

DE LA RECHERCHE À L'INDUSTRIE



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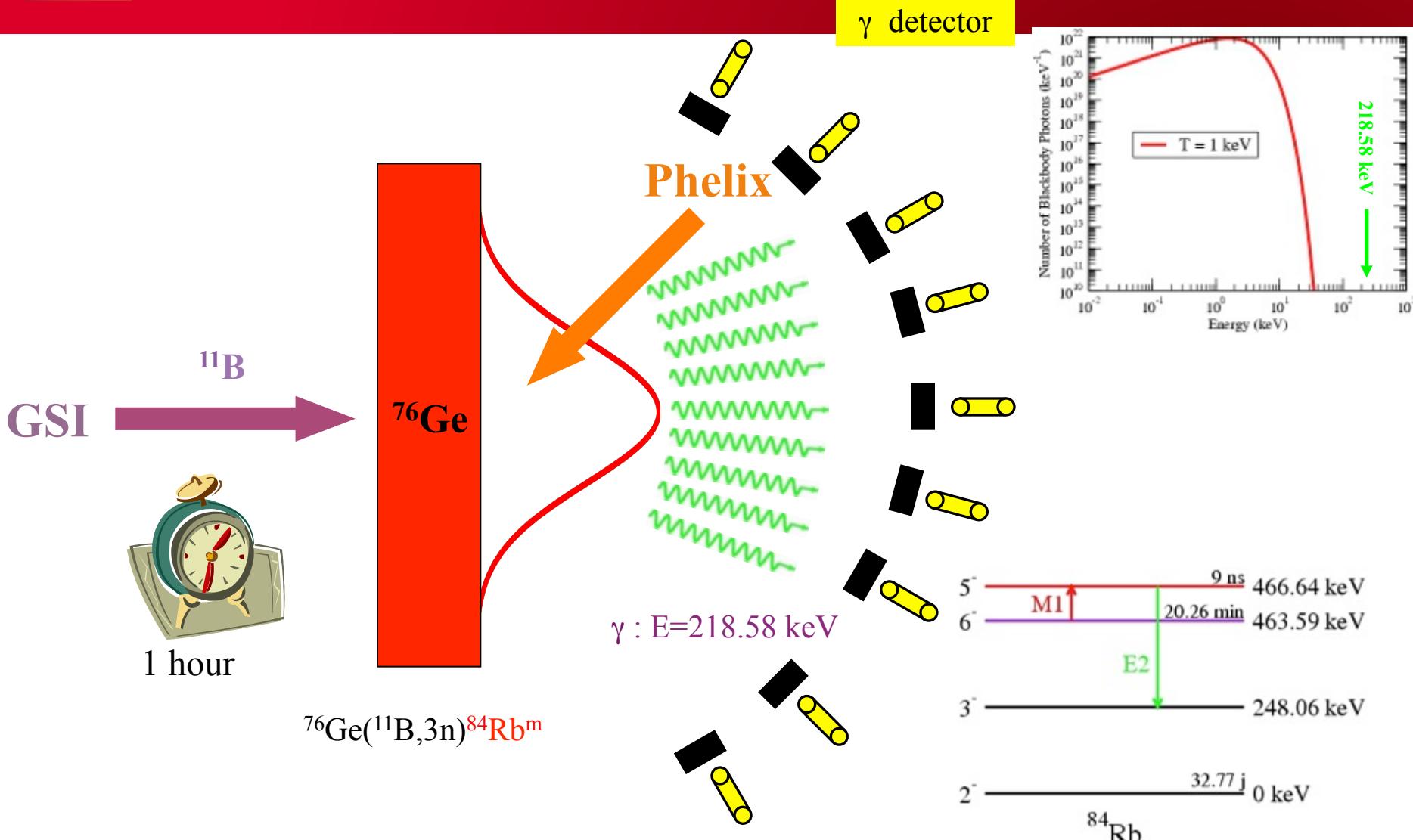
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Indirect Deexcitation Of ^{84}Rb in a Plasma Created at PHELIX

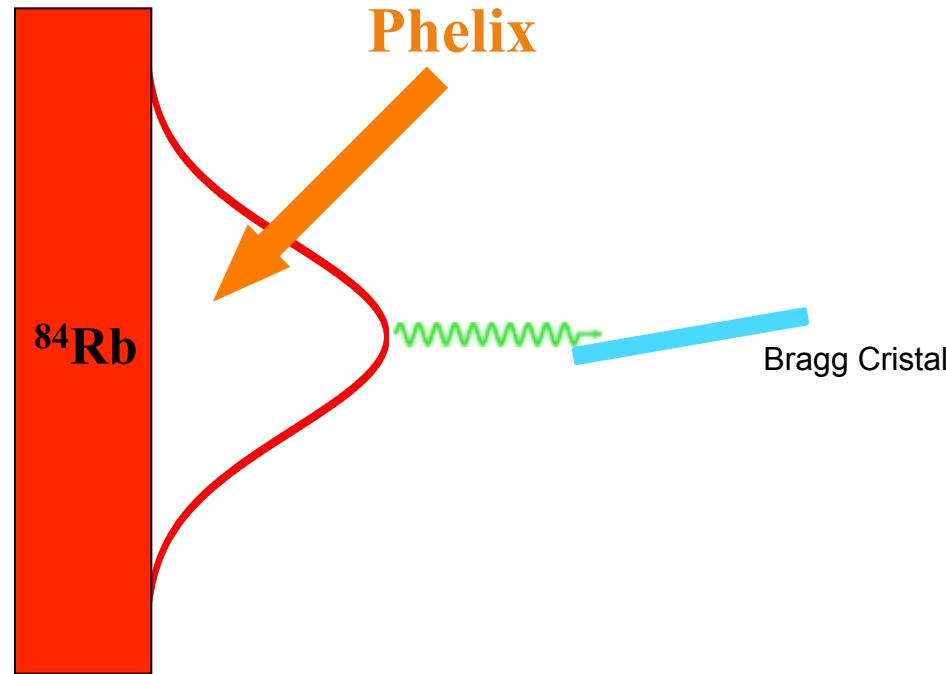
The Final Experiment ?



CEA-CENBG-GSI Collaboration

Gilbert GOSSELIN San Francisco 2014

The Preliminary Experiment



CEA-CENBG-GSI Collaboration

Spectrum Evaluation

■ NEET Evaluation

- Nuclear Transition Energy : 3.05 keV now 3.50 keV
- Requires precise knowledge of atomic transition energy

■ MCDF (Multi-Configuration Dirac-Fock)

- Hamiltonian diagonalization for each J
- Precise atomic energies $\frac{\Delta E}{E} \approx 10^{-3}$
- Very Long Calculation Times
- Not the best way to get a spectrum
- Is probably best to get line energies for NEET calculations

Spectrum Evaluation

■ Spectrum

$$S(E) = \sum_Q P_Q \sum_i P_i \frac{\Gamma}{(E - \Delta E_i)^2 + \frac{\Gamma^2}{4}}$$

■ Configuration Probability : Grand Canonical Partition Function

$$P_Q P_i = \frac{(2j_i + 1)e^{-\frac{E_i}{kT} - Q\eta}}{\sum_k (2j_k + 1)e^{-\frac{E_k}{kT} - Q\eta}}$$

η : reduced chemical potential

Configuration Interaction

Configuration Interaction (CI)	With	Without
Definition	(n,l) (not j) $(1s)^2 (2s)^1 (4p)^1 \rightarrow (1s)^2 (2s)^2$	(n,l,j) $(1s_{1/2})^2 (2s_{1/2})^1 (4p_{3/2})^1 \rightarrow (1s_{1/2})^2 (2s_{1/2})^2$
Calculation Time	Long (very long...)	Long (much less so...)
Configuration Number	Not so Huge	Huge
Precision	Even Better	Quite Good

Spectrum Evaluation

■ Configuration Numbers

- Electrons from n=1 to n=6
- Transitions : n=3,4,5,6 → n=2
- Initial Configurations : 1s filled

Charge State	With CI	Without CI
	(All Transitions)	(3s _{1/2} to 2p _{1/2} only)
34+	19	1
33+	Configuration Selection is mandatory	
32+		559
31+		6,741
30+	32,699	57,520
29+	127,956	418,359
28+	444,310	2,591,331
27+	1,395,835	14,049,302
26+	4,026,185	68,016,688

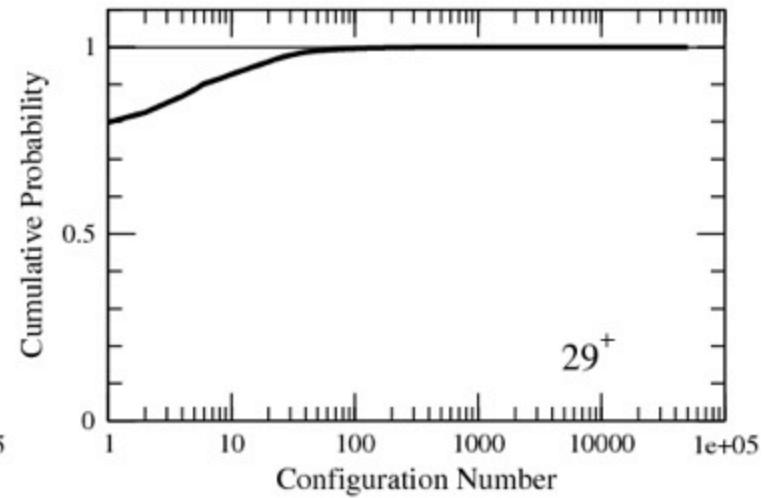
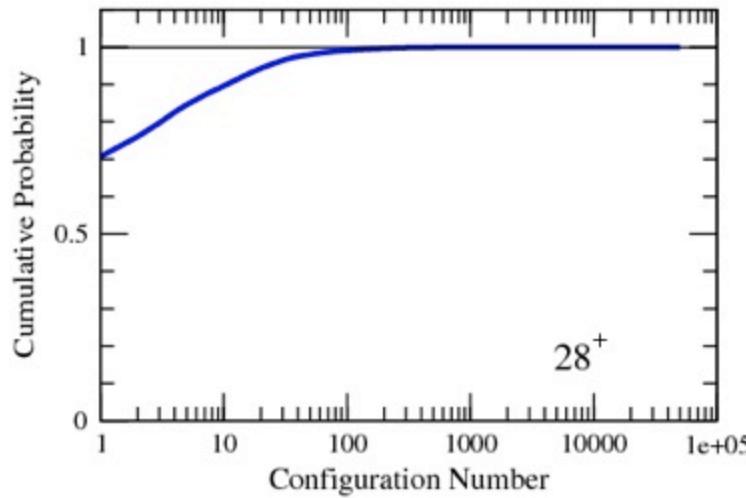
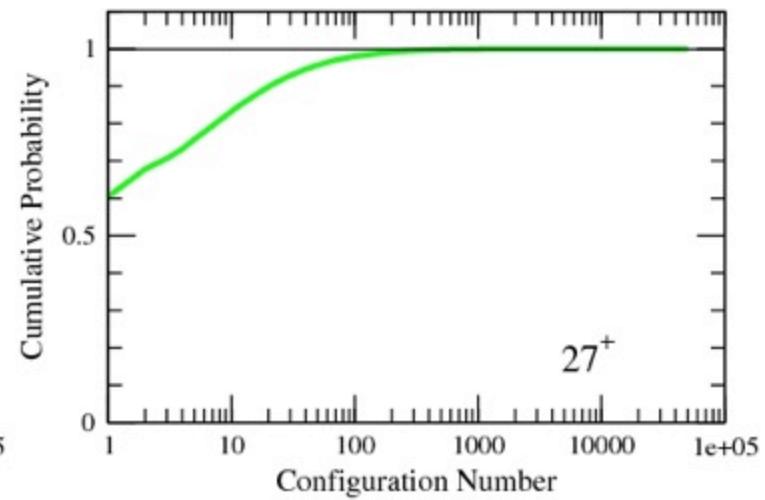
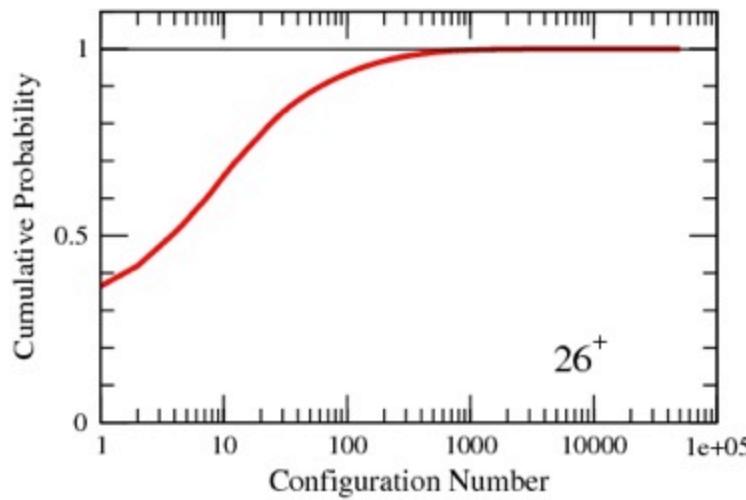
Configuration Selection

- Goal : Eliminate the less probable configurations
 - Problem : Partition function cannot be evaluated yet
 - Configurations probabilities are unknown
 - Configuration probability estimation: Bernoulli
 - Sub-shells occupation from average atom model
 - Configurations are ordered by decreasing probability
$$P_i \approx \prod_k C_{D_k}^{n_k} (p_k)^{n_k} (1 - p_k)^{D_k - n_k}$$
 - Configurations selection under cumulated $P_{\text{threshold}}$

$$\sum_{k=1}^{N_{\text{sel}}} P_k \geq P_{\text{threshold}}$$

Configuration Selection

$$T_e = 270 \text{ eV}$$



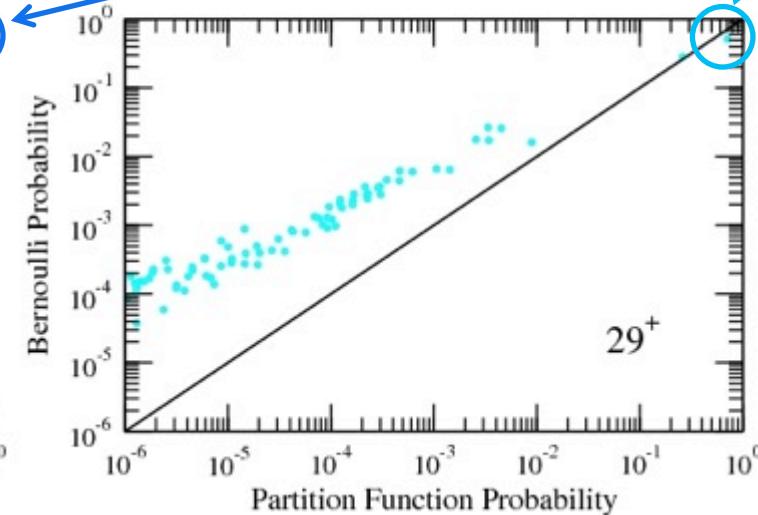
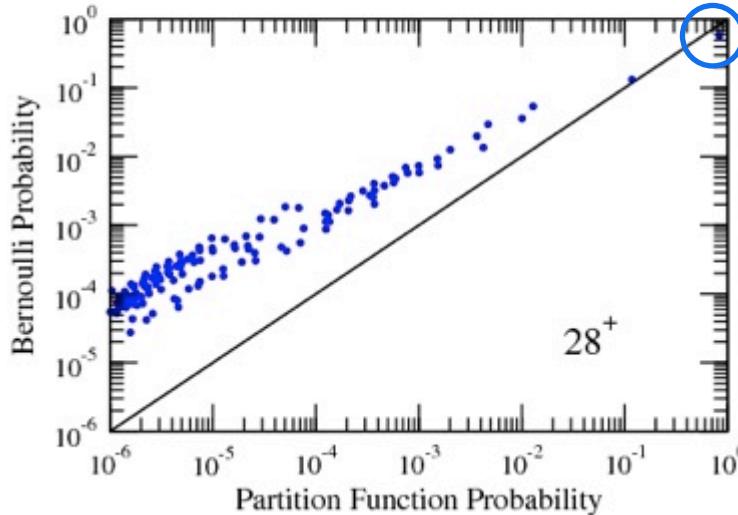
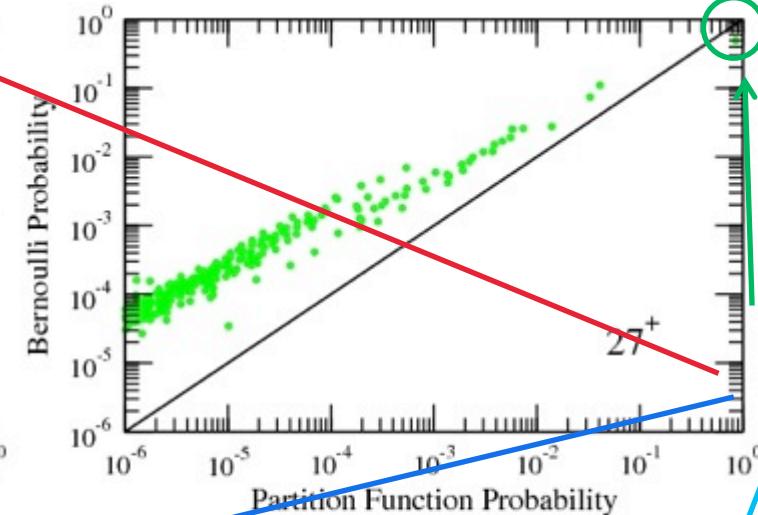
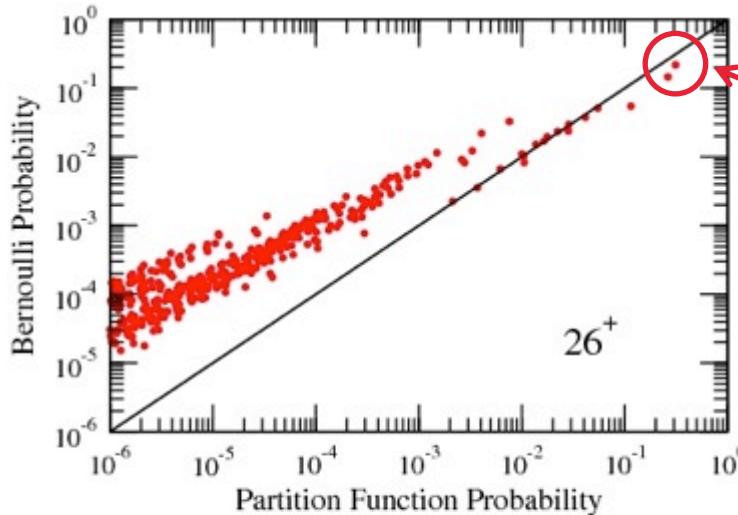
Configuration Selection

■ Configuration Numbers

■ Initial Configurations : 1s full, electrons from n=1 to n=6

Charge State	With CI		Without CI	
	(All Transitions)		(3s _{1/2} to 2p _{1/2} only)	
	Total	Selected (99,9 %)	Total	Selected (99 %)
34+	19	19	1	1
33+	190	180	33	3
32+	1,325	397	559	5
31+	7,220	869	6,741	6
30+	32,699	1,529	57,520	12
29+	127,956	1,956	418,359	19
28+	444,310	1,704	2,591,331	30
27+	1,395,835	2,821	14,049,302	37
26+	4,026,185	5,225	68,016,688	87

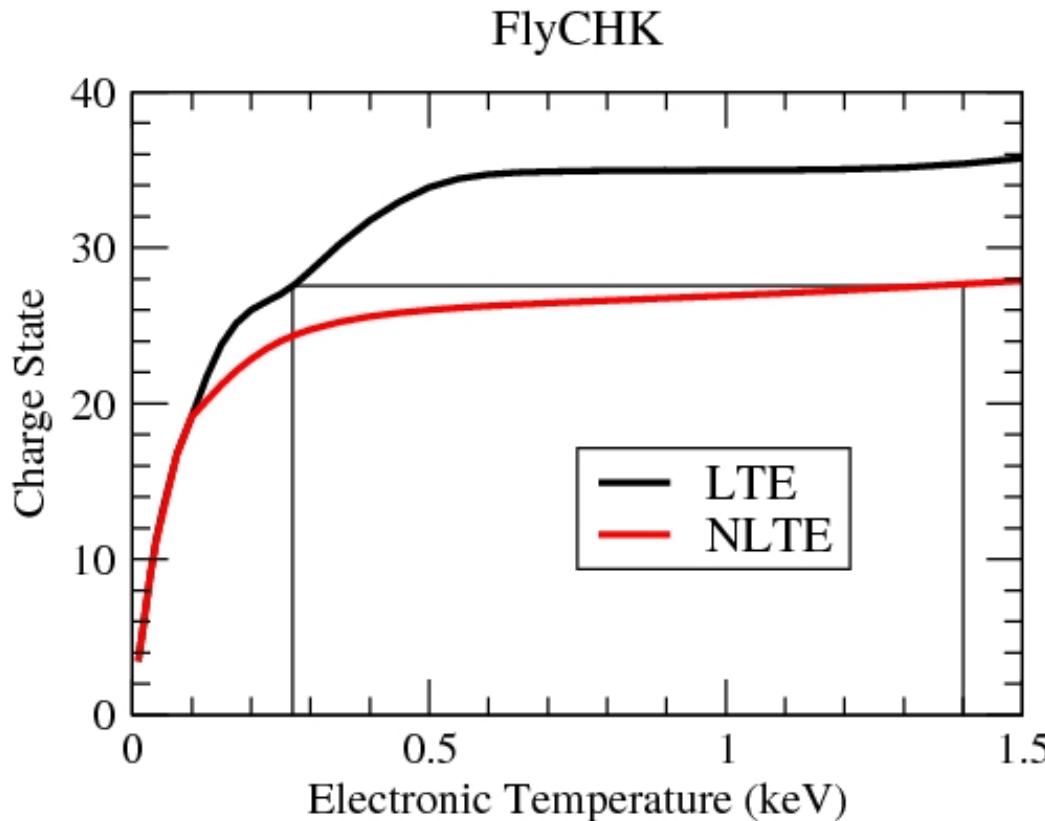
Bernoulli vs Partition Function



$T_e = 270 \text{ eV}$

Fondamental Configurations

Charge States under Non LTE Conditions



$$T_z = 270 \text{ eV}$$

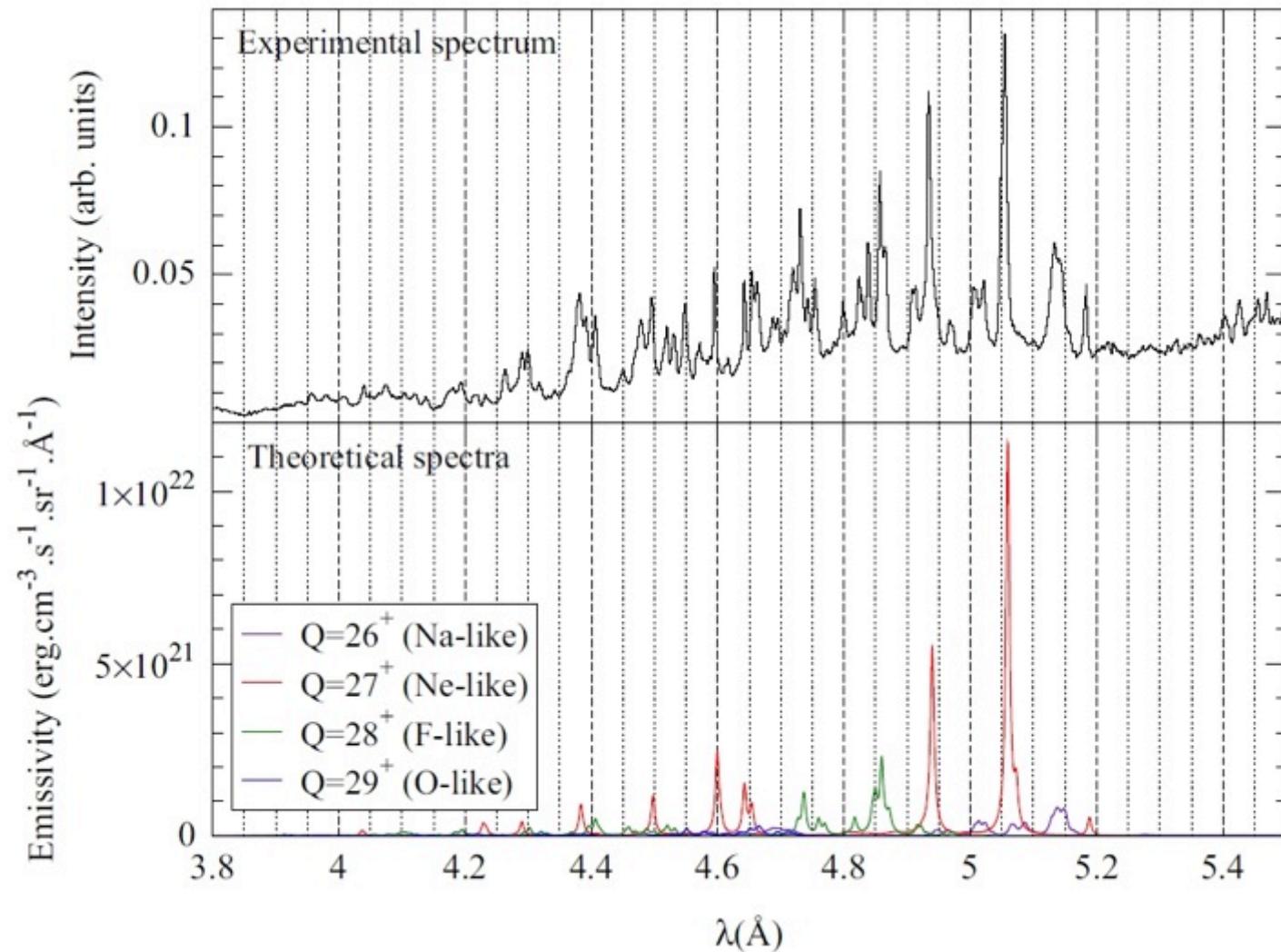
$$T_{\text{HETL}} = 1.4 \text{ keV}$$

Ionic Fraction

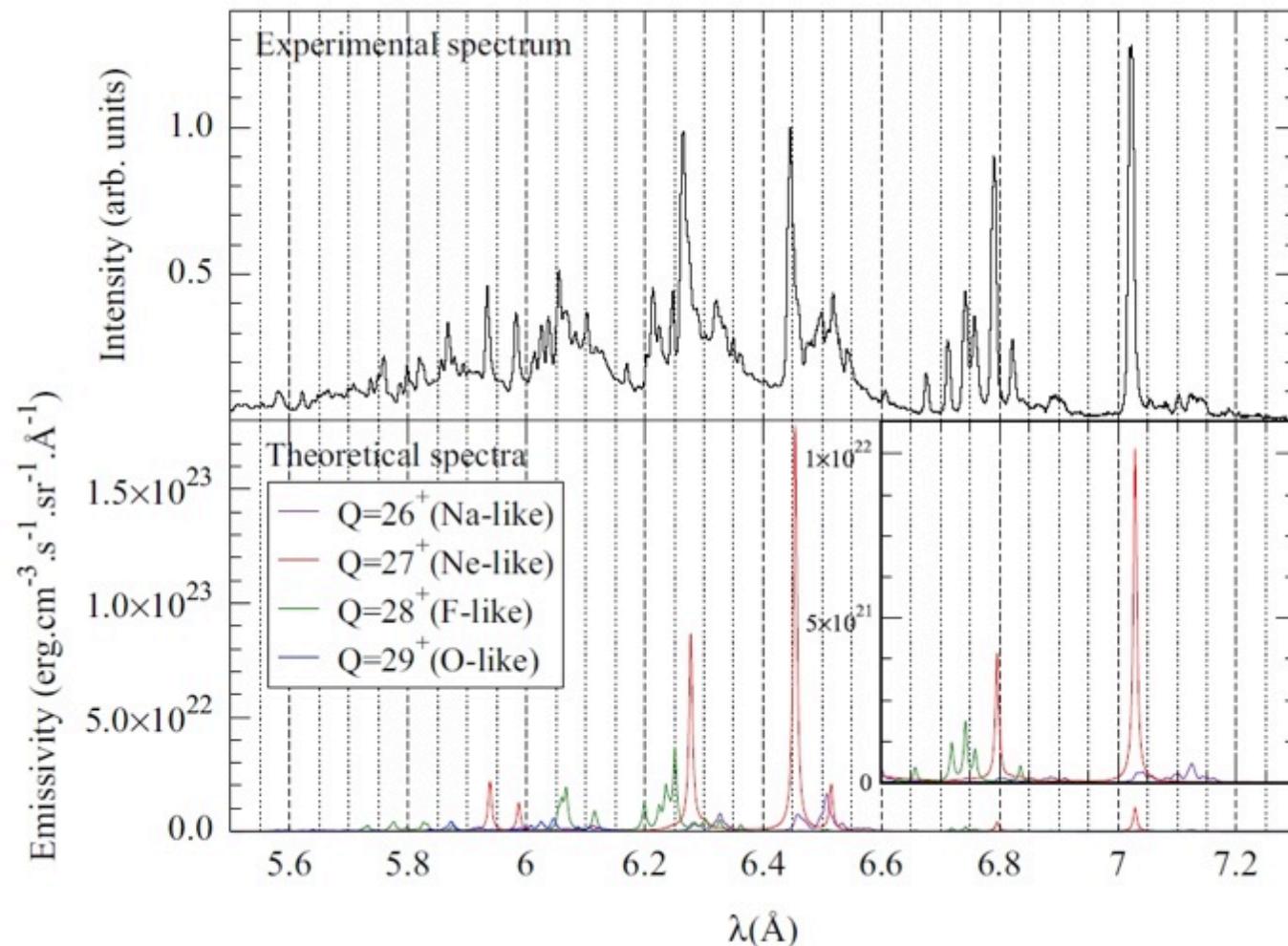
Q	P_Q
26 ⁺	8.48 %
27 ⁺	39.5 %
28 ⁺	39.1 %
29 ⁺	11.0 %
30 ⁺	1.05 %

From AVERROES & FlyCHK

Experimental Spectrum vs MCDF Spectrum (no CI)



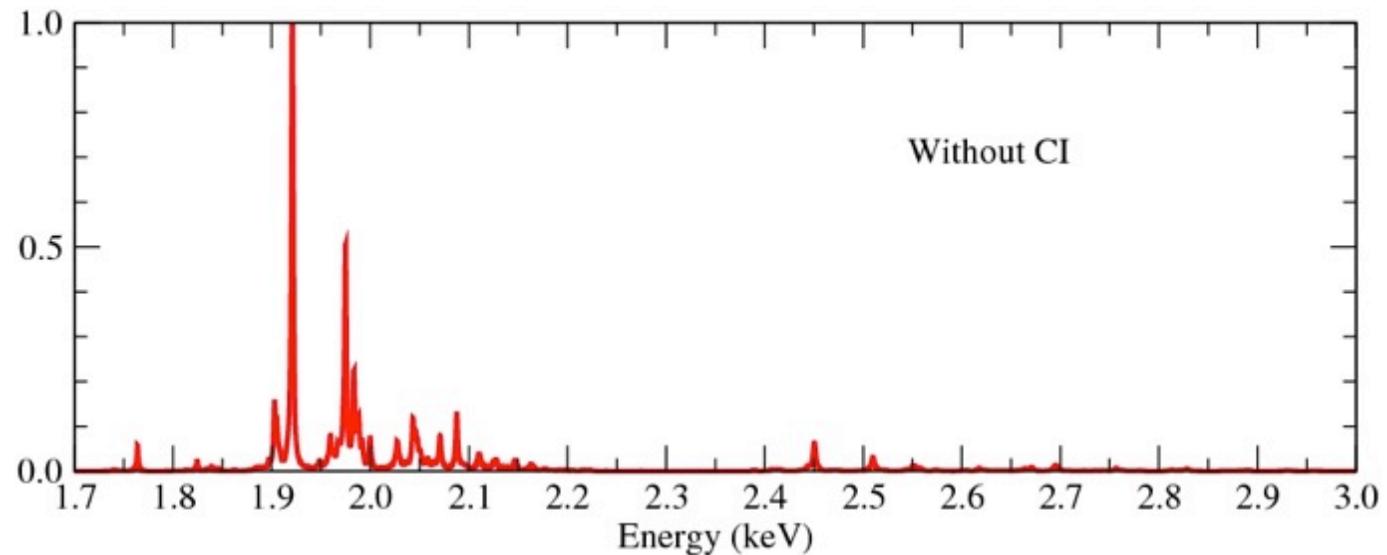
Experimental Spectrum vs MCDF Spectrum (no CI)



Spectrum Analysis

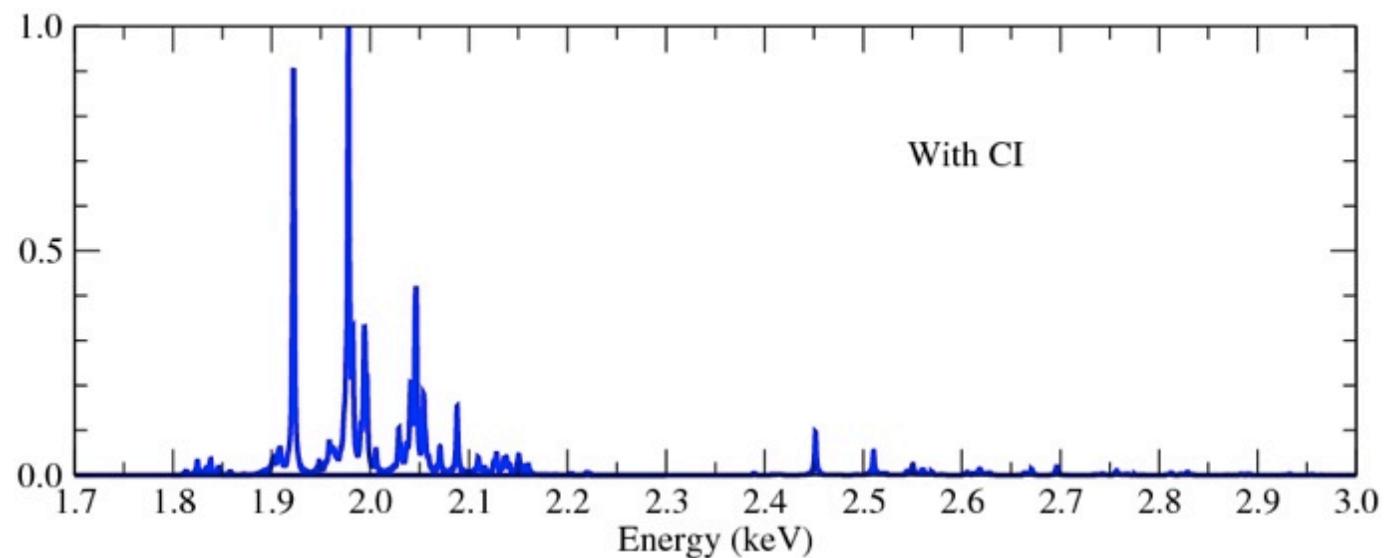
- Most lines have been identified
 - Energy, initial configuration, angular momentum
 - More than 50 new lines previously unidentified
- Charge states distribution
 - Ionization temperature model is fine
- Line intensities are globally good within a factor of 2 or 3
 - Exception around 7 Å

Spectrum with CI vs without CI



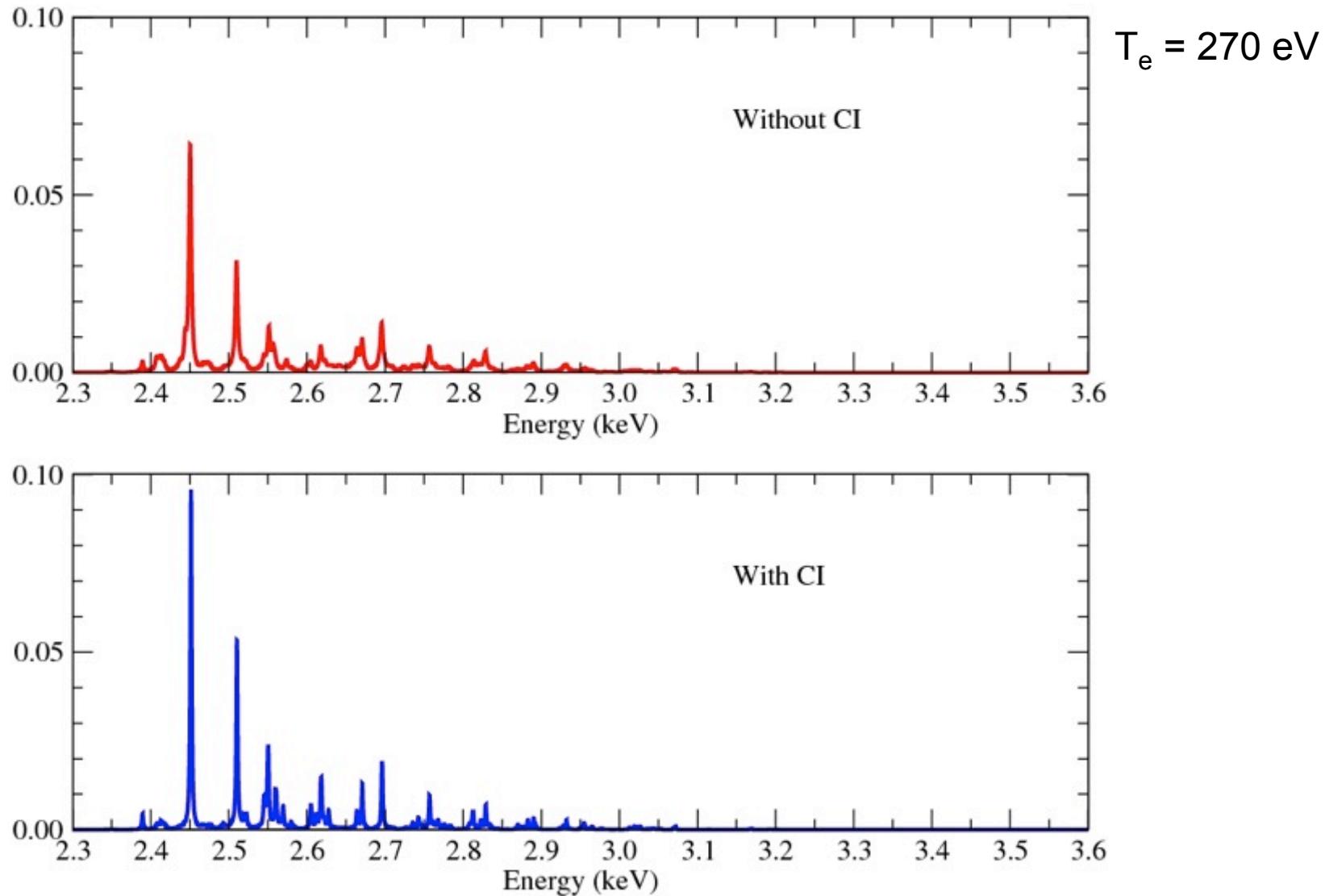
Without CI

$T_e = 270 \text{ eV}$



With CI

Spectrum with CI vs without CI



Alternative Atomic Physics Models

■ AVERROES

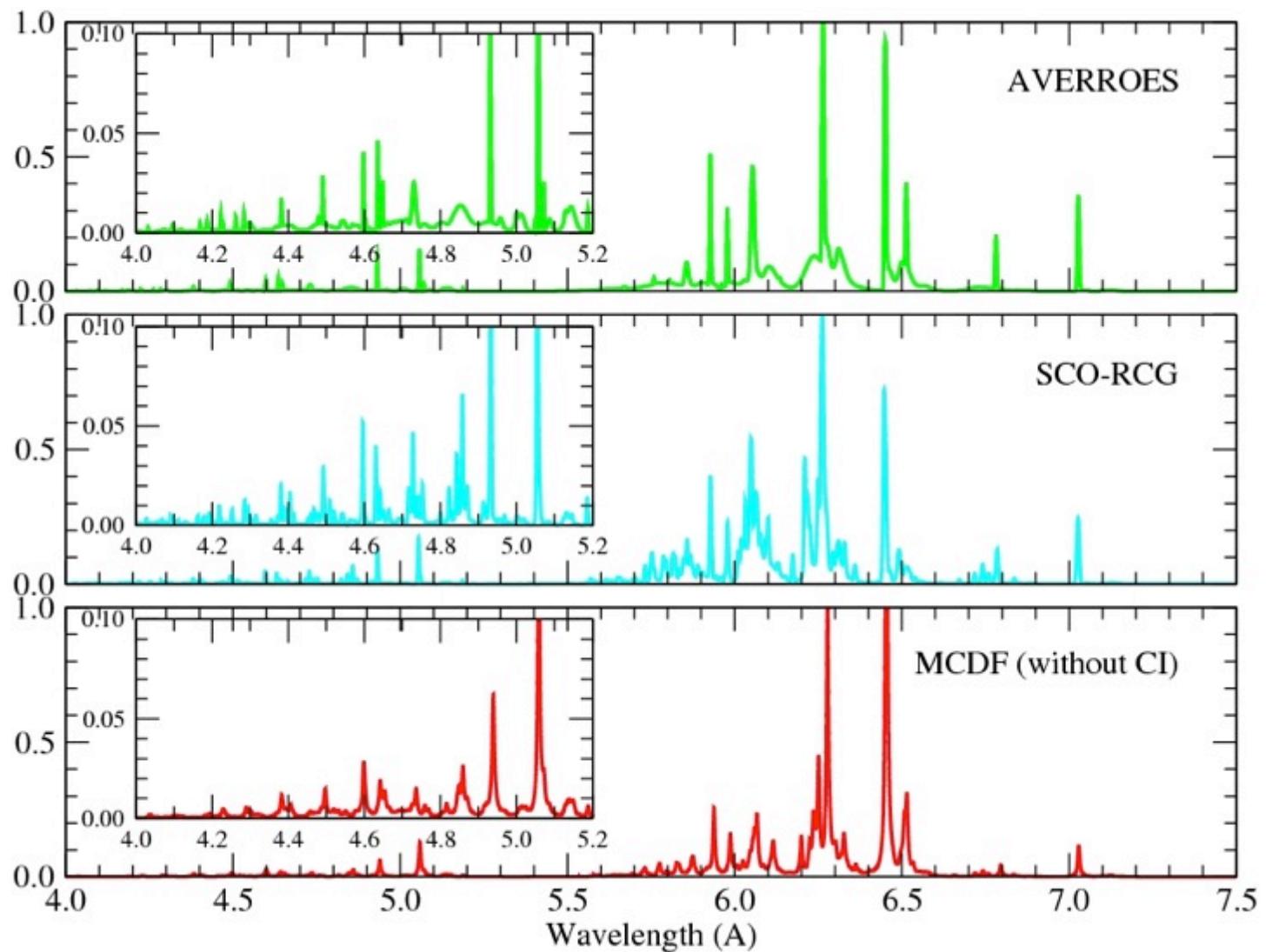
- Superconfigurations approach
- Native non-LTE
- Partial LTE within superconfigurations

■ SCO-RCG

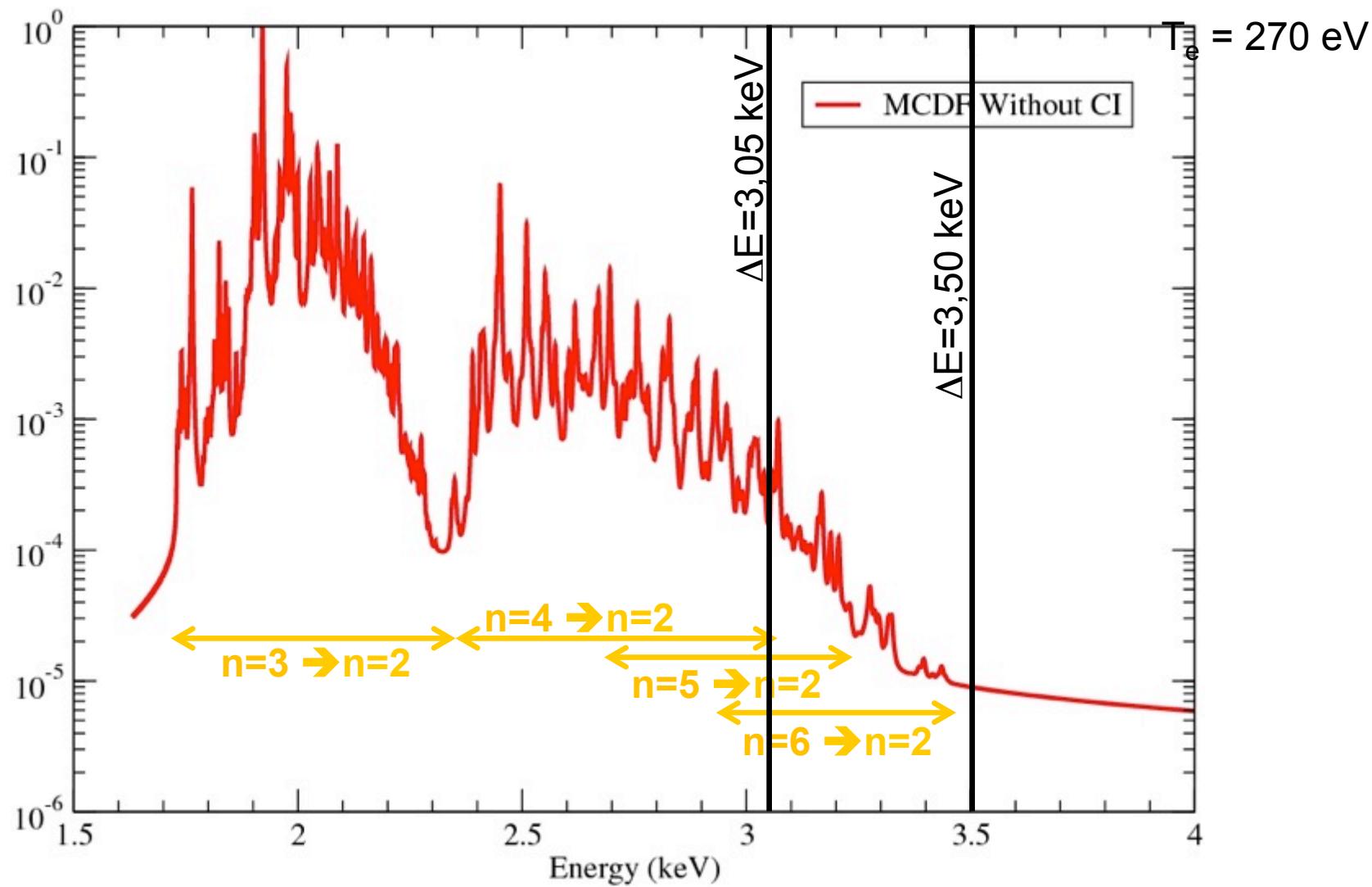
- Combines statistical and detailed approach
- SOSA (Spin Orbit Split Array)
- Transition arrays subdivided into sub arrays (SO effect)

Spectrum

$T_e = 270 \text{ eV}$



What about the new transition energy ?



Conclusion & Perspectives

- Experimental spectrum is well restituted
 - MCDF calculations with or without CI
 - Very time consuming
 - Agreement with AVERROES calculations
- Rubidium 84 is probably not the best candidate
 - $n=4,5,6 \rightarrow n=2$ nearly impossible with $\Delta E = 3,50$ keV
 - Higher transition energy than expected
 - Optimum Charge state for NEET is now $30^+/32^+$
- Future NEET calculations
 - Will require MCDF with CI
 - Alternate ADAM model (see next talk with M. Comet)

Thank you
for your
attention

Questions
are welcome

