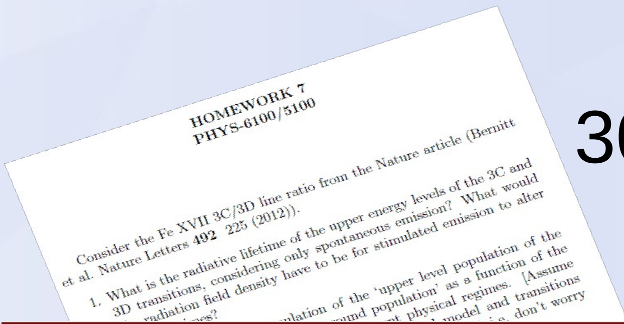
The long-standing discrepancy of Fe XVII spectral emission

S.D. Loch, C.P. Ballance, Ye Li,
C.J. Fontes, and M. Fogle

30th September 2014



HOMEWORK 7
PHYS-6100/5100

Consider the Fe XVII 3C/3D line ratio from the Nature article (Bernitt et al. Nature Letters **492** 225 (2012)).

1. What is the radiative lifetime of the upper energy levels of the 3C and 3D transitions, considering only spontaneous emission? What would the radiation field density have to be for stimulated emission to alter

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NATURE | LETTER

日本語要約

An unexpectedly low oscillator strength as the origin of the Fe XVII emission problem

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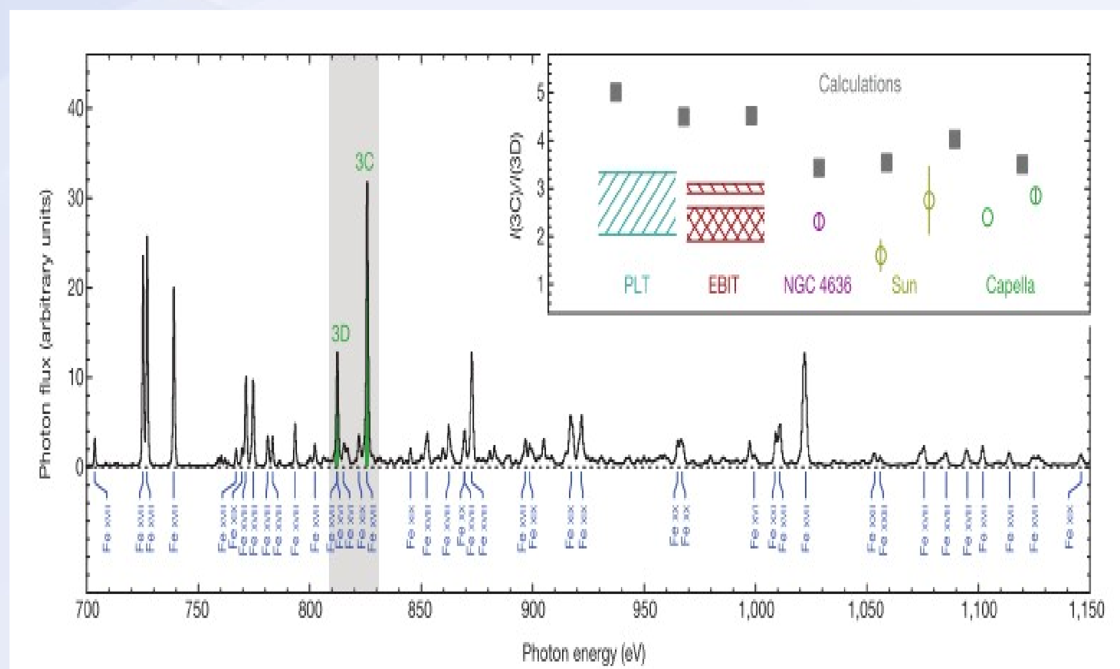
Affiliations | Contributions | Corresponding author

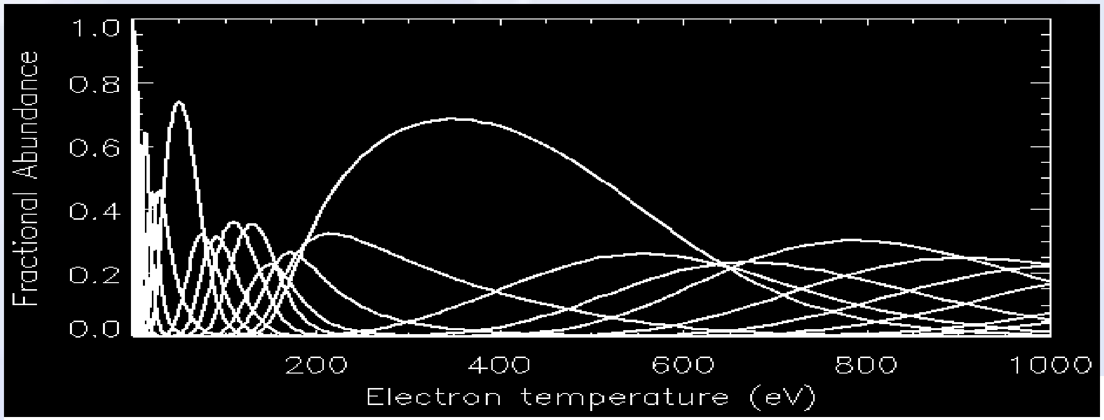
Nature **492**, 225–228 (13 December 2012) | doi:10.1038/nature11627



Outline

- Example of Fe XVII spectral diagnostics
- Very brief history of the discrepancies
- Electron-Beam Ion Trap (EBIT) measurements
- The new X-ray Free Electron Laser (XFEL) experiment
- The resolution to the discrepancy

Fe^{16+} spectral emission



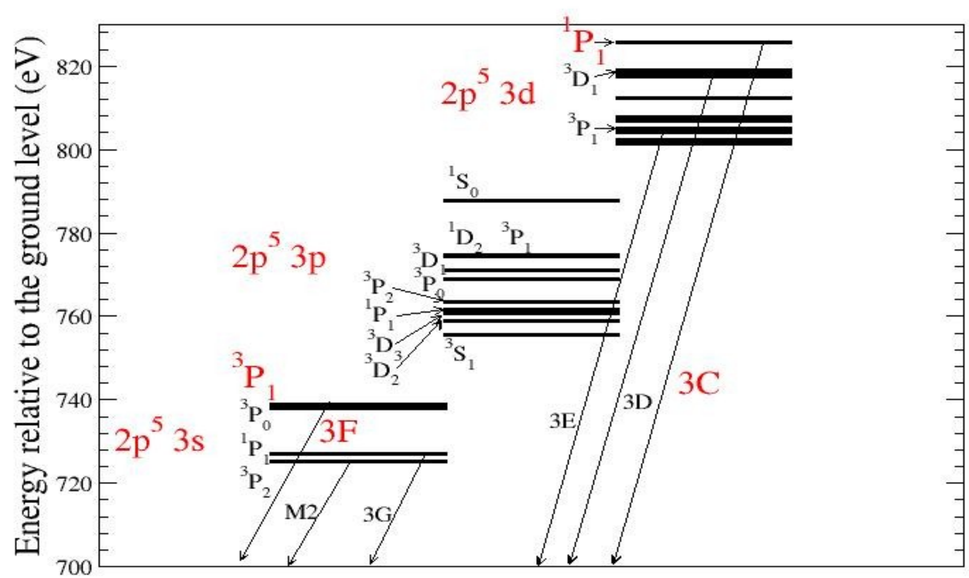
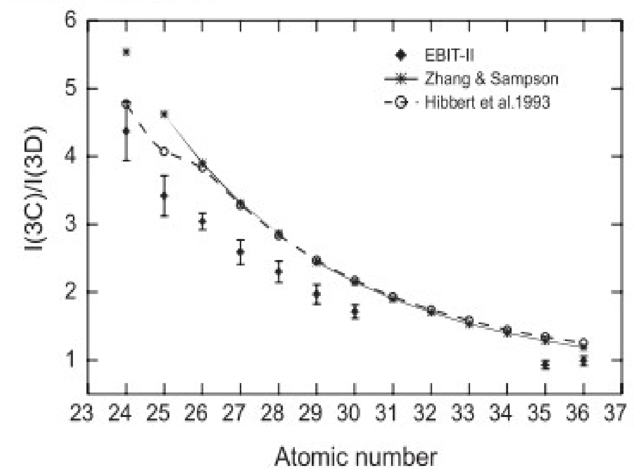


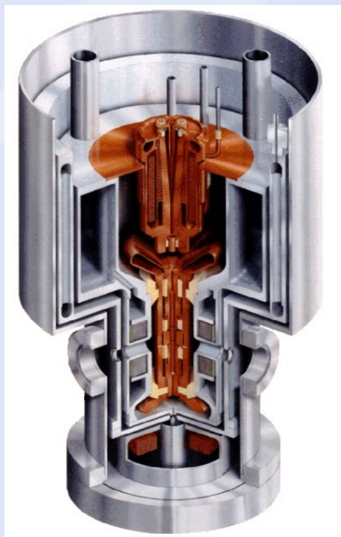
Fig. 5. Comparison of measured and calculated relative intensity R as a function of Z along the neon-like isoelectronic sequence. Measured values, labeled EBIT-II, are compared with calculations of Hibbert et al. [27] and Zhang and Sampson [55]. This figure is adopted from ref. 54.

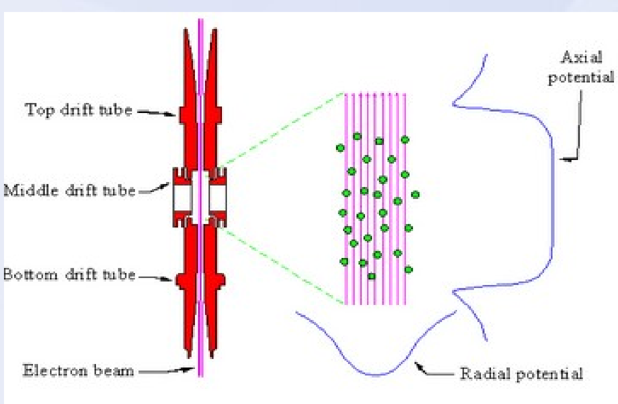


Brown, Can. J. Phys. ***86*** *199 (2008)*

The EBIT measurement

The EBIT experiments trapped Fe^{16+} ions and excited them with an electron-beam.



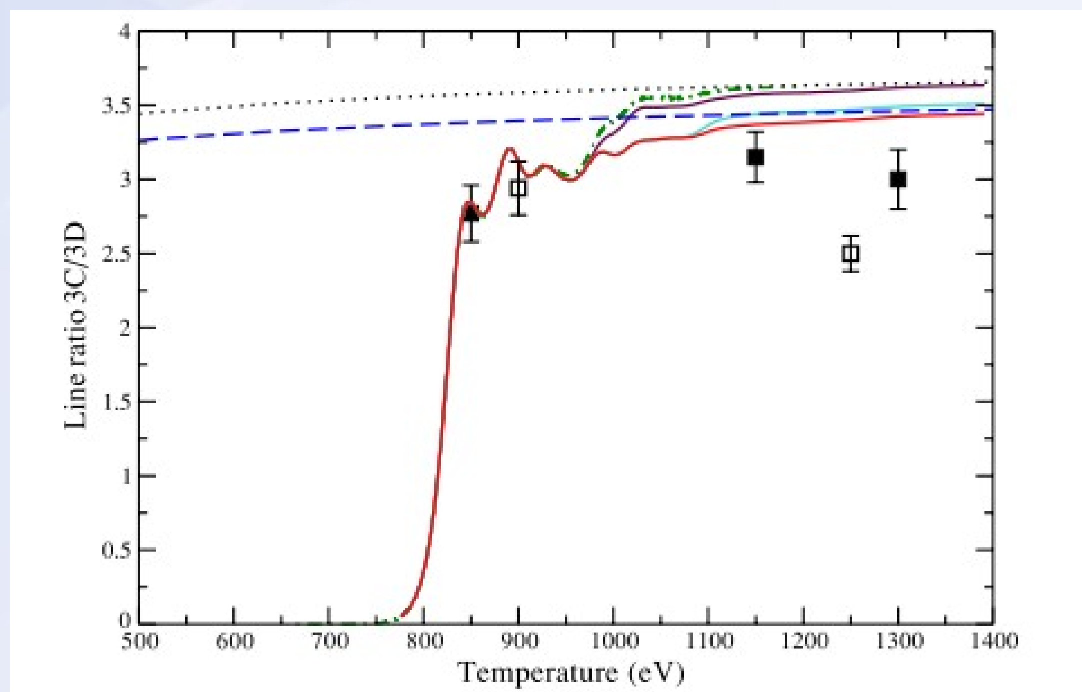


$$\frac{I_{i\to g}}{I_{j\to g}} = \frac{Q_{g\to i}}{Q_{g\to j}} \frac{B_{i\to g}}{B_{j\to g}}.$$

The collisional rate coefficient is given by

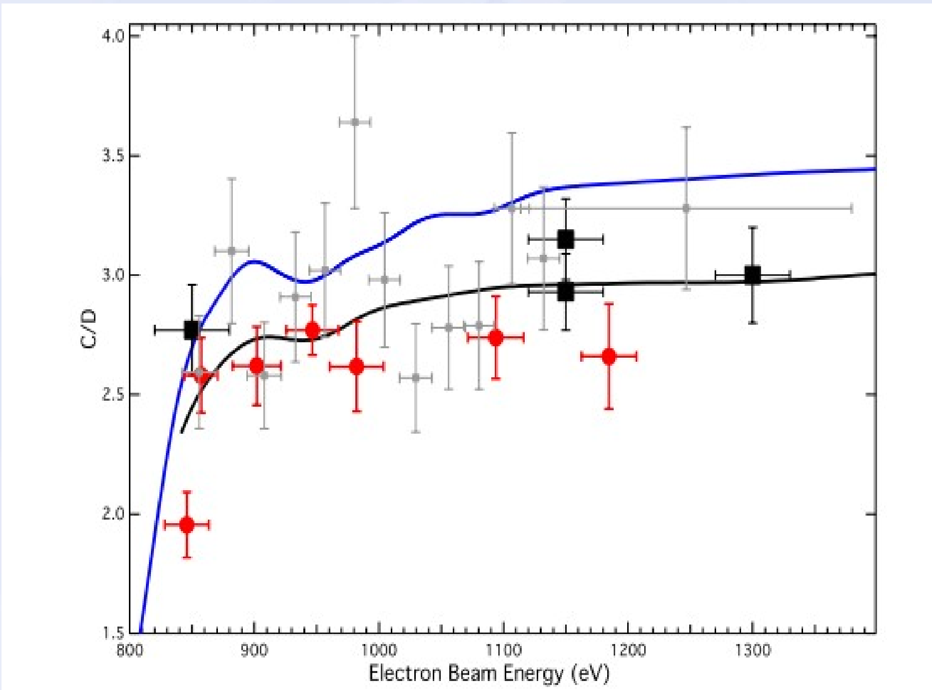
$$Q_{i\to j} = \int_0^\infty \sigma_{i\to j}(E) v f(E)\, \mathrm{d}E,$$

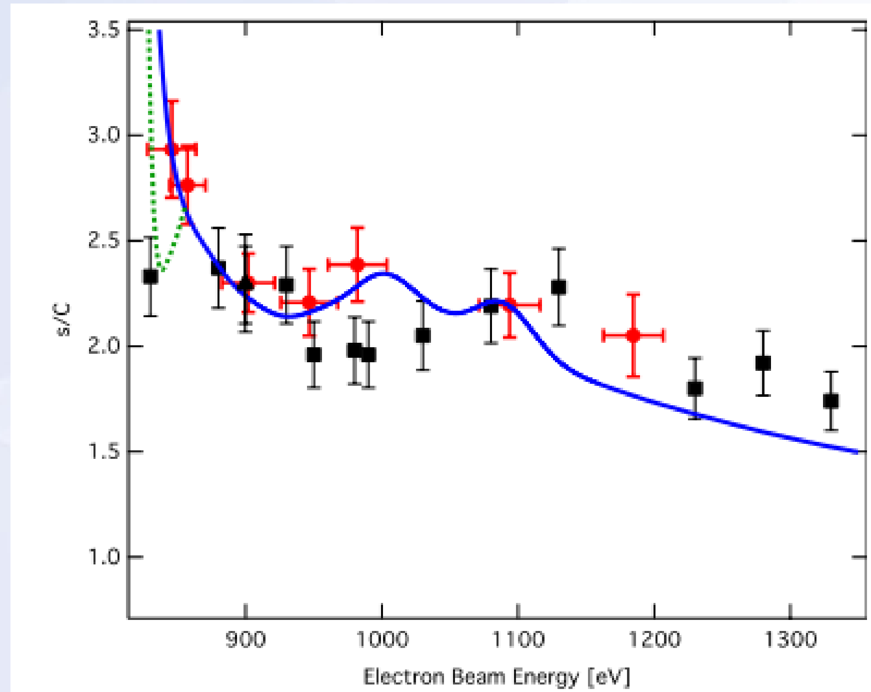
Simple coronal model



*Loch et al. J. Phys. B, **39** : 85 (2006)*

Recent EBIT measurements (NIST)





*Gillaspy et al. ApJ **728** : 132 (2011)*

In modeling these EBIT experiments one needs to include
- Non-Maxwellian electron distribution functions
- Cascades from higher energy levels.
- Resonance contributions to the excitation cross sections.

The many explanations for the discrepancies

Reference	Method or description	Effect or cross section, σ in units of 10^{-20} cm^2	3C $\%\Delta_{E_1}$	3C $\%\Delta_{E_2}$	3D $\%\Delta_{E_1}$	3D $\%\Delta_{E_2}$
2002 [2]	Extensive set of resonances and excitation channels	$\sigma_{E_1}^{3C} = 12.5$, $\sigma_{E_2}^{3C} = 13.3$, $\sigma_{E_1}^{3D} = 3.41$, $\sigma_{E_2}^{3D} = 3.93$	−32	−33	−9	−24
2006 [1]	Measurement	$\sigma_{E_1}^{3C} = 8.49 \pm 1.6$, $\sigma_{E_2}^{3C} = 8.88 \pm 0.93$, $\sigma_{E_1}^{3D} = 3.10 \pm 0.64$, $\sigma_{E_2}^{3D} = 2.98 \pm 0.33$	0	0	0	0
2006 [1]	FAC DW with cascades and RE	3C is essentially unchanged; 3D increases by 17% and 8%.	−33	−32	−26	−32
2006 [3]	*R* matrix with additional cascades	3C decreases by 5%; 3D increases by 11% at 910 eV and remains unchanged at 964 eV.	−28	−27	−20	−25
2007 [4]	Dirac *R* matrix with improved convergence	3C decreases by 12 and 15%; 3D increases by 10% at 910 and remains unchanged at 964 eV.	−20	−17	−19	−24
2008 [5]	RDW with pseudostates	3C decreases by 14 and 19%; 3D decreases by 5 and 17%.	−18	−14	−4	−7
2008 [6]	Recalculates RR cross section onto 3*d* levels.	The measured cross sections normalized to RR onto 3*d* levels increase by 24% and are brought into agreement with [4].	−19	−19	−19	−19
2008 [7]	Recalculates RR cross sections at 964 eV.[a]	The measured cross section decreases by ~6%, on average.	?	6	?	6
2009 [8]	MBPT with improved atomic structure	3C decreases by 9 and 13%; 3D increases by 14% at 910 eV and 2% at 964 eV.	−23	−20	−23	−26
2009 [9]	Calculates the polarization of 3C and 3D to be 20% higher than previous calculations.	Effect not given	?	?	?	?
2010 [10,11]	The polarization calculation of [9] is incorrect; previous calculations are correct.	No effect	...	...	...	...
2011 [12]	States that [7]'s RR onto 3*s* is 35% lower than used in [1]. 3*d* and 3*p* are the same as quoted by [7].	If normalized to 3*s*, cross sections go down by 35%.	54	54	54	54
2012 [13]	Includes PRR.	Raises RR cross sections by 20%.	−17	−17	−17	−17

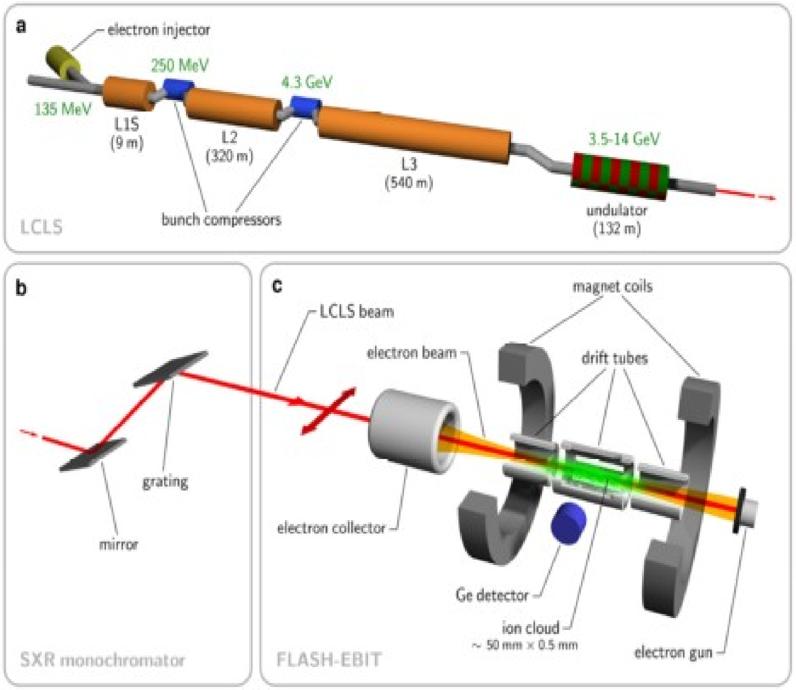
[a]RR cross sections decrease by 5, 6, and 7% for 3*s*, 3*p*, and 3*d*, respectively.

*Taken from Brown and Beiersdorfer, PRL **108** 239302 (2012)*

The big question!

- So what if the atomic physics theoretical calculations are wrong?
  - Perhaps the underlying atomic structure is wrong, leading to inaccuracies in the Fe^{16+} wave functions.
  - If this is the case, then we should be able to see it in the oscillator strength.
  - If the oscillator strength is wrong, it would be an indication that the electron-impact excitation data could also be wrong.
- **So an experiment was designed to <u>measure the oscillator strength ratio for the 3C/3D transitions in Fe XVII</u>.**

The Linear Coherent Light Source (LCLS) + EBIT experiment



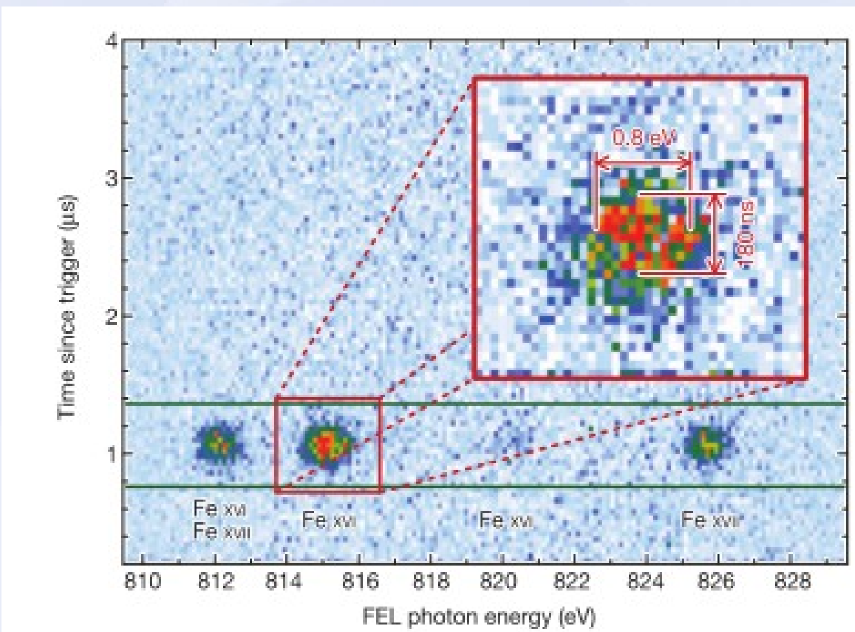
Supplementary Figure S1. Experimental setup. Photons are produced with the Linac Coherent Light Source free-electron laser (a). Electrons are accelerated by the last kilometre of the SLAC 3 km linear accelerator (L1S, L2, L3). Typical electron energies are shown in green. Radiation is generated in an undulator, and the photon energy is selected by a monochromator (b). Ions are produced in the FLASH-EBIT (c) by electron-impact ionization and trapped in a cloud by the electron beam space charge, a strong magnetic field, and an additional electrostatic potential. The FEL photon beam enters the trap and overlaps axially with the ion cloud. Fluorescence is detected with a high-purity Ge detector. A double-ended arrow indicates the plane of FEL polarization. The elements in the figure are not drawn to scale.

*From Bernitt et al. Nature Letts., **492** 225 (2012)*

The idea was as follows:

- Use an XFEL to excite just one transition at a time. So there can be no cascades.
- Remove the free electrons so there can be no collisional-redistribution.
- The measured spectral line 3C/3D ratio should be the ratio of the 3C/3D oscillator strength.

Over many sets of XFEL pulses they gathered the data for an Fe XVII spectrum



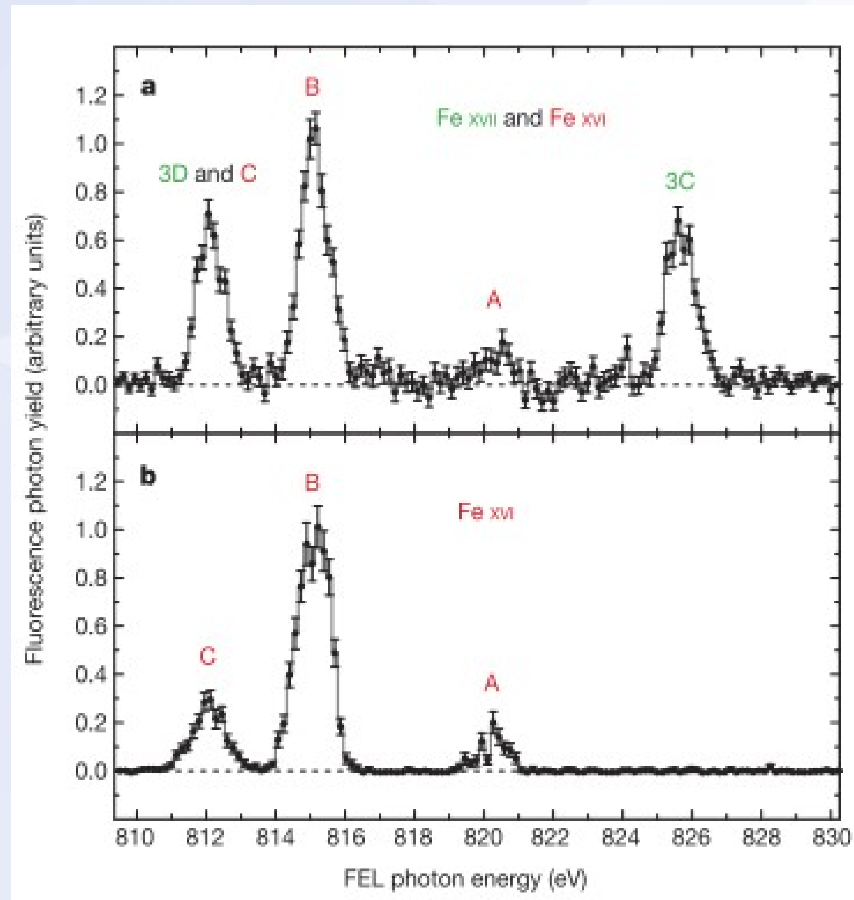


Figure 3 | Measured X-ray fluorescence spectra. **a**, A typical fluorescence

*From Bernitt et al. Nature Letts., **492** 225 (2012)*

The results – very large differences with theory!

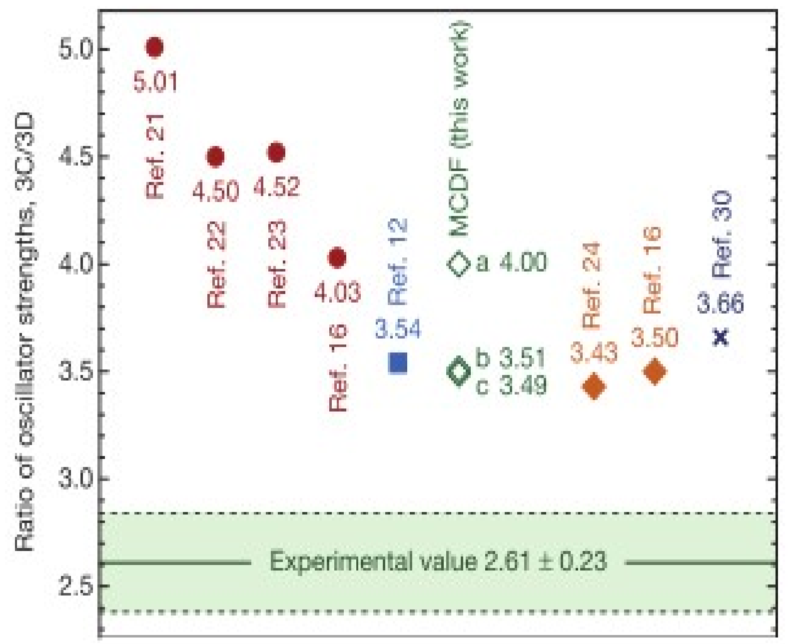
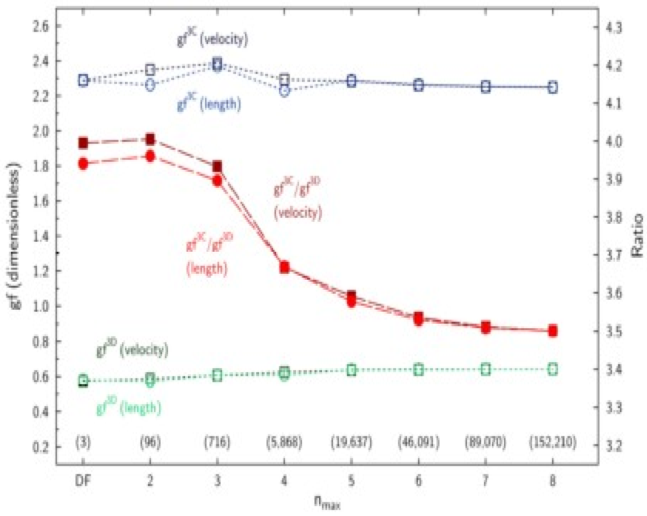


Figure 4 | Predicted and measured intensity ratios of lines 3C and 3D. The



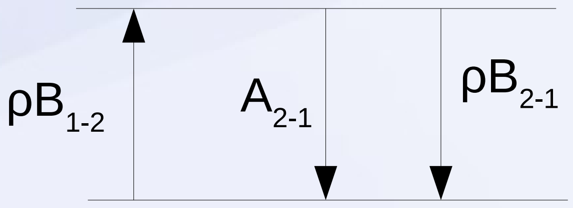
Supplementary Figure S4. MCDF Calculations. Convergence of the calculated weighted oscillator strengths $gf = -g_i f_{i\to l} = -g_e f_{i\to e}$ as function of the maximal principal quantum number n_{max} used in the configuration expansion. The numbers in parentheses indicate the number of *jj*-coupled configurations taken into account in the representation of the excited-state wave function. Results are given in the relativistic length and velocity gauges.

*From Bernitt et al. Nature Letts., **492** 225 (2012)*

Modeling

$$\begin{aligned}\frac{dN_1}{dt} &= -N_1\rho B_{1\to 2} + N_2(A_{2\to 1} + \rho B_{2\to 1})\\ \frac{dN_2}{dt} &= N_1\rho B_{1\to 2} - N_2(A_{2\to 1} + \rho B_{2\to 1})\end{aligned}$$

- Simple two level system.



- The intensity was modeled via

$$\frac{I^{3C}_{i\to 1}}{I^{3D}_{k\to 1}} = \frac{\int\int N_i(x,t)A_{i\to 1}dxdt}{\int\int N_k(x,t)A_{k\to 1}dxdt},$$

- The equilibrium population is
- The line ratio reduces to the ratio of the Einstein A-coefficients

$$N_i = \frac{N_1\rho(\omega_o)B_{1\to i}}{A_{i\to j} + \rho(\omega_o)B_{i\to 1}}$$

$$N_i^{low\,\rho} = \frac{N_1\rho B_{1\to i}}{A_{i\to 1}}.$$

$$N_i^{high\,\rho} = \frac{N_1 B_{1\to i}}{B_{i\to 1}} = N_1$$

Undergraduate Quantum Mechanics II Spring 2014: the homework assignment!

HOMEWORK 7
PHYS-6100/5100

Consider the Fe XVII 3C/3D line ratio from the Nature article (Bernitt et al. Nature Letters **492** 225 (2012)).

1. What is the radiative lifetime of the upper energy levels of the 3C and 3D transitions, considering only spontaneous emission? What would the radiation field density have to be for stimulated emission to alter these lifetimes?
2. Make a plot of the population of the 'upper level population of the 3C transition divided by the ground population' as a function of the radiation density. Describe the different physical regimes. [Assume the populations are described by the coronal model and transitions only happen between the ground and the upper level, i.e. don't worry about radiative branching]
3. Explore whether the addition of stimulated emission in the population modeling for this laser-excited plasma can alter the line ratio from the oscillator strength ratio that the article assumes.

Timescales and radiation field densities

- The XFEL laser pulse conditions:
  - durations of 200-500 fs, lifetimes of the levels are 3C ~45 fs, 3D ~ 163 fs. So it isn't safe to assume quasi-static equilibrium.
  - We estimate a range of radiation field densities of ρ=2.6 – 6.6 x 10^{-6} J/m^3/Hz.
- There will be significant emission once the pulse has left the plasma, the emission in each spectral line should be
- We evaluation N_2 using the time-dependent collisional-radiative equations.

$$\frac{N_{2\rightarrow 1}^{photons}}{\Delta V} = \int_0^{t_{pulse}} N_2(t) A_{2\rightarrow 1} dt + N_2(t_{pulse})$$

Emission during the pulse interaction with the plasma volume

Emission from the volume after the pulse has left.

Results : excited populations

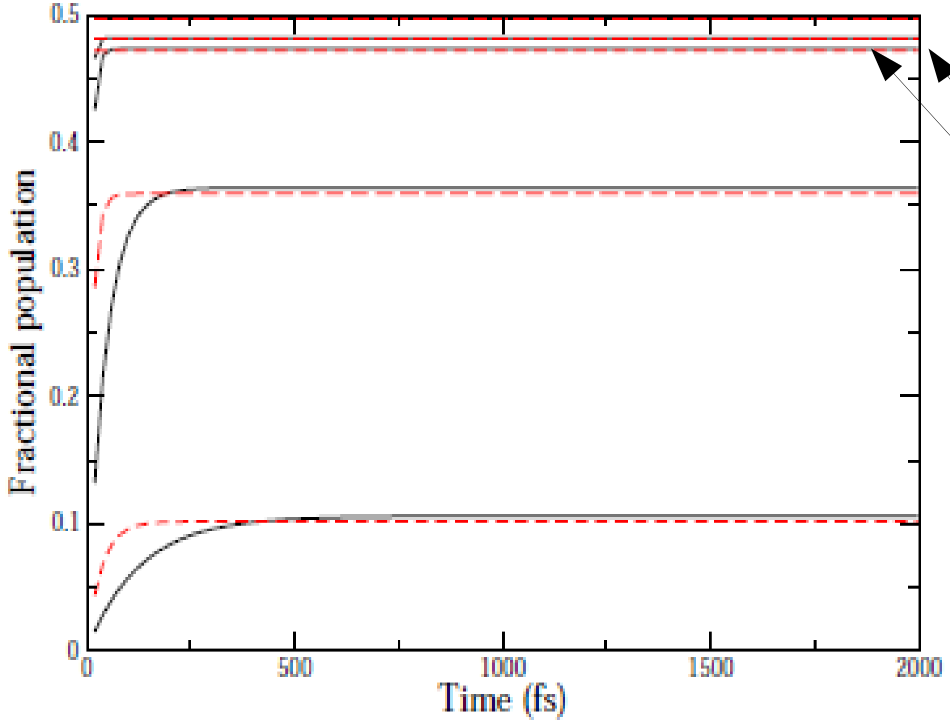


Fig. 1.— Fractional population in the excited state as a function of time, i.e., N_2/N_{tot}: results for the 3D transition (solid line) and the 3C transition (dashed line). Reading from the lowest to the highest set of lines the results are for: $\rho=1\times10^{-7}$, 1×10^{-6}, 6.6×10^{-6}, 1×10^{-5}, and 1×10^{-4} $J/m^3/Hz$.

- It seems likely that the populations are close to the limit of the high radiation field density for the majority of the pulse interaction with the plasma.
- Remember, we estimate ρ=2.6 – 6.6 x 10^{-6} J/m^3/Hz
- Note that the at high rho, the line ratio reduces to a simple function of A-values and pulse duration.

$$
\begin{aligned}
\frac{I^{3C}_{i\to1}}{I^{3D}_{k\to1}} &= \frac{\int_0^{t_{pulse}} N_i(t)A^{3C}_{i\to1}dt + N_i(t_{pulse})}{\int_0^{t_{pulse}} N_k(t)A^{3D}_{k\to1}dt + N_k(t_{pulse})} \\
&= \frac{N_i^{high\,\rho}A^{3C}_{i\to1}t_{pulse} + N_i^{high\,\rho}}{N_k^{high\,\rho}A^{3D}_{k\to1}t_{pulse} + N_k^{high\,\rho}} \\
&= \frac{A^{3C}_{i\to1}t_{pulse} + 1}{A^{3D}_{k\to1}t_{pulse} + 1}.
\end{aligned}
$$

Results : excited populations

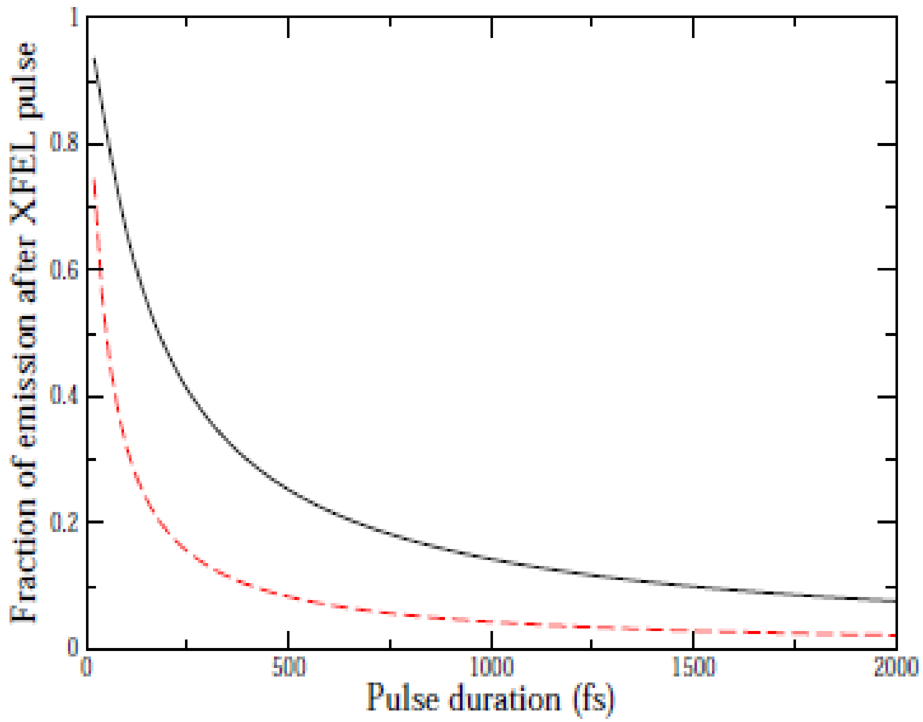


Fig. 2.— The fraction of the emission coming after the XFEL pulse has left the plasma volume, as a function of pulse duration and for $\rho = 4.6 \times 10^{-6}$ J/m^3/Hz: 3D (solid line) and the 3C (dashed line).

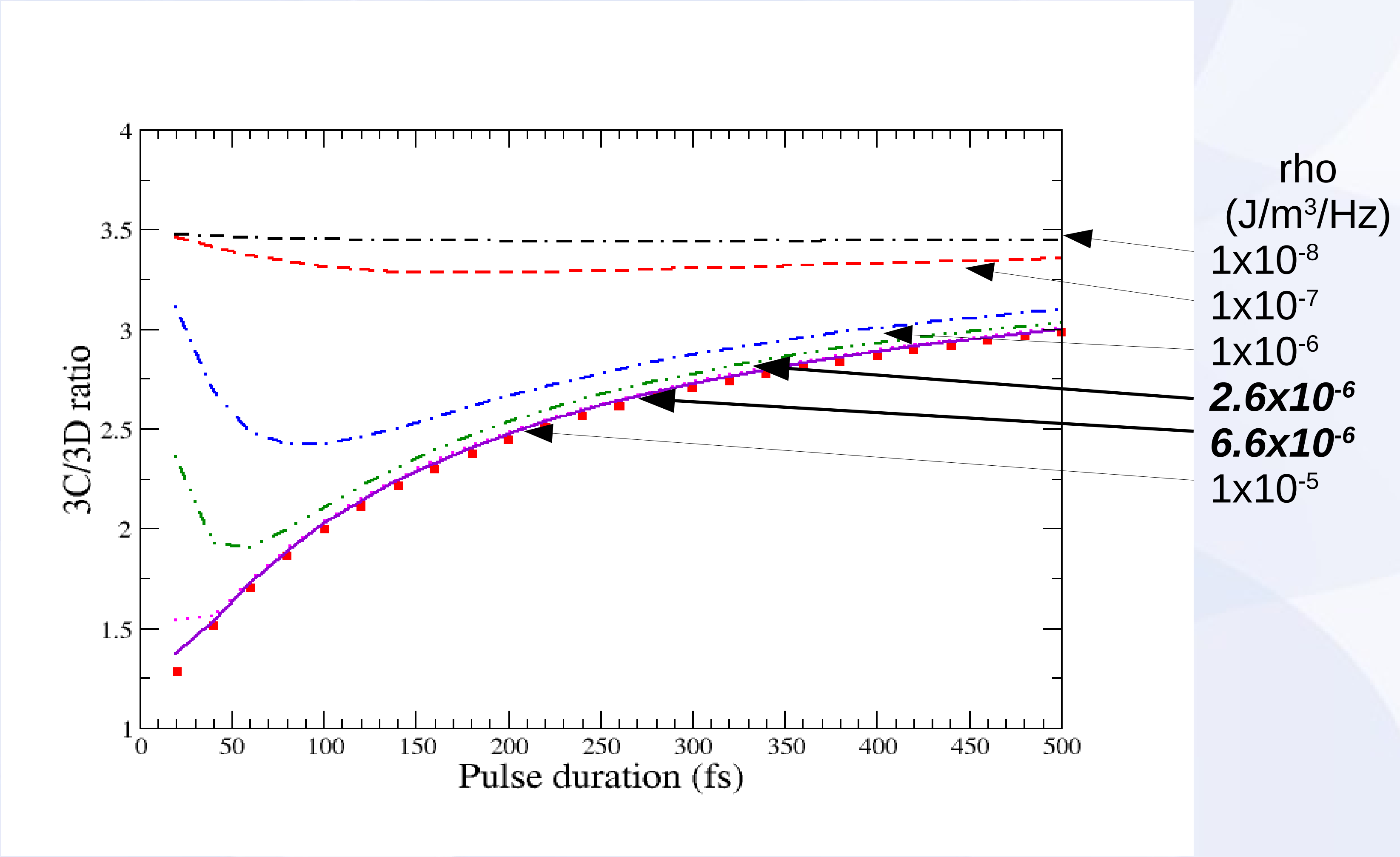
- It seems likely that the populations are close to the limit of the high radiation field density for the majority of the pulse interaction with the plasma.
- Remember, we estimate ρ=2.6 – 6.6 x 10^{-6} J/m^3/Hz
- Note that the at high rho, the line ratio reduces to a simple function of A-values and pulse duration.

$$\frac{I^{3C}_{i\to 1}}{I^{3D}_{k\to 1}} = \frac{\int_0^{t_{pulse}} N_i(t) A^{3C}_{i\to 1} dt + N_i(t_{pulse})}{\int_0^{t_{pulse}} N_k(t) A^{3D}_{k\to 1} dt + N_k(t_{pulse})}$$

$$= \frac{N_i^{high\,\rho} A^{3C}_{i\to 1} t_{pulse} + N_i^{high\,\rho}}{N_k^{high\,\rho} A^{3D}_{k\to 1} t_{pulse} + N_k^{high\,\rho}}$$

$$= \frac{A^{3C}_{i\to 1} t_{pulse} + 1}{A^{3D}_{k\to 1} t_{pulse} + 1}.$$

Results: the line ratio



Results: Stochastic pulses

- In the experiment, the radiation field density is not homogeneous in time.
- It is a stochastic set of 1-2 fs spikes, with 1-2 fs gaps.
- So we generated our own set of stochastic field densities.

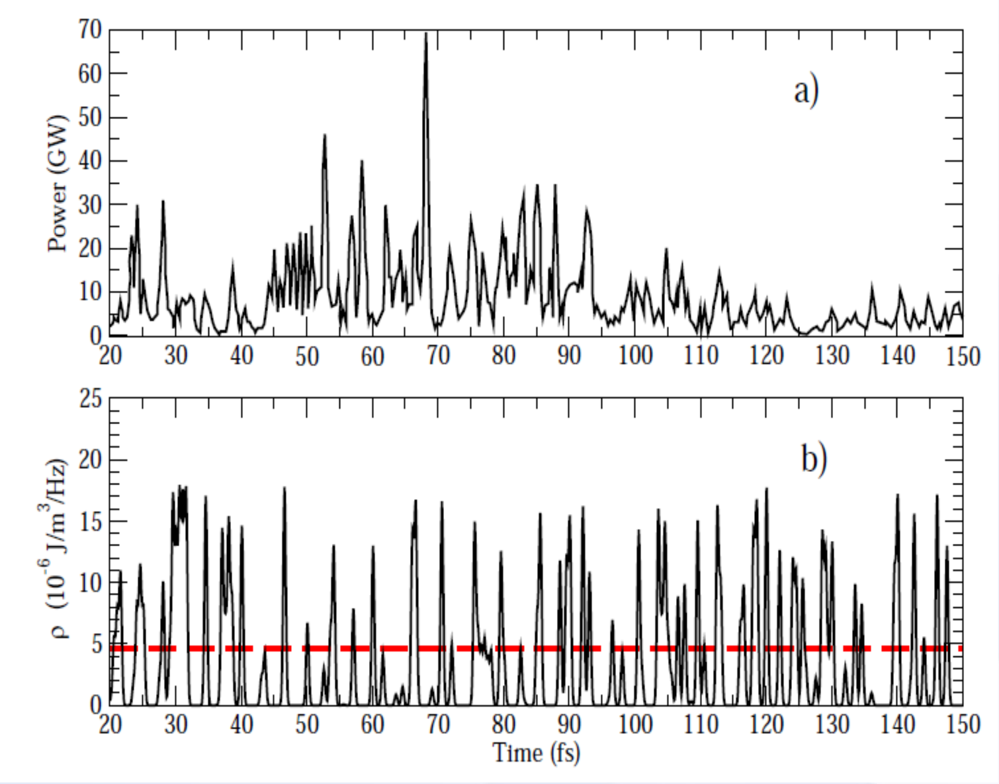
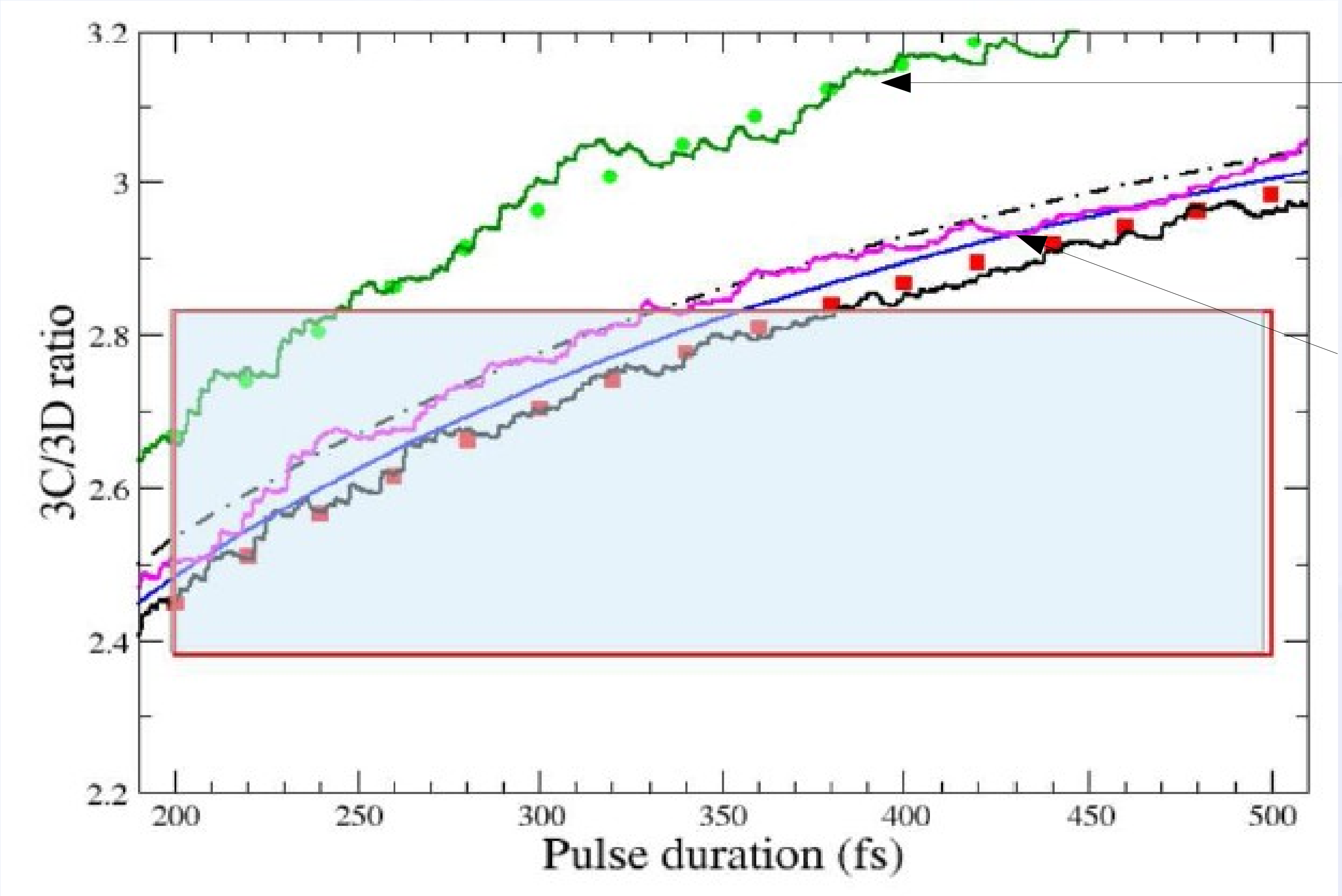


Fig. 4.— *Figure a) shows a typical experimentally measured XFEL profile for an 800 eV pulse. Figure b) shows one of our simulated stochastic pulses as a function of time for an average ρ of 4.6×10^{-6} J/m^3/Hz. The dashed line shows a homogeneous ρ of 4.6×10^{-6} J/m^3/Hz. The stochastic pattern continues for the duration of the pulse.*

Comparison with experiment

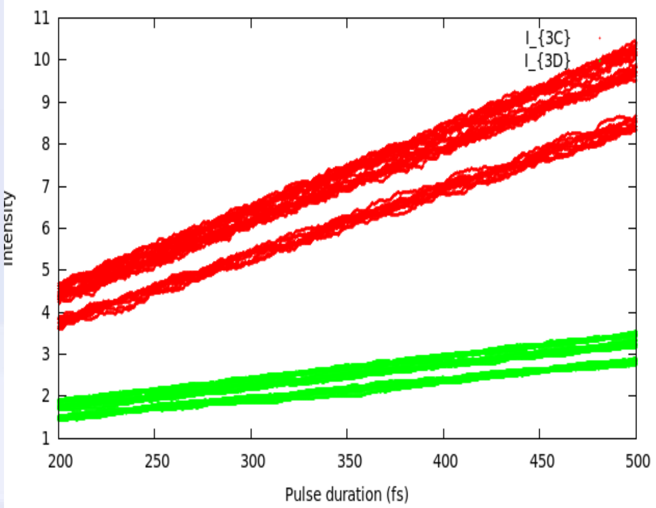


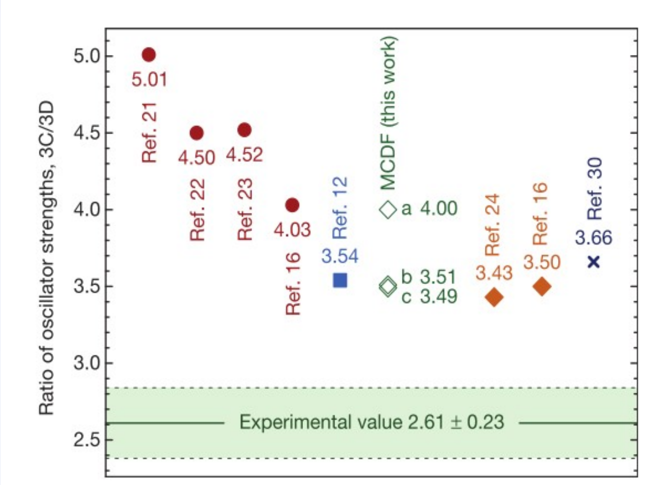
Results using an f-ratio of 3.9

Results using an f-ratio of 3.5

The final values

- One last thing: The experiment does necessarily have the same pulse duration that excited the 3C and the 3D. The previous plot assumes that it does.
- So really we should perform a large number of simulations for a given rho, storing the average I_{3C}, I_{3D}, along with their standard deviations.
- **We did this and get a final value for the experiment of 2.8 ± 0.12**
- **This compares with an experimental ratio of 2.61 ± 0.23.**





Conclusions

- It appears that time-dependent effects are causing the LCLS measurements to become lower than the oscillator strength ratio.
- Once the experimental parameters are accounted for, an oscillator strength ratio of 3.5 produced good agreement with the measurements.
- Note that this is consistent with the largest atomic structure calculations, but does imply that a further look at the collision cross sections should be undertaken.