

# Fully microscopic scission-point model to predict fission fragment observables : SPY model

J.-F. Lemaître

Institut d'Astronomie et d'Astrophysique - Brussels University

Collaborators: S. Goriely, S. Hilaire, J.-L. Sida

# Energy production applications

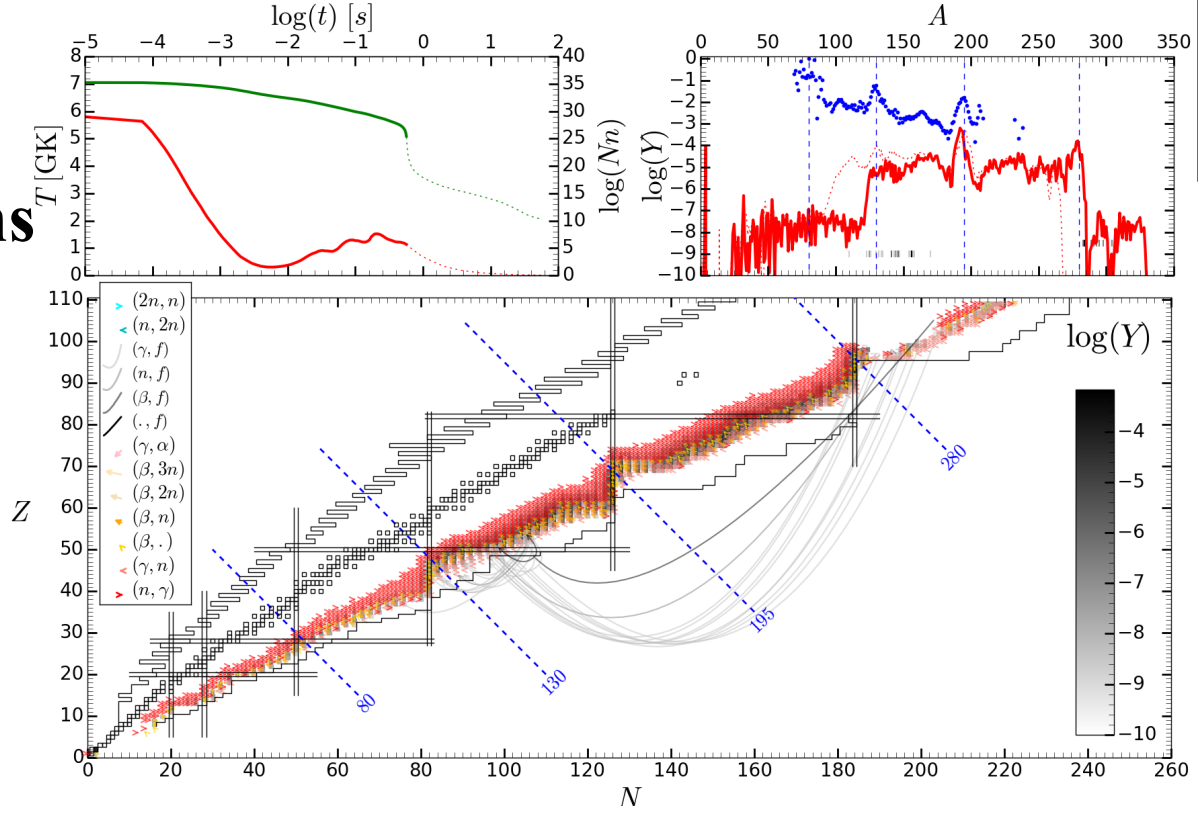
- nuclear power reactors
- nuclear waste recycling

# Astrophysics (NS ejecta)

- rapid neutron-capture process

# Nuclear physics

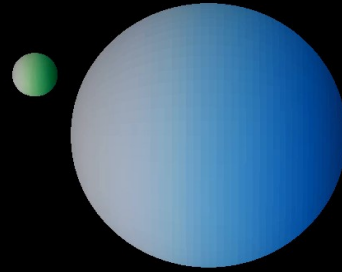
- static & dynamic properties
- neutron rich nuclei production



- \* **Fission process**
- \* **SPY model**
- \* **Results**
- \* **Pu240**
- \* **Systematic**

# Fission process

neutron capture

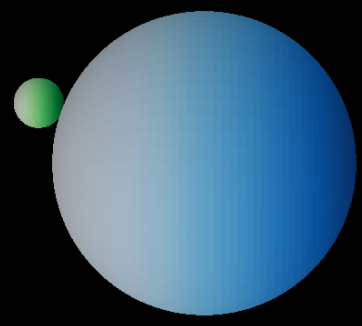


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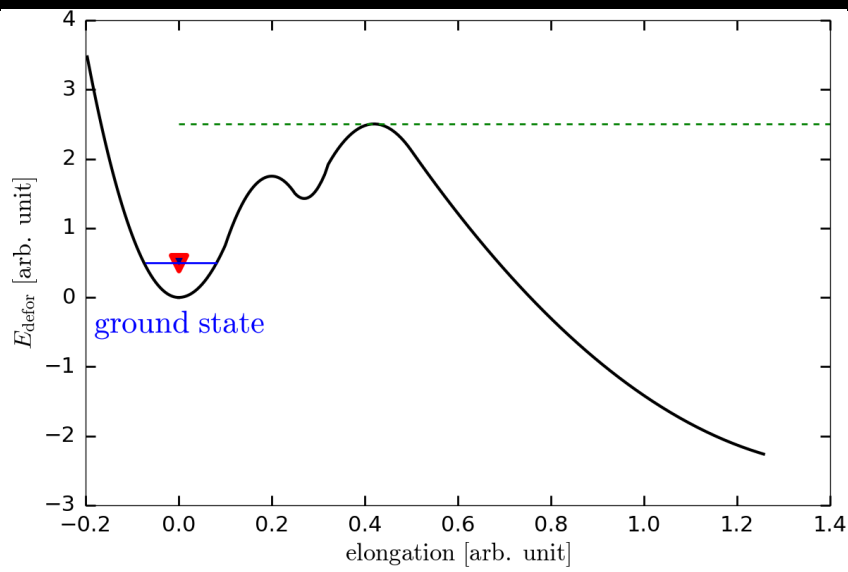
# Fission process

compound nucleus formation

$t = 0$  [s]

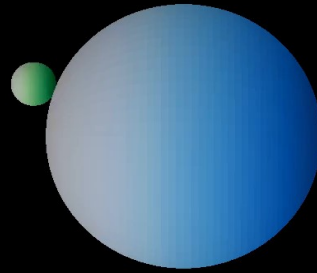


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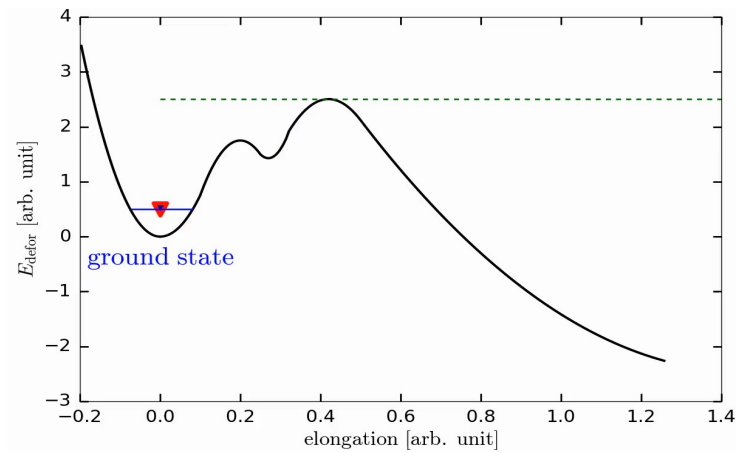


compound nucleus formation

$t = 0$  [s]

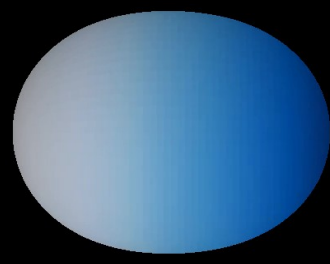


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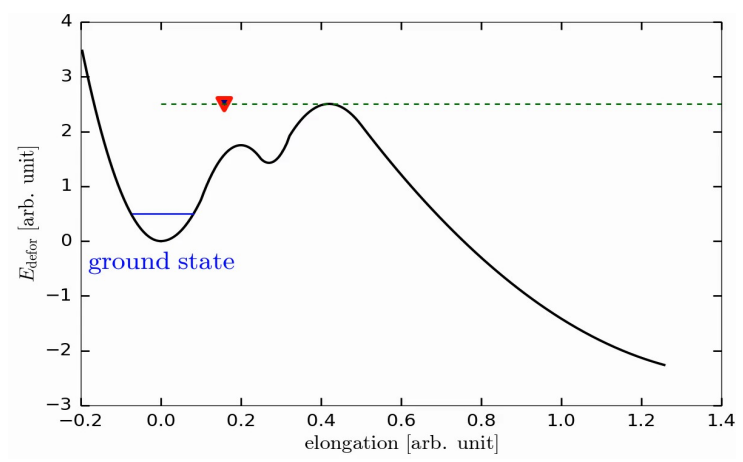


# Fission process

compound nucleus deformation  $0 < t < 10^{-19}$  [s]



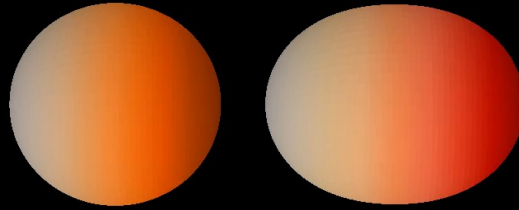
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# Fission process

nucleus scission

$t = 10^{-19}$  [s]



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# Fission process

fragments flying away from one another



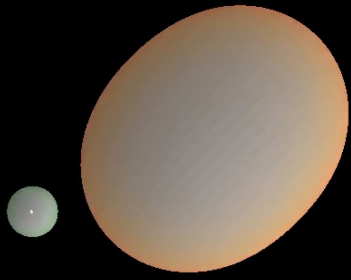
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# Fission process

neutron evaporation

$$t = 10^{-17} \text{ [s]}$$



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# Fission process

gamma evaporation

$t = 10^{-14}$  [s]



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# Fission process

beta evaporation

$t > 10^{-6}$  [s]

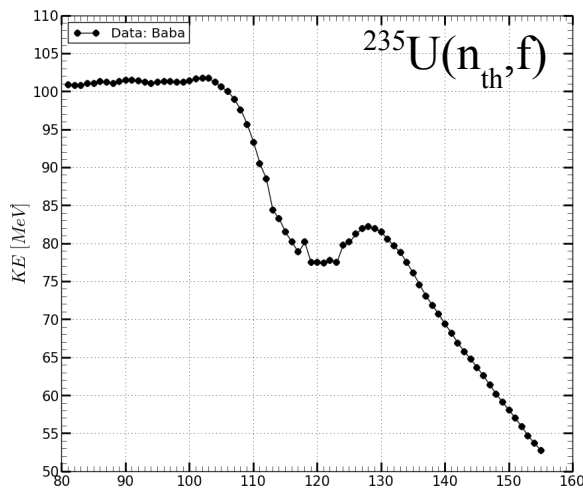


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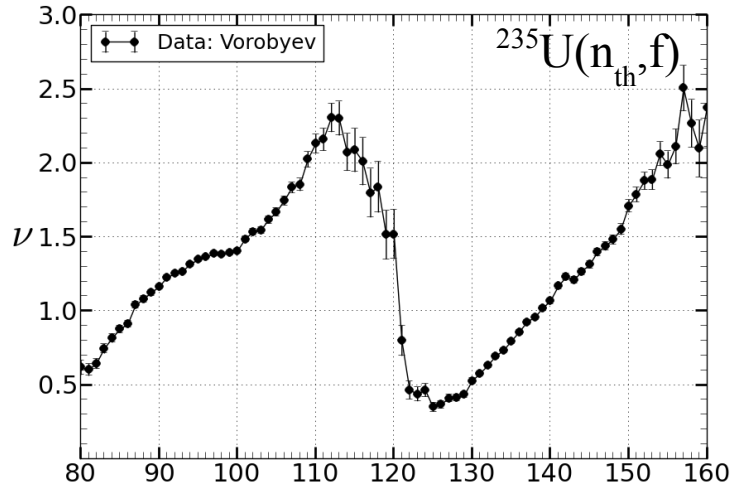
# SPY model presentation

What is the role of the **nuclear structure** of fission fragments during the fission process ?

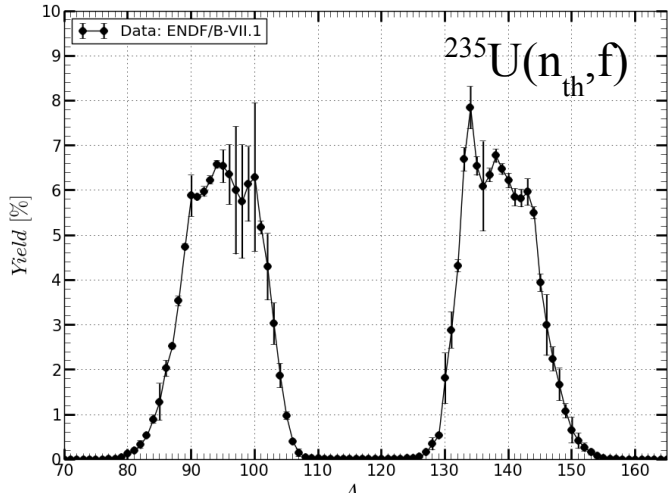
Can **experimental data** be understood/reproduced considering only the nuclear structure of the fission fragments ?



kinetic energy

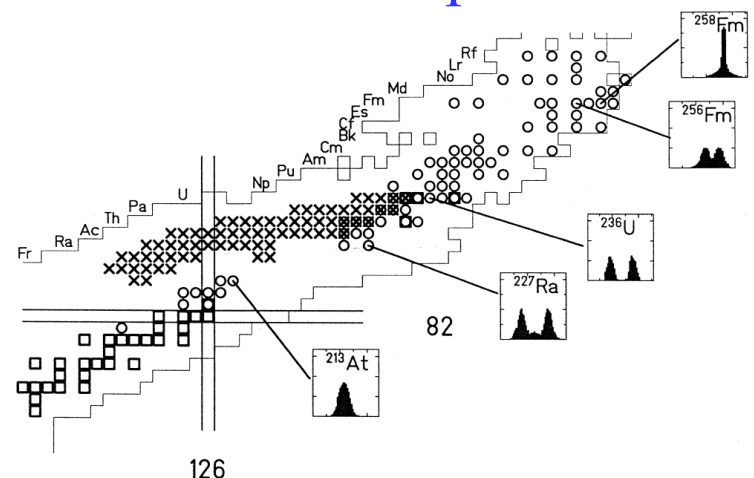


neutron evaporation



yields

symmetric/asymmetric fission



# SPY model

## a scission point model

**Hypo. to determine the frag. properties** : fission process ( $CN \rightarrow \text{frag.}$ )  $\approx$  scission line

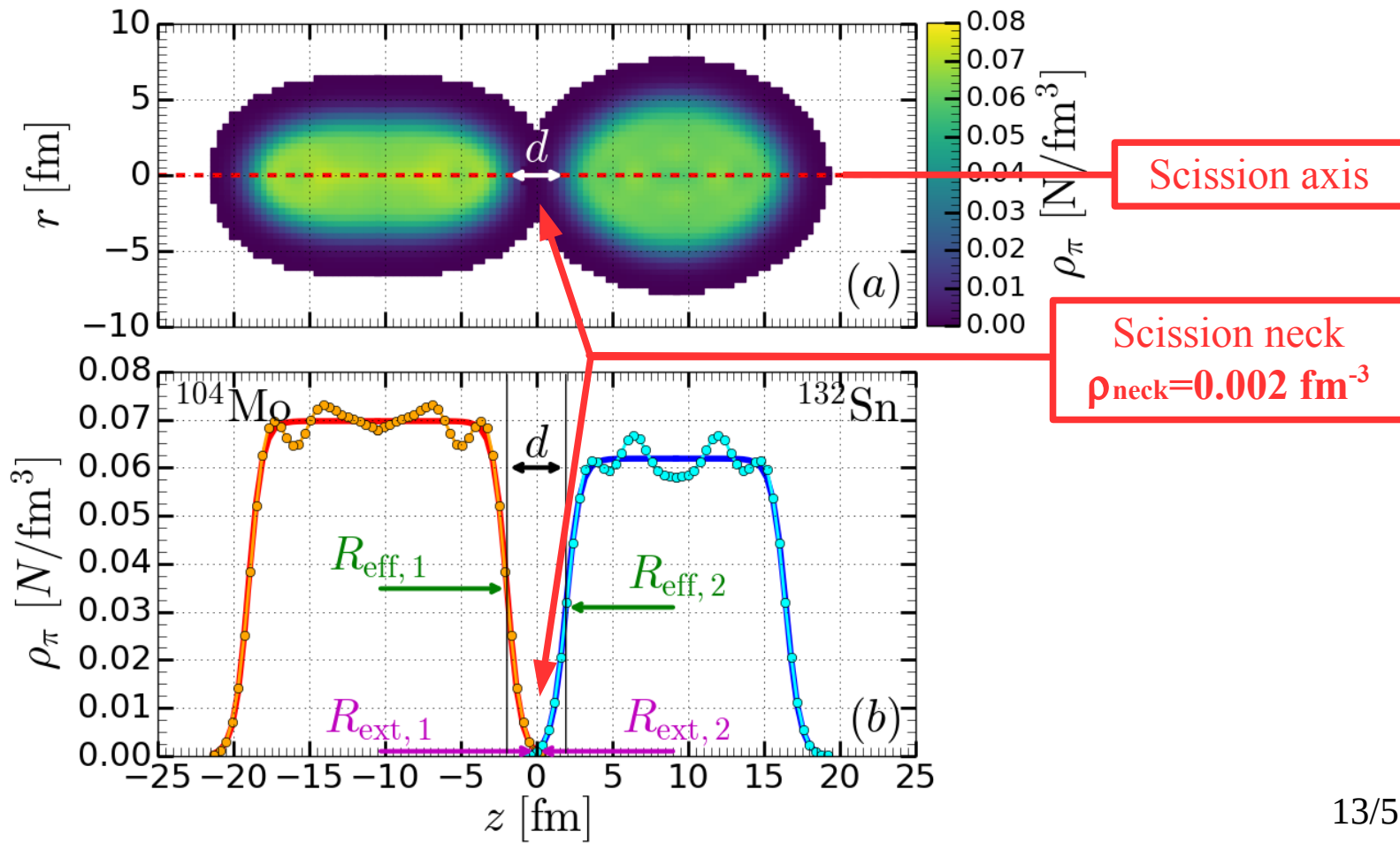
**Scission configuration** : defined by the proton density at scission neck between 2 frag.

Fragments are at rest (no prescission kinetic energy)

Fragments are axially symmetric

**Inputs** : frag.  $E_{\text{ind}}$ , spl & proton density from HFB calculations (Gogny or Skyrme)

Proton density distribution  
 $^{104}\text{Mo}(\beta=1.2) + ^{132}\text{Sn}(\beta=0.4)$



Proton density along scission axis

# SPY model

## a statistical model

- **ONLY based on fission fragments & first-chance fission**
- Evolution (quasi static) between saddle point to scission point is neglected
- Isolated fragments
- Well defined fragments characteristics ( $Z$ ,  $N$ ,  $\beta$ )
- **Fragmentation probability  $\propto$  number of available states**
  - ↳ Fragments observables

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Two quantities are needed to compute physical quantities

- **available energy** for each fragmentation of the system : **AE**
- the number of **available states** for each fragmentation of the system : **AS**

# SPY model

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$^{235}\text{U}(n_{\text{th}}, f)$  :  $\sim 500$  fragmentations

1 fragmentation  $\rightarrow 57 \times 57$  deformations

↳ Ecoul : the most time-consuming numerically computed

↳  $AE \approx 20 \text{ MeV} \rightarrow 20 \text{ AS/fragmentation}$

}

1,6 million AE

}

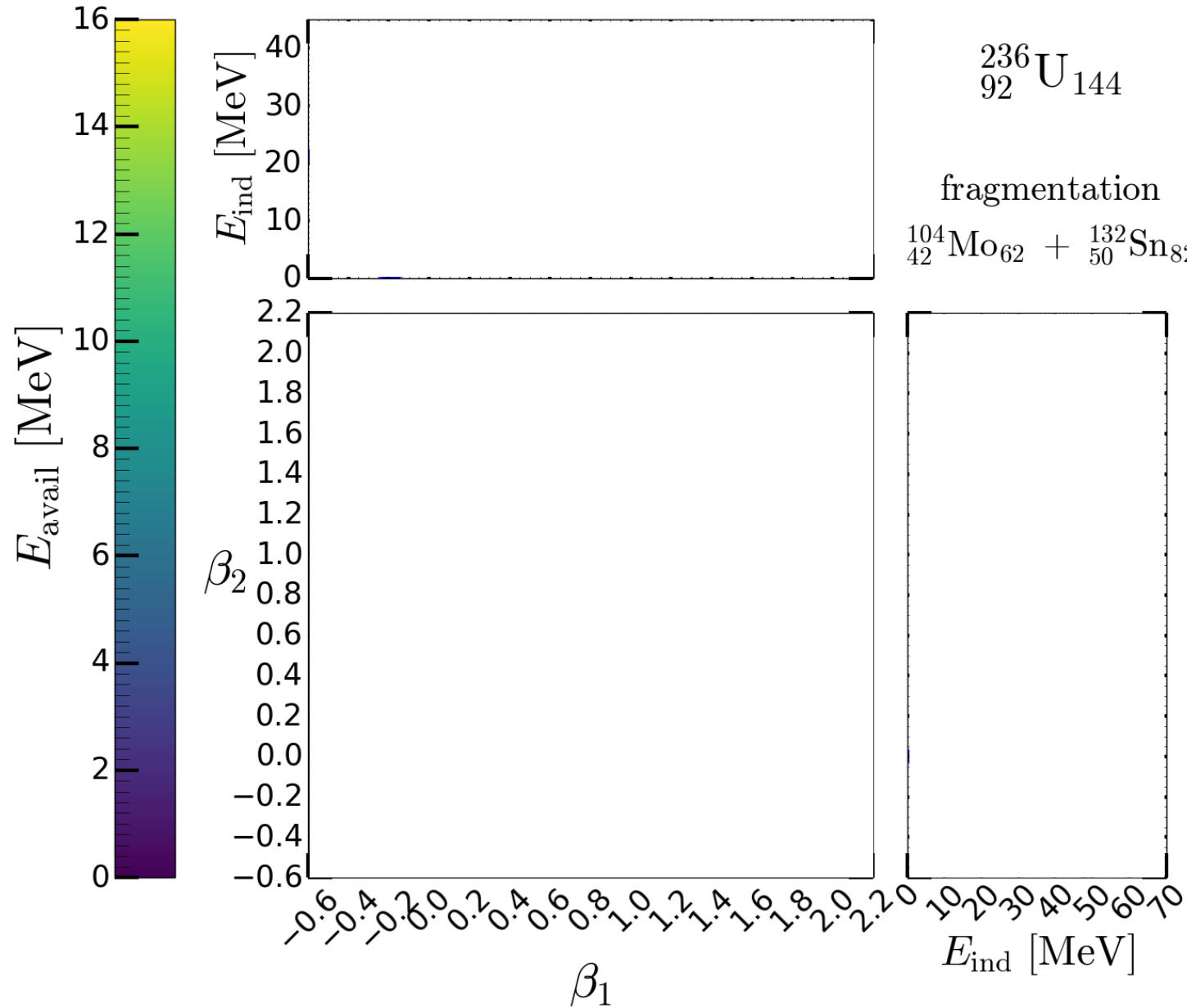
32 million AS



# SPY model

## available energy & available states

$$AE = |E_{\text{ind}1} + E_{\text{ind}2} + E_{\text{coul}} + E_{\text{nucl}} - E_{\text{CN}}|$$

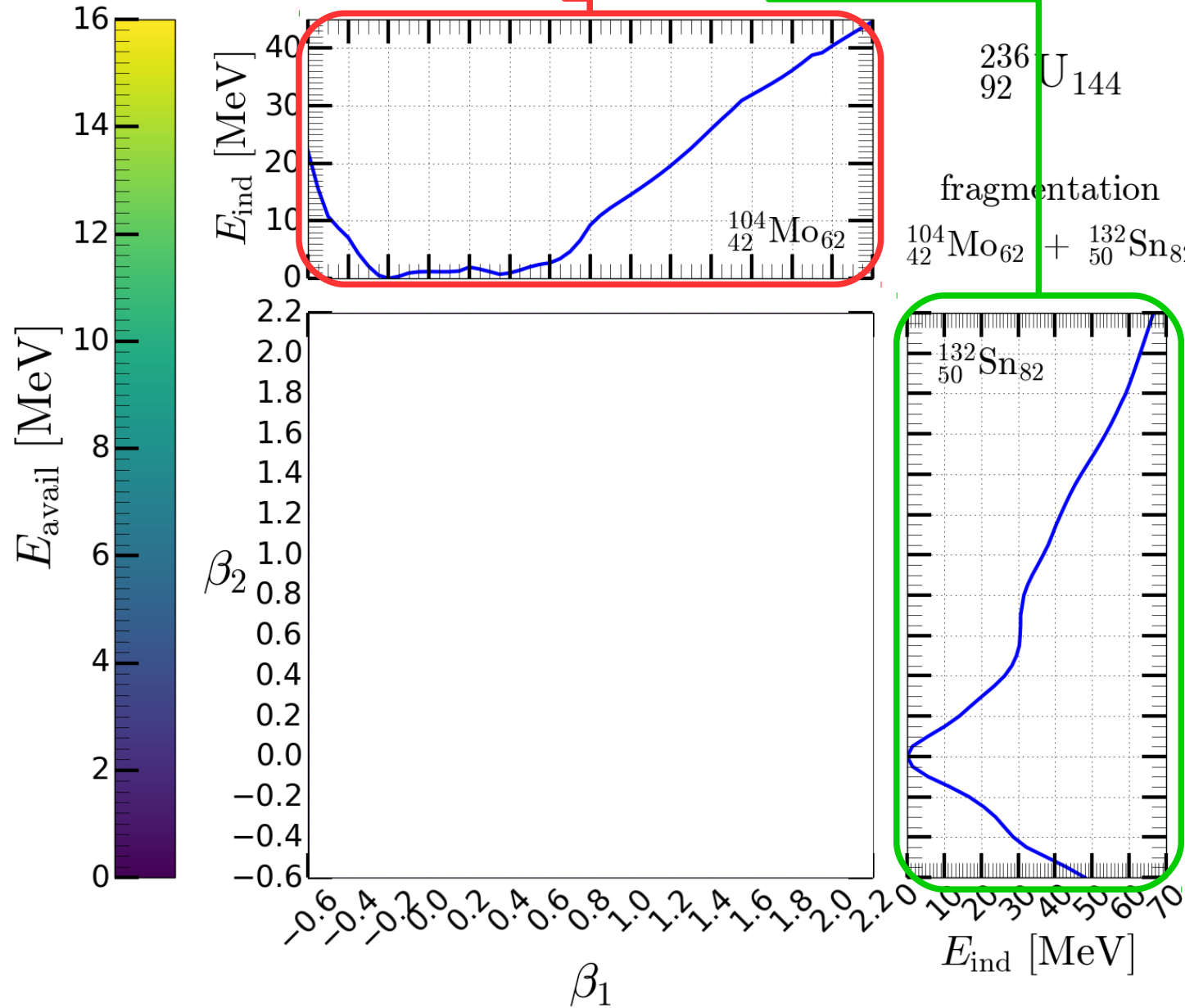


# SPY model

## available energy & available states

$$AE = |E_{\text{ind } 1} + E_{\text{ind } 2} + E_{\text{coul}} + E_{\text{nucl}} - E_{\text{CN}}|$$

\* Individual energies :  
HFB with eff. N-N int.  
Gogny or Skyrme

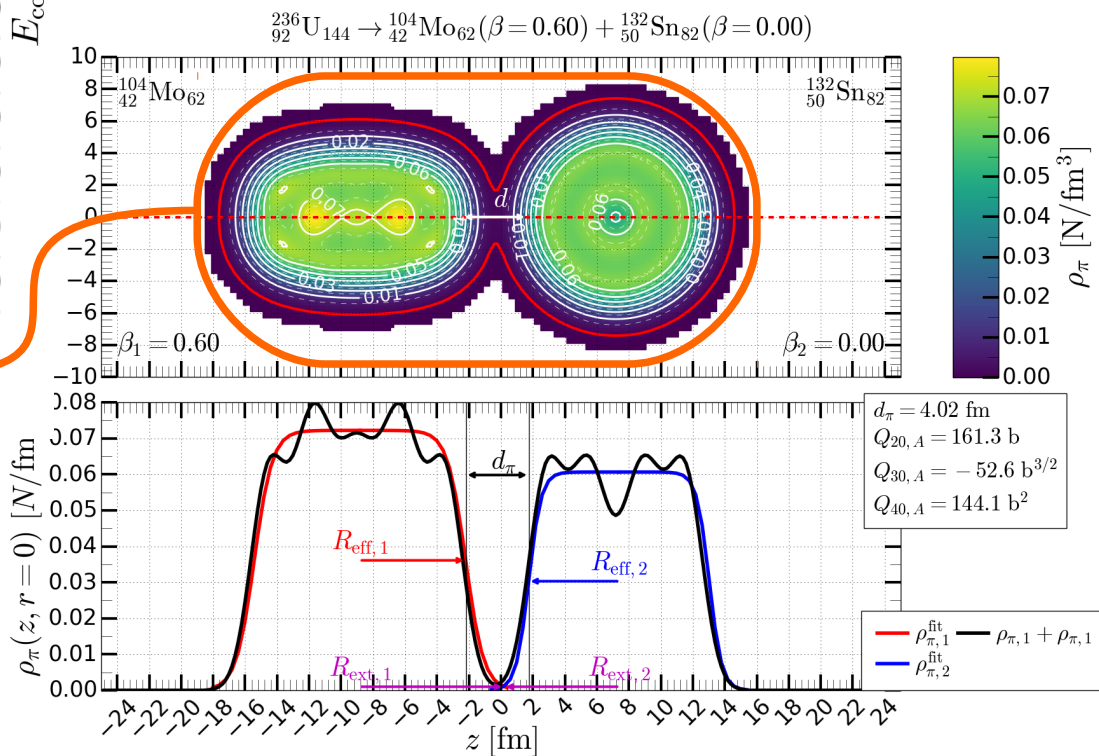
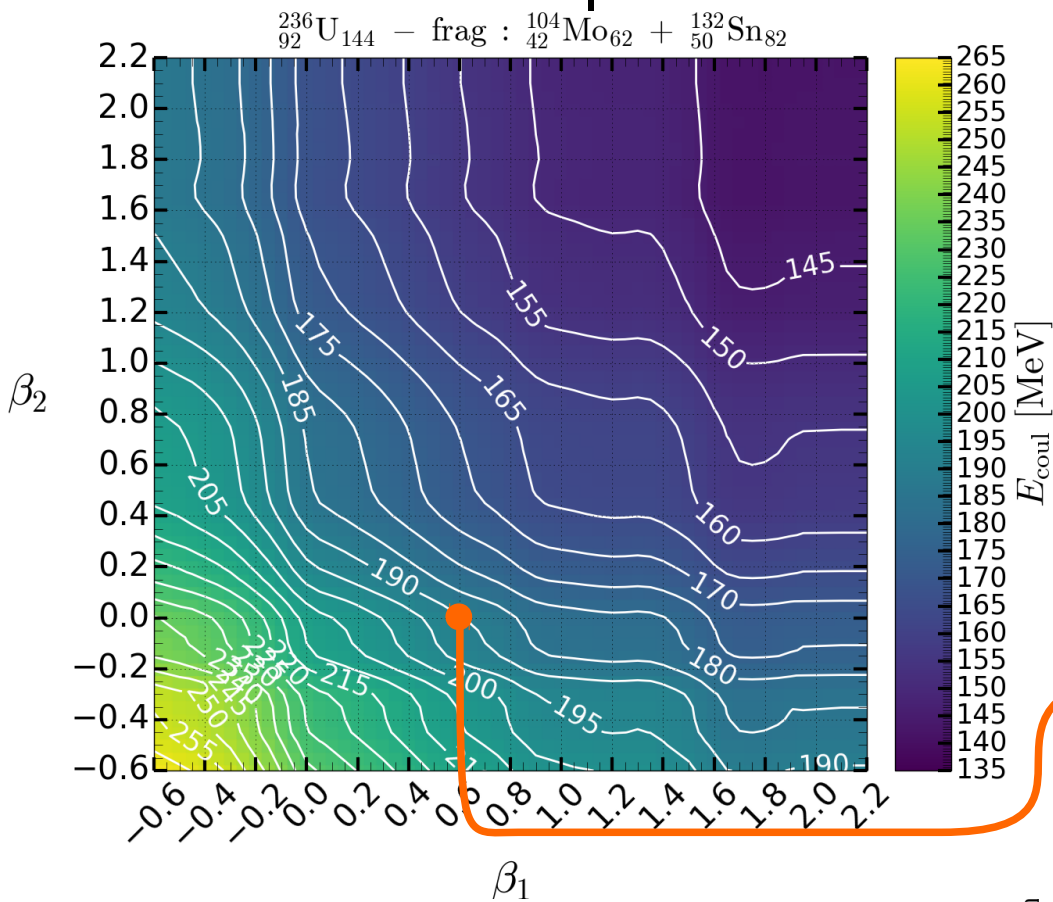


# SPY model

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- \* Individual energies :  
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Gogny or Skyrme
- \* Coulomb repulsion energy :  
numerically computed  
using HFB proton density

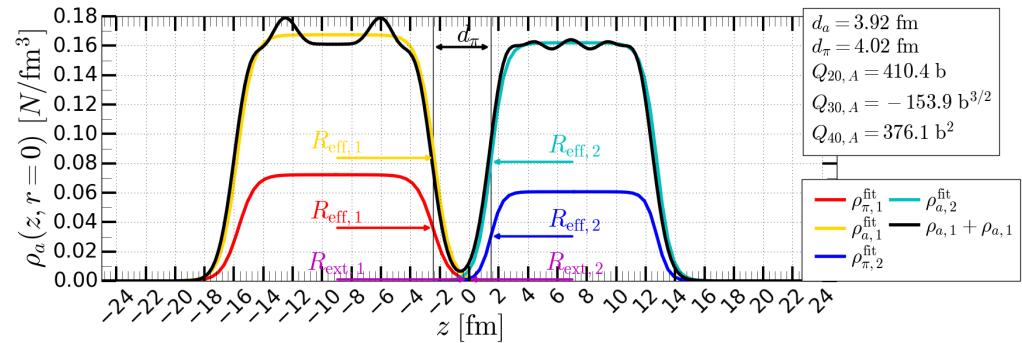
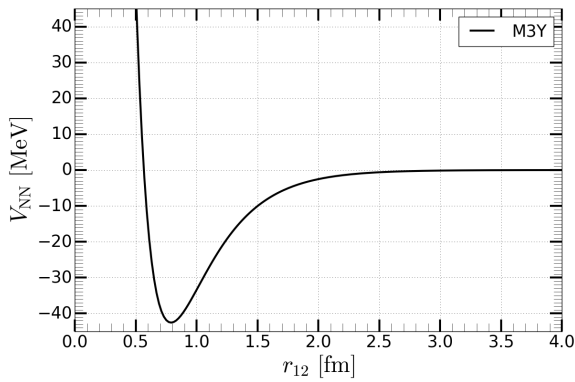
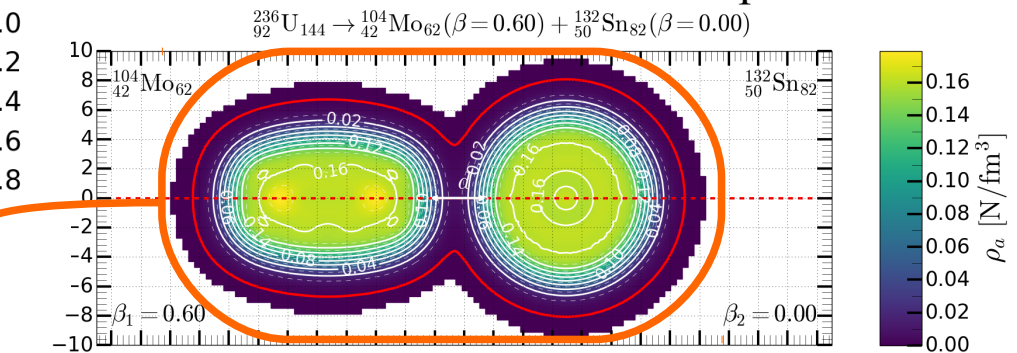
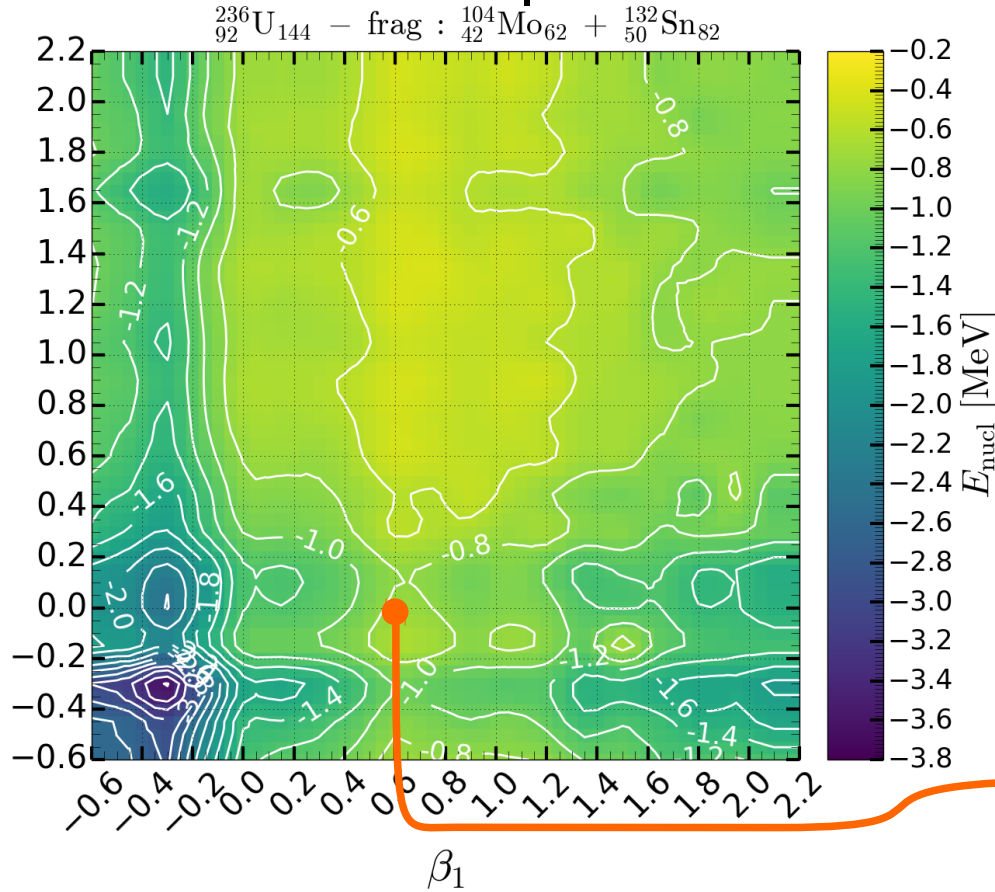


# SPY model

## available energy & available states

$$AE = |E_{\text{ind } 1} + E_{\text{ind } 2} + E_{\text{coul}} + E_{\text{nucl}} - E_{\text{CN}}|$$

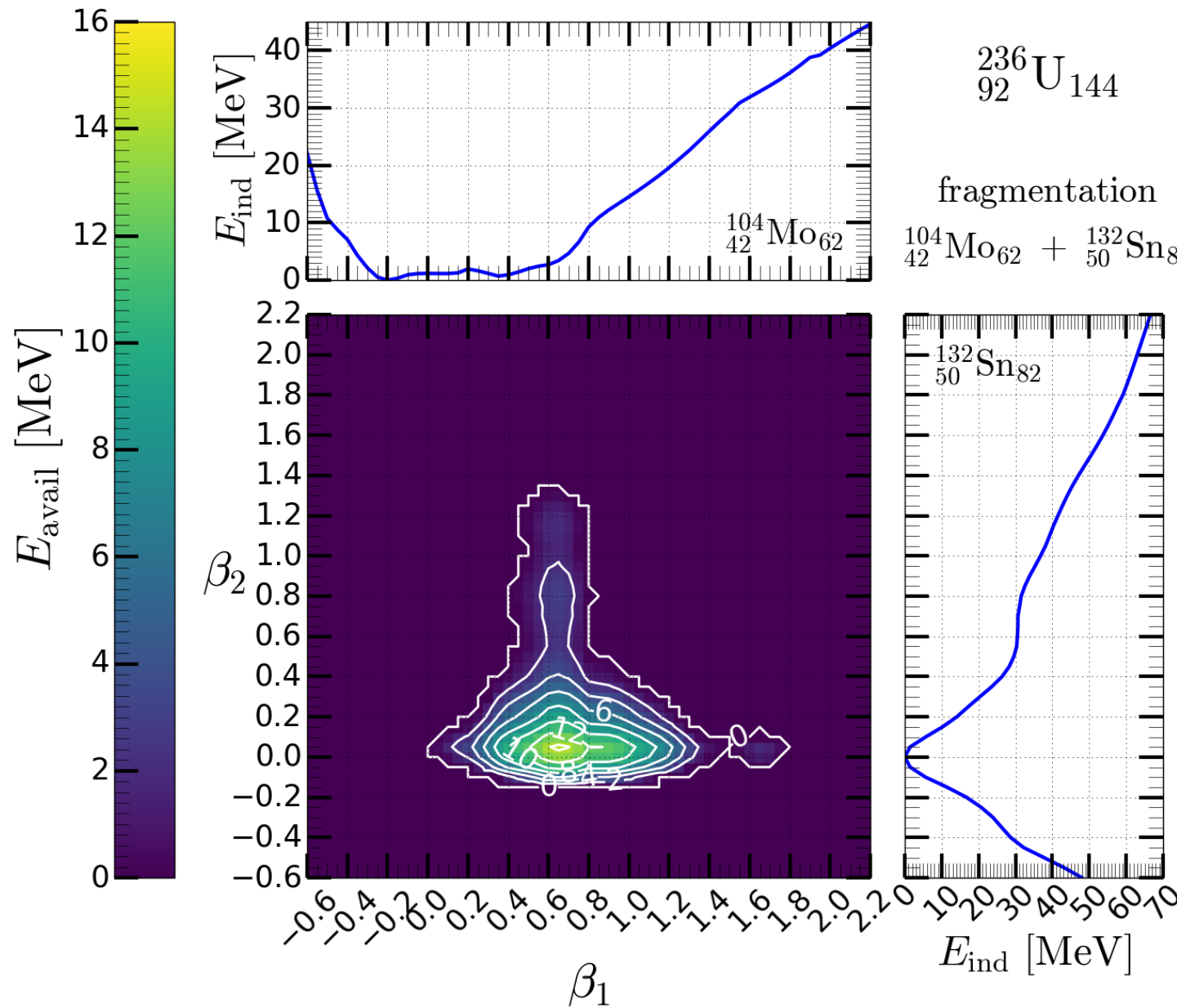
- \* Individual energies :  
HFB with eff. N-N int.  
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- \* Nuclear attraction energy :  
numerically computed  
using HFB nucleon density  
or Blocki prox. Pot.



# SPY model

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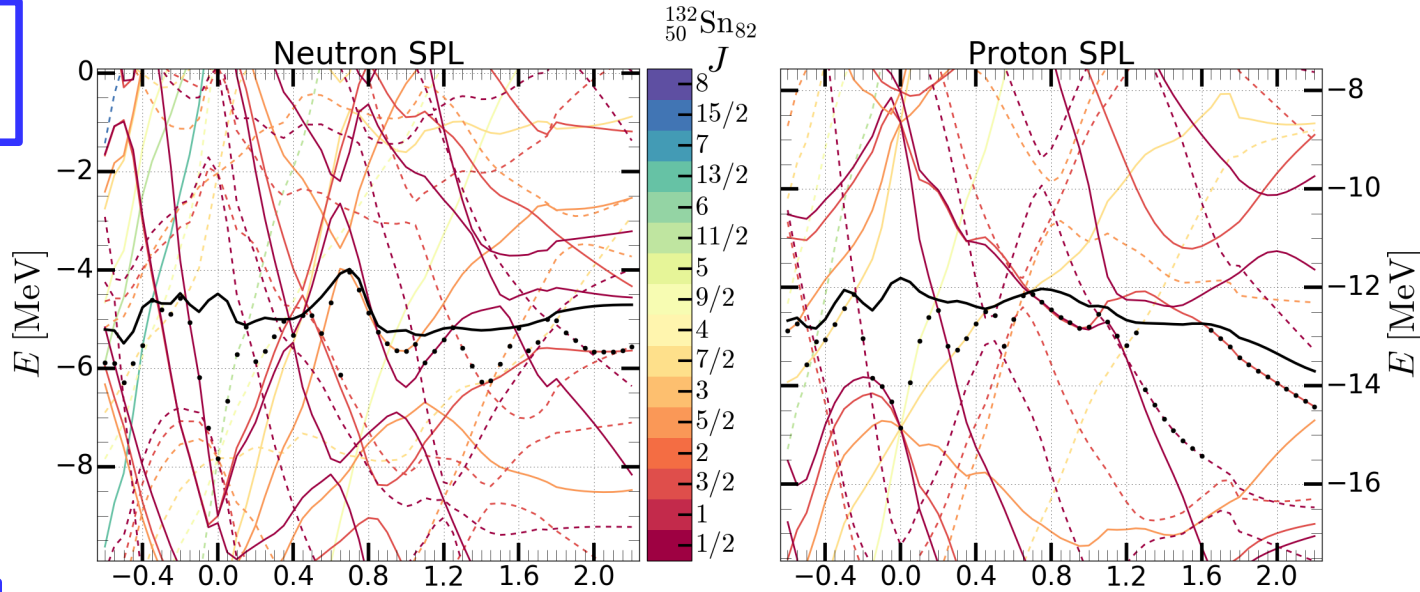
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# SPY model

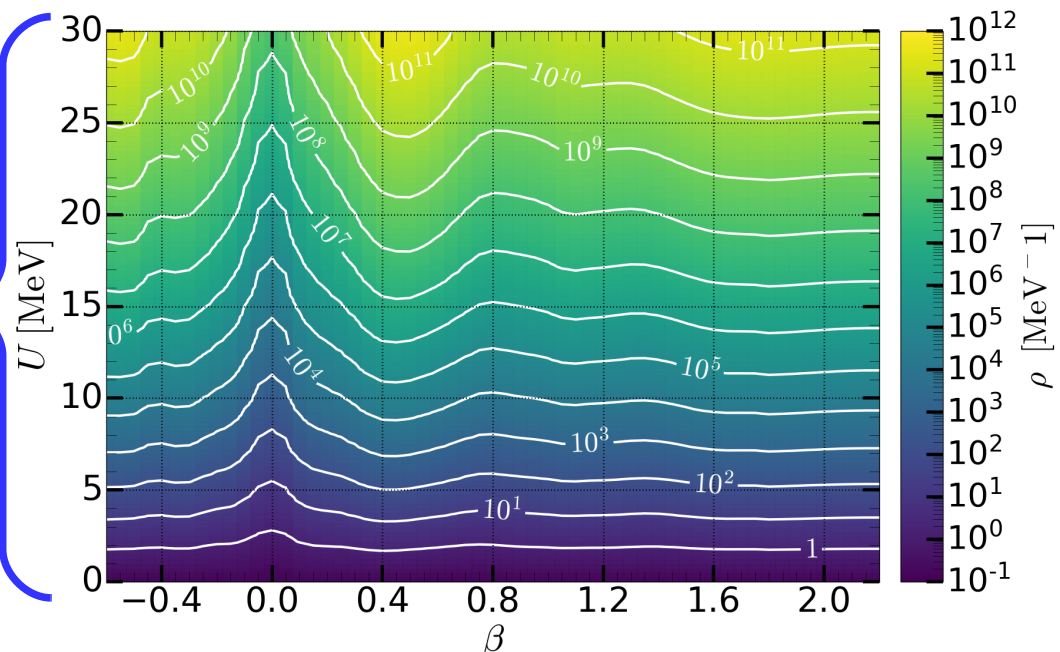
available energy & available states

$$AS = \rho_1 (x AE) \rho_2 ((1-x) AE) \delta E^2$$

HFB single particle levels



statistical description of NSD : BCS theory

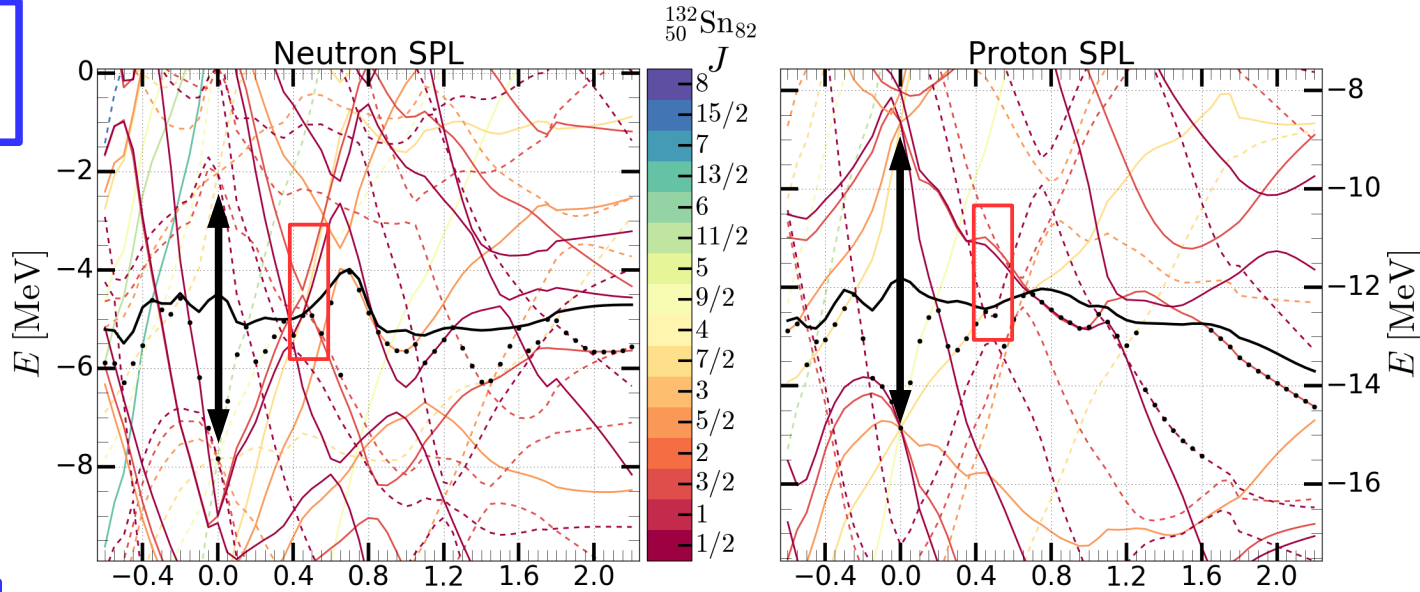


# SPY model

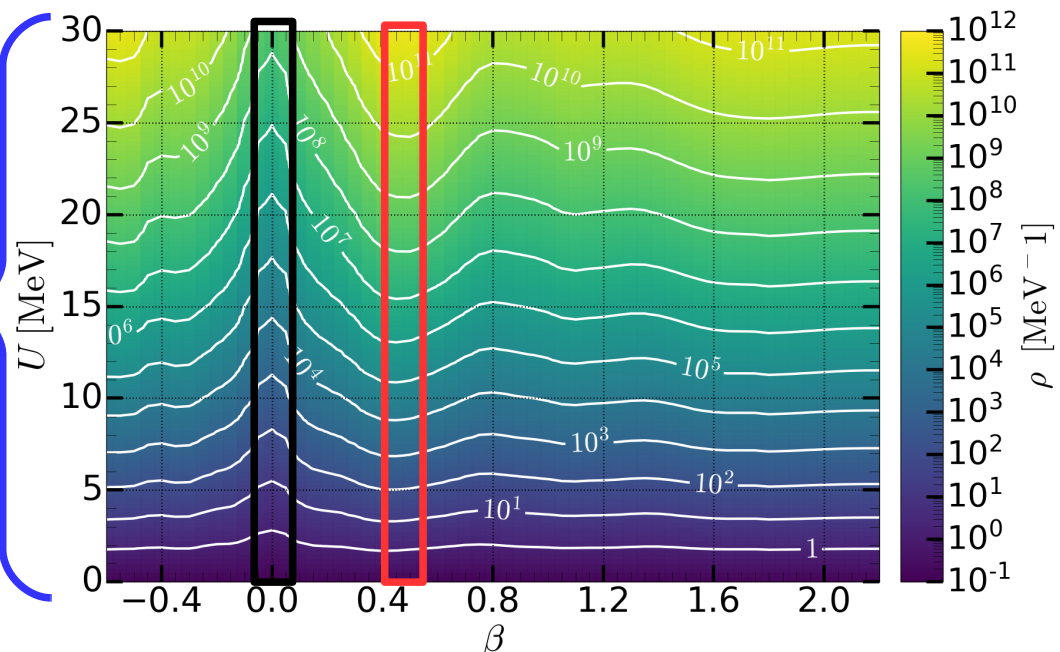
available energy & available states

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HFB single particle levels



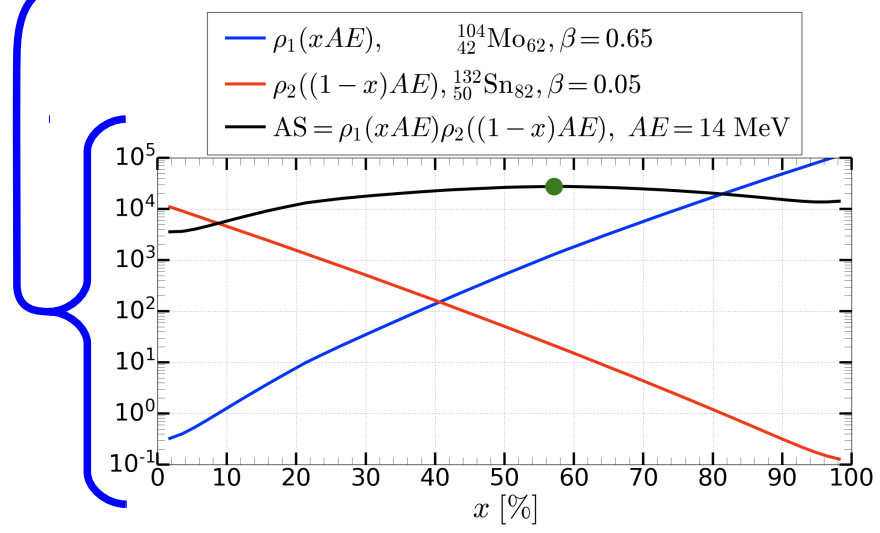
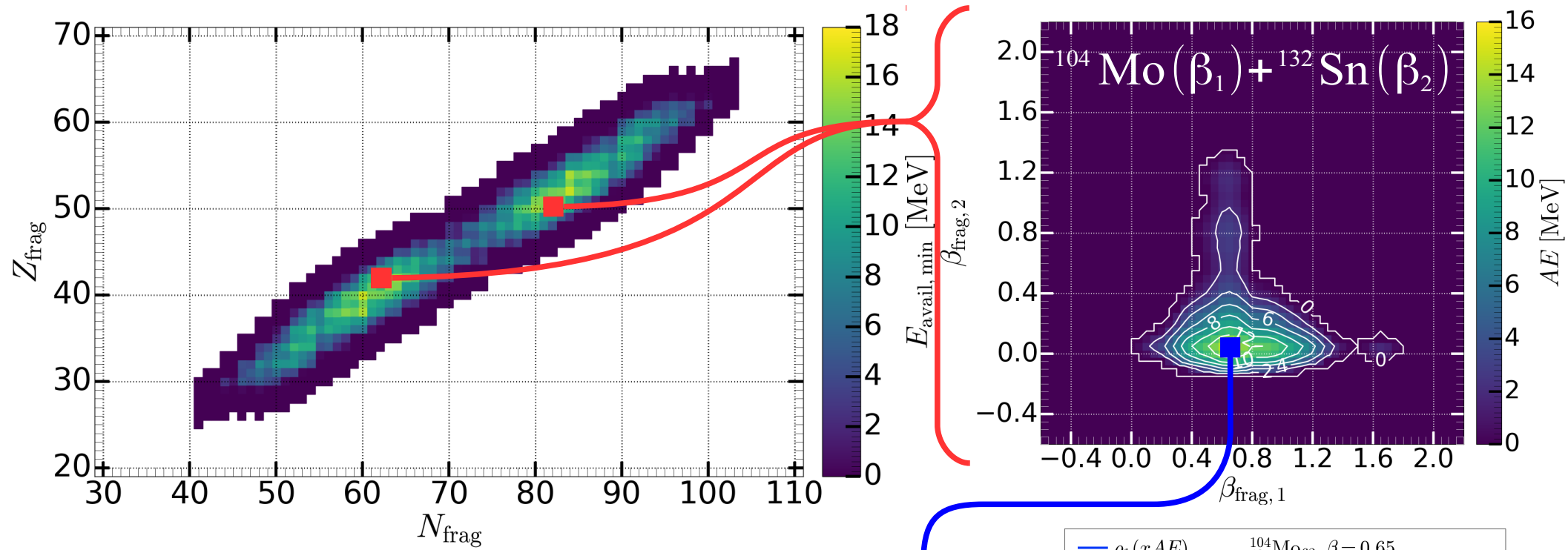
statistical description of NSD : BCS theory



double shell closure  
open shell

# SPY model

## available energy & available states



Probability of a given fragmentation

All deformation couples  $(\beta_1, \beta_2)$

All energy shares

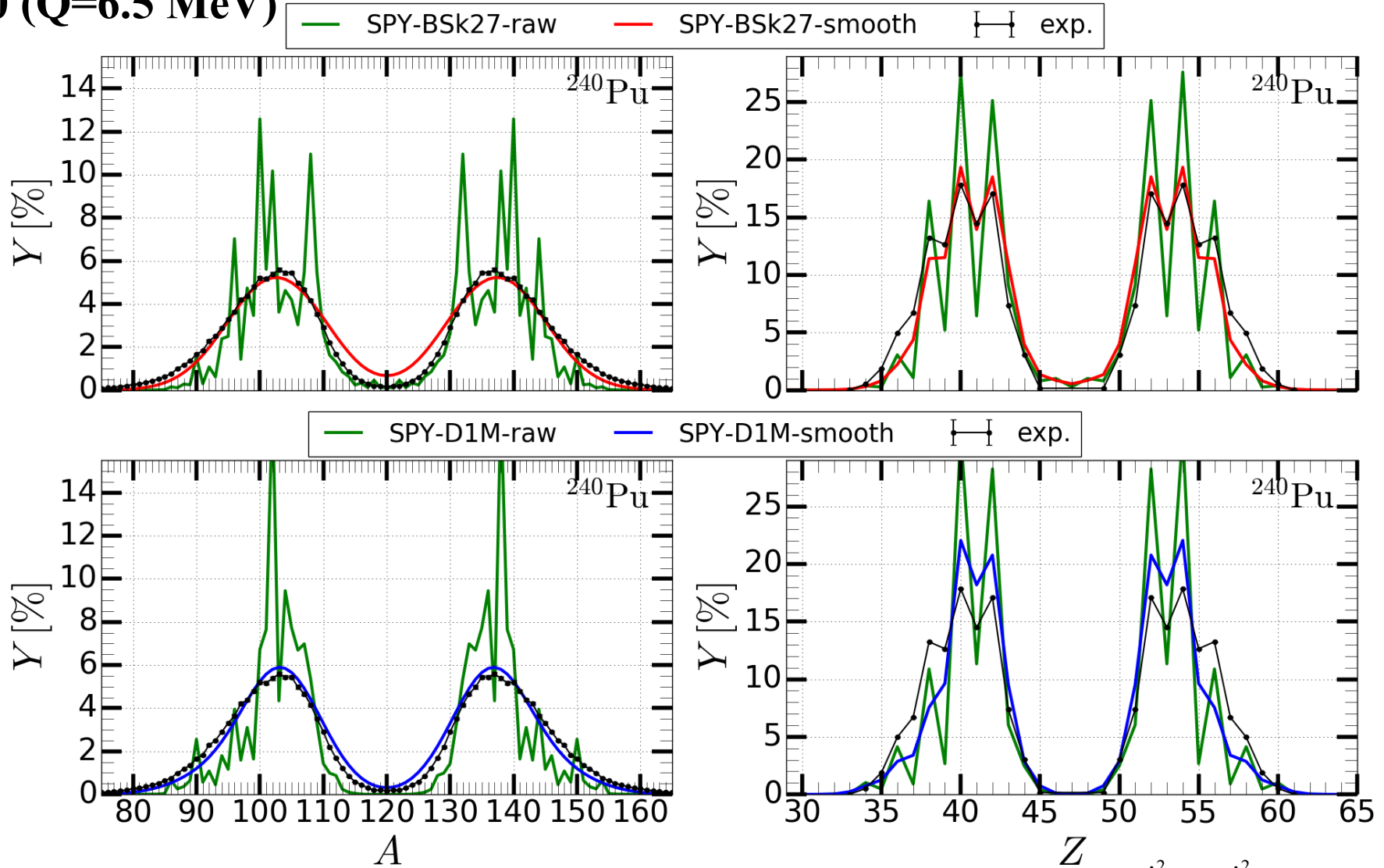
$$Y(Z_1, N_1, Z_2, N_2) = \iint_{\beta_1, \beta_2} \int_0^1 \rho_1(x \overbrace{AE}^{AE(\beta_1, \beta_2)}, \beta_1) \rho_2((1-x) \overbrace{AE}^{AE(\beta_1, \beta_2)}, \beta_2) \delta E^2 dx d\beta_1 d\beta_2$$



# SPY model

## raw yields VS smoothed yields

Pu240 (Q=6.5 MeV)

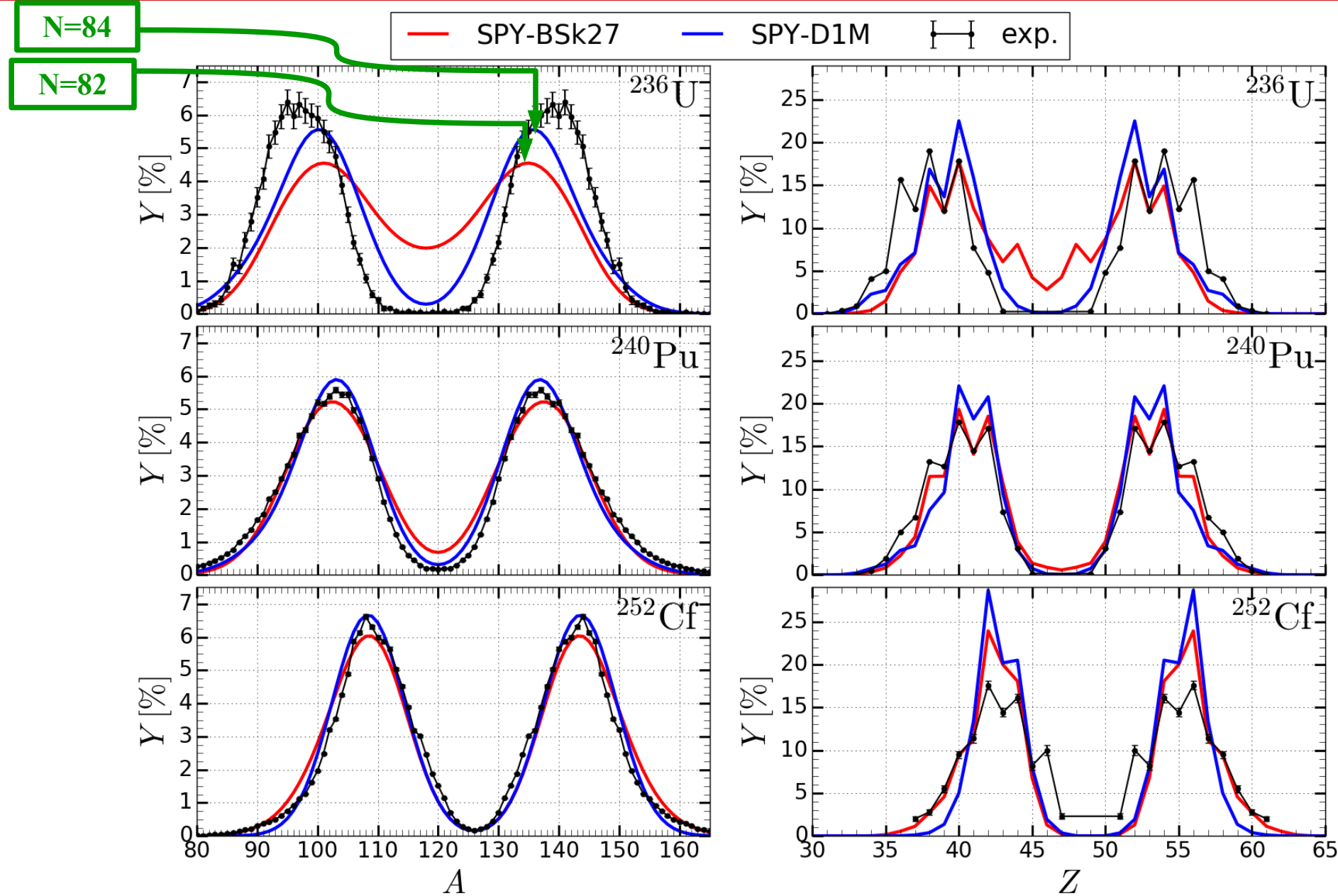


$$Y_{\text{smooth}}(Z, N) = \sum_{i=-4}^4 \sum_{j=-15}^{15} Y_{\text{raw}}(Z+i, N+j) C_z C_n e^{-\frac{i^2}{2\sigma_z^2} - \frac{j^2}{2\sigma_n^2}}$$

$$\sigma_n = 5 \text{ and } \sigma_z = 0.65$$

# Results

## Fission of U236, Pu240 & Cf252



Exp data : U236 → C. Romano et al, PRC81, 014607 (2010)

// W. Lang et al, NPA345, 34 (1980)

Pu240 → C. Tsuchiya et al, J. Nucl. Sci. Technol. 37, 941 (2000) // C. Schmitt et al, NPA430, 21 (1984)

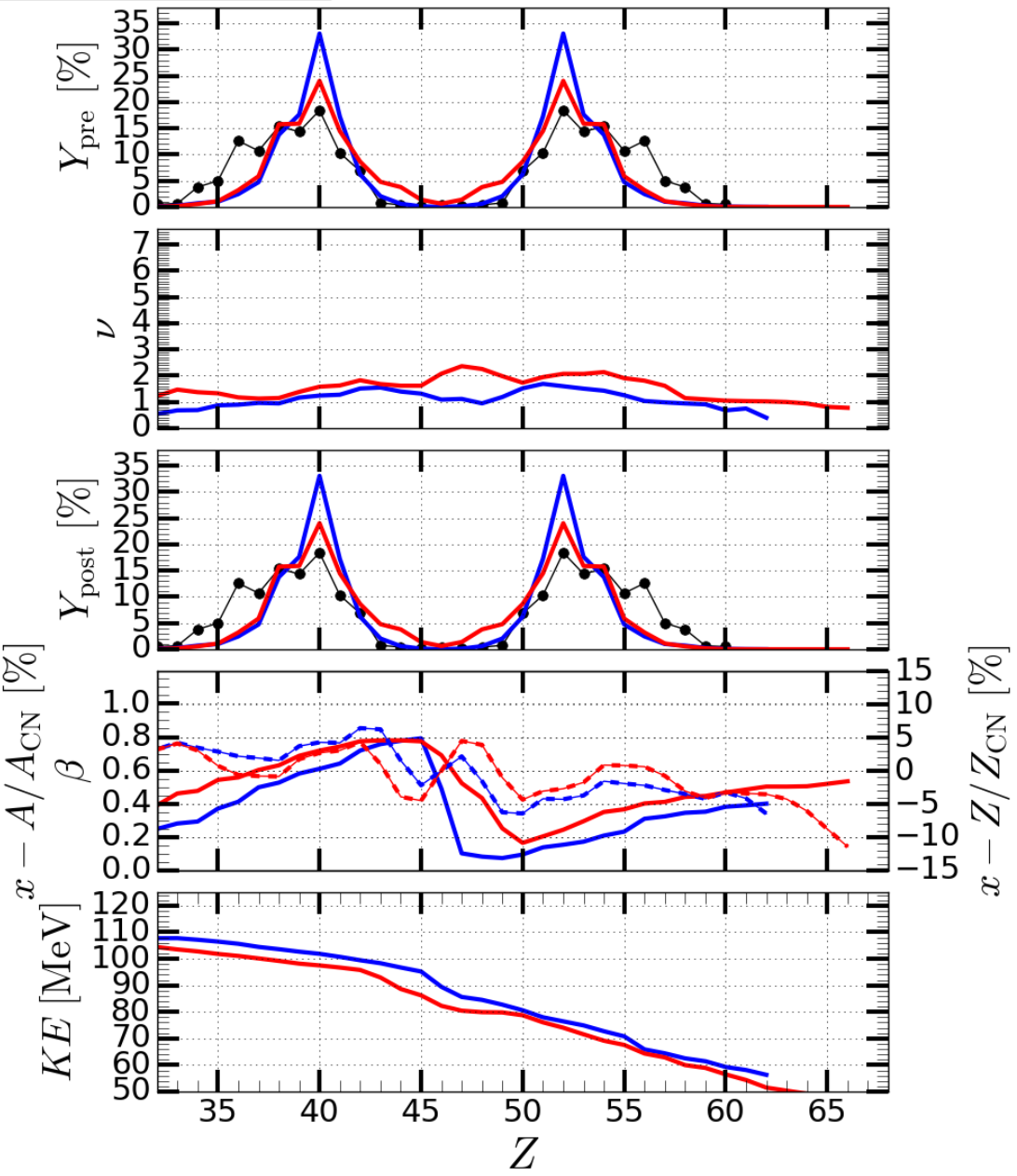
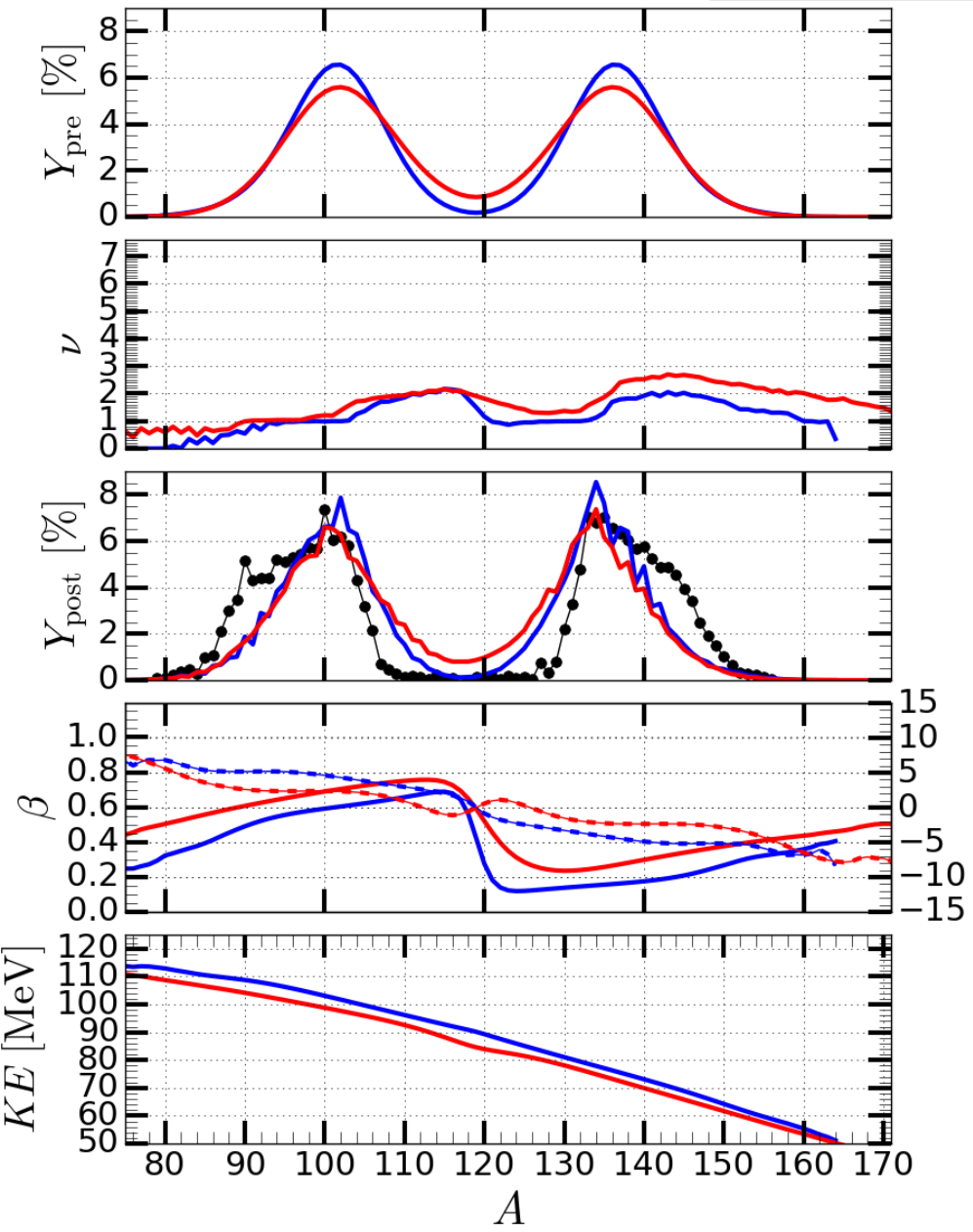
Cf252 → Sh. Zeynalov et al, J. Korean Phy. Soc. 59, 1396 (2011) // G. Mariolopoulos et al, NPA361, 213 (1981) 26/53



# Results

## Fission of U238 – Q=7.4 MeV

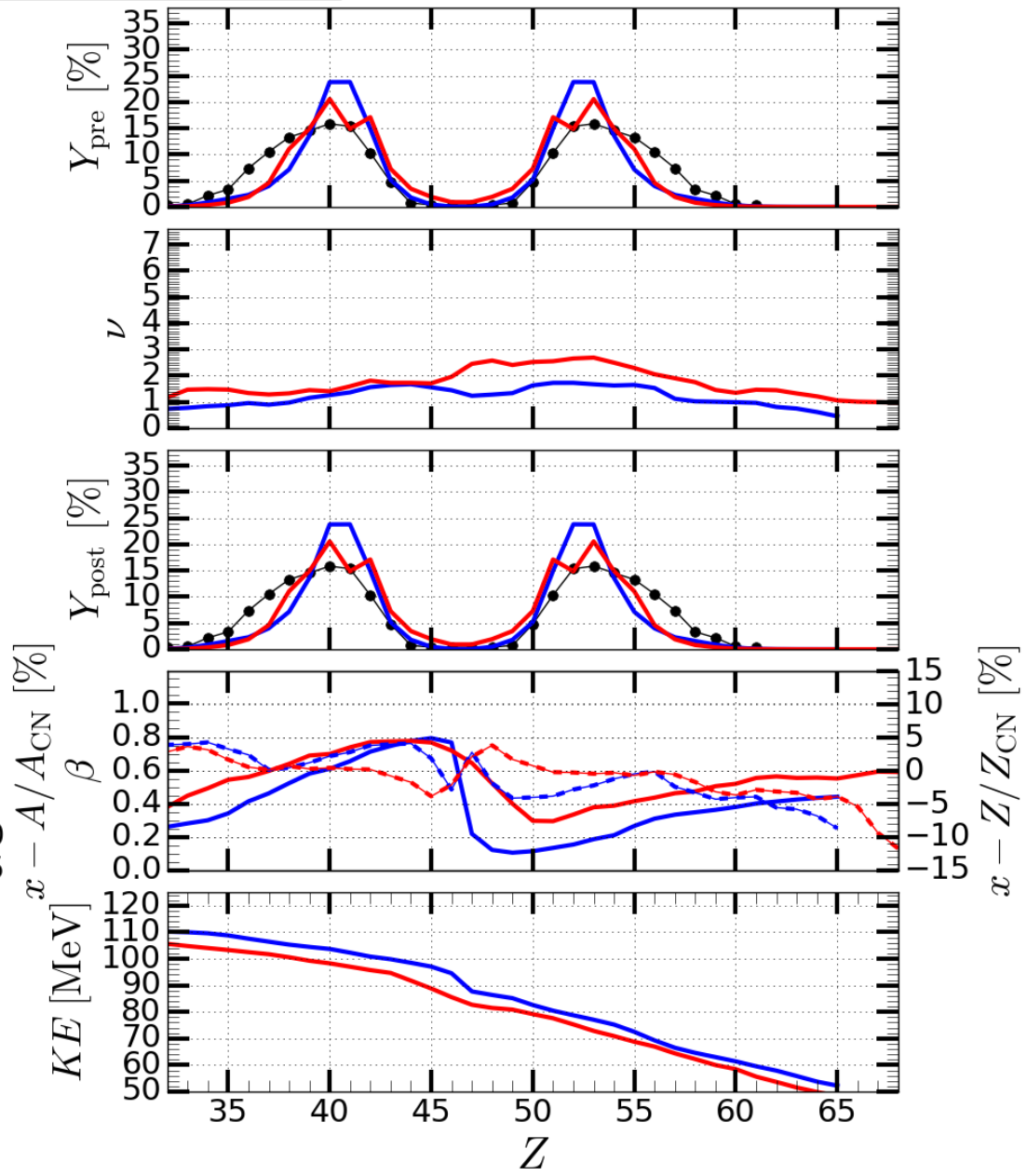
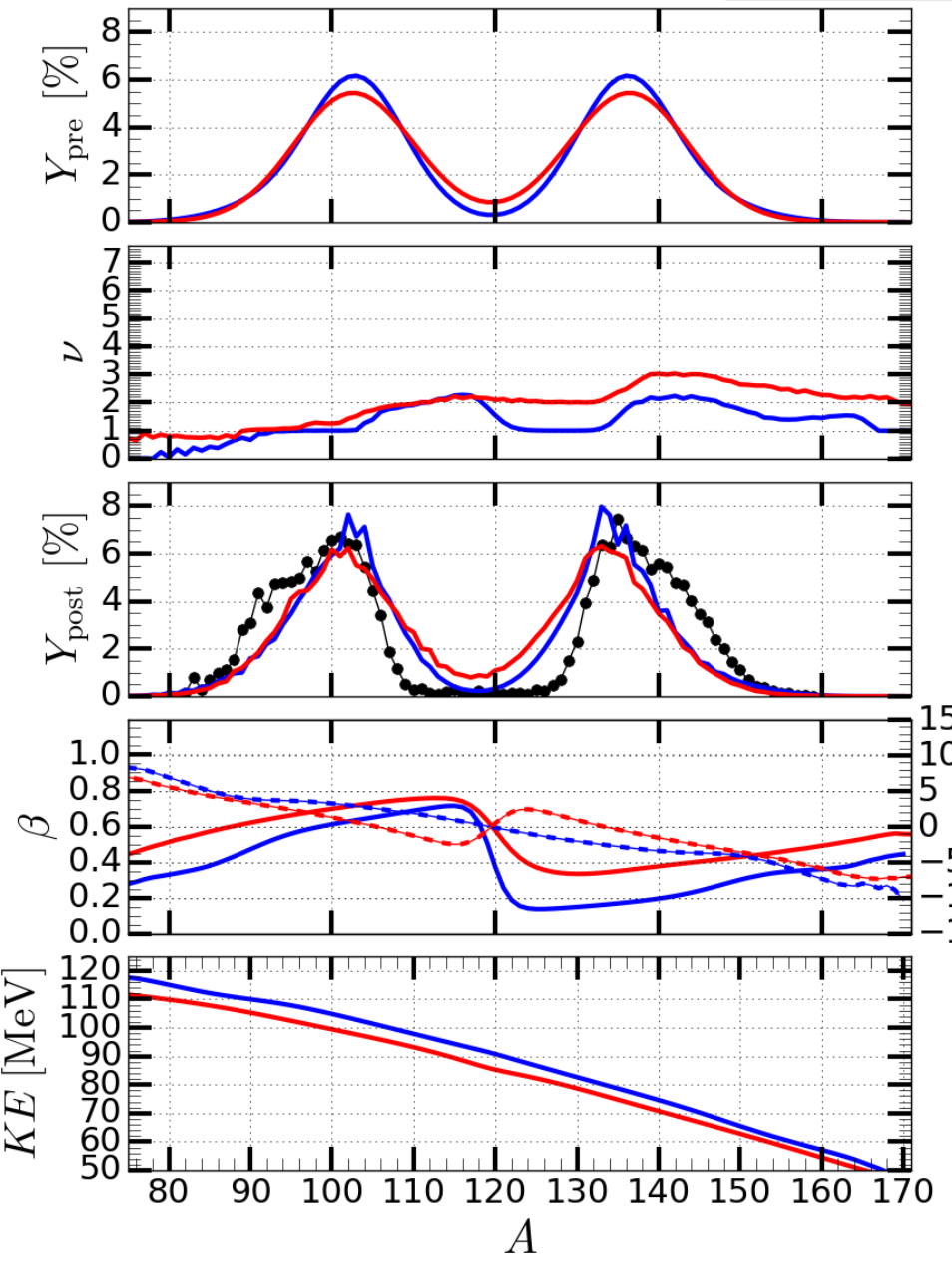
— D1M — BSk27



# Results

## Fission of Np239 – Q=7.5 MeV

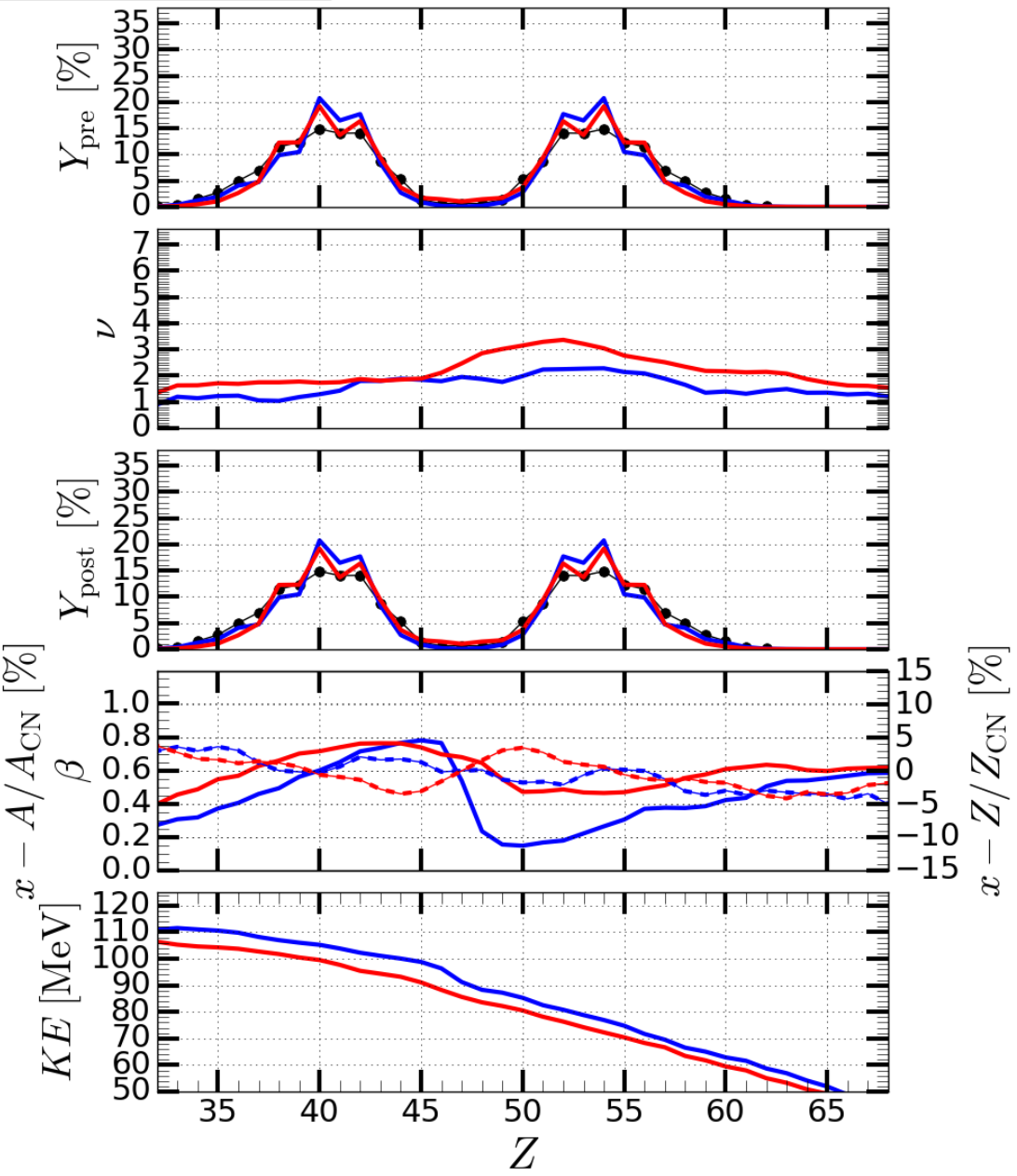
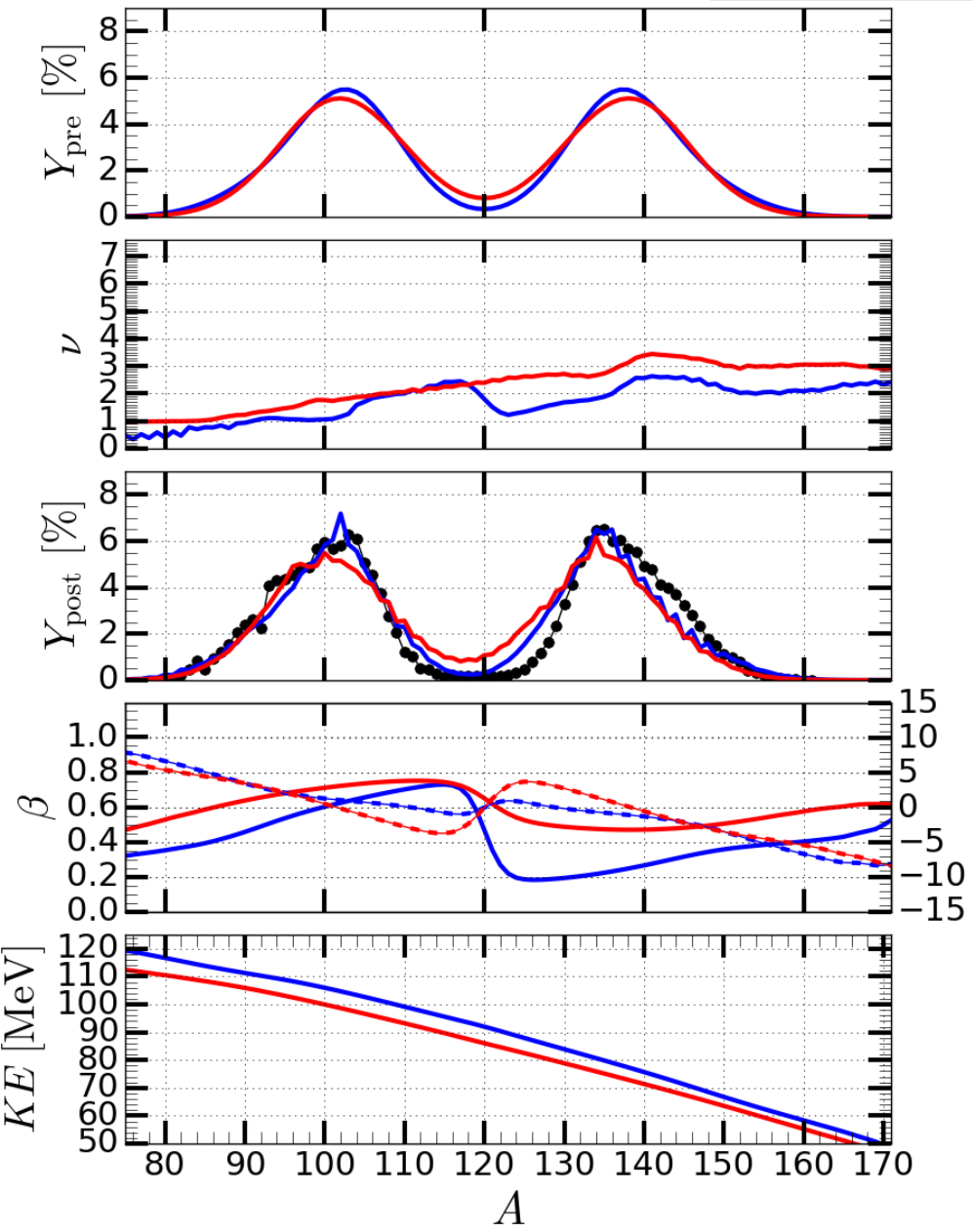
— D1M — BSk27



# Results

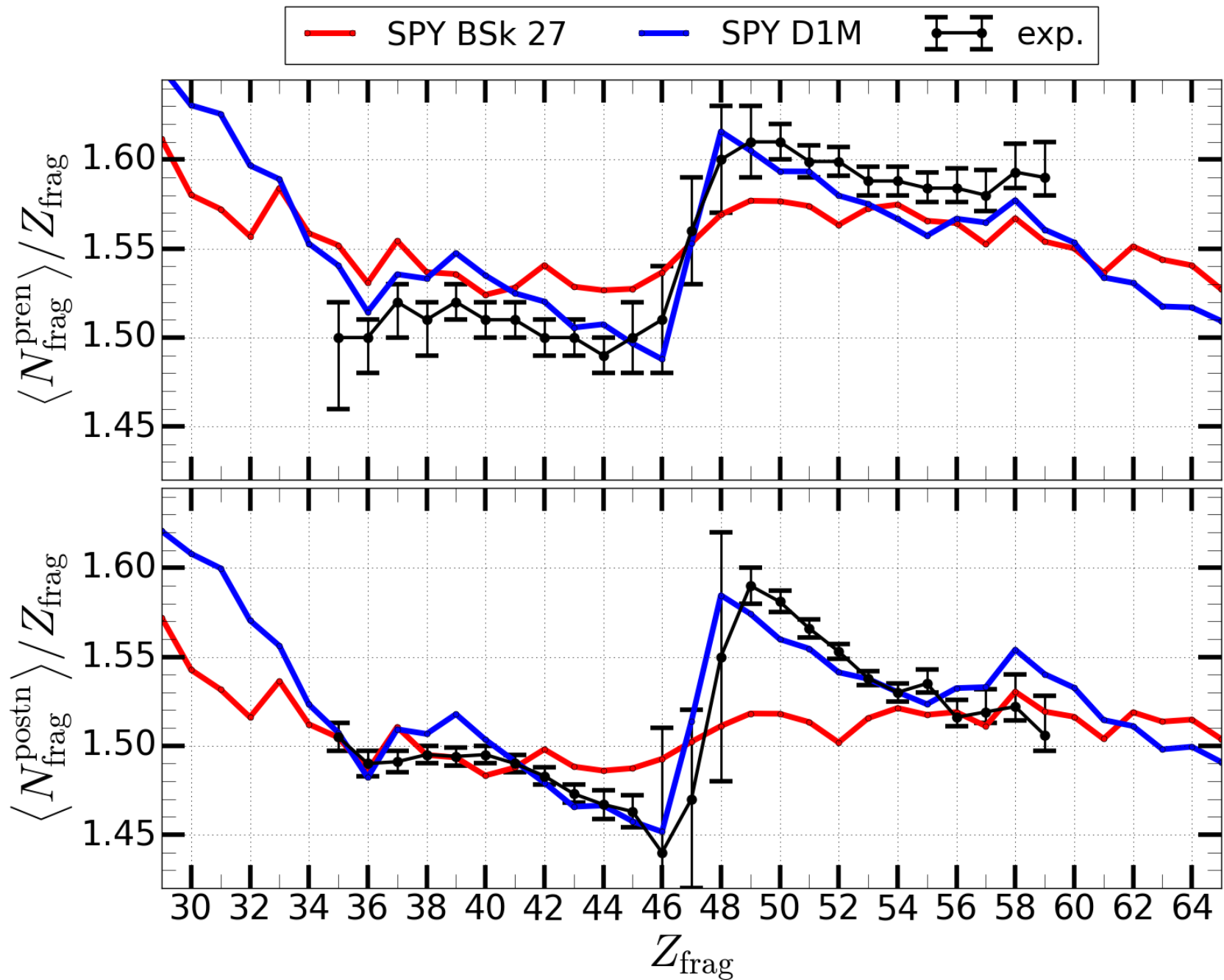
## Fission of Pu240 – Q=10.7 MeV

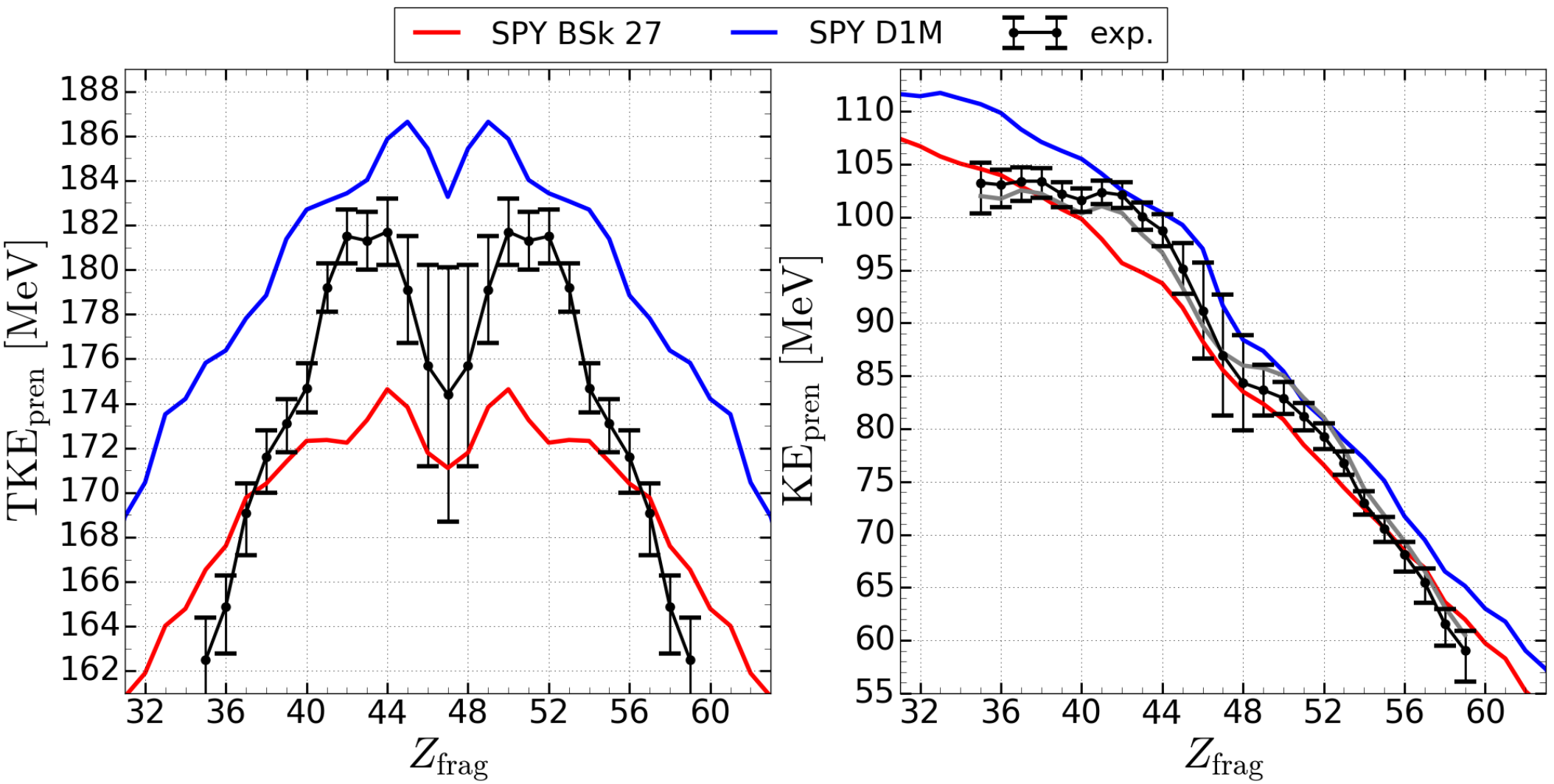
— D1M — BSk27



# Pu240

## $\langle N \rangle / Z - Q = 9 \text{ MeV}$





In gray, exp. TKE + Z<sub>UCD</sub>  
 In black, exp. TKE + exp. <N>/Z

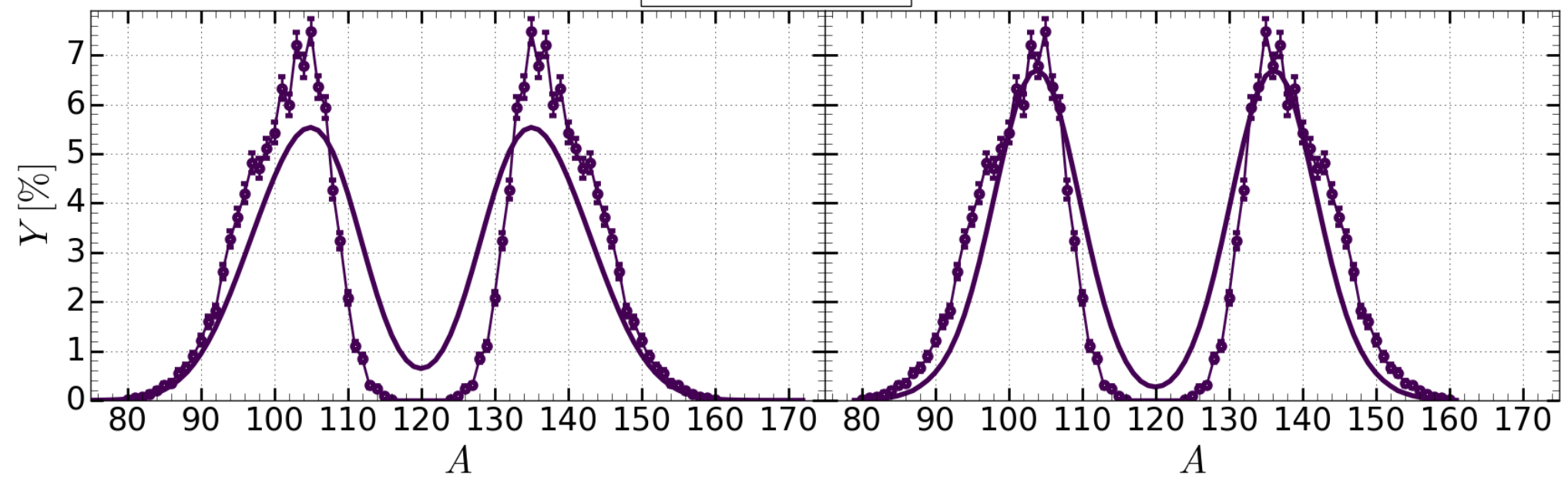
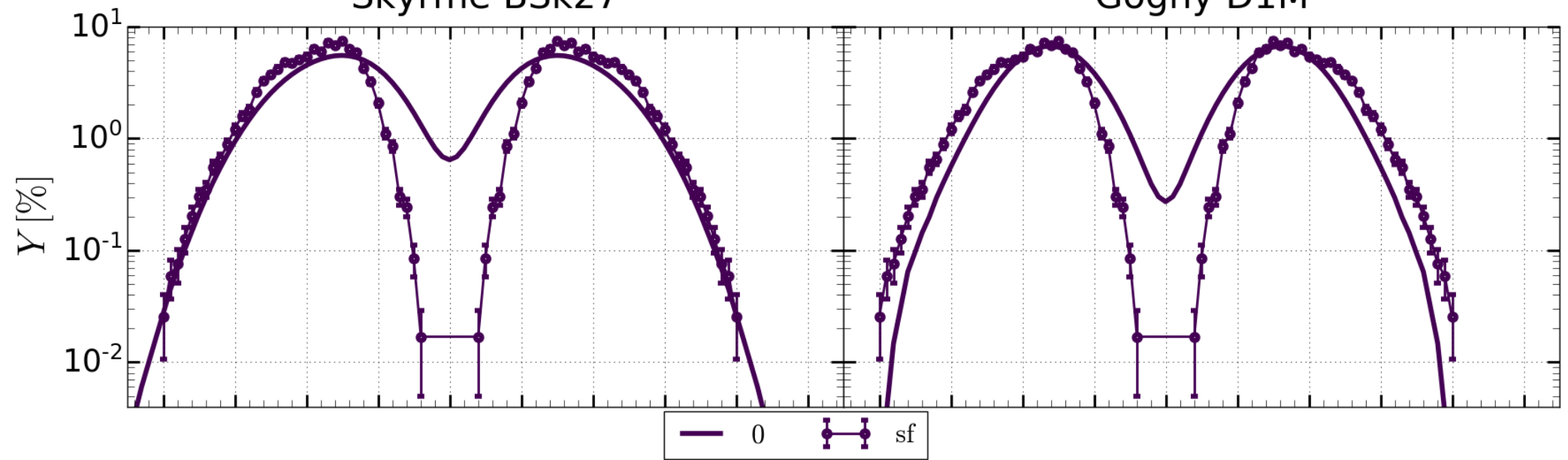


# Pu240

## Q=0 MeV

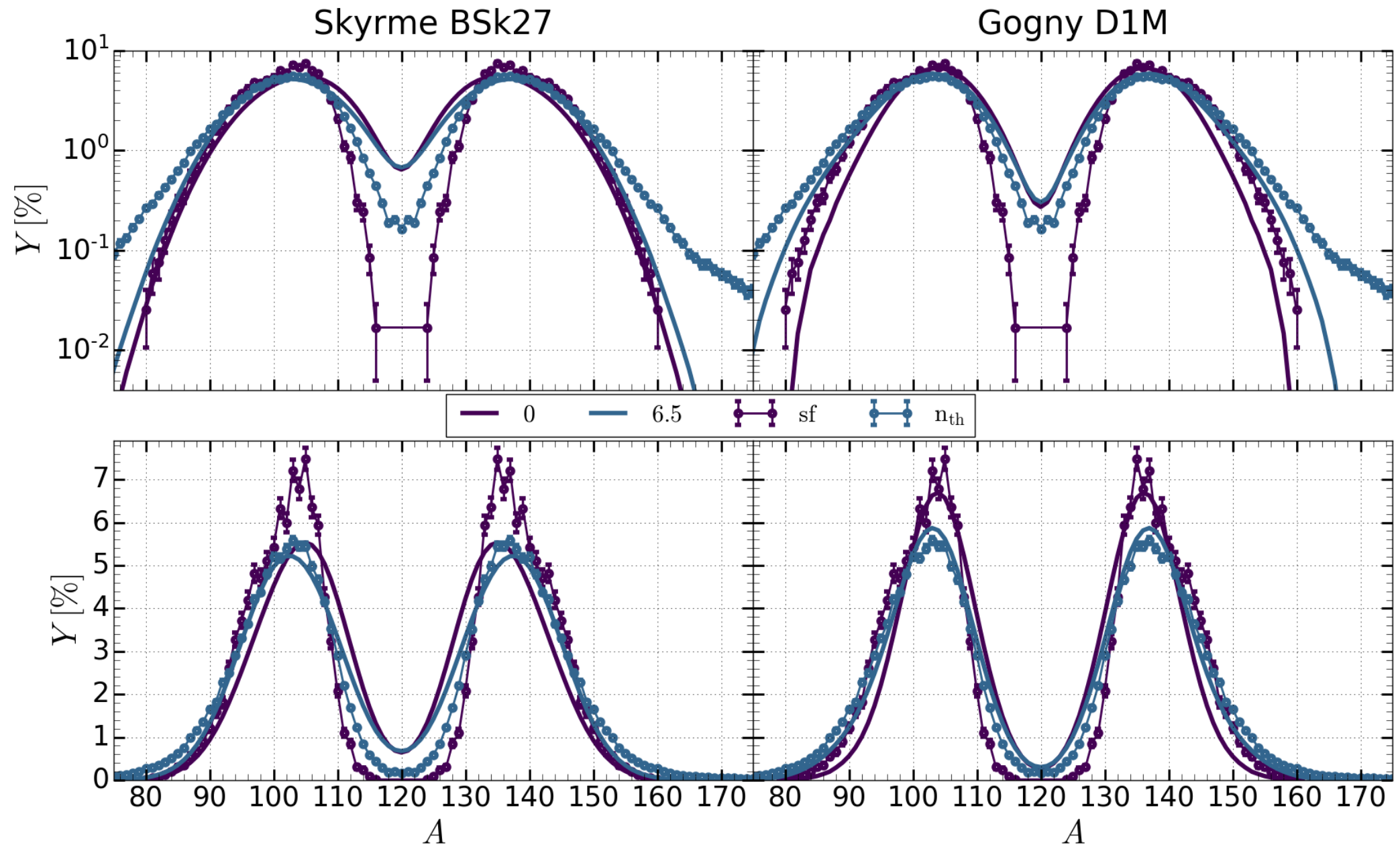
Skyrme BSk27

Gogny D1M



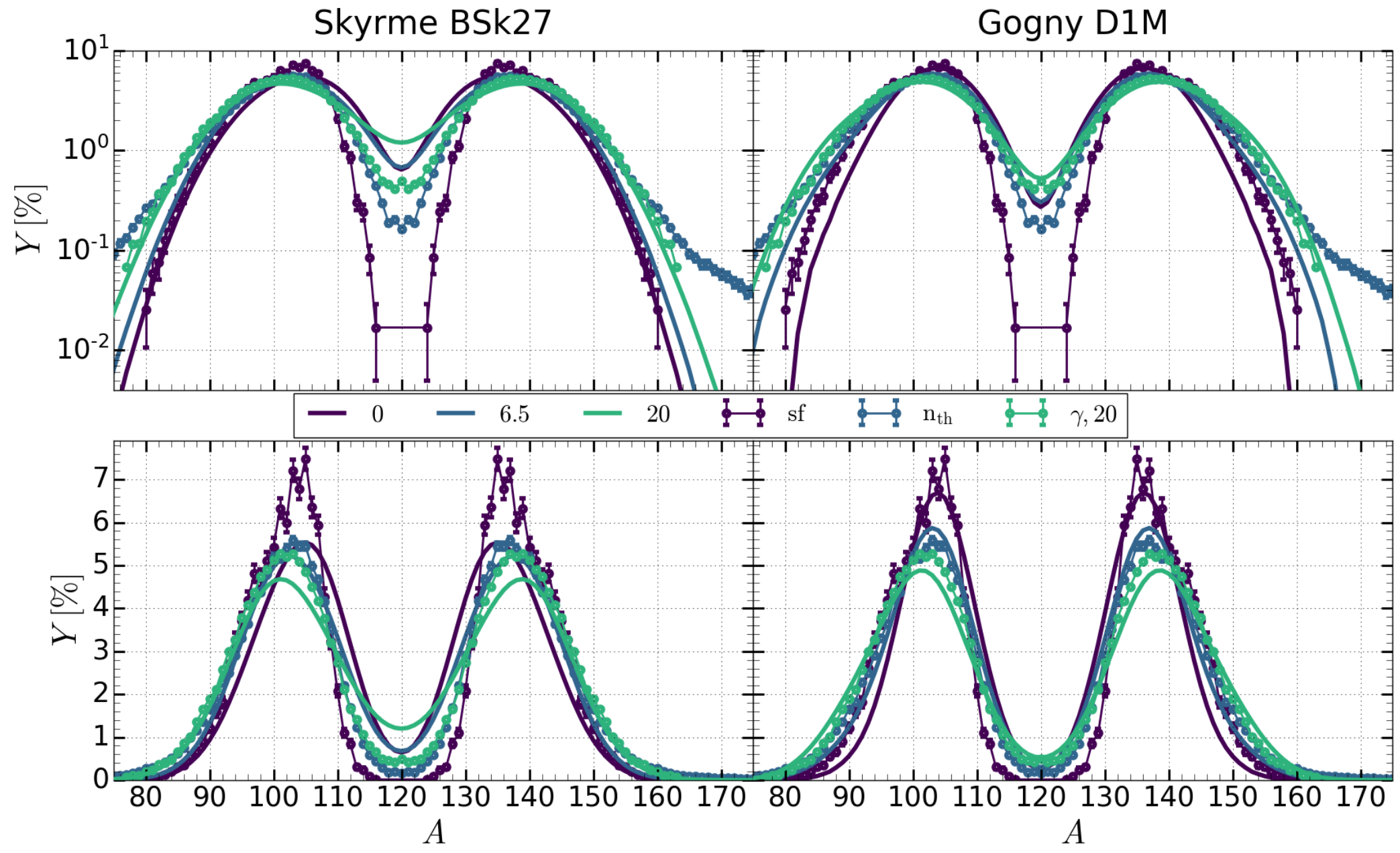
# Pu240

## Q=0/6.5 MeV



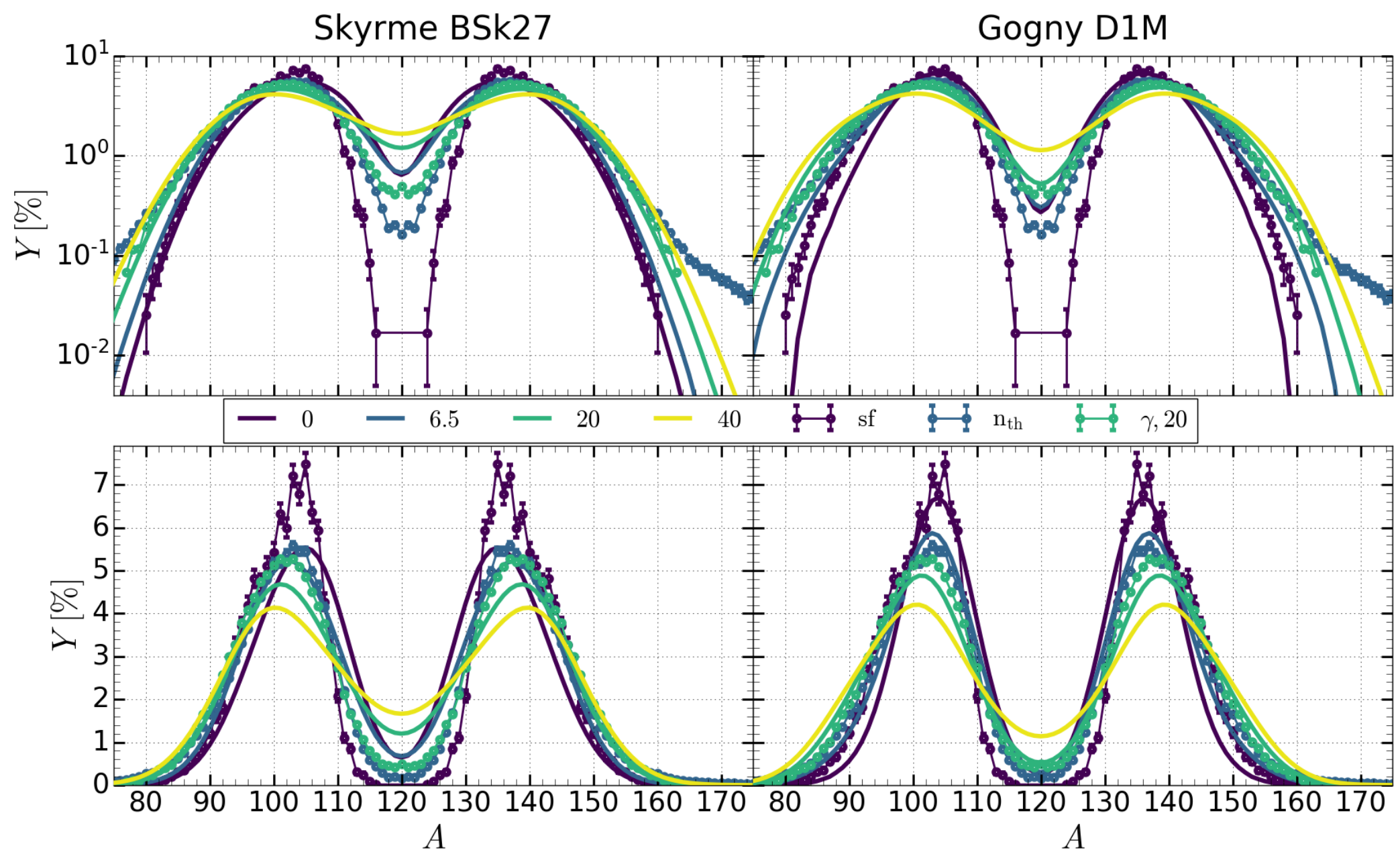
# Pu240

## Q=0/6.5/20 MeV



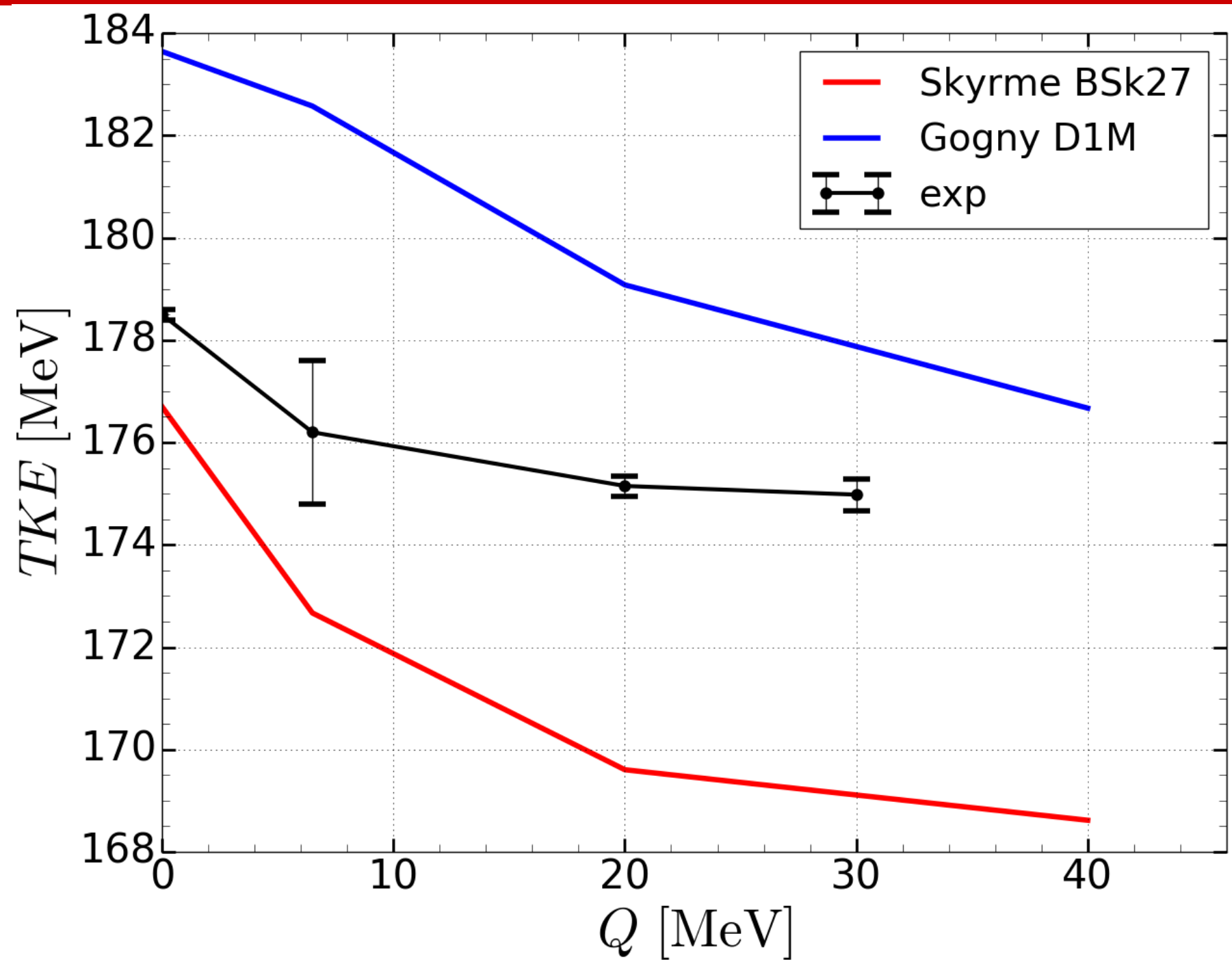
# Pu240

## Q=0/6.5/20/40 MeV

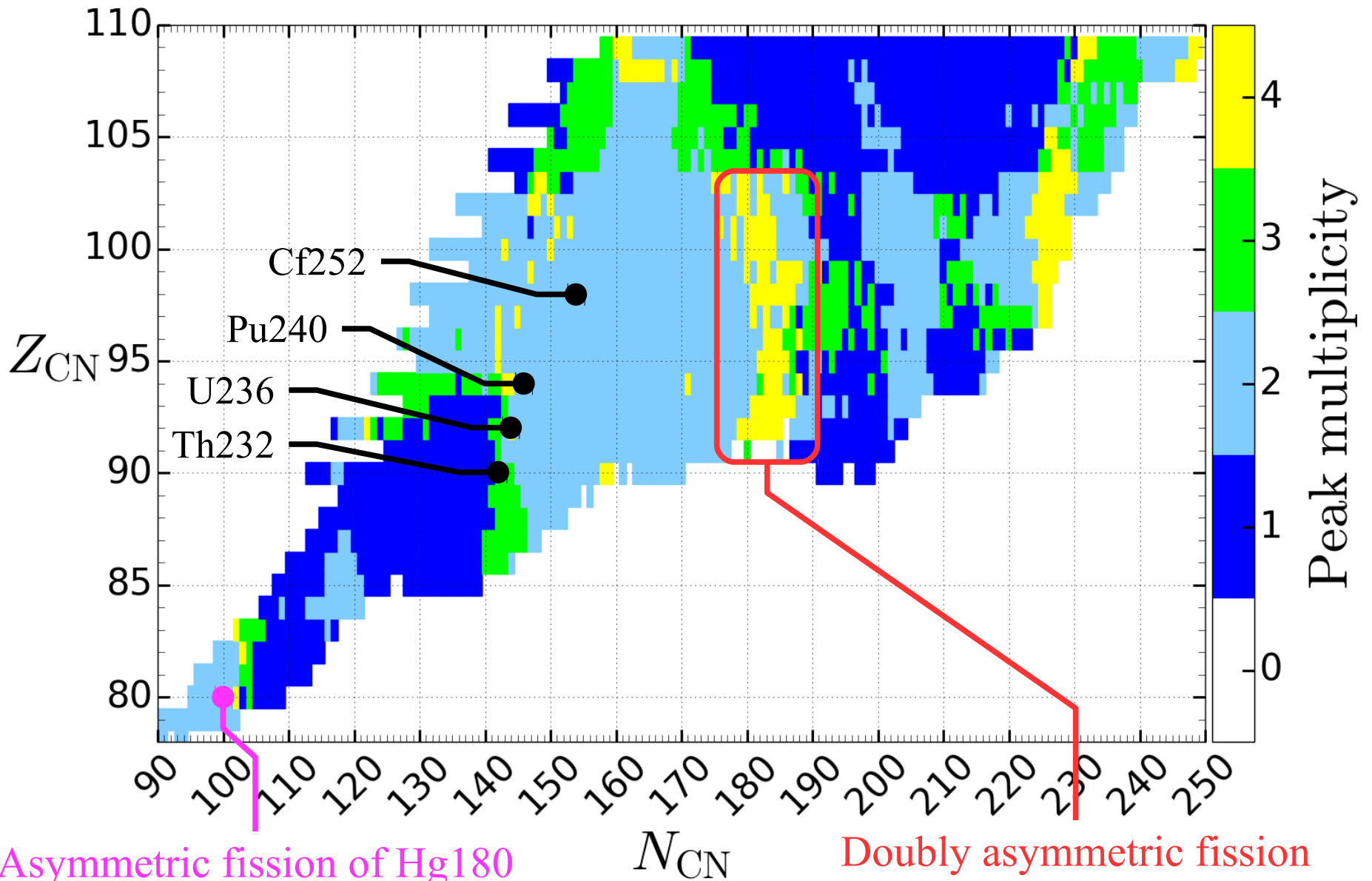


# Pu240

Q=0/6.5/20/40 MeV



# Systematic Peak multiplicity



Asymmetric fission of Hg180

(S. Panebianco et al, Phys. Rev. C 86, 064601 (2012))

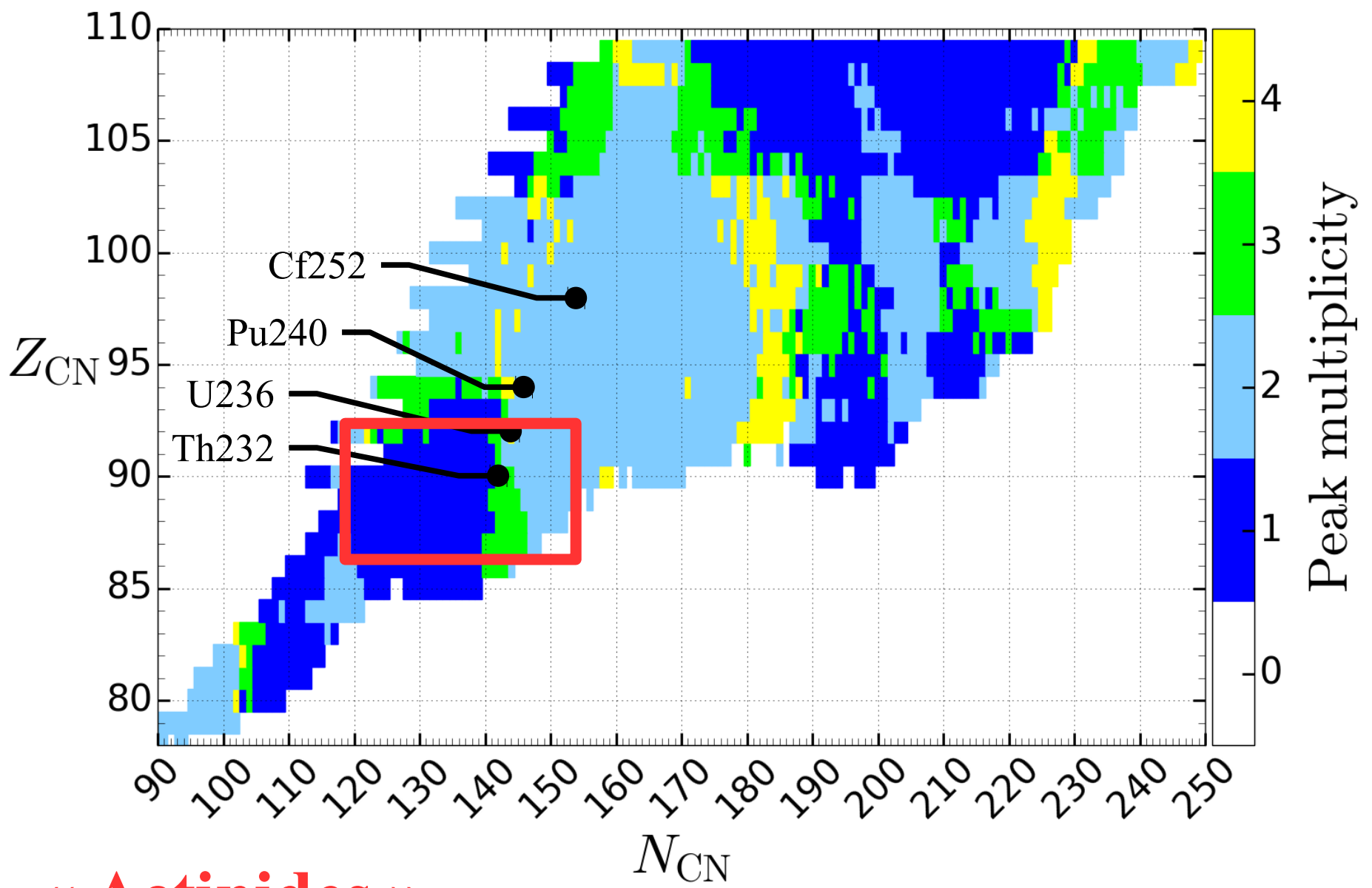
Doubly asymmetric fission

→ production of r-process elements  $A \sim 165$

(S. Goriely et al, Phys. Rev. Lett. 111, 242502 (2013))

SPY-BSk27 \*  $Q=8$  MeV \*  $\rho_{\text{neck}}=0.002$  fm<sup>-3</sup>

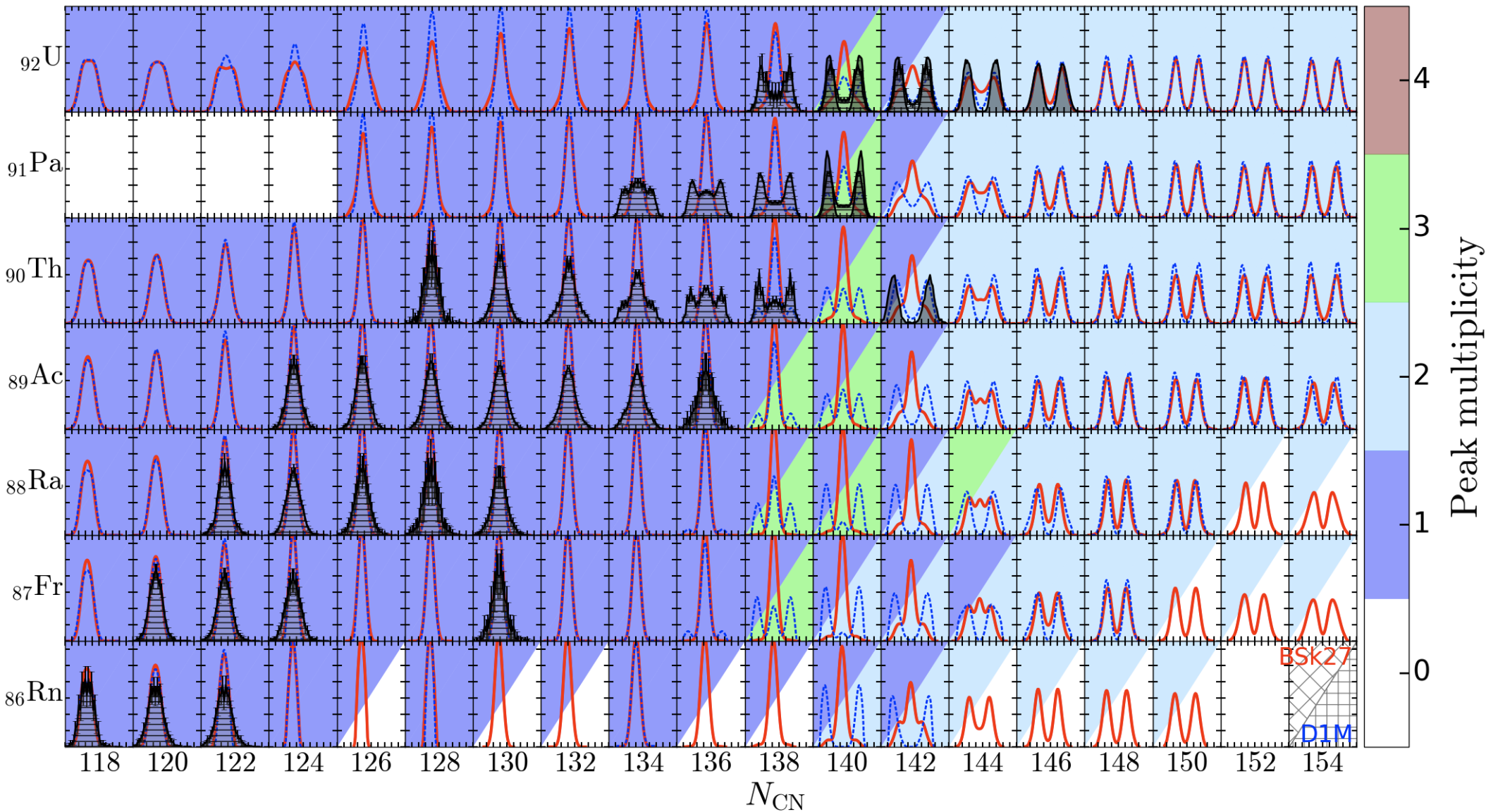
# Systematic Peak multiplicity



« Actinides »

# Systematic, BSk27+D1M

nuclei : Rn  $\rightarrow$  U,  $Q=10$  MeV,  $\rho_{\text{neck}}=0.002$  fm $^{-3}$



Disparity of the location of sym/asym fission for Fr, Rn (6 neutrons)  
 Transition sym/asym occurs for a too neutron rich isotope wrt exp. data  
 Exp. Data, curve with a striped filling : Coulex induced fission,  $E^*$  around 11 MeV (GDR) (NPA655 p221(2000))  
 QEC transition sym/asym of U at low  $E^*$  ( $< E_{\text{barr}} + 2$  MeV) ? transition sym/asym location for  $Z < 90$



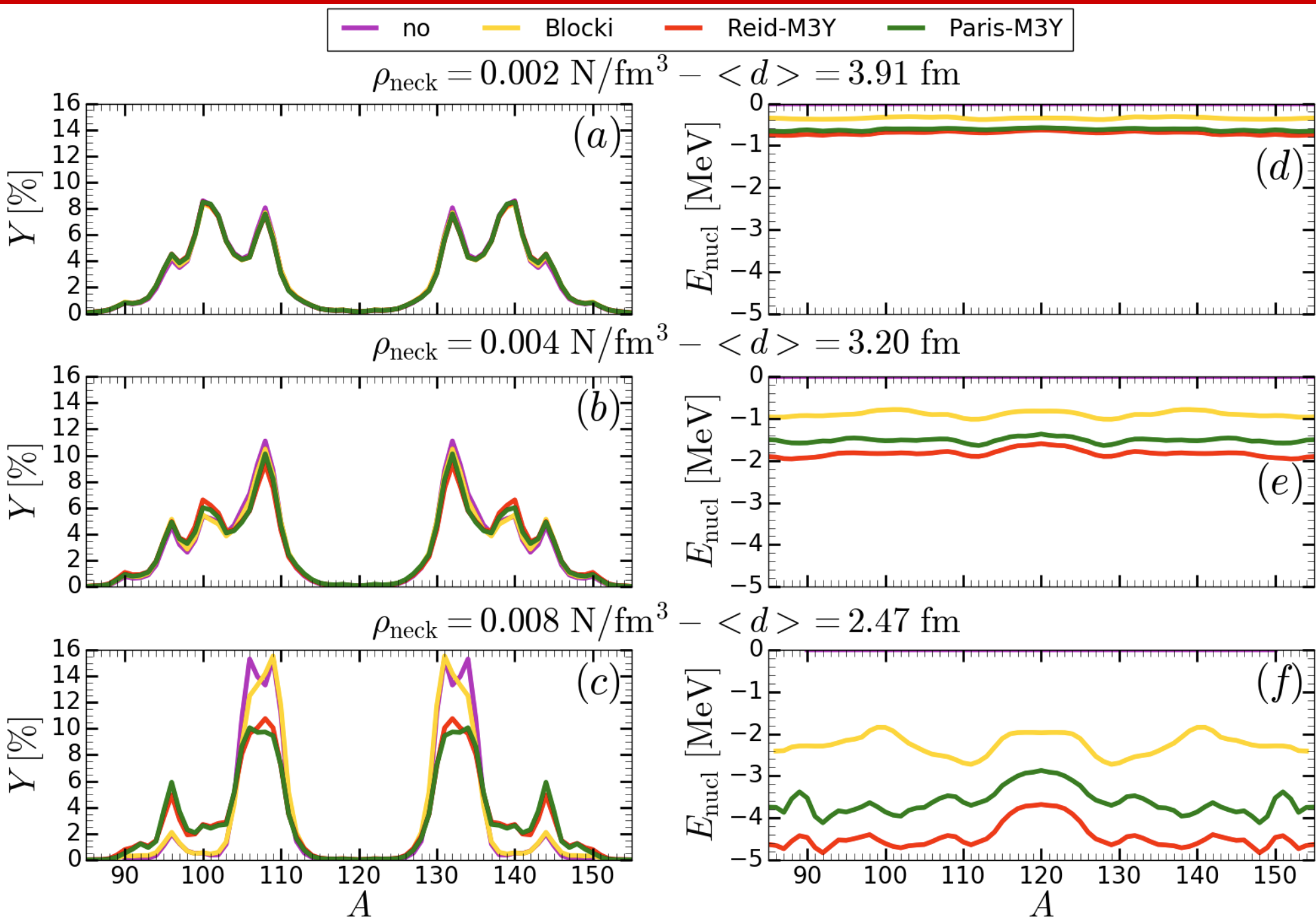
## Conclusions

- Scission point, static frag., statistical (microcanonical description)
- Definition of the scission point based on realistic proton distribution
- All ingredients are calculated coherently in the same microscopic framework  
(Skyrme BSk27 eff. N-N interaction ; J.-F. Lemaître et al, Phys Rev C 99, 034612 (2019) )
- Applied to the r-process, doubly asymm. fission (S. Goriely et al, Phys. Rev. Lett. 111, 242502 (2013))

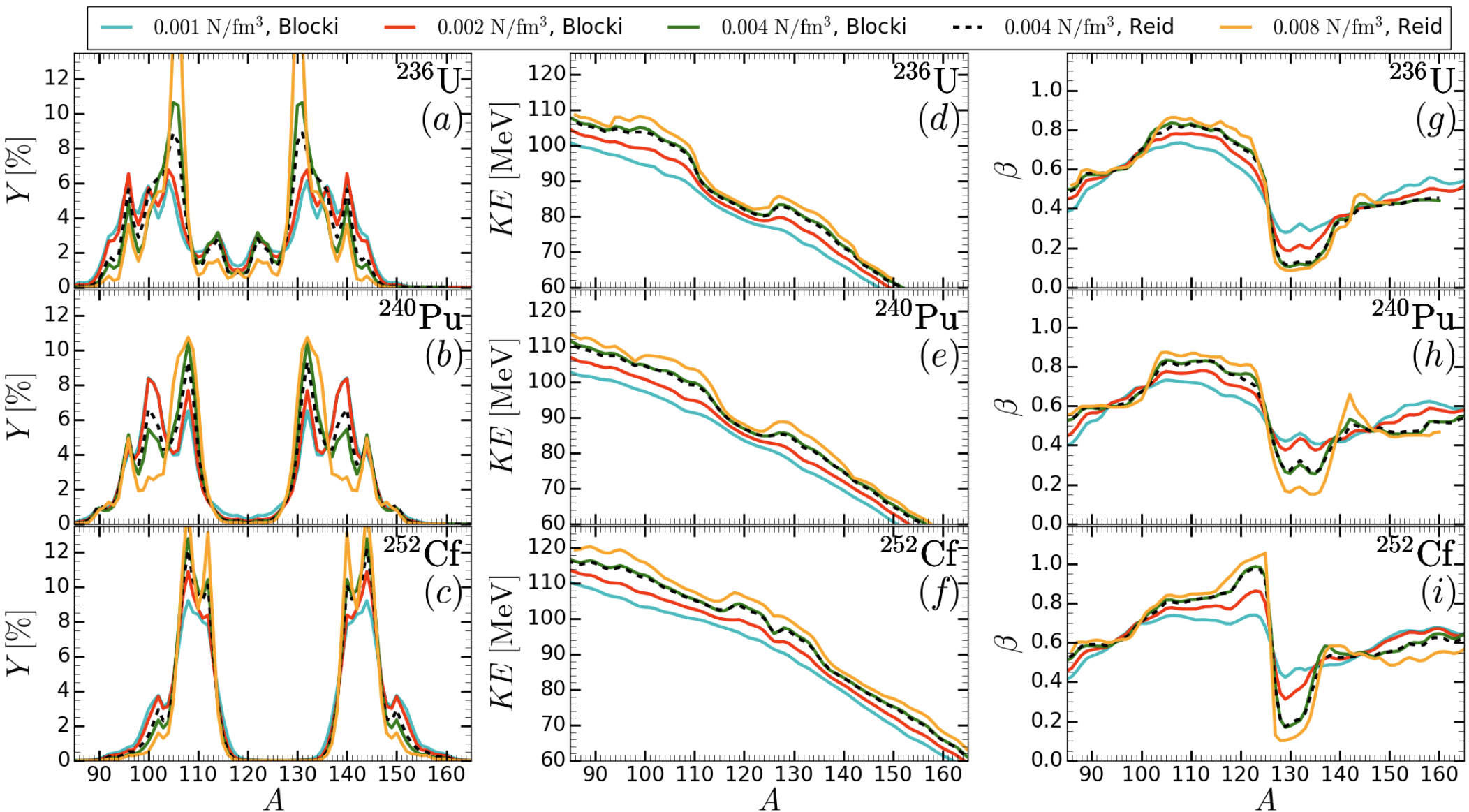
## Outlooks

- \* Improve the description of the kinetic energy
- \* Improve the neutron evaporation
- \* Improve  $Y$  evolution with  $Q$
- \* Octupole deformations
- \* Explore the odd-even effects in observables
- \* States densities including pairing gap ( $\Delta$ ) fluctuations
- \* New version with Gogny-D1M eff. N-N interaction  $\rightarrow$  link with PES

# Impact of $E_{\text{nucl}}$ & $\rho_{\text{neck}}$ on Pu240

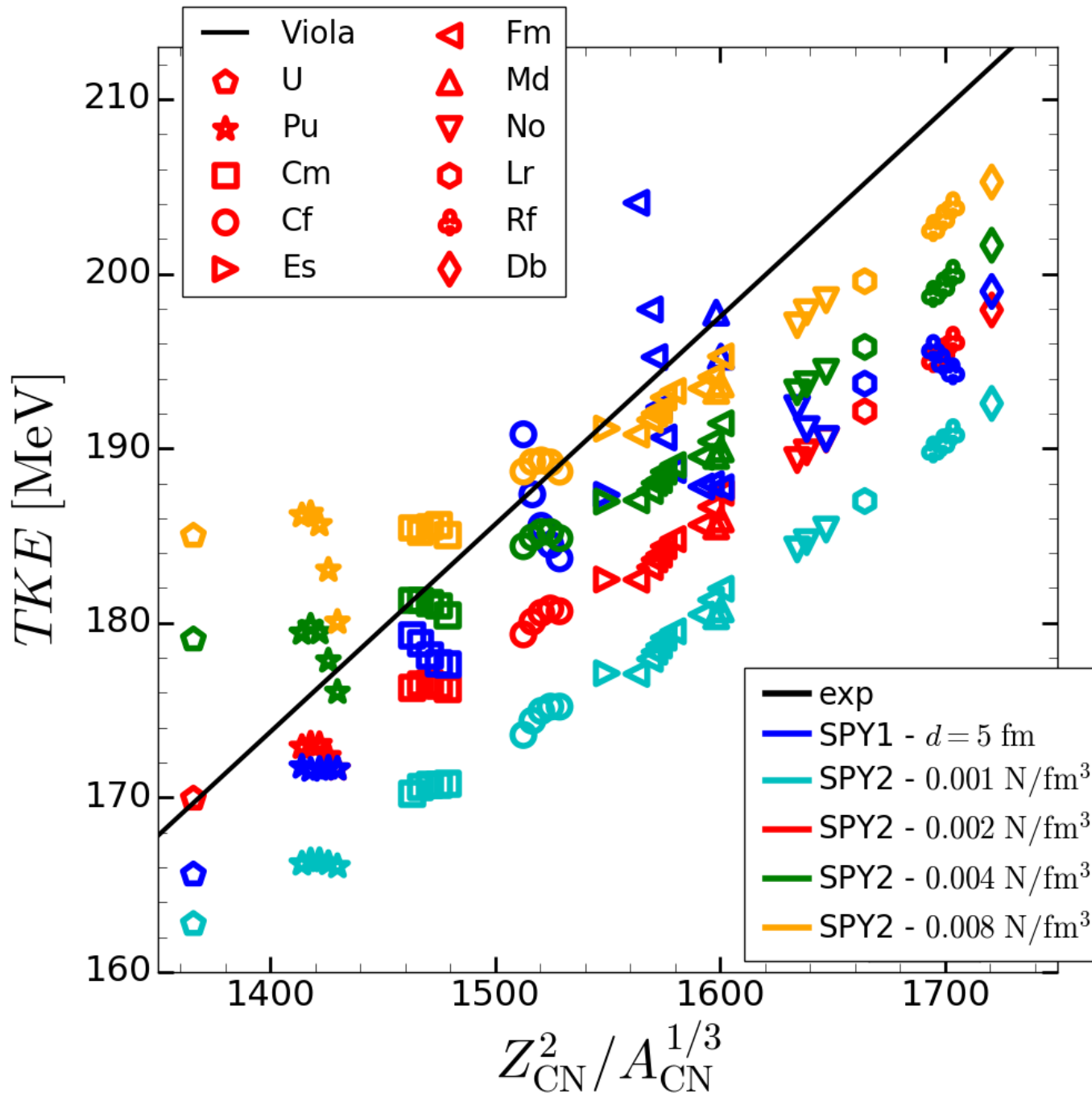


# Impact of $\rho_{\text{neck}}$ on yields

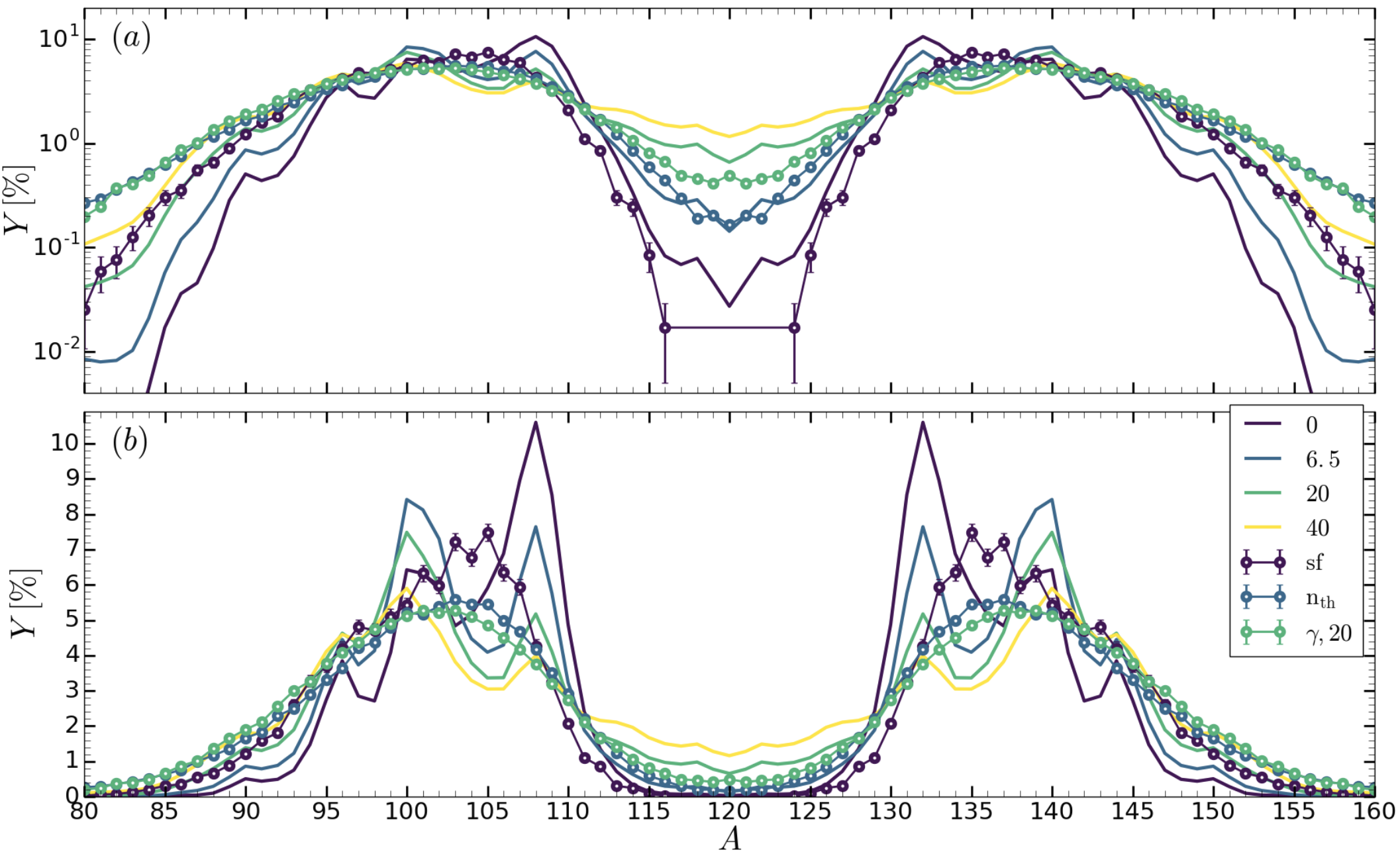


# Impact of $\rho_{\text{neck}}$ on TKE

BSk 27  
Q=8MeV



$$\sigma_z = \sigma_n = 0.65$$



particle number equation :

$$N_q = \sum_k 1 - \frac{\varepsilon_q^k - \lambda_q}{E_q^k} \tanh\left(\frac{E_q^k}{2T}\right) \text{ with } N_q = Z \text{ or } N$$

gap equation :

$$\frac{2}{G_q} = \sum_k \frac{1}{E_q^k} \tanh\left(\frac{E_q^k}{2T}\right) \text{ with } G_q \text{ the pairing strength}$$

where :

$$E_q^k = \sqrt{(\varepsilon_q^k - \lambda_q)^2 + \Delta_q^2} \text{ the quasiparticle energy}$$

$\varepsilon_q^k$  : energy of the kth level of the SPL scheme

$\lambda_q$  : chemical potential ;  $\Delta_q$  : pairing gap ;  $T$  : temperature

$$E_{\text{tot}}(T) = \sum_{q=n,p} \sum_k \left[ 1 - \frac{\varepsilon_q^k - \lambda_q}{E_q^k} \tanh\left(\frac{E_q^k}{2T}\right) \right] - \frac{\Delta_q^2}{G_q}$$

$$S(T) = 2 \sum_{q=n,p} \sum_k \ln(1 + e^{-E_q^k/T}) + \frac{E_q^k/T}{1 + e^{E_q^k/T}}$$

finally we have :

$$\frac{1}{\rho(\mathbf{U})} = (2\pi)^{3/2} \left[ \frac{\sqrt{D(\mathbf{U})}}{e^{S(\mathbf{U})}} + \frac{1}{\omega_0(\mathbf{U})} \right]$$

with :

$$\omega_0(\mathbf{U}) = \frac{\pi^2 e}{12} \frac{S(\mathbf{U})^2}{T \sqrt{S_n(\mathbf{U}) S_z(\mathbf{U})}} e^{S_n(\mathbf{U}) S_z(\mathbf{U})} \text{ to avoid unphysical divergence}$$

where

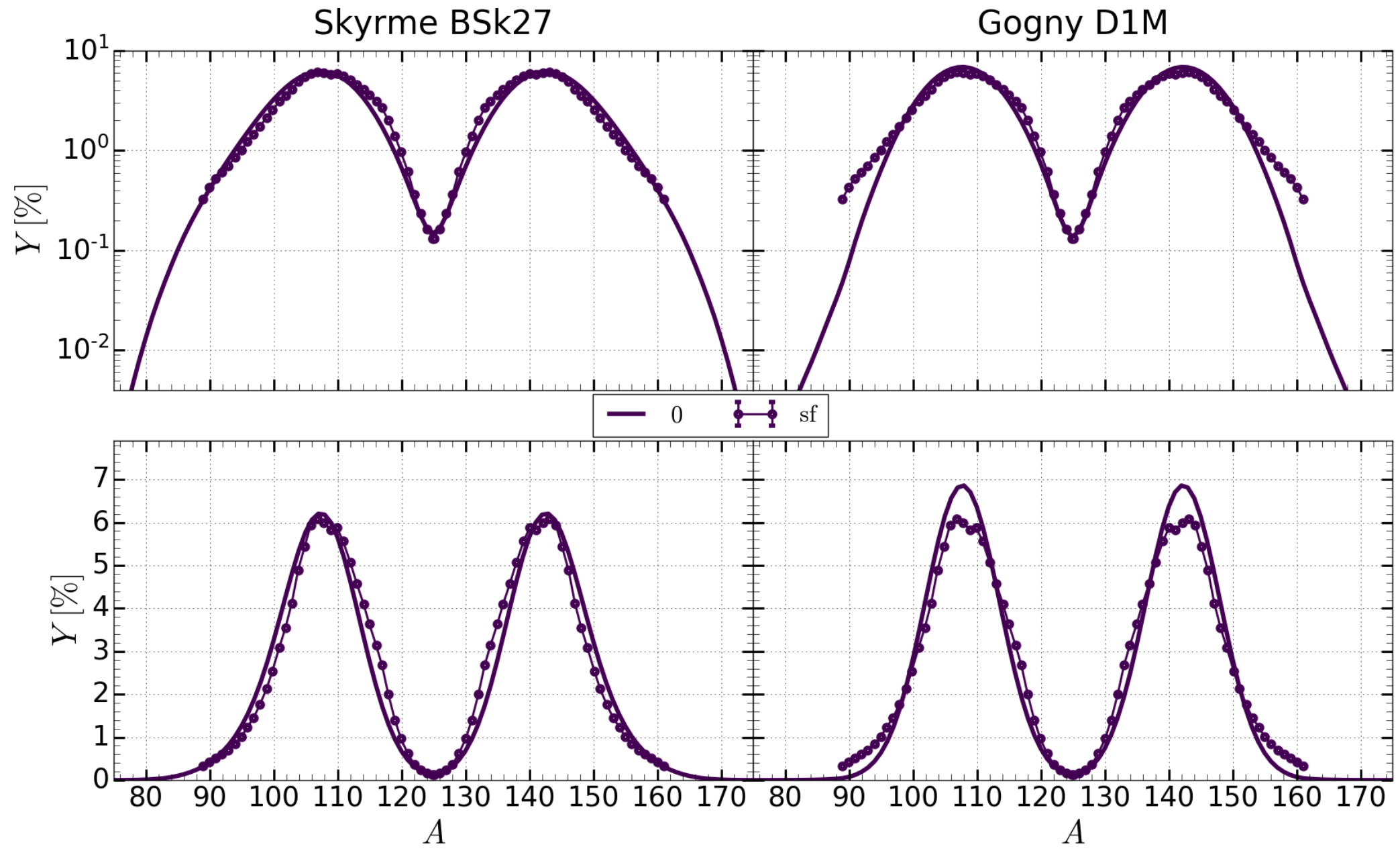
$$U = U(T) = E(T) - E(T=0)$$

$$S(U) = S_n(U) + S_z(U)$$

$D(U)$  is the determinant of the 2nd derivatives of  $\Xi$

# Cf250

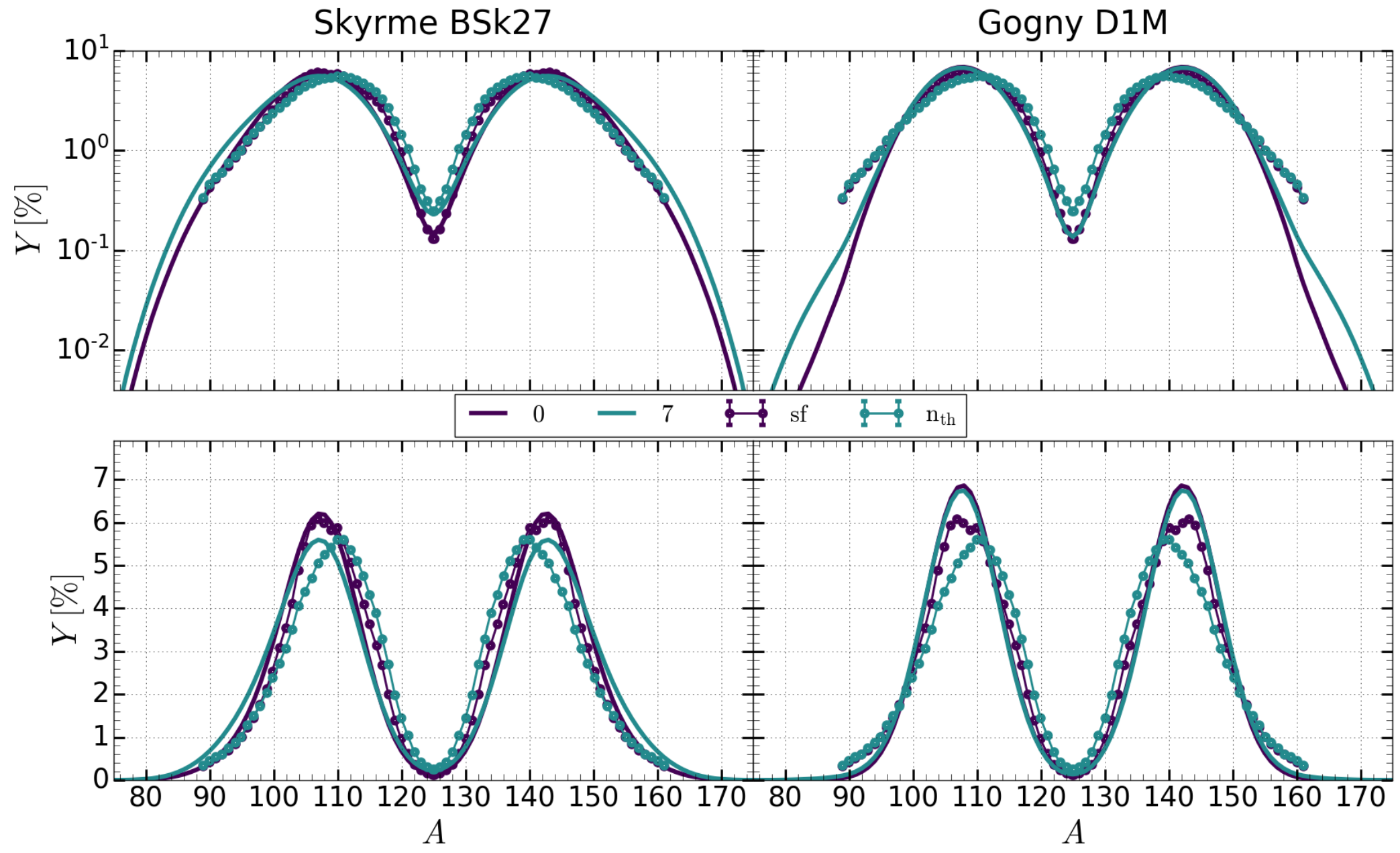
## Fission of Cf250 – Q=0/7/46 MeV





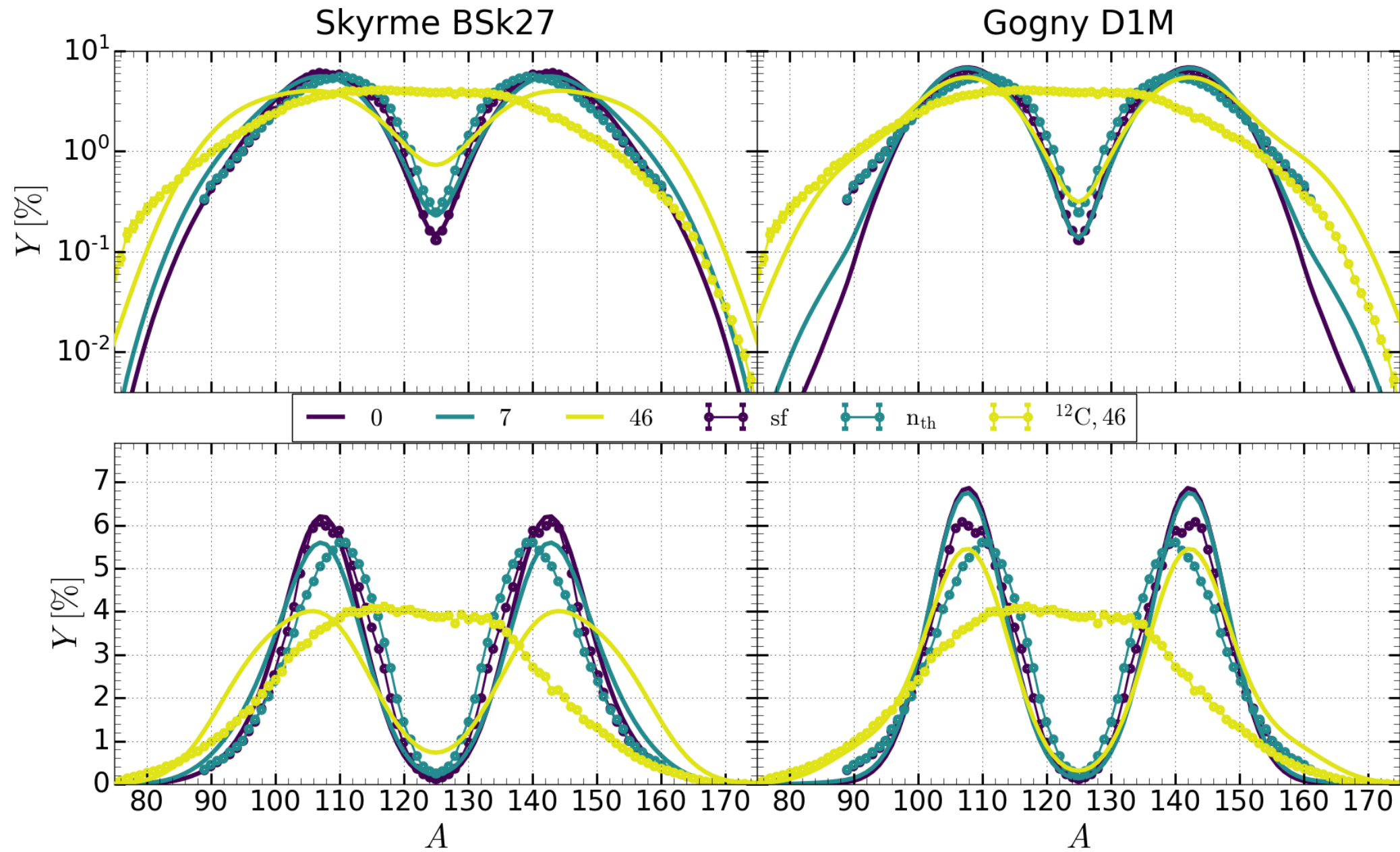
# Cf250

## Fission of Cf250 – Q=0/7/46 MeV



# Cf250

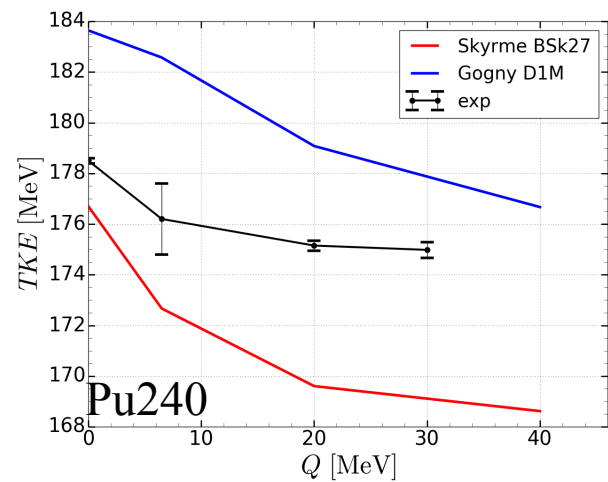
## Fission of Cf250 – Q=0/7/46 MeV



# Pu240 VS Cf250

## <TKE> evolution with Q

**Pu240** : increase of the symm. part of the yields distribution with Q  
 <TKE> decreases, from sf to nif **-1 MeV**  
 (D1M) & -4 MeV (BSk27)  
 Wagemans, ch8 : **-1.4 ± 0.1 MeV**



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 Wagemans, ch8 : **<TKE> increase**

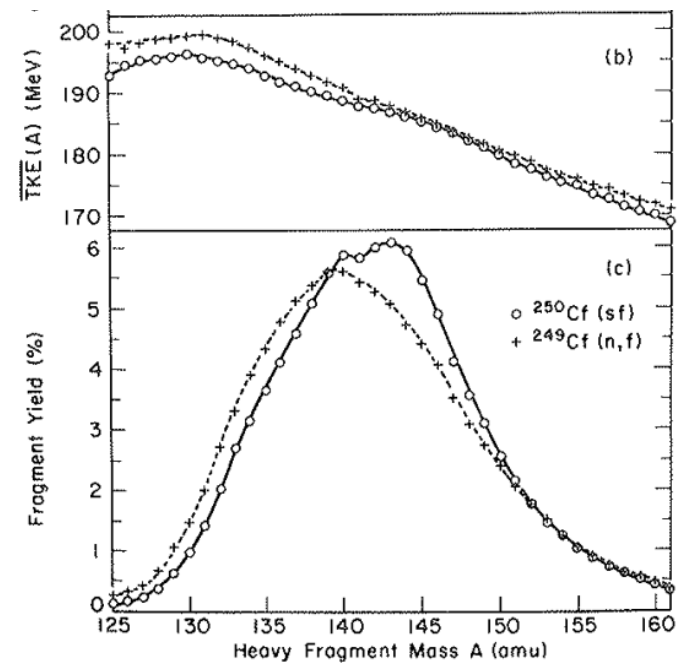
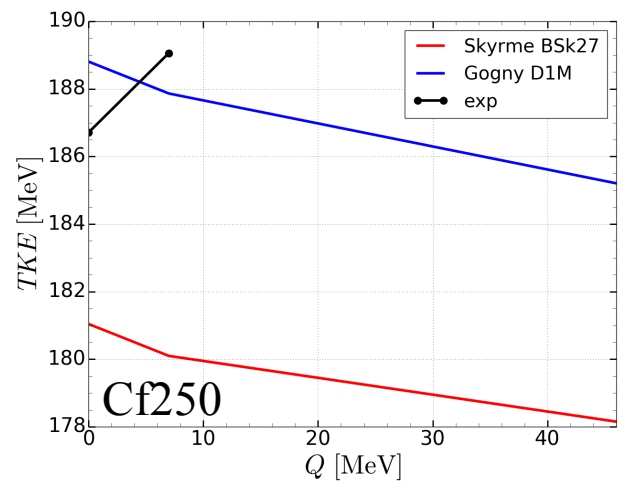
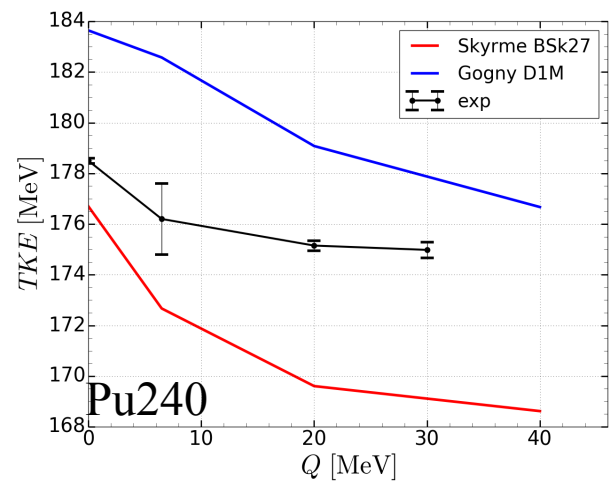


FIGURE 59. Spontaneous fission of <sup>250</sup>Cf (open points) and thermal neutron fission of <sup>249</sup>Cf(n,f) (crosses): preneutron mass yield (bottom), average total kinetic energy (middle), and rms width of total kinetic energy distribution (top) vs. heavy fragment mass. (From Unik, J. P., Gindler, J. E., Glendenin, L. E., Flynn, K. F., Gorski, A., and Sjoblom, R. K., in *Proc. Symp. Physics and Chemistry of Fission*, Vol. 2, IAEA, Vienna, 1974, 20. With permission.)

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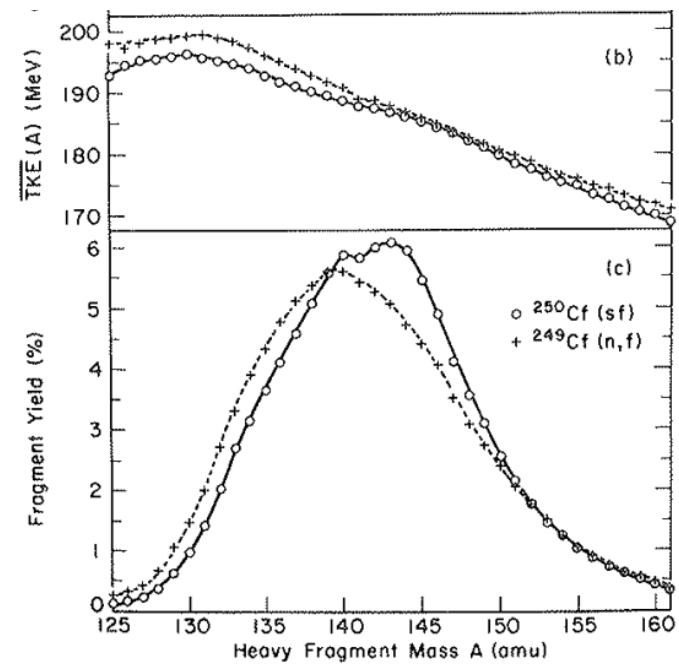
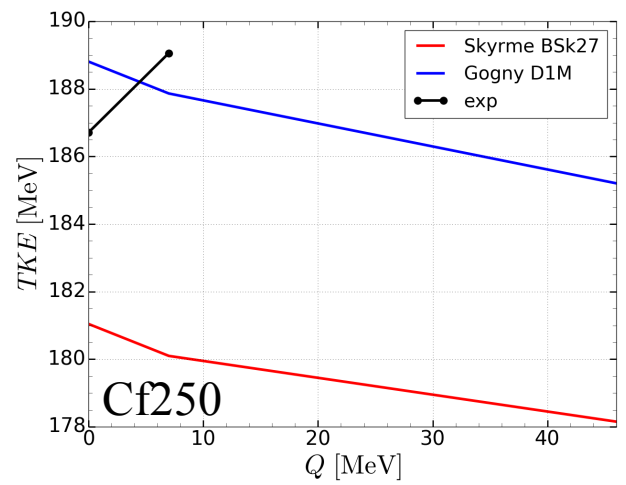
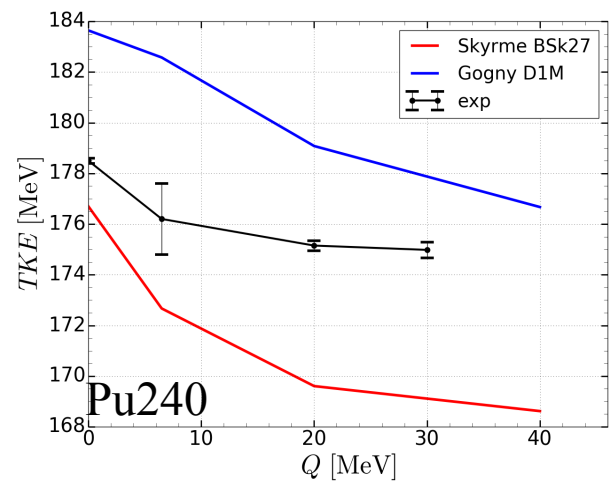


FIGURE 59. Spontaneous fission of <sup>250</sup>Cf (open points) and thermal neutron fission of <sup>249</sup>Cf(n,f) (crosses): preneutron mass yield (bottom), average total kinetic energy (middle), and rms width of total kinetic energy distribution (top) vs. heavy fragment mass. (From Unik, J. P., Gindler, J. E., Glendenin, L. E., Flynn, K. F., Gorski, A., and Sjoblom, R. K., in *Proc. Symp. Physics and Chemistry of Fission*, Vol. 2, IAEA, Vienna, 1974, 20. With permission.)

- \* too strong structure effects ? → no shell closure in frag.
- \* state density evolution with E\*
- \* <sup>238</sup>U(<sup>12</sup>C,f) ≠ <sup>249</sup>Cf(n,f) or <sup>250</sup>Cf(γ,f)
- \* Why <TKE> increases with Q for Cf250 case ? (multi-chance?)

Wagemans, ch8 ‘The interpretation of the above results [TKE evolution with Q] is not obvious. The change of sign in the average shift of KE release when moving from spontaneous to induced fission is, however, a strong indication that the question whether superfluidity in the nuclear system is preserved in the fission process is not at stake. [...]’

→ **Measure Y & <TKE> of Pu240 & Cf250 with Q ?**