

# Radioactive decay simulation of superheavy nuclei in Geant4

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Grand Accélérateur National d'Ions Lourds (GANIL)

27th Geant4 collaboration meeting  
September 2022



A Big  
Thank you

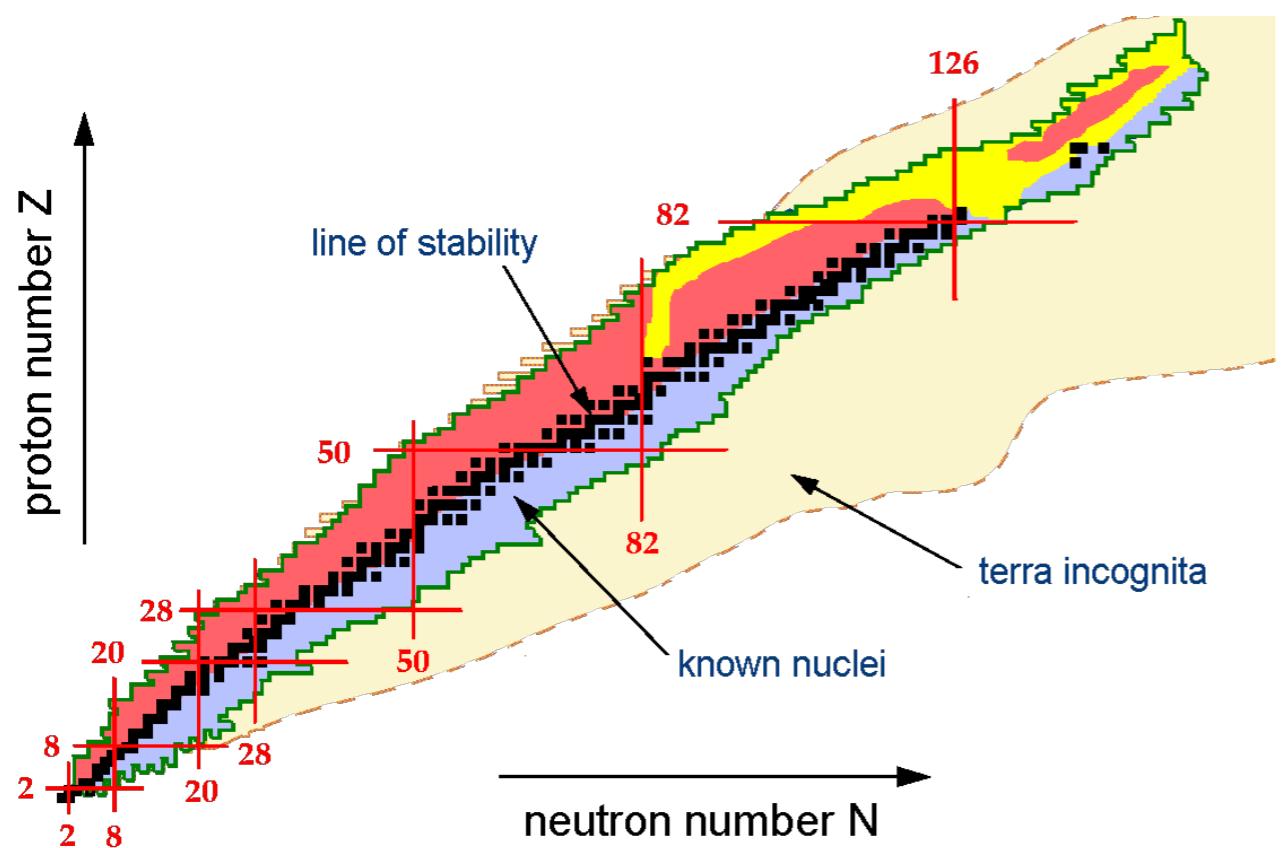
To the Geant4 collaboration



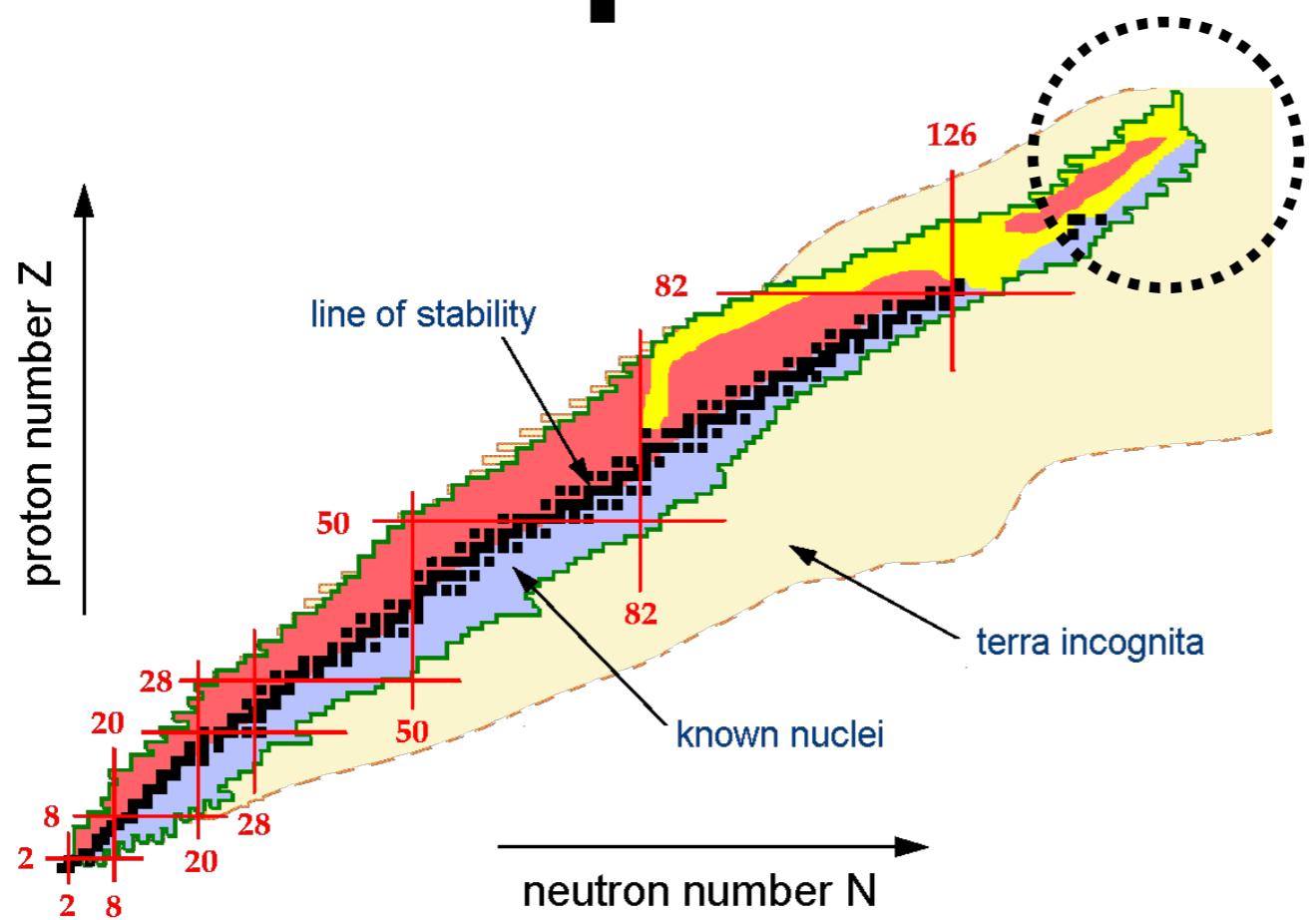
# Outline

- Context
- Experimental setup
- Radioactive decays in Geant4
- Extrapolation of Atomic Data
- Modifications in the code
- Test of the code and its use in the analysis of  $^{255}\text{Rf}$
- Conclusions and outlook

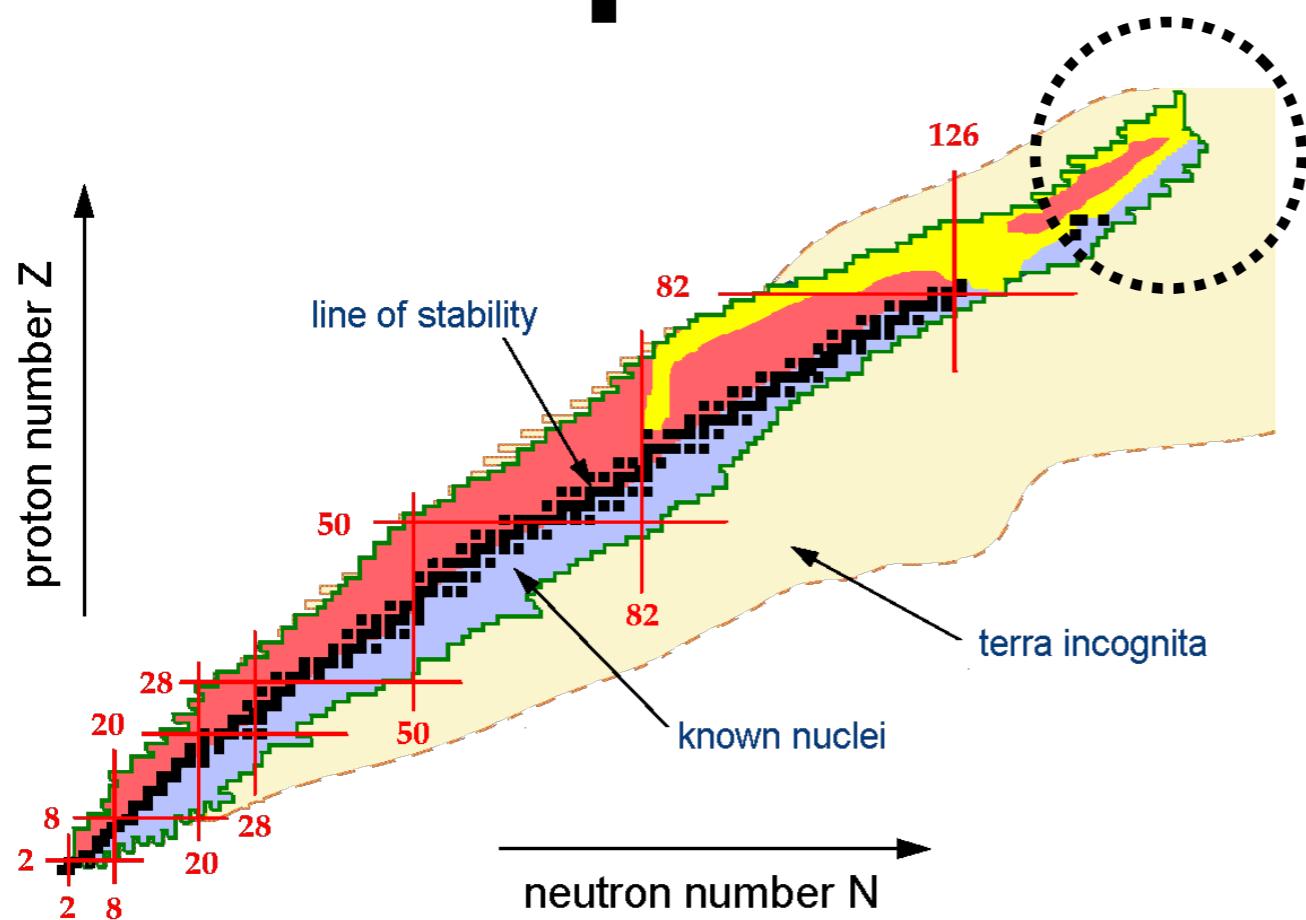
# Superheavy Nuclei



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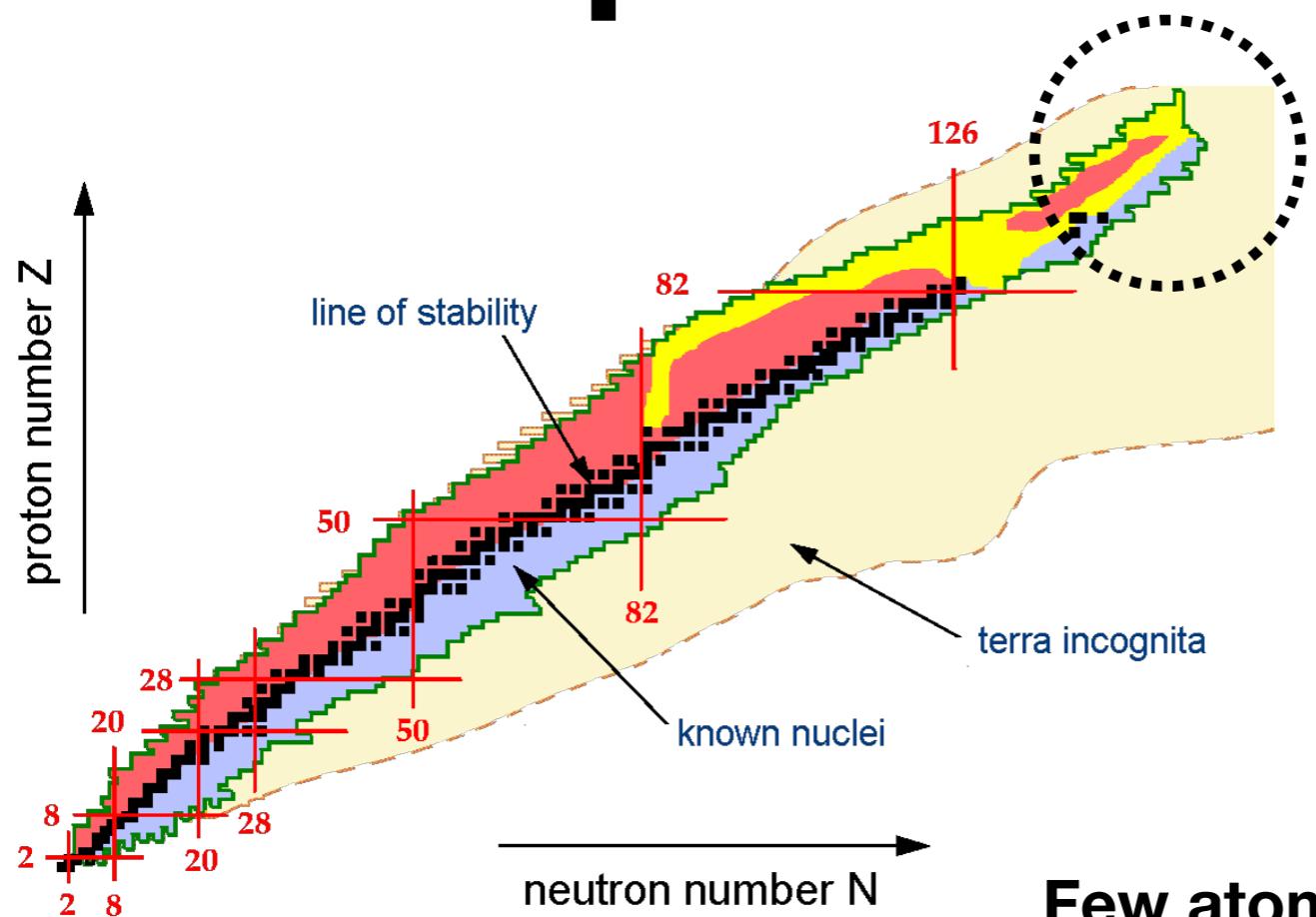


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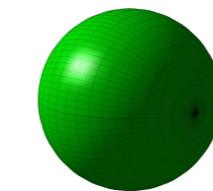
- What are the maximum number of protons and neutrons a nucleus can attain?
- Where exactly is the island of stability ?

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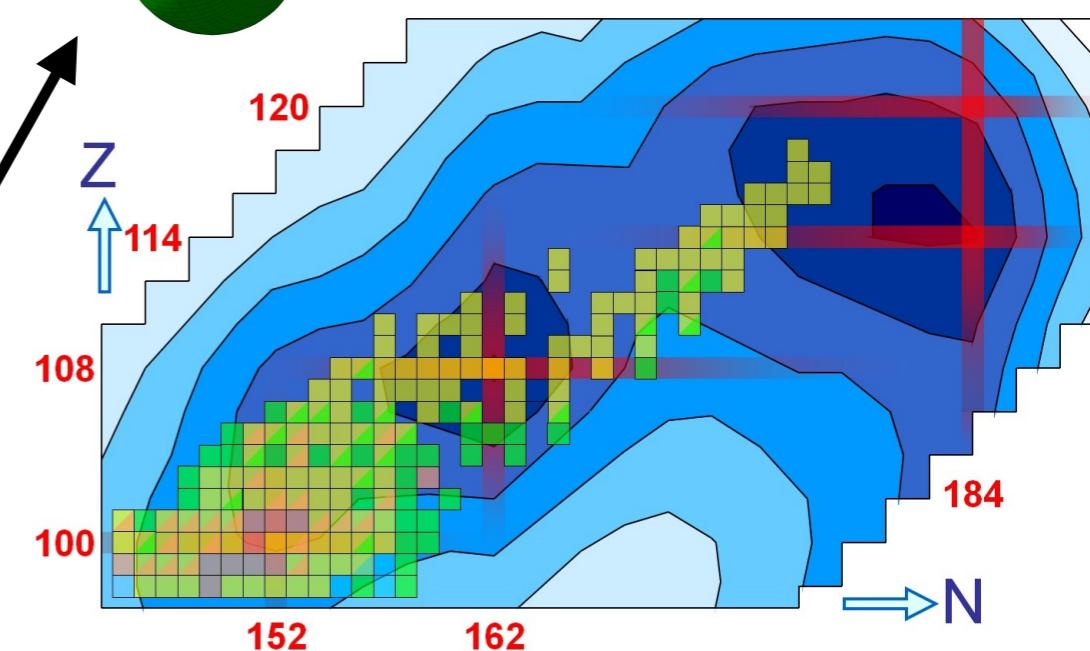
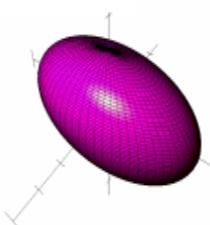
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**Few atoms/week**

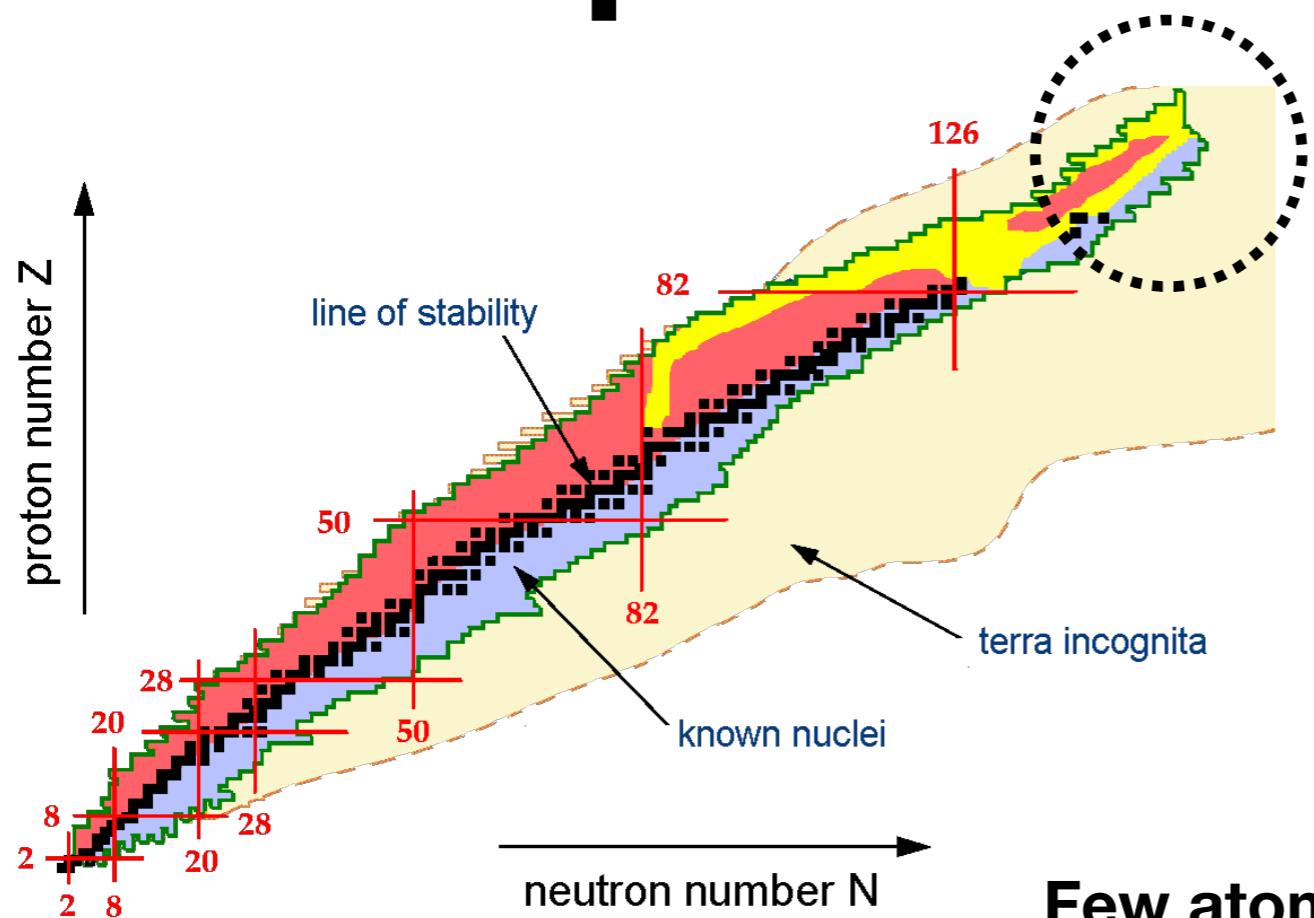


**Produced in Fusion-evaporation reactions**

**Few atoms/s**



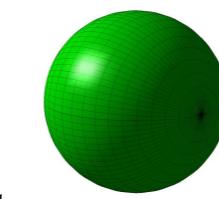
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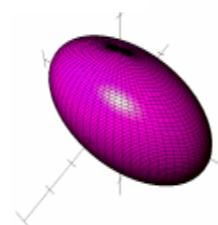
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Identification of superheavy nuclei by detecting their X rays

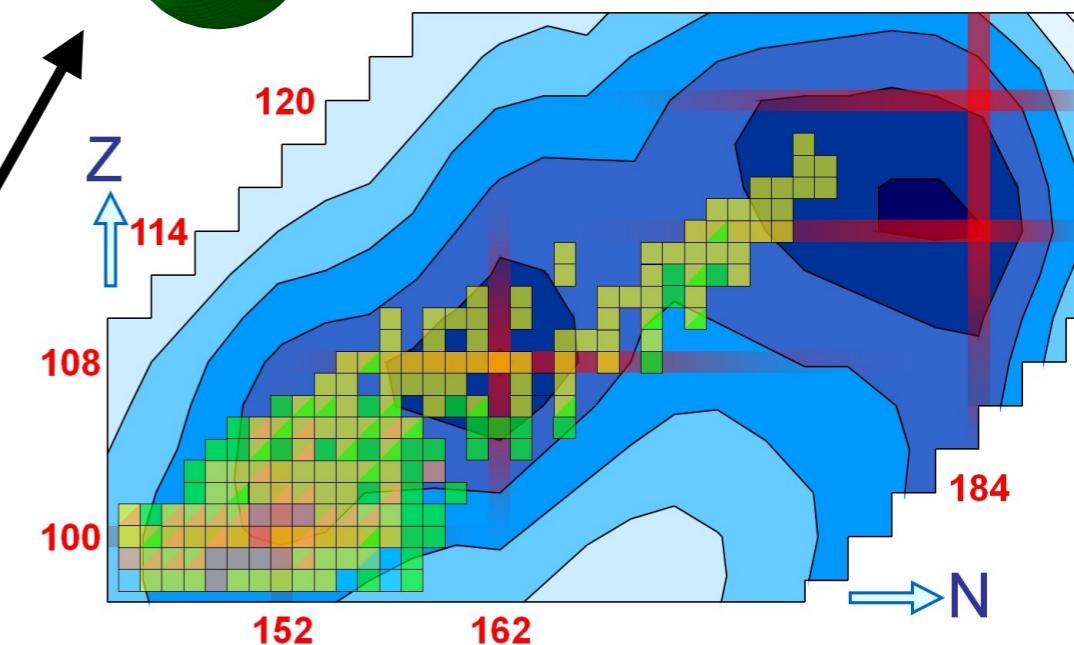
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Produced in Fusion-evaporation reactions



**Few atoms/s**



# Geant4-assisted data analysis

PRL 111, 112502 (2013)

PHYSICAL REVIEW LETTERS

week ending  
13 SEPTEMBER 2013

## Spectroscopy of Element 115 Decay Chains

D. Rudolph,<sup>1,\*</sup> U. Forsberg,<sup>1</sup> P. Golubev,<sup>1</sup> L. G. Sarmiento,<sup>1</sup> A. Yakushev,<sup>2</sup> L.-L. Andersson,<sup>3</sup> A. Di Nitto,<sup>4</sup> Ch. E. Düllmann,<sup>2,3,4</sup> J. M. Gates,<sup>5</sup> K. E. Gregorich,<sup>5</sup> C. J. Gross,<sup>6</sup> F. P. Heßberger,<sup>2,3</sup> R.-D. Herzberg,<sup>7</sup> J. Khuyagbaatar,<sup>3</sup> J. V. Kratz,<sup>4</sup> K. Rykaczewski,<sup>6</sup> M. Schädel,<sup>2,8</sup> S. Åberg,<sup>1</sup> D. Ackermann,<sup>2</sup> M. Block,<sup>2</sup> H. Brand,<sup>2</sup> B. G. Carlsson,<sup>1</sup> D. Cox,<sup>7</sup> X. Derkx,<sup>3,4</sup> K. Eberhardt,<sup>3,4</sup> J. Even,<sup>3</sup> C. Fahlander,<sup>1</sup> J. Gerl,<sup>2</sup> E. Jäger,<sup>2</sup> B. Kindler,<sup>2</sup> J. Krier,<sup>2</sup> I. Kojouharov,<sup>2</sup> N. Kurz,<sup>2</sup> B. Lommel,<sup>2</sup> A. Mistry,<sup>7</sup> C. Mokry,<sup>3,4</sup> H. Nitsche,<sup>5</sup> J. P. Omtvedt,<sup>9</sup> P. Papadakis,<sup>7</sup> I. Ragnarsson,<sup>1</sup> J. Runke,<sup>2</sup> H. Schaffner,<sup>2</sup> B. Schausten,<sup>2</sup> P. Thörle-Pospiech,<sup>3,4</sup> T. Torres,<sup>2</sup> T. Traut,<sup>4</sup> N. Trautmann,<sup>4</sup> A. Türler,<sup>10</sup> A. Ward,<sup>7</sup> D. E. Ward,<sup>1</sup> and N. Wiehl<sup>3,4</sup>

<sup>1</sup>Lund University, 22100 Lund, Sweden

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<sup>6</sup>Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA

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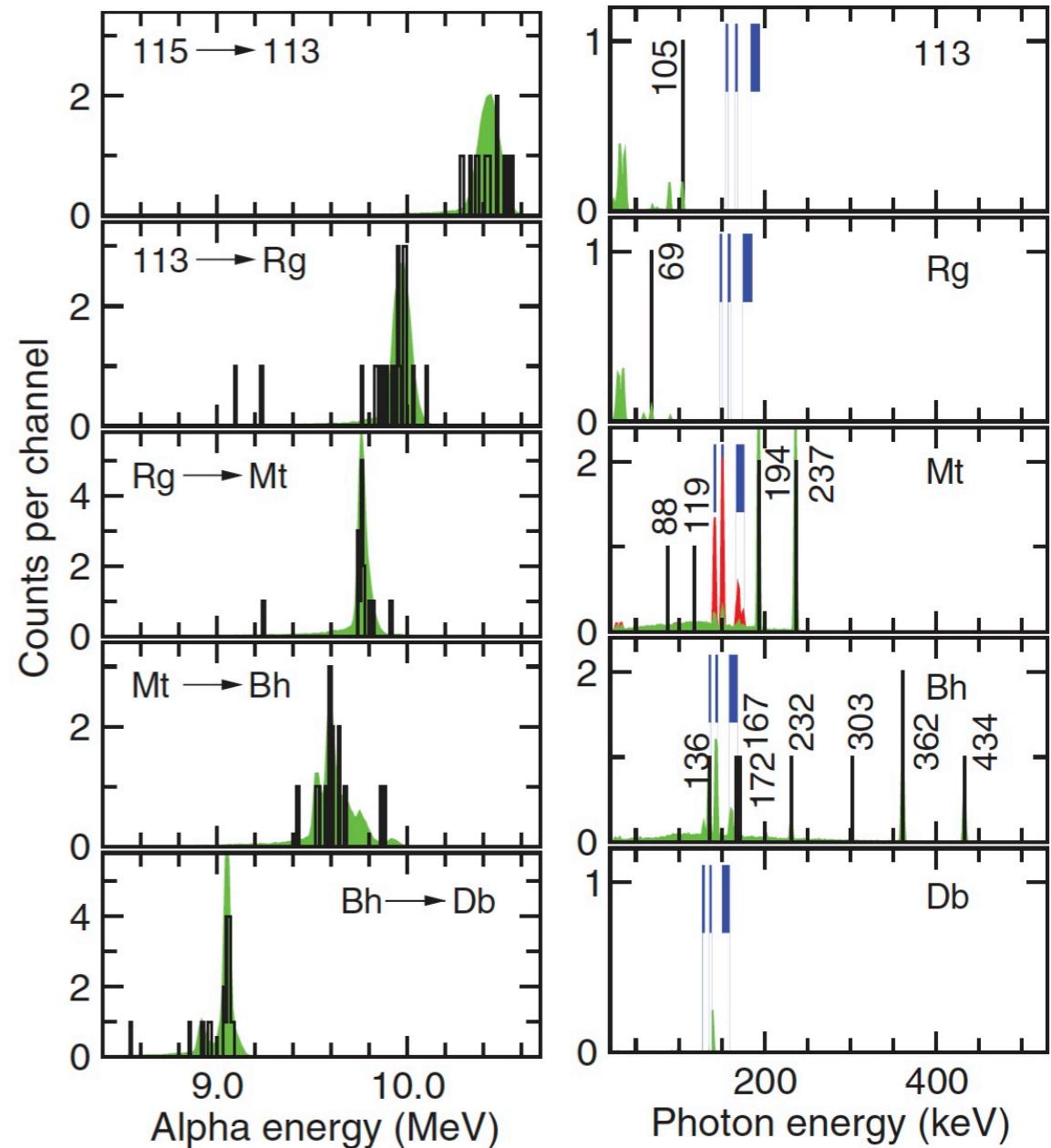
<sup>8</sup>Advanced Science Research Center, Japan Atomic Energy Agency, Tokai, Ibaraki 319-1195, Japan

<sup>9</sup>University of Oslo, 0315 Oslo, Norway

<sup>10</sup>Paul Scherrer Institute and University of Bern, 5232 Villigen, Switzerland

(Received 11 June 2013; published 10 September 2013)

$K_{\alpha 2}, K_{\alpha 1}, K_{\beta}$  Xrays



Green and Red lines are from Geant4 simulation

# Geant4-assisted data analysis

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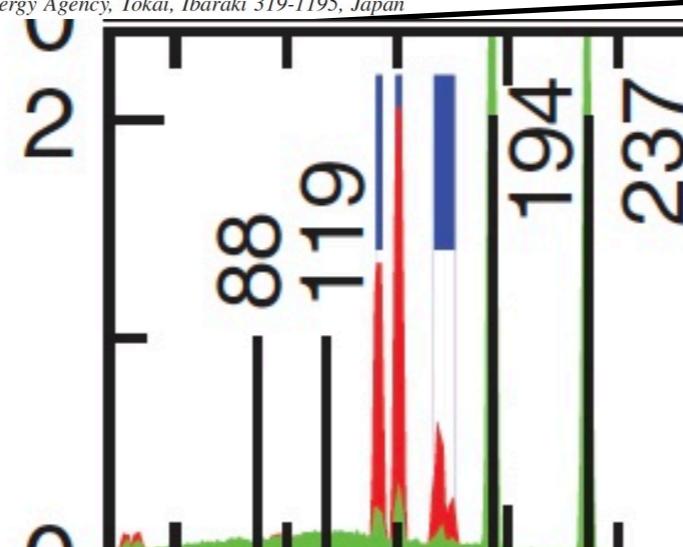
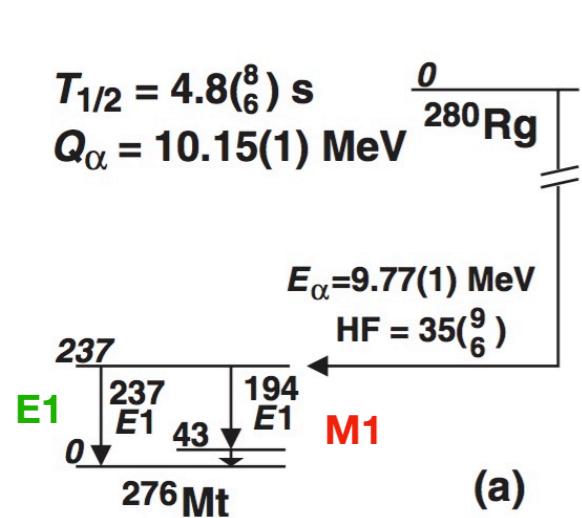
<sup>7</sup>University of Liverpool, Liverpool L69 7ZE, United Kingdom

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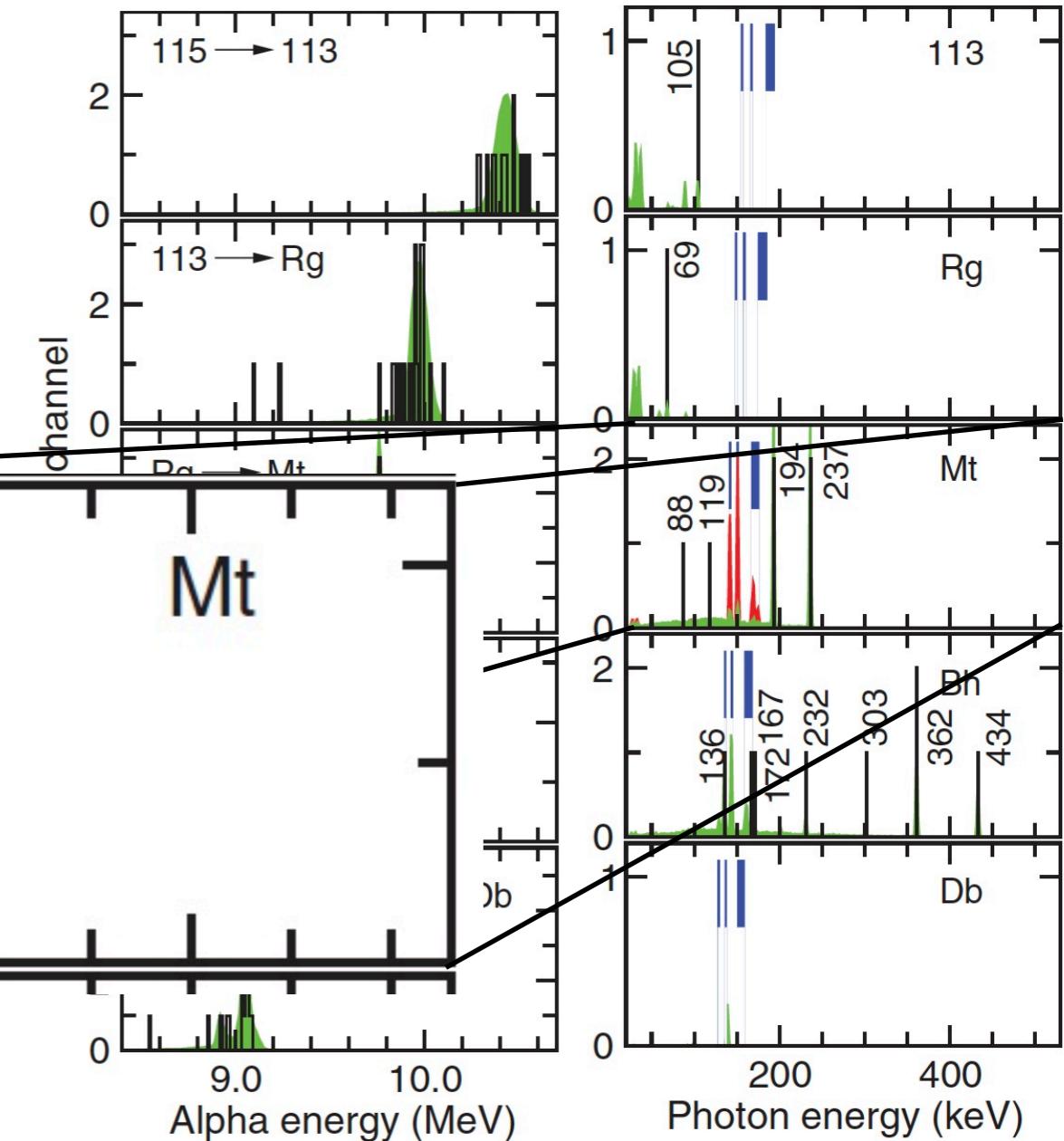
<sup>9</sup>University of Oslo, 031.

<sup>10</sup>Paul Scherrer Institute and University of

(Received 11 June 2013; publish



(a)



Geant4 can be used to interpret data

Green and Red lines are from Geant4 simulation

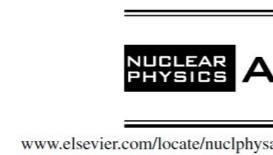
# Another example



Available online at [www.sciencedirect.com](http://www.sciencedirect.com)



Nuclear Physics A 852 (2011) 15–35



[www.elsevier.com/locate/nuclphysa](http://www.elsevier.com/locate/nuclphysa)

## Spectroscopy of $^{253}\text{No}$ and its daughters

A. Lopez-Martens<sup>a,b,\*</sup>, T. Wiborg-Hagen<sup>c</sup>, K. Hauschild<sup>a,b</sup>, M.L. Chelnokov<sup>d</sup>, V.I. Chepigin<sup>d</sup>, D. Curien<sup>e</sup>, O. Dorvaux<sup>e</sup>, G. Drafta<sup>f</sup>, B. Gall<sup>c</sup>, A. Görzen<sup>c,g</sup>, M. Guttormsen<sup>b</sup>, A.V. Isaev<sup>d</sup>, I.N. Izosimov<sup>d</sup>, A.P. Kabachenko<sup>d,l</sup>, D.E. Katrasev<sup>d</sup>, T. Kutsarova<sup>h</sup>, A.N. Kuznetsov<sup>d</sup>, A.C. Larsen<sup>c</sup>, O.N. Malyshev<sup>d</sup>, A. Minkova<sup>i</sup>, S. Mullins<sup>j</sup>, H.T. Nyhus<sup>c</sup>, D. Pantelica<sup>f</sup>, J. Piot<sup>e</sup>, A.G. Popeko<sup>d</sup>, S. Saro<sup>k</sup>, N. Scintee<sup>f</sup>, S. Siem<sup>c</sup>, N.U.H. Syed<sup>c</sup>, E.A. Sokol<sup>d</sup>, A.I. Svirikhin<sup>d</sup>, A.V. Yeremin<sup>d</sup>

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<sup>b</sup> Department of Physics, University of Jyväskylä, Finland

<sup>c</sup> Department of Physics, Oslo University, 0316 Oslo, Norway

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<sup>g</sup> DAPNIA/SPhN, CEA-Saclay, France

<sup>h</sup> INRNE, Bulgarian Academy of Sciences, 1784 Sofia, Bulgaria

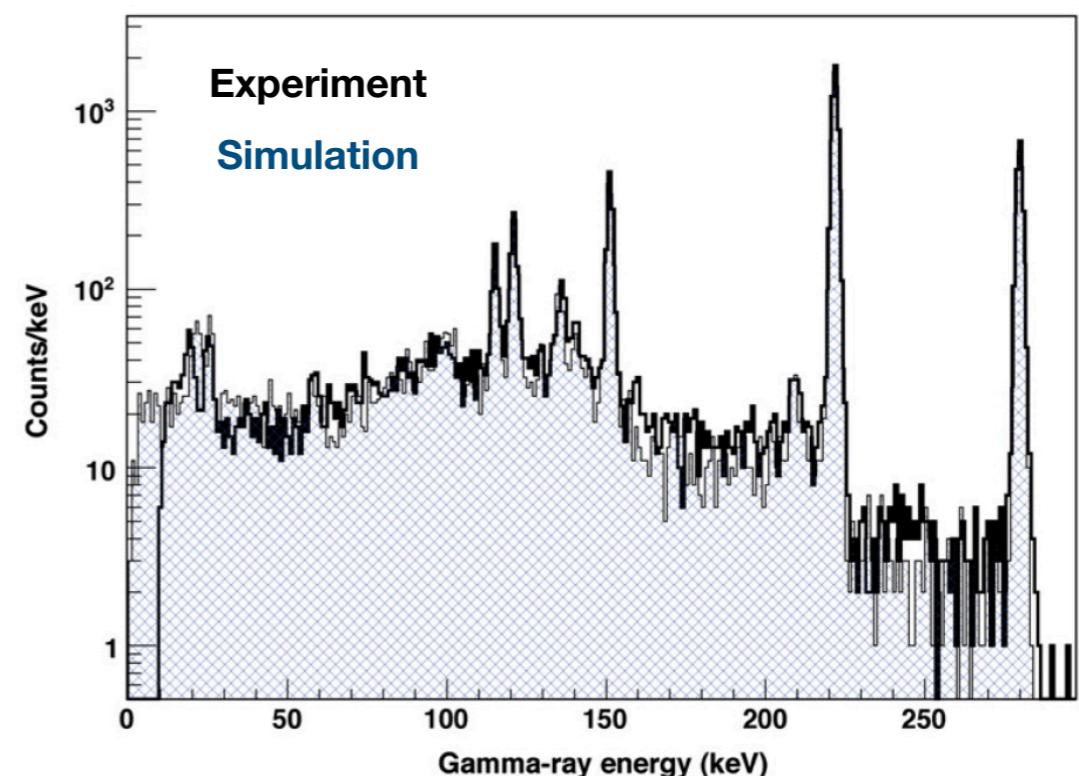
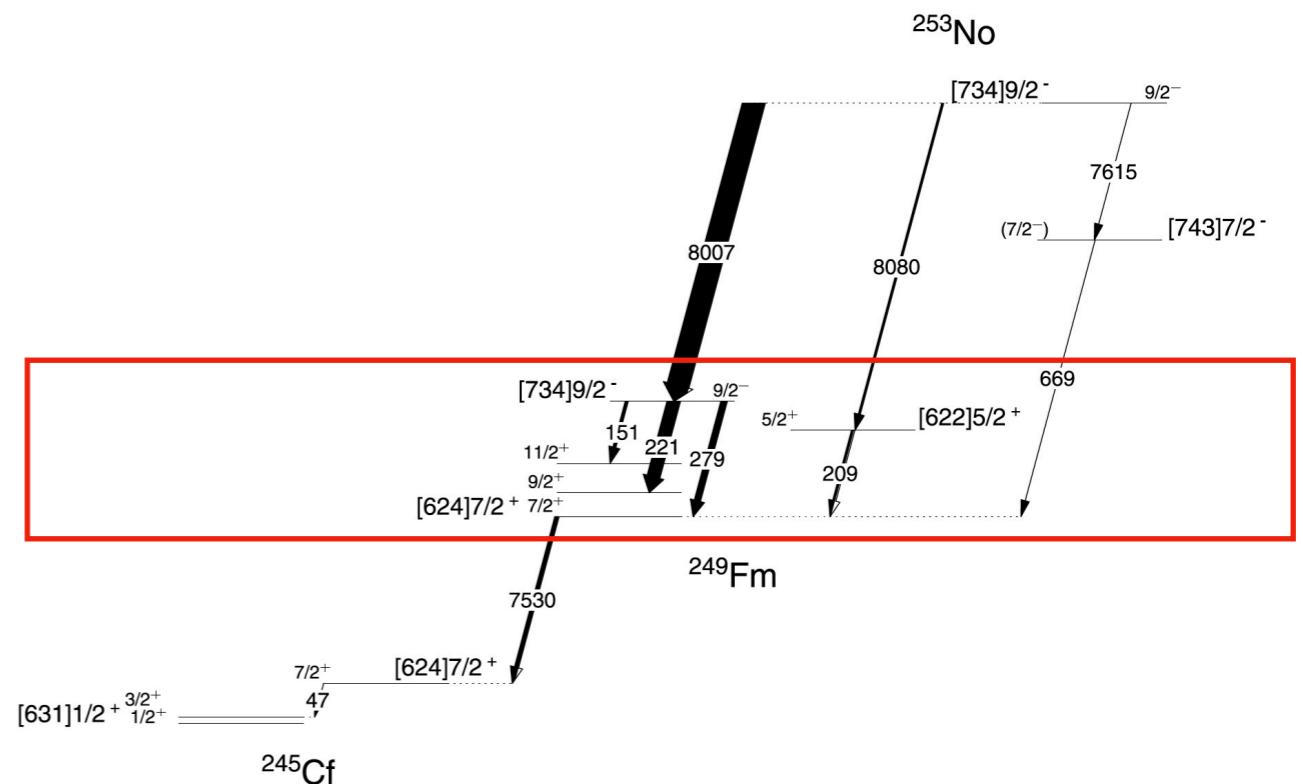
<sup>i</sup> Department of Atomic Physics, University of Sofia, 1164 Sofia, Bulgaria

<sup>j</sup> iThemba Labs, South Africa

<sup>k</sup> Department of Physics, Comenius University, SK-84215, Bratislava, Slovakia

Received 19 October 2010; received in revised form 10 January 2011; accepted 10 January 2011

Available online 20 January 2011



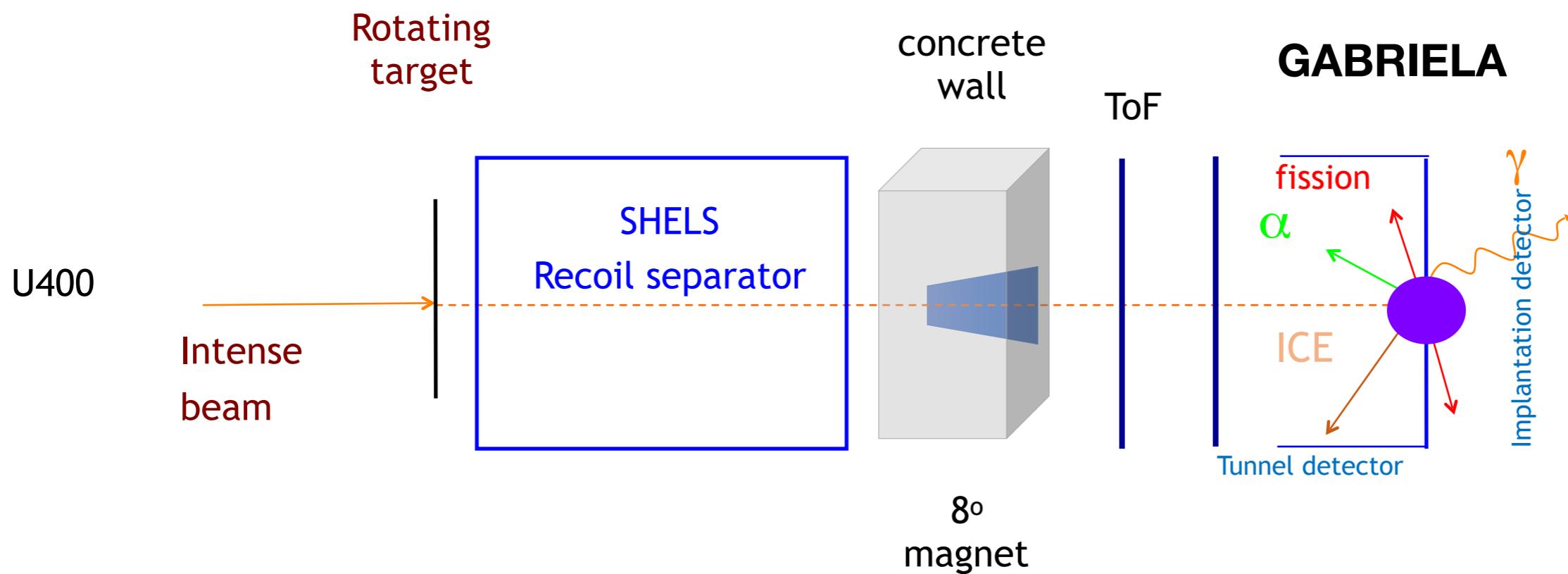
## Consistency of the decay scheme

# Experiment

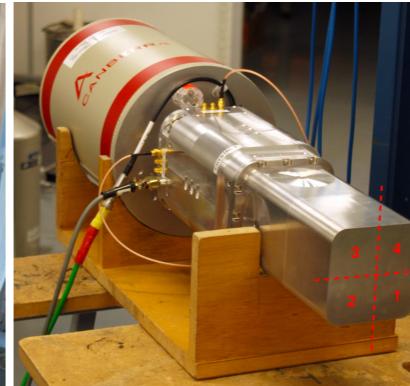
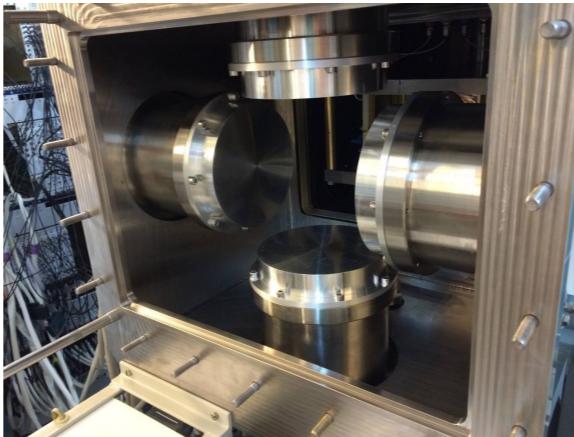
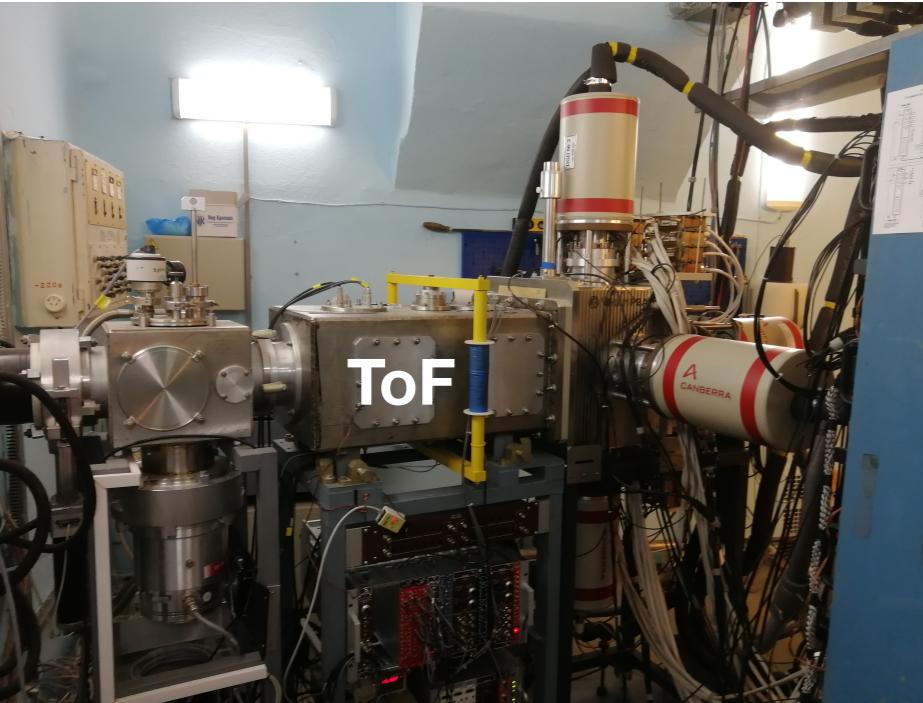
ANR-CLODETTE  
 (2013-2017) & RFBR



Gamma Alpha Beta Recoil Investigations with  
 the ELectromagnetic Analyser

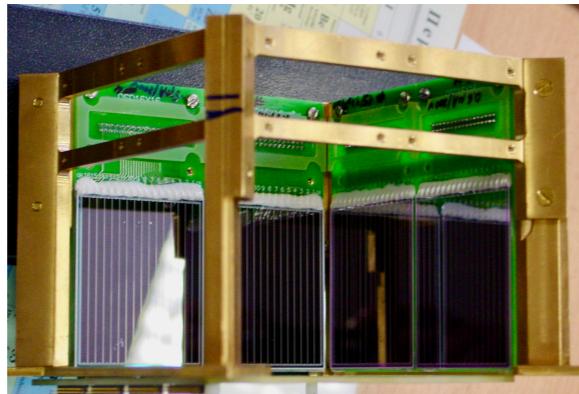
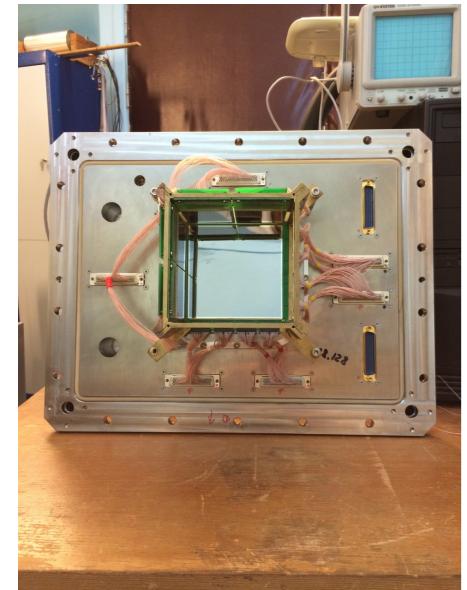


# GABRIELA



~1 mm thin Al window inserts  
for Ge detectors

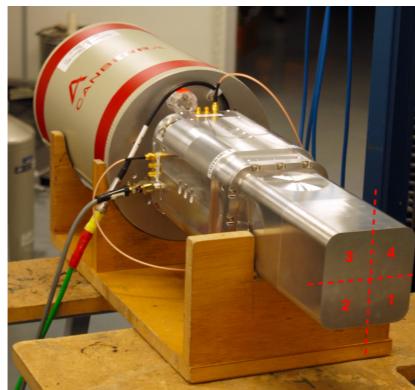
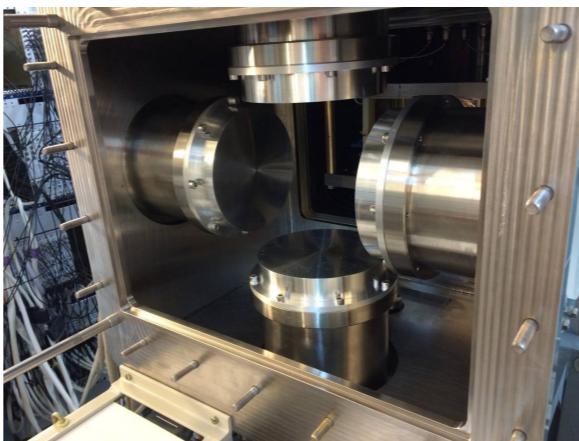
Clover



Tunnel : 8 detectors x 16x16 strips  
Thickness: 750  $\mu\text{m}$

DSSD : 128x128 strips  
Thickness: 300  $\mu\text{m}$  -  
500  $\mu\text{m}$

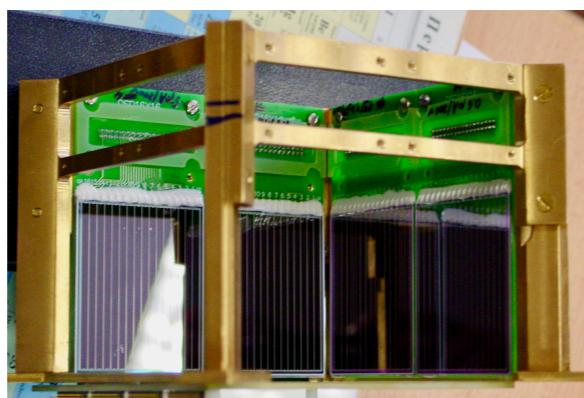
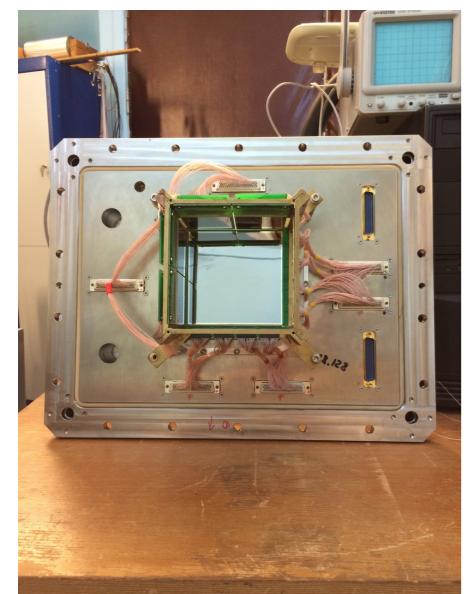
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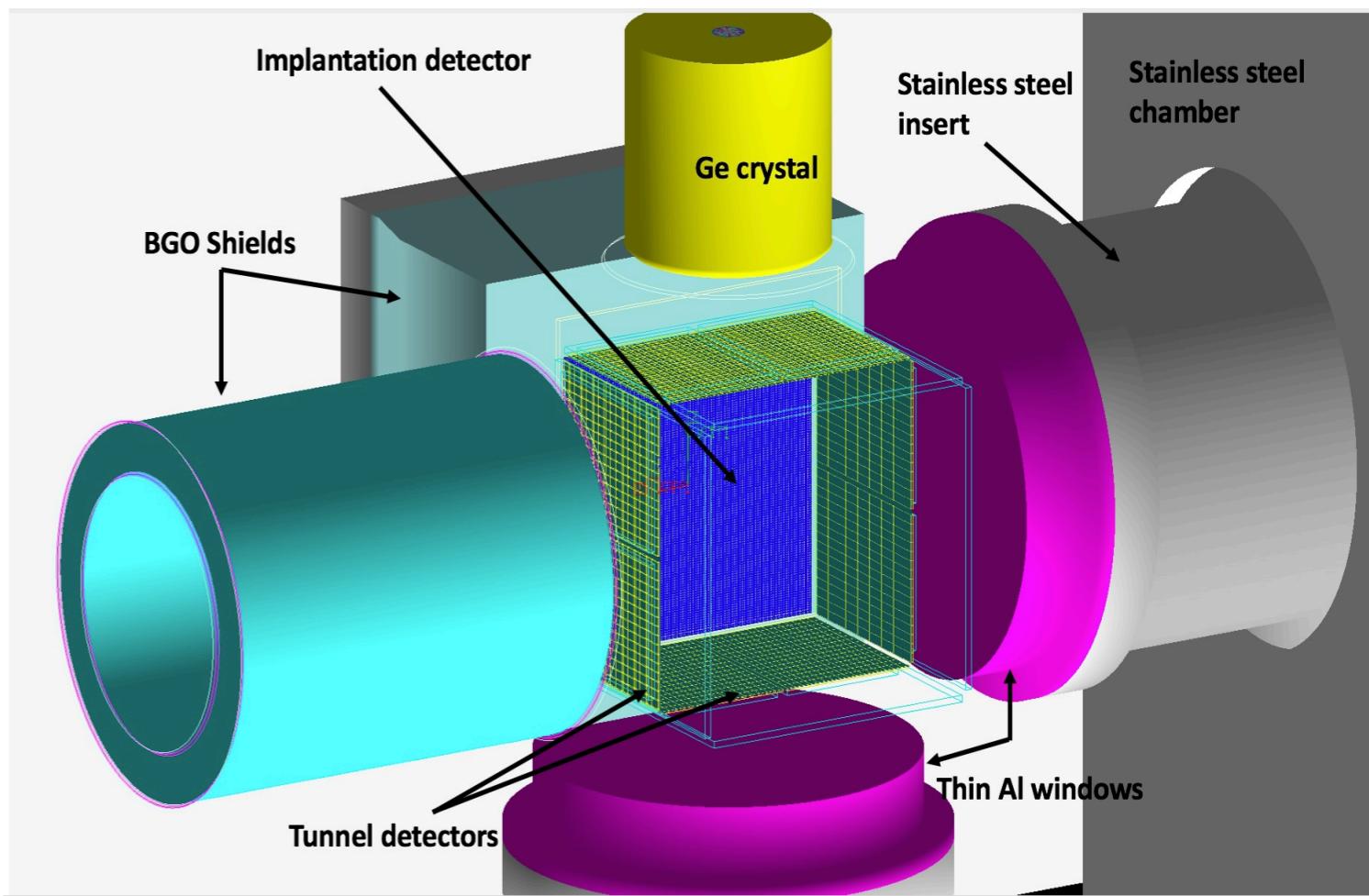
Clover

**GABRIELA in Geant4**



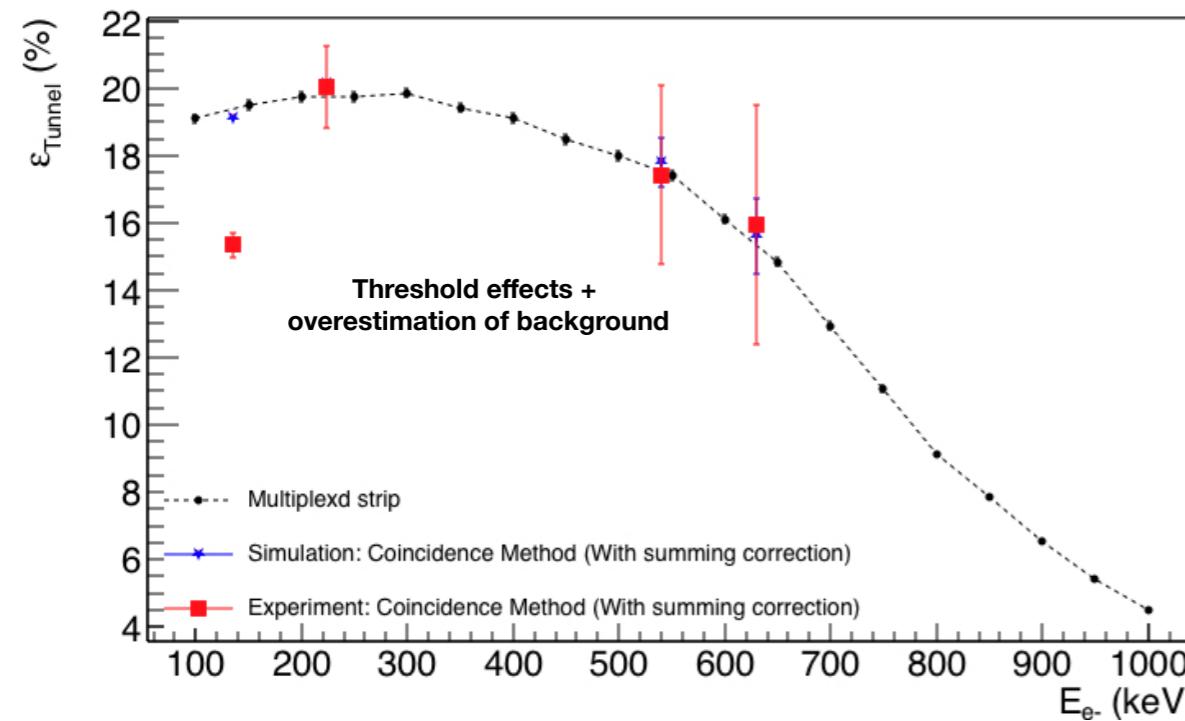
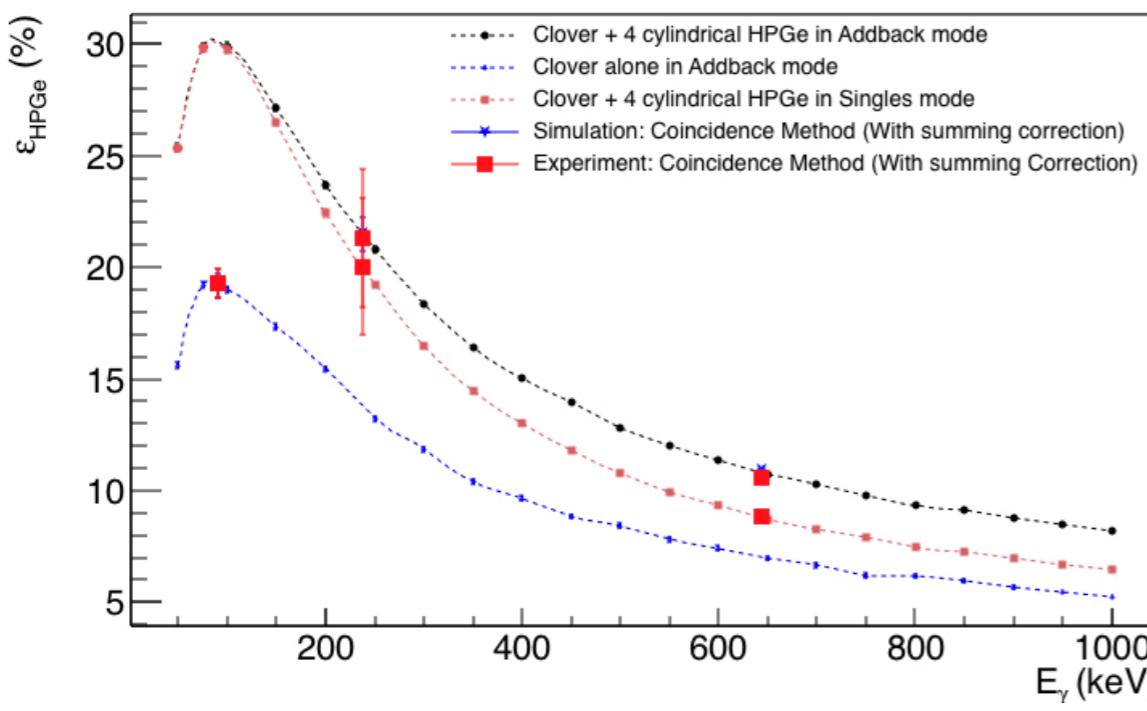
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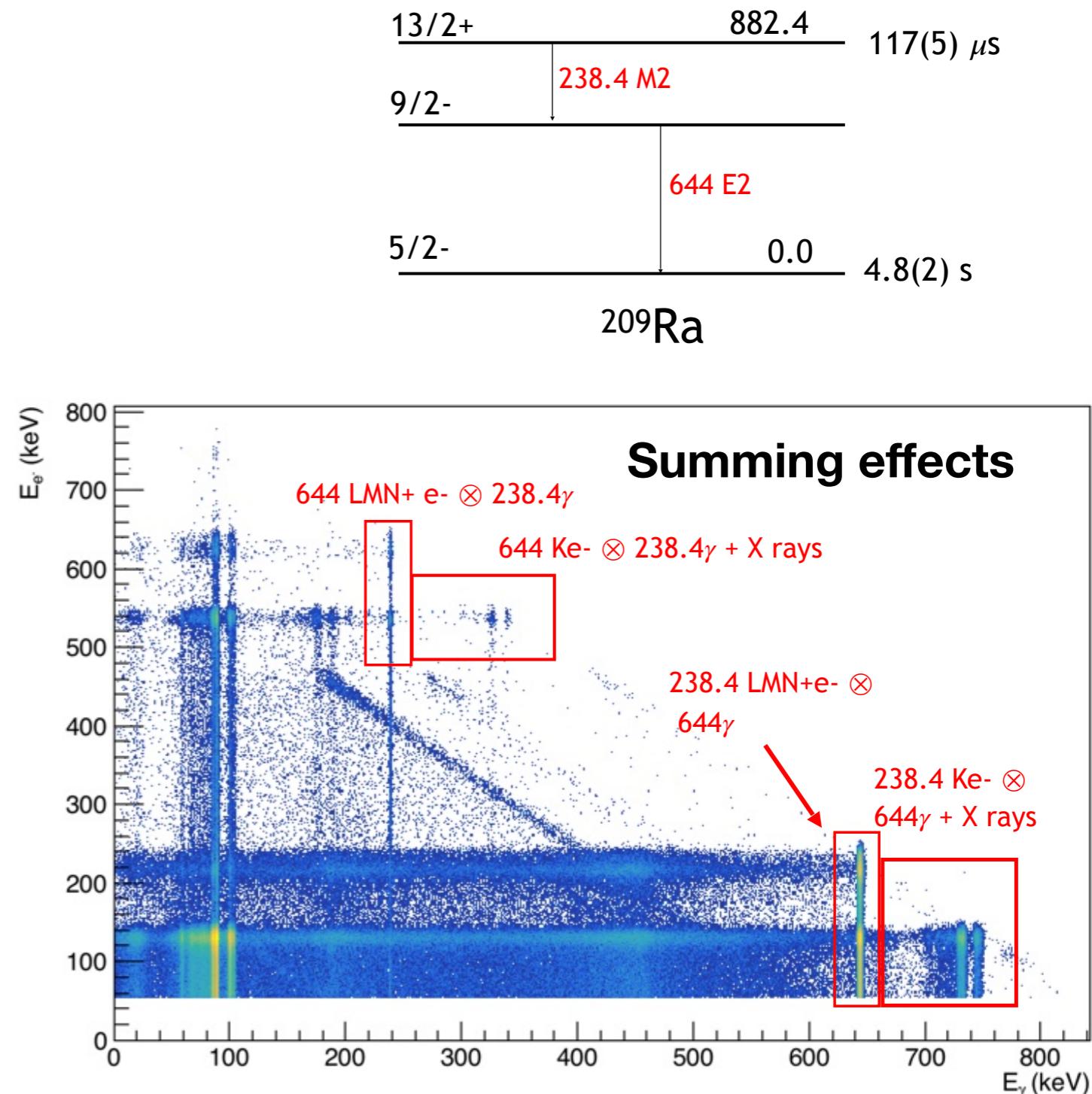
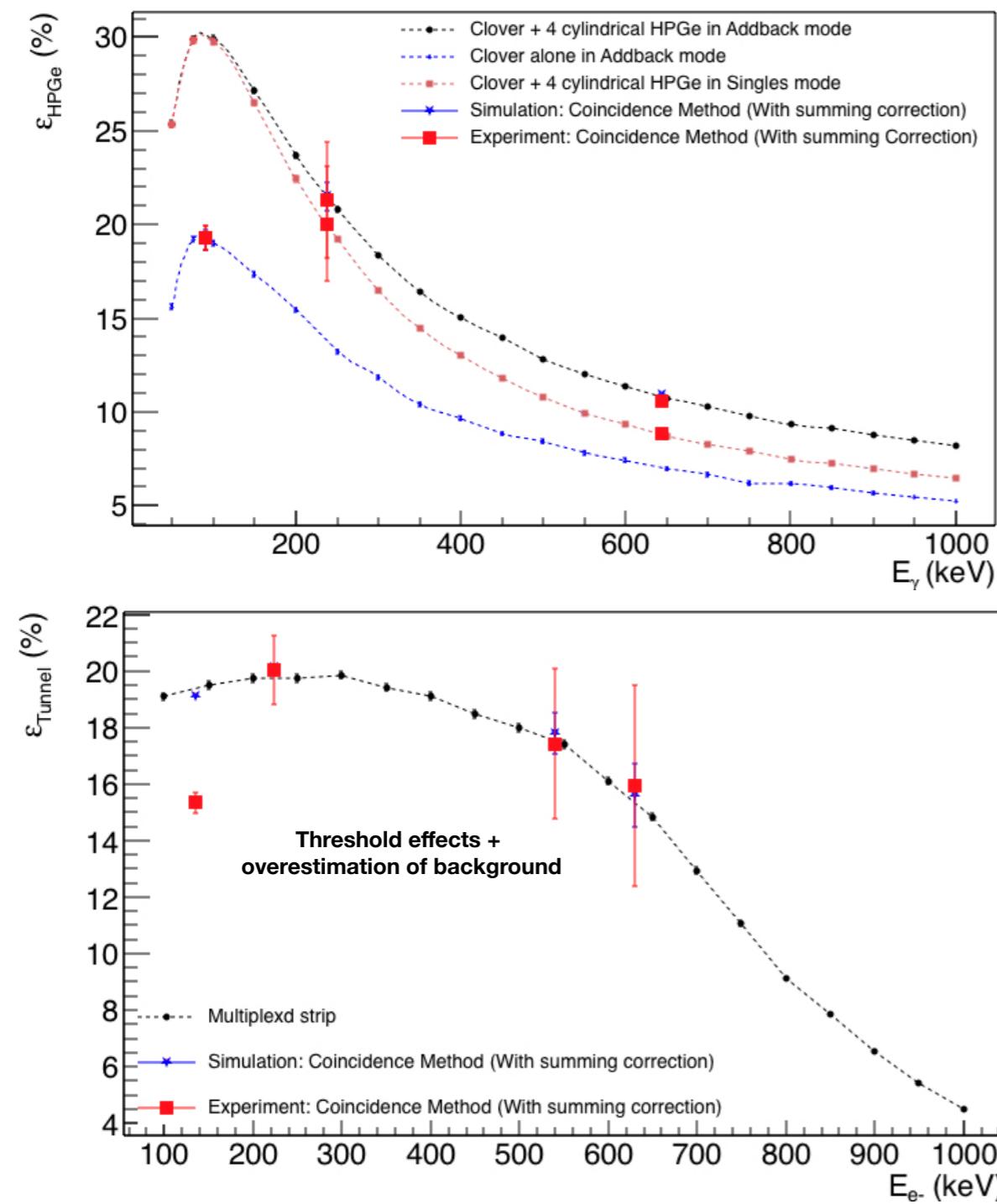


Courtesy of K. HAUSCHILD

# Characterisation of GABRIELA



# Characterisation of GABRIELA



# Radioactive decays in Geant4 for $Z > 100$

Geant4 allows addition of:

- ❖ Nuclear level data (photon evaporation) using  
`AddPrivateData(Z,A,"fileName_zZ.aA")`
- ❖ Radioactive decay data using  
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## *Limitations:*

For  $Z > 100$  internal conversion processes (important for heavy elements) are not simulated. Hence, no X-ray or Auger e- emission.

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- Hard code limits on  $Z = 100$

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## *Solutions:*

- Add atomic relaxation process in the simulations (event generator)  
[A. Lopez-Martens et al., Nucl. Phys. A852, 15 (2011)].
- Use the built-in Geant4 libraries (but, disguise heavy nuclei as lighter ones by modifying the atomic properties such as electron binding energies, occupancy, X-ray and Auger energies)  
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## *This work:*

- ✓ Using data from  $Z = 90$  to  $Z = 100$ , extrapolated Auger and Fluorescence data up to Rf
- ✓ Modify Geant4 source code: change the atomic number limits in the relevant classes, addition of atomic shell data, electron binding energies and so on.

# Extrapolation of Fluorescence Data

| 1  | 1           | 1        | Initial<br>vacancy<br>subshell         |
|----|-------------|----------|--|
| 5  | 0.297058    | 0.115888 |  |
| 6  | 0.454157    | 0.121786 |  |
| 10 | 0.0533827   | 0.135896 |  |
| 11 | 0.106009    | 0.137287 |  |
| 13 | 0.00223099  | 0.137919 |  |
| 14 | 0.00240819  | 0.138187 |  |
| 18 | 0.0136759   | 0.140941 |  |
| 19 | 0.0286788   | 0.14132  | Radiative<br>transition<br>probability |
| 21 | 0.000699076 | 0.141618 |  |
| 22 | 0.000760166 | 0.141686 |  |
| 29 | 0.00354388  | 0.142312 |  |
| 30 | 0.00736636  | 0.142411 |  |
| 32 | 0.000160799 | 0.142526 | Final<br>vacancy<br>subshell           |
| 33 | 0.000172719 | 0.142541 |  |
| 43 | 0.000596927 | 0.142639 |  |
| 44 | 0.00105819  | 0.142654 |  |
| -1 | -1          | -1       | End of data set                        |

TABLE VI. Atomic Subshell Designators

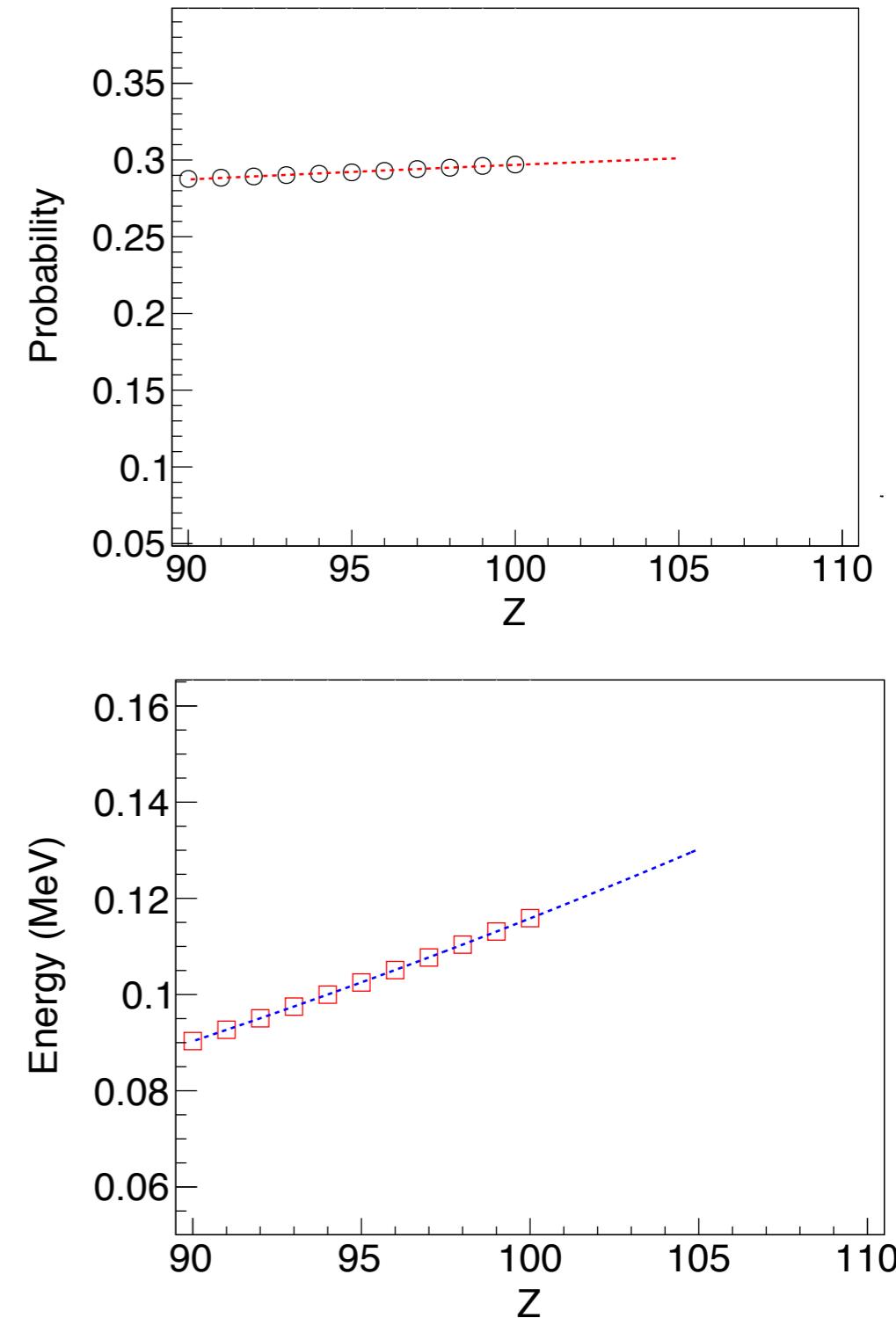
| Designator | Subshell   | Designator | Subshell   | Designator | Subshell     |
|------------|------------|------------|------------|------------|--------------|
| 1.         | K (1s1/2)  | 21.        | N4 (4d3/2) | 41.        | P1 (6s1/2)   |
| 2.         | L (2)      | 22.        | N5 (4d5/2) | 42.        | P23 (6p)     |
| 3.         | L1 (2s1/2) | 23.        | N67 (4f)   | 43.        | P2 (6p1/2)   |
| 4.         | L23 (2p)   | 24.        | N6 (4f5/2) | 44.        | P3 (6p3/2)   |
| 5.         | L2 (2p1/2) | 25.        | N7 (4f7/2) | 45.        | P45 (6d)     |
| 6.         | L3 (2p3/2) | 26.        | O (5)      | 46.        | P4 (6d3/2)   |
| 7.         | M (3)      | 27.        | O1 (5s1/2) | 47.        | P5 (6d5/2)   |
| 8.         | M1 (3s1/2) | 28.        | O23 (5p)   | 48.        | P67 (6f)     |
| 9.         | M23 (3p)   | 29.        | O2 (5p1/2) | 49.        | P6 (6f5/2)   |
| 10.        | M2 (3p1/2) | 30.        | O3 (5p3/2) | 50.        | P7 (6f7/2)   |
| 11.        | M3 (3p3/2) | 31.        | O45 (5d)   | 51.        | P89 (6g)     |
| 12.        | M45 (3d)   | 32.        | O4 (d3/2)  | 52.        | P8 (6g7/2)   |
| 13.        | M4 (3d3/2) | 33.        | O5 (5d5/2) | 53.        | P9 (6g9/2)   |
| 14.        | M5 (3d5/2) | 34.        | O67 (5f)   | 54.        | P1011 (6h)   |
| 15.        | N (4)      | 35.        | O6 (5f5/2) | 55.        | P10 (6h9/2)  |
| 16.        | N1 (4s1/2) | 36.        | O7 (5f7/2) | 56.        | P11 (6h11/2) |
| 17.        | N23 (4p)   | 37.        | O89 (5g)   | 57.        | Q (7)        |
| 18.        | N2 (4p1/2) | 38.        | O8 (5g7/2) | 58.        | Q1 (7s1/2)   |
| 19.        | N3 (4p3/2) | 39.        | O9 (5g9/2) | 59.        | Q23 (7p)     |
| 20.        | N45 (4d)   | 40.        | P (6)      | 60.        | Q2 (7p1/2)   |
|            |            |            |            | 61.        | Q3 (7p3/2)   |

Perkins, S T, and Cullen, D E. *ENDL type formats for the LLNL Evaluated Atomic Data Library, EADL, for the Evaluated Electron Data Library, EEDL, and for the Evaluated Photon Data Library, EPDL*. United States: N. p., 1994. Web. doi: 10.2172/10172308.

# Extrapolation of Fluorescence Data

| 1  | 1           | 1        | Initial<br>vacancy<br>subshell         |
|----|-------------|----------|--|
| 5  | 0.297058    | 0.115888 | Energy<br>in MeV                       |
| 6  | 0.454157    | 0.121786 |  |
| 10 | 0.0533827   | 0.135896 |  |
| 11 | 0.106009    | 0.137287 |  |
| 13 | 0.00223099  | 0.137919 |  |
| 14 | 0.00240819  | 0.138187 |  |
| 18 | 0.0136759   | 0.140941 |  |
| 19 | 0.0286788   | 0.14132  | Radiative<br>transition<br>probability |
| 21 | 0.000699076 | 0.141618 |  |
| 22 | 0.000760166 | 0.141686 |  |
| 29 | 0.00354388  | 0.142312 |  |
| 30 | 0.00736636  | 0.142411 |  |
| 32 | 0.000160799 | 0.142526 | Final<br>vacancy<br>subshell           |
| 33 | 0.000172719 | 0.142541 |  |
| 43 | 0.000596927 | 0.142639 |  |
| 44 | 0.00105819  | 0.142654 |  |
| -1 | -1          | -1       | End of data set                        |

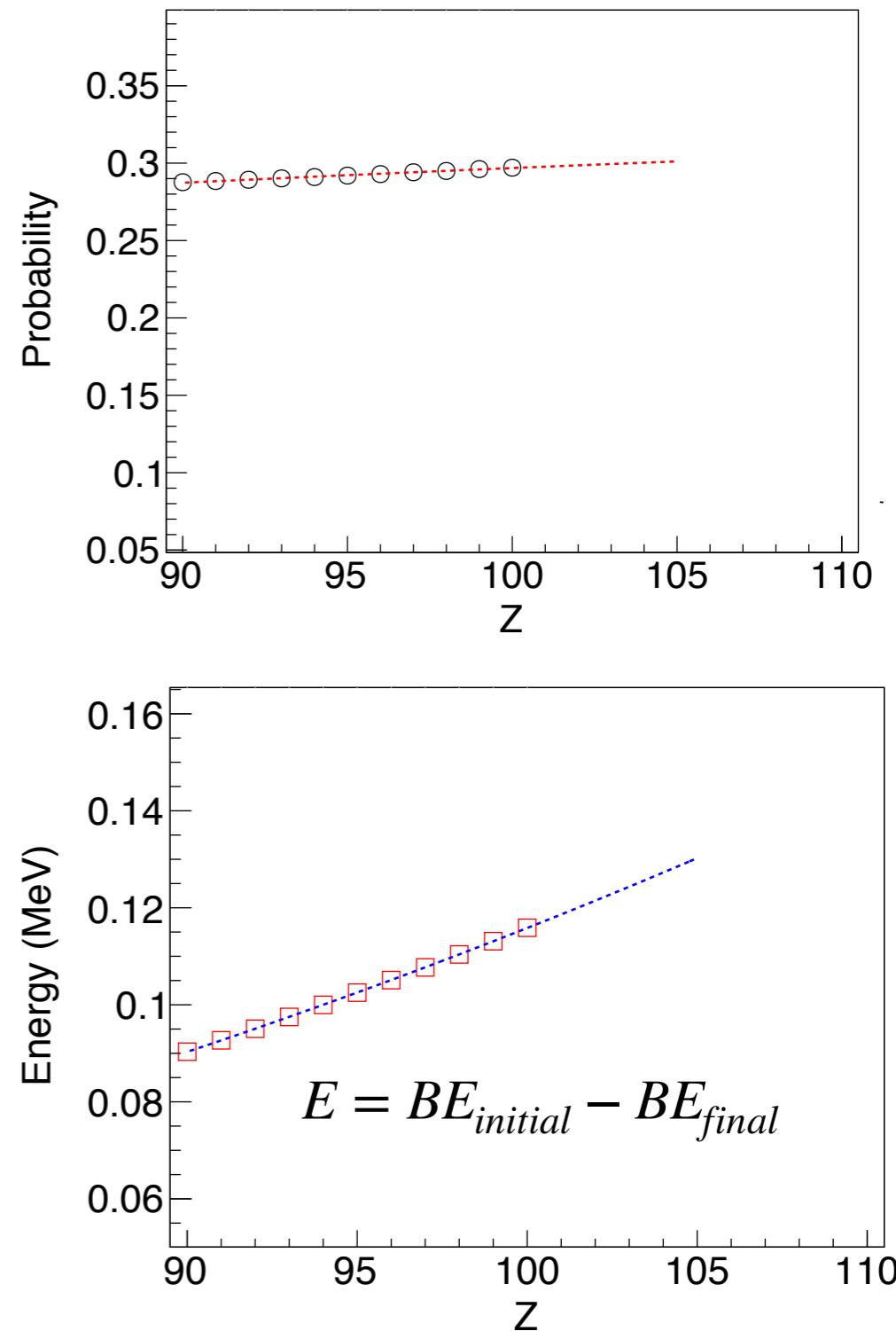
Evaluated Atomic Data Library notation



# Extrapolation of Fluorescence Data

| 1  | 1           | 1        | Initial<br>vacancy<br>subshell         |
|----|-------------|----------|--|
| 5  | 0.297058    | 0.115888 | Energy<br>in MeV                       |
| 6  | 0.454157    | 0.121786 |  |
| 10 | 0.0533827   | 0.135896 |  |
| 11 | 0.106009    | 0.137287 |  |
| 13 | 0.00223099  | 0.137919 |  |
| 14 | 0.00240819  | 0.138187 |  |
| 18 | 0.0136759   | 0.140941 |  |
| 19 | 0.0286788   | 0.14132  | Radiative<br>transition<br>probability |
| 21 | 0.000699076 | 0.141618 |  |
| 22 | 0.000760166 | 0.141686 |  |
| 29 | 0.00354388  | 0.142312 |  |
| 30 | 0.00736636  | 0.142411 |  |
| 32 | 0.000160799 | 0.142526 |  |
| 33 | 0.000172719 | 0.142541 |  |
| 43 | 0.000596927 | 0.142639 | Final<br>vacancy<br>subshell           |
| 44 | 0.00105819  | 0.142654 |  |
| -1 | -1          | -1       | End of data set                        |

Evaluated Atomic Data Library notation

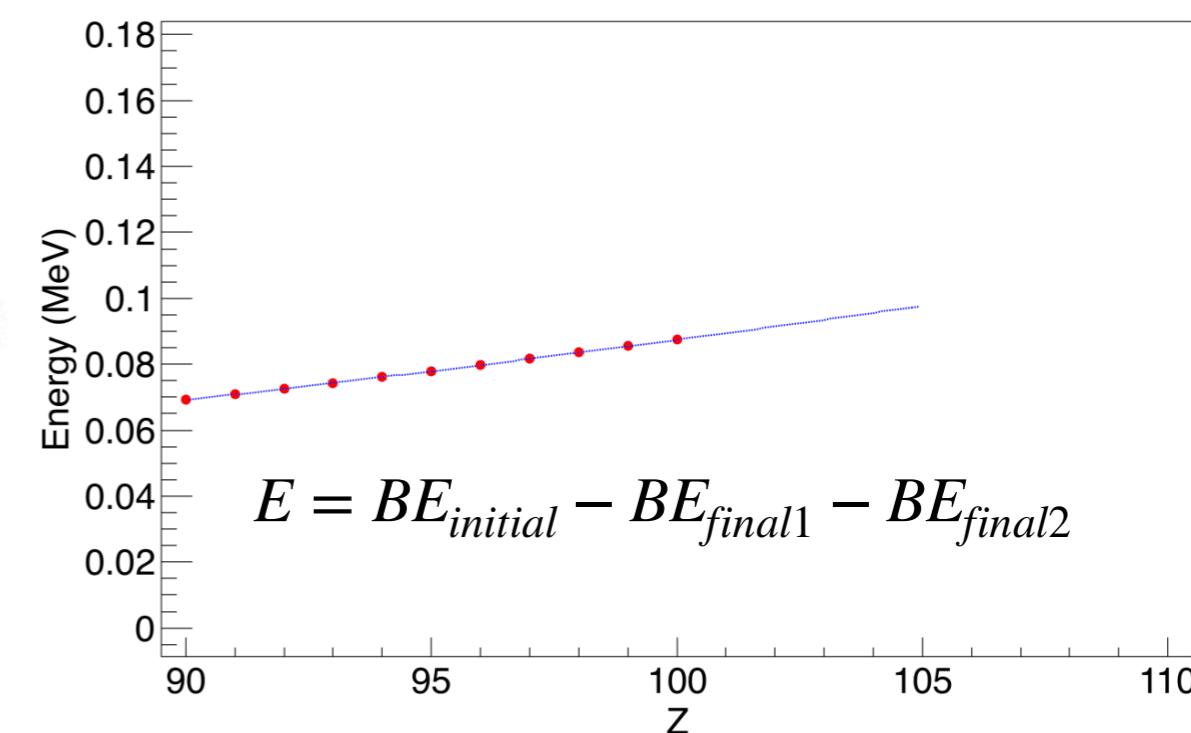
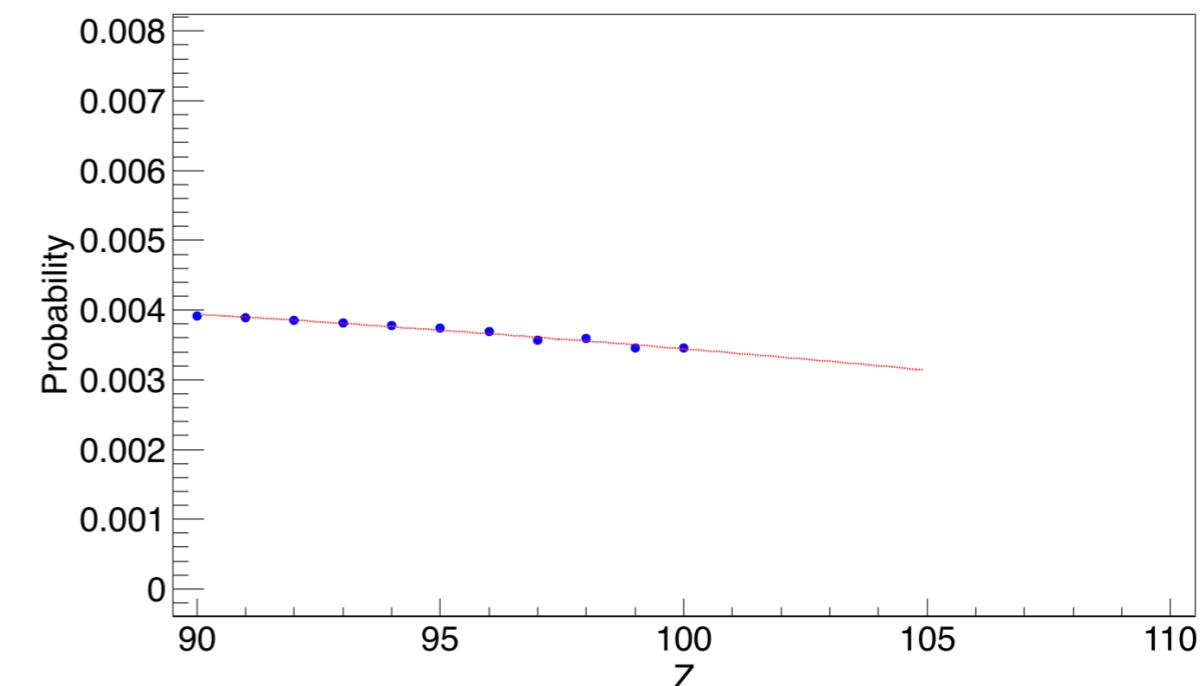


# Extrapolation of Auger Data

| 1  | 1  | 1              | 1              |                 |
|----|----|----------------|----------------|-----------------|
| 3  | 3  | 0.34565300E-02 | 0.87436000E-01 | Initial         |
| 3  | 5  | 0.70246600E-02 | 0.88266000E-01 | vacancy         |
| 3  | 6  | 0.19702200E-02 | 0.94164000E-01 | subshell        |
| .  | .  | .              | .              |                 |
| 5  | 5  | 0.18830300E-03 | 0.89096000E-01 | Energy          |
| 5  | 6  | 0.30001900E-02 | 0.94994000E-01 | in MeV          |
| 5  | 8  | 0.13242500E-02 | 0.10870800E+00 | Non-            |
| .  | .  | .              | .              | Radiative       |
| .  | .  | .              | .              | transition      |
| 6  | 6  | 0.11558800E-02 | 0.10089200E+00 | probability     |
| 6  | 8  | 0.32593500E-03 | 0.11460600E+00 | Subshell of     |
| 6  | 10 | 0.54621400E-03 | 0.11500200E+00 | relaxing        |
| .  | .  | .              | .              | electron        |
| 30 | 33 | 0.62100000E-07 | 0.14227200E+00 | Subshell of     |
| -1 | -1 | -1             | -1             | Auger           |
|    |    |                |                | electron        |
|    |    |                |                | End of data set |

# Extrapolation of Auger Data

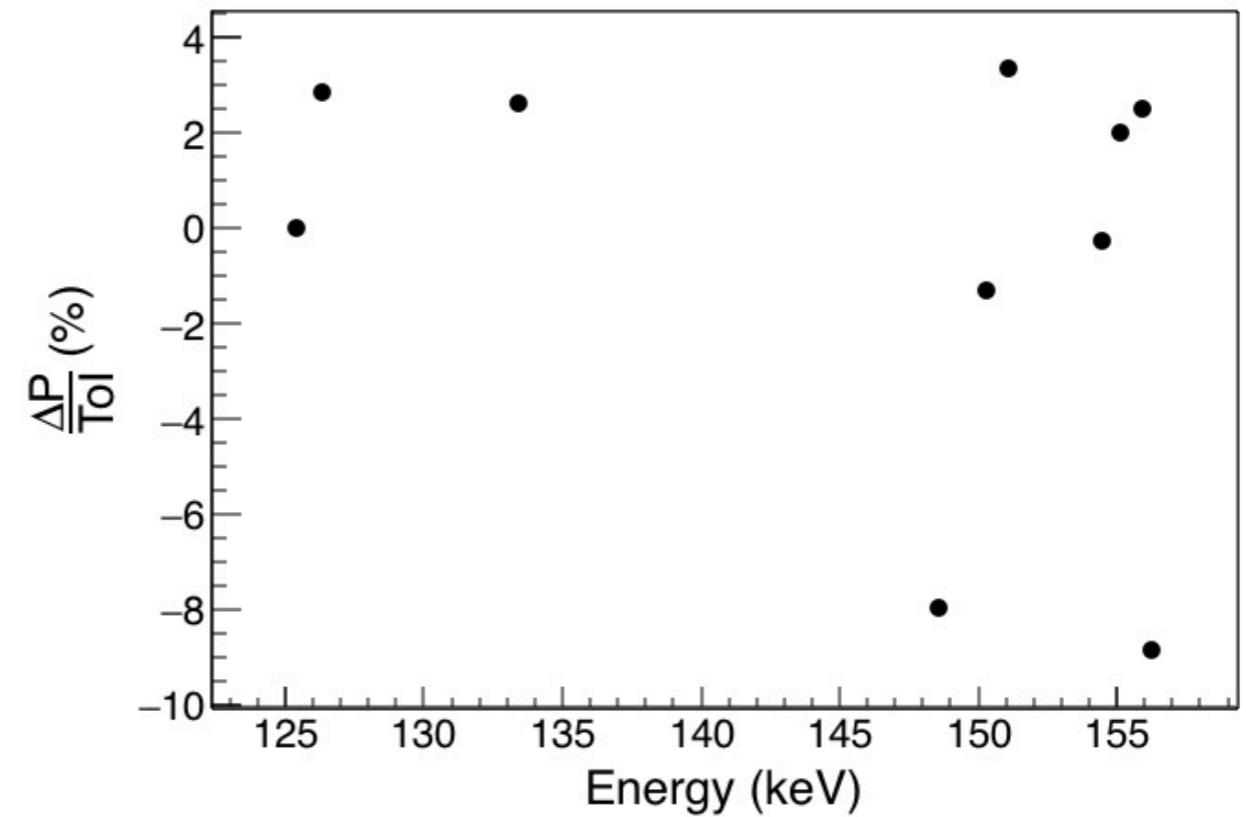
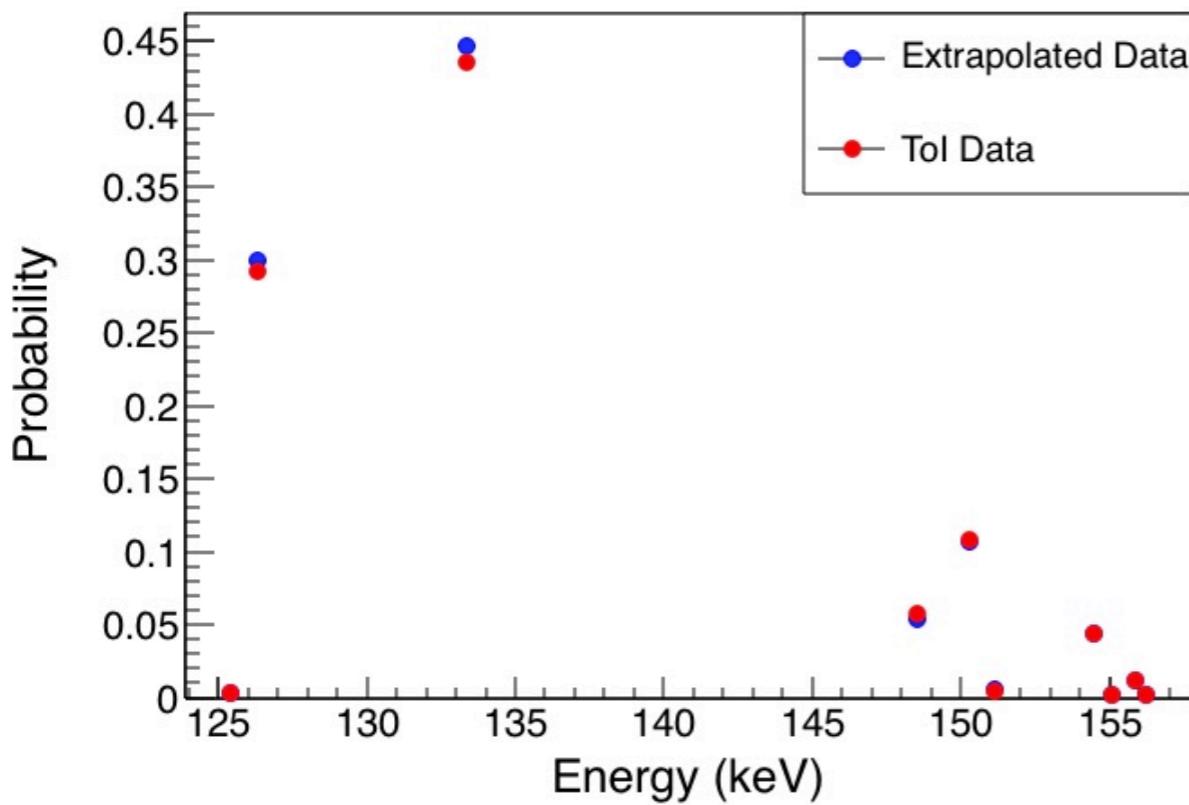
| Initial<br>vacancy<br>subshell | Energy<br>in MeV | Non-<br>Radiative<br>transition<br>probability | Subshell of<br>relaxing<br>electron | Subshell of<br>Auger<br>electron | End of data set |
|--------------------------------|------------------|--|-------------------------------------|----------------------------------|-----------------|
| 1                              | 1                | 1  | 1                                   | 1                                |                 |
| 3                              | 3                | 0.34565300E-02                                 | 0.87436000E-01                      |                                  |                 |
| 3                              | 5                | 0.70246600E-02                                 | 0.88266000E-01                      |                                  |                 |
| 3                              | 6                | 0.19702200E-02                                 | 0.94164000E-01                      |                                  |                 |
| .                              | .                | .  | .                                   |                                  |                 |
| .                              | .                | .  | .                                   |                                  |                 |
| 5                              | 5                | 0.18830300E-03                                 | 0.89096000E-01                      |                                  |                 |
| 5                              | 6                | 0.30001900E-02                                 | 0.94994000E-01                      |                                  |                 |
| 5                              | 8                | 0.13242500E-02                                 | 0.10870800E+00                      |                                  |                 |
| .                              | .                | .  | .                                   |                                  |                 |
| .                              | .                | .  | .                                   |                                  |                 |
| 6                              | 6                | 0.11558800E-02                                 | 0.10089200E+00                      |                                  |                 |
| 6                              | 8                | 0.32593500E-03                                 | 0.11460600E+00                      |                                  |                 |
| 6                              | 10               | 0.54621400E-03                                 | 0.11500200E+00                      |                                  |                 |
| .                              | .                | .  | .                                   |                                  |                 |
| .                              | .                | .  | .                                   |                                  |                 |
| 30                             | 33               | 0.62100000E-07                                 | 0.14227200E+00                      |                                  |                 |
| -1                             | -1               | -1   | -1                                  |                                  |                 |



# Comparison with the values given in the Table of Isotopes

## Z=104

$$\Delta P = \text{Extrapolated} - \text{Tol}$$

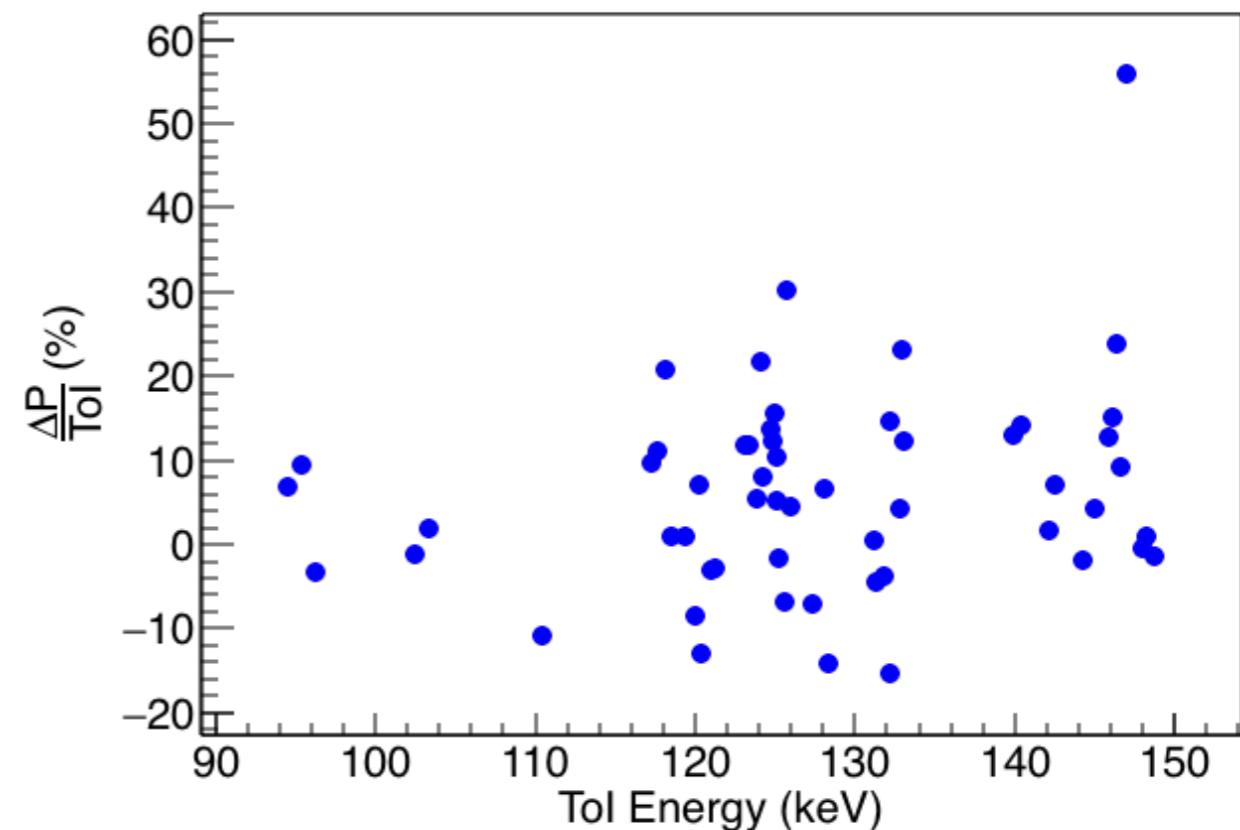
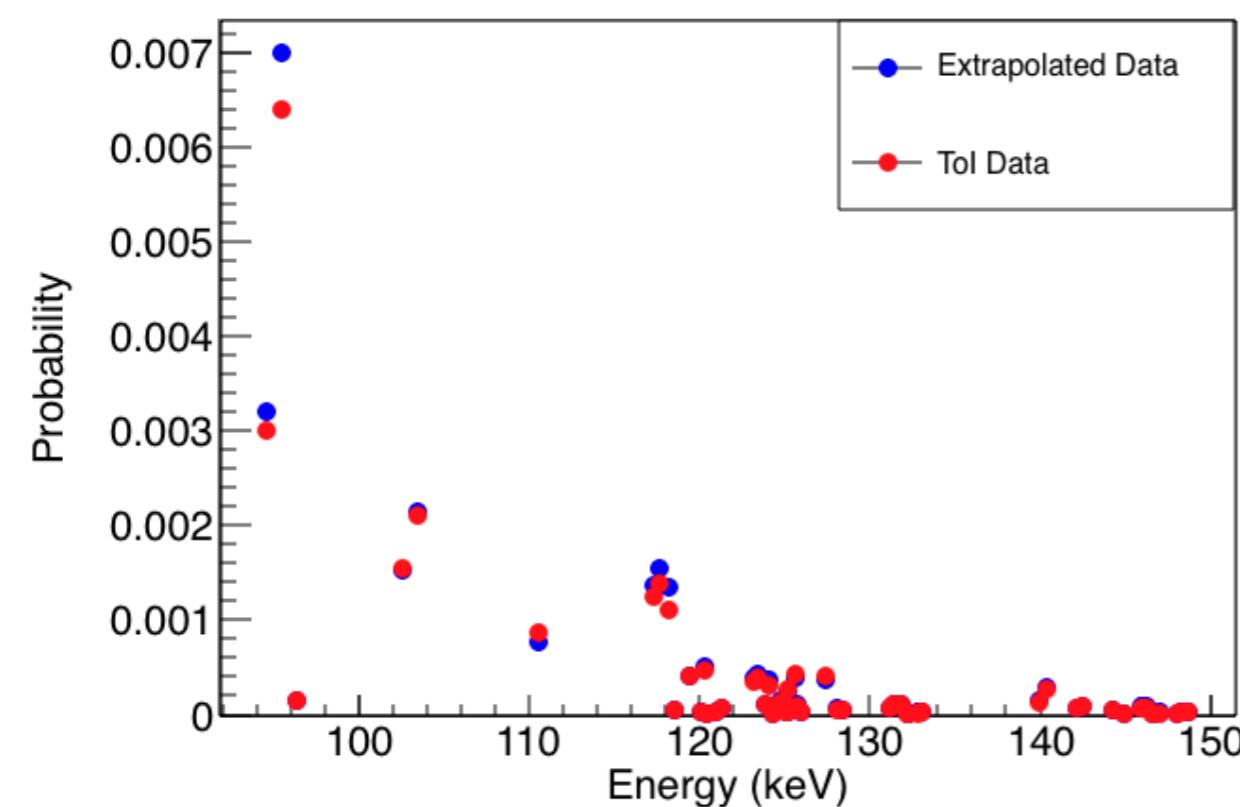


Fluorescence probabilities for a K-shell vacancy in Rf

# Comparison with the values given in the Table of Isotopes

## Z=104

$$\Delta P = \text{Extrapolated} - \text{Tol}$$

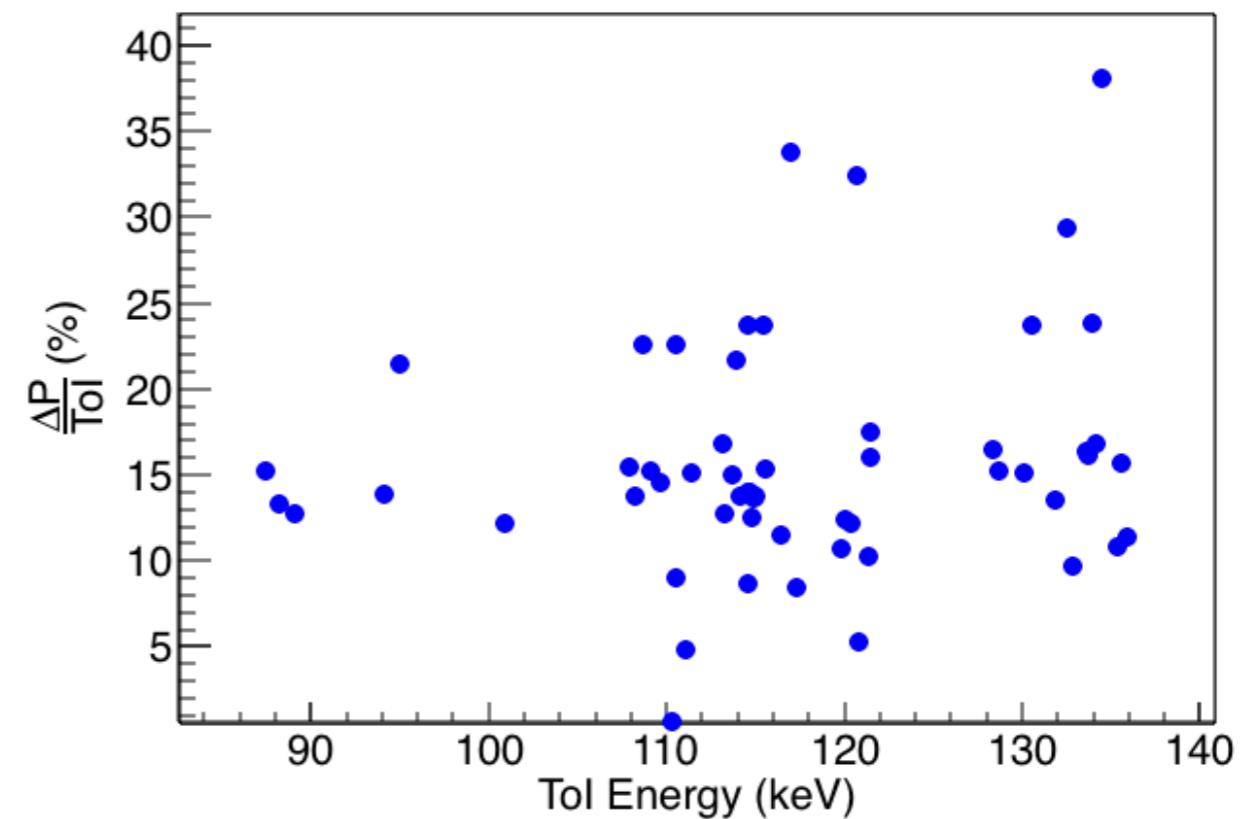
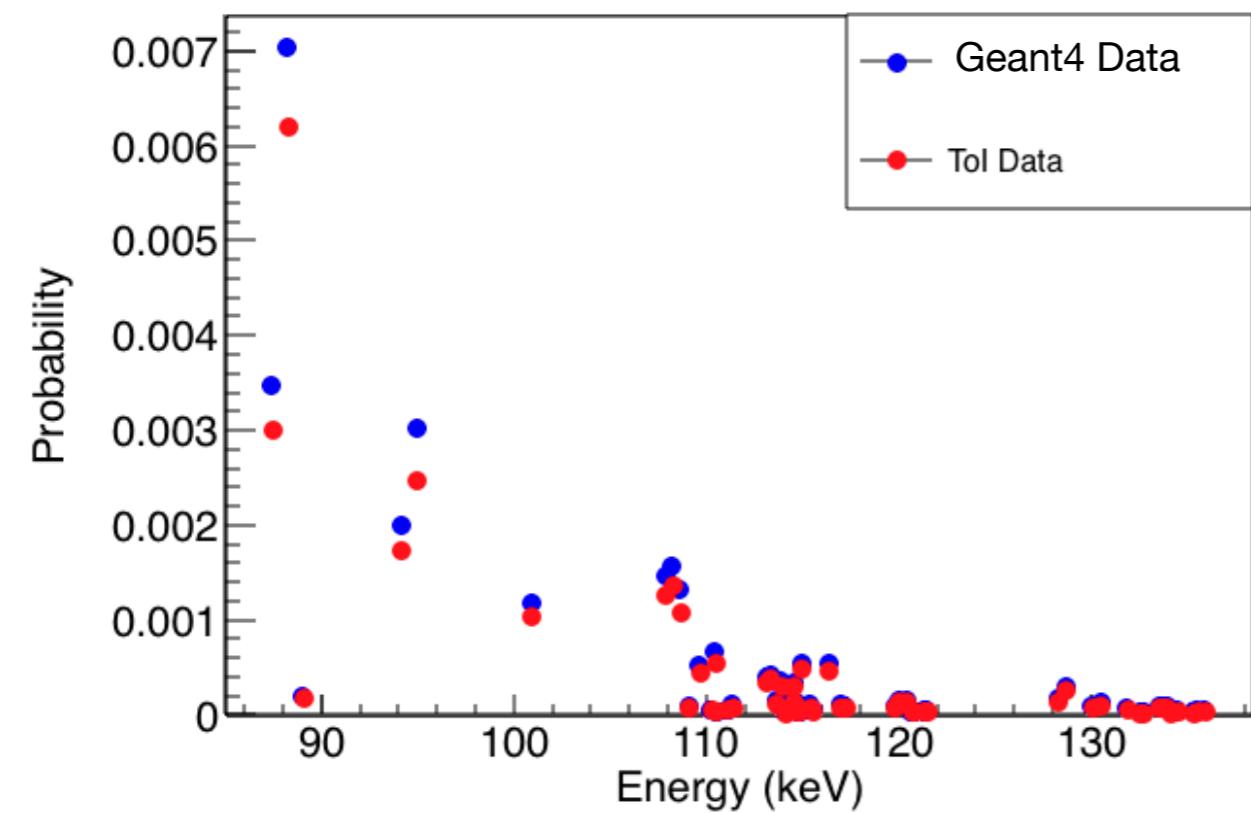


Auger probabilities for a K-shell vacancy in Rf

# Comparison with the values given in the Table of Isotopes

## Z=100

$$\Delta P = Geant4 - ToI$$

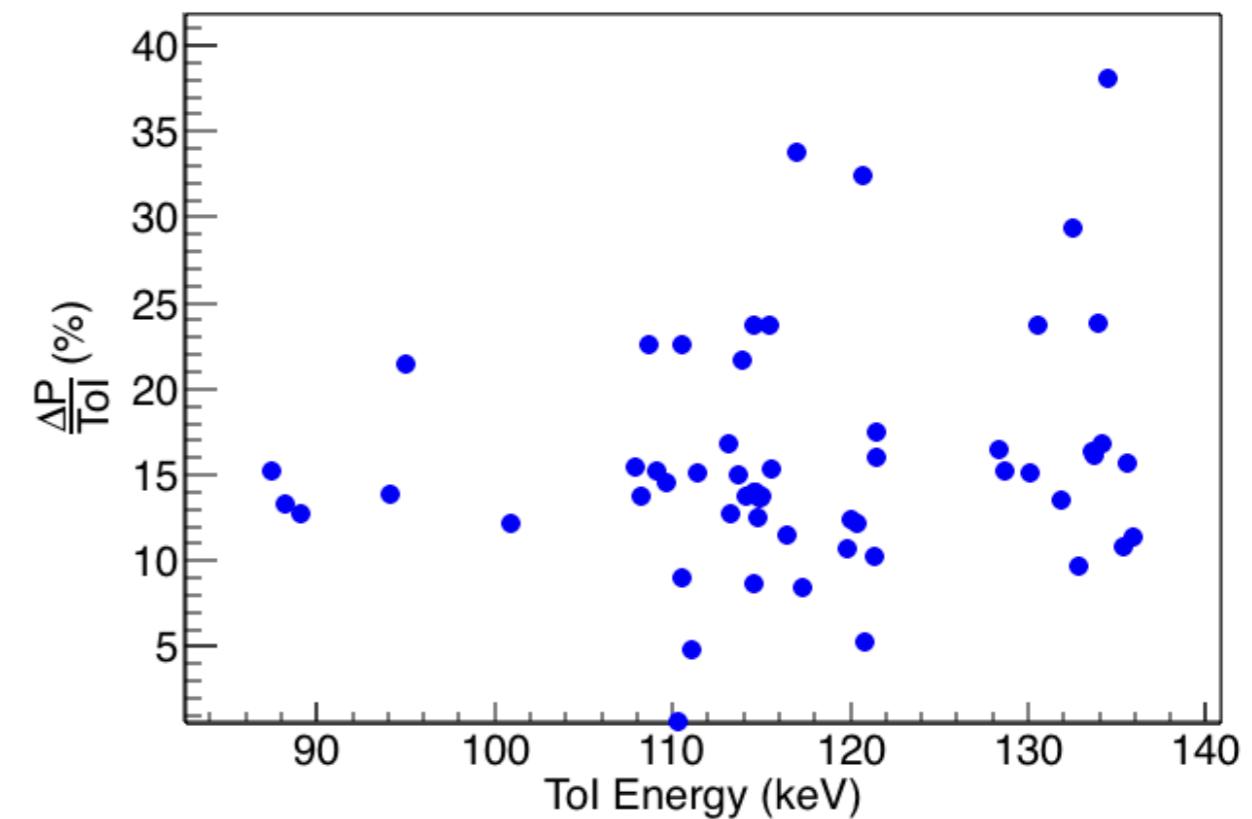
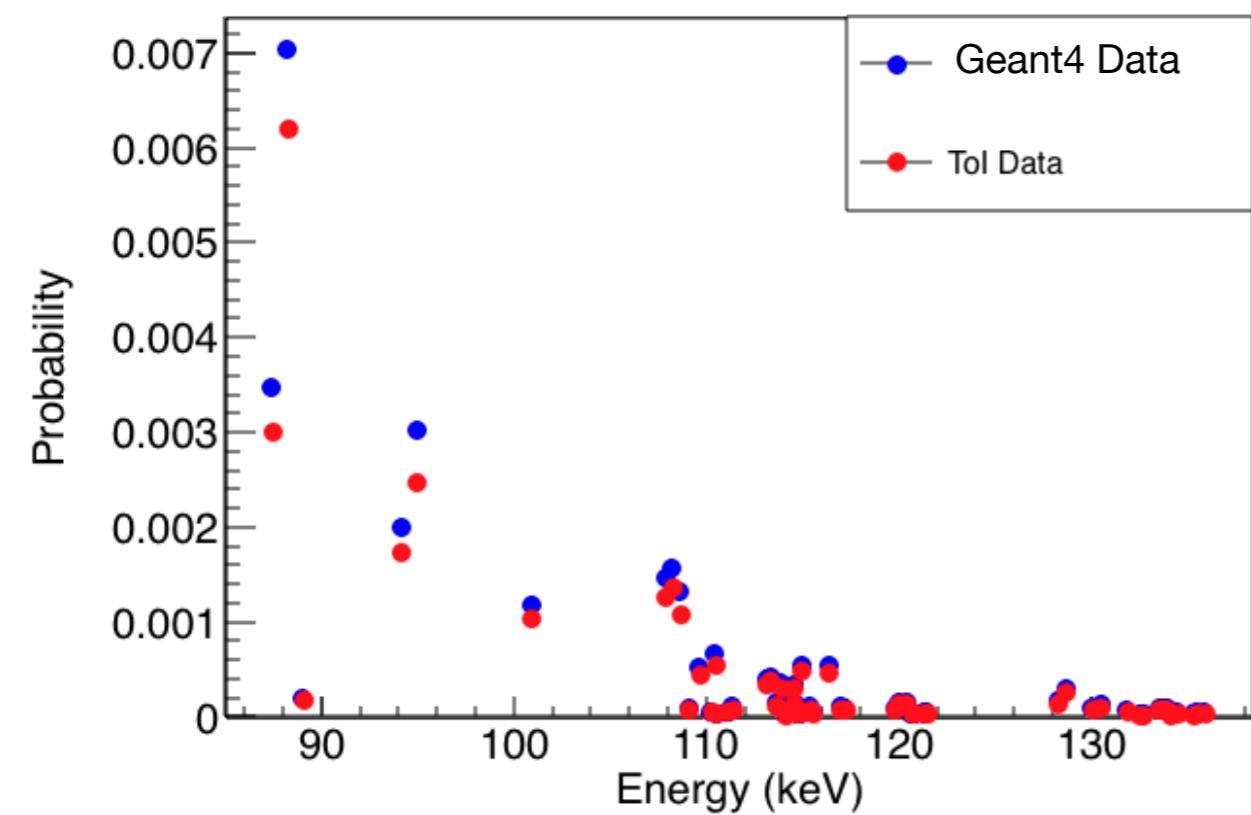


Auger probabilities for a K-shell vacancy in Fm

# Comparison with the values given in the Table of Isotopes

## Z=100

$$\Delta P = Geant4 - ToI$$



Auger probabilities for a K-shell vacancy in Fm

In Geant4

Auger = Auger + Coster-Kronig

# Data Addition

- binding energy information form Tol in G4EMLOW/flour(\_Bearden)/binding.dat
- Fluorescence data in G4EMLOW/flour/ and flour\_Barden/

fl-tr-pr-101.dat

fl-tr-pr-102.dat

fl-tr-pr-103.dat

fl-tr-pr-104.dat

- Auger data in G4EMLOW/auger/

au-tr-pr-101.dat

au-tr-pr-102.dat

au-tr-pr-103.dat

au-tr-pr-104.dat

# Modifications in the source code

## G4ECDecay.cc

```
G4DecayProducts* G4ECDecay::DecayIt(G4double)
{...
.
.
.
if (applyARM) {
    if (atomDeex) {
        G4int aZ = G4MT_daughters[0]->GetAtomicNumber();
        G4int nShells = G4AtomicShells::GetNumberOfShells(aZ);
        if (shellIndex >= nShells) shellIndex = nShells;
        G4AtomicShellEnumerator as = G4AtomicShellEnumerator(shellIndex);
        const G4AtomicShell* shell = atomDeex->GetAtomicShell(aZ, as);
        eBind = shell->BindingEnergy();
        if (atomDeex->IsFluoActive() && aZ > 5 && aZ < 105) {
```

## G4ITDecay.cc

```
G4DecayProducts* G4ITDecay::DecayIt(G4double)
{...
.
.
.
if (applyARM) {
    G4int shellIndex = photonEvaporation->GetVacantShellNumber();
    if (shellIndex > -1) {
        G4VAtomDeexcitation* atomDeex =
            G4LossTableManager::Instance()->AtomDeexcitation();
        if (atomDeex->IsFluoActive() && parentZ > 5 && parentZ < 105) {
```

# Modifications in the source code

## G4ShellData.hh

```
G4ShellData(G4int minZ = 1, G4int maxZ = 104, G4bool isOccupancy = false);
```

## G4AtomicTransitionManager.cc

```
G4AtomicTransitionManager::G4AtomicTransitionManager()
: augerData(0),
zMin(1),
zMax(104),
infTableLimit(6),
supTableLimit(104),
isInitialized(false),
verboseLevel(0)
```

## G4AugerData.cc

```
G4AugerData::G4AugerData()
{
    G4int n = 0;
    G4int pos = 0;

    for (pos = 0 ; pos < 105; pos++)
    {
        number0fVacancies.push_back(n);
    }

    BuildAugerTransitionTable();
}

void G4AugerData::BuildAugerTransitionTable()
{
    for (G4int element = 6; element < 105; element++)
    {
        augerTransitionTable.insert(trans_Table::value_type(element, LoadData(element)));
    }
}
```

# Modifications in the source code

## G4UAtomicDeexcitation.cc

```
void G4UAtomicDeexcitation::GenerateParticles(
    std::vector<G4DynamicParticle*>*> vectorOfParticles,
    const G4AtomicShell* atomicShell,
    G4int Z,
    G4double gammaCut,
    G4double eCut)
{..
    // let's check that 5<Z<100
    if (Z>5 && Z<105) {
        ...
        if (IsAugerCascadeActive())
        {
            //-----
            vacancyArray.push_back(givenShellId);

            // let's check that 5<Z<100
            if (Z<6 || Z>104){
                //G4Exception("G4UAtomicDeexcitation::GenerateParticles()", "de0001", JustWarning, "Energy
deposited locally");
                return;
            }
        }
    }
}
```

# Modifications in the source code

## G4GammaTransition.cc

```
G4Fragment*  
G4GammaTransition::SampleTransition(G4Fragment* nucleus,  
                                     G4double newExcEnergy,  
                                     G4double mpRatio,  
                                     G4int  JP1,  
                                     G4int  JP2,  
                                     G4int  MP,  
                                     G4int  shell,  
                                     G4bool isDiscrete,  
                                     G4bool isGamma)  
{  
    G4Fragment* result = nullptr;  
    G4double bond_energy = 0.0;  
  
    if (!isGamma) {  
        if(0 <= shell) {  
            G4int Z = nucleus->GetZ_asInt();  
            if(Z <= 104) {
```

# Modifications in the source code

G4AtomicShells.hh

```
static const G4int fNumberOfShells[105];
static const G4int fIndexOfShells[105];
static const G4int fNumberOfElectrons[1650];
static const G4double fBindingEnergies[1650];
```

G4AtomicShells.cc

```
G4AtomicShells::fNumberOfShells[105]{
...
}
const G4int G4AtomicShells::fIndexOfShells[105] =
{
...
1540, 1567, 1594, 1622
}
const G4double G4AtomicShells::fBindingEnergies[1650] =
{
...
// Md -----
146526.0 , 28387.0 , 27438.0 , 21356.0 , 7440.0 , 7001.0 , 5552.0 , 4889.0 ,
4615.0 , 2024.0 , 1816.0 , 1424.0 , 1105.0 , 1034.0 , 618.0 , 597.0 ,
471.0 , 389.0 , 272.0 , 154.0 , 137.0 , 12.9 , 10.5 , 61.0 ,
37.0 , 17.0 , 5.9 , -----
// No -----
149208.0 , 29221.0 , 28255.0 , 21851.0 , 7678.0 , 7231.0 , 5702.0 , 5028.0 ,
4741.0 , 2097.0 , 1885.0 , 1469.0 , 1145.0 , 1070.0 , 645.0 , 624.0 ,
490.0 , 406.0 , 280.0 , 161.0 , 142.0 , 13.6 , 11.1 , 63.0 ,
38.0 , 18.0 , 6.0 , -----
// Lr -----
152970.0 , 30083.0 , 29103.0 , 22359.0 , 7930.0 , 7474.0 , 5860.0 , 5176.0 ,
4876.0 , 2180.0 , 1963.0 , 1523.0 , 1192.0 , 1112.0 , 680.0 , 658.0 ,
516.0 , 429.0 , 296.0 , 174.0 , 154.0 , 19.9 , 17.0 , 71.0 ,
44.0 , 21.0 , 3.9 , 6.9 , -----
// Rf -----
156288.0 , 30881.0 , 29986.0 , 22907.0 , 8161.0 , 7738.0 , 6009.0 , 5336.0 ,
5014.0 , 2237.0 , 2035.0 , 1554.0 , 1233.0 , 1149.0 , 725.0 , 701.0 ,
535.0 , 448.0 , 319.0 , 190.0 , 171.0 , 26.0 , 22.8 , 82.0 ,
55.0 , 33.0 , 5.0 , 7.5
}
```

```
const G4int G4AtomicShells::fNumberOfElectrons[1650] =
```

```
{
...
// Md --
2, 2, 2, 4, 2, 2, 4, 4, 6, 2, 2, 4, 4, 6, 6, 8, 2, 2, 4, 4, 6, 6, 7, 2, 2, 4, 2, //=101
// No -
2, 2, 2, 4, 2, 2, 4, 4, 6, 2, 2, 4, 4, 6, 6, 8, 2, 2, 4, 4, 6, 6, 8, 2, 2, 4, 2, //=102
// Lr -
2, 2, 2, 4, 2, 2, 4, 4, 6, 2, 2, 4, 4, 6, 6, 8, 2, 2, 4, 4, 6, 6, 8, 2, 2, 4, 1, 2, //=103
// Rf -
2, 2, 2, 4, 2, 2, 4, 4, 6, 2, 2, 4, 4, 6, 6, 8, 2, 2, 4, 4, 6, 6, 8, 2, 2, 4, 2, 2 //=104
}
```

```
G4int G4AtomicShells::GetNumberOfElectrons(G4int Z, G4int ShellNb), G4double G4AtomicShells::GetTotalBindingEnergy(G4int Z)
if(Z<0 || Z>104)
```

Electron Binding energy from Table of Isotopes 8th  
Electron Configuration from CRC Handbook of Chemistry and Physics 8th Ed

# EM classes that do (not) work after modifications

| c1                          | c2                          |
|-----------------------------|-----------------------------|
| G4EmStandardPhysics_option4 | G4EmStandardPhysics_option1 |
| G4EmLivermorePhysics        | G4EmStandardPhysics_option2 |
| G4EmLowEPPhysics            | G4EmStandardPhysics_option3 |
|                             | G4EmStandardPhysics         |
|                             | G4EmStandardPhysicsGS       |
|                             | G4EmStandardPhysicsSS       |
|                             | G4EmStandardPhysicsWVI      |
|                             | G4EmPenelopePhysics         |

Table C.1: Built-in EM physics lists that can (c1) and cannot (c2) be used.

| EM process            | c1   | c2   |
|-----------------------|--|--|
| Photo-electric effect | G4PolarizedPEEffectModel   | G4PEEffectFluoModel<br>G4LivermorePhotoElectricModel<br>G4LivermorePolarizedPhotoElectricModel<br>G4PenelopePhotoElectricModel   |
| Compton scattering    | G4LivermoreComptonModel<br>G4LivermorePolarizedComptonModel<br>G4LowEPComptonModel<br>G4LivermoreComptonModelRC* | G4KleinNishinaCompton<br>G4KleinNishinaModel<br>G4PenelopeComptonModel<br>G4PolarizedComptonModel  |
| Gamma conversion      | G4BetheHeitler5DModel*   | G4BetheHeitlerModel<br>G4PairProductionRelModel<br>G4LivermoreGammaConversionModel<br>G4BoldyshevTripletModel<br>G4LivermoreNuclearGammaConversionModel<br>G4LivermorePolarizedGammaConversionModel<br>G4PolarizedGammaConversionModel |
| Rayleigh scattering   | G4JAEAElasticScatteringModel*  | G4LivermoreRayleighModel<br>G4PenelopeRayleighModel<br>G4LivermorePolarizedRayleighModel   |
| e-ionization          | G4PAIModel<br>G4PAIPhotModel   | G4PenelopeIonisationModel<br>G4MollerBhabhaModel<br>G4LivermoreIonisationModel<br>G4PolarizedMollerBhabhaModel   |
| $\mu$ ionisation      |  | G4MuBetheBlochModel  |
| ion Ionisation        | G4LindhardSorensenIonModel*<br>G4AtimaEnergyLossModel*   | G4IonParametrisedLossModel<br>G4BetheBlochModel<br>G4BetheBlochIonGasModel<br>G4BraggIonModel<br>G4BraggIonGasModel  |
| eBremsstrahlung       | G4PolarizedBremsstrahlungModel*  | G4PenelopeBremsstrahlungModel<br>G4SeltzerBergerModel<br>G4eBremsstrahlungRelModel<br>G4LivermoreBremsstrahlungModel   |

Table C.2: Models that can (c1) and cannot (c2) be used for  $Z > 100$ . The models indicated by '\*' do not exist in the GEANT4 version used for this work.

# EM classes that do (not) work after modifications

| c1                          | c2                          |
|-----------------------------|-----------------------------|
| G4EmStandardPhysics_option4 | G4EmStandardPhysics_option1 |
| G4EmLivermorePhysics        | G4EmStandardPhysics_option2 |
| G4EmLowEPPhysics            | G4EmStandardPhysics_option3 |
|                             | G4EmStandardPhysics         |
|                             | G4EmStandardPhysicsGS       |
|                             | G4EmStandardPhysicsSS       |
|                             | G4EmStandardPhysicsWVI      |
|                             | G4EmPenelopePhysics         |

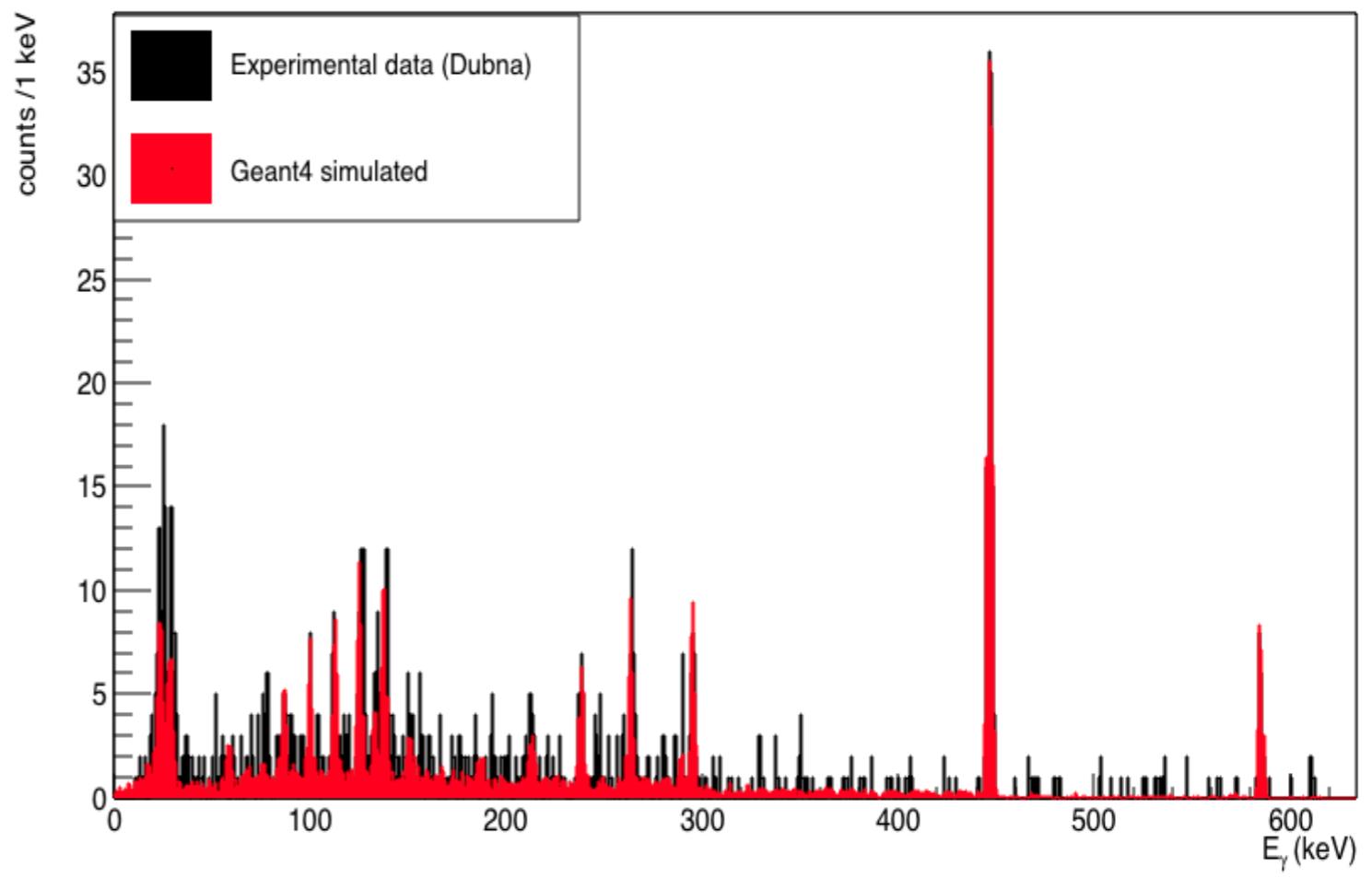
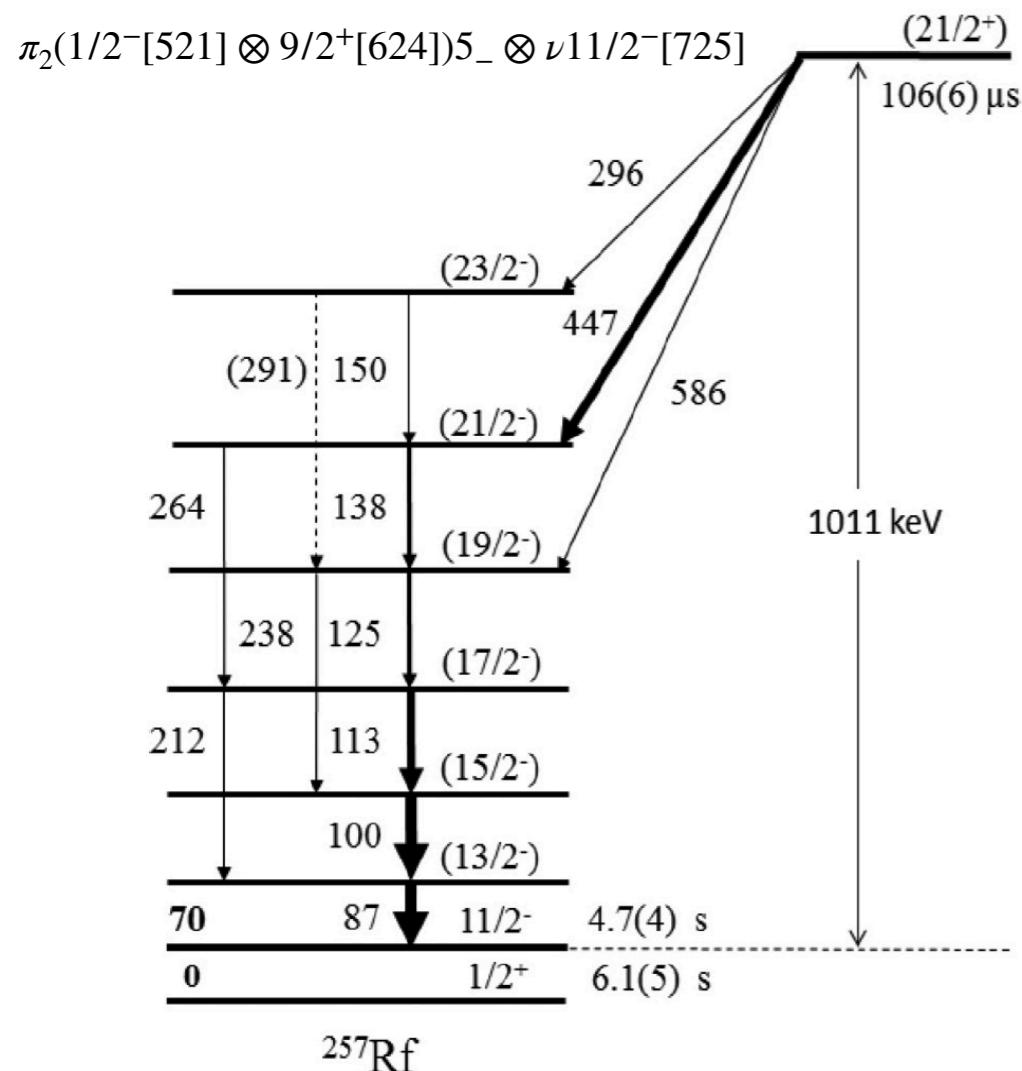
Table C.1: Built-in EM physics lists that can (c1) and cannot (c2) be used.

## Build your own EM Physics list

| EM process            | c1   | c2   |
|-----------------------|--|--|
| Photo-electric effect | G4PolarizedPEEffectModel   | G4PEEffectFluoModel<br>G4LivermorePhotoElectricModel<br>G4LivermorePolarizedPhotoElectricModel<br>G4PenelopePhotoElectricModel   |
| Compton scattering    | G4LivermoreComptonModel<br>G4LivermorePolarizedComptonModel<br>G4LowEPComptonModel<br>G4LivermoreComptonModelRC* | G4KleinNishinaCompton<br>G4KleinNishinaModel<br>G4PenelopeComptonModel<br>G4PolarizedComptonModel  |
| Gamma conversion      | G4BetheHeitler5DModel*   | G4BetheHeitlerModel<br>G4PairProductionRelModel<br>G4LivermoreGammaConversionModel<br>G4BoldyshevTripletModel<br>G4LivermoreNuclearGammaConversionModel<br>G4LivermorePolarizedGammaConversionModel<br>G4PolarizedGammaConversionModel |
| Rayleigh scattering   | G4JAEAElasticScatteringModel*  | G4LivermoreRayleighModel<br>G4PenelopeRayleighModel<br>G4LivermorePolarizedRayleighModel   |
| e-ionization          | G4PAIModel<br>G4PAIPhotModel   | G4PenelopeIonisationModel<br>G4MollerBhabhaModel<br>G4LivermoreIonisationModel<br>G4PolarizedMollerBhabhaModel   |
| $\mu$ ionisation      |  | G4MuBetheBlochModel  |
| ion Ionisation        | G4LindhardSorensenIonModel*<br>G4AtimaEnergyLossModel*   | G4IonParametrisedLossModel<br>G4BetheBlochModel<br>G4BetheBlochIonGasModel<br>G4BraggIonModel<br>G4BraggIonGasModel  |
| eBremsstrahlung       | G4PolarizedBremsstrahlungModel*  | G4PenelopeBremsstrahlungModel<br>G4SeltzerBergerModel<br>G4eBremsstrahlungRelModel<br>G4LivermoreBremsstrahlungModel   |

Table C.2: Models that can (c1) and cannot (c2) be used for  $Z > 100$ . The models indicated by '\*' do not exist in the GEANT4 version used for this work.

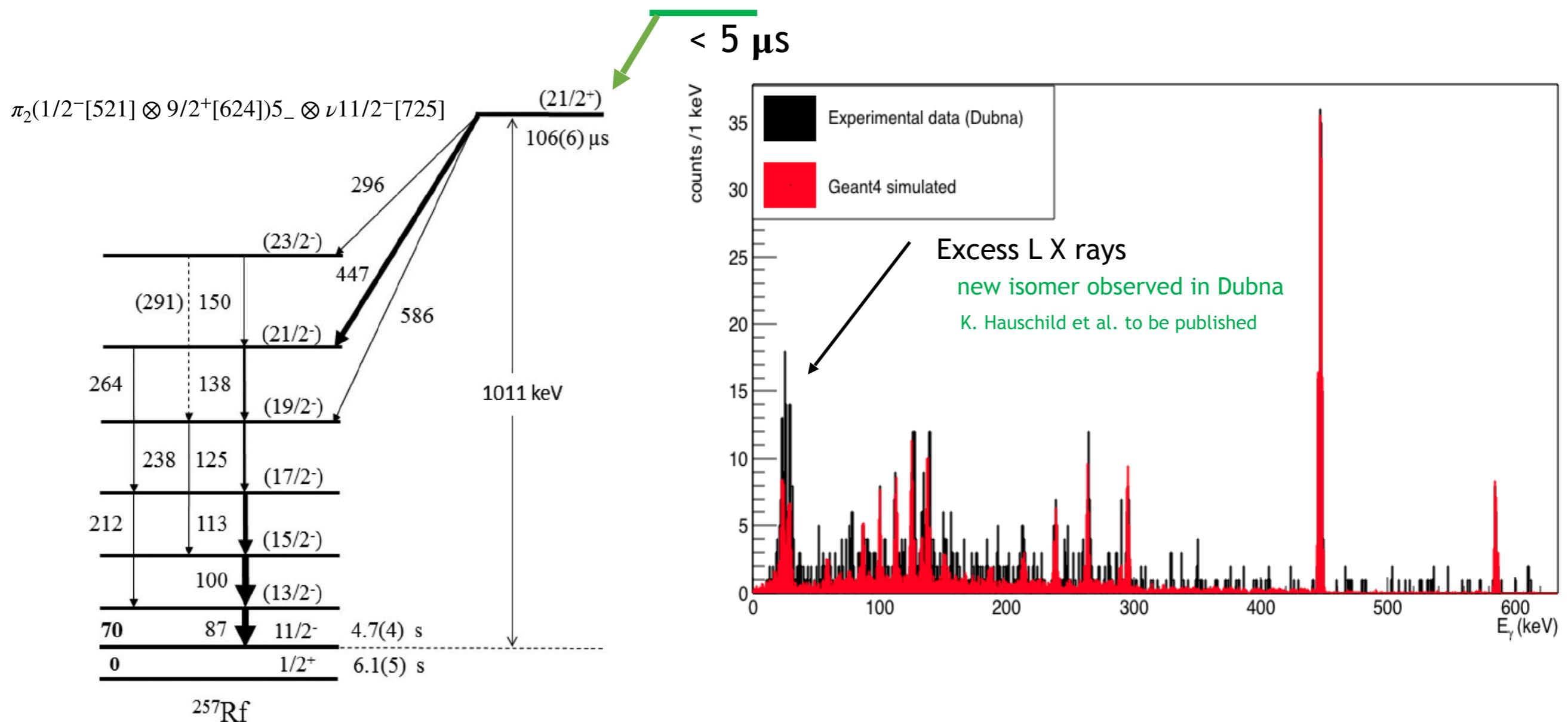
# Test of the modified code



J. Rissanen et al., Phys. Rev C **88**, 044313 (2013)

Geant4 simulations of the isomer decay observed in Dubna confirm the Berkeley decay scheme.

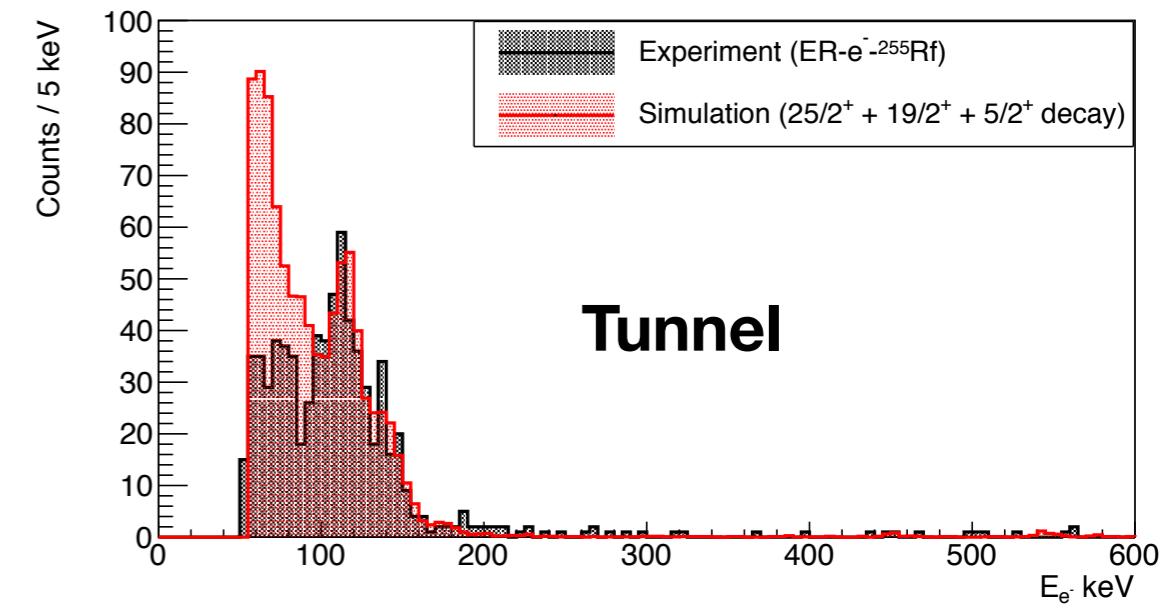
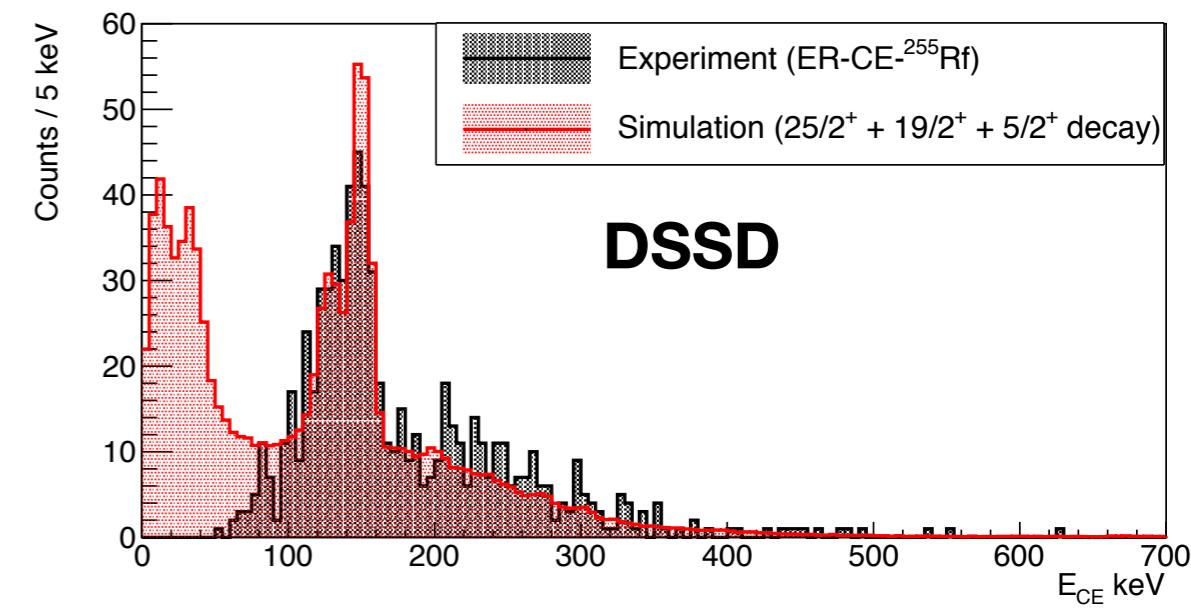
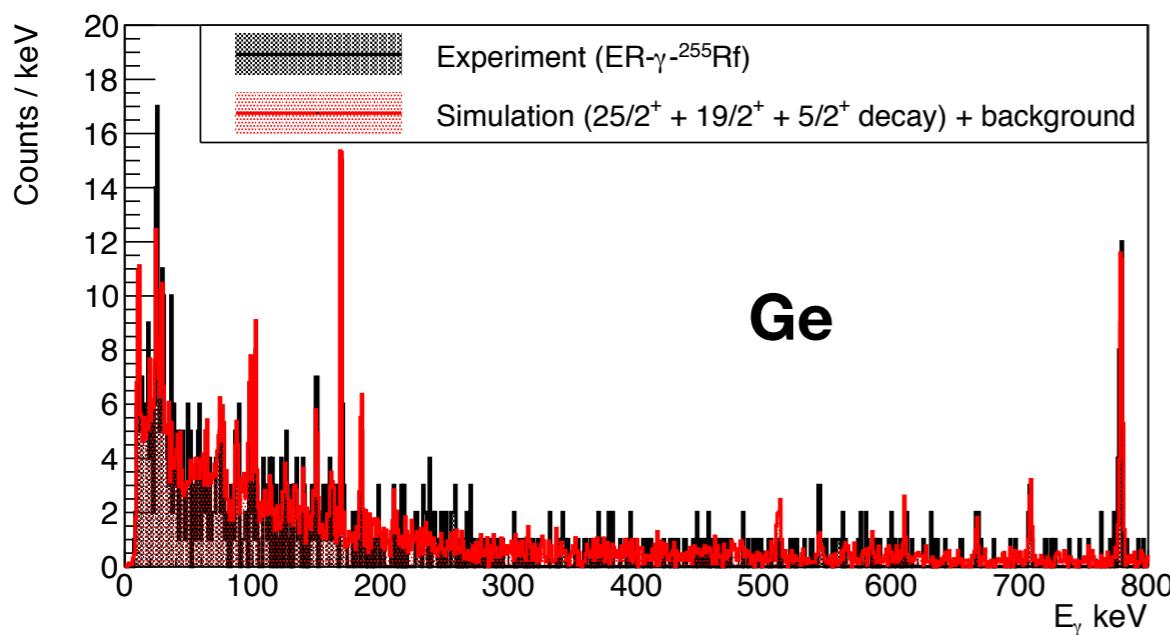
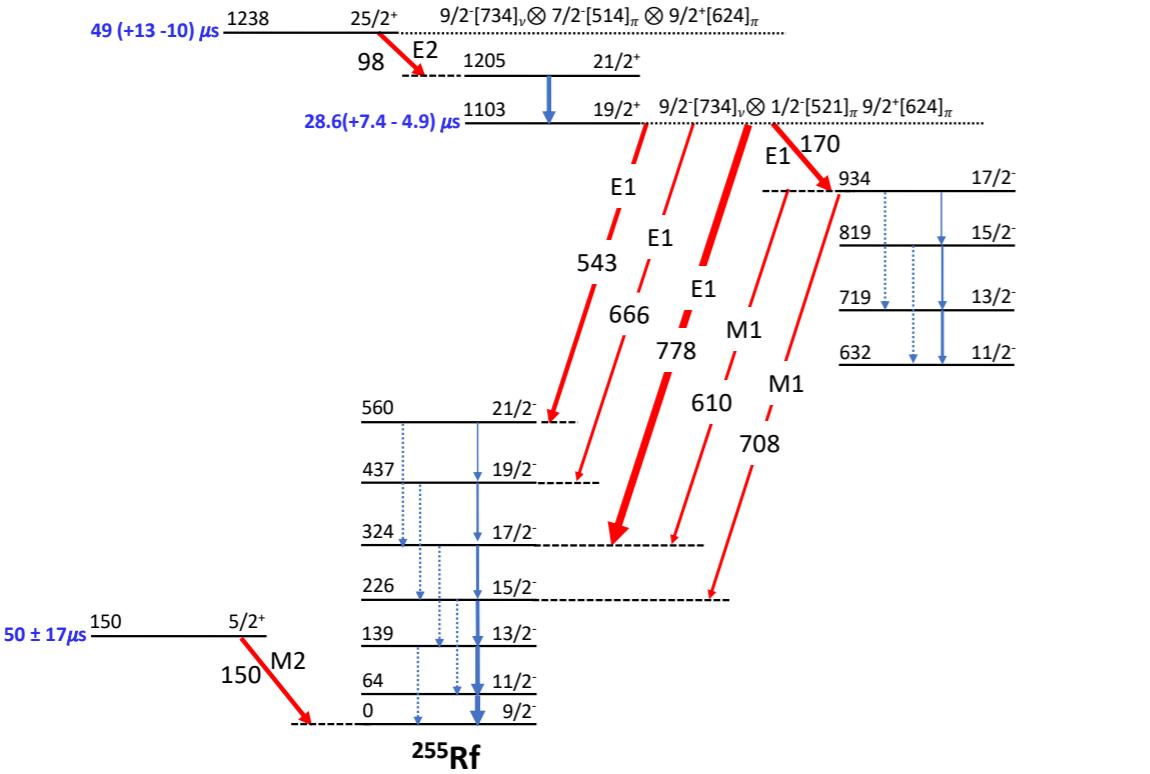
# Test of the modified code



J. Rissanen et al., Phys. Rev C **88**, 044313 (2013)

Geant4 simulations of the isomer decay observed in Dubna confirm the Berkeley decay scheme.

# Geant4 Simulation of isomeric decays in $^{255}\text{Rf}$



# Conclusions and outlook

- Geant4 is very useful in analysing data
- Extrapolated Auger and Fluorescence data and made some modifications in the source code
- Modified code tested against experimental data
- Use JAC to calculate the atomic properties for superheavy elements
- Extend the code for  $Z > 104$

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## Atomic properties

- Hyperfine splitting & representation
- Zeeman splitting; Lande factors
- Isotope shifts
- Atomic form factors
- Plasma shifts,  $\alpha$ -variations, ...

## Atomic processes

- Photon emission & transition probabilities
- Photoexcitation, ionization & recombinat.
- Auger emission & di-electr. recombination
- Rayleigh-Compton scattering
- Multiphoton (de-) excitation, ...

## Atomic cascades

- Average singe-configuration approach
- Multiple-configuration approach
- Incorporation of shake-up & shake-off
- Ion & electron distributions, ...

## Interactive High-Level Language

### JAC

#### Jena Atomic Calculator

A Julia implementation for atomic computations.

## Atomic responses

- Field-induced processes & ionization
- High-harmonic generation
- Particle-impact processes
- Charge exchange

## Time evolution

- Liouville equation for statistical tensors & atomic density matrices
- Atoms in intense light pulses
- Angle- & polarization-dependent observables

## Semi-empirical estimates

- Weak-field ionization rates
- Asymptotic behaviour & formulas
- Stopping powers
- Plasma Stark broadening, ...

Open-source applications  
in physics, science and  
technology.

# Thank you for your attention

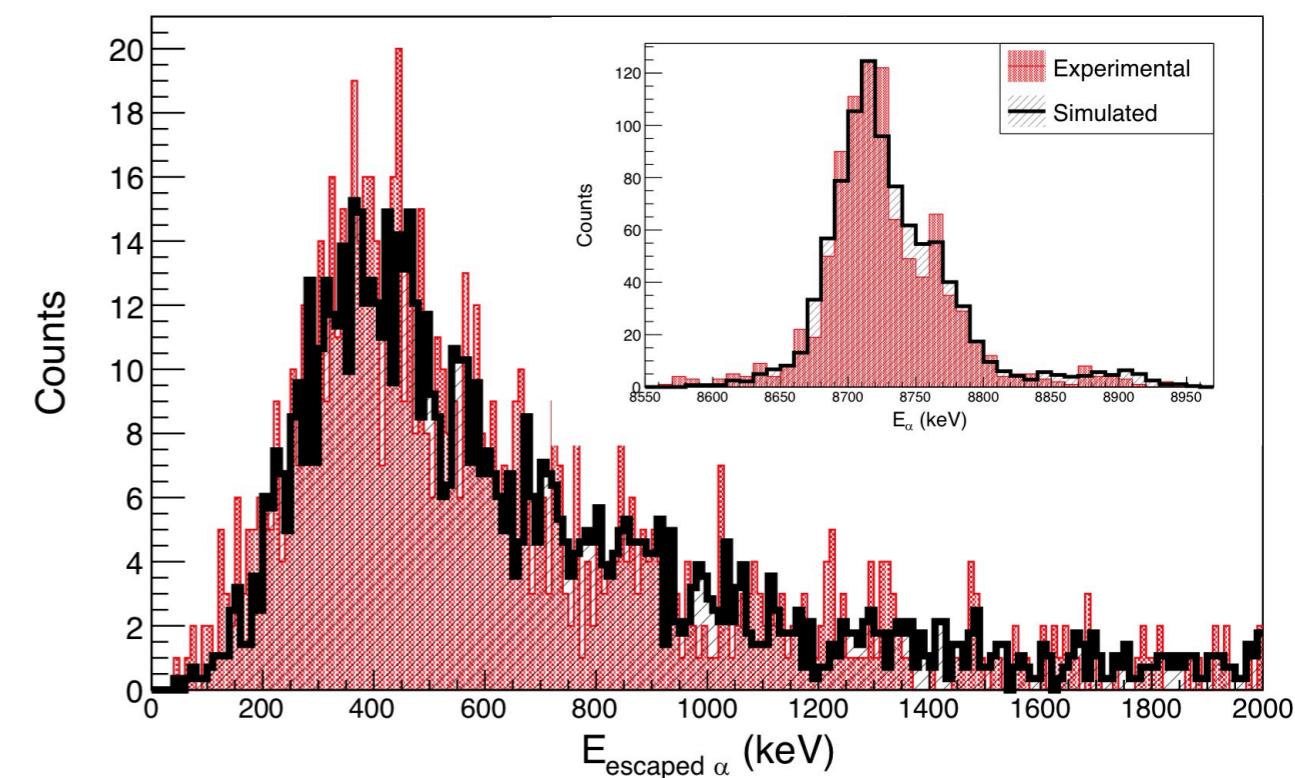
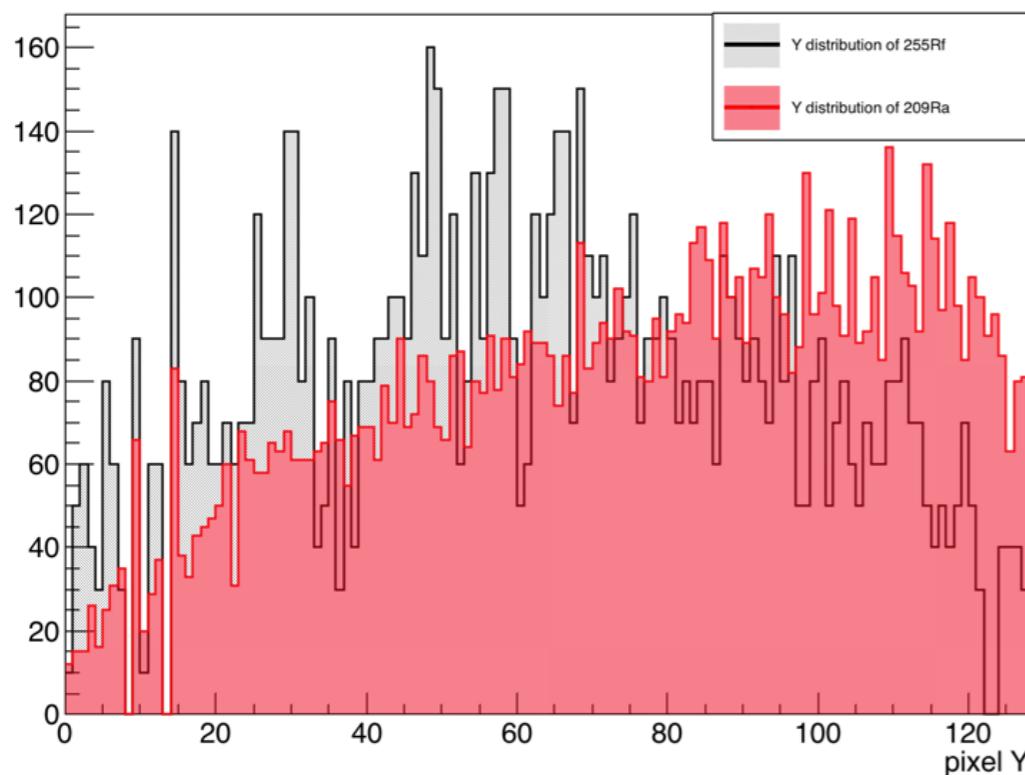
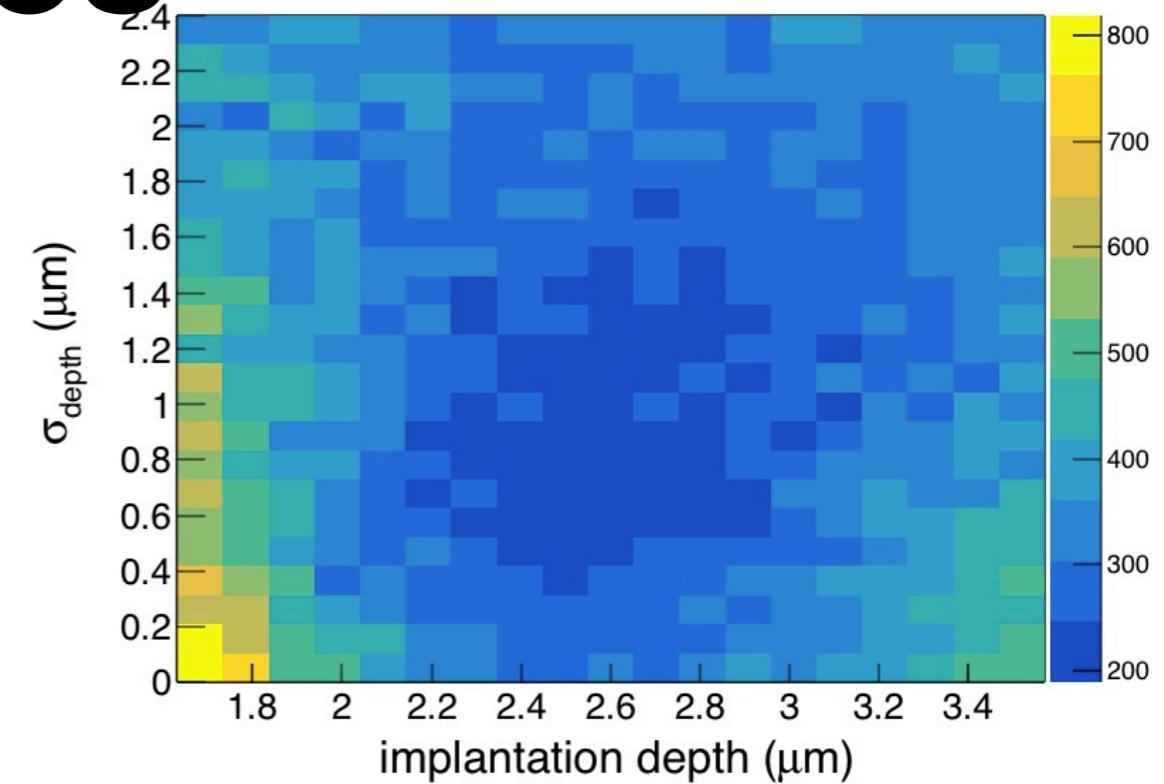
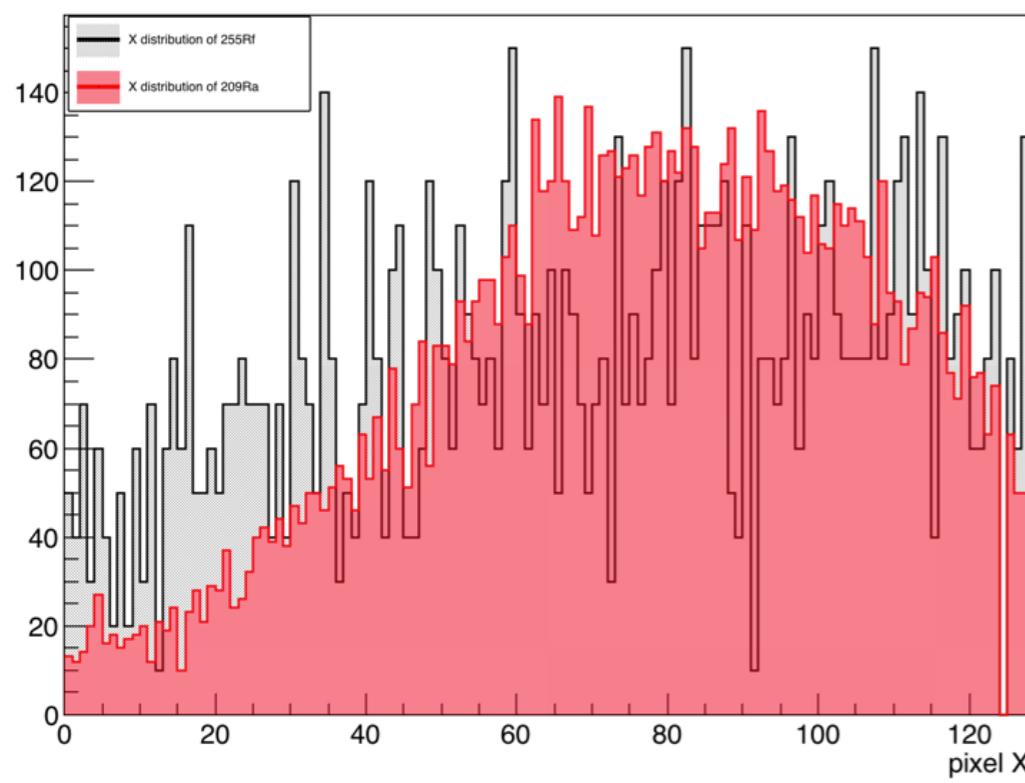


Araceli Lopez-Martens



Karl Hauschild

# Position distribution of the sources



# Radioactive decays in Geant4

