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Balancing Completeness and Detail in Opacity Calculations

S.B. Hansen and C.A. Iglesias

Sandia National Laboratories and Lawrence Livermore National Laboratory

Workshop on Astrophysical Opacities

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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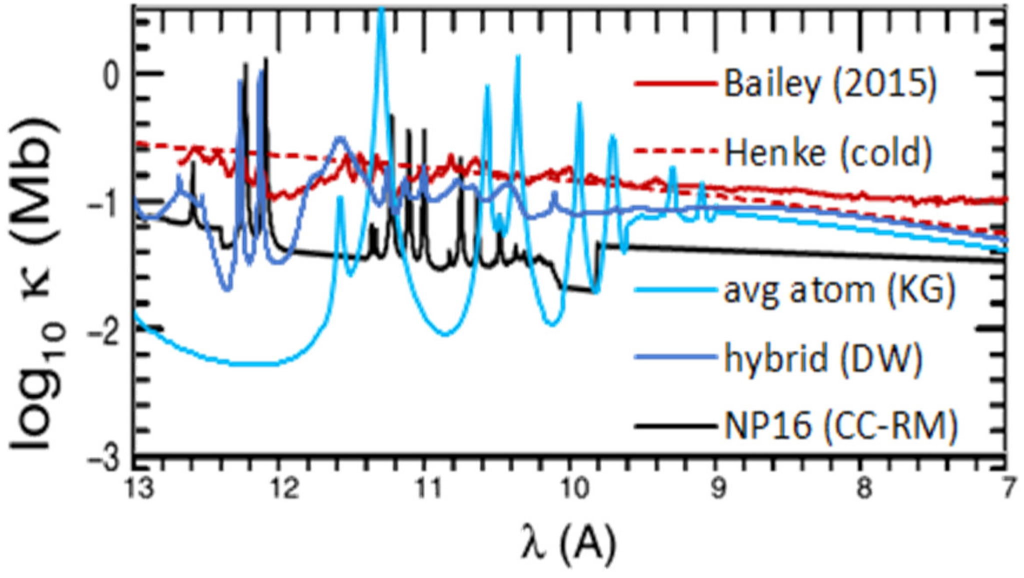
Outline

- What do we know from experiments about the opacity of iron?
  - Cold opacities
  - High-energy-density experiments: the outstanding puzzle

- What do we know from fundamental theory?

More complete ↕ More detailed

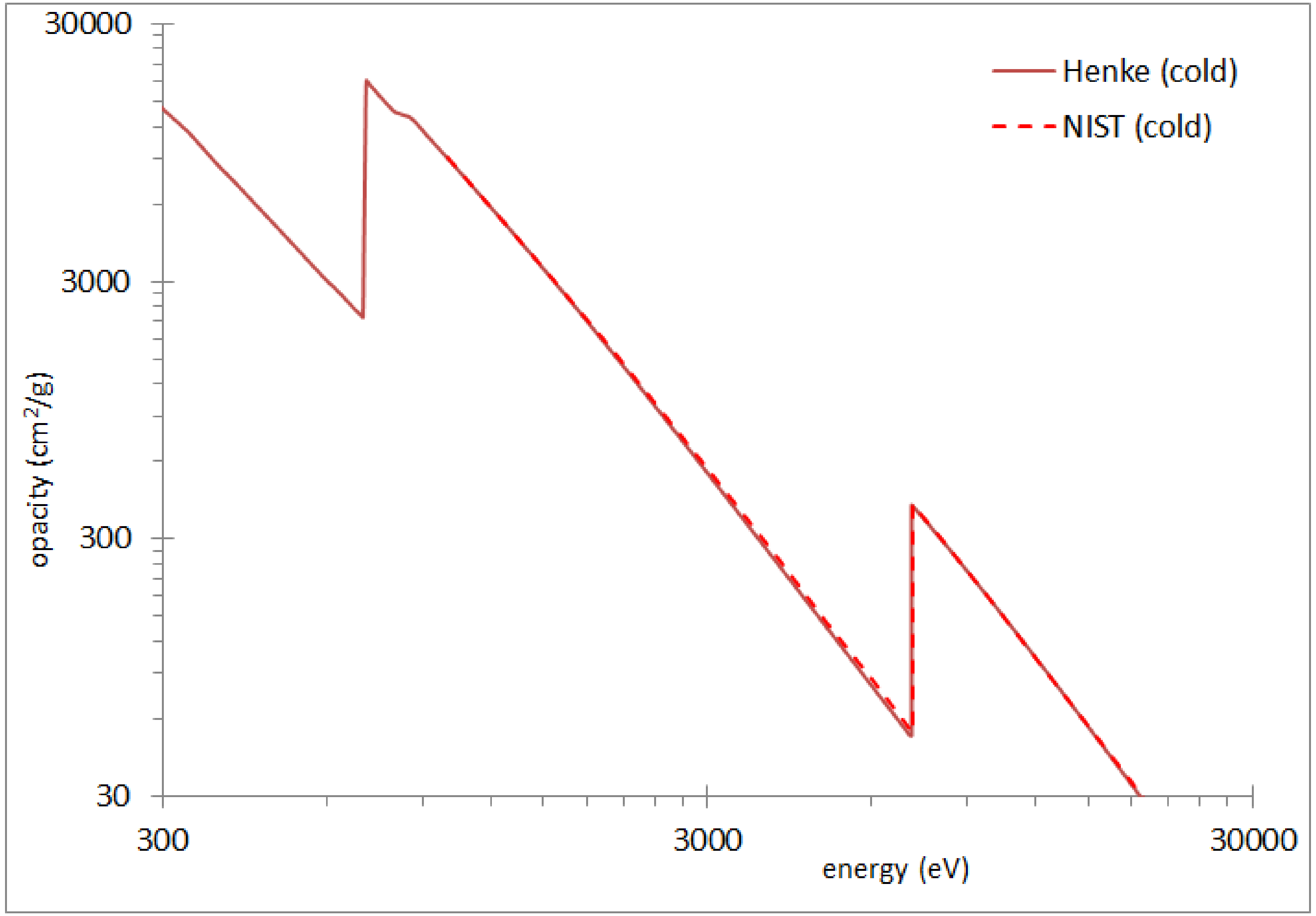
  - Average atom models
  - Unresolved transition arrays
  - Fine-structure models
  - Close-coupling/R-matrix



- Can *refining* theory help us resolve the iron opacity puzzle?
  - It appears not: neither model detail nor completeness is lacking

- Can *extending* theory help us resolve the iron opacity puzzle?
  - Perhaps, but much more work is needed – and that work must acknowledge completeness and consistency as *first-order requirements* of opacity calculations

Cold opacities are more or less settled



NIST and CXRO provide databases of cold opacities [1,2] informed by x-ray absorption measurements; agree to within < 5%

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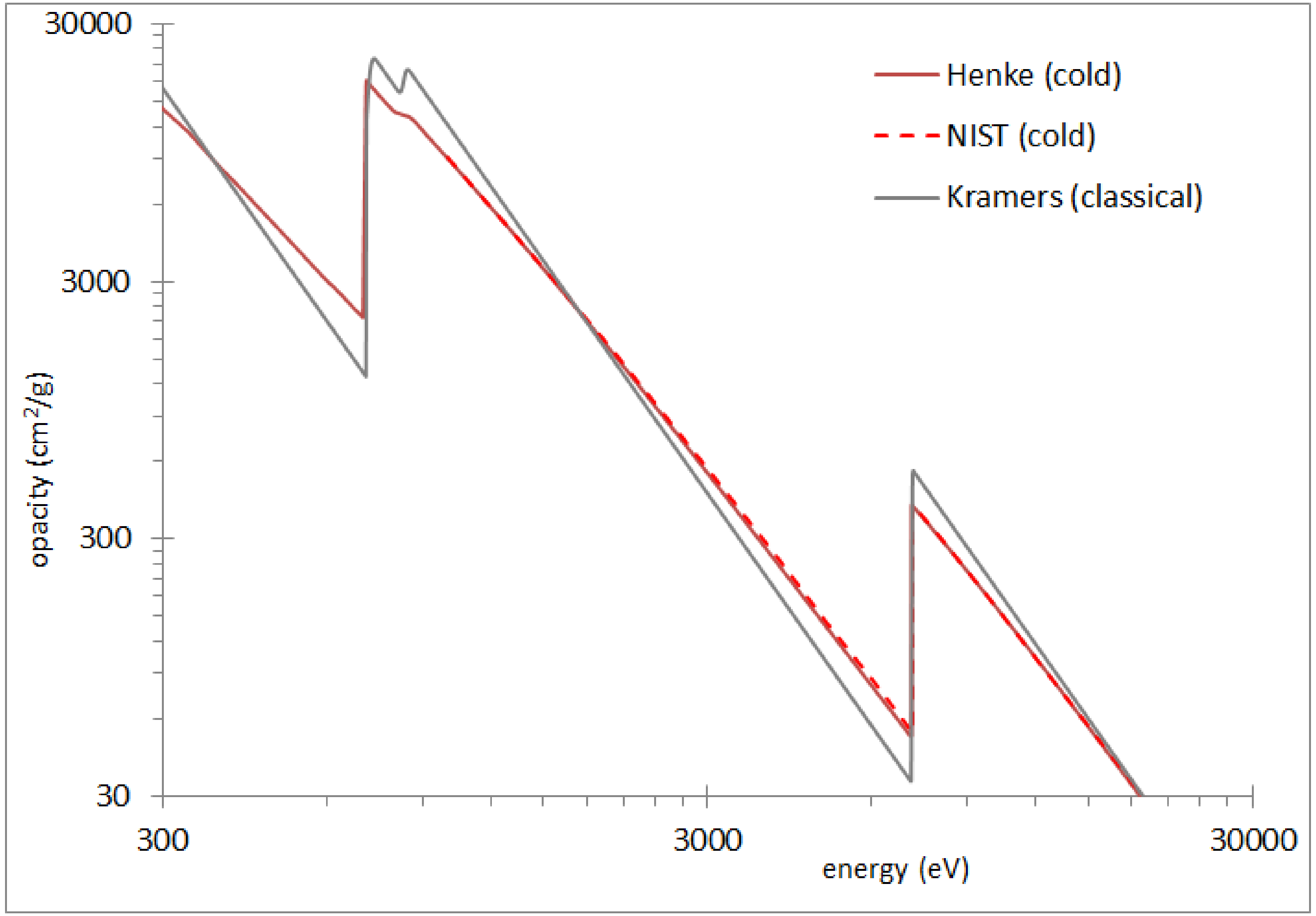

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Classical approximations for bound-free cross sections $\sigma^{\text{Kramers}} = \frac{32\alpha}{3\sqrt{3}} \frac{\text{Ry}^2}{m_e} \frac{Z^4 Q}{n^5 \varepsilon}$ roughly reproduce the standard data, and can be corrected by quantum Gaunt factors

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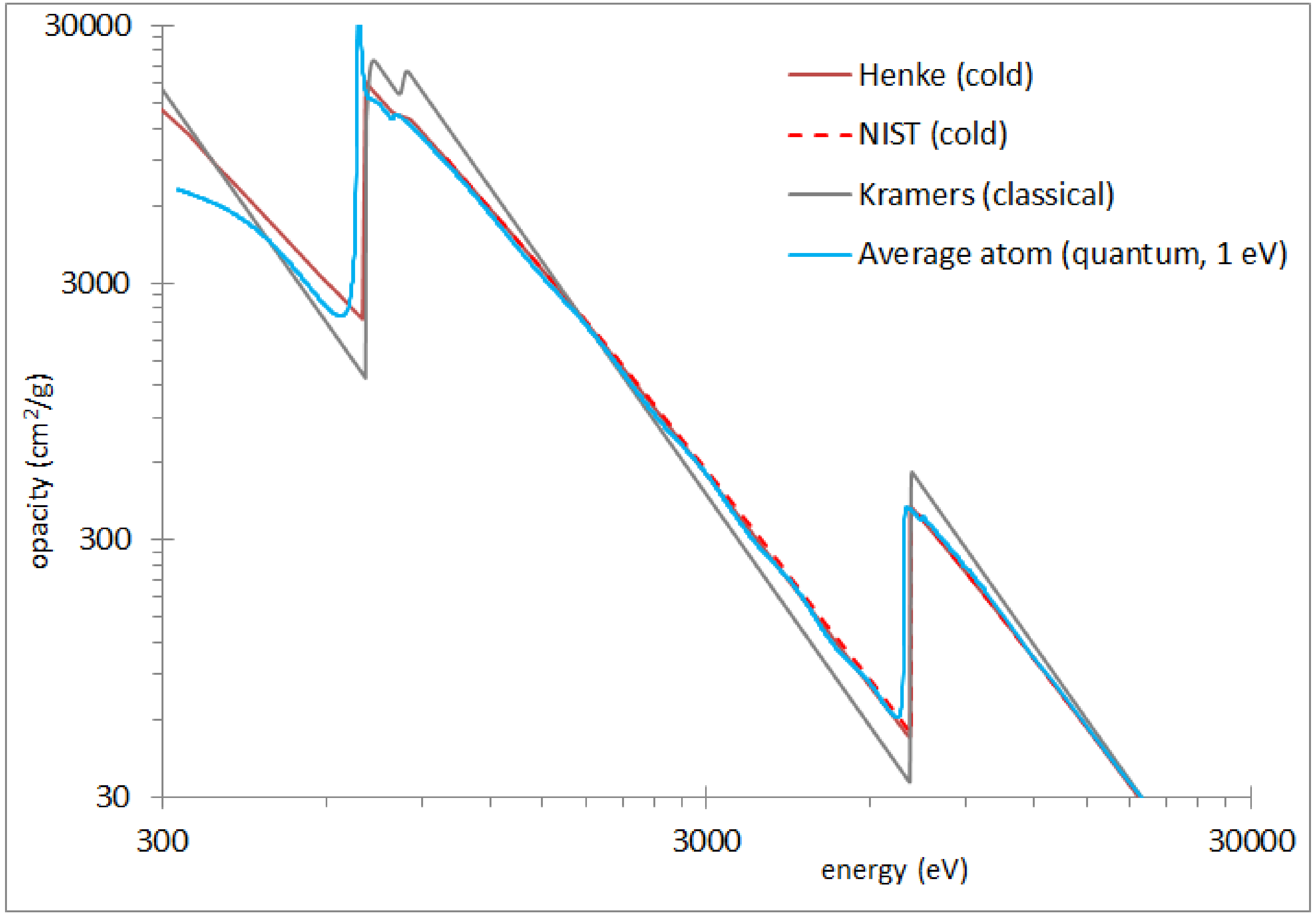

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Quantum average-atom calculations strictly obey sum rules [1] and match standard data well, especially after correcting the DFT energies

1. C Iglesias. *HEDP* **15**, 4 (2015)

Opacity modeling at HED conditions is more challenging

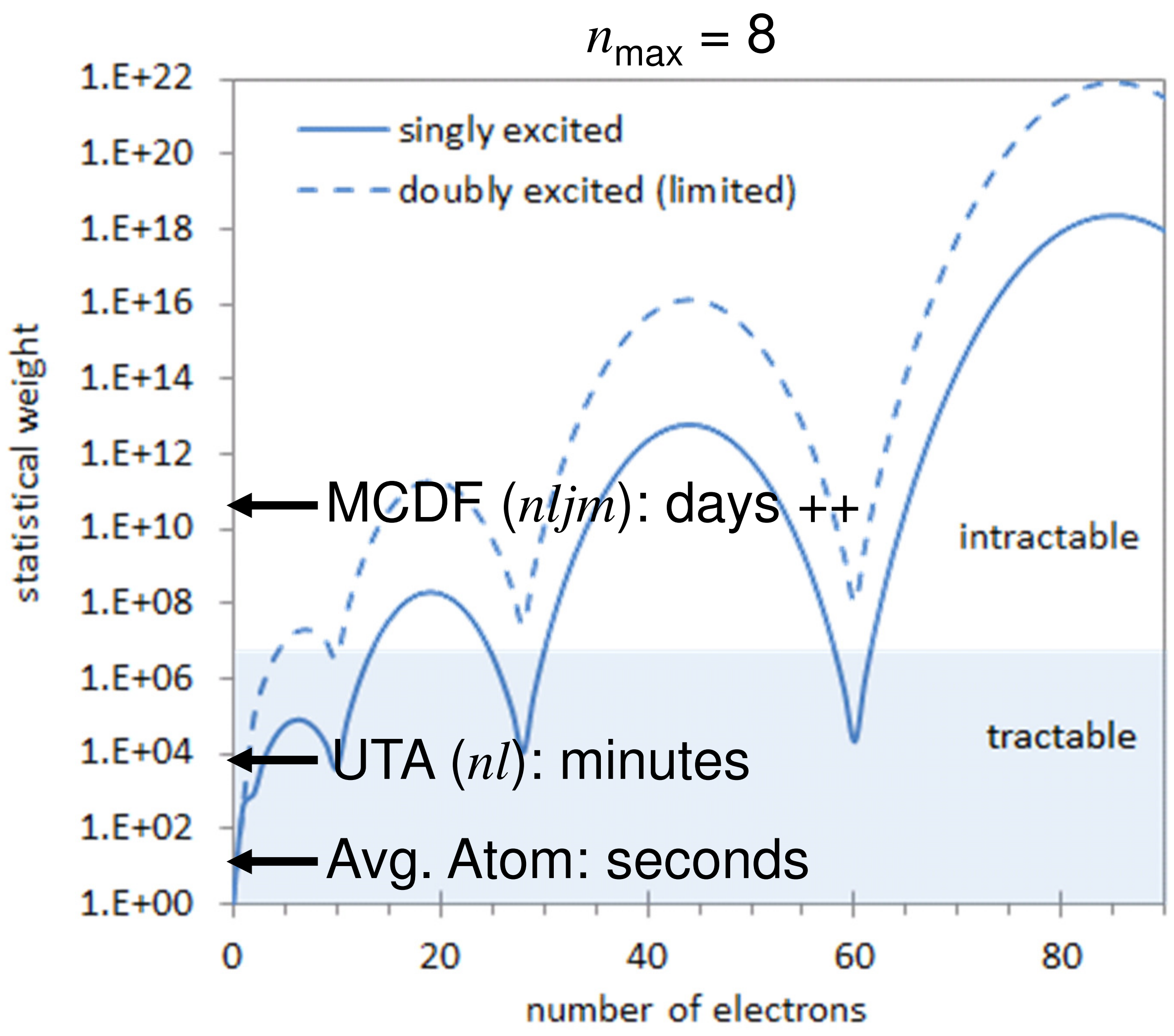
- High temperatures move electrons into excited states, which may or may not be in Local Thermodynamic Equilibrium (LTE); this leads to additional processes and divergence in $X_n \sim g_n\, e^{-E_n/T}$
- High densities lead to collisions and strong fields, which truncate the state space via continuum lowering/ IPD, can enforce LTE, and leads to collisional line broadening and Stark line splitting

Opacity models <u>must:</u>

1) Completely account for all occupied states in accessible ions (a complete and consistent EOS)
2) Completely account for all photon absorption processes from those states (bound-bound, bound-free, free-free… and multiphoton?)
3) Be computationally tractable

Opacity models <u>should:</u>

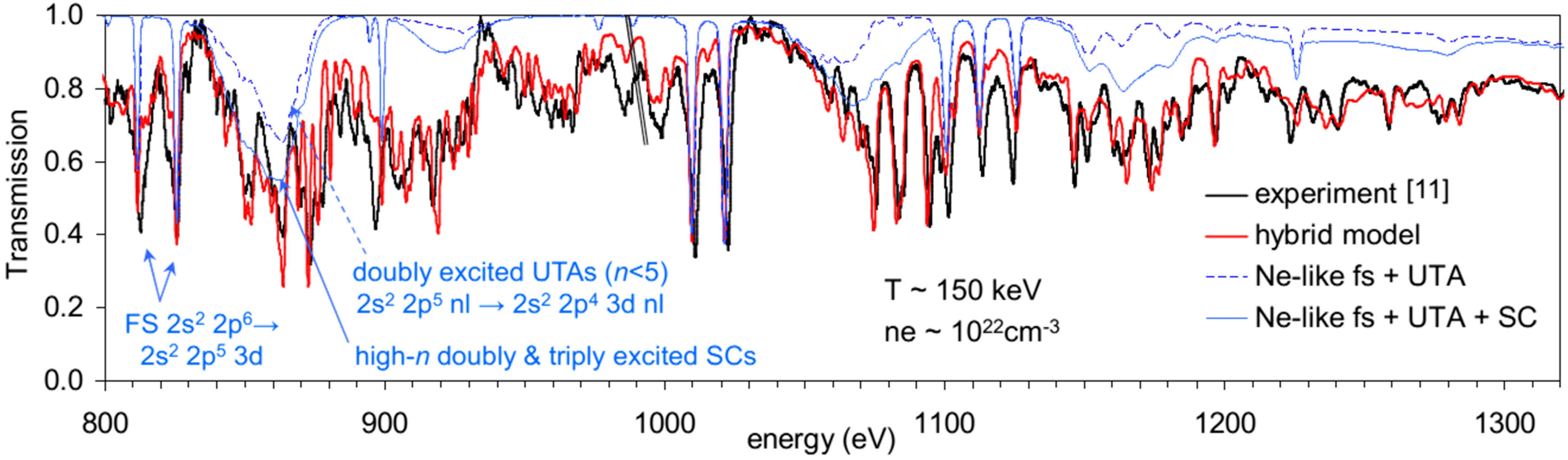
1) Have a “sufficient” and consistent treatment of line broadening
2) Have “sufficient” detail in the atomic structure



Until recently, balancing enforced completeness with "sufficient" detail appeared to be a sound approach

We know what we need to do:
get complete atomic structure from extensive MCDF or CC calculations, and then calculate all cross sections with the best methods available, ensuring that the line-shapes and EOS are consistent with the atomic structure and that the structure is complete… unfortunately we also know that's impossible.

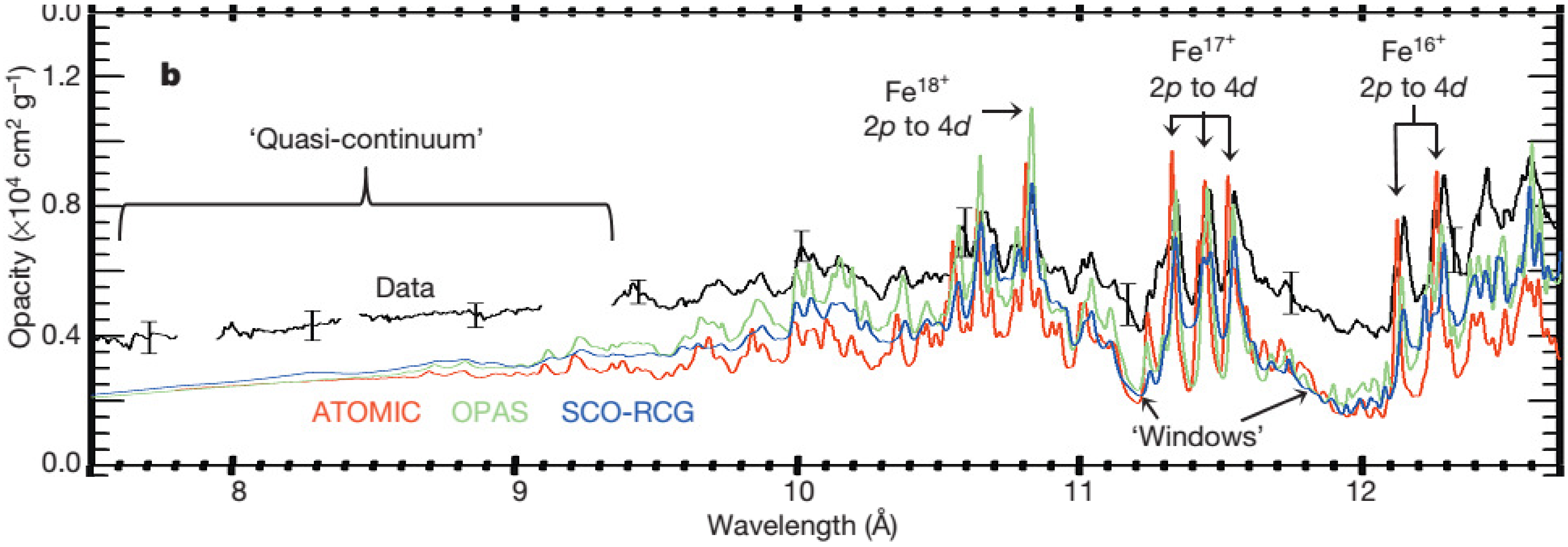
However, we can make informed choices that effectively balance completeness, accuracy, and tractability



1. Bailey et al. *PRL* **99**, 265002 (2007)

In 2015, that approach failed

In 2015, Bailey et al. published experimental results for iron opacity at T_e =183 eV and n_e = $3x10^{22}$ e/cm^3 showing lines that were much broader than theory predicts and continuum opacities that were much higher than any model – and higher than the cold opacities.

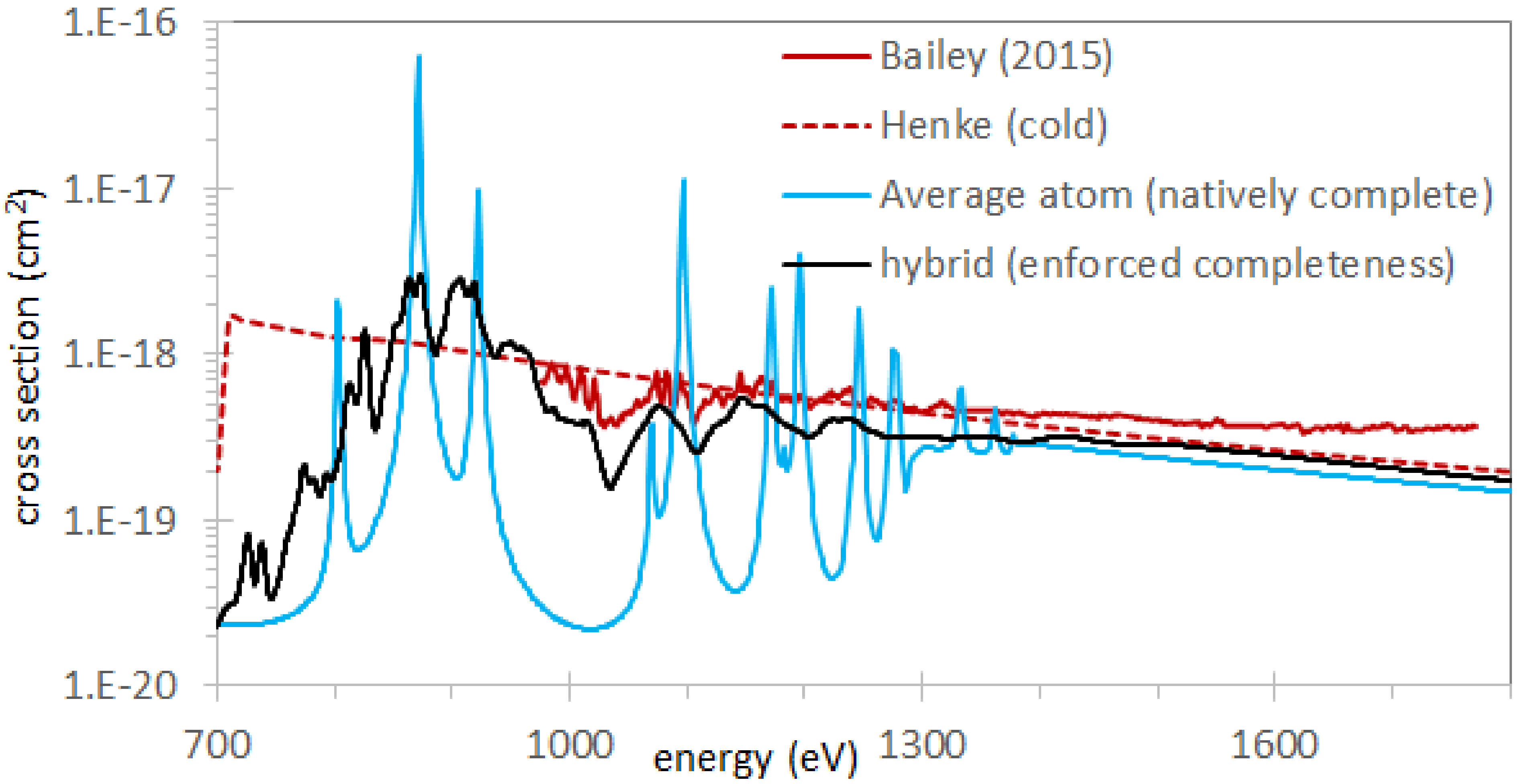


1. Bailey et al. *Nature* **517**, 56 (2015)

Were the calculations incomplete?

In general, no.

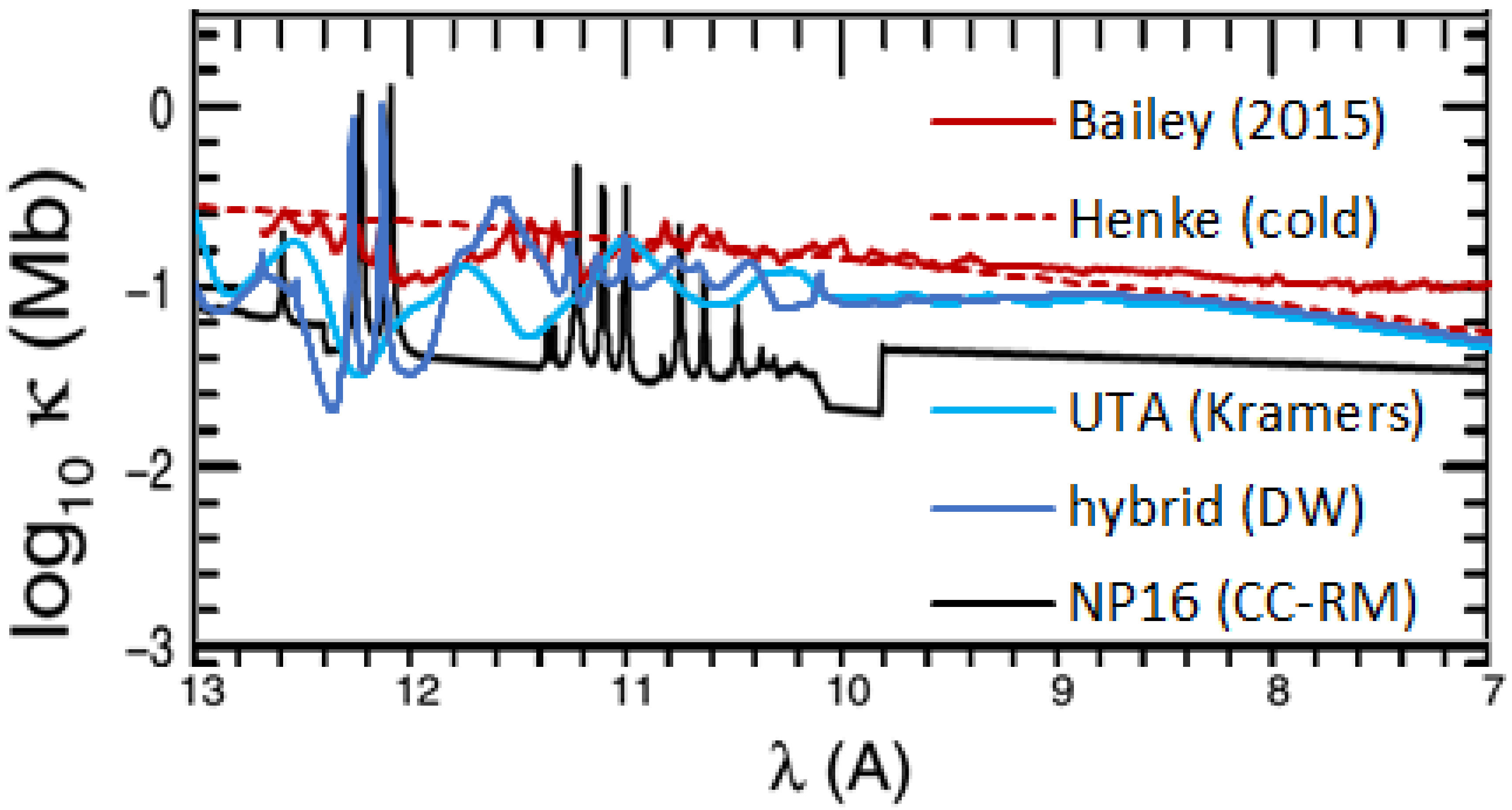
Most standard opacity models explicitly enforce completeness. Comparisons with simple average-atom models that natively possess strict completeness show that the disagreement in the continuum region cannot be resolved by adding more states.



Even with enhanced broadening, the enforced-complete "best effort" models that matched the low-density data with incredible fidelity cannot reproduce the measured high-density continuum region.

Were the calculations insufficiently detailed?

No. Unsurprisingly, models that sacrifice completeness for detail disagree <u>more</u> with the measured continuum than models that either explicitly or natively enforce completeness.



NP16: Nahar and Pradhan, *PRL* **116**, 235003 (2016); *cf*. PRL **117**, 249501 (2016), *ibid* 249502 and Ap J **835**, 284 (2017)

Revisiting the requirements for HED opacity models

Opacity models should:

1) Have a “sufficient” and consistent treatment of line broadening

2) Have “sufficient” detail in the atomic structure

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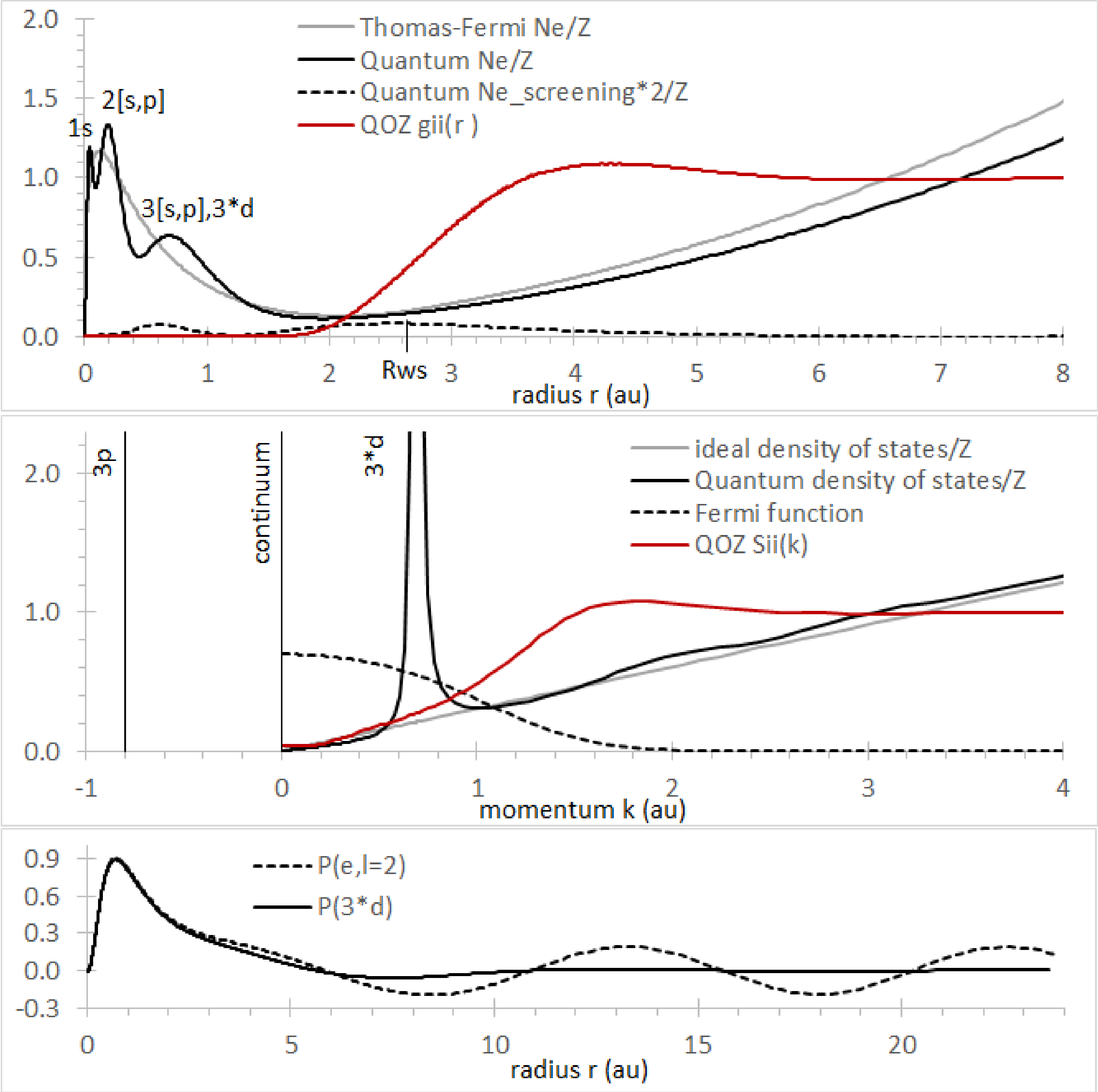
Simple but strict consistency: Extended average-atom models



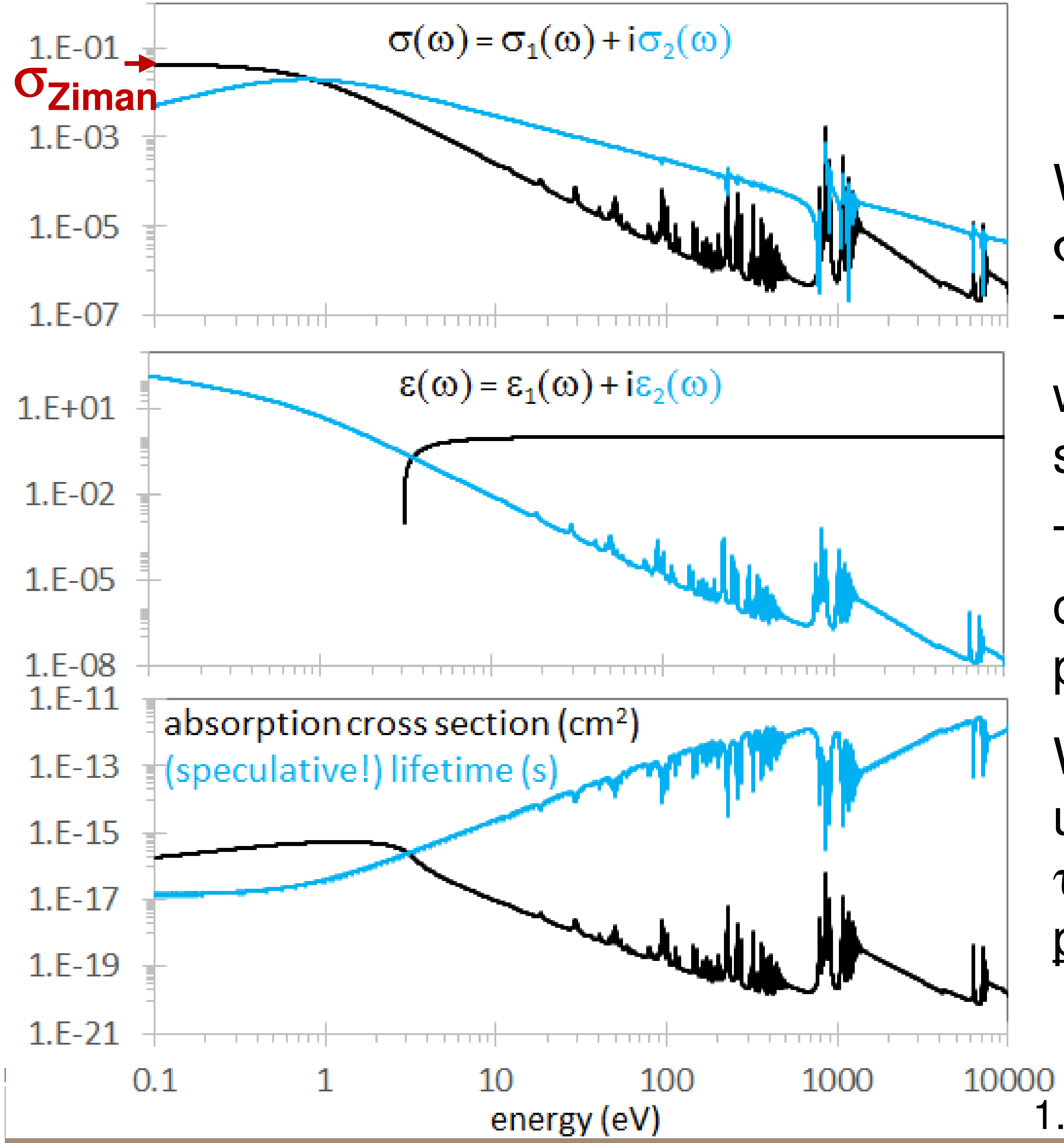
Electrons are treated quantum mechanically in a self-consistent field much like Purgatorio[1], within an ion correlation sphere instead of muffin-tin. Ions are treated with the quantum Ornstein-Zernike equations[2] using a potential generated from the self-consistent electronic structure.

To ensure smooth transitions under pressure ionization, we define quasi-bound wavefunctions P(n*l) = $\langle P(e,l) \rangle_k$ and assign them to the ion. This collapses multiple definitions of Z* into a single value

The EOS, continuum lowering, and potentially even line broadening derived from this model are all fully self-consistent and natively complete.

1. B.G. Wilson *et al*, *JQSRT* **99**, 658 (2006) 2. C. Starrett & D. Saumon, *HEDP* **10**, 35 (2014)

Optical properties can be generated from the wavefunctions



$$\sigma(\omega) = \frac{2}{3}\frac{n_a e^2}{\omega^2}\int v^3 \sigma_{tr}\left(-\frac{\partial f}{\partial E}\right)\frac{d^3p}{(2\pi\hbar)^3}$$

We use Kubo-Greenwood[1] to generate $\sigma(\omega) \rightarrow \varepsilon(\omega), n(\omega), \alpha(\omega), \tau(\omega)$

This provides rough but *strictly complete* opacities which account for all electronic states and obey all sum rules.

The model is also *natively consistent*, with continuum lowering and EOS derived from the same potential and wavefunctions that produce $\alpha(\omega)$.

We are exploring ways to increase consistency by using $S_{ii}(k)$ to generate P(E) for Stark splitting and $\tau(\omega)$ for both collisional broadening and multi-photon processes.

1. M. Yu Kuchiev and W.R. Johnson *et al*, *PRE* **78**, 026401 (2008)

A first step: two-photon processes in a rough approximation

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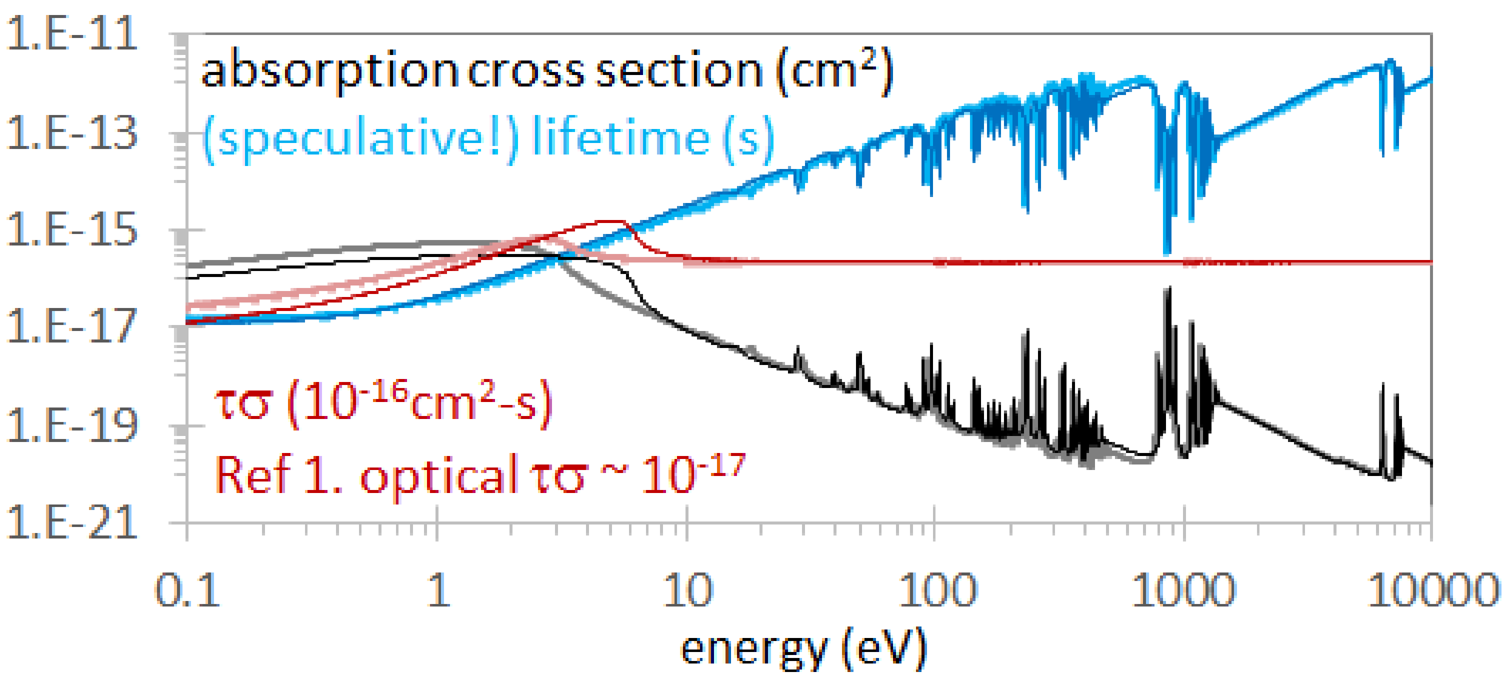
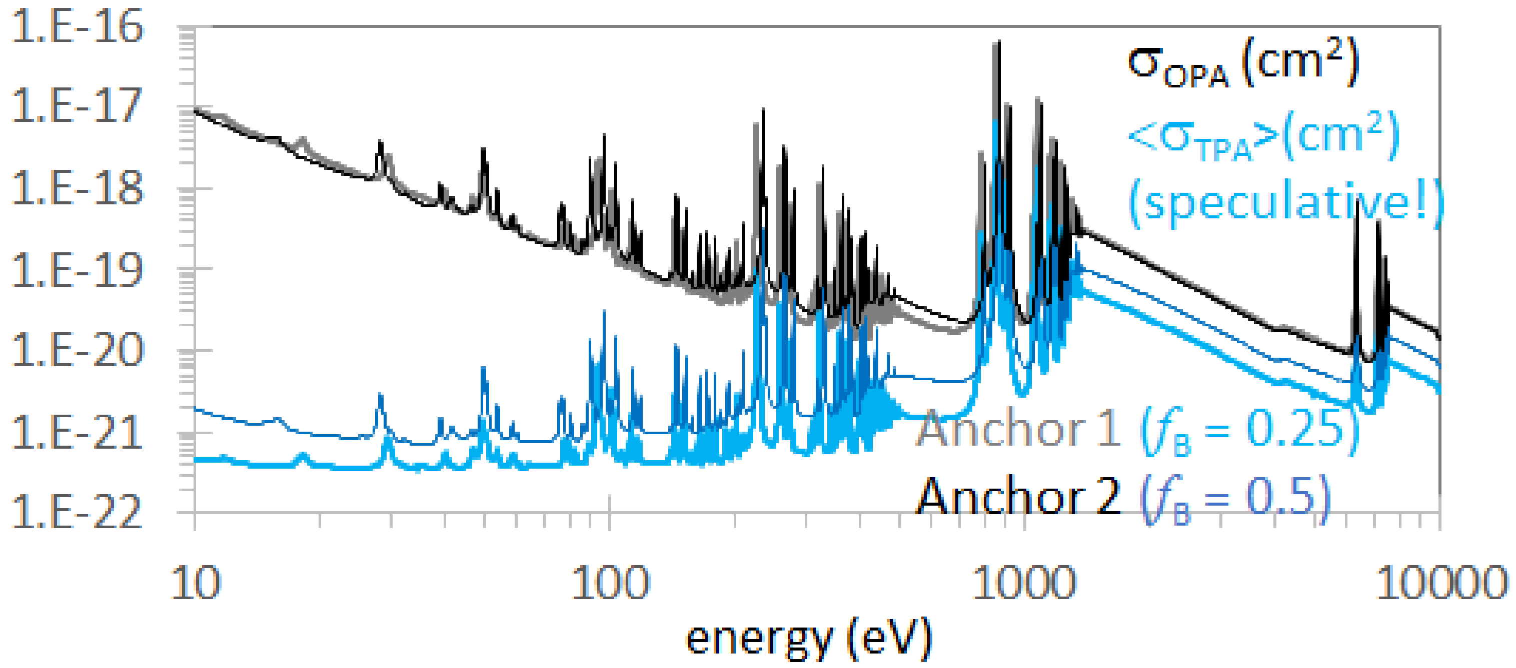




Following Lambropolous & Tang [1], we approximate the two-photon process as a series of one-photon processes, and integrate over the backlighter intensity $f_B\, B(\omega)$:

$\sigma_{TPA} = \sigma_{i\text{-}j}\ \tau_j\ \sigma_{j\text{-}f}$ [cm^4 s]

$\langle\sigma_{TPA}\rangle = \sigma_{OPA} \int_0^Q (\tau_j\ \sigma_{j\text{-}f})(\omega)\ f_B\, B(\omega)\ d\omega$ [cm^2]

With the *speculation* that $\tau(\omega) = n_i / [\varepsilon_2(\omega) d\omega]$ (?), from [2], we find that $\langle\sigma_{TPA}\rangle$ can plausibly account for the iron data – and it will not be a factor for NIF experiments!

Please note that this is highly preliminary. See recent work from R. More (forthcoming HEDP) and M. Kruze for more rigorous (but as-yet less complete!) approaches.

1. Lambropolous & Tang, *J. Opt. Soc. Am. B* **4**, 821 (1987)   2. F. Wooten, Optical Properties of Solids, NY Ac.Press Eq. 3.108

Conclusions

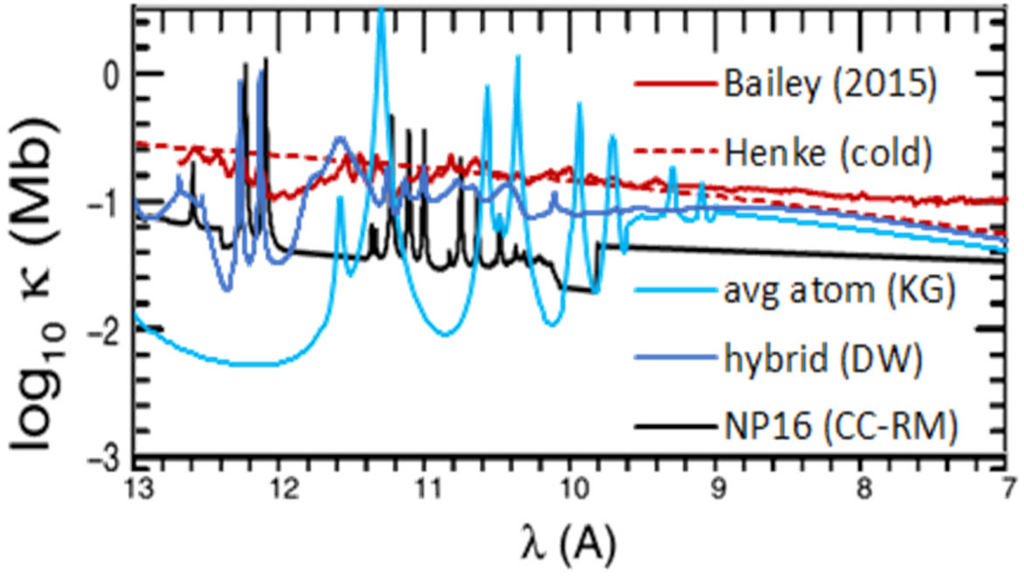
- Z experimental opacities remain a significant and unresolved puzzle

- Opacity models must balance completeness and detail:

More complete

- Average atom models
- Unresolved transition arrays
- Fine-structure models
- Close-coupling/R-matrix

More detailed



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Back-up

The Astrophysical Journal, 835:284 (5pp), 2017 February 1

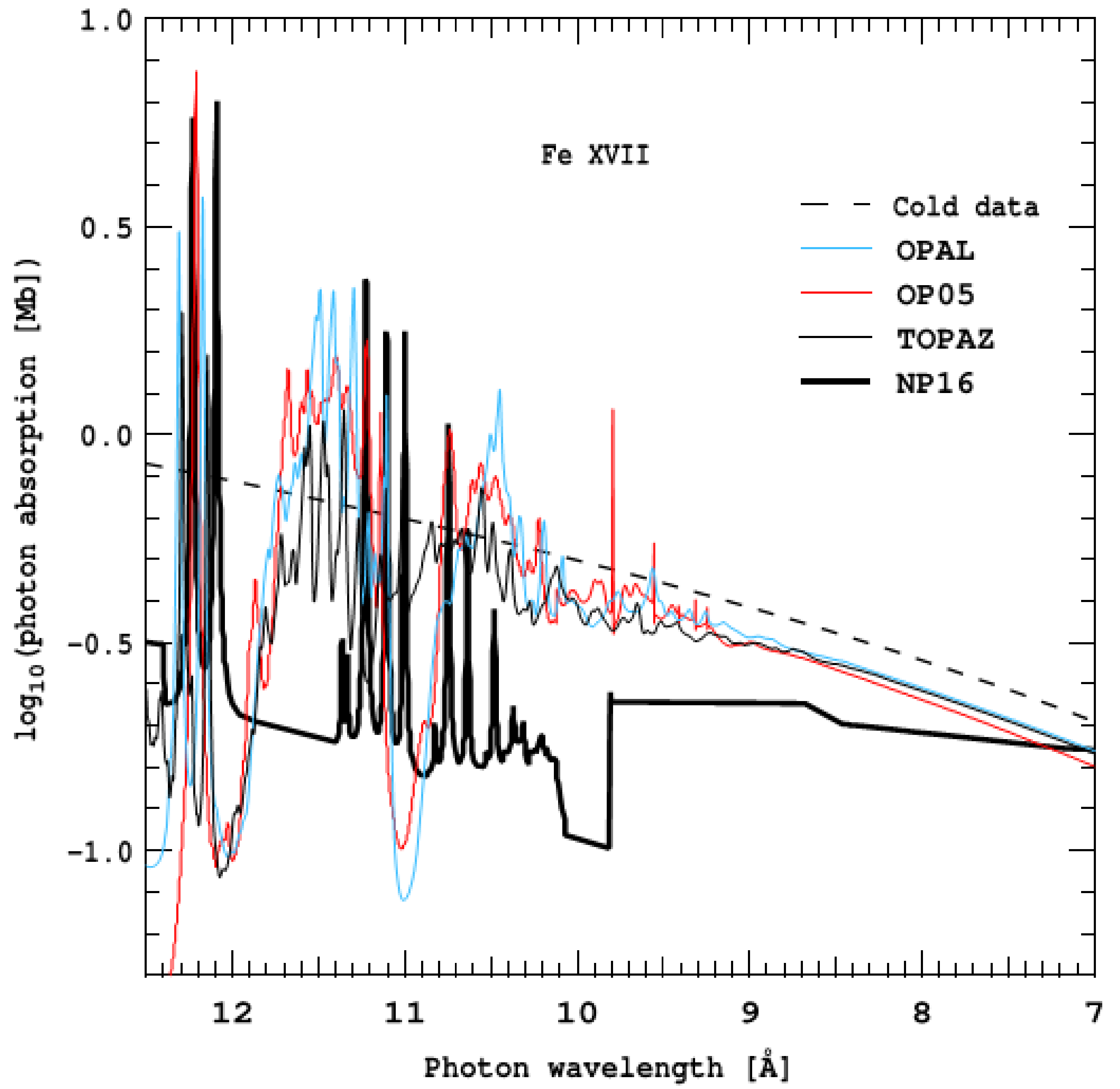

Figure 1. Fe XVII monochromatic opacities in the spectral range and conditions of the Sandia experiments from several codes and the cold solid density data.

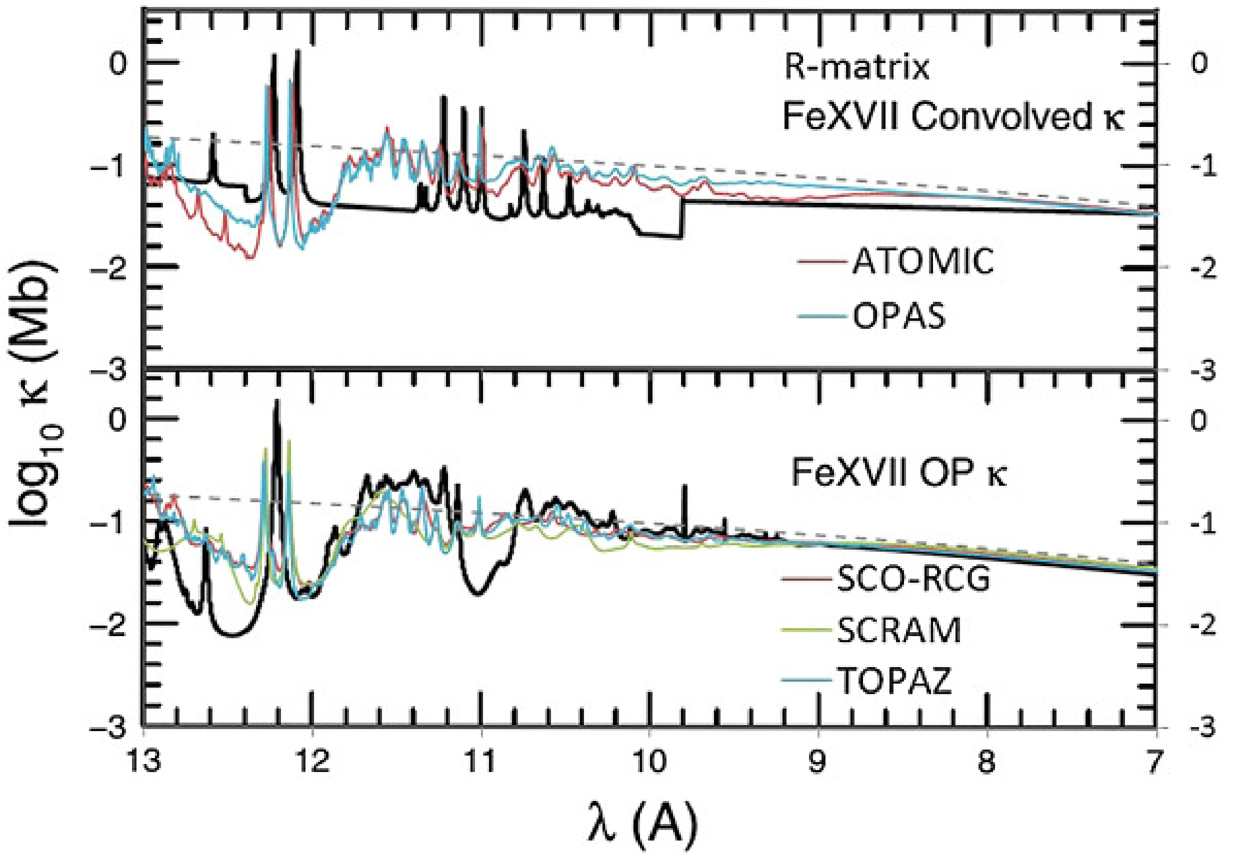

FIG. 1. (Adapted from Fig. 5 of Ref. [1].) Opacities of FeXVII at a temperature of 2.1×10^6 K, free electron number density of 3.1×10^{22} cm^{-3}, and abundance of 0.195. Dashed lines are 0.195× the cold reference opacity [10], representing a fully occupied *L* shell.

which generate 99 LS-terms. It follows that NP16 omitted the photon ionizations:

$$\begin{aligned} &2s^2 2p^5 n\ell + h\nu \rightarrow 2s2p^5 n\ell\varepsilon p \quad n\ell = 4d, 4f, \\ &\quad \text{and} \quad n \geqslant 5 \\ &2s2p^6 n\ell + h\nu \rightarrow 2p^6 n\ell\varepsilon p \quad \text{all } n \\ &2s^2 2p^5 n\ell + h\nu \rightarrow 2s^2 2p^4 n\ell\varepsilon\ell' \quad n \geqslant 5 \\ &2s2p^6 n\ell + h\nu \rightarrow 2s2p^5 n\ell\varepsilon\ell' \quad n\ell = 4d, 4f, \\ &\quad \text{and} \quad n \geqslant 5 \end{aligned} \tag{5}$$

with $\ell' = s, d$ for dipole allowed transitions.

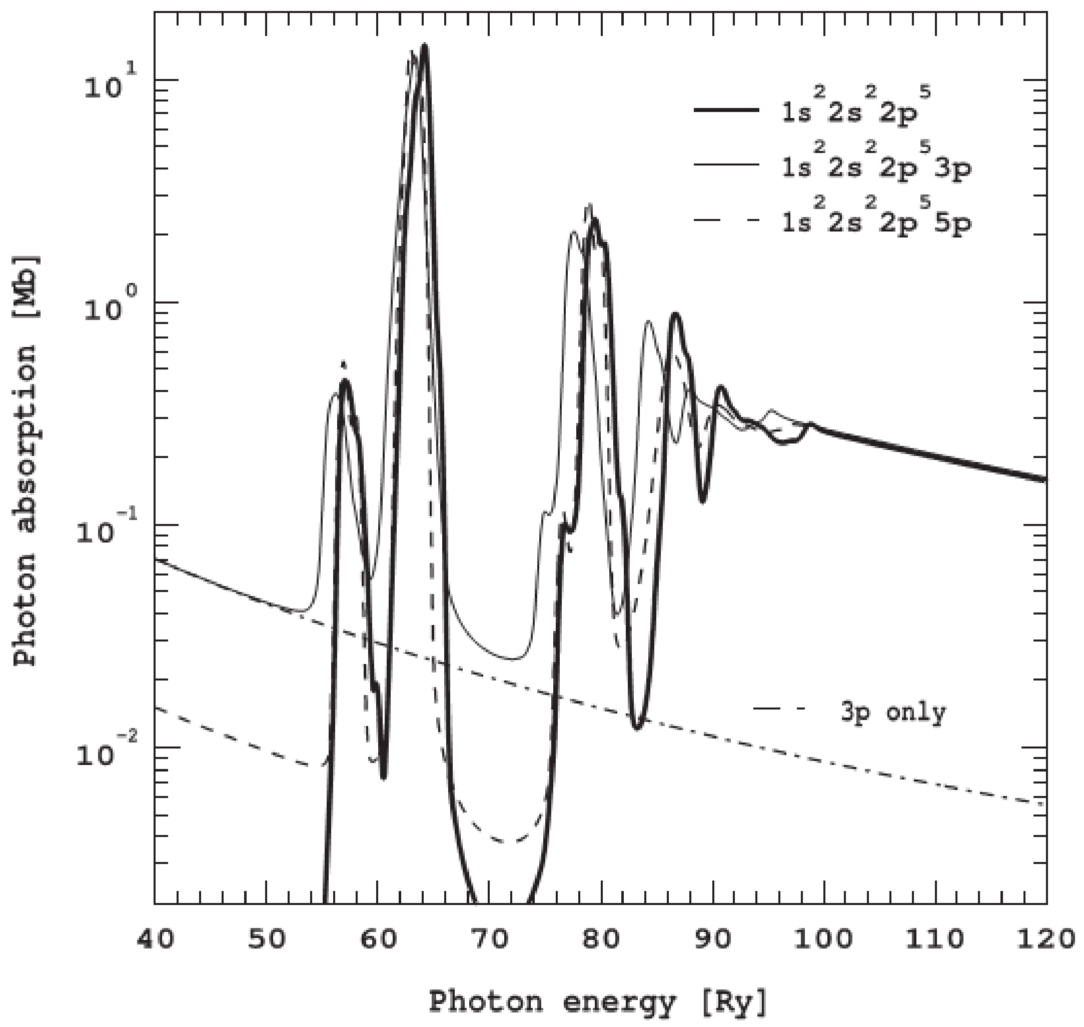

Figure 2. TOPAZ total photon absorption cross-section for the Fe XVIII ground configuration (thick line), the Fe XVII singly excited configuration with $3p$ (thin line) and $5p$ (dash line) spectators, plus only ionization by the $3p$ spectator (dot–dashed line). Results are convolved with a Gaussian with 8 eV FWHM for clarity.

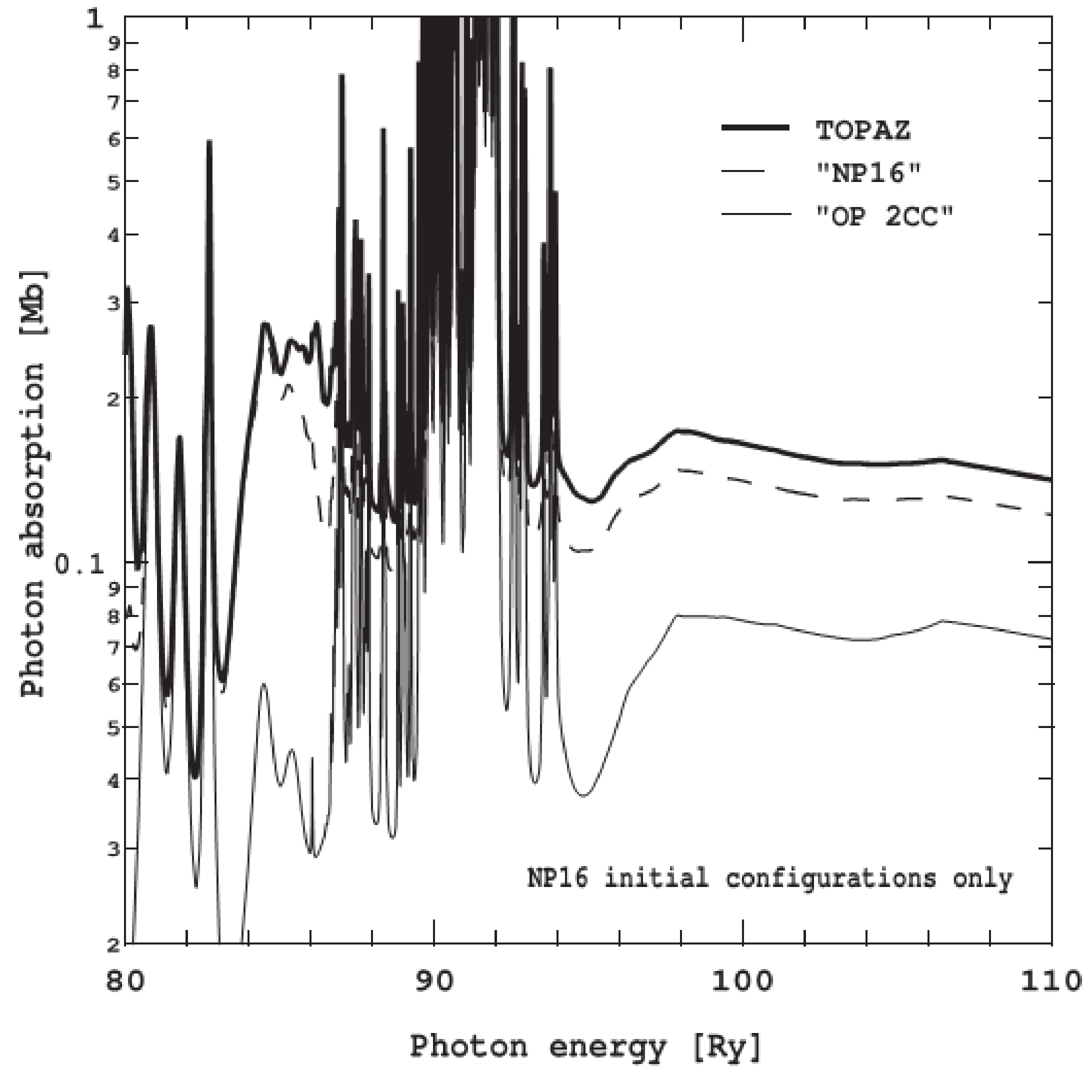

Figure 3. TOPAZ photon absorption at conditions of Figure 1 for the initial configurations included in NP16: total absorption (thick line), with only cross-sections included by NP16 (dash line), and with only cross-sections included in OP 2CC (thin line).