Predicting stability of heaviest nuclei

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- equilibrium shapes
- masses, separation energies, Q alpha values
- saddle point shapes and fission barrier heights

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Properties of heaviest nuclei with $98 \leq Z \leq 126$ and $134 \leq N \leq 192$

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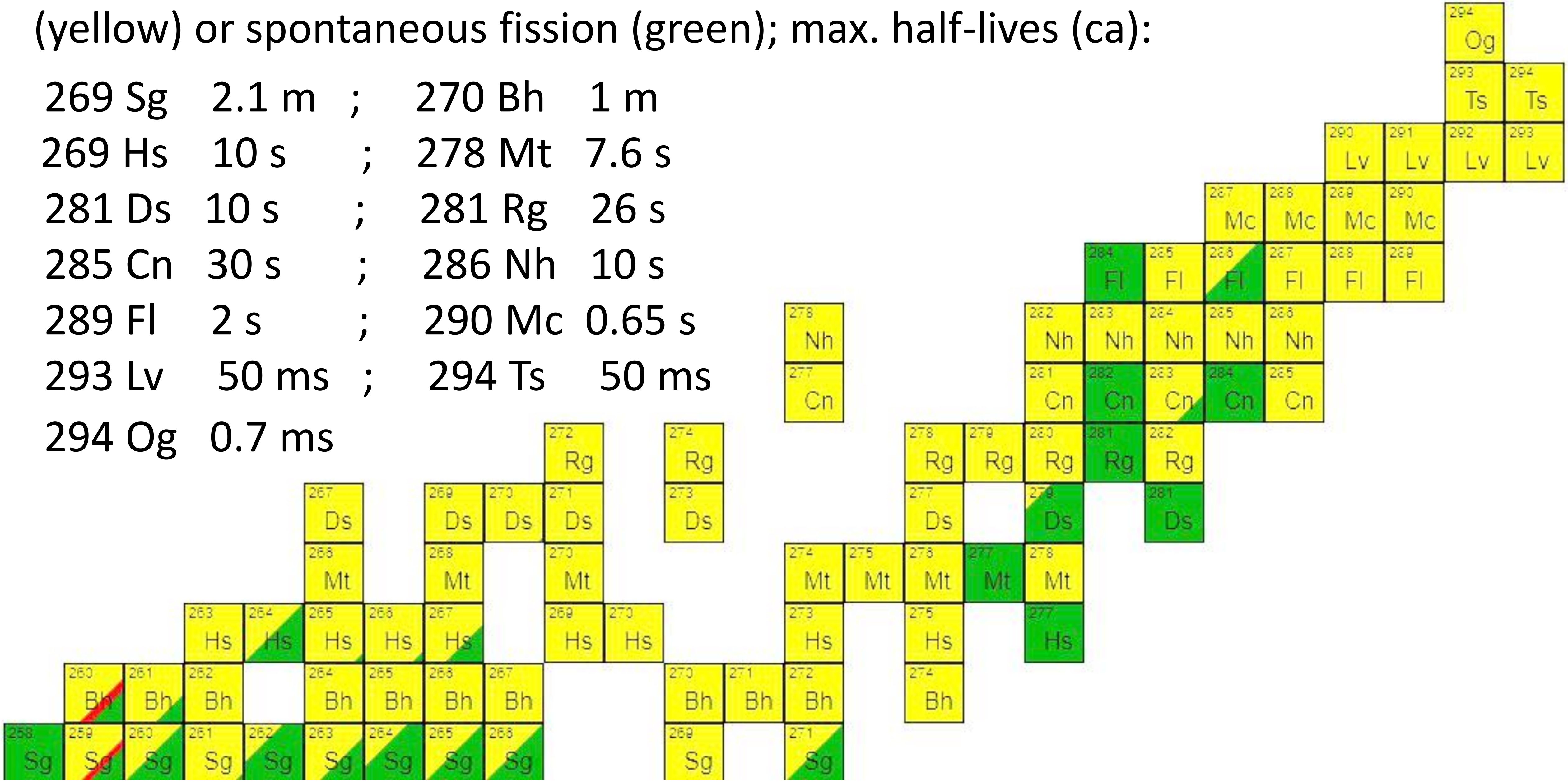
ABSTRACT

We systematically determine ground-state and saddle-point shapes and masses for 1305 heavy and superheavy nuclei with Z = 98–126 and N = 134–192, including odd-A and odd–odd systems. From these we derive static fission barrier heights, one- and two-nucleon separation energies, and Q_α values for g.s. to g.s. transitions. Our study is performed within the microscopic–macroscopic method with the deformed Woods–Saxon single-particle potential and the Yukawa-plus-exponential macroscopic energy taken as the smooth part. We use parameters of the model that were fitted previously to masses of even–even heavy nuclei. For systems with odd numbers of protons, neutrons, or both, we use a standard BCS method with blocking. Ground-state shapes and energies are found by the minimization over seven axially-symmetric deformations. A search for saddle-points was performed by

North-east of the table of nuclides: decay via alpha-emission (yellow) or spontaneous fission (green); max. half-lives (ca):

269 Sg	2.1 m	;	270 Bh	1 m	
269 Hs	10 s	;	278 Mt	7.6 s	
281 Ds	10 s	;	281 Rg	26 s	
285 Cn	30 s	;	286 Nh	10 s	
289 Fl	2 s	;	290 Mc	0.65 s	
293 Lv	50 ms	;	294 Ts	50 ms	
294 Og	0.7 ms				

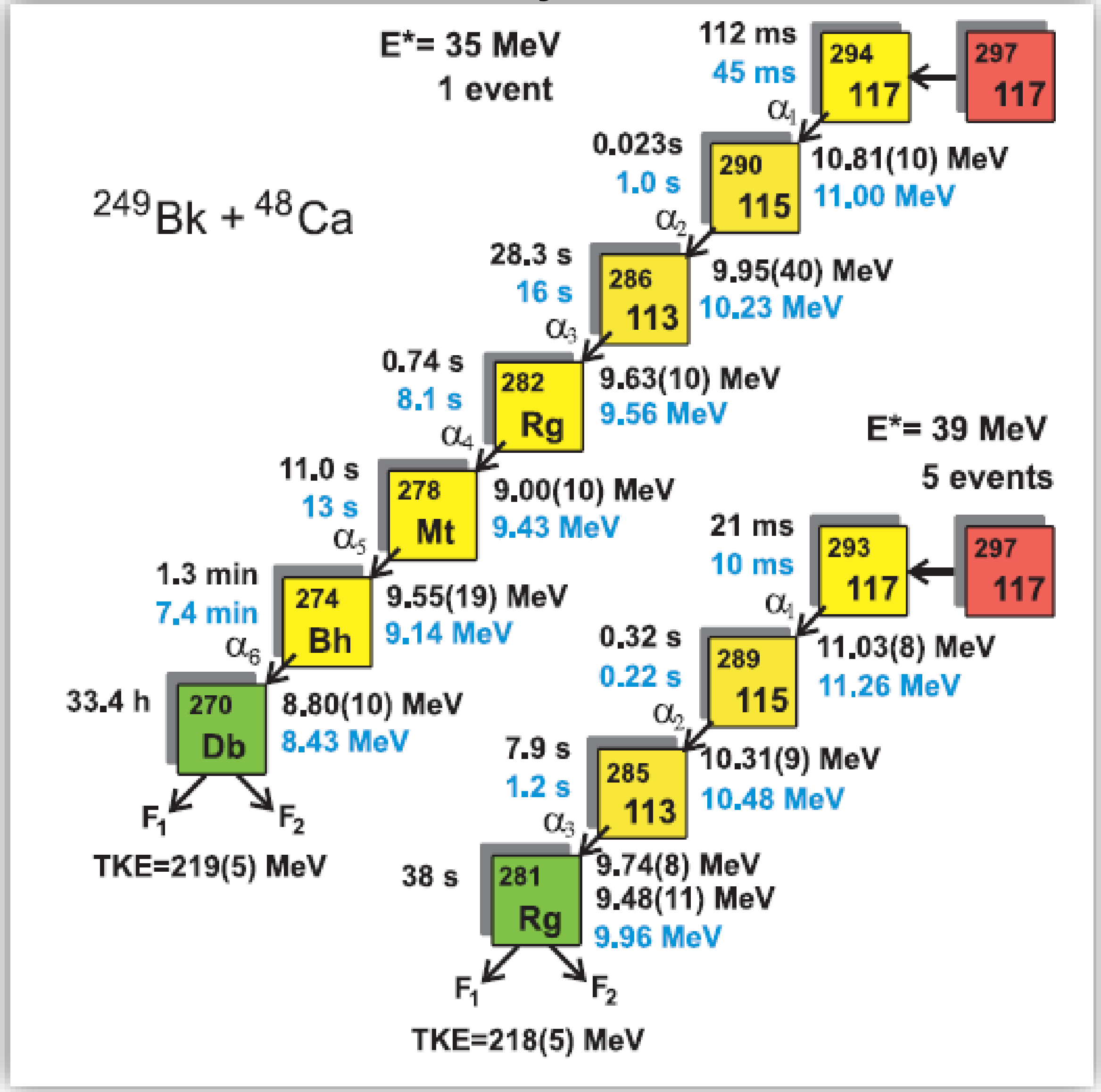


Main interests of the study:

- limits of nuclear stability;
- possible new structural effects;
- possible influence of SHN on nucleosynthesis via r-process in supernovae and neutron star mergers – its assessment requires fission barriers, alpha-decay rates etc;
- access to chemical properties of new elements.

Involves a serious extrapolation of theory – there is uncertainty concerning magic numbers beyond lead.

Example of exp. data: observed decay chains for Z=117



Alpha – decay energies which are nuclear mass differences can be converted into alpha half-lives by means of simple formulas valid to ca 1 order of magnitude.

Fission barriers (in actinides the first and second barriers are experimentally evaluated) give probability of fission at sizable (over the barrier) excitation energy. These quantities are useful for estimates of various reactions.

Spontaneous fission half-lives require more knowledge then the barrier height alone. However, together with the overall energy landscape they give clue about it.

Selfconsistent mean-field theory with effective density – dependent interaction: HF or HFB   (or RMF); schematically:

$$\hat{\rho} = \sum_{n\ occ} |\phi_n\rangle\langle\phi_n|,$$ density made shape-dependent via constraints on moments

$$E(\{\phi_k\}) = E(\rho) = \sum_{\mu\nu} t_{\mu\nu}\rho_{\nu\mu} + \frac{1}{2}\sum_{\mu\nu\gamma\delta}(v_{\mu\nu\gamma\delta} - v_{\mu\nu\delta\gamma})\rho_{\delta\nu}\rho_{\gamma\mu},$$

$$\delta E(\{\phi_k\})/\delta\phi_m^* = \hat{h}(\rho)\,|\phi_m\rangle, \qquad \hat{h}(\rho)\phi_\mu = (\hat{t}+\hat{V})\phi_\mu = e_\mu\phi_\mu,$$

Micro-macro method: idea that macroscopic energy formulas are 99% correct while the remnant is due to bunching of s.p. levels into shells – hence shell correction.

a density $\tilde{\rho}$, obtained from ρ by a procedure of averaging over the shell structure, $\hat{h}(\tilde{\rho})\psi_\mu = (\hat{t}+\hat{\tilde{V}})\psi_\mu = \varepsilon_\mu\psi_\mu.$

$$\rho^S = \sum_{n\ occ} |\psi_n\rangle\langle\psi_n|$$

$$E_{HF}(\rho) - E(\tilde{\rho}) = \mathrm{Tr}\,\hat{h}(\tilde{\rho})(\rho^S - \tilde{\rho}^S) \; + \; \text{terms} \sim (\delta\rho)^2.$$

Based on this, one assumes: $$E_{HF}(\rho) \approx E_{LD} + \mathrm{Tr}\,\hat{h}(\rho^S - \tilde{\rho}^S) = E_{LD} + \delta E.$$

Micro-macro method may use various geometric deformations of nuclear surface

$$R(\vartheta,\varphi) = c(\{\beta\})R_0\{1 + \sum_{\lambda\geq 1} \beta_{\lambda 0} Y_{\lambda 0}(\vartheta,\varphi) + \sum_{\lambda\geq 1,\mu>0} \beta_{\lambda\mu} Y^r_{\lambda\mu}(\vartheta,\varphi)\},$$

$$E_{tot}(\beta_{\lambda\mu}) = E_{macro}(\beta_{\lambda\mu}) + E_{micro}(\beta_{\lambda\mu})$$

$$E_{macro}(\beta_{\lambda\mu}) = \text{Yukawa} \; + \text{exponential}$$

$$E_{micro}(\beta_{\lambda\mu}) = \text{Woods-Saxon} + \text{pairing BCS}$$

- energy on maps: $$E = E_{tot}(\beta_{\lambda\mu}) - E_{macro}(\beta_{\lambda\mu} = 0)$$

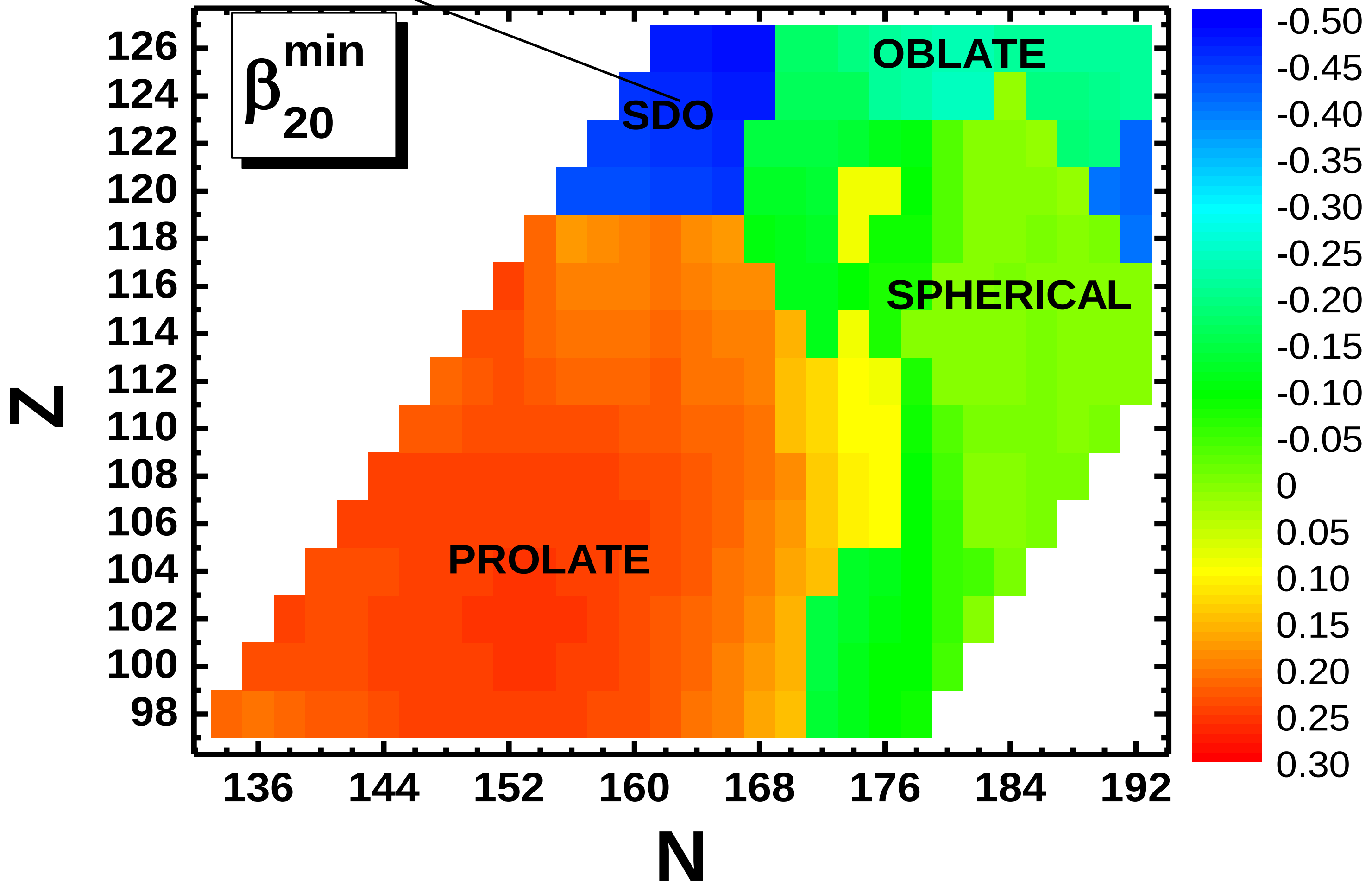
Ground state shapes

$SDO:$

$\beta_{20} \approx -0.5$

$Axis.ratio \approx \frac{3}{2}$

Micro-macro results; mostly four - dimensional minimization



In contrast to many Skyrme forces, Woods-Saxon micro-macro model gives lower barriers and mostly oblate ground states for Z>=124,126 (no magic gap for 126 protons).

Fit to experimental masses

- Z>82, N>126,
- Number of nuclei: 252
- For odd and odd-odd systems there are 3 additional parameters – macroscopic energy shifts (they have no effect on Q alpha).

Predictions for SHE:

88 Q_{alpha} values, Z=101-118,

7 differ from exp. by more than 0.5 MeV;

the largest deviation: 730 keV (blocking).

Slight underestimate for Z=108;

Overestimate: 109-113

Statistical parameters of the fit to masses in the model with blocking in separate groups of even-even, odd-even, even-odd and odd-odd heavy nuclei:

	e - e	o - e	e - o	o - o
N	74	56	69	53
h	0.0	1.013	0.824	1.703
$<\mid M^{th} - M^{exp} \mid>$	0.212	0.340	0.356	0.566
$Max \mid M^{th} - M^{exp} \mid$	0.833	0.836	1.124	1.387
δ_{RMS}	0.284	0.425	0.435	0.666

The same but for the method without blocking.

	e - e	o - e	e - o	o - o
N	74	56	69	53
h	0.0	-0.751	0.268	0.234
$<\mid M^{th} - M^{exp} \mid>$	0.187	0.460	0.273	0.295
$Max \mid M^{th} - M^{exp} \mid$	0.652	1.398	0.892	0.853
δ_{RMS}	0.251	0.551	0.343	0.366

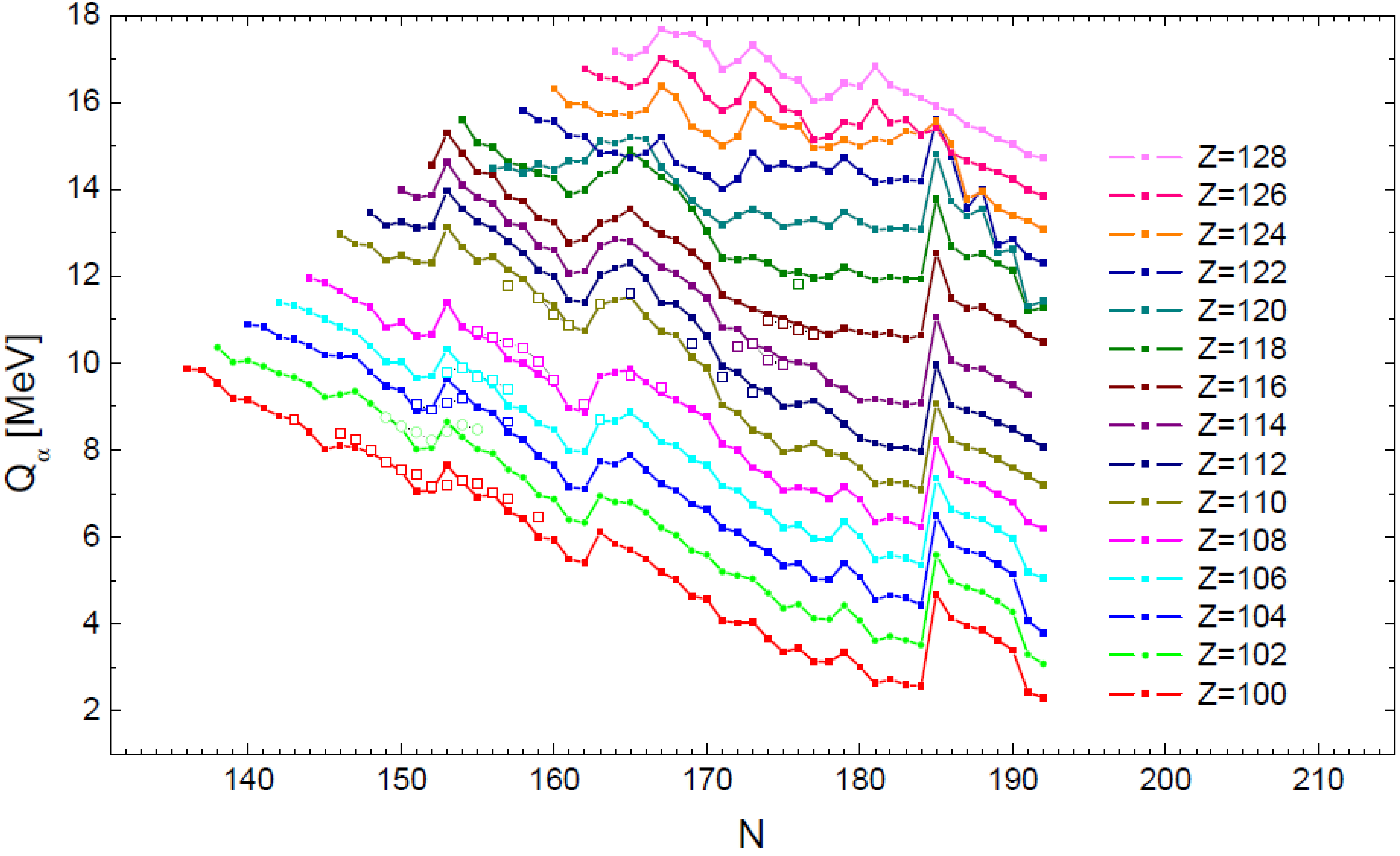
Q alpha

204 nuclei in the fit region

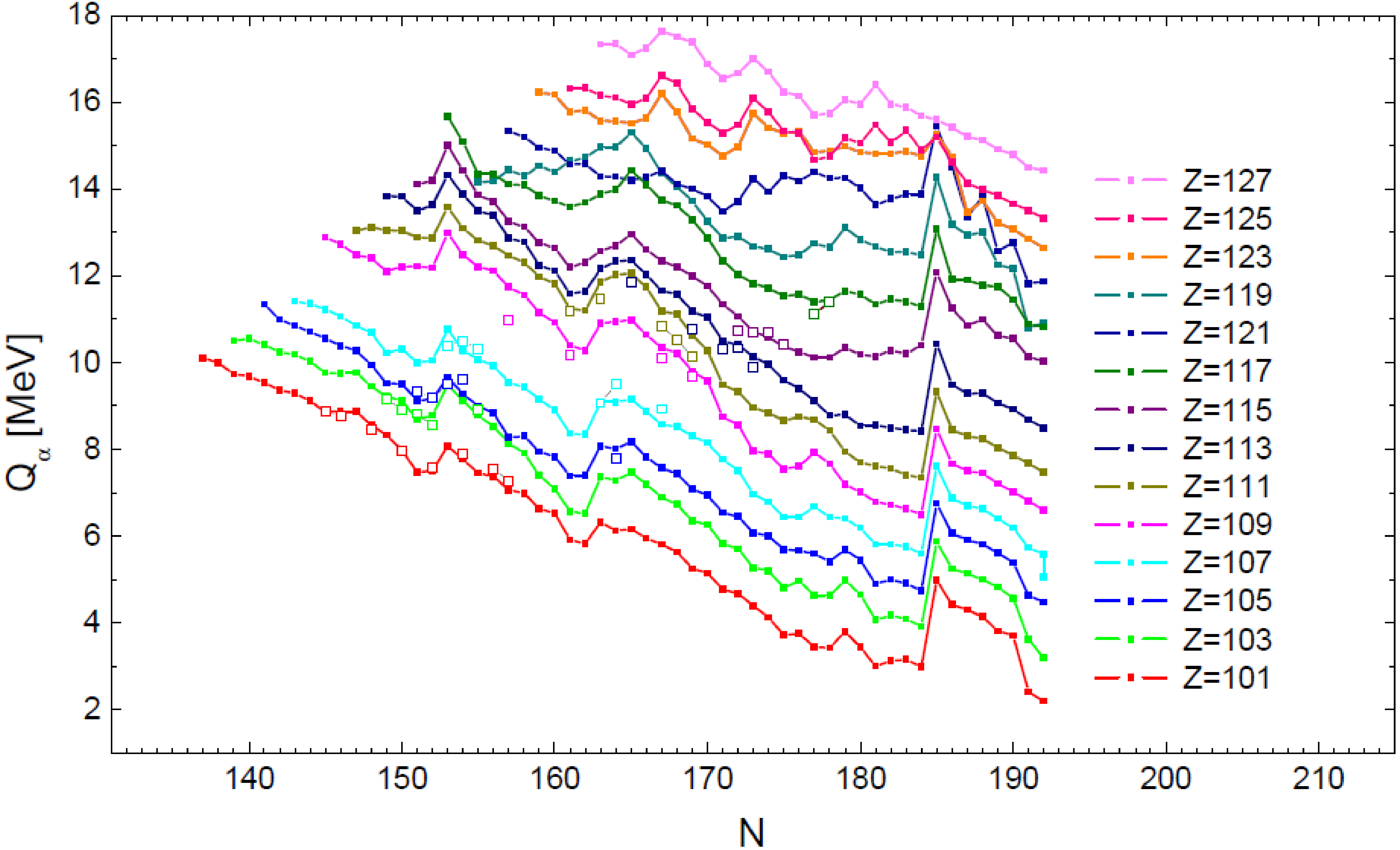
	blocking	q.p.method
mean error	326 keV	225 keV
rms	426 keV	305 keV

88 nuclei Z=101-118

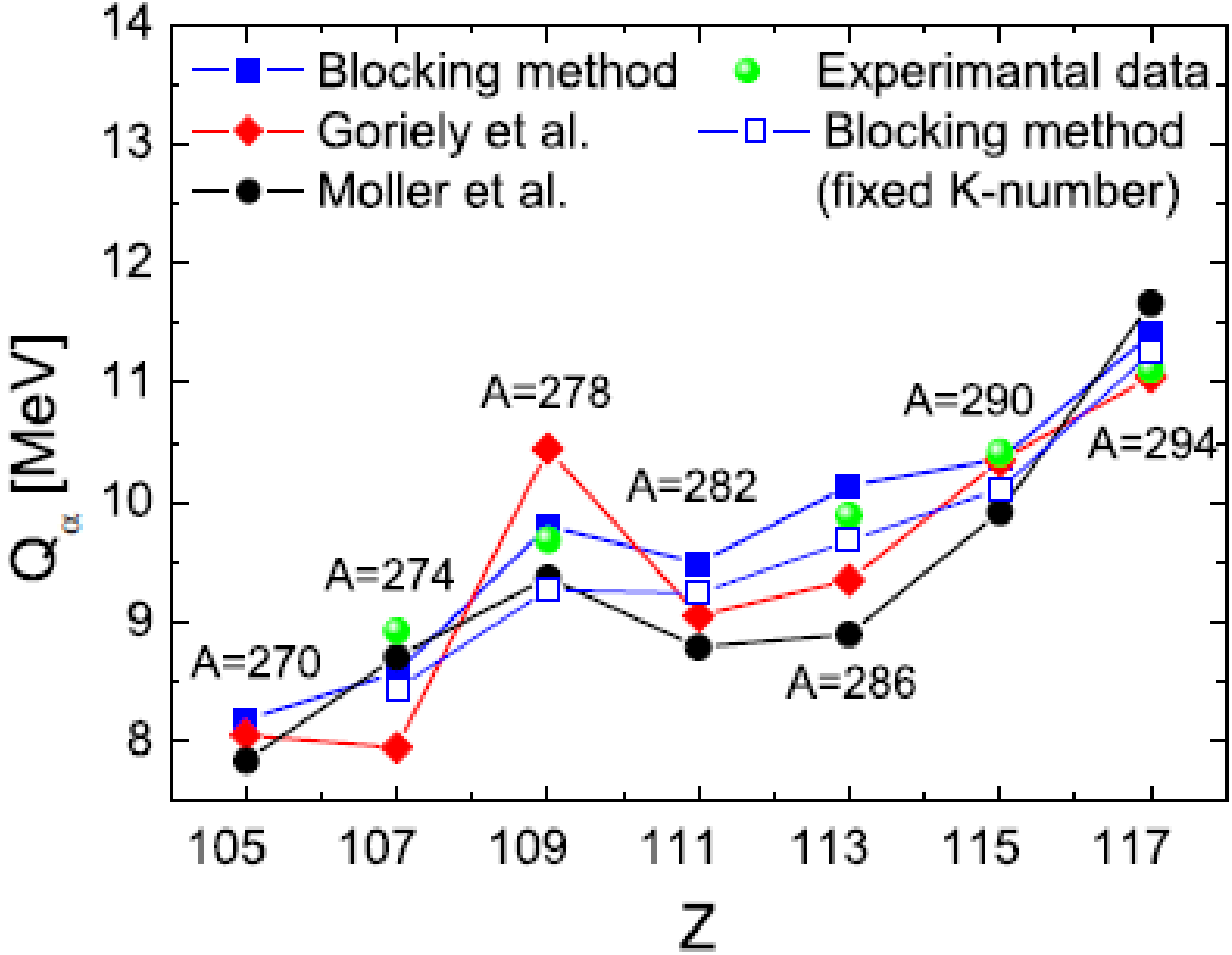
	blocking	q.p.method
mean error	217 keV	196 keV
rms	274 keV	260 keV

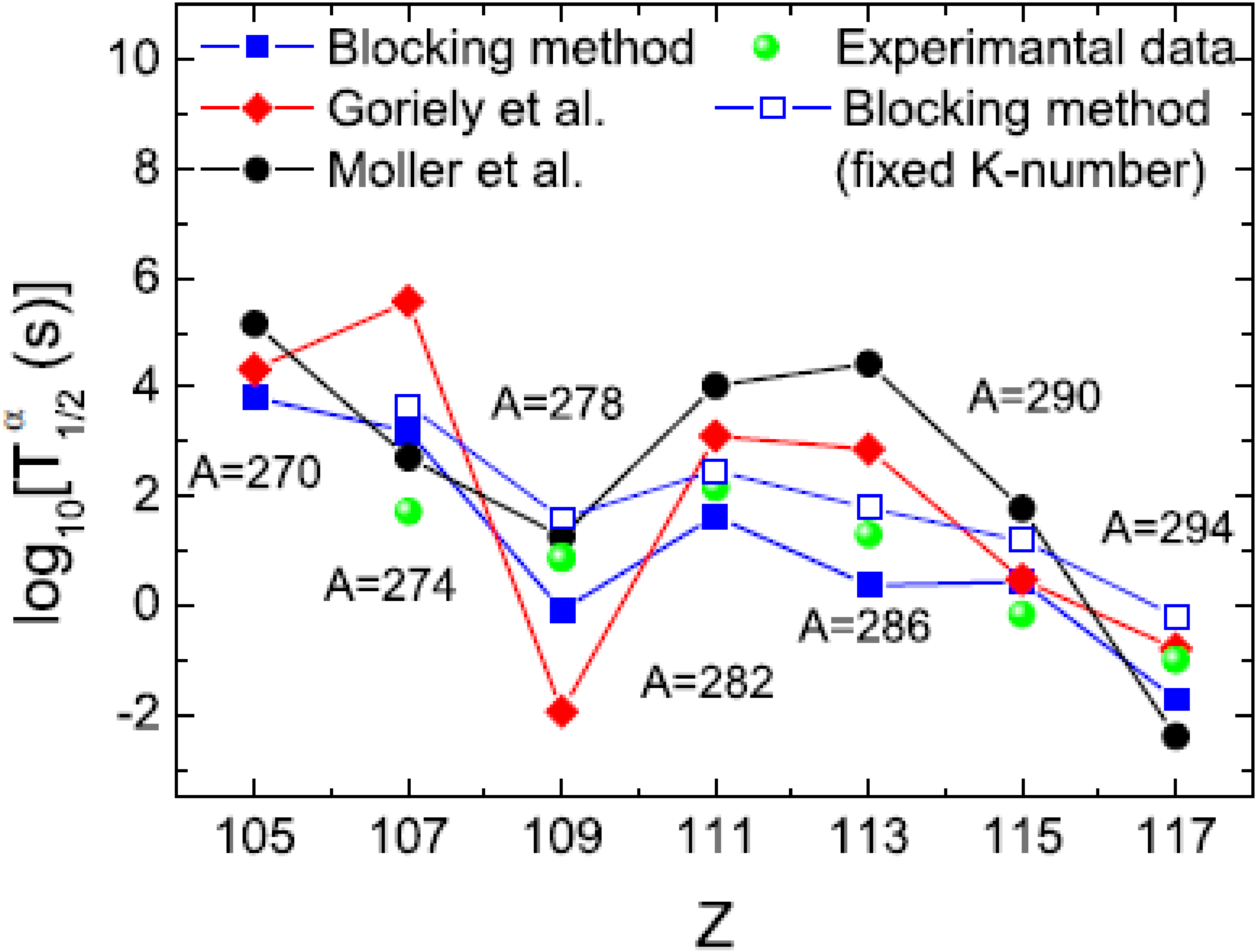


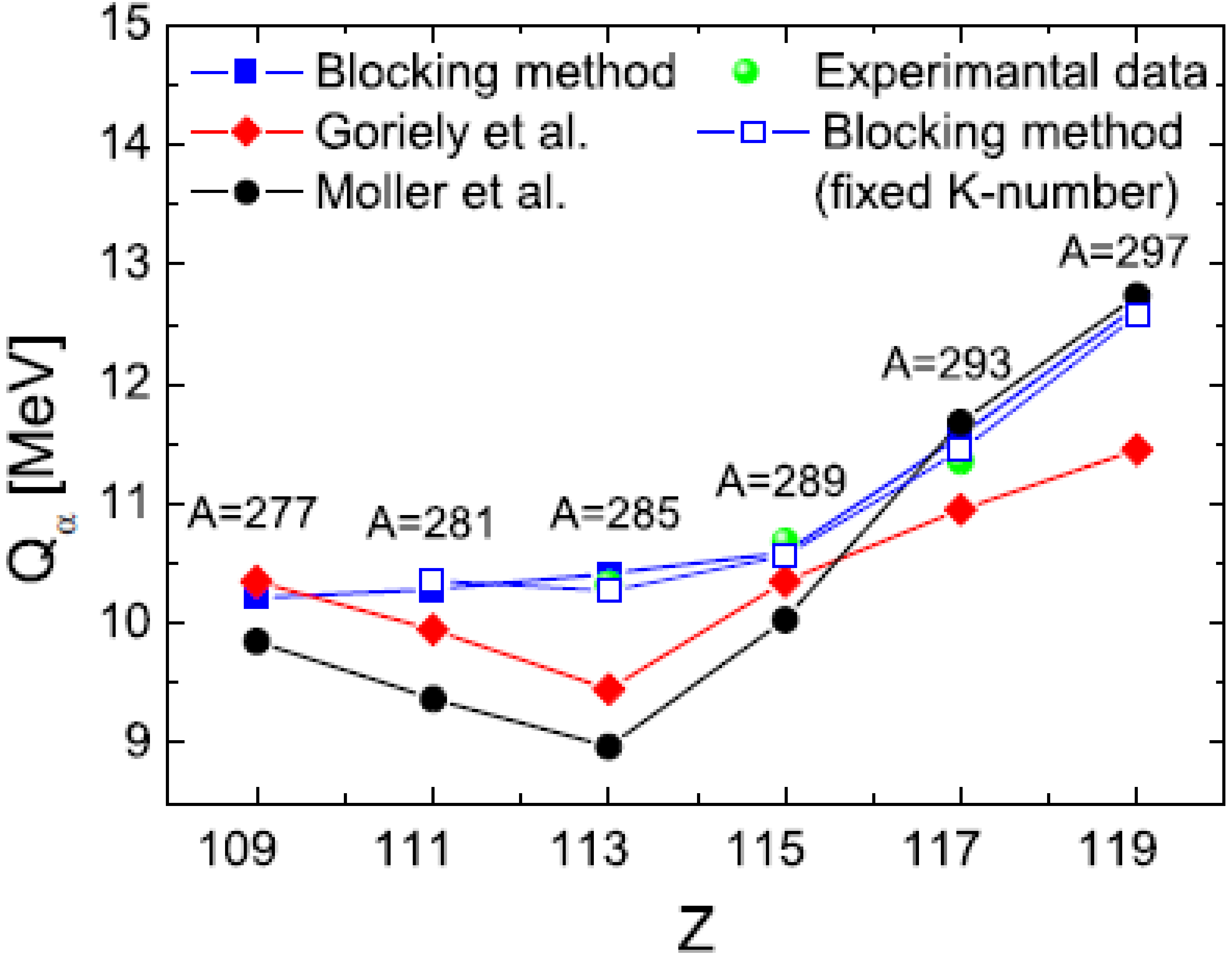
18
16
14
12
10
8
6
4
2
140
150
160
170
180
190
200
210
Q_α [MeV]
N
Z=128
Z=126
Z=124
Z=122
Z=120
Z=118
Z=116
Z=114
Z=112
Z=110
Z=108
Z=106
Z=104
Z=102
Z=100



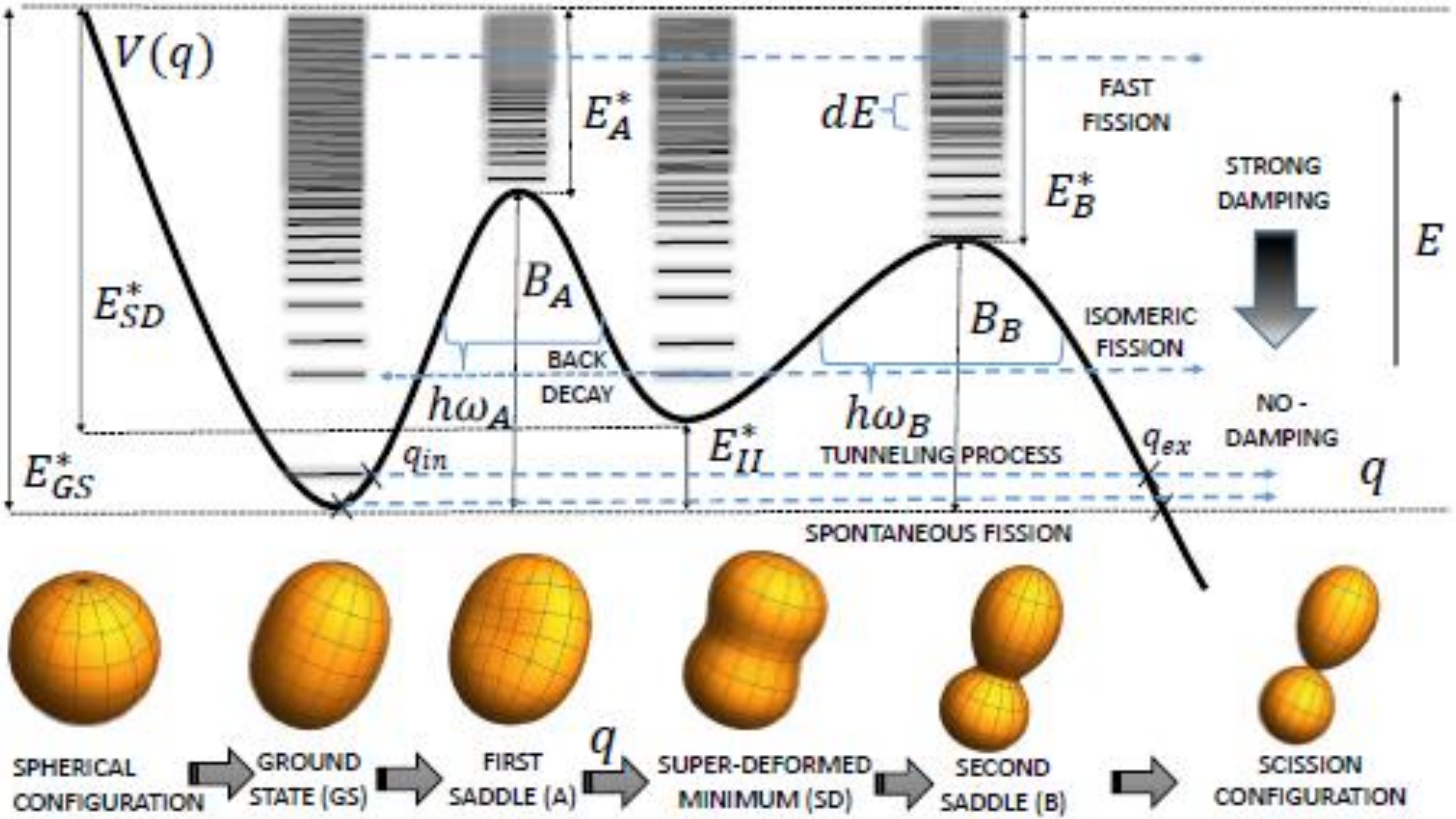
18
16
14
12
10
8
6
4
2
Q_α [MeV]
140
150
160
170
180
190
200
210
N
Z=127
Z=125
Z=123
Z=119
Z=121
Z=117
Z=115
Z=113
Z=111
Z=109
Z=107
Z=105
Z=103
Z=101


Blocking method
Goriely et al.
Moller et al.
Experimantal data
Blocking method
(fixed K-number)
A=270
A=274
A=278
A=282
A=286
A=290
A=294
Q_α [MeV]
Z
8
9
10
11
12
13
14
105
107
109
111
113
115
117


Blocking method
Experimantal data
Goriely et al.
Blocking method
(fixed K-number)
Moller et al.
A=270
A=274
A=278
A=282
A=286
A=290
A=294
$\log_{10}[T^{\alpha}_{1/2}(s)]$
Z
10
8
6
4
2
0
-2
105
107
109
111
113
115
117



Blocking method
Experimantal data
Goriely et al.
Blocking method
(fixed K-number)
Moller et al.
A=277
A=281
A=285
A=289
A=293
A=297
Q_α [MeV]
Z
15
14
13
12
11
10
9
109
111
113
115
117
119



V(q)
E*_A
dE
FAST FISSION
STRONG DAMPING
E*_B
E
B_A
E*_SD
B_B
ISOMERIC FISSION
BACK DECAY
hω_A
hω_B
NO - DAMPING
E*_II
TUNNELING PROCESS
q_ex
q_in
E*_GS
q
SPONTANEOUS FISSION
SPHERICAL CONFIGURATION
GROUND STATE (GS)
FIRST SADDLE (A)
q
SUPER-DEFORMED MINIMUM (SD)
SECOND SADDLE (B)
SCISSION CONFIGURATION

Finding fission barrier heights requires a whole landscape.

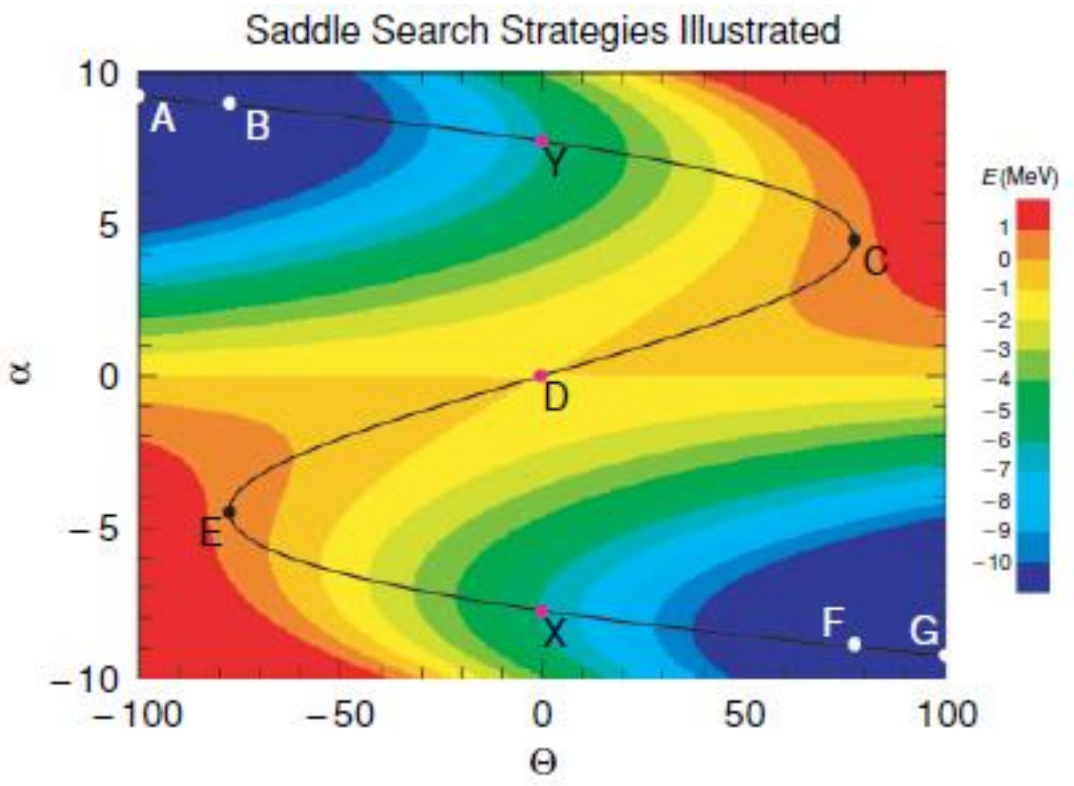
1) One needs n = 5 - 6 deformation variables (at least).
2) Saddles cannot be obtained by minimization (that is inherent in selfconsistent methods). Energy on n – dimensional grids is required, and usually a subsequent interpolation.
3) Inclusion of odd-A and odd-odd nuclei multiplies effort by 25 – 100 due to various possible configurations.

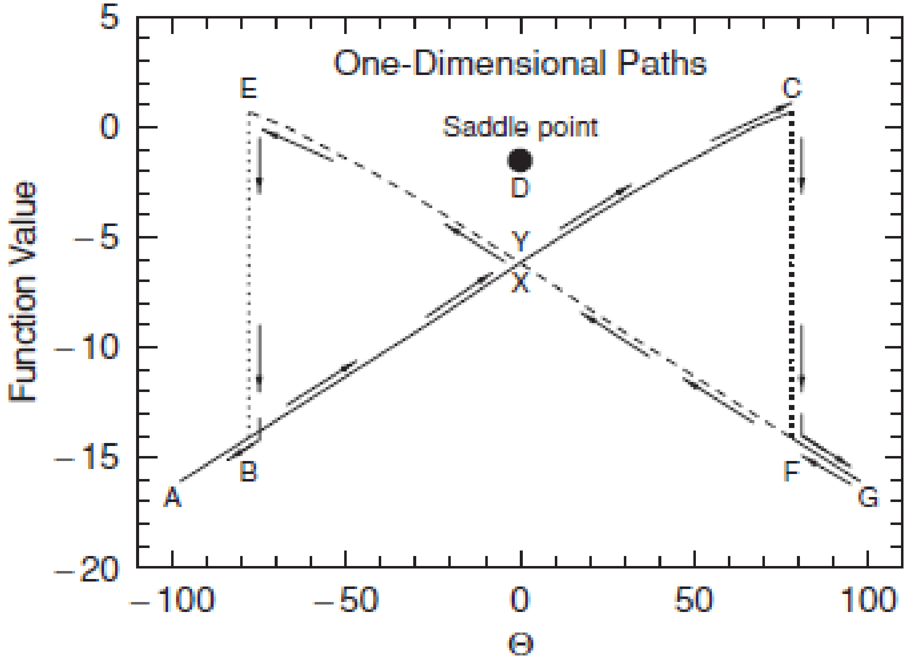
Because of the above there are very few systematic calculations of fission barriers, and even less satisfactory ones.

Selfconsistent type (inherently relying on minimization):
- too many symmetries imposed;
- no sufficient control on multiple minima & valley-to-valley switching => no certainty about saddles

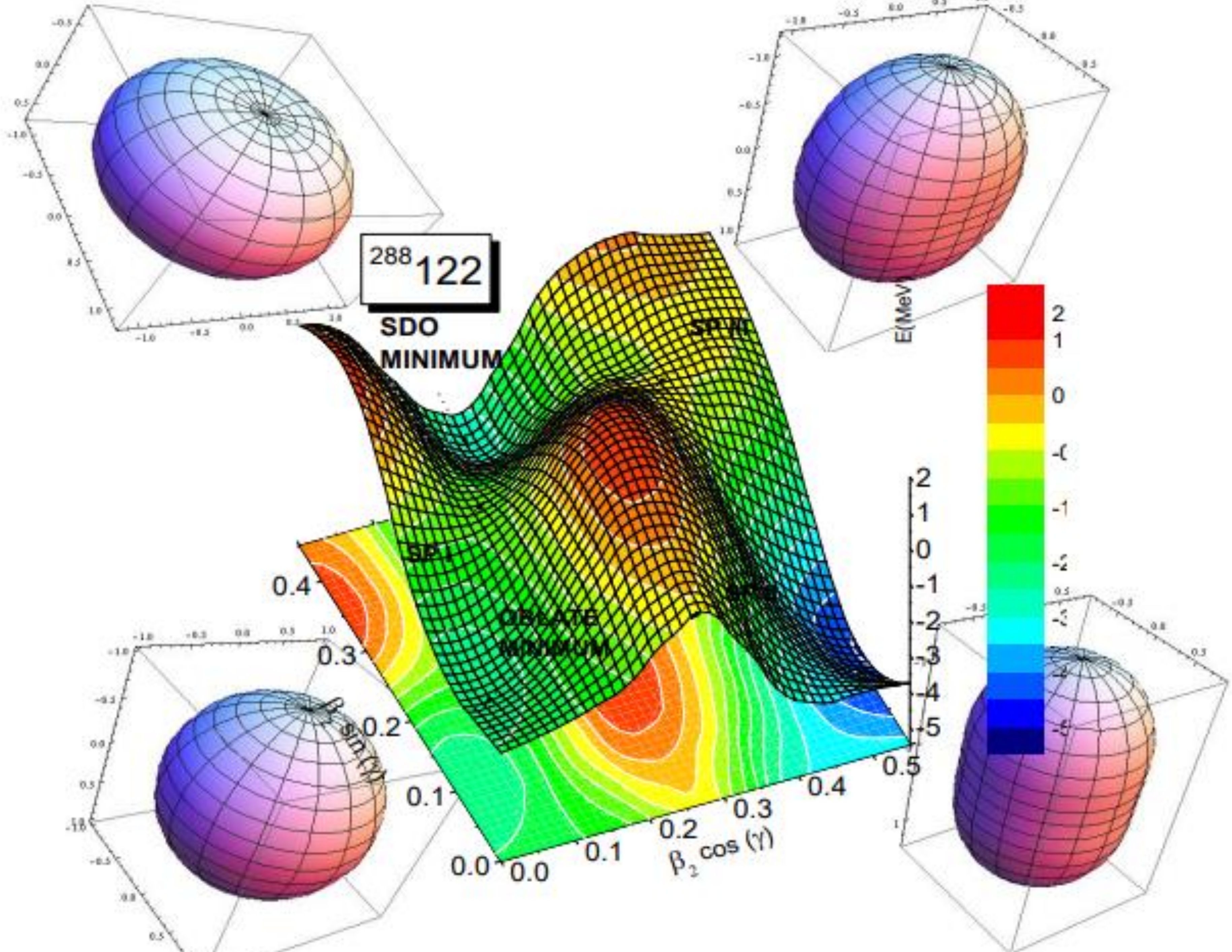
Micro-macro type:
- too few deformations or
- the use of the minimization in the saddle search.

Example of misleading minimization - P. Moller et al, Phys. Rev. C 79 (2009) 064304

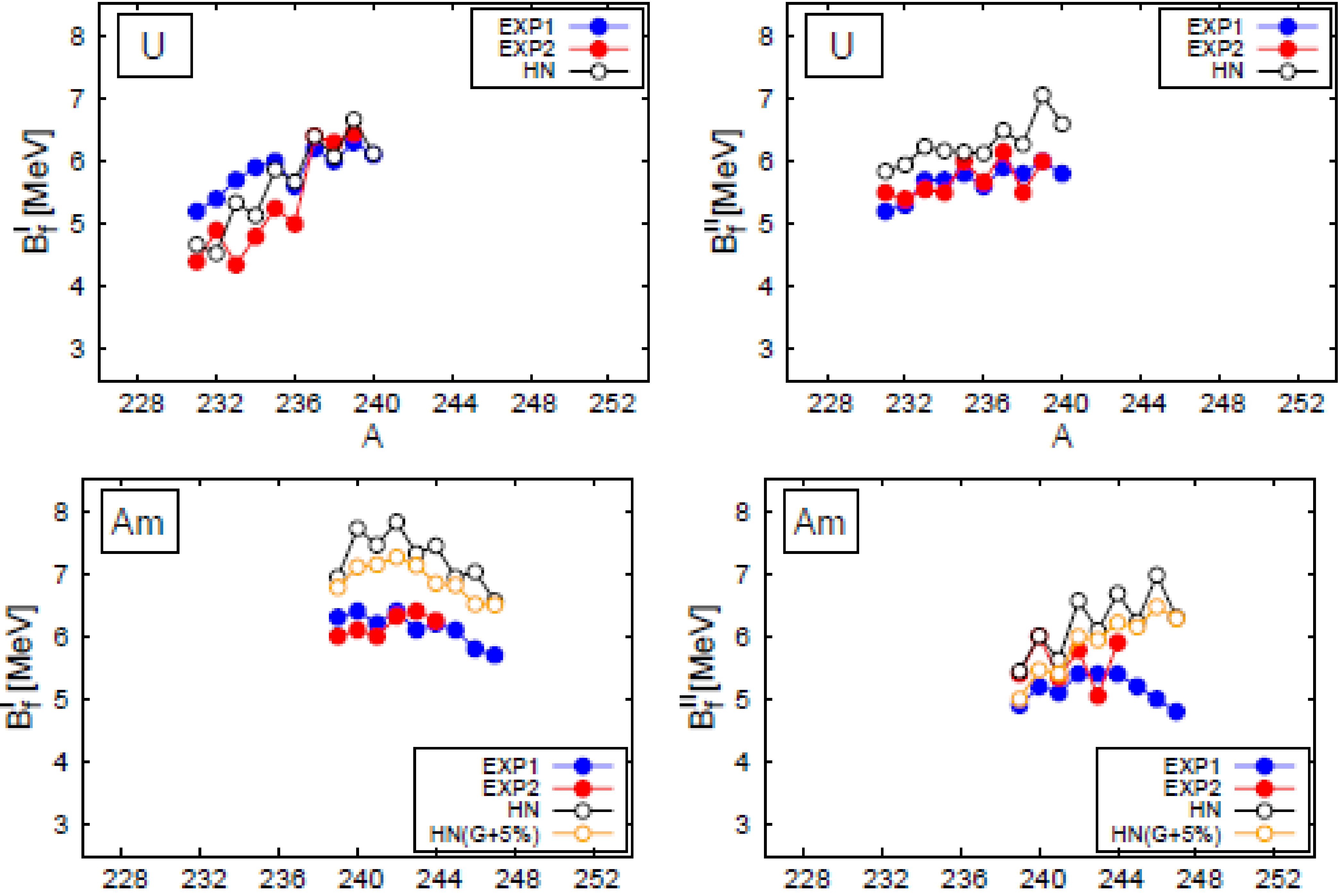




We used 5 or 7 – dimensional energy grids; the shapes included either nonaxiality or mass-asymmetry;
calculations including both non-axiality and mass-asymmetry were done for a check.
Immersion Water Flow method was used for finding (multiple) saddles.
Interpolated grids for IWF included ca 10 millions of points.
Finally, the (not automated) selection of proper saddles was done.

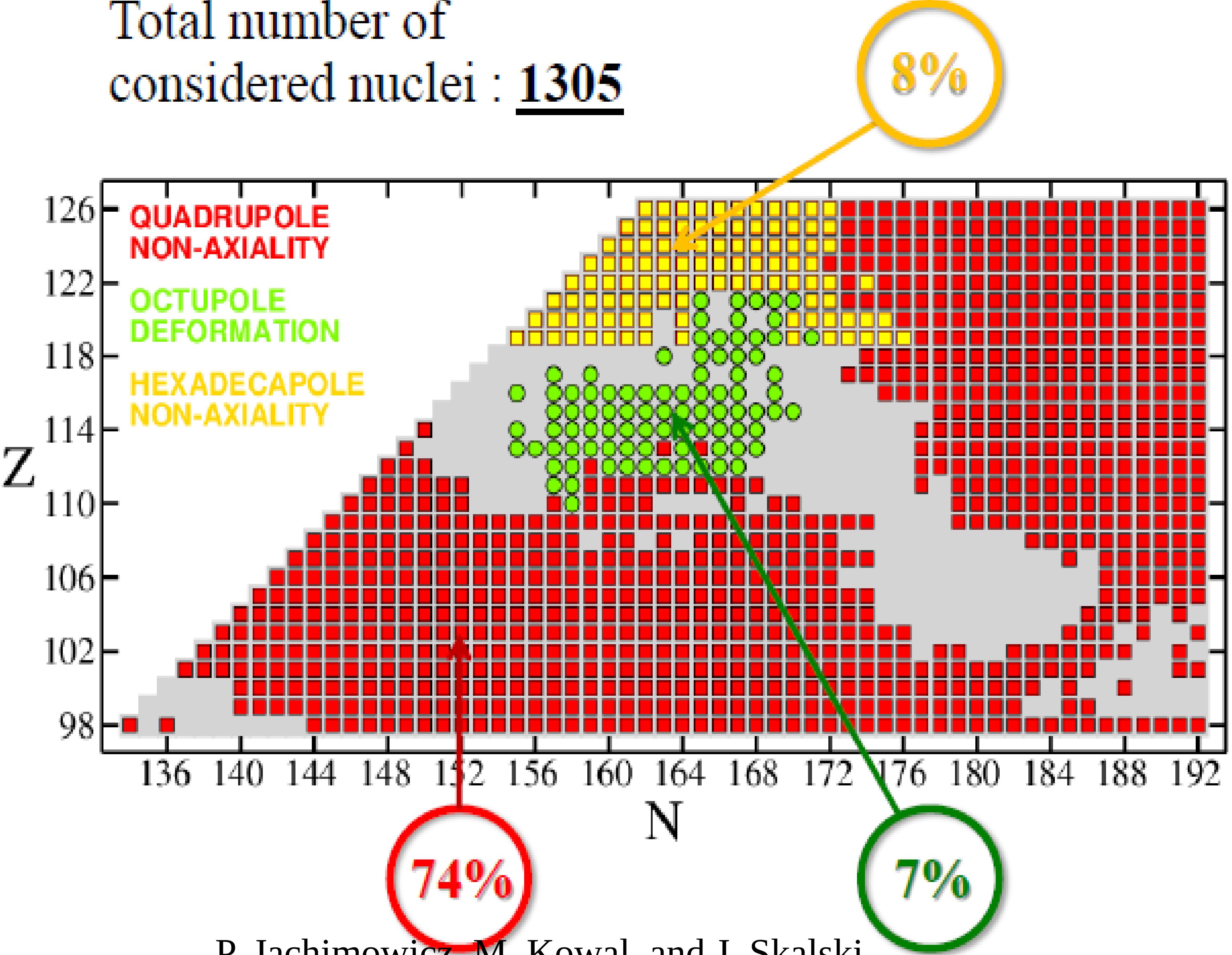


288122
SDO
MINIMUM
OBLATE
MINIMUM
E(MeV)
β2 cos (γ)
β2 sin (γ)



rms deviation in barriers for 72 actinides: ca 0.9 MeV

Total number of considered nuclei : **1305**



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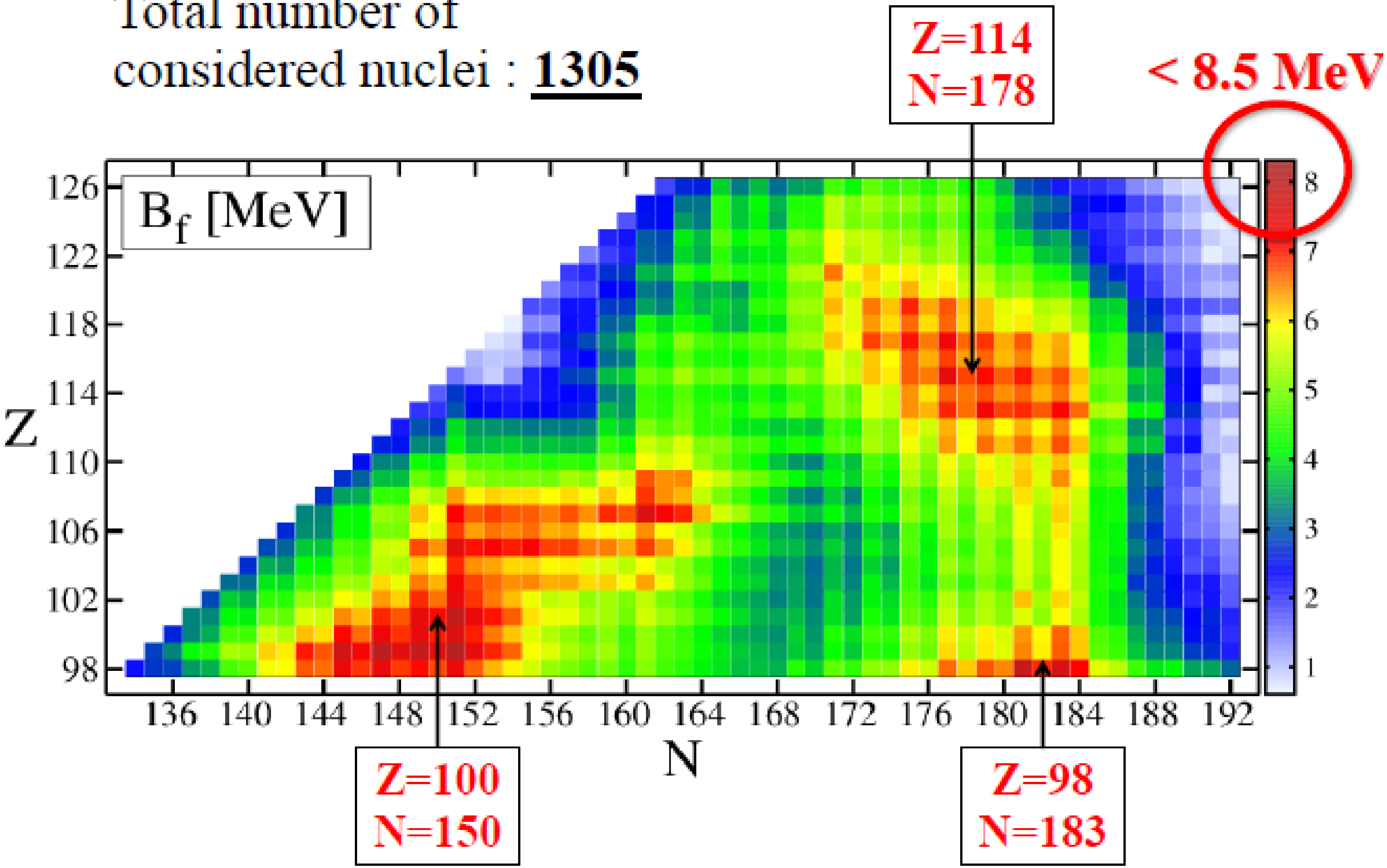
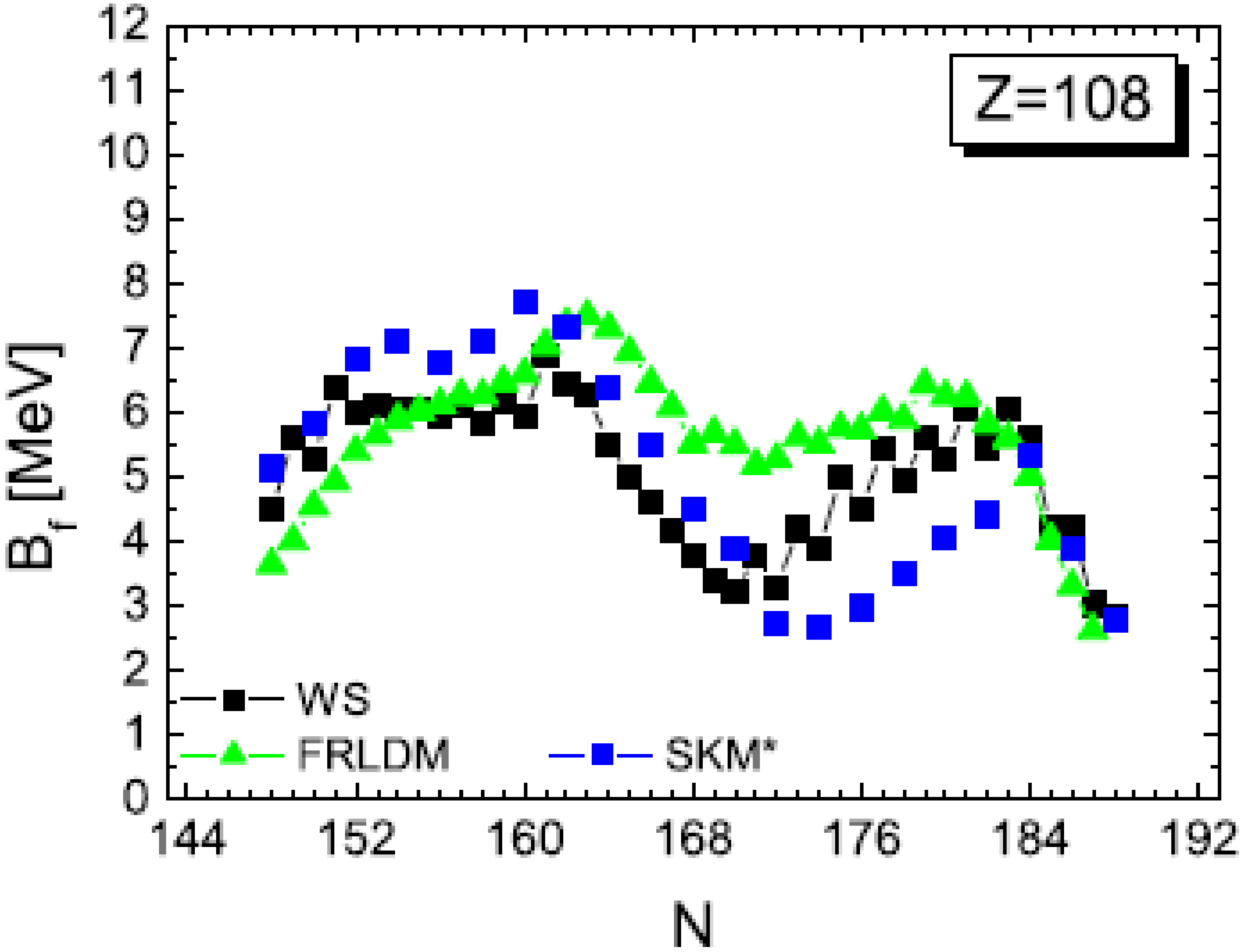
Phys. Rev. C 95, 014303 (2017)

CALCULATED FISSION BARRIER HEIGHTS

Total number of considered nuclei : **1305**





Z=108
B_f [MeV]
N
WS
FRLDM
SKM*
0
1
2
3
4
5
6
7
8
9
10
11
12
144
152
160
168
176
184
192

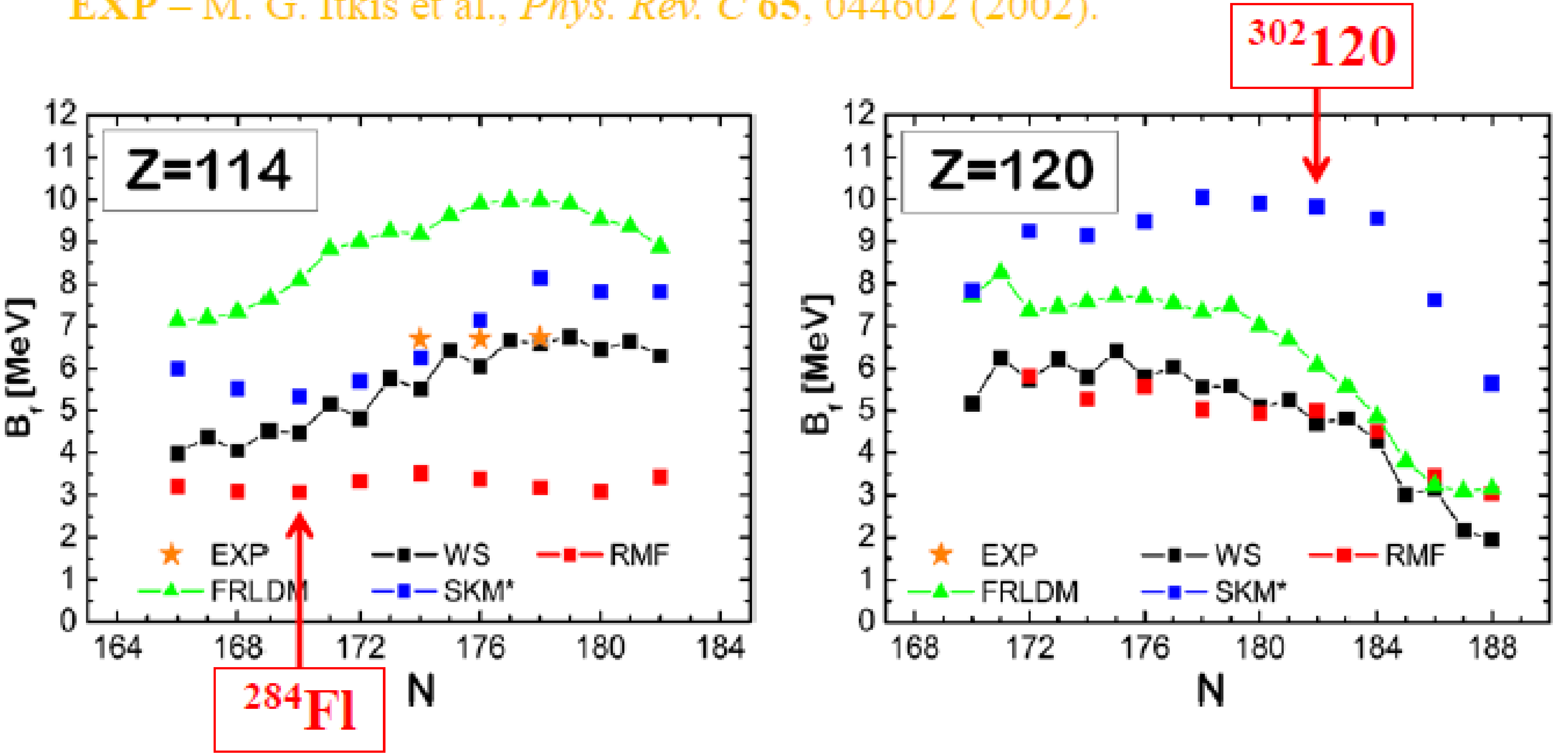
WS – our results

FRLDM – P. Möller et al., *Phys. Rev. C* **91**, 024310 (2015).

SKM* – A. Staszczak et al., *Phys. Rev. C* **87**, 024320 (2013).

RMF – H. Abusara et al. : *Phys. Rev. C* **85**, 024314 (2012); **82**, 044303 (2010).

EXP – M. G. Itkis et al., *Phys. Rev. C* **65**, 044602 (2002).



Thank you for your attention