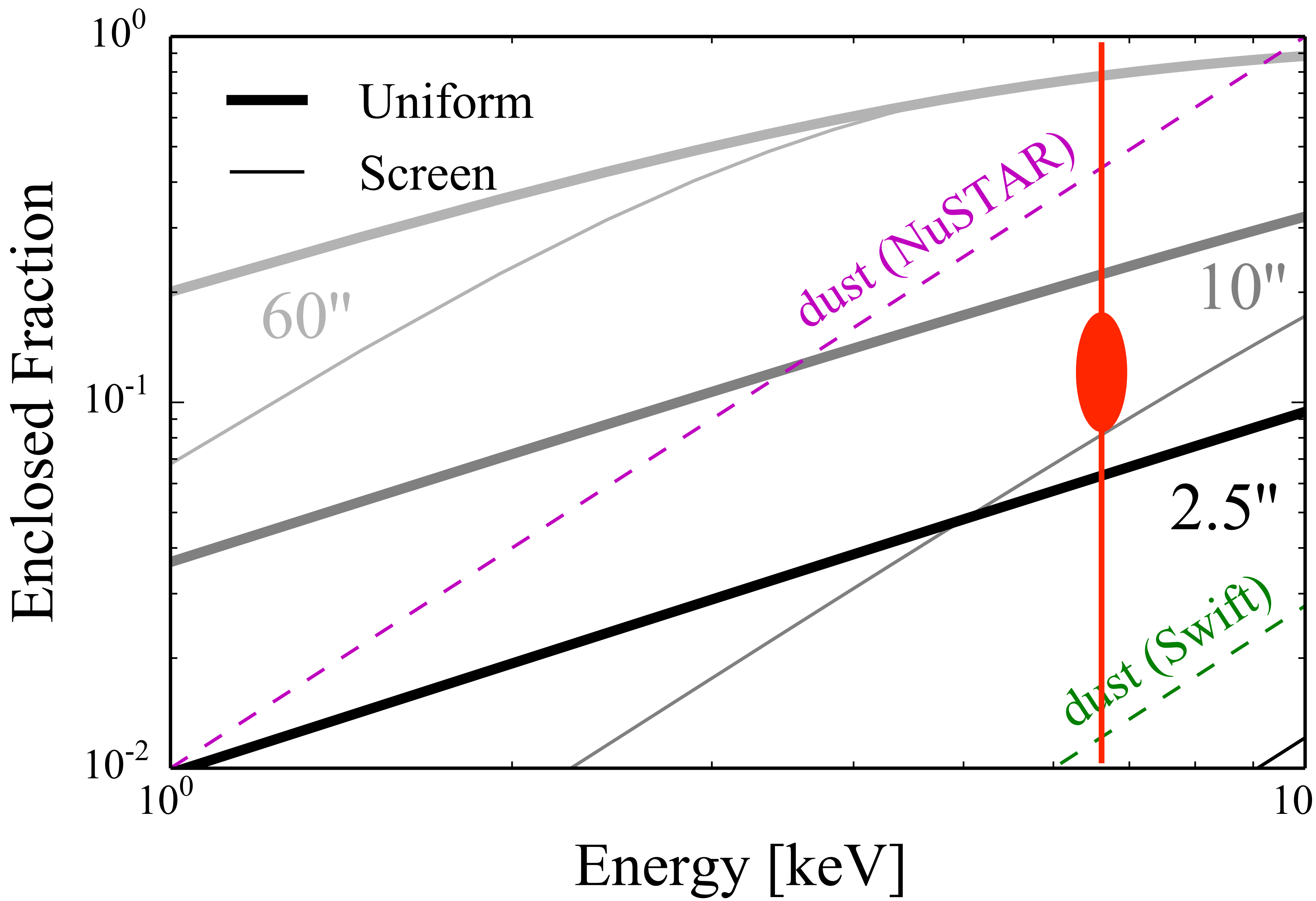


Rule of thumb: **Is** $\tau_{\rm sca}\ (1 - f_{\rm encl}) \geq$ **desired accuracy?**

$$\tau_{\rm sca} \sim 5\% \left(\frac{\rm NH}{10^{21}\ {\rm cm}^{-2}}\right) \left(\frac{E}{\rm keV}\right)^{-2}$$

For example:
6.7 keV Fe line complex,
NH = 10^{23} cm^{-2},
observed with *Swift*

$\tau_{\rm sca}\ (1 - f_{\rm encl}) \approx 10\%$



Are you worried about dust grains > 0.3 μm?

Intrinsic to source?

Are you worried about dust grains > 0.3 μm?

Intrinsic to source?

yes

Use **tbabs** with larger dust grain size parameters (self-blanketing)

Are you worried about dust grains > 0.3 μm?

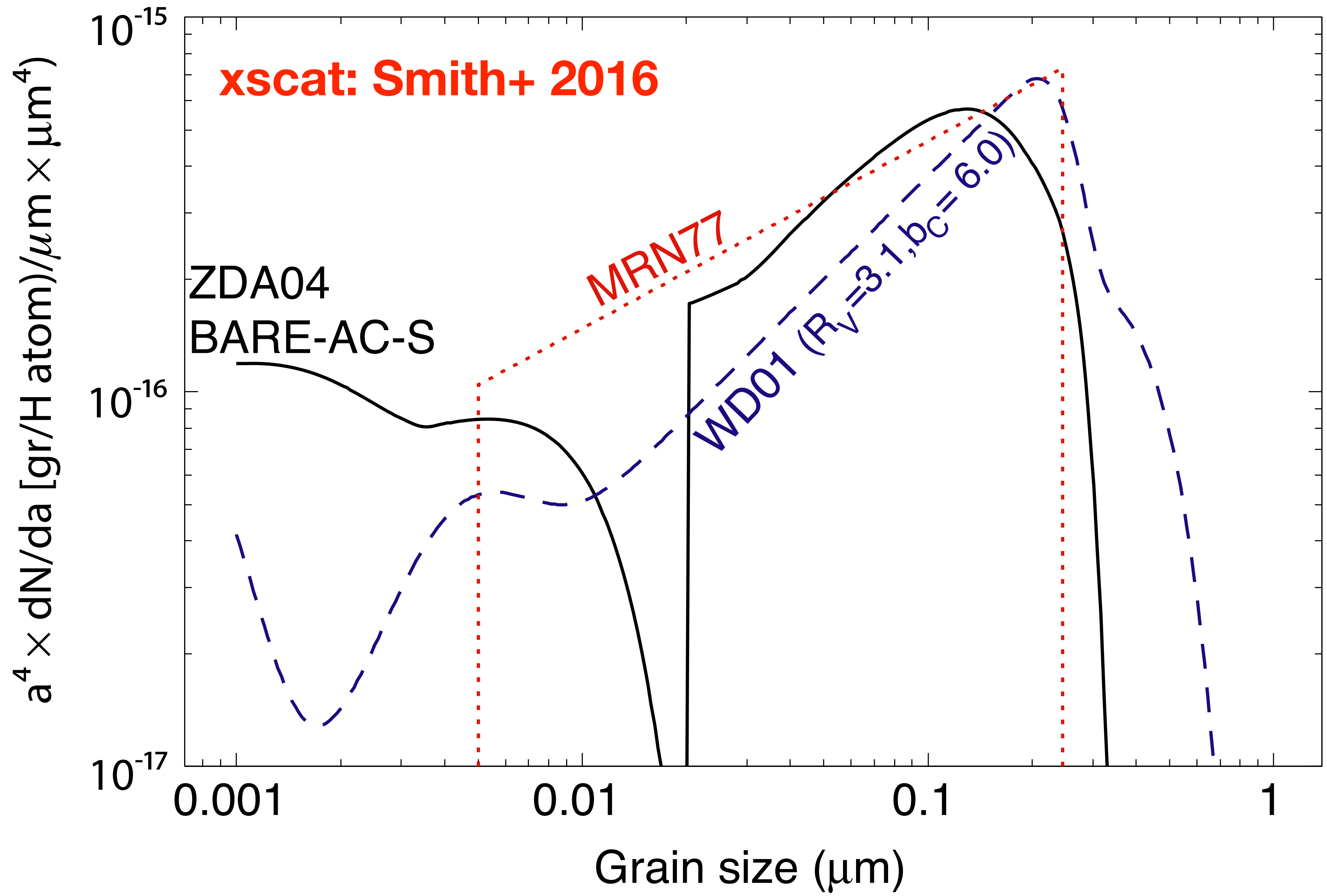
Intrinsic to source?

yes

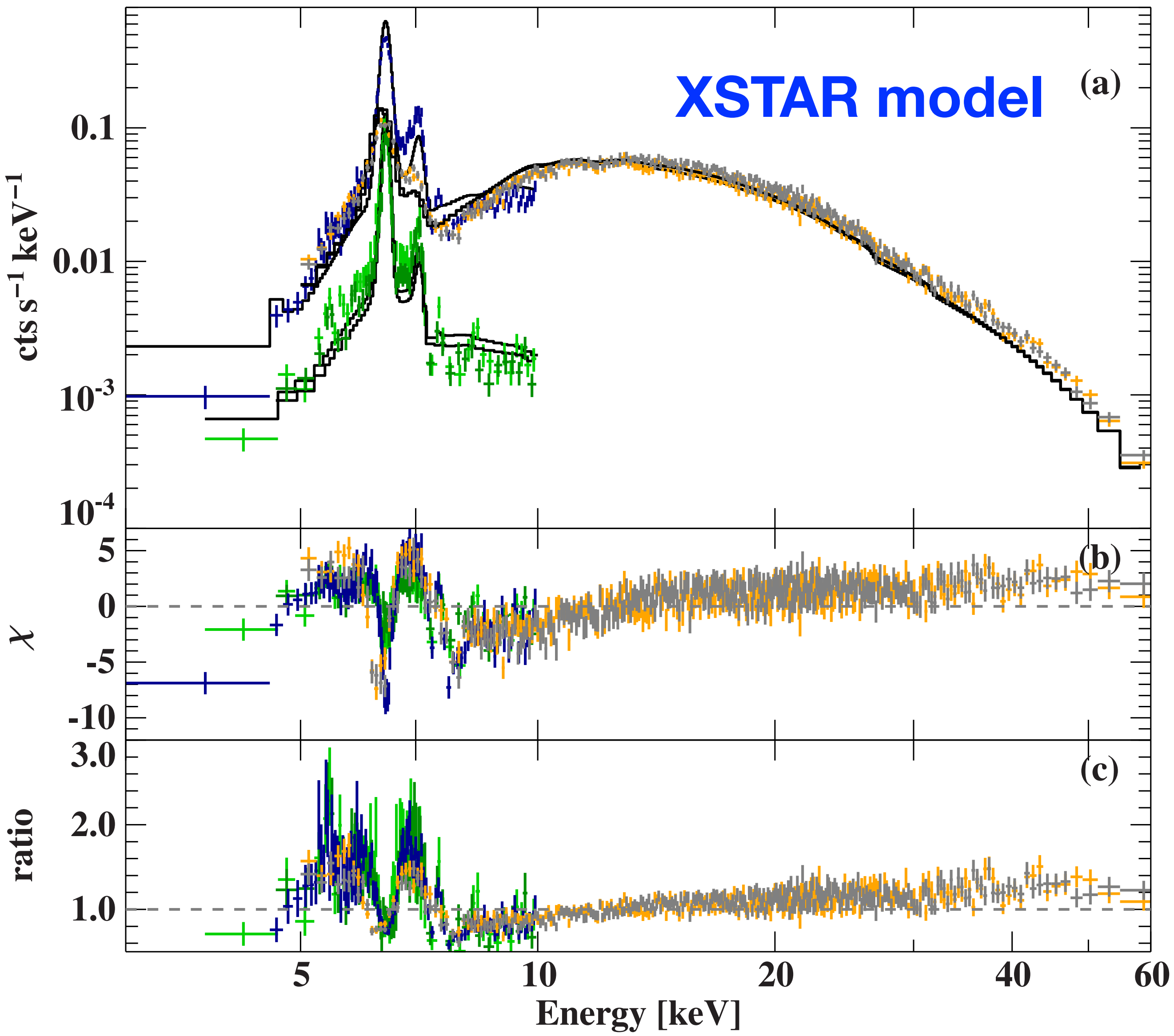
no

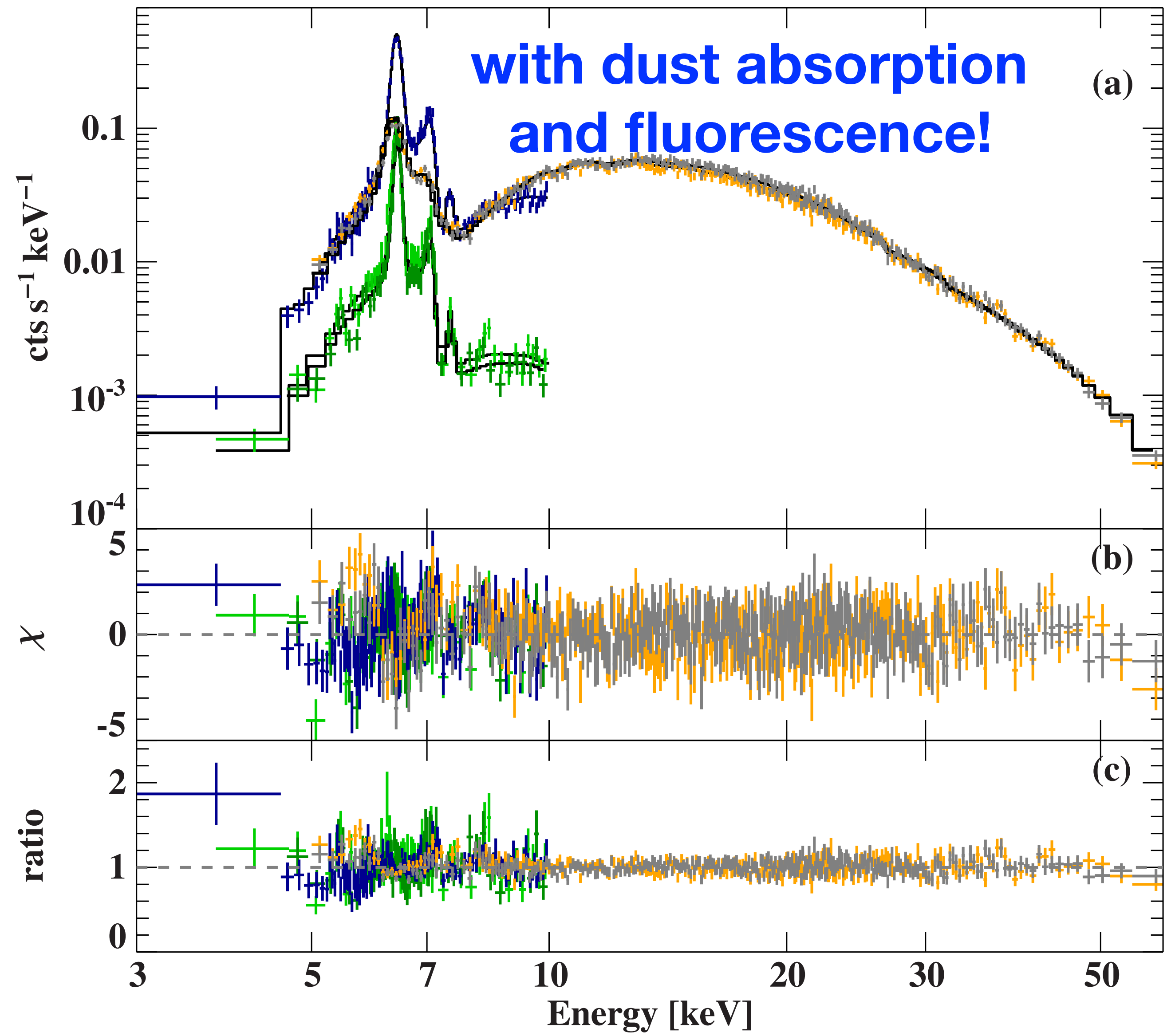
Use **tbabs** with larger dust grain size parameters (self-blanketing)

Use **xscat** or ***eblur/newdust***



HMXB IGR J16318–4848





Ballhausen+ (2020, accepted)

Choose your own dust model adventure at github.com/eblur/newdust

dust grain population
- optical constants
- dust grain size distribution
- scattering physics (Mie, Rayleigh-Gans)

input to →

- UniformGalHalo
- ScreenGalHalo

- Calculate enclosed fractions
- Simulate halo images
- Simulate dust echoes

Collaboration welcome