Ground states, competing minima & fission barriers in SHN

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1. Introduction
2. Method of calculation of Potential energy surfaces (PES)

3. First minima - ground state properties
4. Saddle points - fission barriers
   - A check: actinides (first & second barriers)
   - SHN
5. Competing minima - shape coexistence
6. SDO – minima (YpE, LSD, Sly6, Gogny)

Macroscopic-microscopic approach:

$$E = \underbrace{E_{tot}(\beta_{\lambda\mu})}_{E_{MACRO}(\beta_{\lambda\mu}) + E_{MICRO}(\beta_{\lambda\mu})} - E_{MACRO}(\beta_{\lambda\mu}=0)$$

- ○ **$E_{MACRO}(\beta_{\lambda\mu})$ = Yukawa + exp**
- ○ **$E_{MICRO}(\beta_{\lambda\mu})$ = Woods – Saxon + pairing BCS**

Shape Parametrization:

$$R(\Theta,\Phi)=\{1+a_{20}Y_{20}+a_{40}Y_{40}+a_{60}Y_{60}+a_{80}Y_{80}$$

$$+a_{22}Y^{(+)}_{22}+a_{42}Y^{(+)}_{42}+a_{44}Y^{(+)}_{44}$$

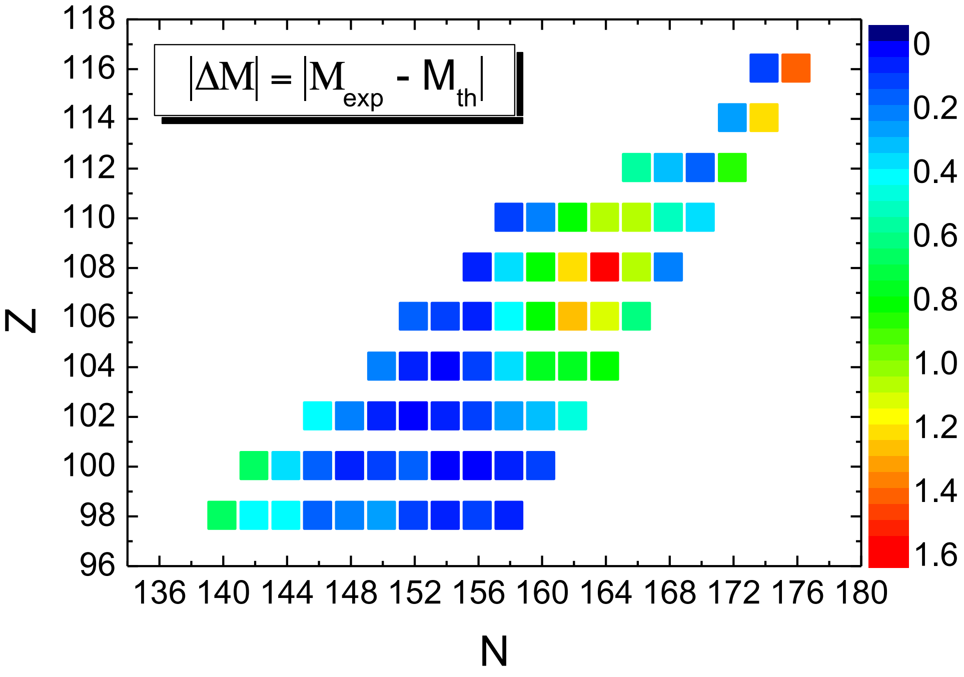
$$+a_{32}Y^{(+)}_{32}+a_{52}Y^{(+)}_{52}$$

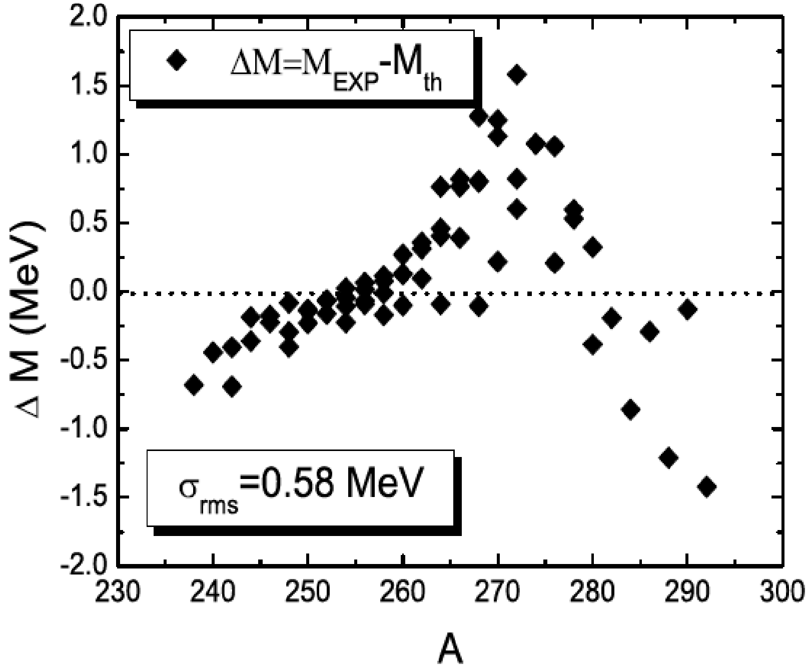
$$+a_{30}Y_{30}+a_{50}Y_{50}+a_{70}Y_{70}\}$$

12-DIM !

$$Y^{(+)}_{\lambda\mu}=\frac{1}{\sqrt{2}}(Y_{\lambda\mu}+Y_{\lambda-\mu})$$

N	$<\| M_{gs}^{th} - M_{gs}^{exp} \|>$	$Max \| M_{gs}^{th} - M_{gs}^{exp} \|$	r.m.s
67	0.43	1.58	0.58





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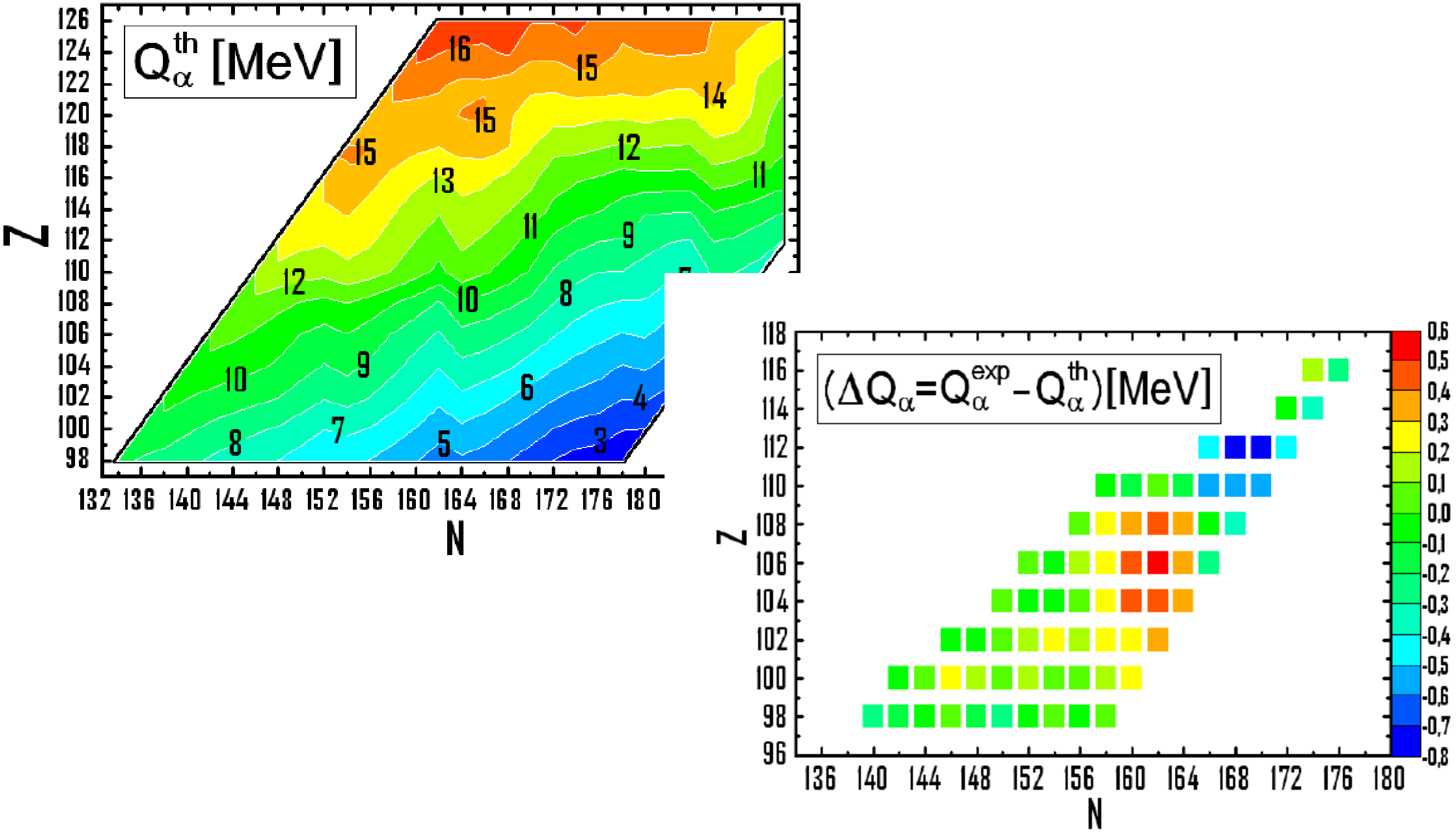
N	$<\mid Q_{\alpha}^{th} - Q_{\alpha}^{exp} \mid>$	$Max \mid Q_{\alpha}^{th} - Q_{\alpha}^{exp} \mid$	r.m.s
67	0.02	0.74	0.29



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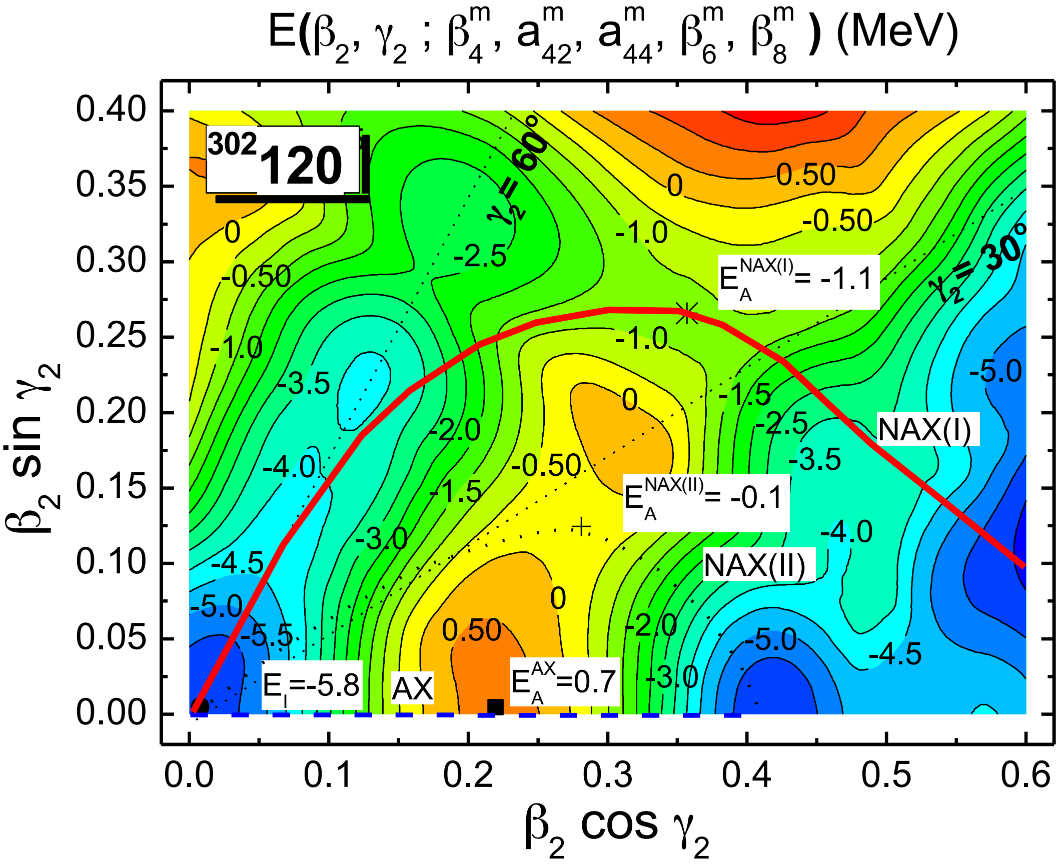
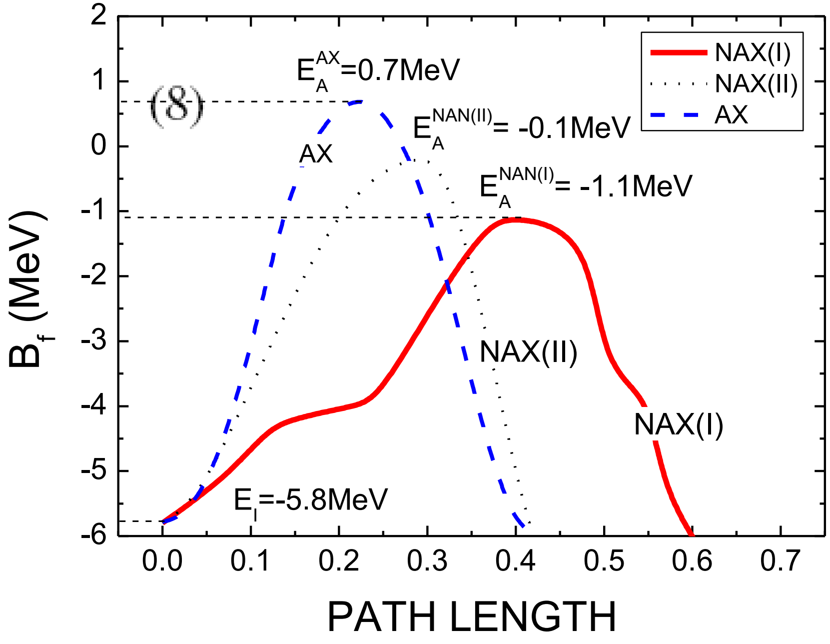
The potential energy is calculated in the following grid points:

$$\beta_2 \cos\gamma_2 = 0(0.05)0.65,$$
$$\beta_2 \sin\gamma_2 = 0(0.05)0.40,$$
$$\beta_4 = -0.20(0.05)0.20.$$



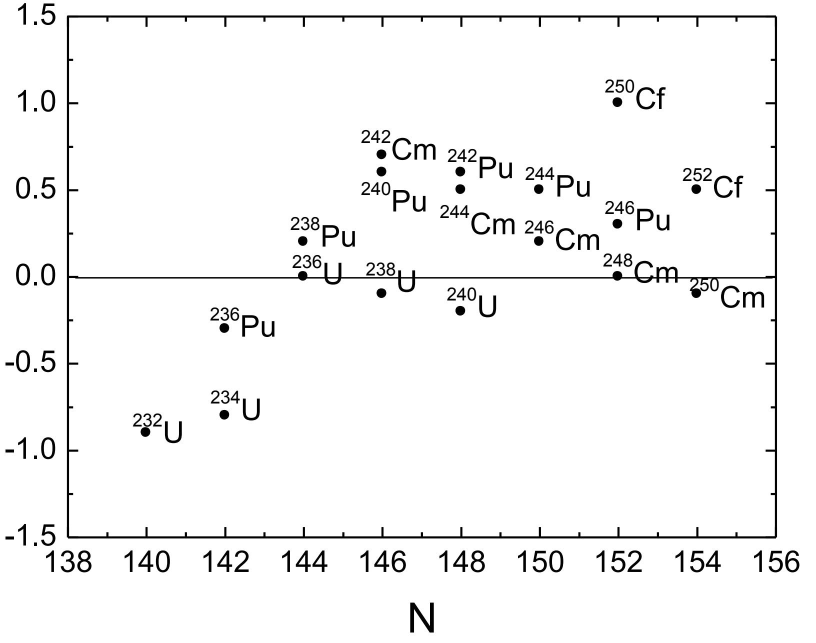
$E(\beta_2, \gamma_2\,;\, \beta_4^m, a_{42}^m, a_{44}^m, \beta_6^m, \beta_8^m)$ (MeV)

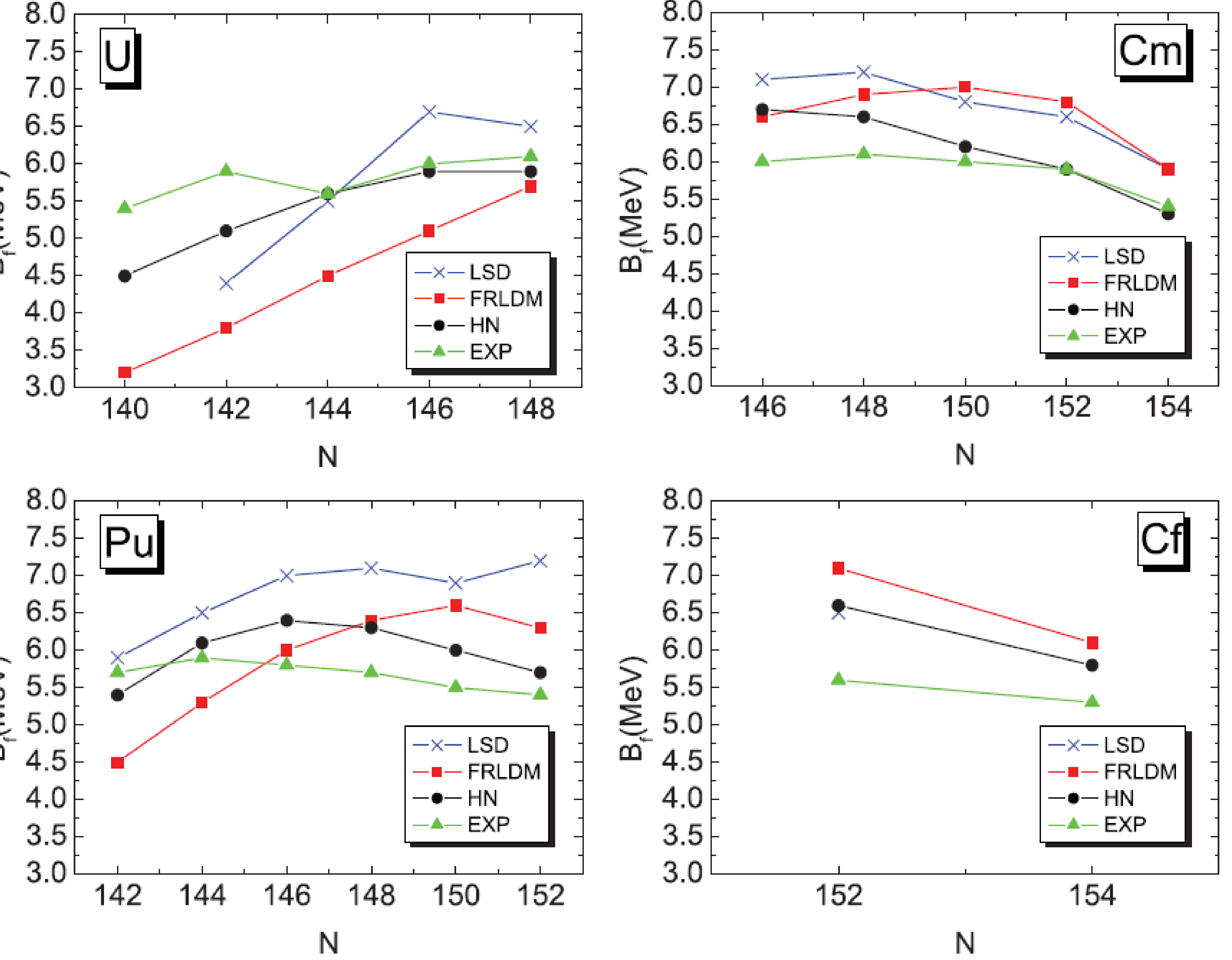


M. Kowal, P. Jachimowicz, and A. Sobiczewski Phys. Rev. C **82**, 014303 (2010)

Z	N	A	LSD	FRLDM	HN	EXP
92	140	232	–	3.2	4.5	5.4
	142	234	4.4	3.8	5.1	5.9
	144	236	5.5	4.5	5.6	5.6
	146	238	6.7	5.1	5.9	6.0
	148	240	6.5	5.7	5.9	6.1
94	142	236	5.9	4.5	5.4	5.7
	144	238	6.5	5.3	6.1	5.9
	146	240	7.0	6.0	6.4	5.8
	148	242	7.1	6.4	6.3	5.7
	150	244	6.9	6.6	6.0	5.5
	152	246	7.2	6.3	5.7	5.4
96	146	242	7.1	6.6	6.7	6.0
	148	244	7.2	6.9	6.6	6.1
	150	246	6.8	7.0	6.2	6.0
	152	248	6.6	6.8	5.9	5.9
	154	250	5.9	5.9	5.3	5.4
98	152	250	6.5	7.1	6.5	5.6
	154	252	–	6.1	5.8	5.3

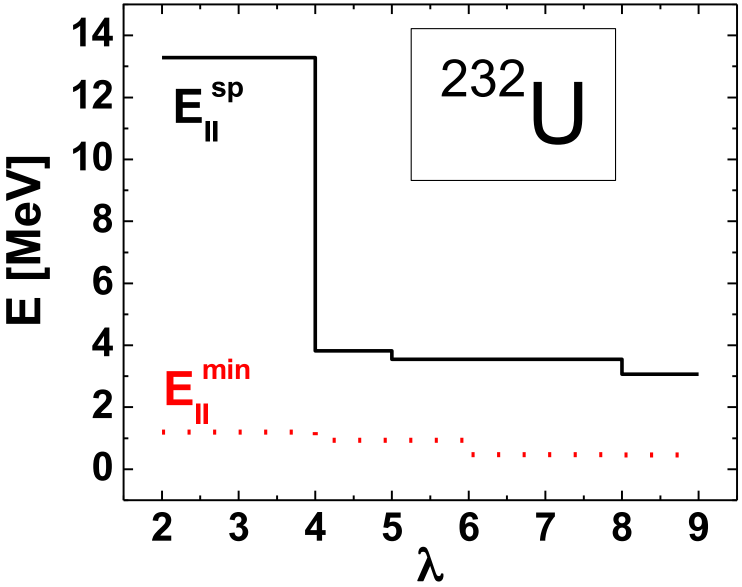
Models	LSD	FRLDM	HN
N	16	18	18
$\langle\lvert B_f^{\mathrm{th}} - B_f^{\mathrm{expt}}\rvert\rangle$	0.9	1.0	0.4
$\mathrm{Max}\lvert B_f^{\mathrm{th}} - B_f^{\mathrm{expt}}\rvert$	1.8	2.2	1.0
rms	1.0	1.1	0.5




U
Cm
Pu
Cf
B_f(MeV)
N
140
142
144
146
148
150
152
154
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
7.0
7.5
8.0
LSD
FRLDM
HN
EXP

Second saddles:

$$\begin{aligned}
\beta_{20} &= 0.65\ (0.05)\ 0.85\\
\beta_{30} &= 0.00\ (0.05)\ 0.30\\
\beta_{40} &= -0.30\ (0.05)\ 0.30\\
\beta_{50} &= 0.00\ (0.05)\ 0.20\\
\beta_{60} &= -0.20\ (0.05)\ 0.20\\
\beta_{80} &= -0.15\ (0.05)\ 0.15.
\end{aligned}$$



Interpolation → 1059926301 grid points !

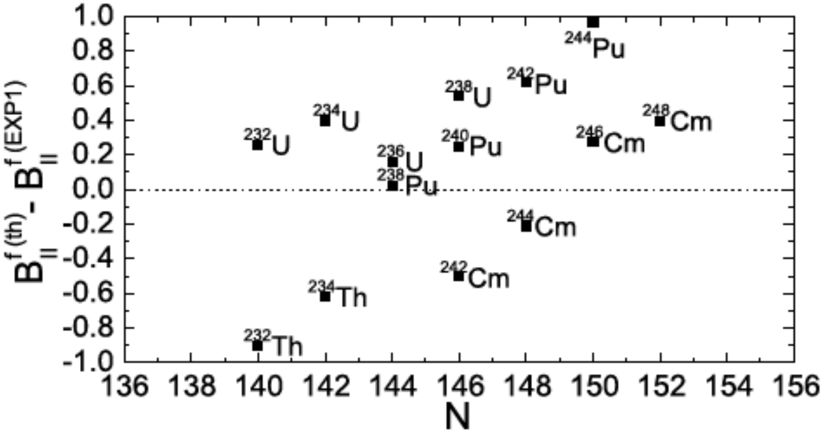
DMP & IWF method has been used

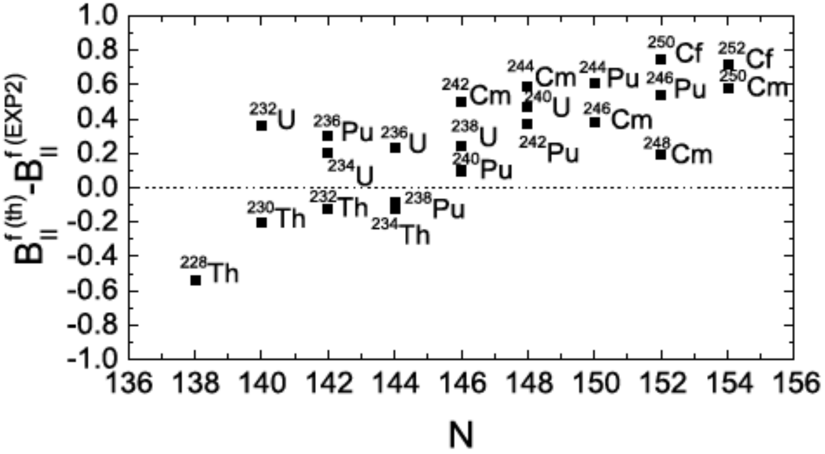
~~Minimization in remaining degrees of freedom~~

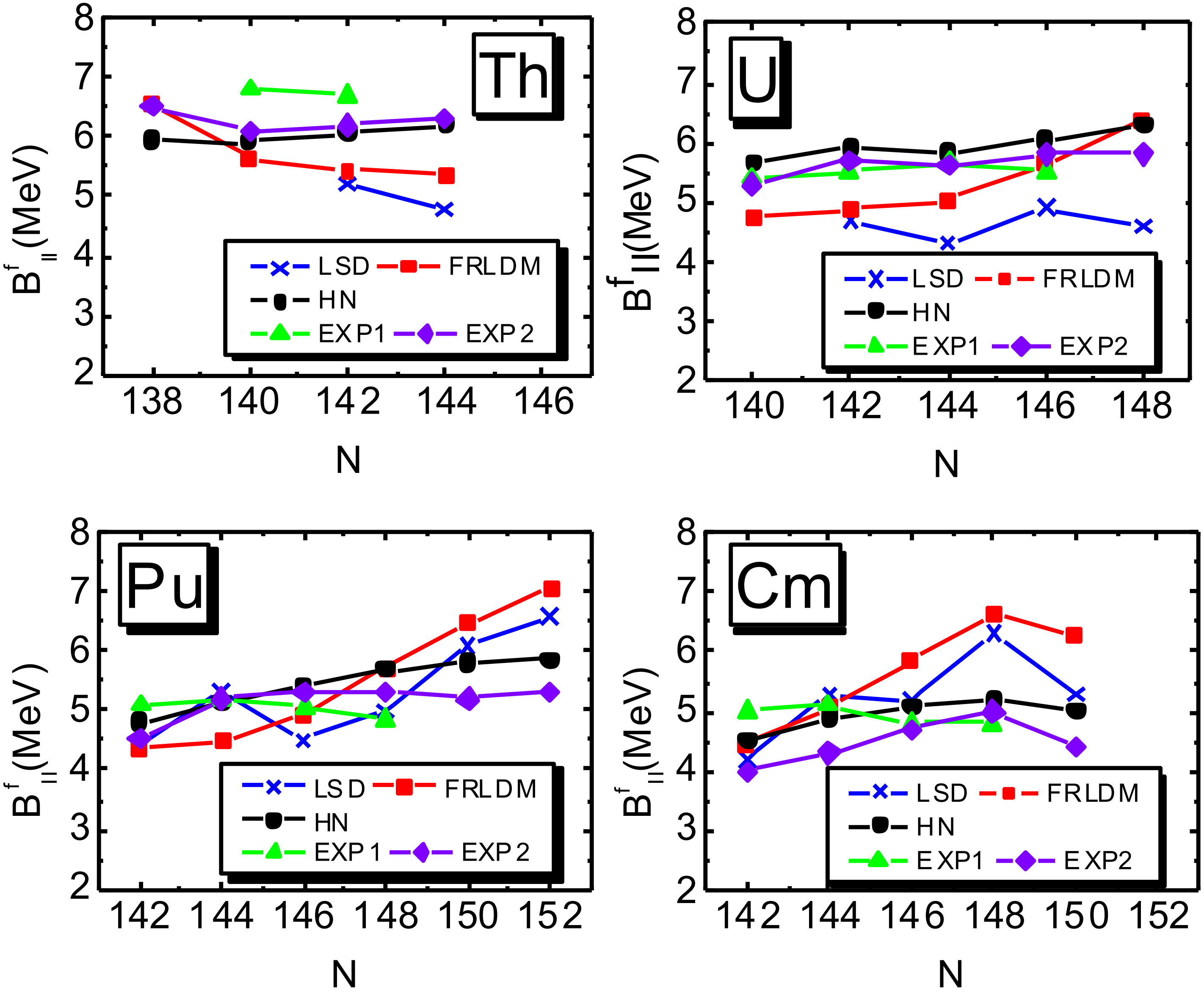
P. Jachimowicz, M. Kowal, and J. Skalski
Phys. Rev. C **85**, 034305 (2012)

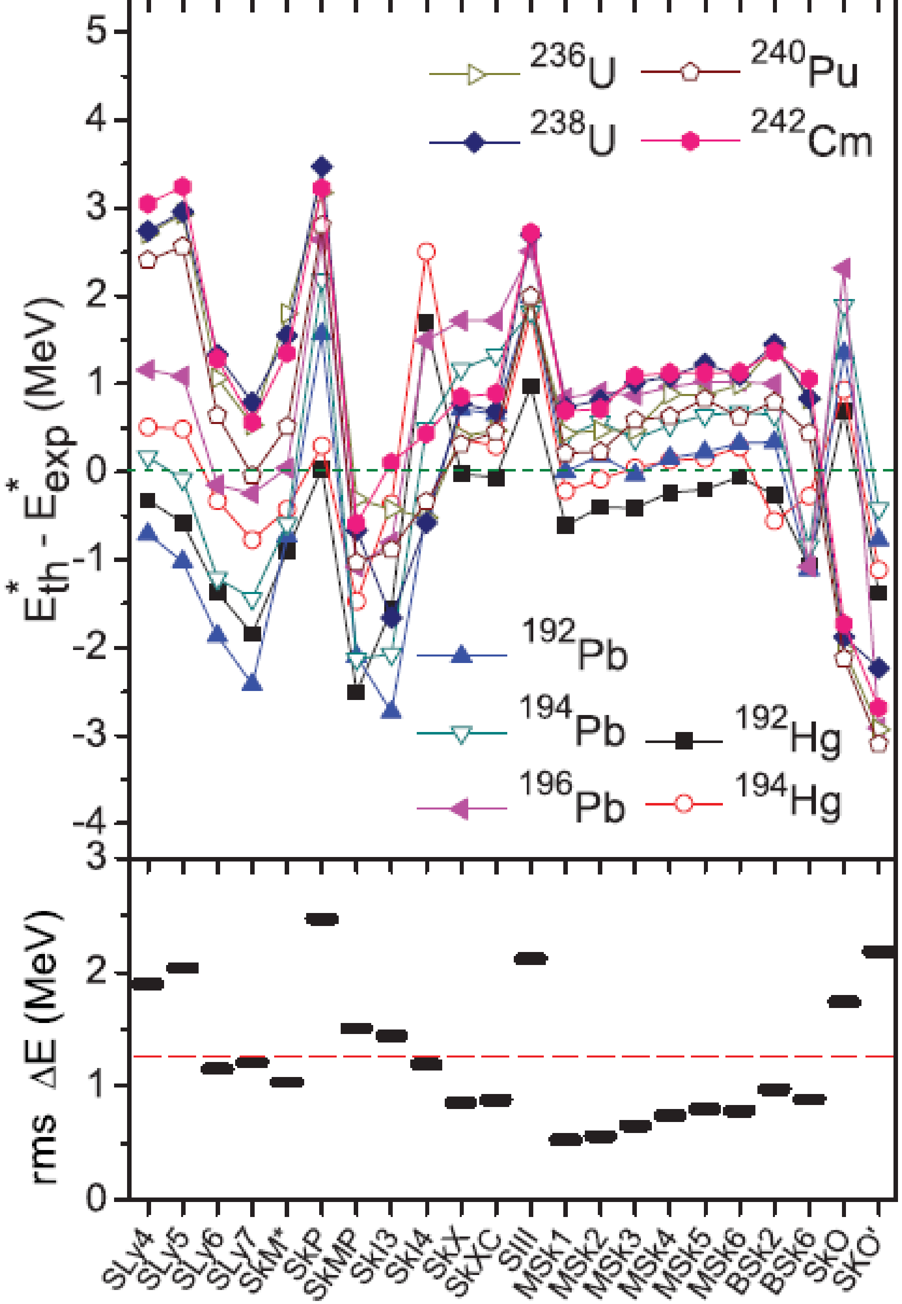
Z	N	A	LSD	FRLDM	HN	EXP1	EXP2
90	136	226	–	7.20	6.26	–	–
	138	228	–	6.53	5.92	–	6.5
	140	230	–	5.65	5.97	6.80	6.1
	142	232	5.2	5.45	6.07	6.70	6.2
	144	234	4.8	5.37	6.07	–	6.3
	146	236	–	6.04	6.35	–	–
92	138	230	–	4.28	5.64	–	–
	140	232	–	4.73	5.66	5.40	5.3
	142	234	4.7	4.89	5.84	5.50	5.7
	144	236	4.3	5.03	5.78	5.67	5.6
	146	238	4.9	5.64	5.93	5.50	5.8
	148	240	4.6	6.37	6.04	–	5.8
	150	242	–	7.10	6.23	–	–
94	140	234	–	–	4.68	–	–
	142	236	4.4	4.36	5.06	–	4.5
	144	238	5.3	4.47	5.15	5.10	5.2
	146	240	4.5	4.91	5.28	5.15	5.3
	148	242	5.0	5.72	5.52	5.05	5.3
	150	244	6.1	6.47	5.63	4.85	5.2
	152	246	6.6	7.07	5.75	–	5.3
	154	248	–	–	5.42	–	–
96	144	240	–	3.92	4.25	–	–
	146	242	4.2	4.45	4.42	5.00	4.0
	148	244	5.3	5.07	4.72	5.10	4.3
	150	246	5.2	5.87	4.98	4.80	4.7
	152	248	6.3	6.65	5.14	4.80	5.0
	154	250	5.3	6.25	4.87	–	4.4
	156	252	–	5.68	4.31	–	–
98	150	248	–	5.18	4.14	–	–
	152	250	4.6	5.92	4.57	–	3.8
	154	252	–	5.83	4.36	–	3.5
	156	254	–	5.27	3.95	–	–

Theoretical models:	LSD		FRLDM		HN	
Experimental data:	[23]	[24]	[23]	[24]	[23]	[24]
N	12	18	14	22	14	22
$<\mid B_f^{th} - B_f^{exp} \mid>$	0.78	0.84	0.79	0.90	0.39	0.33
$Max \mid B_f^{th} - B_f^{exp} \mid$	1.50	1.50	1.85	2.33	0.83	0.86
δ_{RMS}	0.92	0.94	0.95	1.11	0.46	0.40






Th
U
Pu
Cm
B^f_{II}(MeV)
N
2
3
4
5
6
7
8
138
140
142
144
146
148
150
152
LSD
FRLDM
HN
EXP1
EXP2



NIKOLOV, SCHUNCK, NAZAREWICZ, BENDER, AND PEI

PHYSICAL REVIEW C **83**, 034305 (2011)

Z	N	A	$E_{II}^{min}(th)^*$	$E_{II}^{min}(exp)^*$
92	144	236	2.04	2.75
92	146	238	1.94	2.56
94	142	236	2.43	3.00
94	144	238	2.05	2.40
94	146	240	1.95	2.80
94	148	242	1.99	2.20
96	144	240	1.69	2.00
96	146	242	1.64	1.90
96	148	244	1.68	2.20(?)

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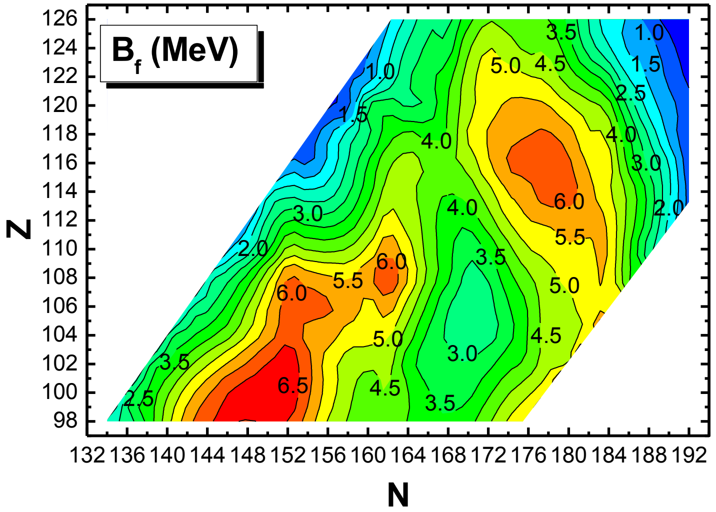
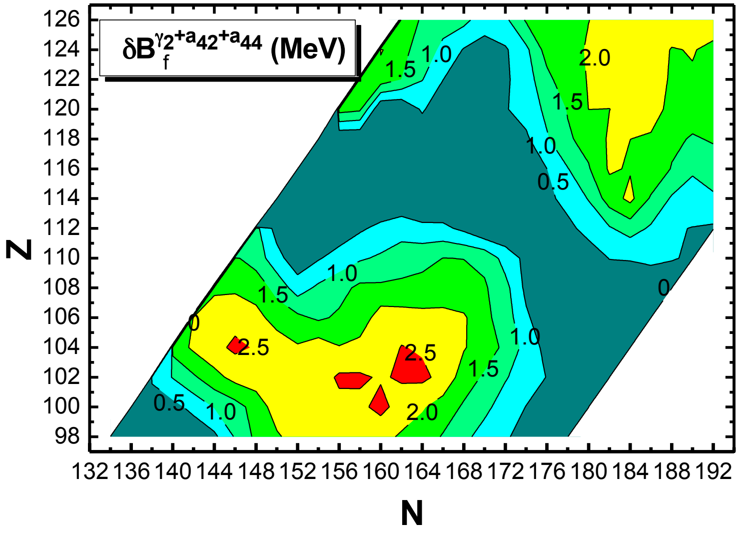
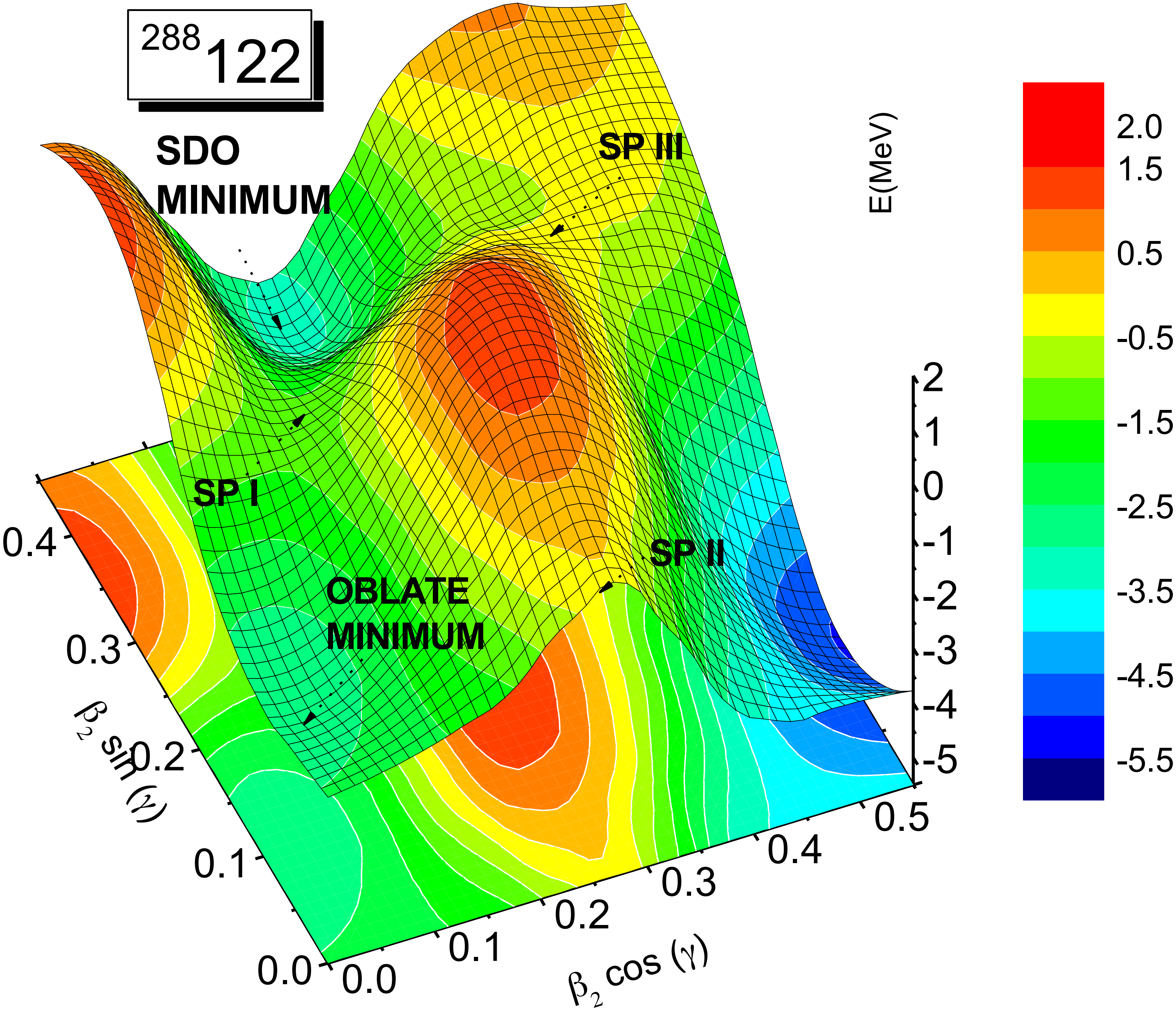
Fission barriers

Nucleus	SHF	FRLDM	ETFSI	HN	EXP
$^{284}112_{172}$	6.06	7.41	2.2	4.29	5.5
$^{286}112_{174}$	6.91	8.24	3.6	5.01	5.5
$^{288}114_{174}$	8.12	9.18	6.1	5.53	6.7
$^{290}114_{176}$	8.52	9.89	6.6	5.83	6.7
$^{292}114_{178}$	–	9.98	7.2	6.34	6.7
$^{292}116_{176}$	9.35	9.26	6.5	6.22	6.4
$^{294}116_{178}$	9.59	9.46	7.2	6.28	6.4
$^{296}116_{180}$	–	9.10	7.2	6.07	6.4
$^{294}118_{176}$	–	8.48	6.6	5.99	–
$^{296}118_{178}$	–	8.36	7.0	6.04	–
$^{298}118_{180}$	–	8.05	7.4	5.72	–
$^{296}120_{176}$	–	7.69	6.2	5.64	–
$^{298}120_{178}$	–	7.33	6.6	5.50	–
$^{300}120_{180}$	–	7.01	6.8	5.05	–
$^{302}120_{182}$	–	6.07	7.2	4.66	–
$^{304}120_{184}$	–	4.86	6.8	4.20	–



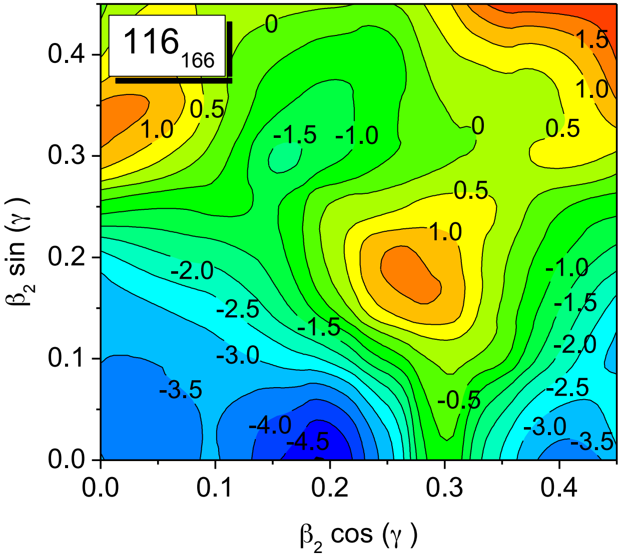




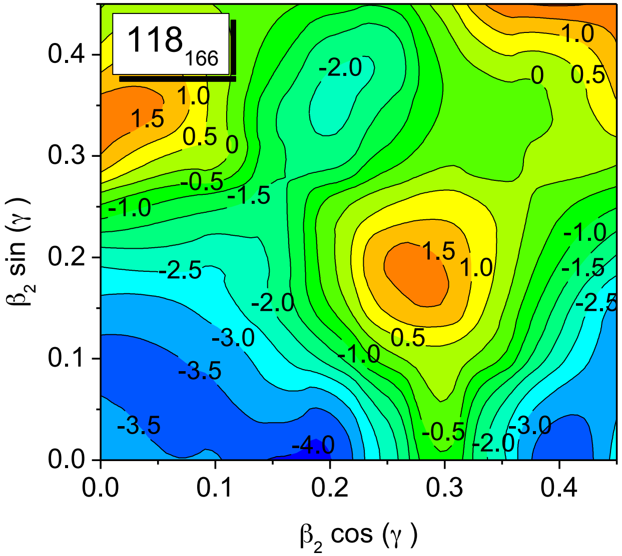
$^{288}122$
SDO MINIMUM
SP III
SP I
SP II
OBLATE MINIMUM
E(MeV)
2.0
1.5
0.5
-0.5
-1.5
-2.5
-3.5
-4.5
-5.5
2
1
0
-1
-2
-3
-4
-5
0.4
0.3
0.2
0.1
0.0
$\beta_2 \sin(\gamma)$
0.0
0.1
0.2
0.3
0.4
0.5
$\beta_2 \cos(\gamma)$

Super Deformed Oblate (SDO) minima

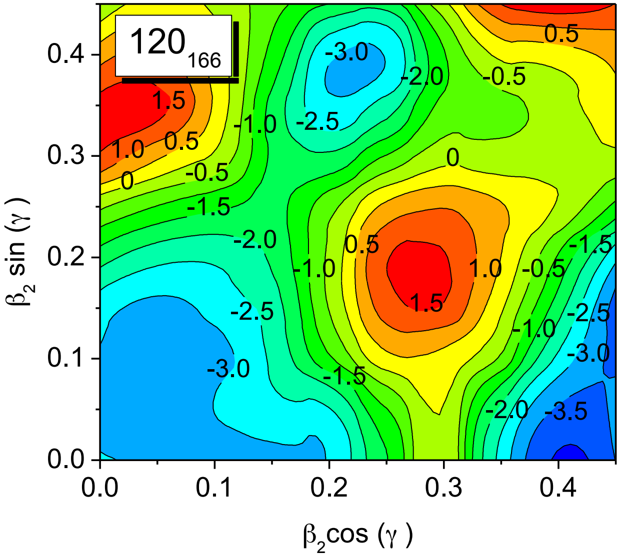
min. in: $(\beta_3, a_{32}, \beta_4, a_{42}, a_{44}, \beta_5, a_{52}, \beta_6, \beta_7, \beta_8)$



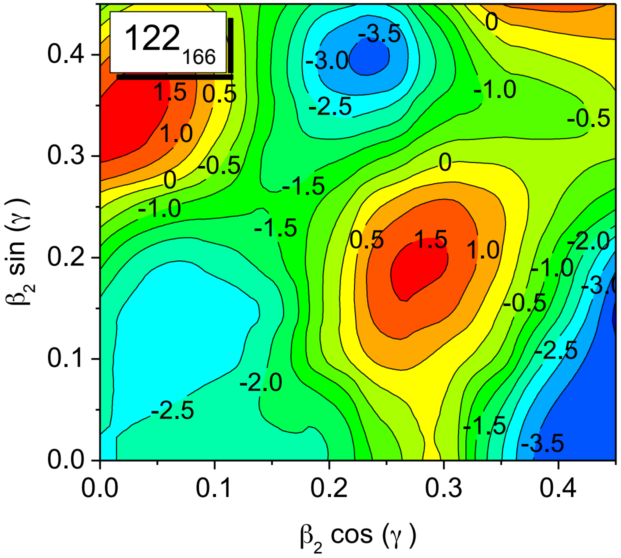
min. in: $(\beta_3, a_{32}, \beta_4, a_{42}, a_{44}, \beta_5, a_{52}, \beta_6, \beta_7, \beta_8)$



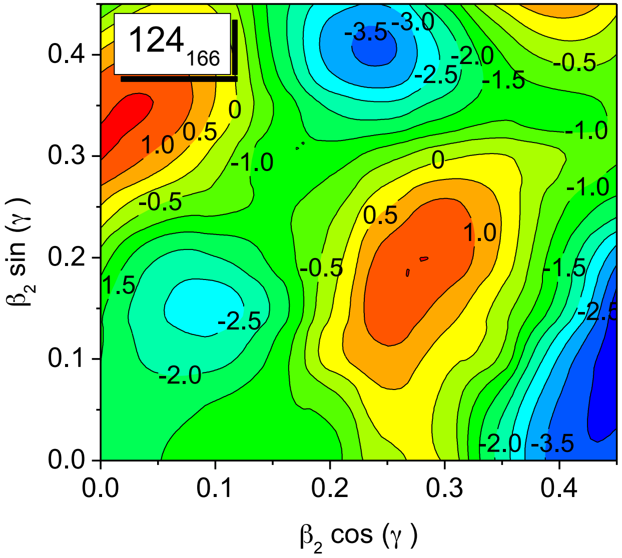
min. in: $(\beta_3, a_{32}, \beta_4, a_{42}, a_{44}, \beta_5, a_{52}, \beta_6, \beta_7, \beta_8)$



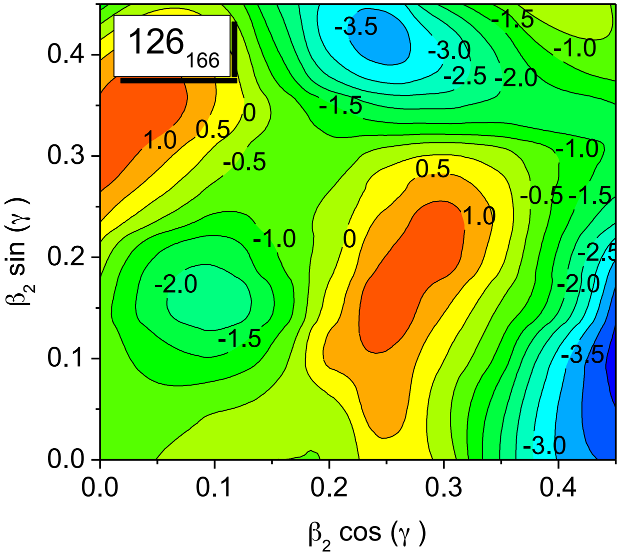
min. in: $(\beta_3, a_{32}, \beta_4, a_{42}, a_{44}, \beta_5, a_{52}, \beta_6, \beta_7, \beta_8)$



min. in: $(\beta_3, a_{32}, \beta_4, a_{42}, a_{44}, \beta_5, a_{52}, \beta_6, \beta_7, \beta_8)$



min. in: $(\beta_3, a_{32}, \beta_4, a_{42}, a_{44}, \beta_5, a_{52}, \beta_6, \beta_7, \beta_8)$

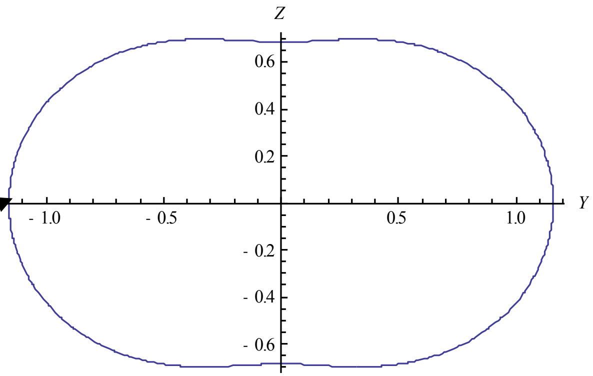


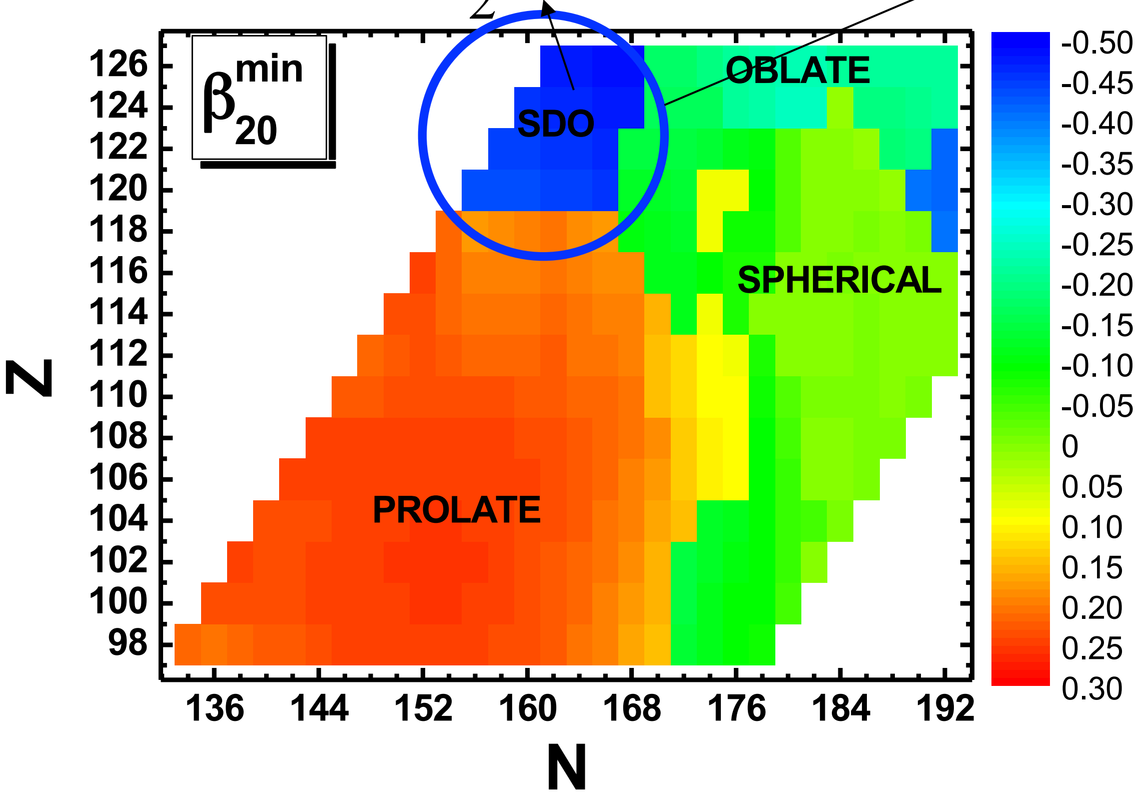
Ground state shapes

$SDO:$

$\beta_{20} \approx -0.5$

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





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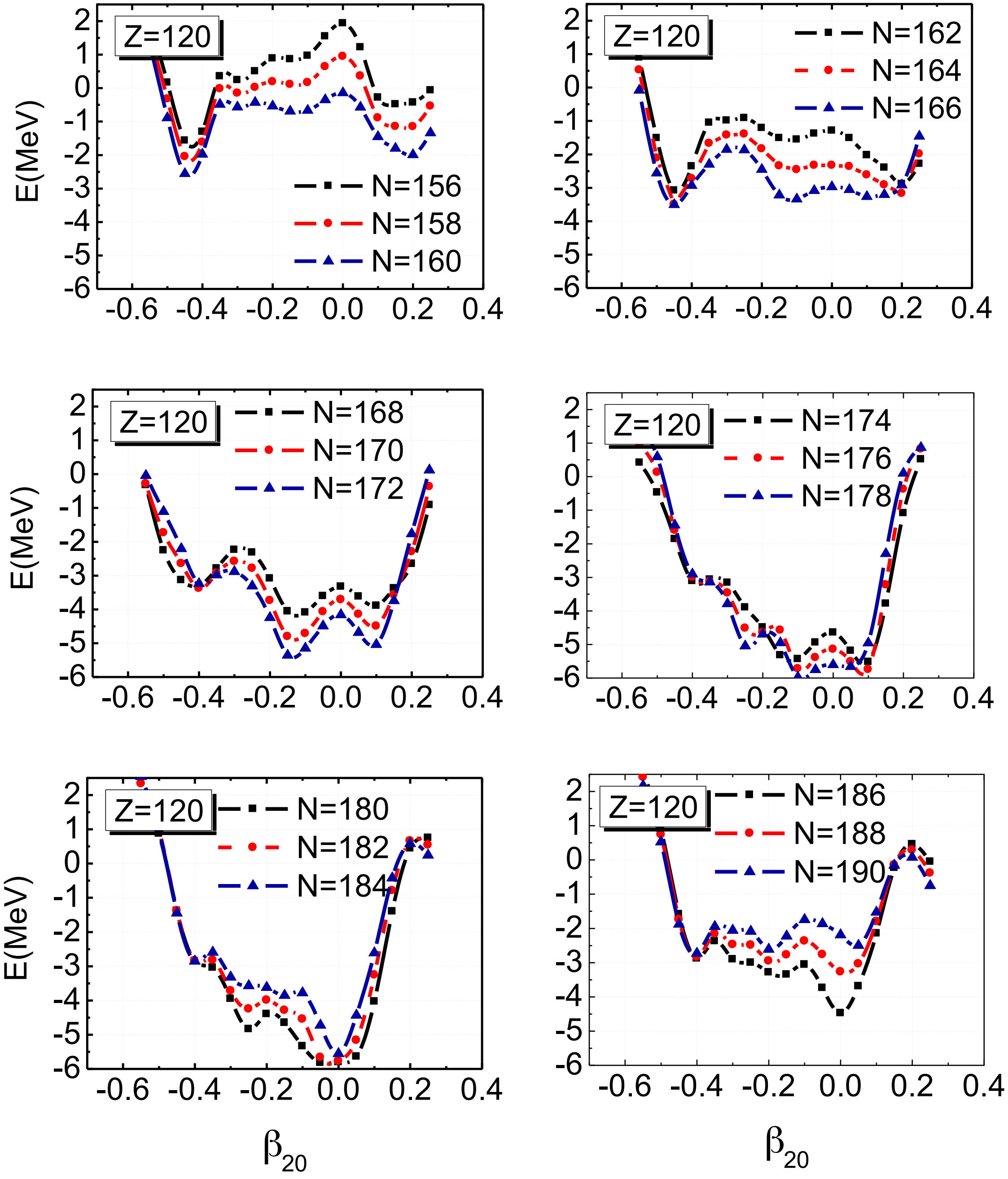
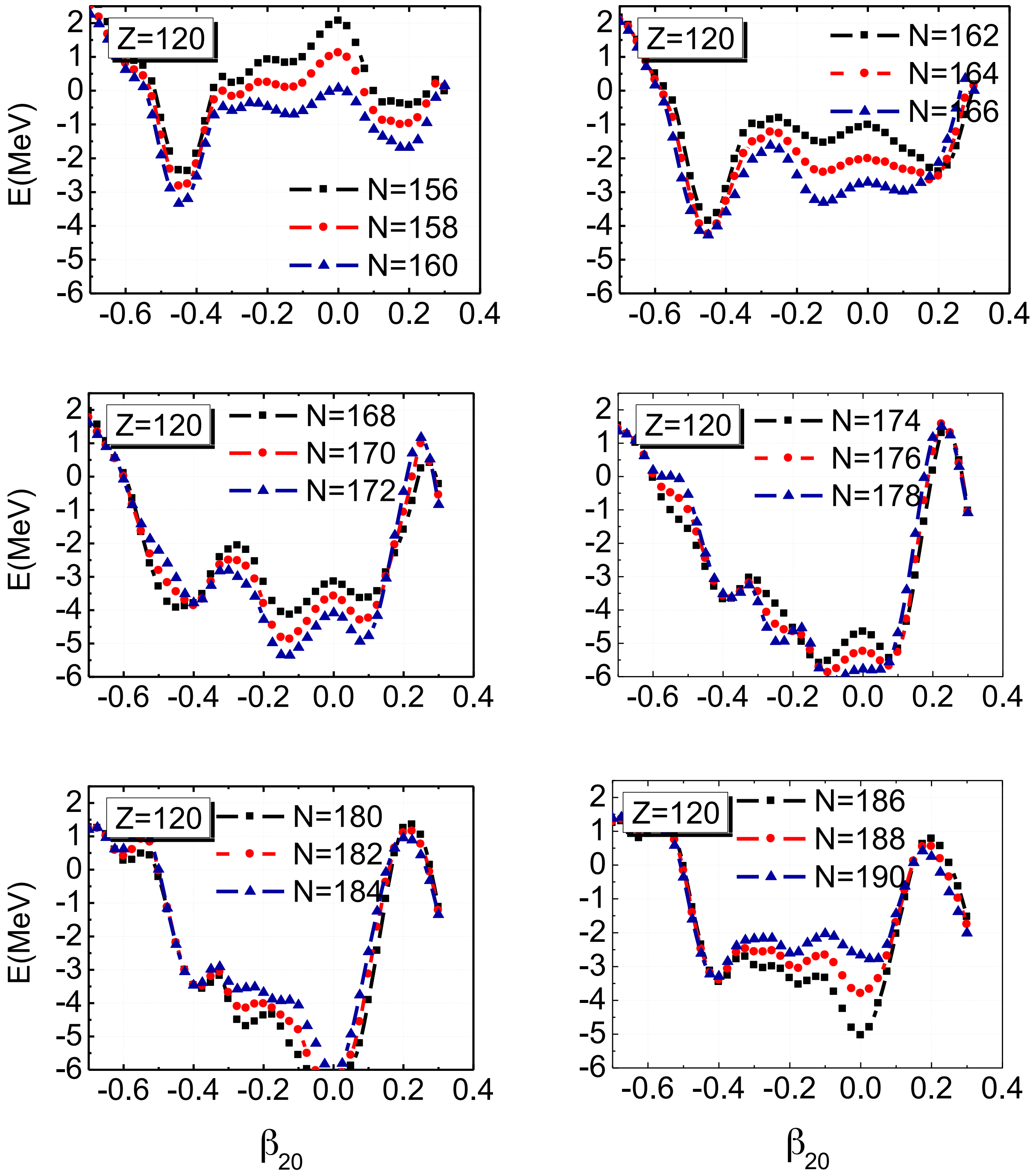
YpE

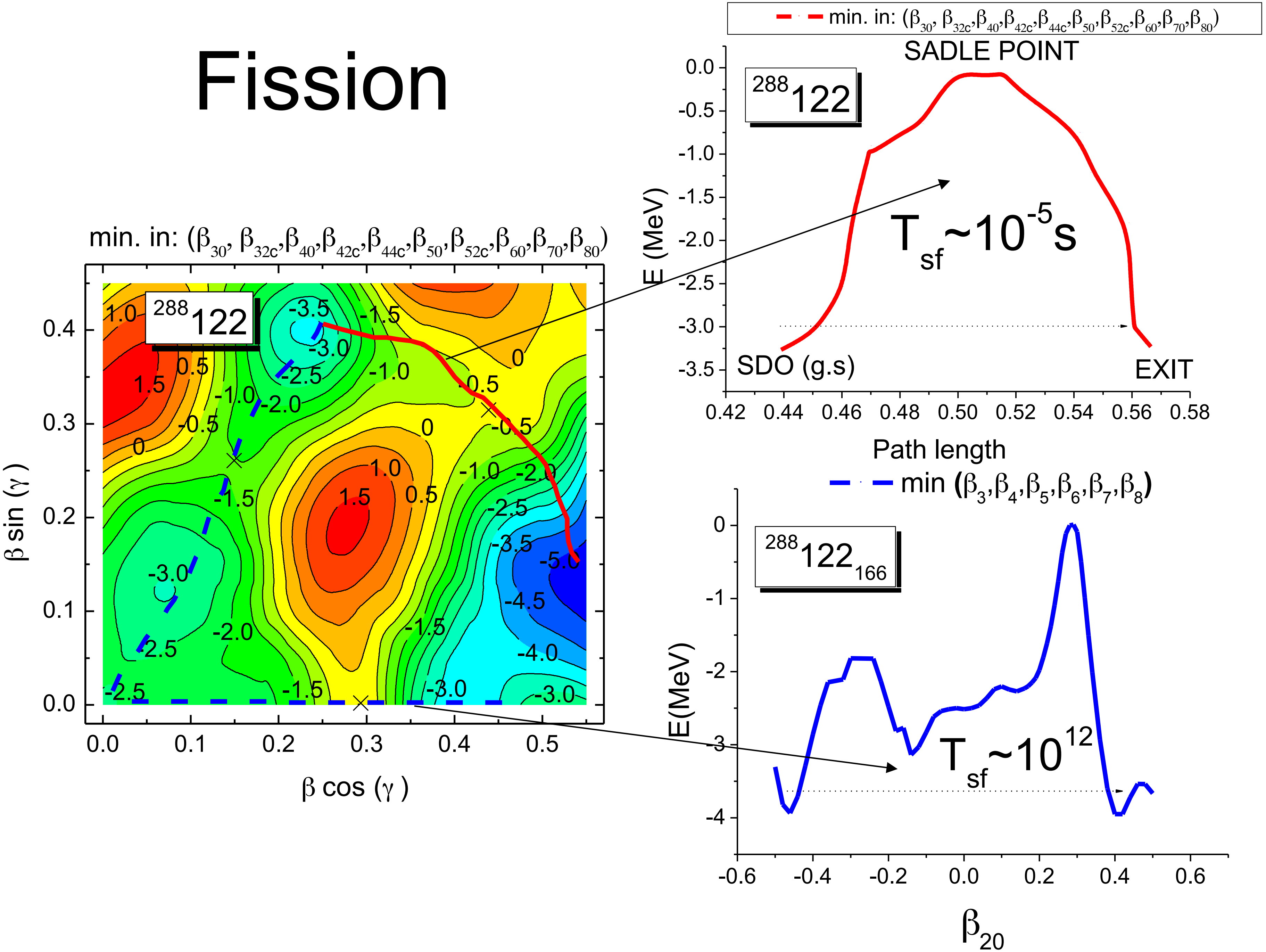

Z=120
N=156
N=158
N=160
Z=120
N=162
N=164
N=166
Z=120
N=168
N=170
N=172
Z=120
N=174
N=176
N=178
Z=120
N=180
N=182
N=184
Z=120
N=186
N=188
N=190
E(MeV)
2
1
0
-1
-2
-3
-4
-5
-6
-0.6
-0.4
-0.2
0.0
0.2
0.4
β_{20}



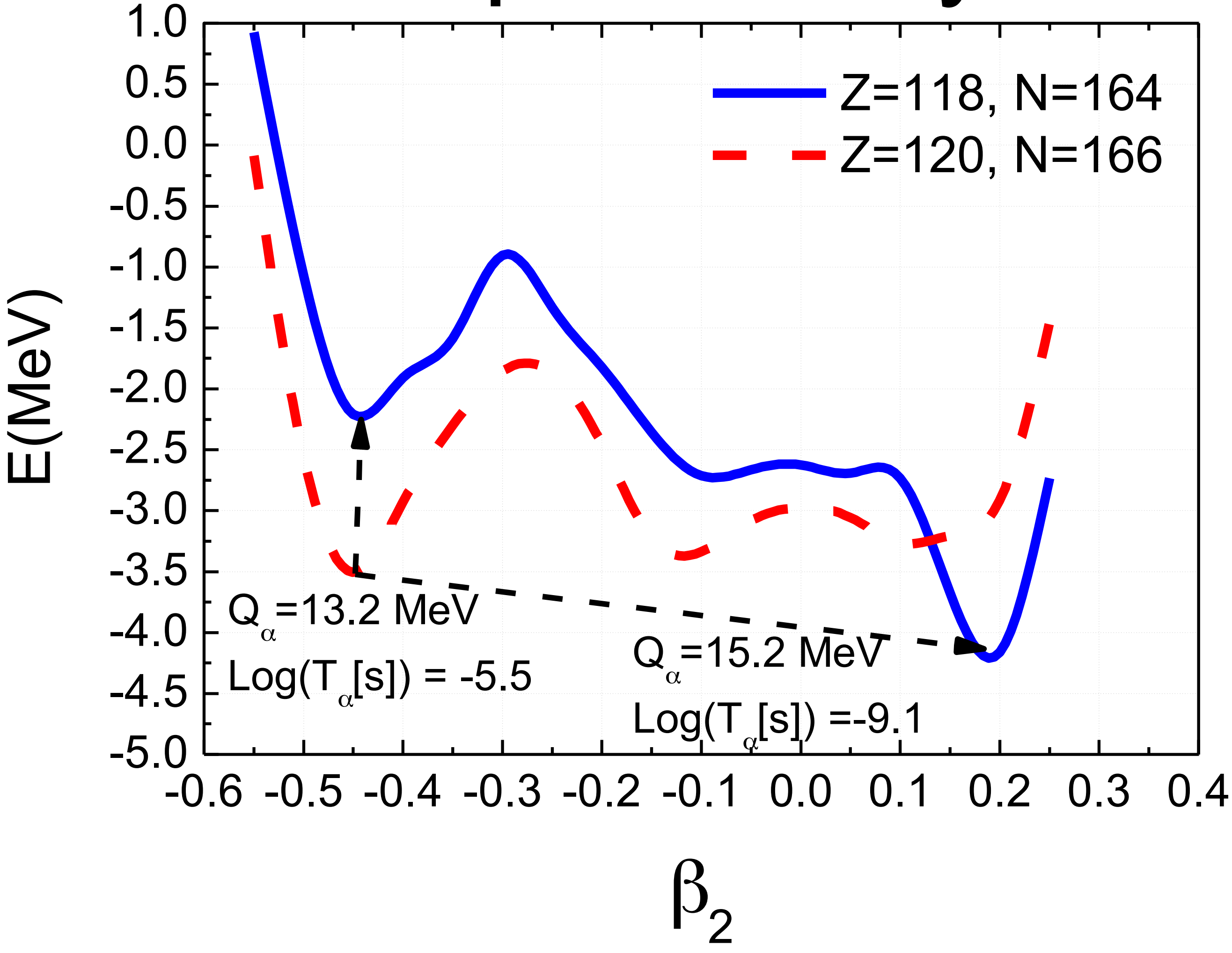
LSD

- LSD → 1 MeV deeper minima!

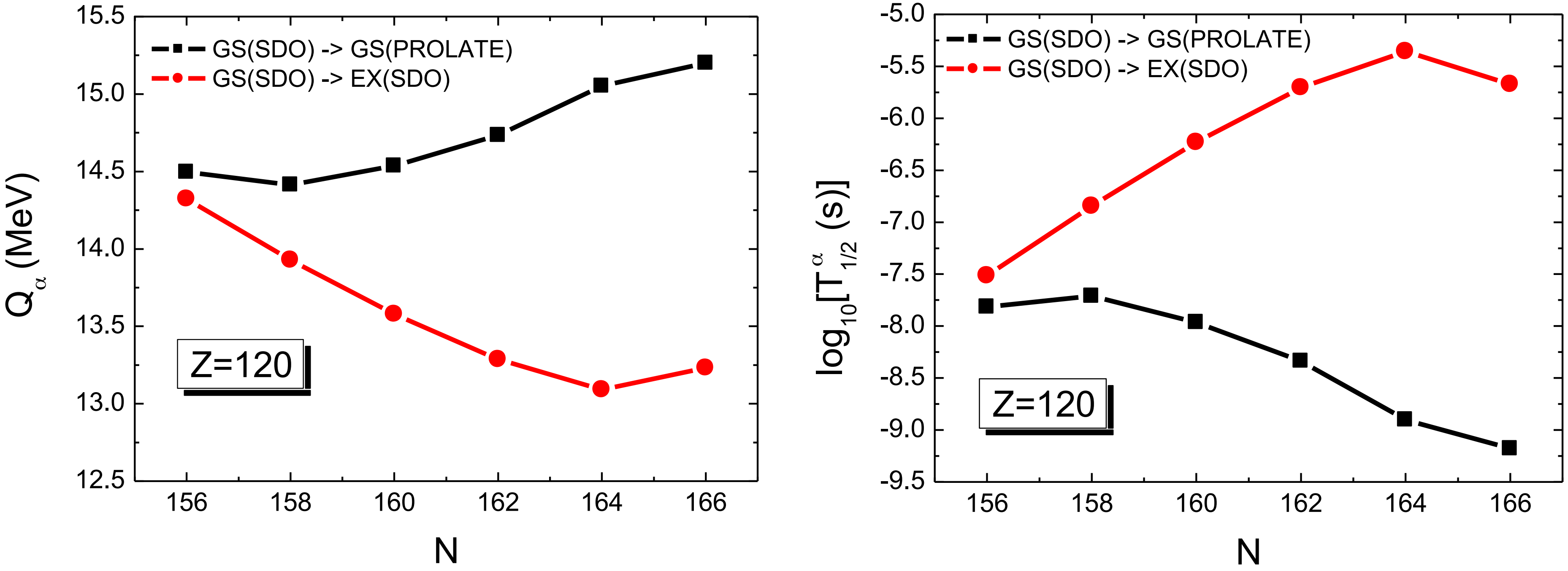
Fission


min. in: (β30, β32c,β40,β42c,β44c,β50,β52c,β60,β70,β80)
288122
1.0
1.5
0.5
0
-0.5
-1.0
-2.0
-2.5
-3.0
-3.5
-1.5
-1.0
0
0.5
-0.5
1.0
1.5
0.5
-1.0
-2.0
-2.5
-3.5
-5.0
-4.5
-4.0
-3.0
-1.5
-3.0
-2.0
-2.5
-1.5
-3.0
-2.5
β sin (γ)
0.0
0.1
0.2
0.3
0.4
β cos (γ)
0.0
0.1
0.2
0.3
0.4
0.5
min. in: (β30, β32c,β40,β42c,β44c,β50,β52c,β60,β70,β80)
SADLE POINT
288122
E (MeV)
0.0
-0.5
-1.0
-1.5
-2.0
-2.5
-3.0
-3.5
Tsf~10-5s
SDO (g.s)
EXIT
0.42
0.44
0.46
0.48
0.50
0.52
0.54
0.56
0.58
Path length
min (β3,β4,β5,β6,β7,β8)
288122166
E(MeV)
0
-1
-2
-3
-4
Tsf~1012
-0.6
-0.4
-0.2
0.0
0.2
0.4
0.6
β20

Alpha decay

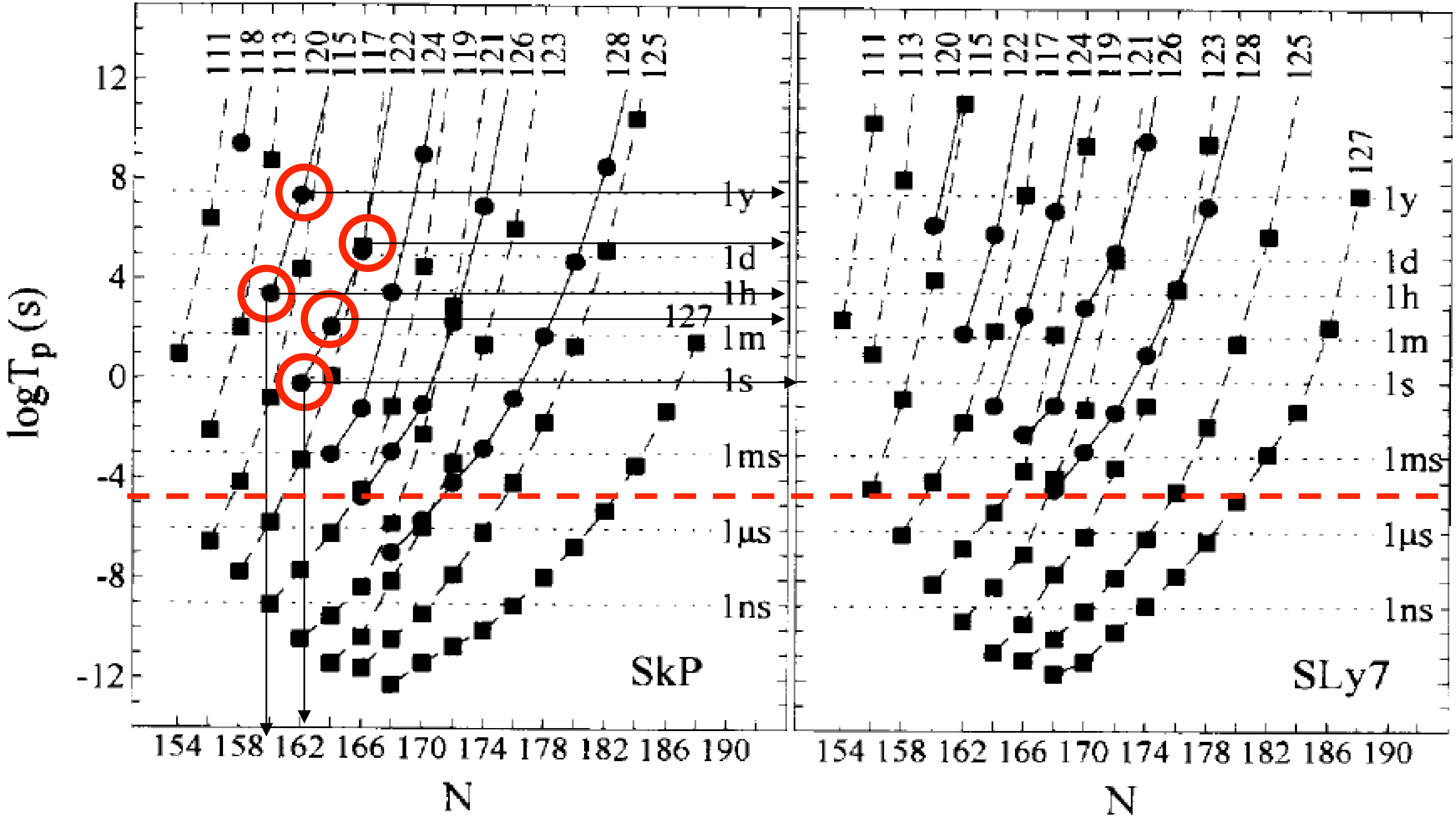


- Formula a’ laViola Seaborg from Royer



15.5
15.0
14.5
14.0
13.5
13.0
12.5
Q_α (MeV)
GS(SDO) -> GS(PROLATE)
GS(SDO) -> EX(SDO)
Z=120
156
158
160
162
164
166
N
-5.0
-5.5
-6.0
-6.5
-7.0
-7.5
-8.0
-8.5
-9.0
-9.5
$\log_{10}[T^{\alpha}_{1/2}$ (s)]
GS(SDO) -> GS(PROLATE)
GS(SDO) -> EX(SDO)
Z=120
156
158
160
162
164
166
N

One proton emission half lives



S. Ćwiok[a,b], J. Dobaczewski[a,c], P.-H. Heenen[d], P. Magierski[b],
W. Nazarewicz[c,e,f]

Beta decay

$$\lambda = \frac{2}{\pi^3 h}\left(\frac{2.4G_F}{(hc)^3}\right)^2 |M|^2 \times \int_{\Delta m_e c^2}^{\Delta mc^2} (\Delta mc^2 - E)^2 \sqrt{E^2 - m_e{}^2 c^4}\, E dE.$$

$$Q_\beta = (\Delta m - m_e), \qquad \Delta m = m_{A,Z} - m_{A,Z\pm 1}$$

$$M = \int \Psi_n{}^*(r)\Psi_p(r) d^3 r$$

$$For \quad Q_\beta ?\ m_e c^2$$

$$\lambda : |M|^2 G_F^2 Q_\beta^5$$

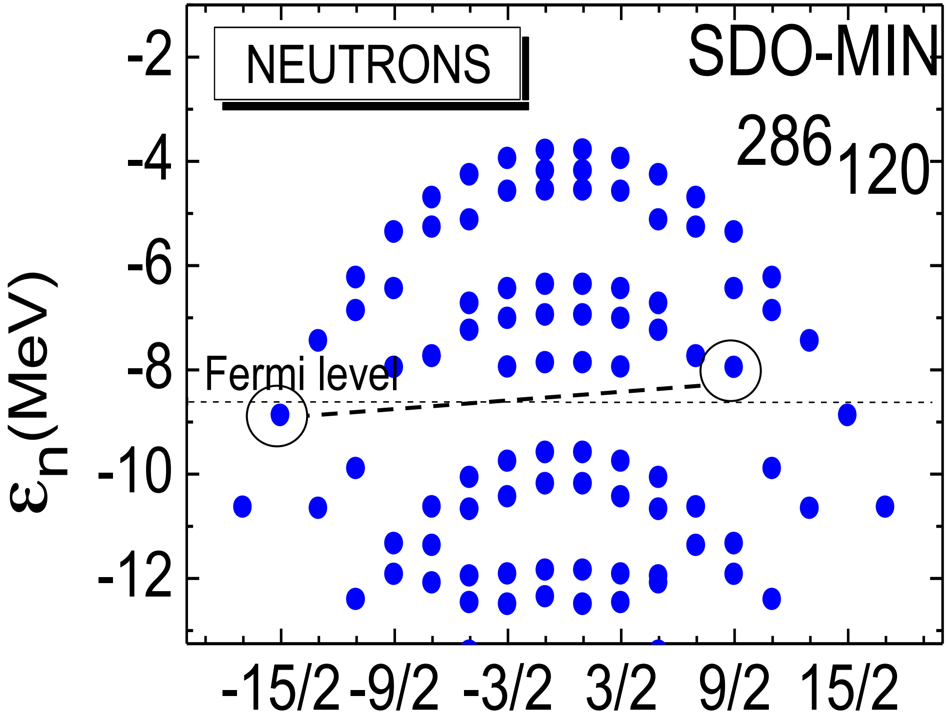
$$and \quad M : 1$$

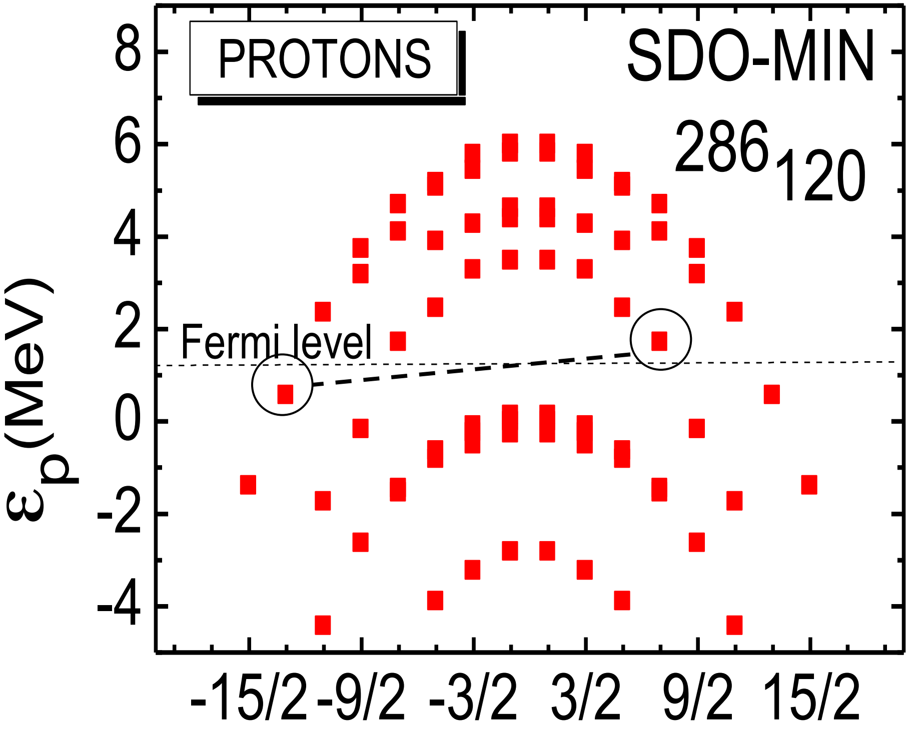
$$\Downarrow \qquad \Downarrow \qquad \Downarrow$$

$$\boxed{T_\beta :\ 0.1 \div 10 s}$$

Since for high-K isomers |M| is reduced, their beta+ decay is even slower.

A fascinating possibility for their longer life-times is related to K-isomerism, high-K configurations at the SDO shape are very likely!!!





Ω OPTIMAL CONFIGURATION: Ω

(15/2+)+(9/2)-=>12-

(13/2-)+(7/2)+=>10-

K-isomerism (discussion) !

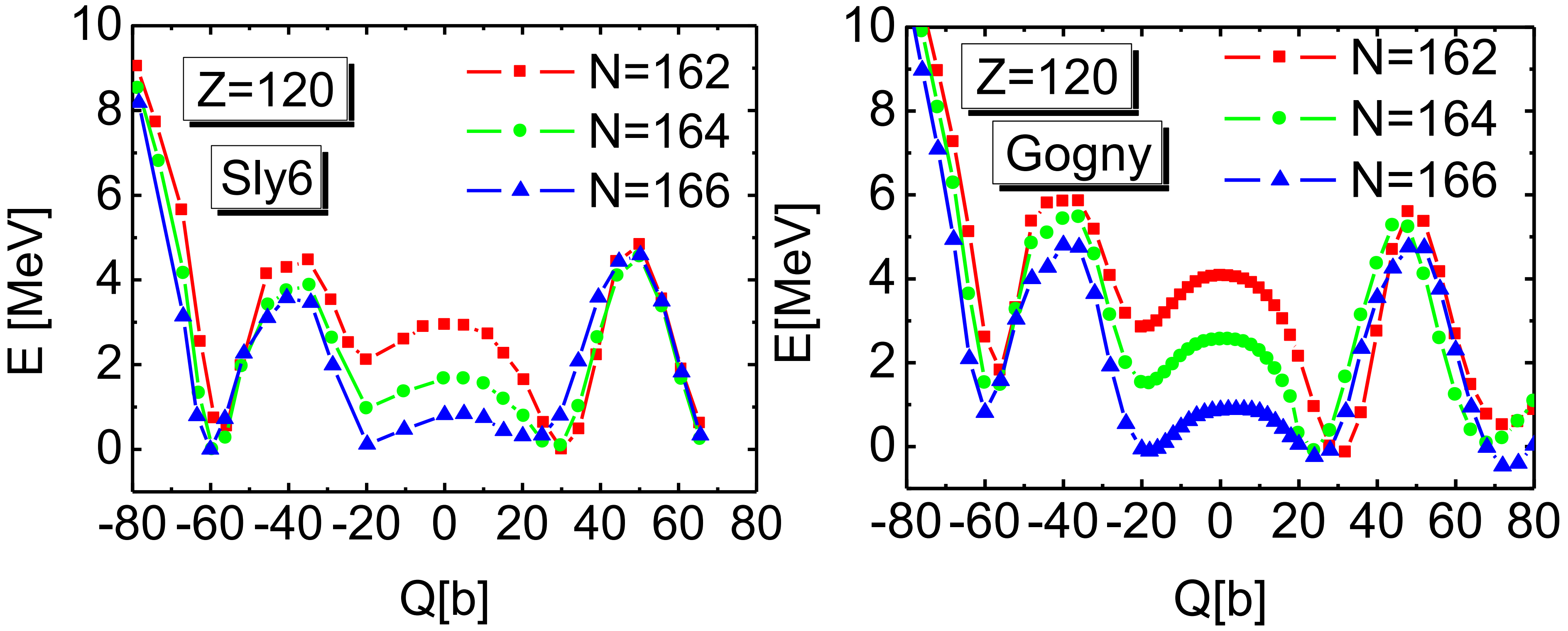
FISSION HINDRANCE:

- T_{sf} for odd and odd-odd heavy and superheavy nuclei are by 3-5 orders longer than for their even-even neighbours.
- Increase was found for high-K isomers, with respect to (prolate) shape isomers on which they are built, in even 240Cm-244Cm.
- For SDO superheavy K-isomers two factors combine to increase fission half-life:
- A) the axial fission path is closed by the conservation of the K quantum number.
- B) triaxial barriers increase due to a decrease in pairing caused by the blocking of two neutrons or protons.
- C) additional hindrance of fission is expected for configurations involving blocked high-Omega intruder states.

ALPHA HINDRANCE:

- High-K isomer in 270Ds has longer (partial) half-live T_{alpha}= 6.0 ms than the g.s., T_{alpha}(g.s.)=100 microsec.
- For SDO nuclei, an additional hindrance may result from a difference between the parent and daughter high-K configuration.
- Extra excitation in the daughter, leading to a smaller Q_{alpha}.

self-consistent calculations



CONCLUSIONS:

- Masses are calculated with rms deviation = 0.58 while Q alpha with rms deviation =0.3
- Taking into account triaxial deformations has been shown to significantly reduce the first fission barrier heights by up to 2.5 MeV. Triaxial deformations do not play a significant role at the second fission barriers. Taking into account octupole deformations has been shown to significantly reduce the second fission barrier heights.
- In comparing our first and second fission barrier calculations with experimental data we find spectacular agreement for investigated nuclei, rms~0.4-0.5
- The results found for DMP and IWM methods are completely consistent with each other in the sense that obtained deformations and energies in both cases are practically the same.

CONCLUSIONS:

- Our calculations indicate that, in contrast to self-consistent mean-field calculations of fission barriers, the barrier height, which is still quite substantial for a nuclei with Z=118 becomes lower than 4.5 MeV for nuclei with Z=126.

- Theoretical evaluations of fission barrier heights based on various models differ between each other significantly. It is obvious that future experiments on superheavy nuclei will constitute a natural benchmark for all theoretical models describing these nuclei.

- The very fact that superdeformed oblate minima (SDO) occur in WS and self-consistent calculations and their geometrical sense points to their universality, as a transitional form between (close to) spherical and toroidal configurations for still heavier hypothetical high-Z systems.

- SDO minima are even by ~1 MeV deeper with the LSD variant of the macroscopic energy.

- In the HFBCS calculations, the energy competition between prolate, oblate and SDO minima and fission barriers come out similar as in the microscopic-macroscopic study.