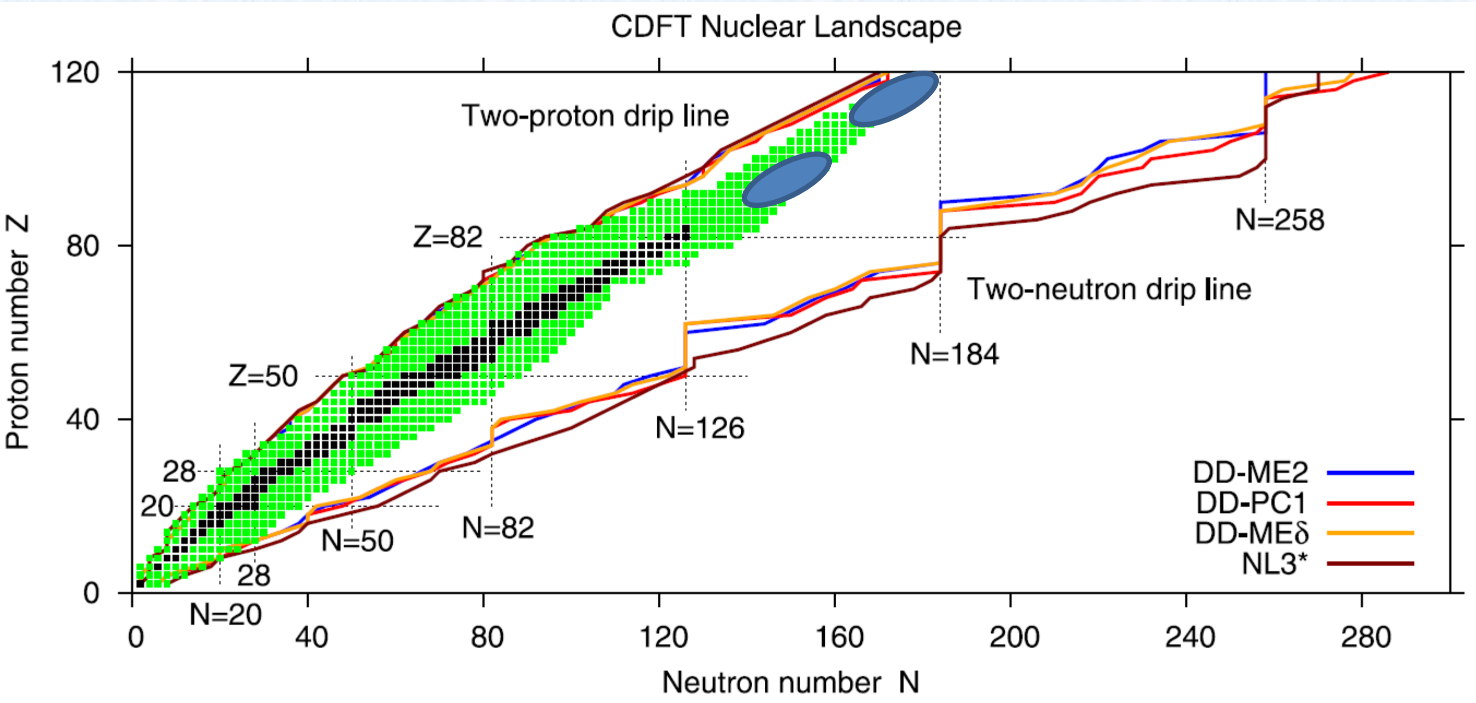
Fission in covariant DFT: status and open questions.

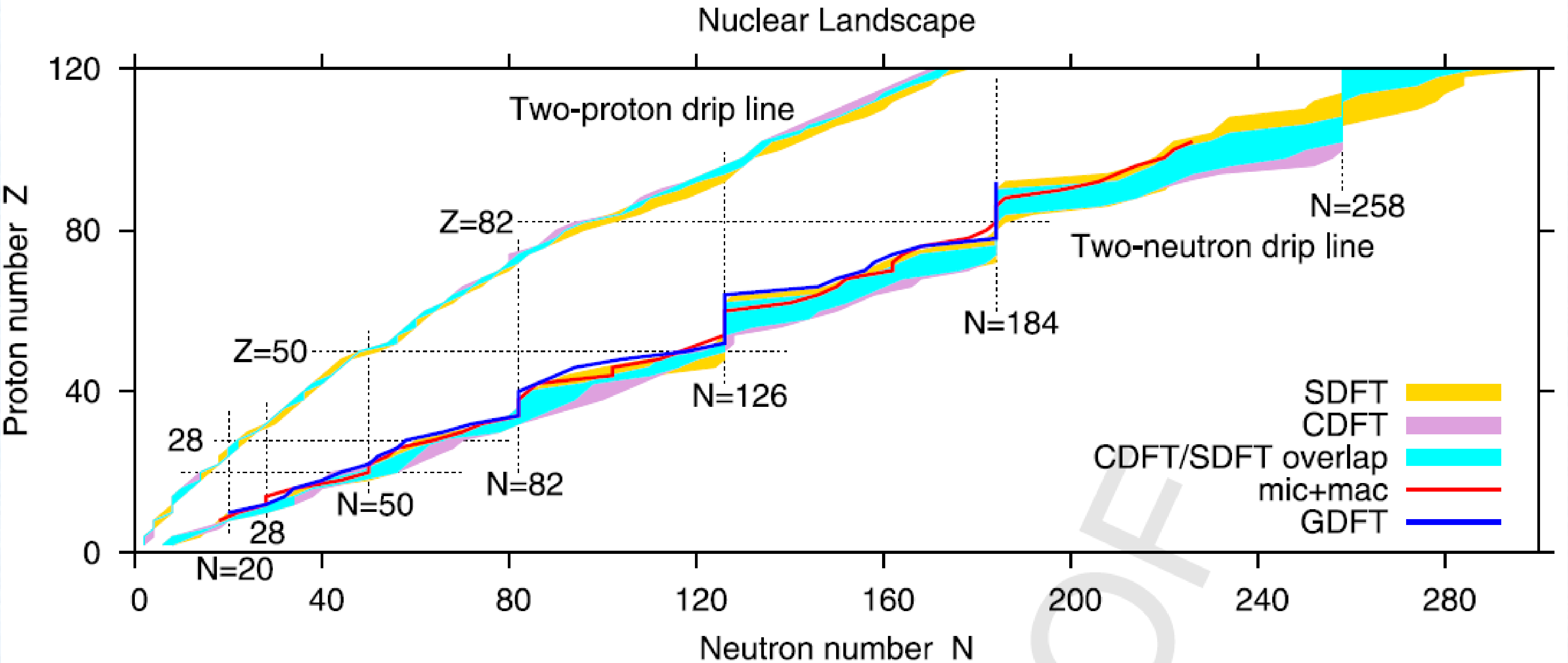
Anatoli Afanasjev
Mississippi State University, USA

1. **Motivation**
2. **Theoretical framework.**
3. **Current status: actinides and superheavy nuclei**
4. **Open questions**
5. **Conclusions**



CDFT
AA et al,
PLB in press

SDFT,
Erler et al,
Nature 486,
509 (2012)



Need for accurate description of fission barriers since they strongly affect:

1. The probability for the **formation** of superheavy nuclei in heavy-ion-fussion reaction (the cross-section very sensitively depends on the fission barrier height).

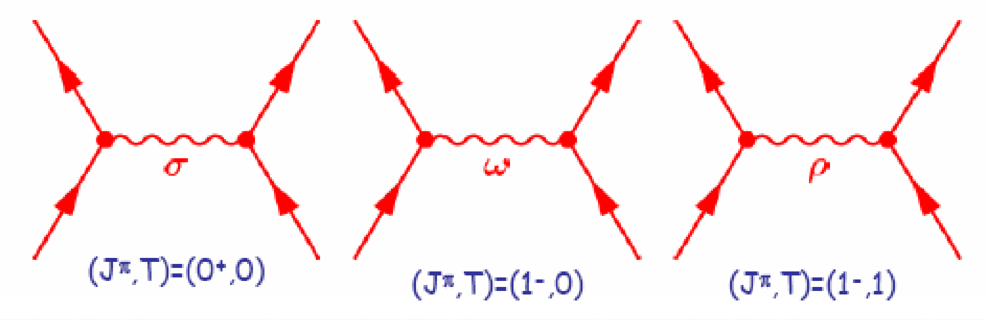
2. **survival probability** of an excited nucleus in its cooling by emitting neutrons and γ-rays in competition with fission (the changes in fission barrier height by 1 MeV changes the calculated survival probability by about one order of magnitude or more)

3. **spontaneous fission lifetimes**

The landscape of PES is an input for the calculations beyond mean field (such as GCM). Fission barriers provide a unique opportunity to test how DFT describe this landscape.

Covariant density functional theory (CDFT)

The nucleons interact via the exchange of effective mesons →
→ **effective Lagrangian**



Long-range attractive scalar field

Short-range repulsive vector field

Isovector field

$$E_{\mathrm{RMF}}[\hat{\rho},\phi_m] = \mathrm{Tr}[(\boldsymbol{\alpha}\boldsymbol{p}+\beta m)\hat{\rho}] \pm \int \left[\frac{1}{2}(\nabla\phi_m)^2 + U(\phi_m)\right] \mathrm{d}^3 r + \mathrm{Tr}[(\Gamma_m \phi_m)\hat{\rho}]$$

density matrix $\hat{\rho}$

$\phi_m \equiv \{\sigma, \omega^\mu, \vec{\rho}^{\,\mu}, A^\mu\}$ - meson fields

$$\boxed{\hat{h} = \frac{\delta E}{\delta \hat{\rho}}}$$

Mean field

$$\boxed{\hat{h}|\varphi_i\rangle = \varepsilon_i |\varphi_i\rangle}$$

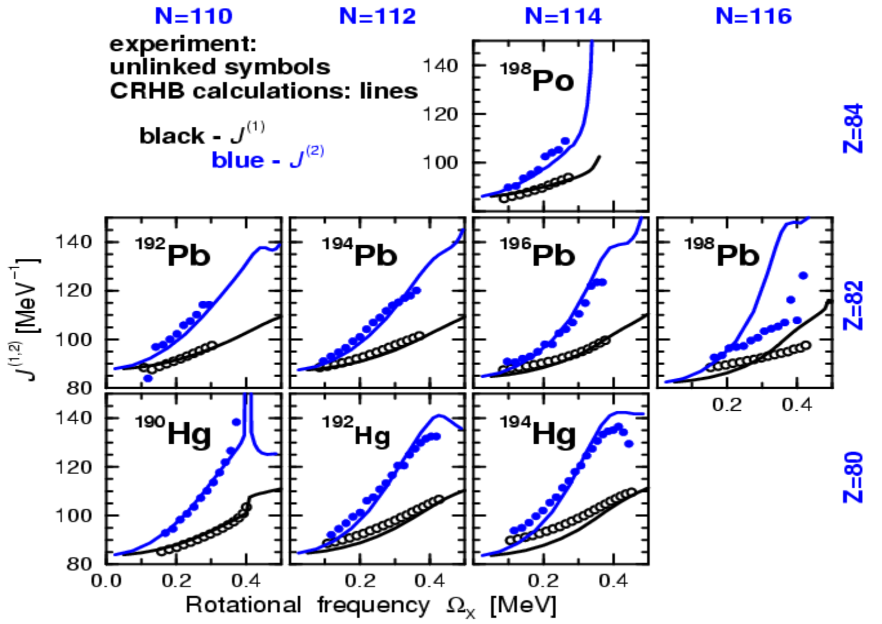
Eigenfunctions

Triaxial RHB code with Gogny force in pairing channel has been developed ~ 10 years ago for the description of rotating nuclei.

However, the calculations in its framework are too computationally expensive.

Use RMF+BCS framework with monopole pairing: required computational time is ~ 20-25 times smaller.

A.V.Afanasjev, P. Ring, J. Konig
Phys. Rev. C60 (1999) 051303; Nucl. Phys. A 676 (2000) 196



$$A \cdot G_n = G_1^n - G_2^n \frac{N-Z}{A} \text{ MeV},$$

$$A \cdot G_p = G_1^p + G_2^p \frac{N-Z}{A} \text{ MeV}$$

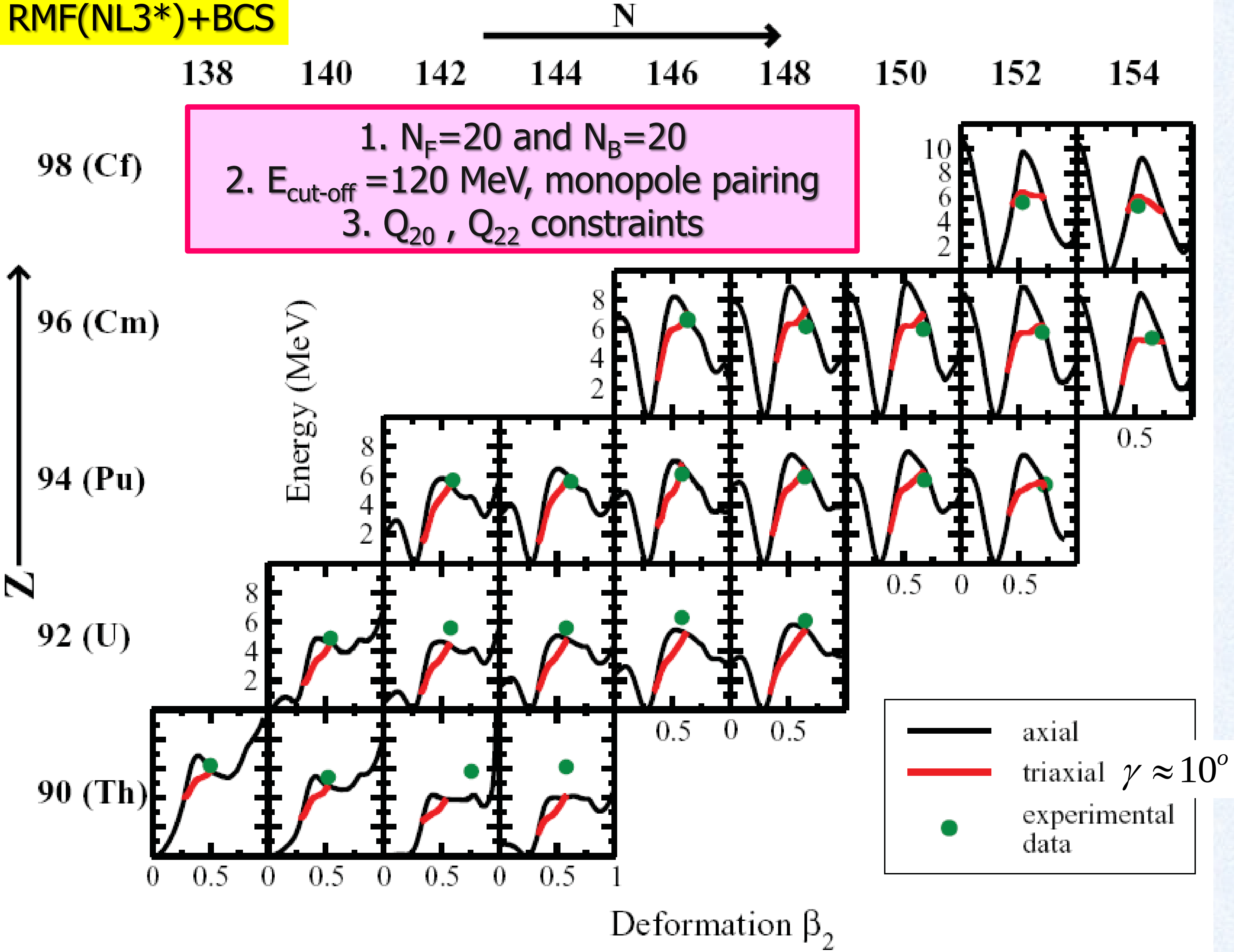
TABLE II. The G_1^n, G_2^n, G_1^p, and G_2^p parameters (in MeV) for different parametrizations of the RMF Lagrangian and cutoff energy $E_{\text{cutoff}} = 120$ MeV.

(Actinides)

Force	G_1^n	G_2^n	G_1^p	G_2^p
NL3*	9.1	6.4	8.1	10.0
DD-PC1	9.2	5.4	8.0	11.4
DD-ME2	9.2	5.8	8.1	11.2

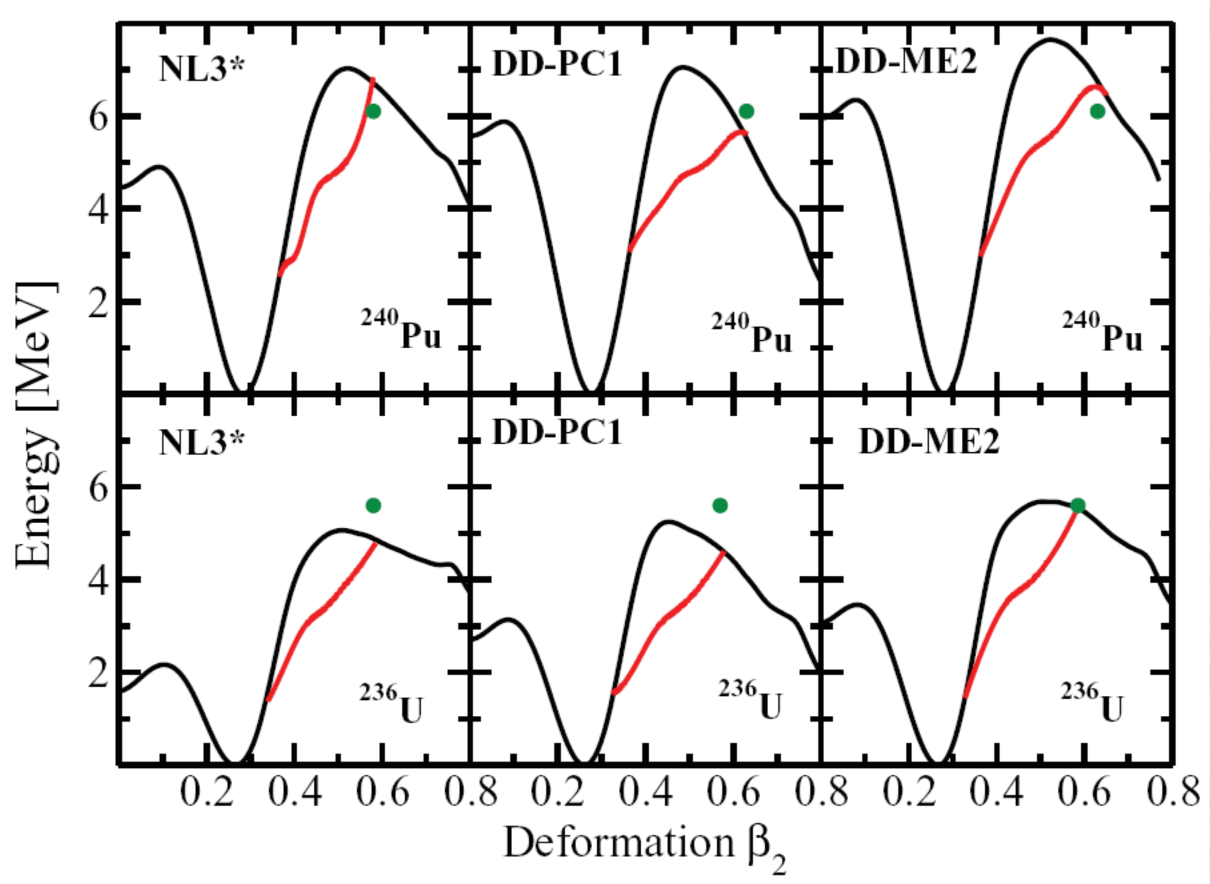
$$\Delta_n = \frac{4.8}{N^{1/3}} \quad \text{MeV}, \qquad \Delta_p = \frac{4.8}{Z^{1/3}} \quad \text{MeV}$$

RMF(NL3*)+BCS

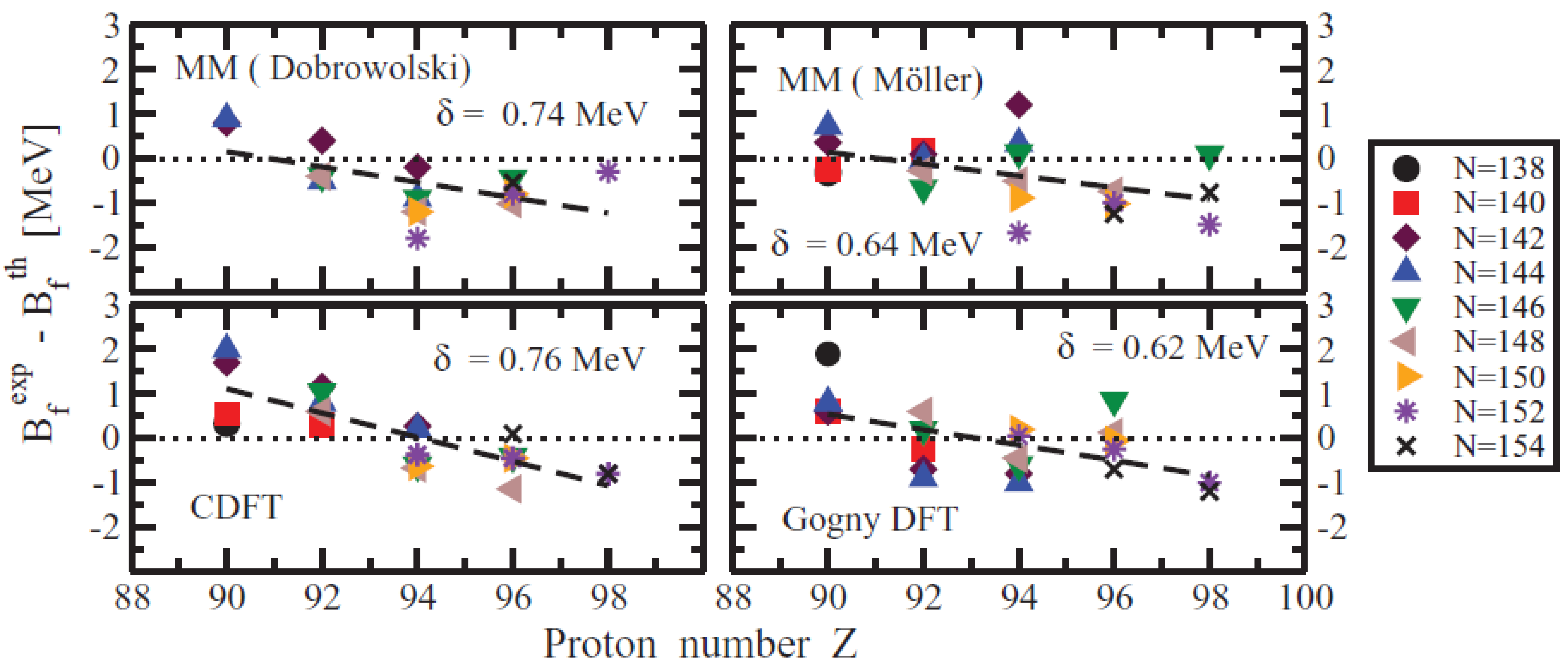


1. N_F=20 and N_B=20
2. $E_{cut\text{-}off}$ =120 MeV, monopole pairing
3. Q_{20} , Q_{22} constraints

Parametrization dependence of fission barriers



Fission barriers: theory versus experiment [state-of-the-art]



Mac+mic, LSD model
A.Dobrowolski et al,
PRC 75, 024613 (2007)

Mac+mic, FRDM model
P. Moller et al,
PRC 79, 064304 (2009)

Gogny DFT,
J.-P. Delaroche et al,
NPA 771, 103 (2006).

CDFT : actinides H. Abusara, AA and P. Ring, PRC 82, 044303 (2010)
superheavies: H. Abusara, AA and P. Ring, PRC 85, 024314 (2012)

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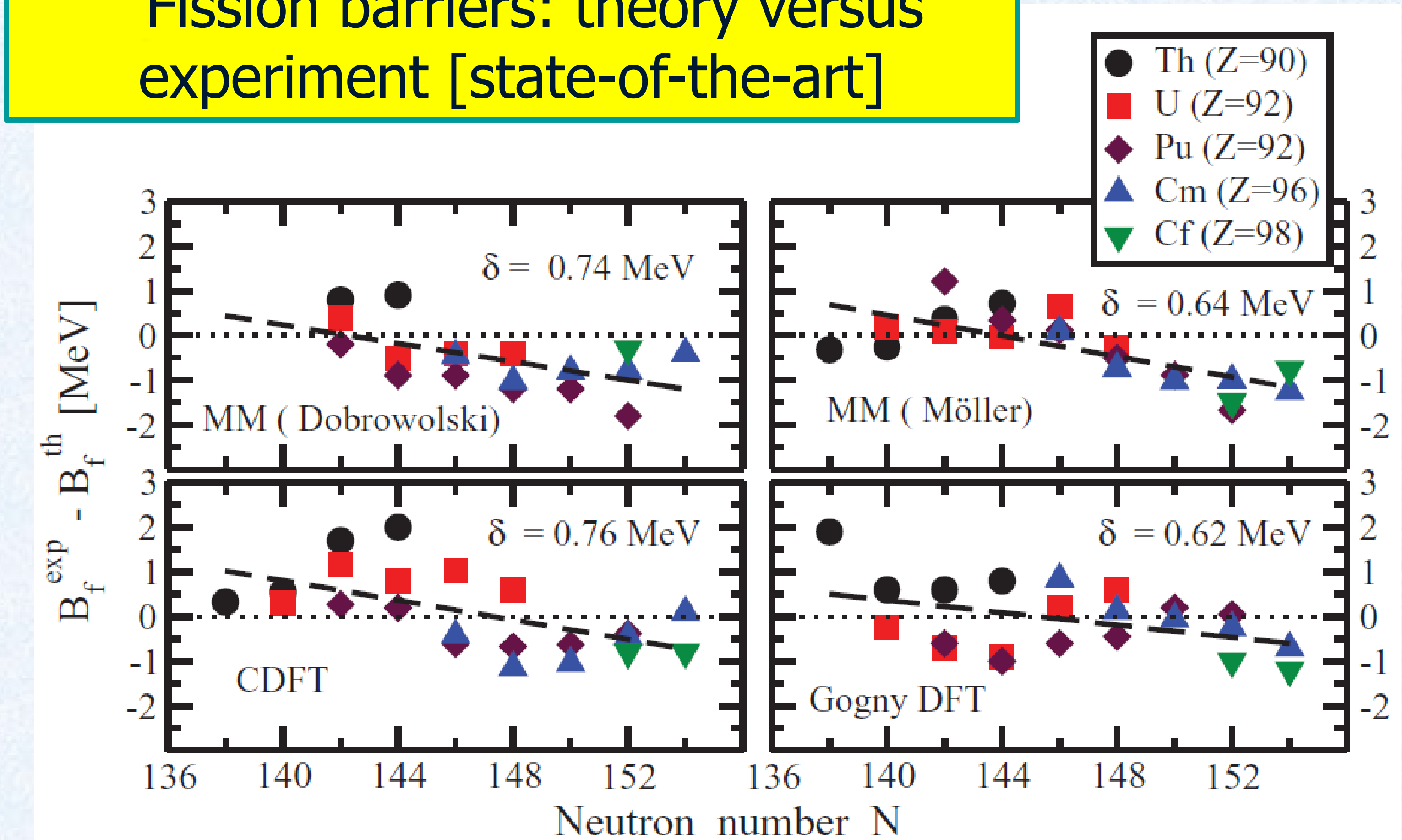

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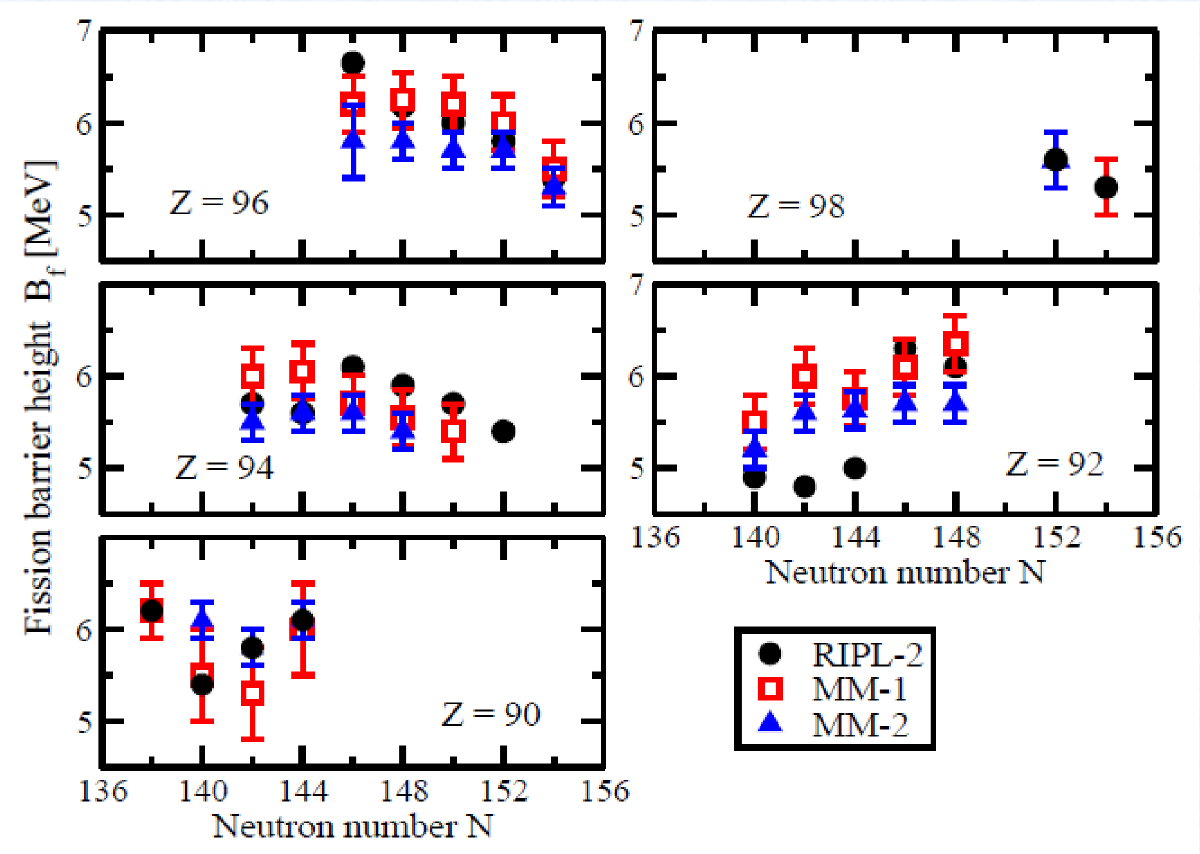
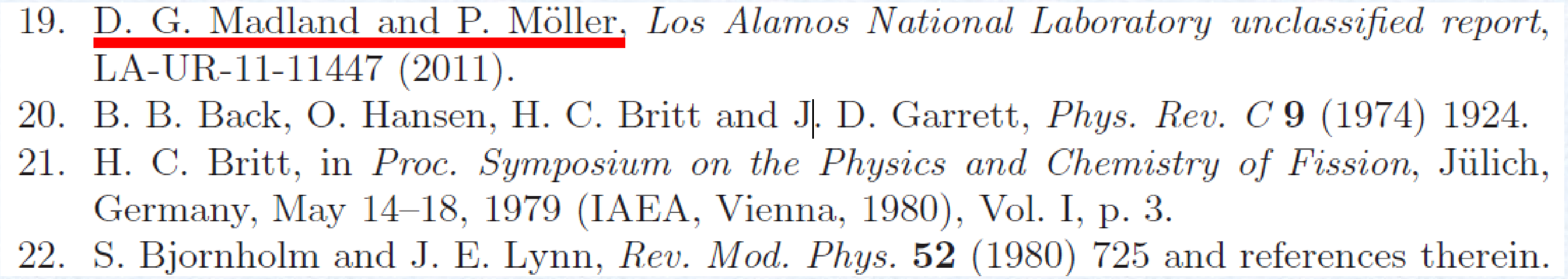
Fission barriers: how accurate are experimental evaluations?



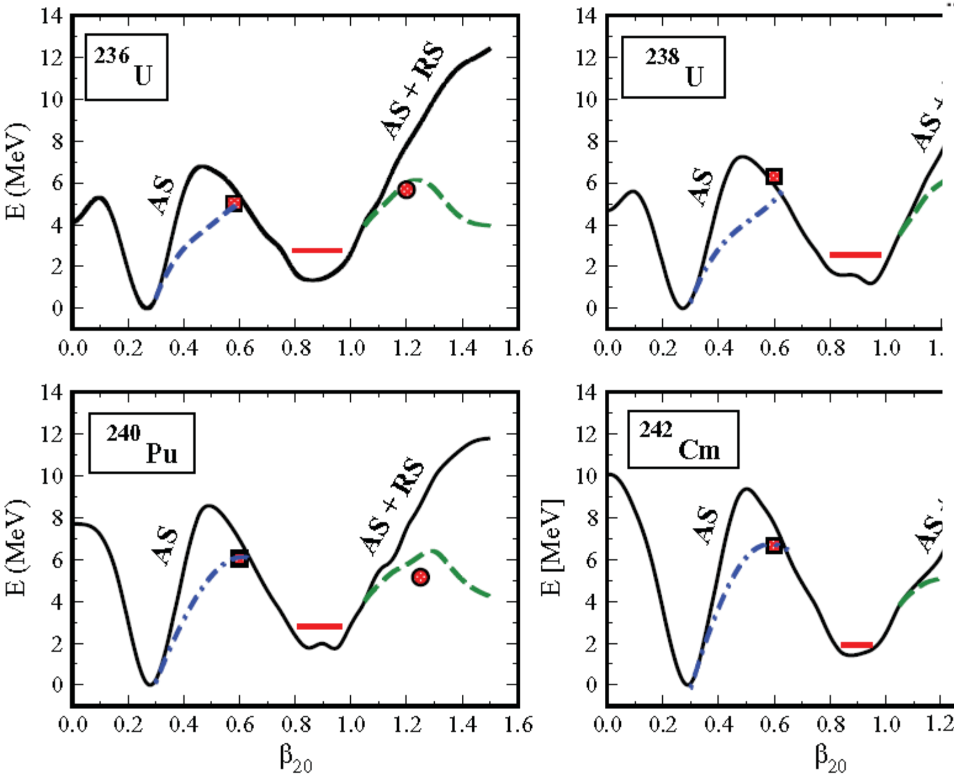
MM-1, MM-2



19. D. G. Madland and P. Möller, *Los Alamos National Laboratory unclassified report*, LA-UR-11-11447 (2011).
20. B. B. Back, O. Hansen, H. C. Britt and J. D. Garrett, *Phys. Rev. C* **9** (1974) 1924.
21. H. C. Britt, in *Proc. Symposium on the Physics and Chemistry of Fission*, Jülich, Germany, May 14–18, 1979 (IAEA, Vienna, 1980), Vol. I, p. 3.
22. S. Bjornholm and J. E. Lynn, *Rev. Mod. Phys.* **52** (1980) 725 and references therein.

Bing-Ban Lu et al,
PRC **85**, 011301(R) (2012)
RMF+BCS based on PC-PK1

V. Prassa et al, PRC **86**, 024317 (2012)
RMF+BCS based on DD-PC1



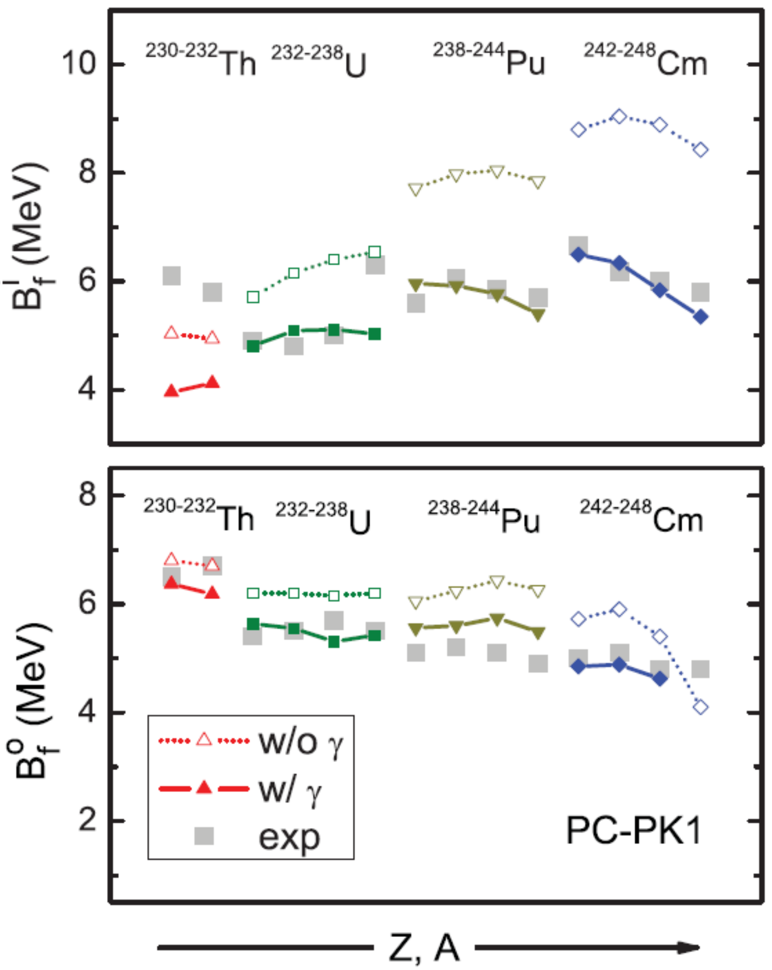


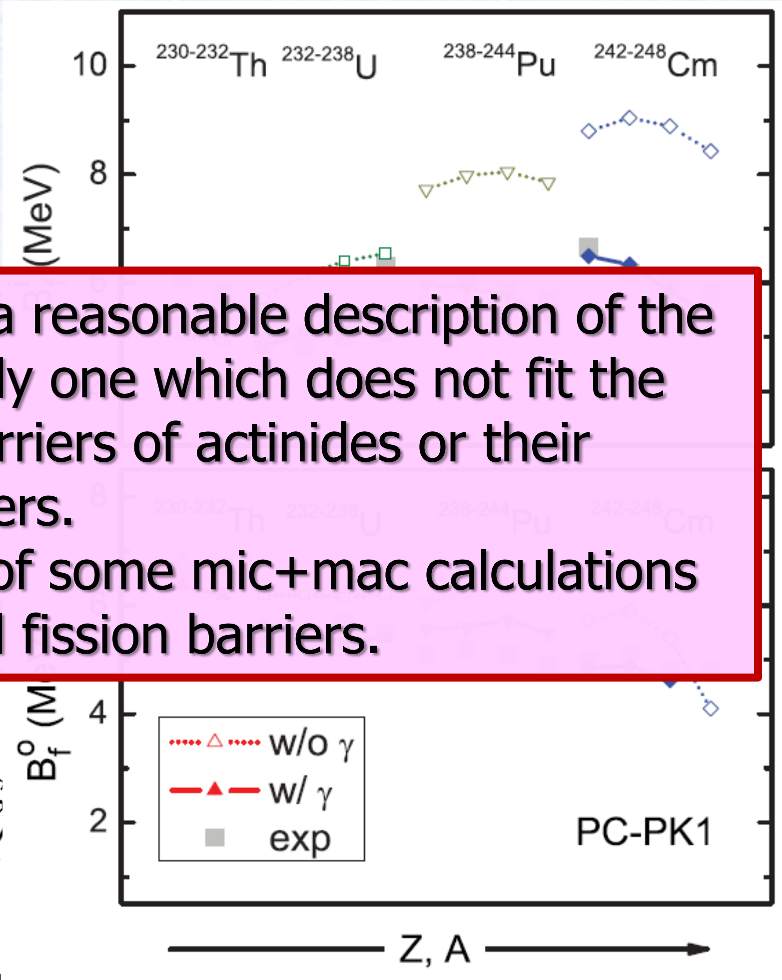
FIG. 2. (Color online) Constrained energy curves of ^{236,238}U, ^{240}Pu, and ^{242}Cm, as functions of the axial quadrupole deforma
sults of self-consistent axially and reflection-symmetric, triaxial, and axially reflection-asymmetric RMF + BCS calculations

Bing-Ban Lu et al,
PRC **85**, 011301(R) (2012)
RMF+BCS based on PC-PK1

V. Prassa et al, PRC **86**, 024317 (2012)
RMF+BCS based on DD-PC1

Among the DFT models which provide a reasonable description of the fission barrier heights, CDFT is the only one which does not fit the parameters to the inner fission barriers of actinides or their fission isomers.

Note also that liquid drop parameters of some mic+mac calculations are fitted to experimental fission barriers.



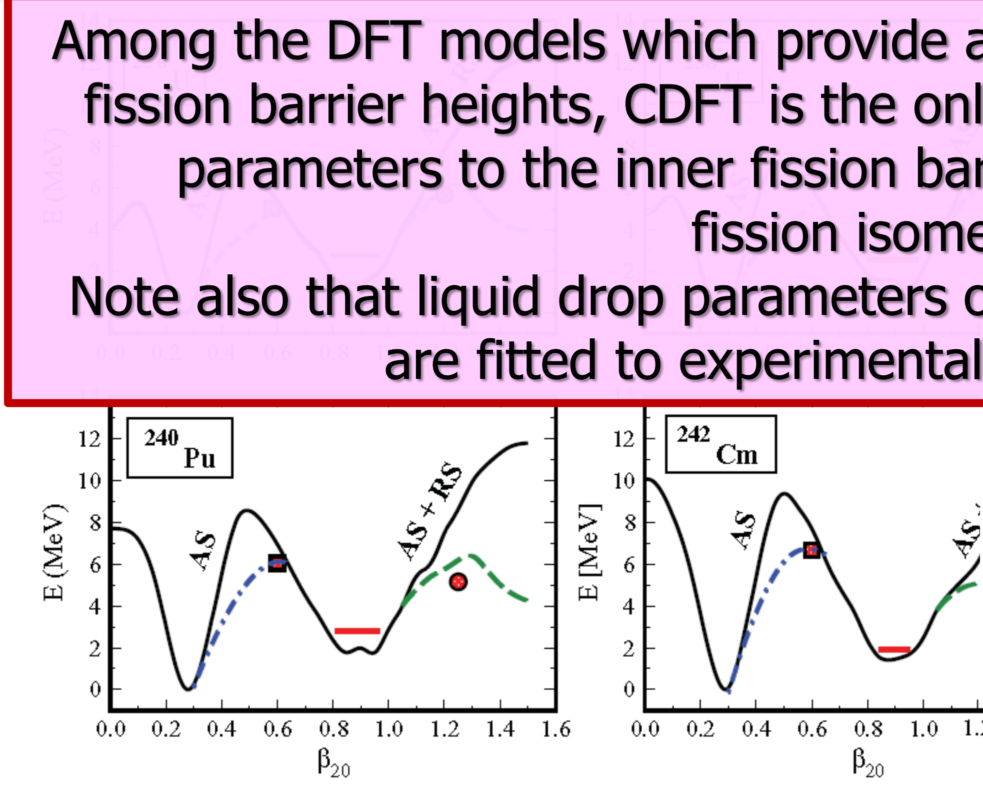


FIG. 2. (Color online) Constrained energy curves of ^{236,238}U, ^{240}Pu, and ^{242}Cm, as functions of the axial quadrupole deforma
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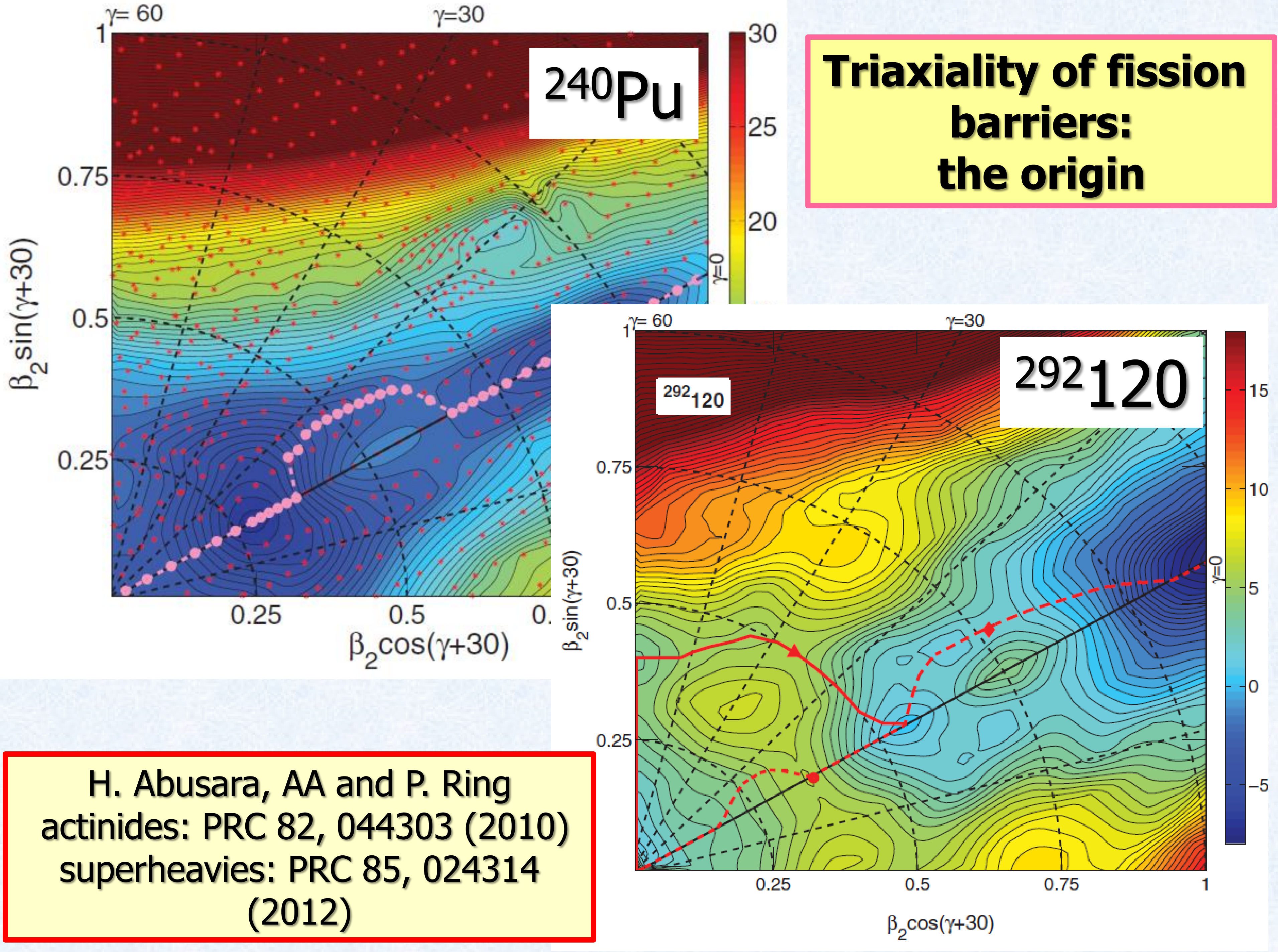
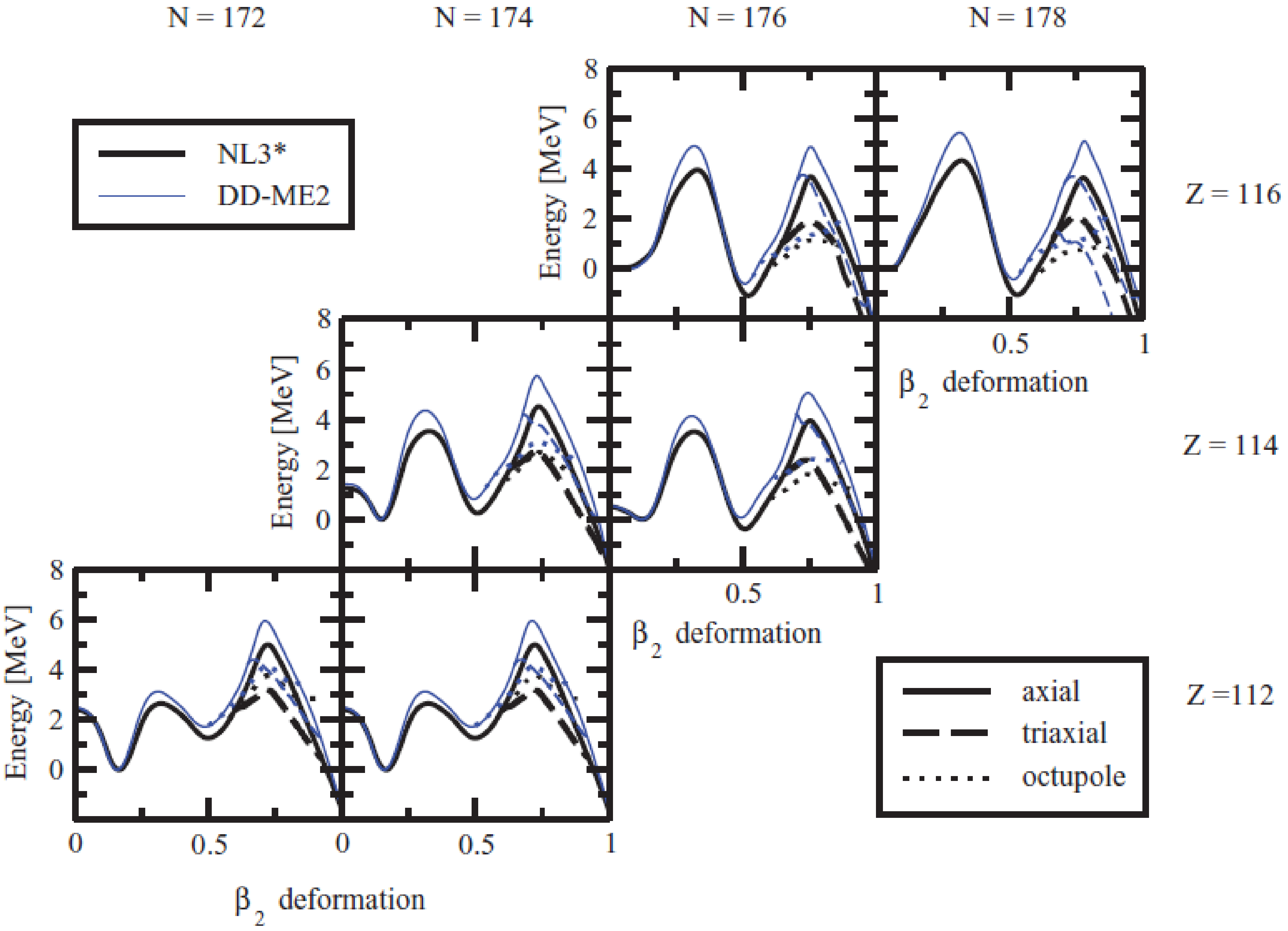
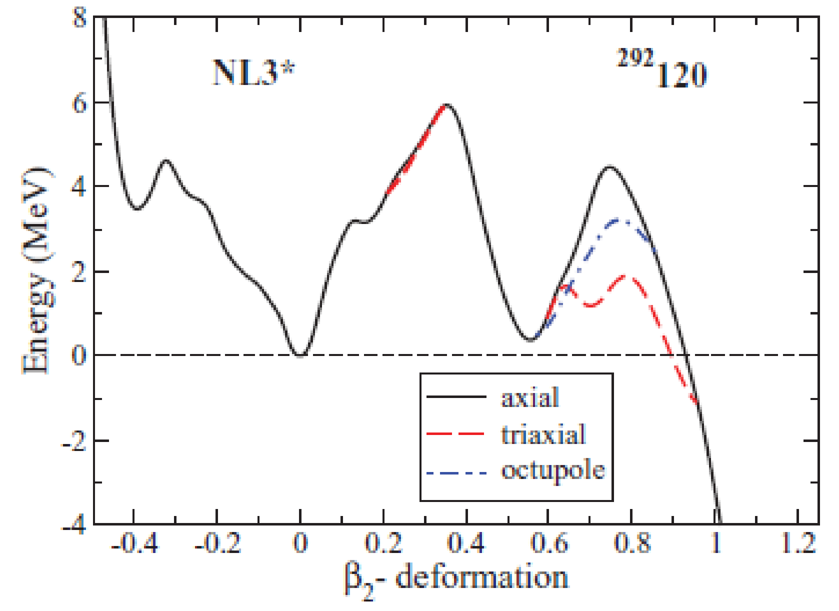
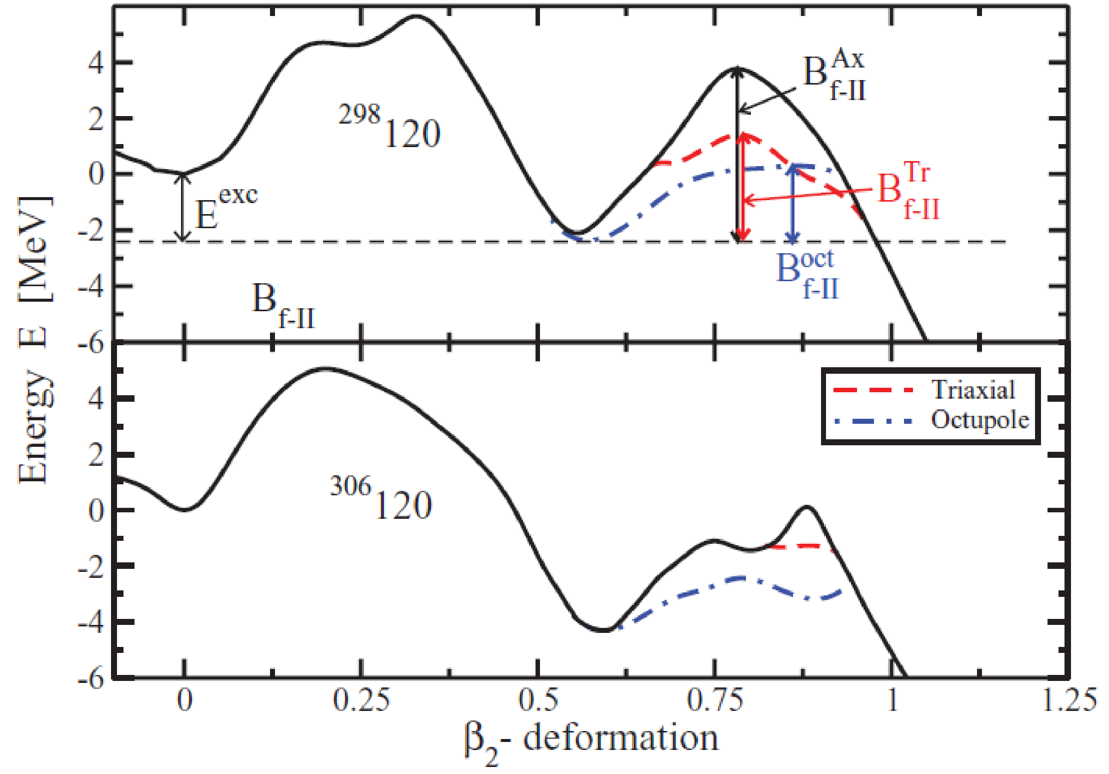
Triaxiality of fission barriers: the origin

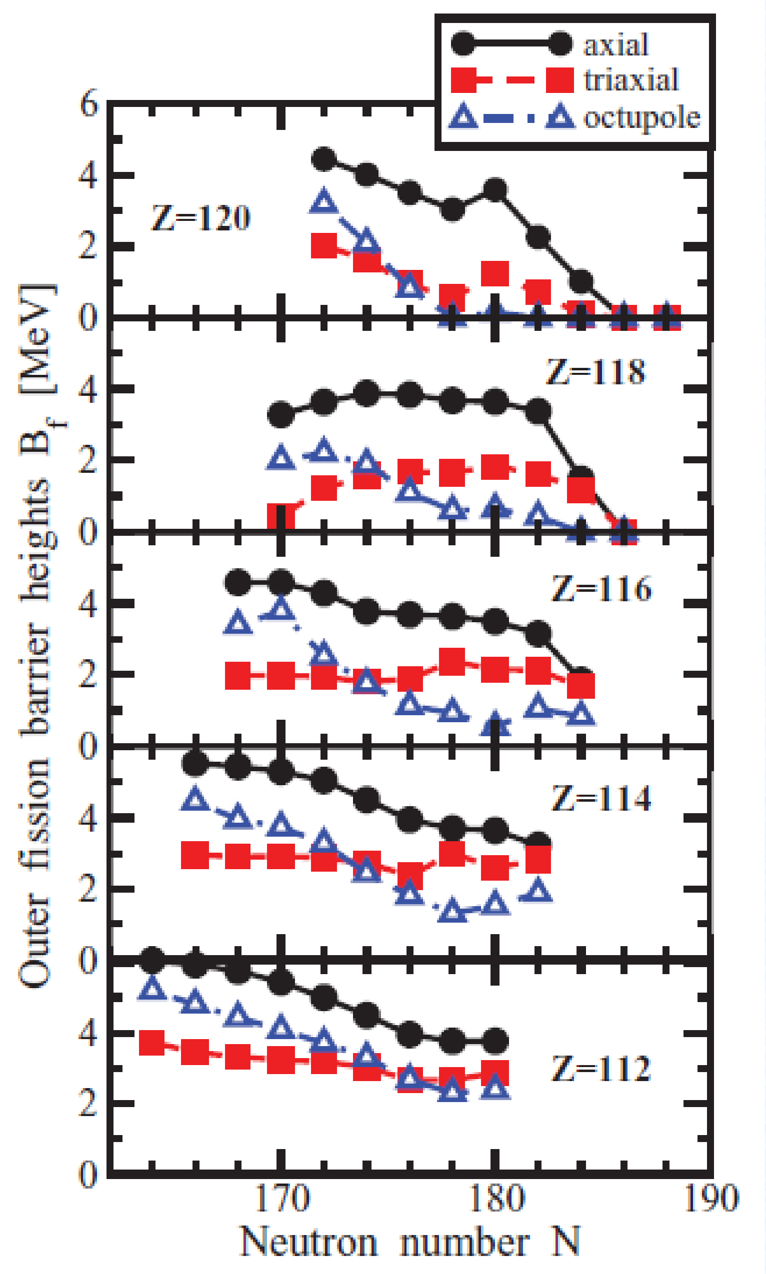


H. Abusara, AA and P. Ring
actinides: PRC 82, 044303 (2010)
superheavies: PRC 85, 024314 (2012)

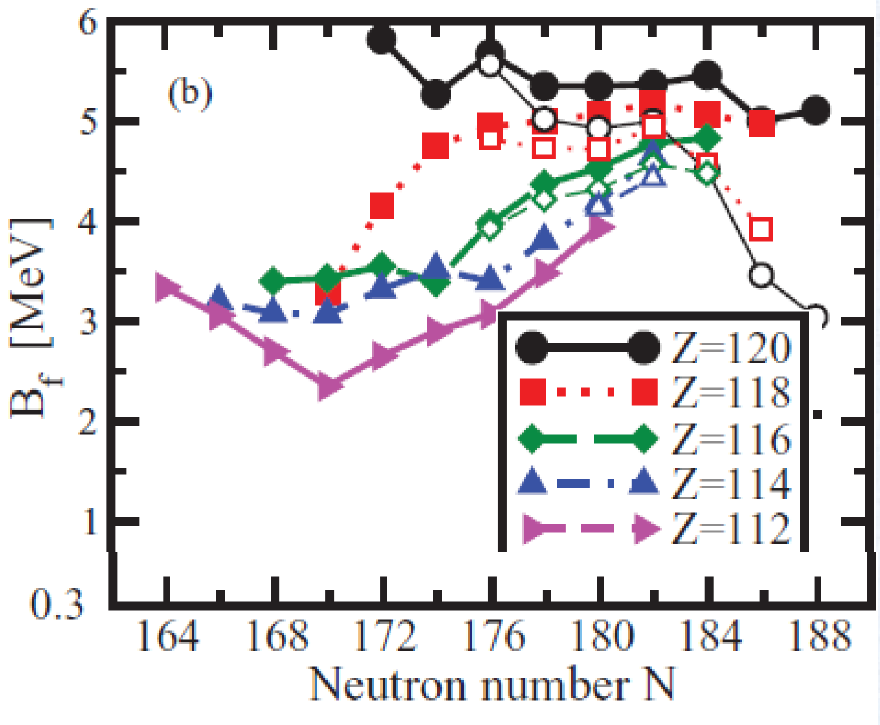

N = 172
N = 174
N = 176
N = 178
NL3*
DD-ME2
Z = 116
Z = 114
Z =112
Energy [MeV]
8
6
4
2
0
0
0.5
1
β$_2$ deformation
axial
triaxial
octupole


NL3*
^{292}120
Energy (MeV)
8
6
4
2
0
-2
-4
-0.4
-0.2
0
0.2
0.4
0.6
0.8
1
1.2
β_2- deformation
axial
triaxial
octupole


^{298}120
E^{exc}
B^{Ax}_{f-II}
B^{Tr}_{f-II}
B^{oct}_{f-II}
B_{f-II}
^{306}120
Triaxial
Octupole
Energy E [MeV]
4
2
0
-2
-4
-6
0
0.25
0.5
0.75
1
1.25
β_2- deformation

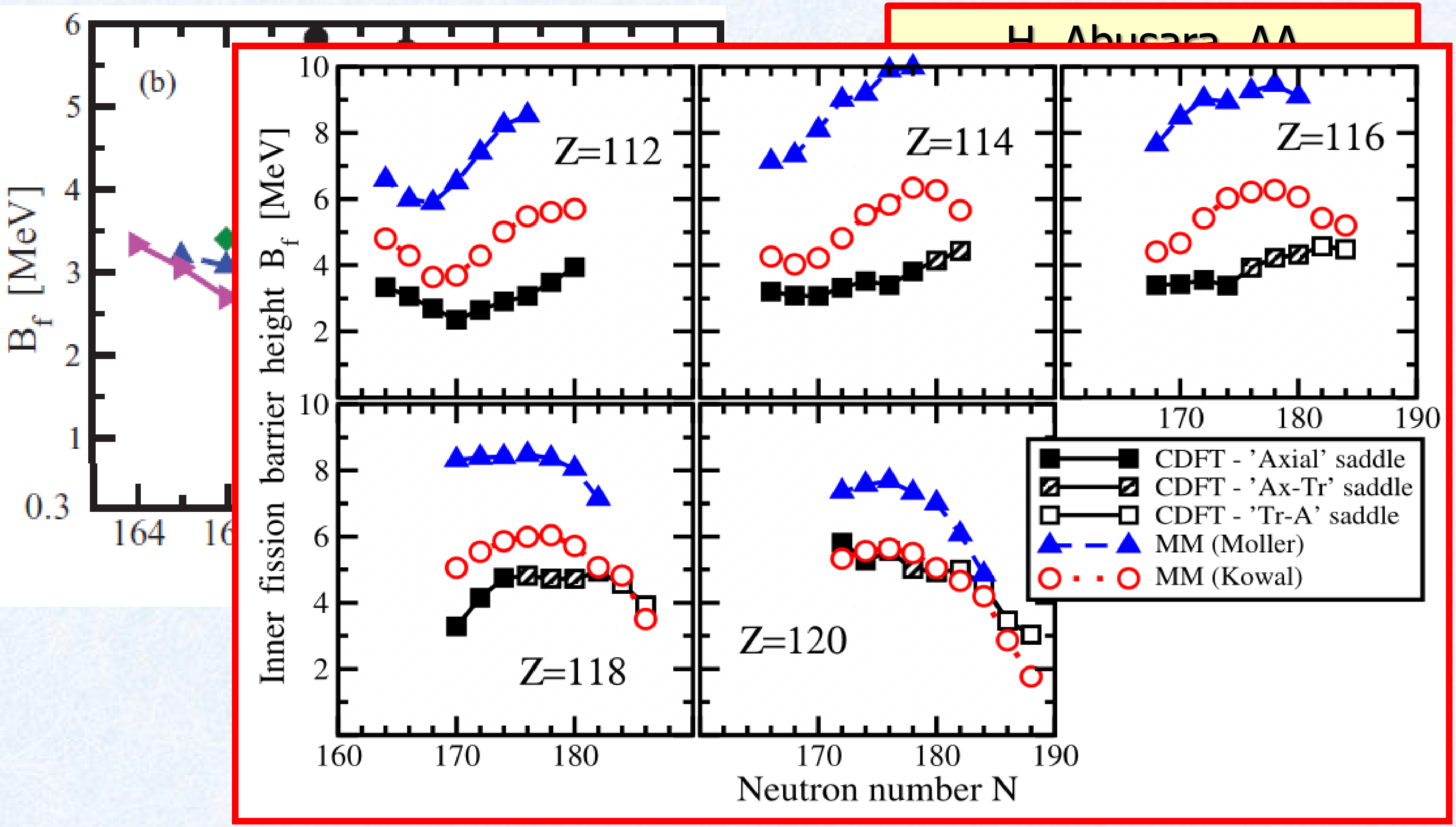

axial
triaxial
octupole
Z=120
Z=118
Z=116
Z=114
Z=112
Outer fission barrier heights B_f [MeV]
6
4
2
0
170
180
190
Neutron number N

Inner fission barrier heights according to different models



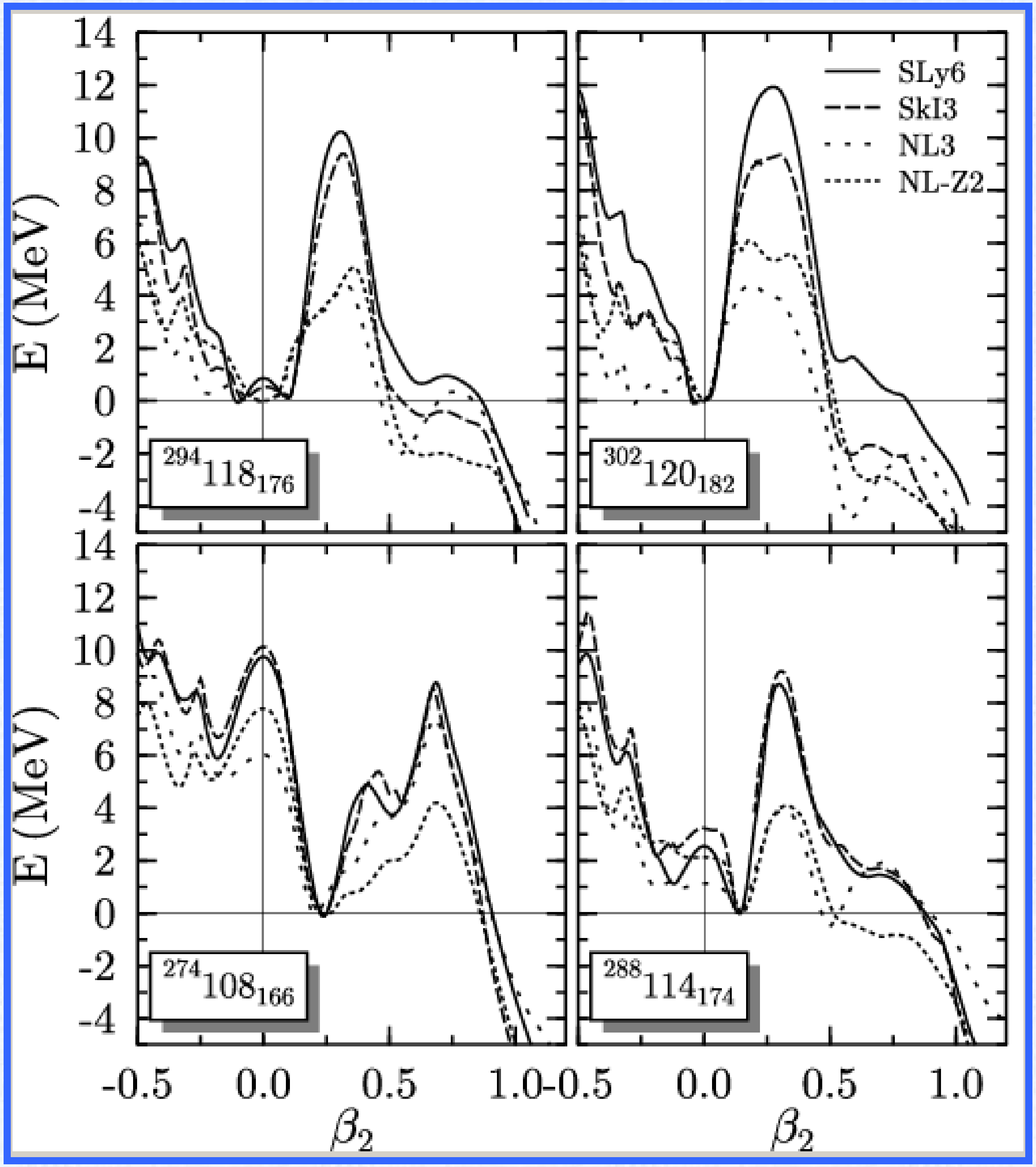
H. Abusara, AA
and P. Ring,
PRC 85, 024314 (2012)

Inner fission barrier heights according to different models



M. Kowal et al, PRC 82, 014303 (2010) - mic=WS potential,
mac=Yukawa+exponential model

P. Moller et al, PRC 79, 064304 (2009) – mic=Folded Yukawa potential
mac =FRDM model.



from Burvenich et al PRC 69, 014307 (2004)

Open questions

Q1. Which criteria to use for the selection of DFT parametrization? Good description of masses? Good description of deformations? Something else?

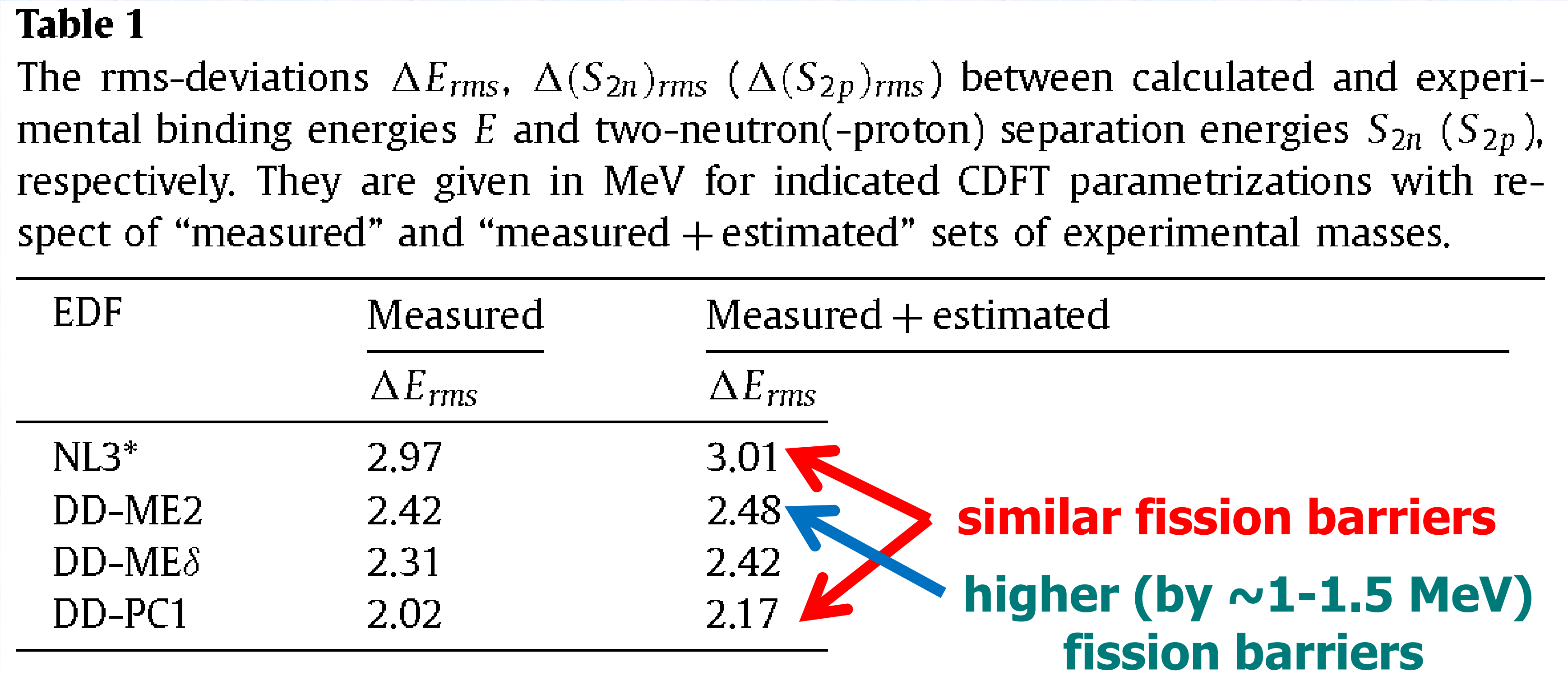


Table 1

The rms-deviations ΔE_{rms}, $\Delta(S_{2n})_{rms}$ ($\Delta(S_{2p})_{rms}$) between calculated and experimental binding energies E and two-neutron(-proton) separation energies S_{2n} (S_{2p}), respectively. They are given in MeV for indicated CDFT parametrizations with respect of "measured" and "measured + estimated" sets of experimental masses.

EDF	Measured	Measured + estimated
	ΔE_{rms}	ΔE_{rms}
NL3*	2.97	3.01
DD-ME2	2.42	2.48
DD-MEδ	2.31	2.42
DD-PC1	2.02	2.17

similar fission barriers

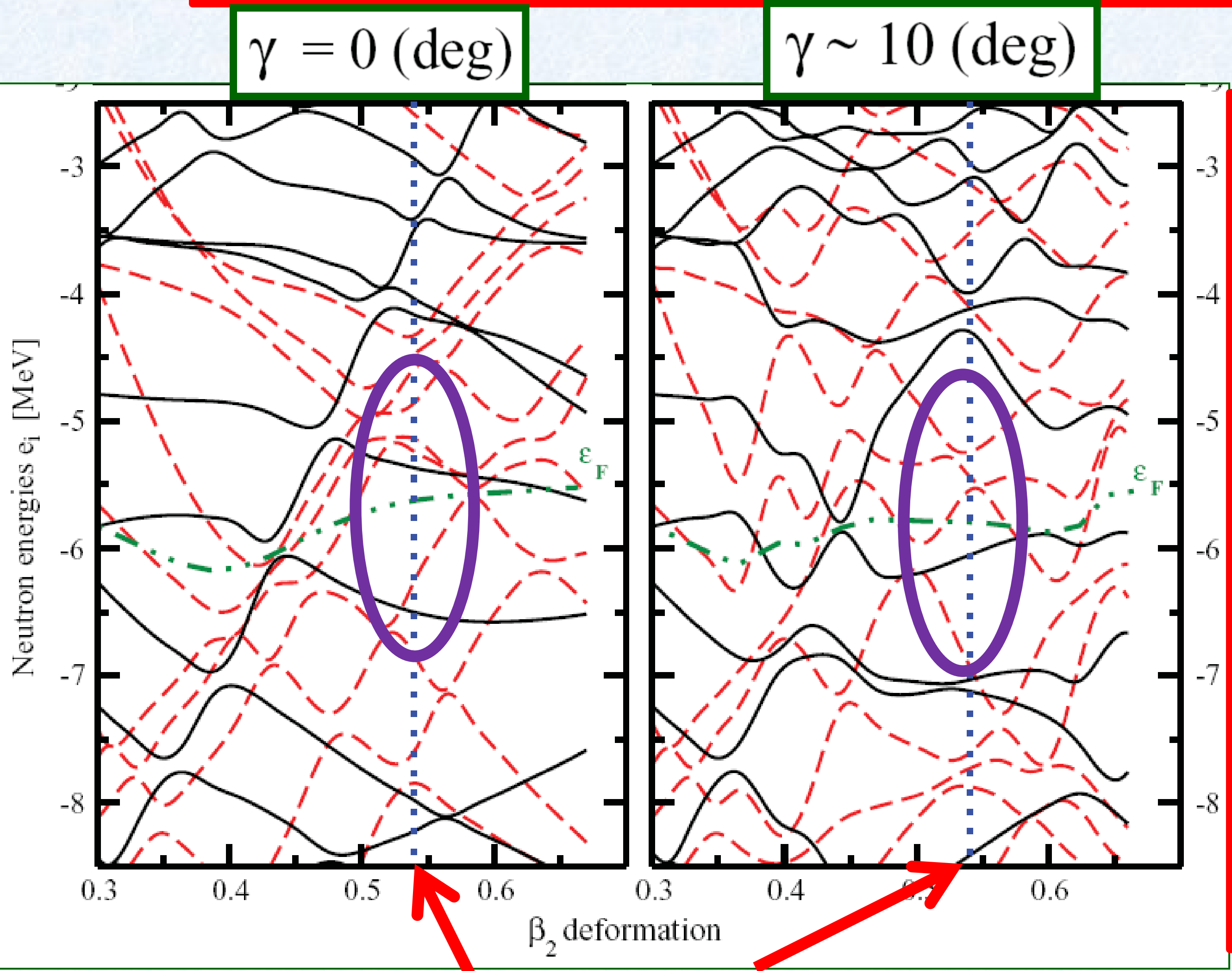
higher (by ~1-1.5 MeV) fission barriers

CDFT - AA et al, PLB in press

Open questions

Q2: How sensitive is the accuracy of the description of fission barrier heights to the accuracy of the description of single-particle energies and the effective mass of nucleon.

The microscopic origin of the lowering of the barrier due to triaxiality

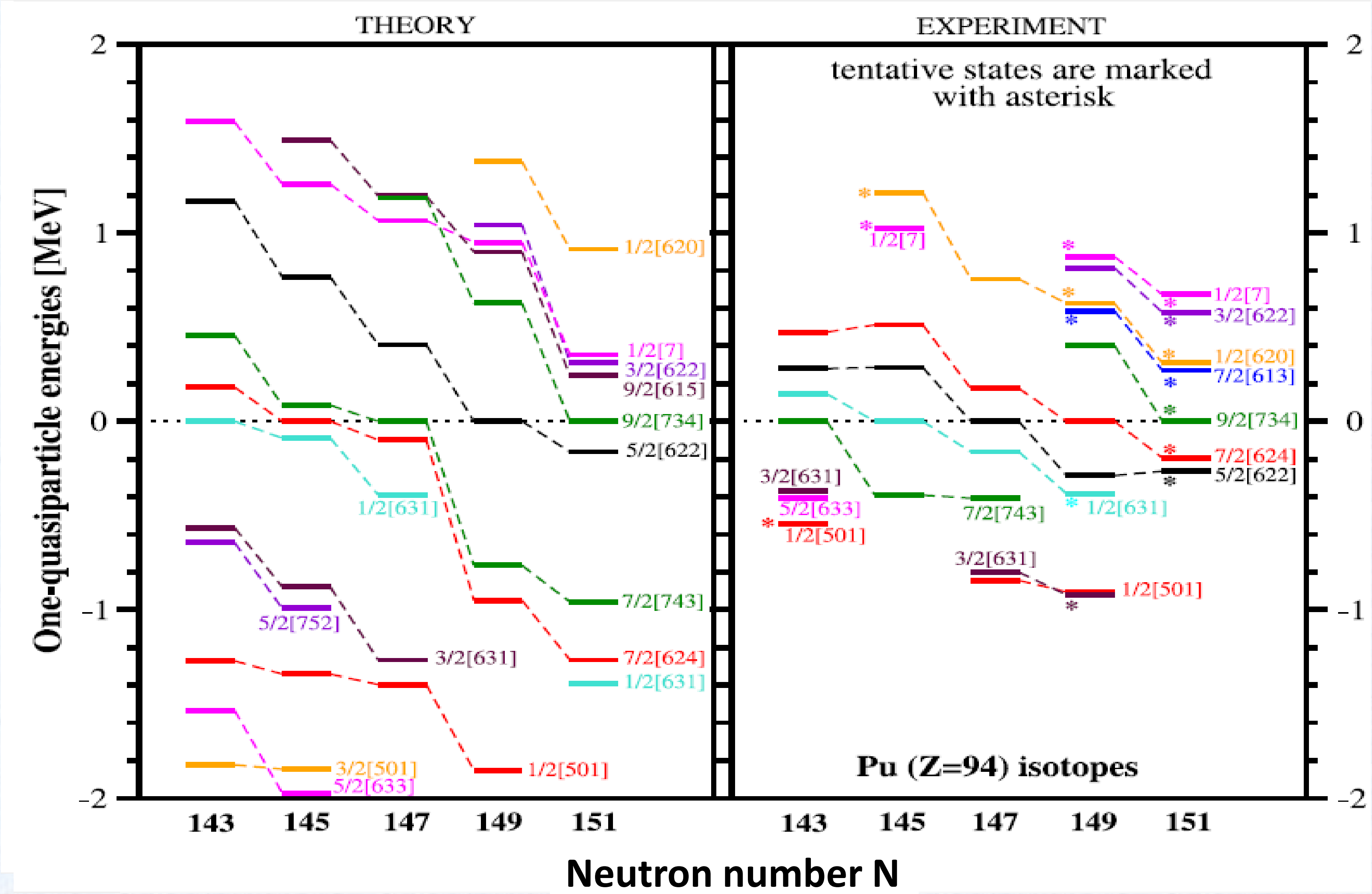


The lowering of the level density at the Fermi surface induced by triaxiality leads to a more negative shell correction energy (as compared with axially symmetric solution), and, as a consequence, to a lower fission barrier.

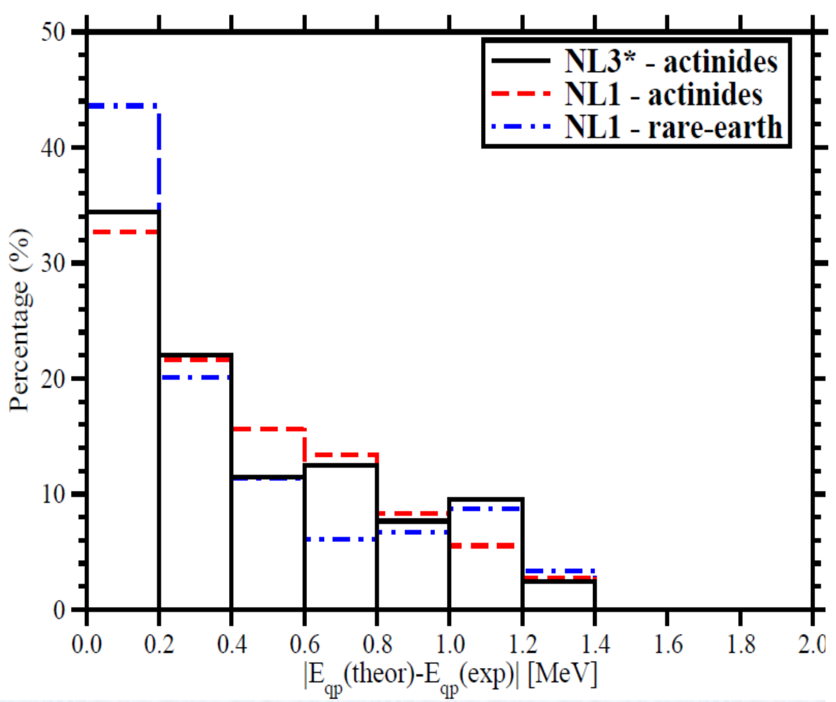
the deformation of the saddle point obtained in the axially symmetric solution.

Systematics of one-quasiparticle states in actinides: the CRHB study

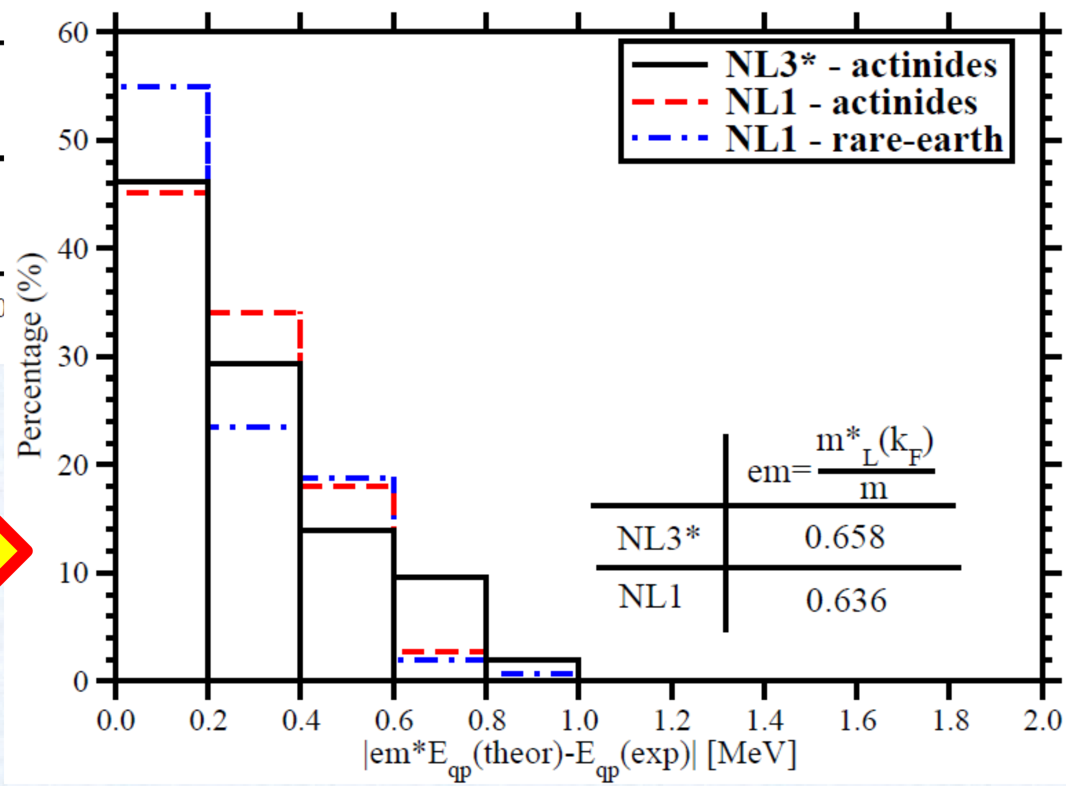
Triaxial CRHB; fully self-consistent blocking, time-odd mean fields included, Gogny D1S pairing, AA and S.Shawaqfeh, PLB 706 (2011) 177



Accuracy of the description of the energies of deformed one-quasiparticle states in actinides in RHB calculations: **correction for low Lorentz effective mass**



Energy scale is corrected for low effective mass



1. 75-80% of the states are described with an accuracy of phenomenological (Nilsson, Woods-Saxon) models
2. The remaining differences are due to incorrect relative energies of the single-particle states

Open questions

Q3: How sensitive are fission barriers to the selection of pairing force and its strengths

S.Karatzikos, AA, G.Lalazissis, P.Ring, PLB 689, 72 (2010)

2. RHB framework

$$\begin{pmatrix} h_D-\lambda & \Delta \\ -\Delta^* & -h_D^*+\lambda \end{pmatrix}\begin{pmatrix} U \\ V \end{pmatrix}_k = E_k\begin{pmatrix} U \\ V \end{pmatrix}_k$$

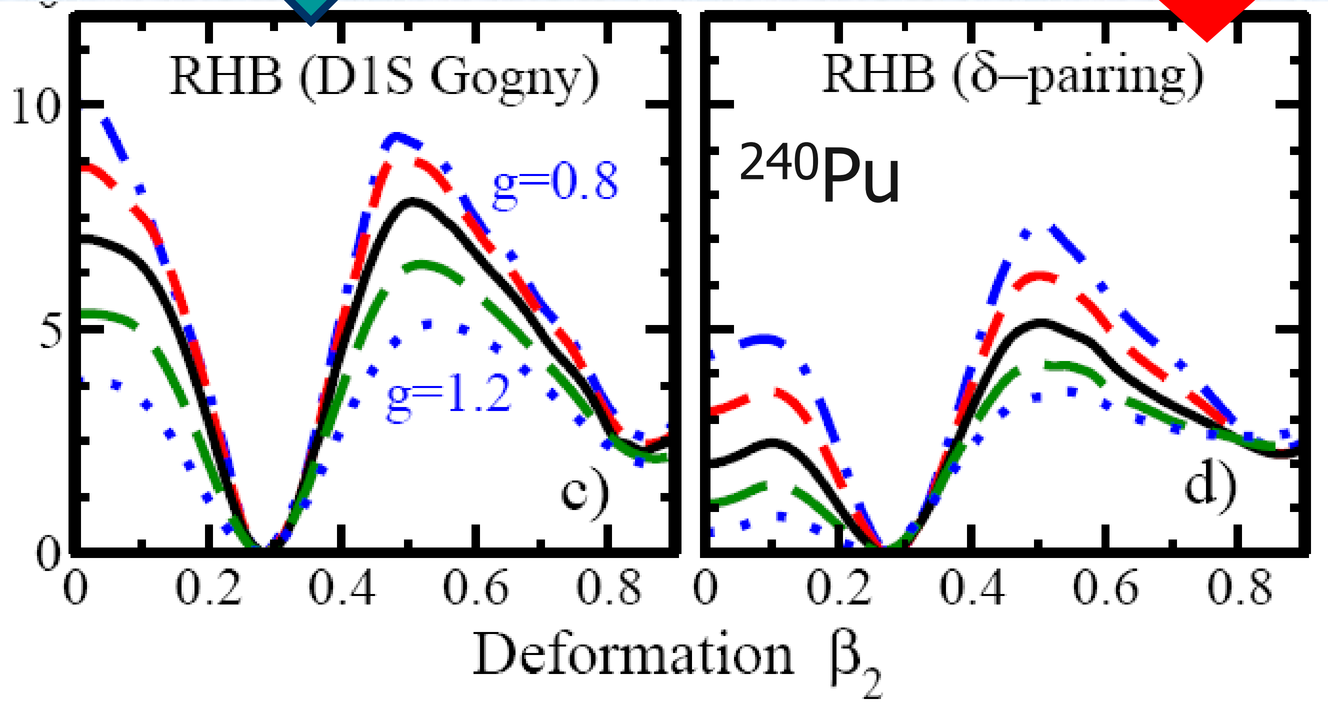
$$\Delta_{12} = \sum_{3<4} V^{\mathrm{pp}}_{1234}\kappa_{34}$$

$$\kappa_{12} = \sum_k V^*_{2k}U_{1k},$$

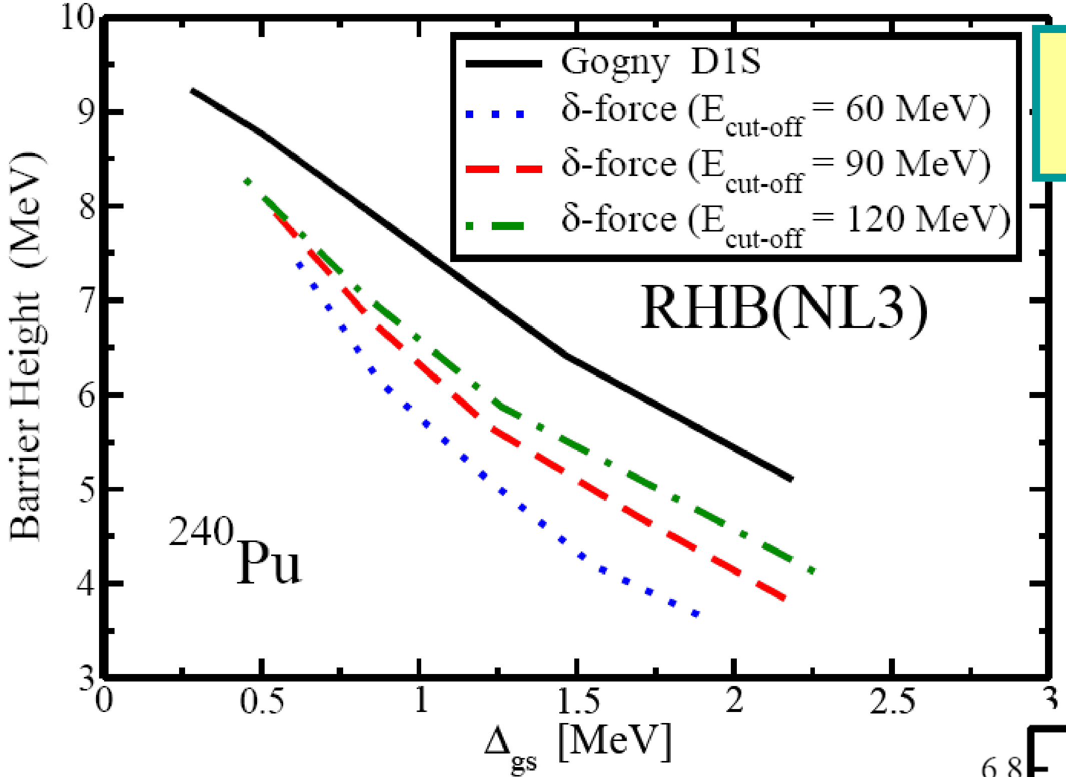
$$E_{\mathrm{pair}} = -\frac{1}{2}\mathrm{Tr}\Delta\kappa.$$

$$V^{\mathrm{pp}}(1,2) = \sum_{i=1,2} e^{-(r/\mu_i)^2}(W_i + B_iP^\sigma - H_iP^\tau - M_iP^\sigma P^\tau)$$

$$V^{\mathrm{pp}}(1,2) = -V_0\delta(\mathbf{r}_1-\mathbf{r}_2)$$



Dependence of the fission barrier height on the cut-off energy $E_{cut\text{-}off}$



Gogny force has finite range, which automatically guarantees a proper cut-off in momentum space

$$\Delta_{gs} = \frac{1}{2}(\langle\Delta\rangle_n + \langle\Delta\rangle_p)$$

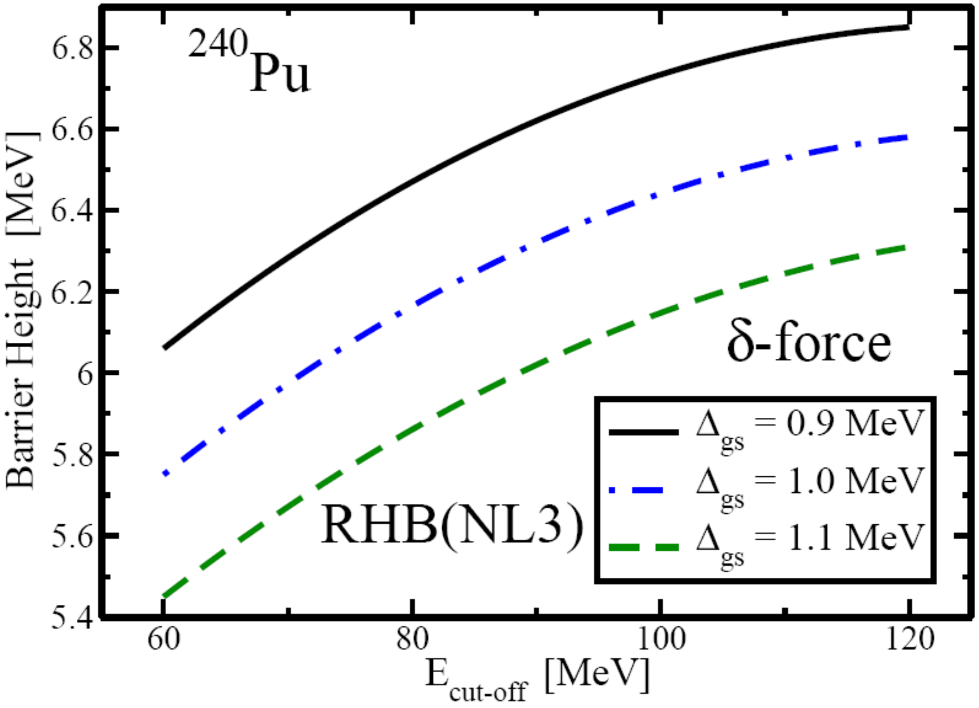
defined in ND-minimum

$\delta - force$

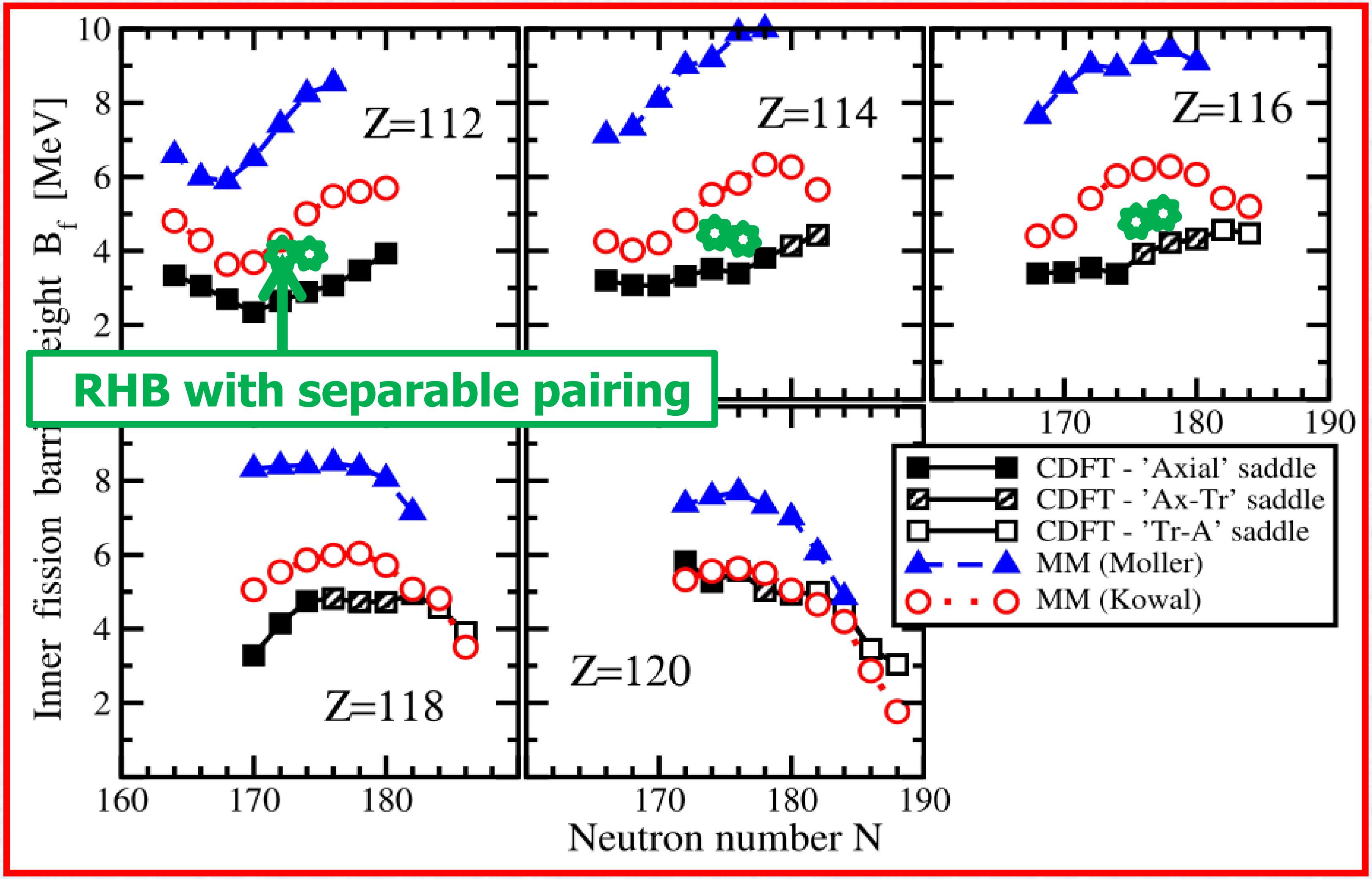
$$\kappa_{12} = \sum_k \underbrace{V_{2k}^* U_{1k}}$$

includes high momenta and leads to a ultra-violet divergence

$E_{cut-off}$ **to avoid divergencies**



Transition from RMF+BCS to RHB with separable pairing (based on Gogny D1S pairing)

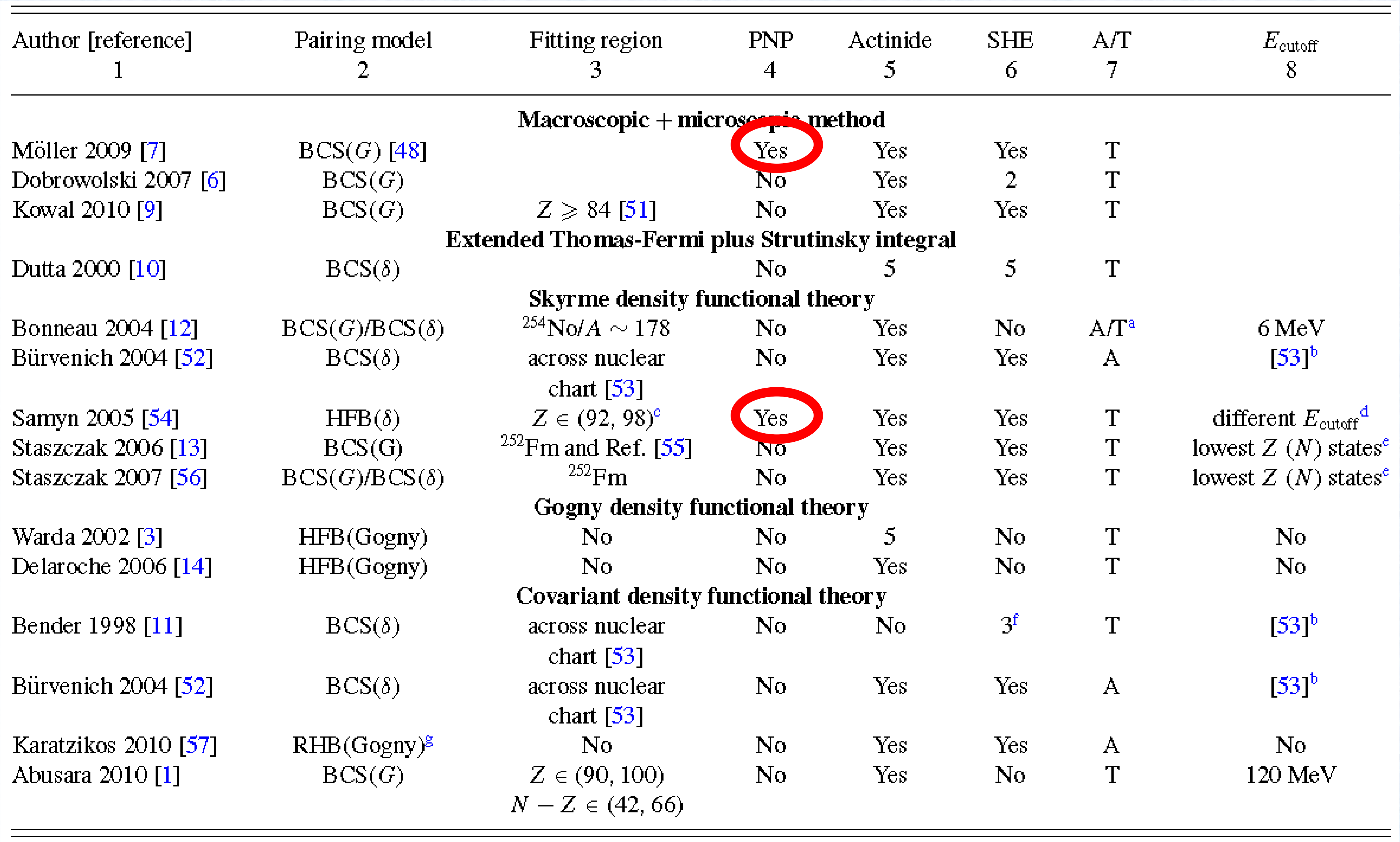


RHB with separable pairing

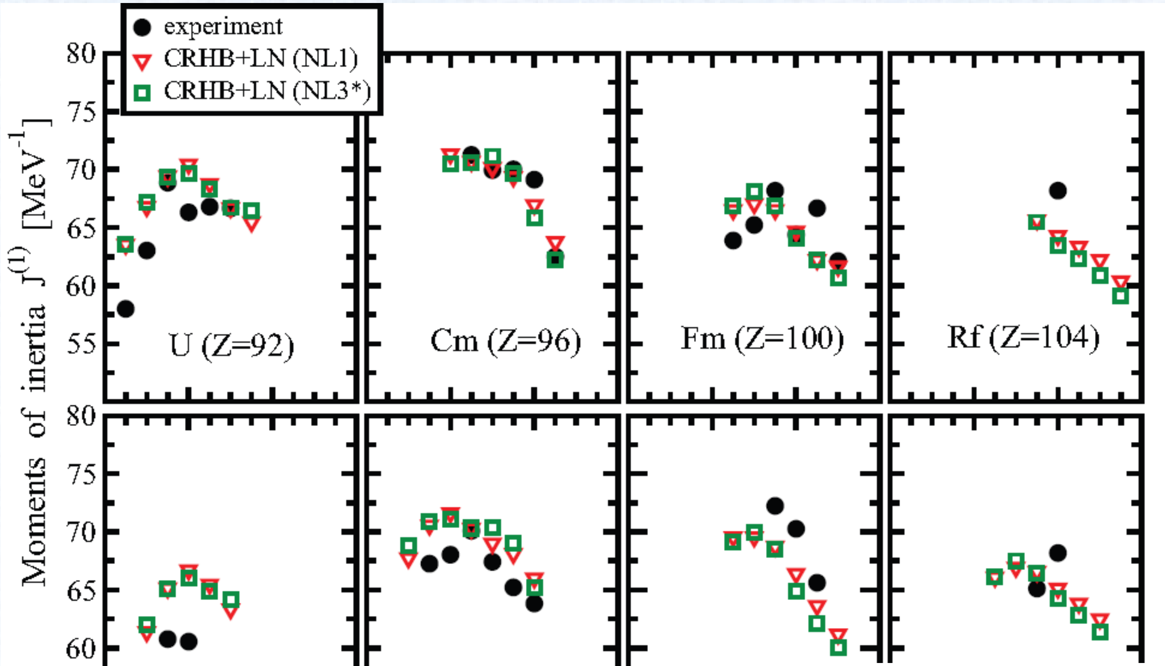
Open questions

Q4. How important is particle number projection for fission barriers?

From H. Abusara, AA and P. Ring, PRC 85, 024314 (2012)



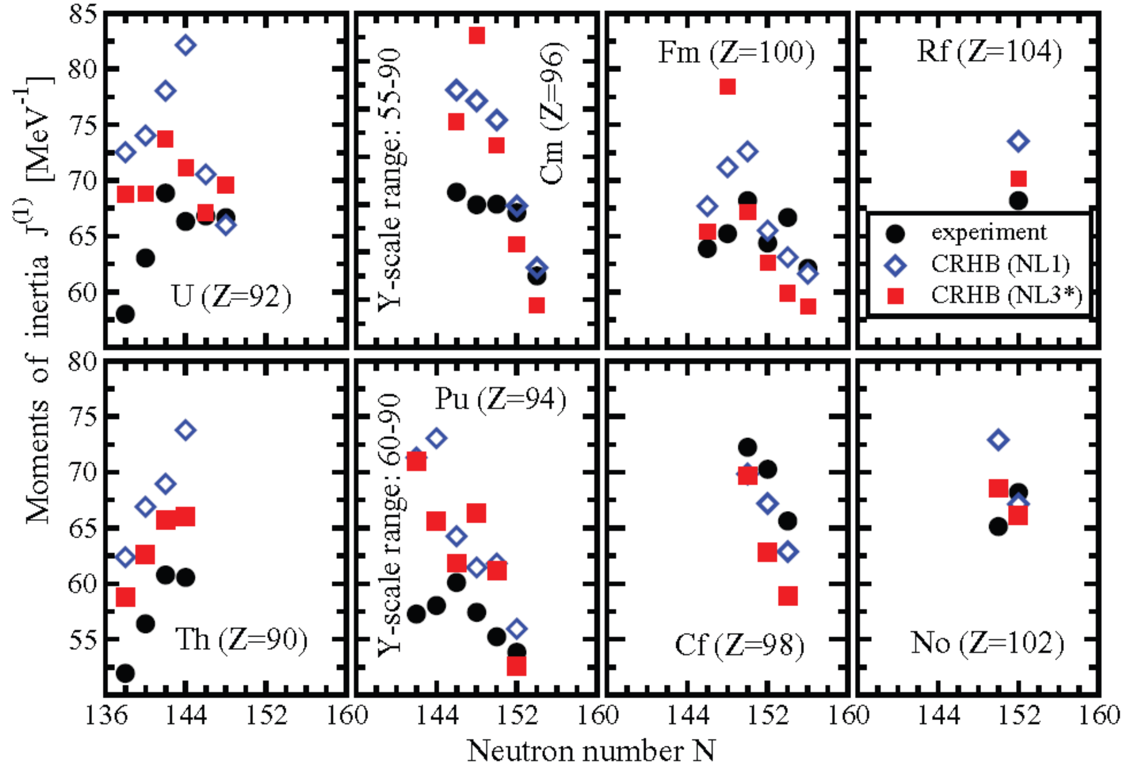
Author [reference] 1	Pairing model 2	Fitting region 3	PNP 4	Actinide 5	SHE 6	A/T 7	E_{cutoff} 8
		Macroscopic + microscopic method					
Möller 2009 [7]	BCS(G) [48]		Yes	Yes	Yes	T	
Dobrowolski 2007 [6]	BCS(G)		No	Yes	2	T	
Kowal 2010 [9]	BCS(G)	$Z \geqslant 84$ [51]	No	Yes	Yes	T	
		Extended Thomas-Fermi plus Strutinsky integral					
Dutta 2000 [10]	BCS(δ)		No	5	5	T	
		Skyrme density functional theory					
Bonneau 2004 [12]	BCS(G)/BCS(δ)	^{254}No/$A \sim 178$	No	Yes	No	A/T[a]	6 MeV
Bürvenich 2004 [52]	BCS(δ)	across nuclear chart [53]	No	Yes	Yes	A	[53][b]
Samyn 2005 [54]	HFB(δ)	$Z \in (92, 98)$[c]	Yes	Yes	Yes	T	different E_{cutoff}[d]
Staszczak 2006 [13]	BCS(G)	^{252}Fm and Ref. [55]	No	Yes	Yes	T	lowest Z (N) states[e]
Staszczak 2007 [56]	BCS(G)/BCS(δ)	^{252}Fm	No	Yes	Yes	T	lowest Z (N) states[e]
		Gogny density functional theory					
Warda 2002 [3]	HFB(Gogny)	No	No	5	No	T	No
Delaroche 2006 [14]	HFB(Gogny)	No	No	Yes	No	T	No
		Covariant density functional theory					
Bender 1998 [11]	BCS(δ)	across nuclear chart [53]	No	No	3[f]	T	[53][b]
Bürvenich 2004 [52]	BCS(δ)	across nuclear chart [53]	No	Yes	Yes	A	[53][b]
Karatzikos 2010 [57]	RHB(Gogny)[g]	No	No	Yes	Yes	A	No
Abusara 2010 [1]	BCS(G)	$Z \in (90, 100)$ $N - Z \in (42, 66)$	No	Yes	No	T	120 MeV

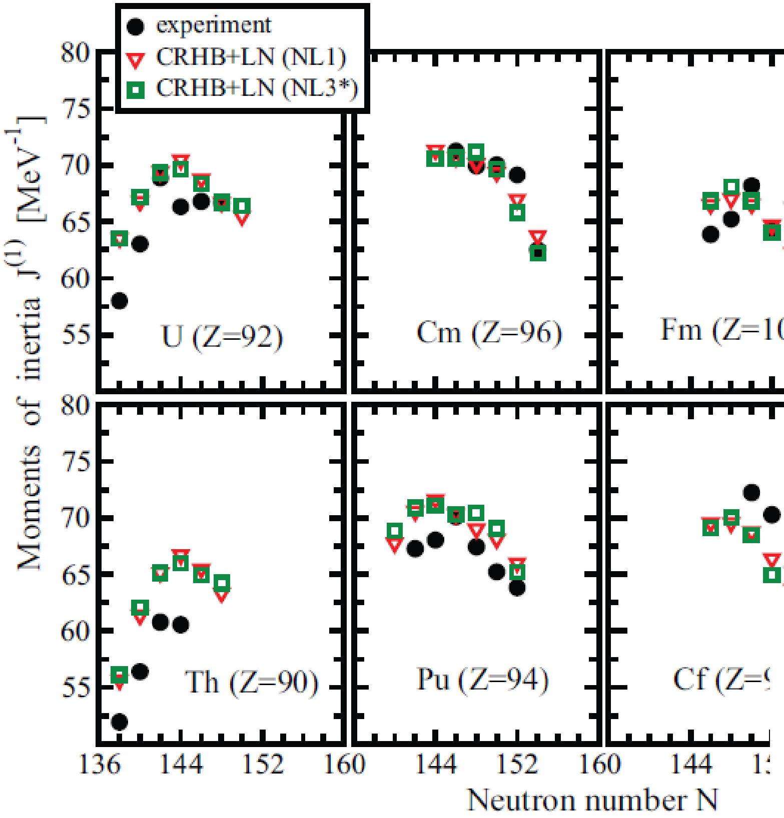


Scaling factor
f=0.915 for NL1
and f= 0.899 for NL3*
In CRHB+LN calculations.

AA and O.Abdurazakov,
PRC 88,014320 (2013).

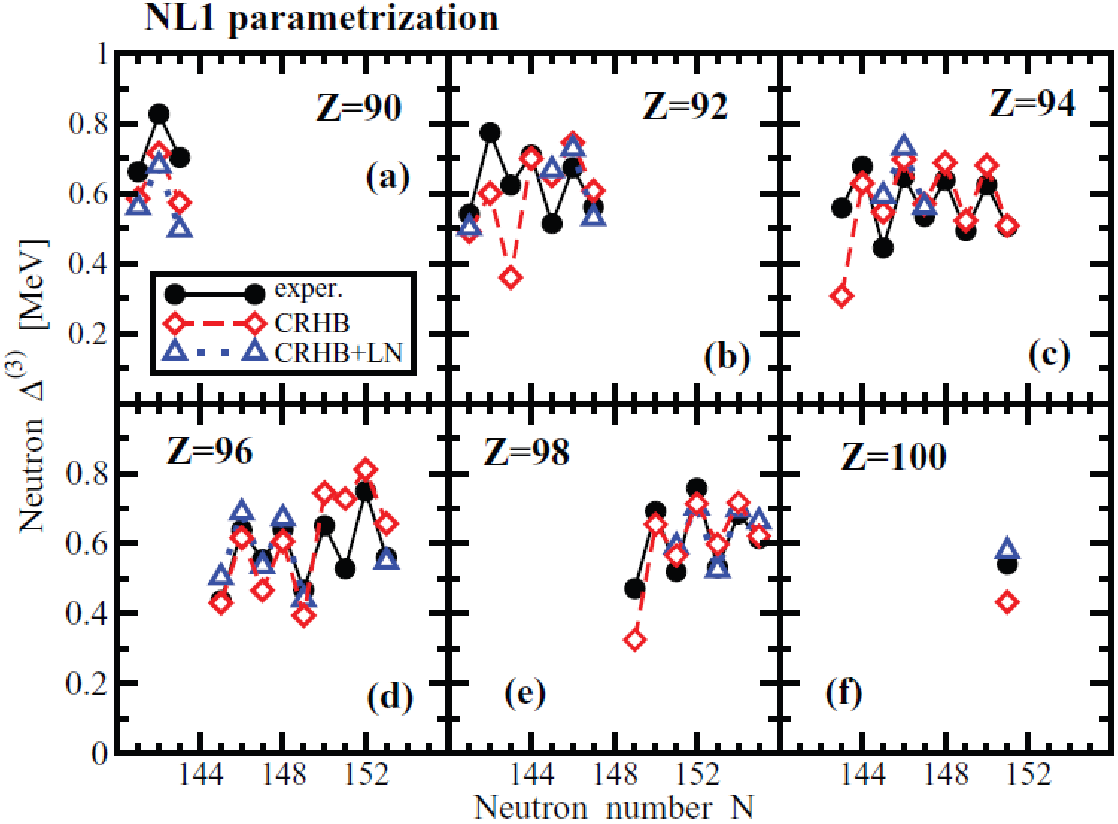
If Lipkin-Nogami (LN) method is neglected then scaling factor f=1.00 is used in the CRHB calculations.



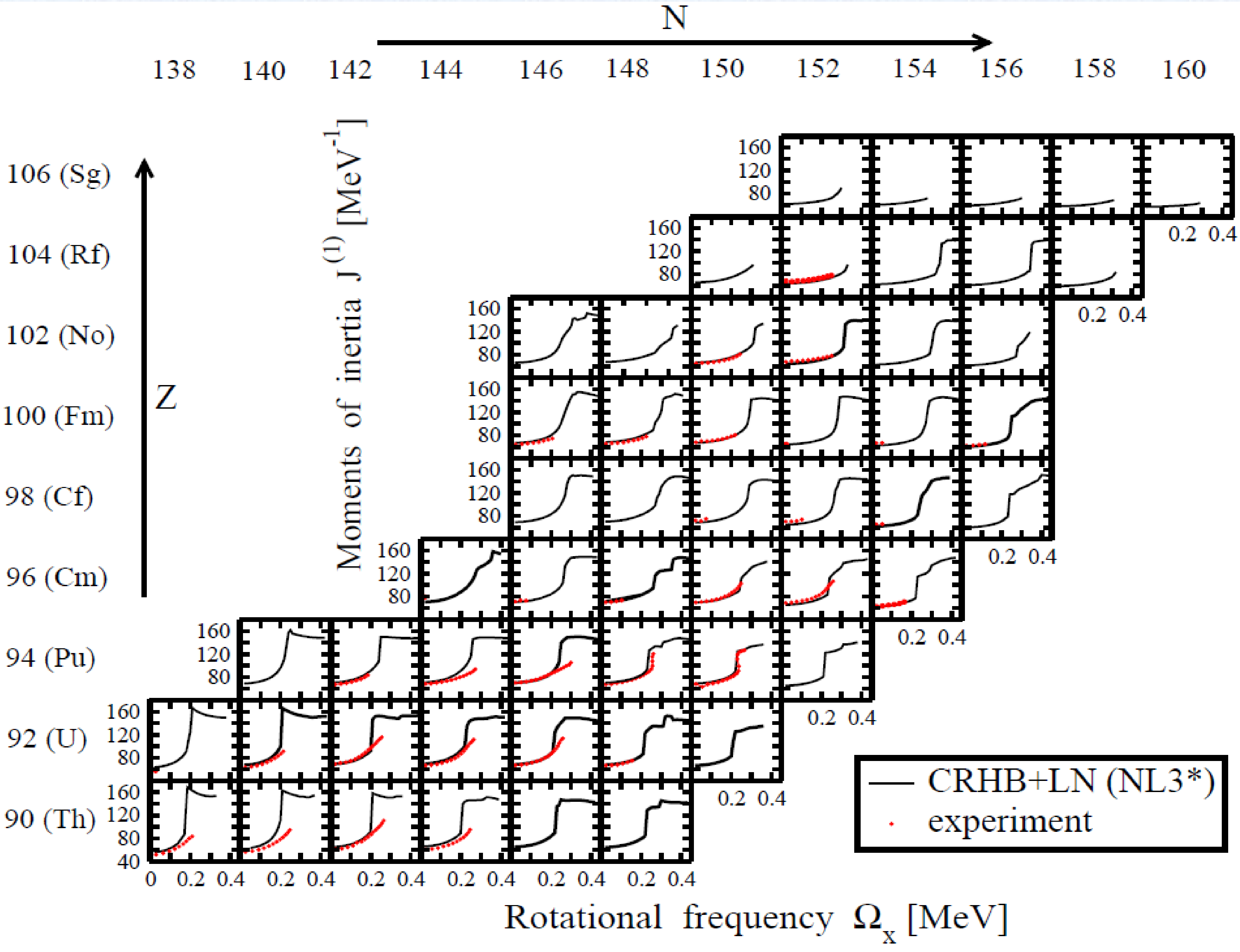


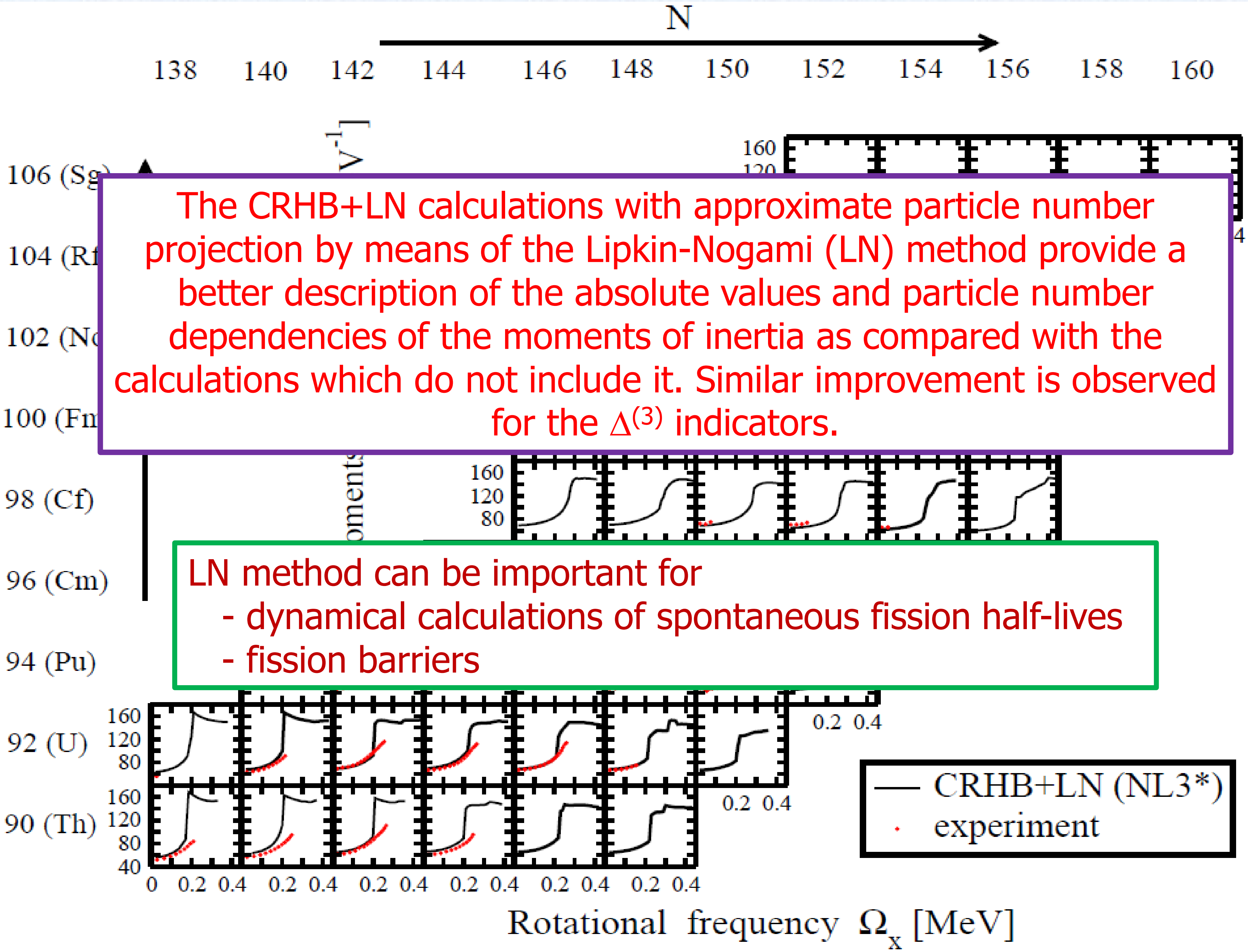
The strength of pairing defined by means of the moments of inertia and three-point $\Delta^{(3)}$ indicators strongly correlate

$$\Delta_{\nu}^{(3)}(N) = \frac{\pi_N}{2}\left[B(N-1) + B(N+1) - 2B(N)\right]$$



If Lipkin-Nogami (LN) method is neglected then scaling factor f=1.00 is used in the CRHB calculations.


N
138
140
142
144
146
148
150
152
154
156
158
160
Z
106 (Sg)
104 (Rf)
102 (No)
100 (Fm)
98 (Cf)
96 (Cm)
94 (Pu)
92 (U)
90 (Th)
Moments of inertia J$^{(1)}$ [MeV^{-1}]
40
80
120
160
0
0.2
0.4
Rotational frequency Ω_x [MeV]
CRHB+LN (NL3*)
experiment



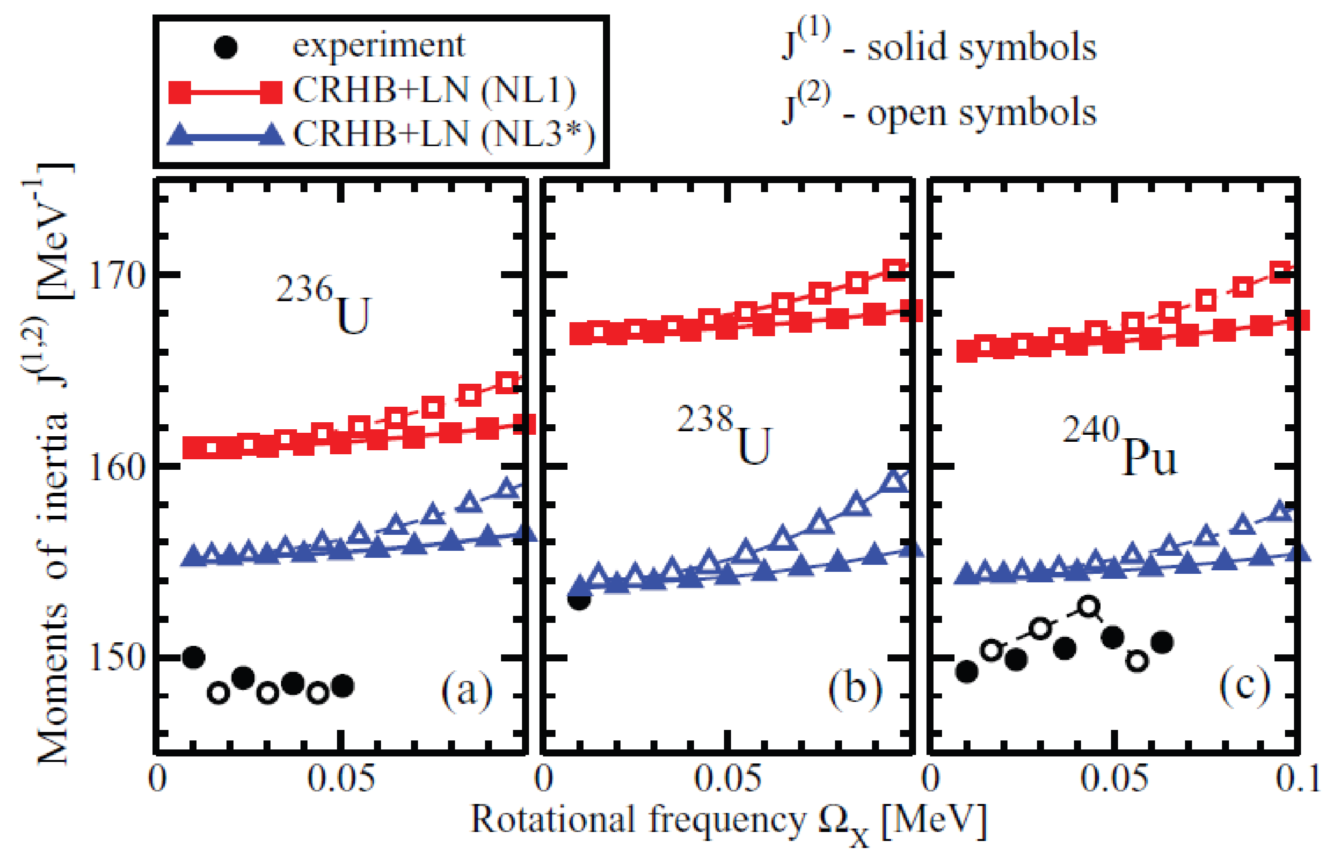
The CRHB+LN calculations with approximate particle number projection by means of the Lipkin-Nogami (LN) method provide a better description of the absolute values and particle number dependencies of the moments of inertia as compared with the calculations which do not include it. Similar improvement is observed for the $\Delta^{(3)}$ indicators.

LN method can be important for
- dynamical calculations of spontaneous fission half-lives
- fission barriers

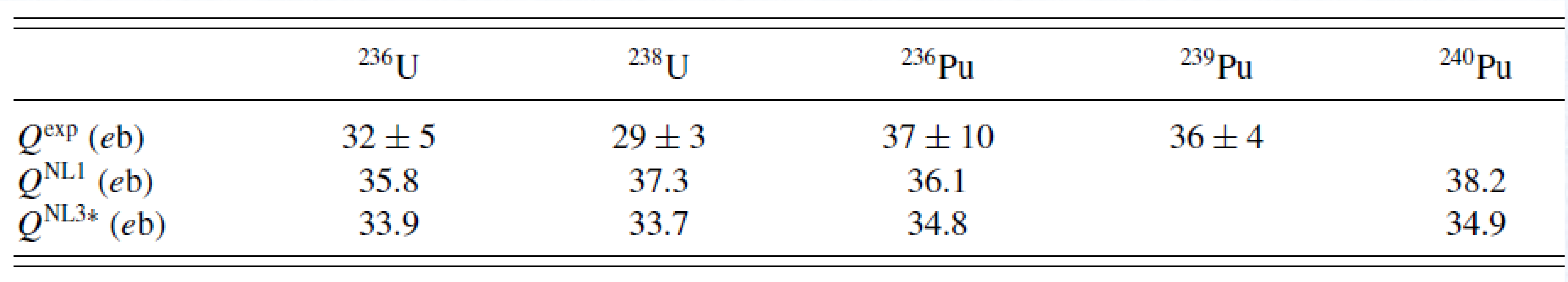
Open questions

Q5: Can we study the variation of pairing with deformation?
Which kind of experimental data to use for that?

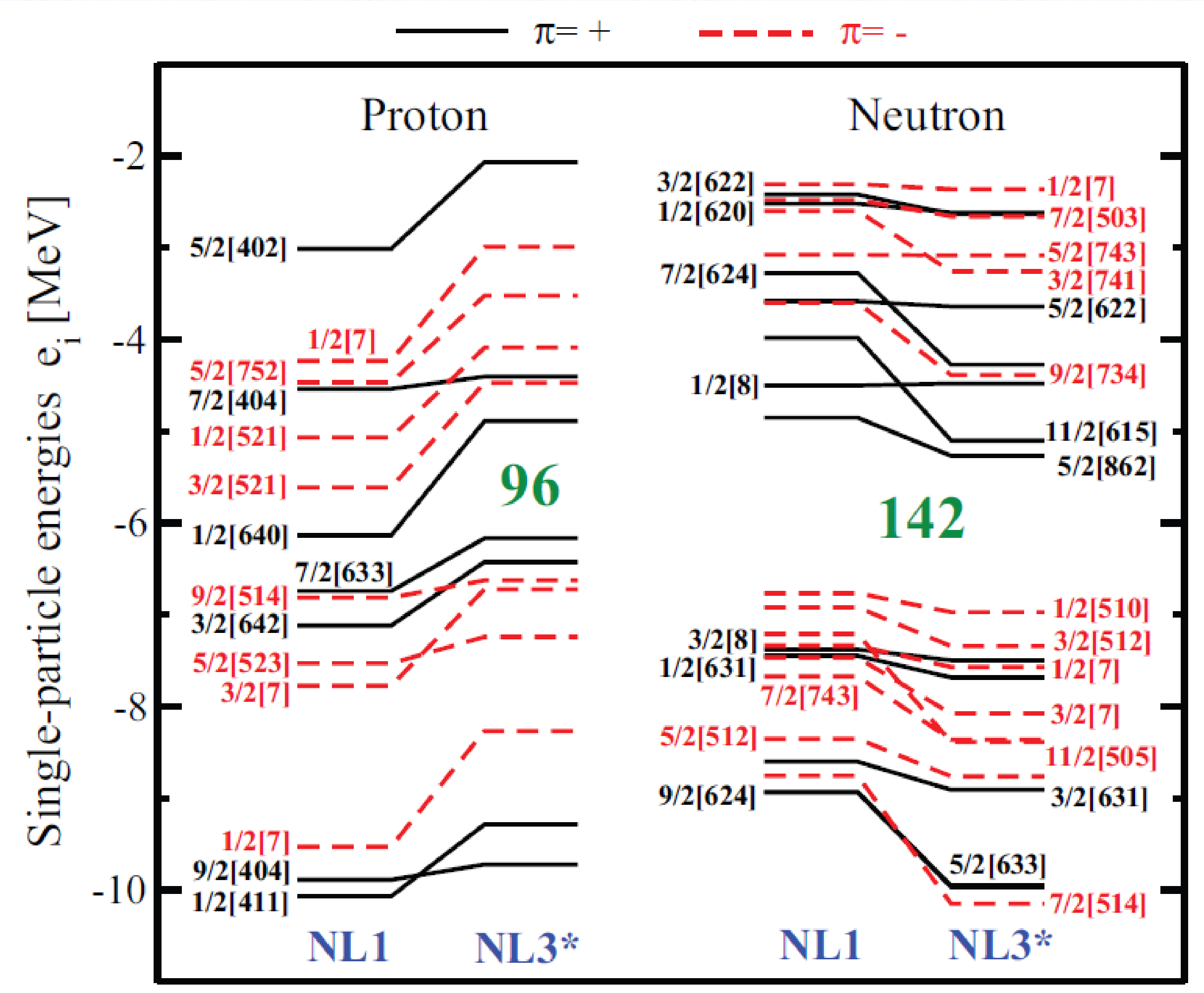
Problem: no experimental information on pairing can be extracted from odd-even mass staggerings for fission isomers (at superdeformation). Such assessment is only possible via moments of inertia.



AA and O.Abdurazakov, PRC 88,014320 (2013).



	^{236}U	^{238}U	^{236}Pu	^{239}Pu	^{240}Pu
Q^{exp} (eb)	32 ± 5	29 ± 3	37 ± 10	36 ± 4	
Q^{NL1} (eb)	35.8	37.3	36.1		38.2
$Q^{\mathrm{NL3*}}$ (eb)	33.9	33.7	34.8		34.9



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Conclusions:

1. Current DFT and mic+mac models provide similar level of the description of fission barrier in actinides.

2. Similarity of the description of fission barriers in actinides does not translate into similarity of predictions for fission barriers in superheavy nuclei. The differences between different classes of the models and the differences within one class of models [dependence on the parametrization] still exists.

3. There are a number of open questions on which we still do not know precise answers.