The uncertainty quantification in covariant density functional theory.

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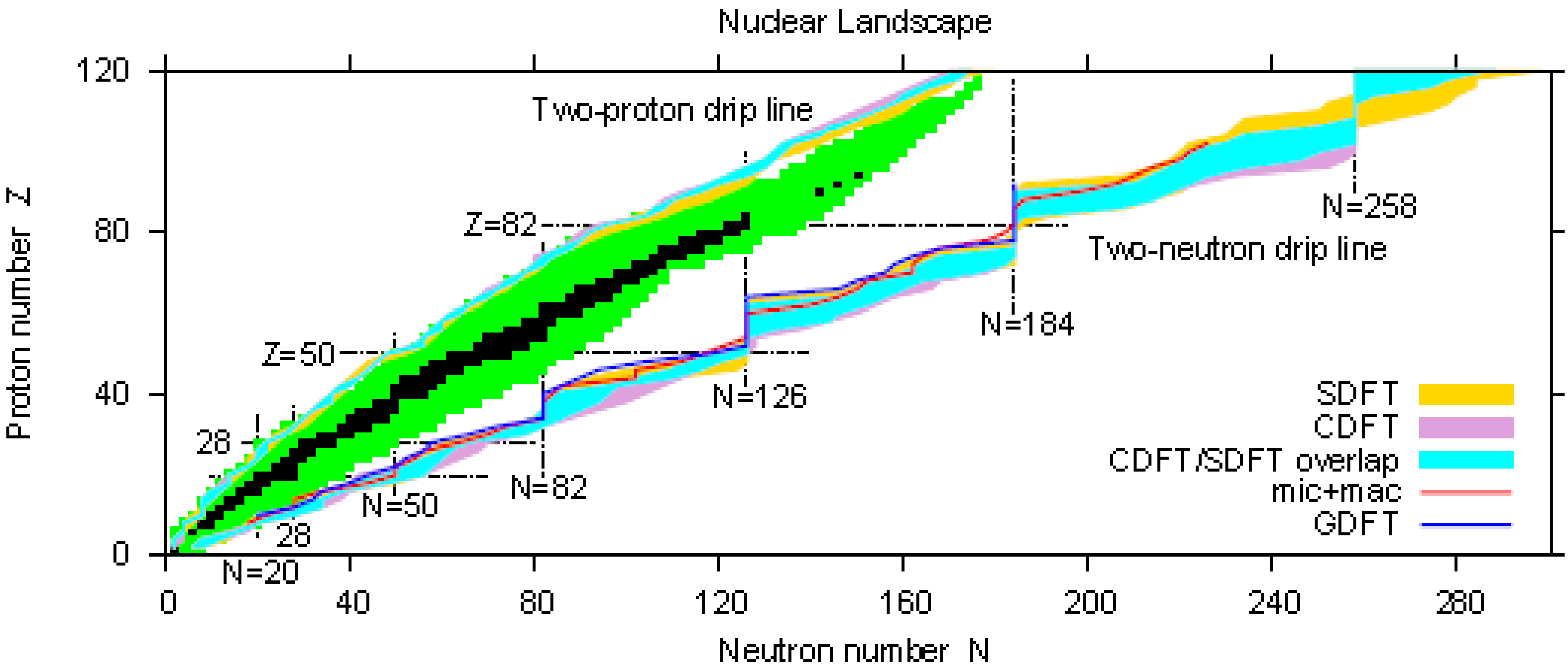
1. **Motivation.**
2. **Basic features of CDFT**
3. **Assessing statistical errors**
4. **Systematic errors/uncertainties and their propagation to unknown regions**
   - **nuclear matter constraints**
   - **neutron-rich nuclei and two-neutron drip line**
   - **superheavy nuclei**
5. **Conclusions**

In collaboration with S.Abgemava, D. Ray (MSU), P. Ring (TU Munich) and T. Nakatsukasa (Tsukuba U)



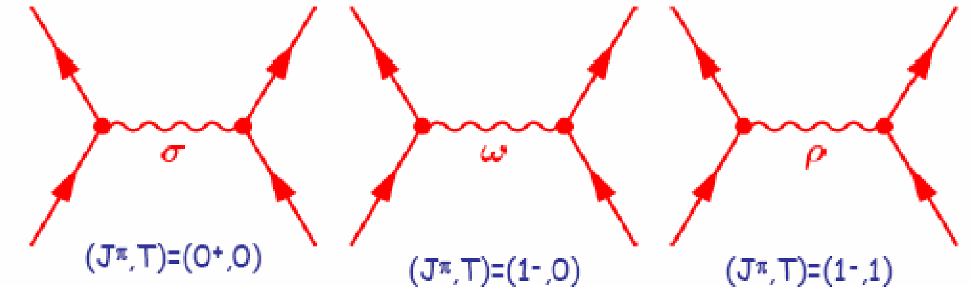
AA, S. Agbemava, D. Ray and P. Ring, PLB 726, 680 (2013)
S. Agbemava, AA, D. Ray and P. Ring, PRC 89, 054320 (2014)
J.Erler et al et al, Nature 486 (2012) 509

How to minimize the uncertainties in theoretical predictions?
Which impact statistical tools could have here?

Basic features of covariant density functional theory

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

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

density matrix $\hat{\rho}$

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

$$\hat{h} = \frac{\delta E}{\delta \hat{\rho}}$$ **Mean field**

$$\hat{h}|\varphi_i\rangle = \varepsilon_i|\varphi_i\rangle$$ **Eigenfunctions**

Dirac equation for fermions

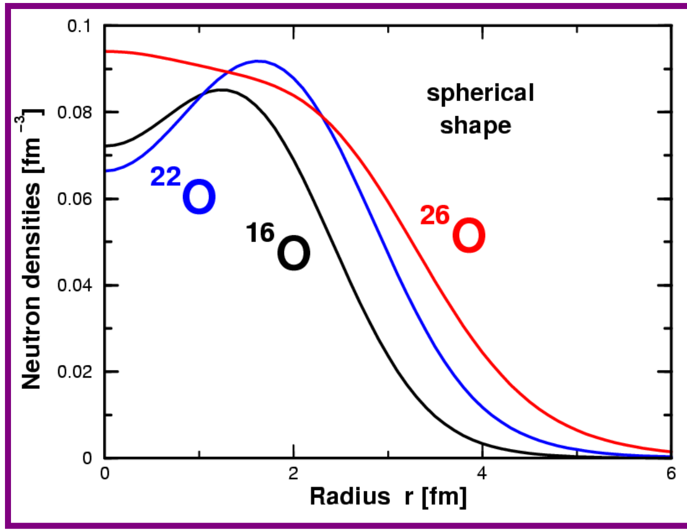
$$\{\vec{\alpha}\vec{p} + V + \beta(m+S)\}\,\Psi_i = \epsilon_i \Psi_i$$

$$\Psi_i = \begin{pmatrix} f_i(r) \\ i g_i(r) \end{pmatrix} = \begin{pmatrix} \text{large} & \text{components} \\ \text{small} & \text{components} \end{pmatrix}$$

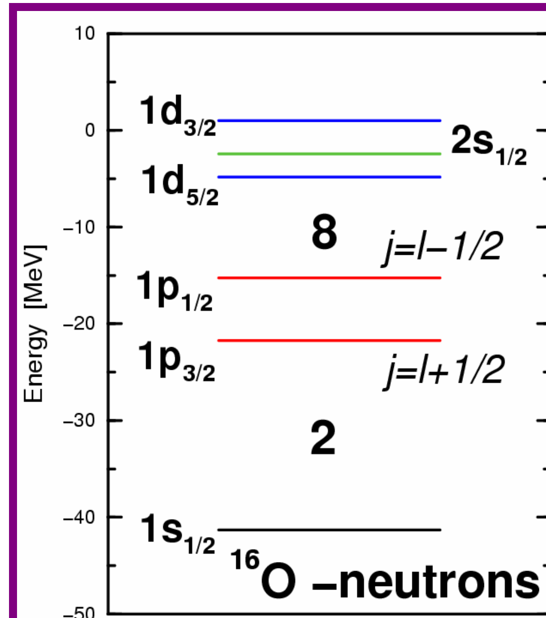
Klein-Gordon equations for bosons

$$\left\{-\Delta + m_\sigma^2\right\}\sigma = -g_\sigma \rho_s - g_2 \sigma^2 - g_3 \sigma^3$$
$$\left\{-\Delta + m_\omega^2\right\}\omega_0 = g_\omega \rho_v$$

Densities

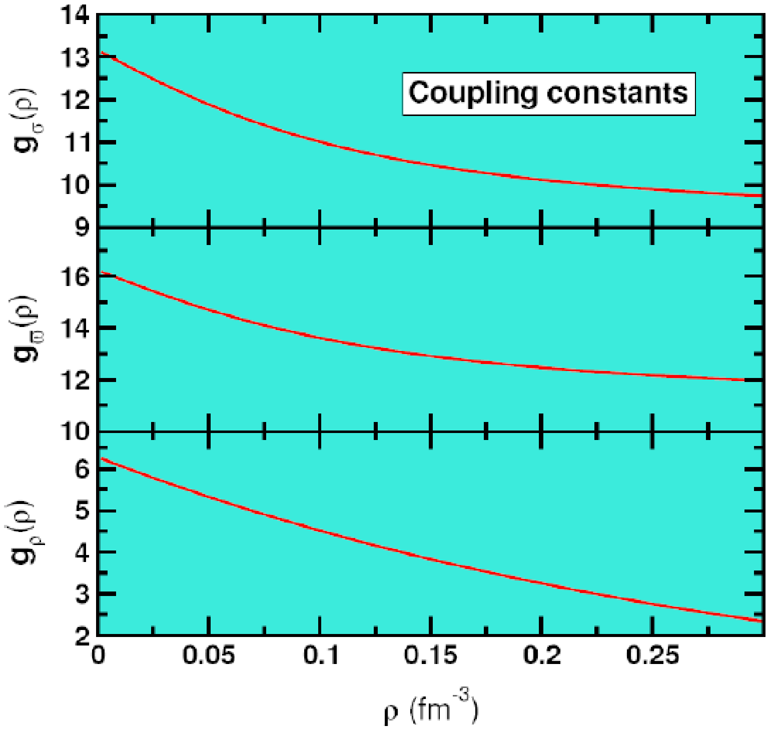


Single-particle energies

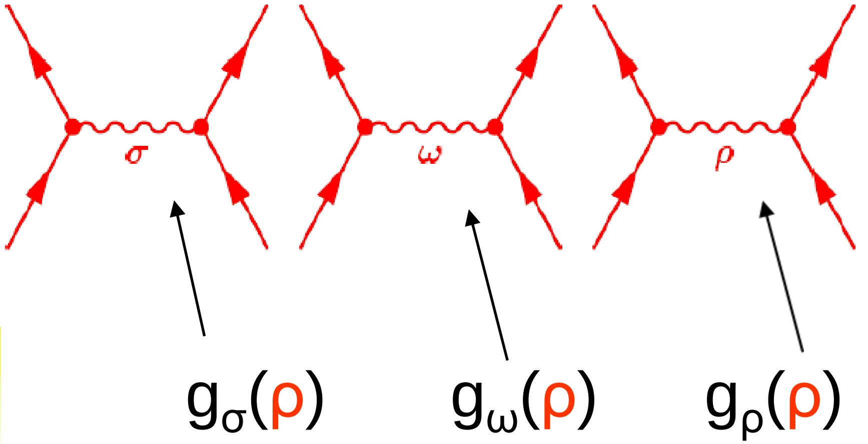


Effective density dependence:

The basic idea comes from ab initio calculations.
Density dependent coupling constants include
Brueckner correlations and three-body forces



Effective interactions with medium-dependent couplings:



Remove mesons → point coupling models with derivative terms

Two major differences between the classes of covariant energy density functionals:

1. **Range of interaction (finite => meson are included)**
   (zero => no meson, point-coupling models)

2. **Effective density dependence**
   - non-linear (through the power of sigma-meson)
   - explicit

Meson-exchange models

$$\mathcal{L} = \bar{\psi}[\gamma(i\partial - g_\omega\omega - g_\rho\vec{\rho}\,\vec{\tau} - eA) - m - g_\sigma\sigma]\psi$$
$$+ \frac{1}{2}(\partial\sigma)^2 - \frac{1}{2}m_\sigma^2\sigma^2 - \frac{1}{4}\Omega_{\mu\nu}\Omega^{\mu\nu} + \frac{1}{2}m_\omega^2\omega^2$$
$$- \frac{1}{4}\vec{R}_{\mu\nu}\vec{R}^{\mu\nu} + \frac{1}{2}m_\rho^2\vec{\rho}^{\,2} - \frac{1}{4}F_{\mu\nu}F^{\mu\nu},$$

Non-linear models

$$U(\sigma) = \frac{1}{2}m_\sigma^2\sigma^2 + \frac{1}{3}g_2\sigma^3 + \frac{1}{4}g_3\sigma^4$$

NL3*

Models with explicit density dependence

no nonlinear terms in the *σ meson*

$$g_i(\rho) = g_i(\rho_{\rm sat})f_i(x) \quad \text{for} \quad i = \sigma, \omega, \rho$$

$$f_i(x) = a_i \frac{1 + b_i(x + d_i)^2}{1 + c_i(x + d_i)^2} \quad \text{for } \sigma \text{ and } \omega$$

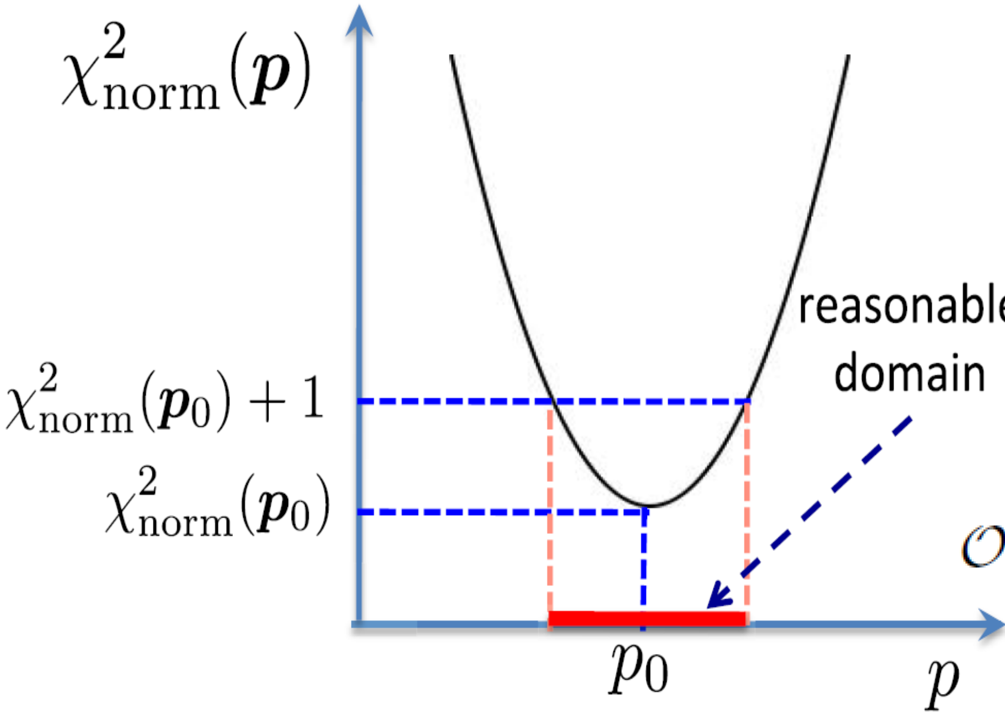
$$f_\rho(x) = \exp[-a_\rho(x - 1)] \quad \text{for } \rho$$

$$x = \rho / \rho_{sat}$$

DD-ME2, DD-MEδ

Assessing statistical errors

Definition of statistical errors



Definition of statistical errors

J. Dobaczewski et al, J. Phys. G, **41** (2014) 074001

$$\chi^2(\boldsymbol{p}) = \sum_{i=1}^{N_d} \frac{\left(\mathcal{O}_i(\boldsymbol{p}) - \mathcal{O}_i^{\rm exp}\right)^2}{\Delta\mathcal{O}_i^2}$$

$\mathcal{O}_i(\boldsymbol{p})$ stands for the calculated values

$\mathcal{O}_i^{\rm exp}$ for experimental data,

$\Delta\mathcal{O}_i$ for adopted errors

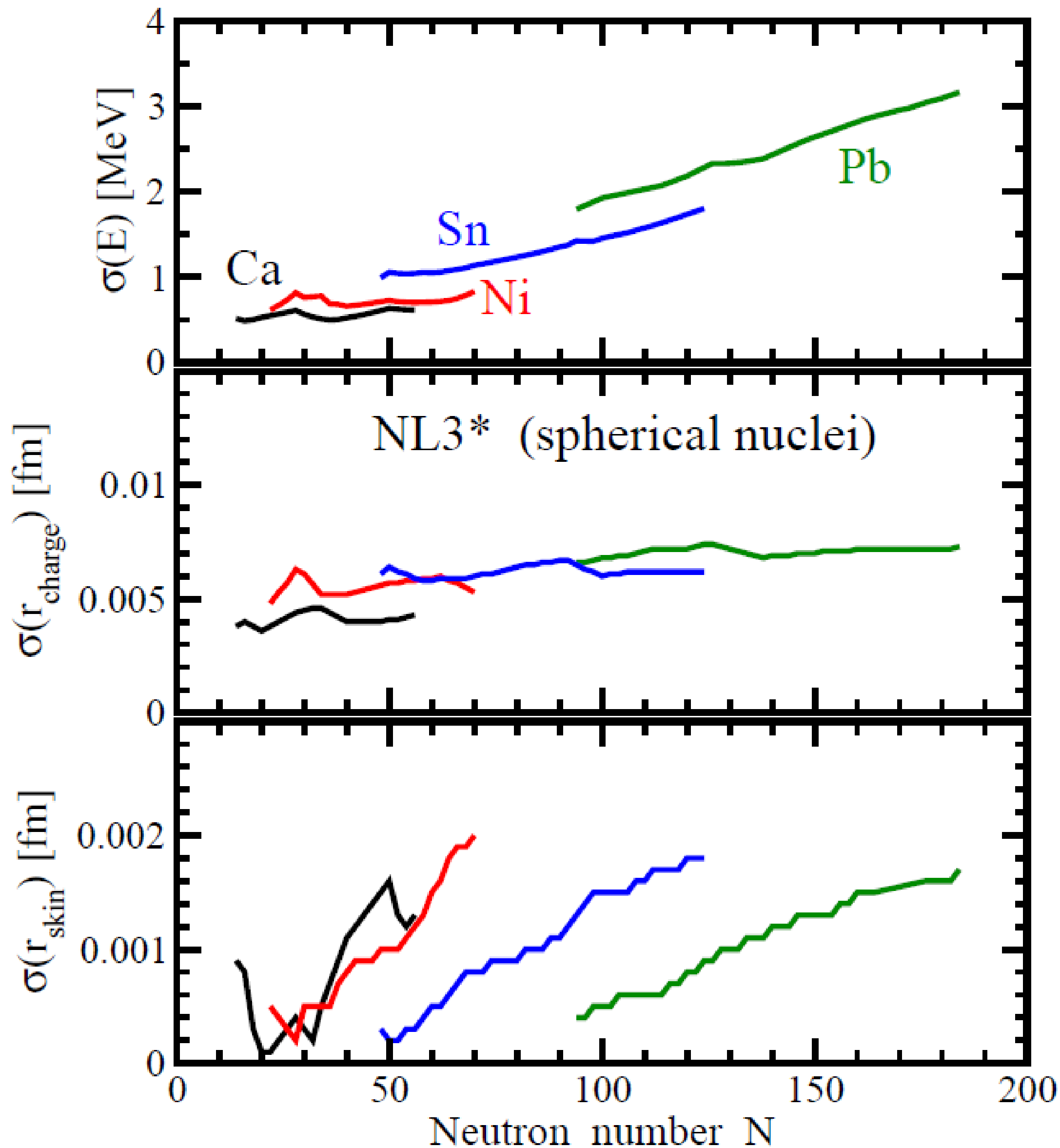
$$\Delta\mathcal{O}_i^2 = \left(\Delta\mathcal{O}_i^{\rm exp}\right)^2 + \left(\Delta\mathcal{O}_i^{\rm num}\right)^2 + \left(\Delta\mathcal{O}_i^{\rm the}\right)^2$$

small — small — subjective

For p_i in a "reasonable domain"

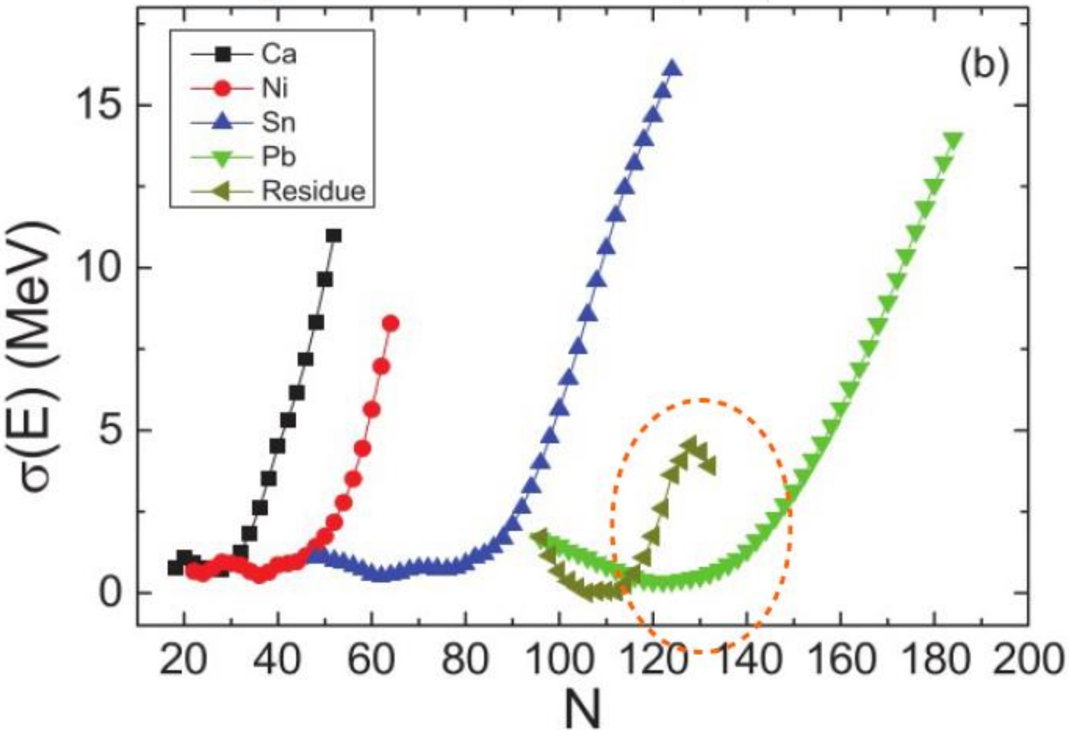
$$\sigma = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(O(p_i) - O(p_0)\right)^2}$$

Statistical errors in the masses, charge radii and neutron skins



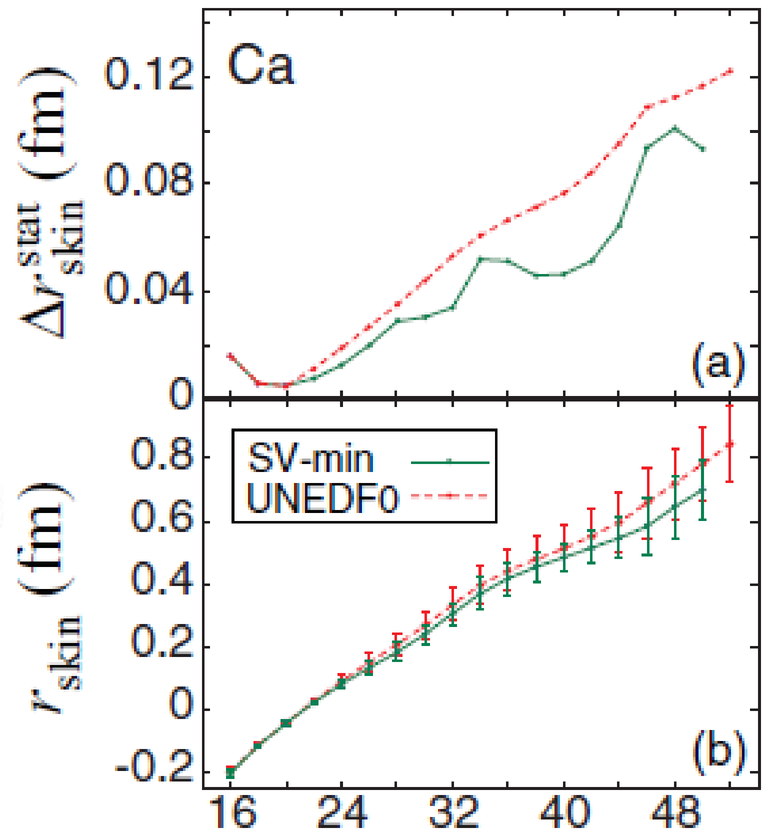
For comparison - statistical errors in Skyrme DFT

Y. Gao, J. Dobaczewski, M. K., J. Toivanen, D. Tarpanov, PRC87, 034324 (2013)



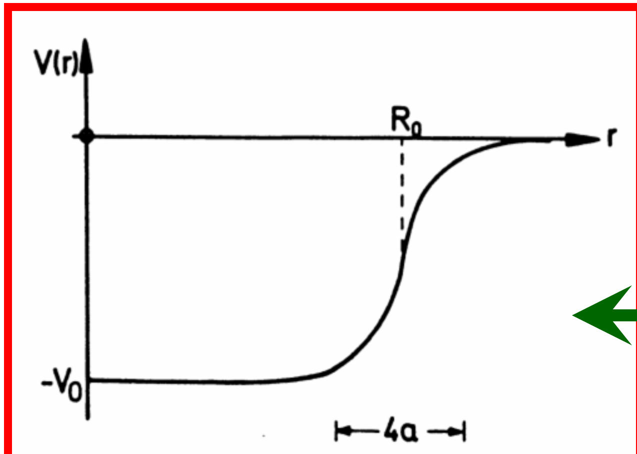
Nucleus	$\Delta r_{\text{skin}}^{\text{stat}}$	
	UNEDF0	SV-min
^{208}Pb	0.058	0.037
^{48}Ca	0.035	0.026

M. Kortelainen et al, PRC 88, 031305(R) (2013)

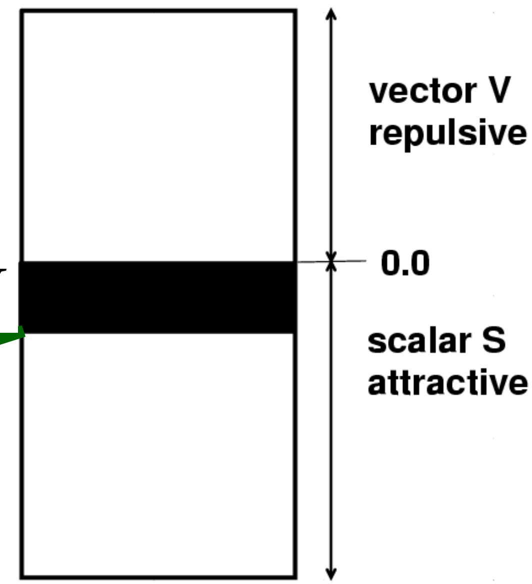


$$V(\mathbf{r}) = g_{\omega}\omega(\mathbf{r})$$

U – nucleonic potential



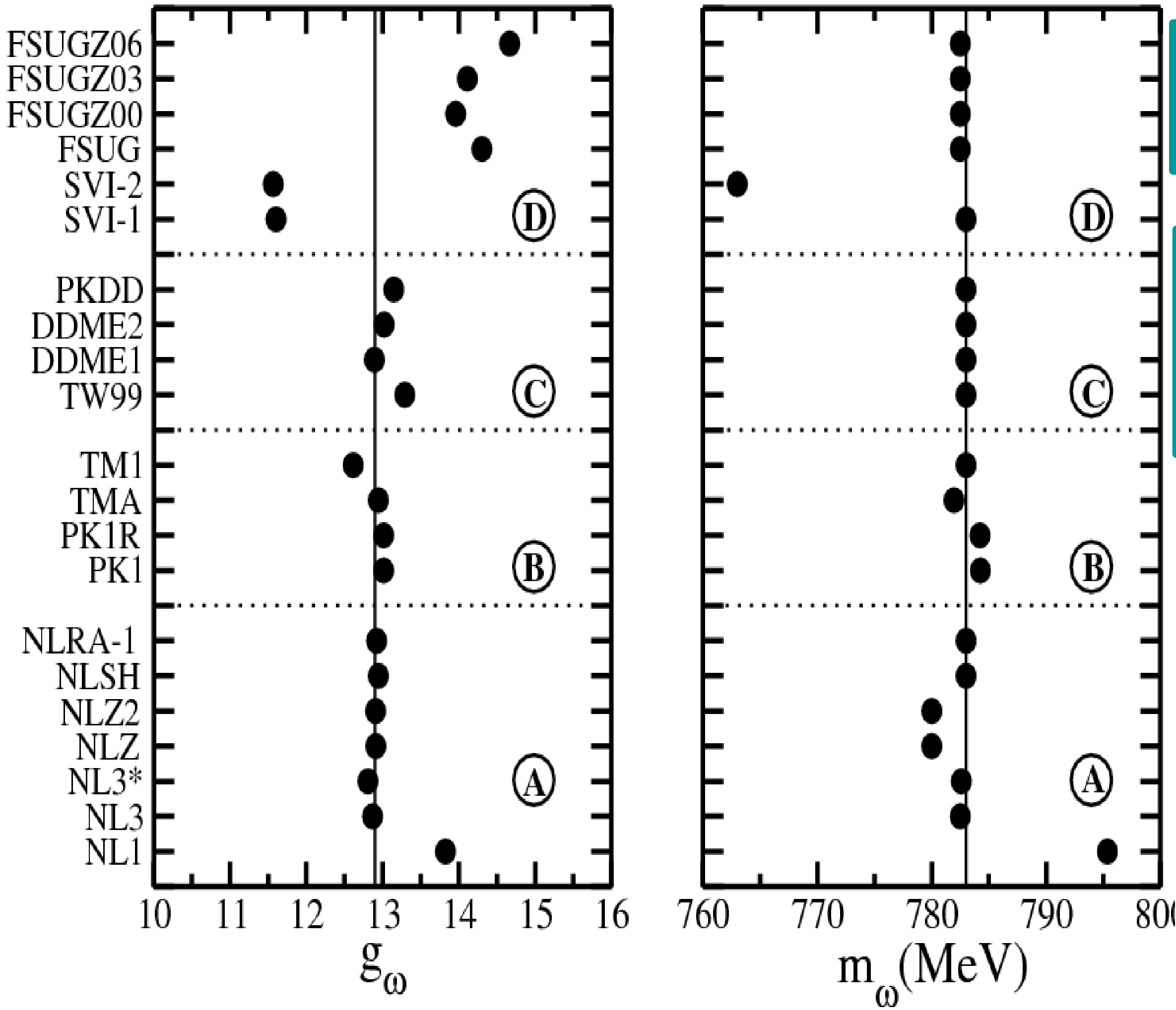
$$U = S + V$$



V ~ 350 MeV/nucleon
S ~ - 400 MeV/nucleon
U ~ - 50 MeV/nucleon

$$S(\mathbf{r}) = g_{\sigma}\sigma(\mathbf{r})$$

Localization of the parameters in the parameter space



include isoscalar-isovector couplings

Density dependence for meson-nucleon couplings for σ-, ω- (ρ-) mesons

Non-linear self-coupling for σ-, ω- (ρ-) mesons

Non-linear self-coupling only for σ-meson

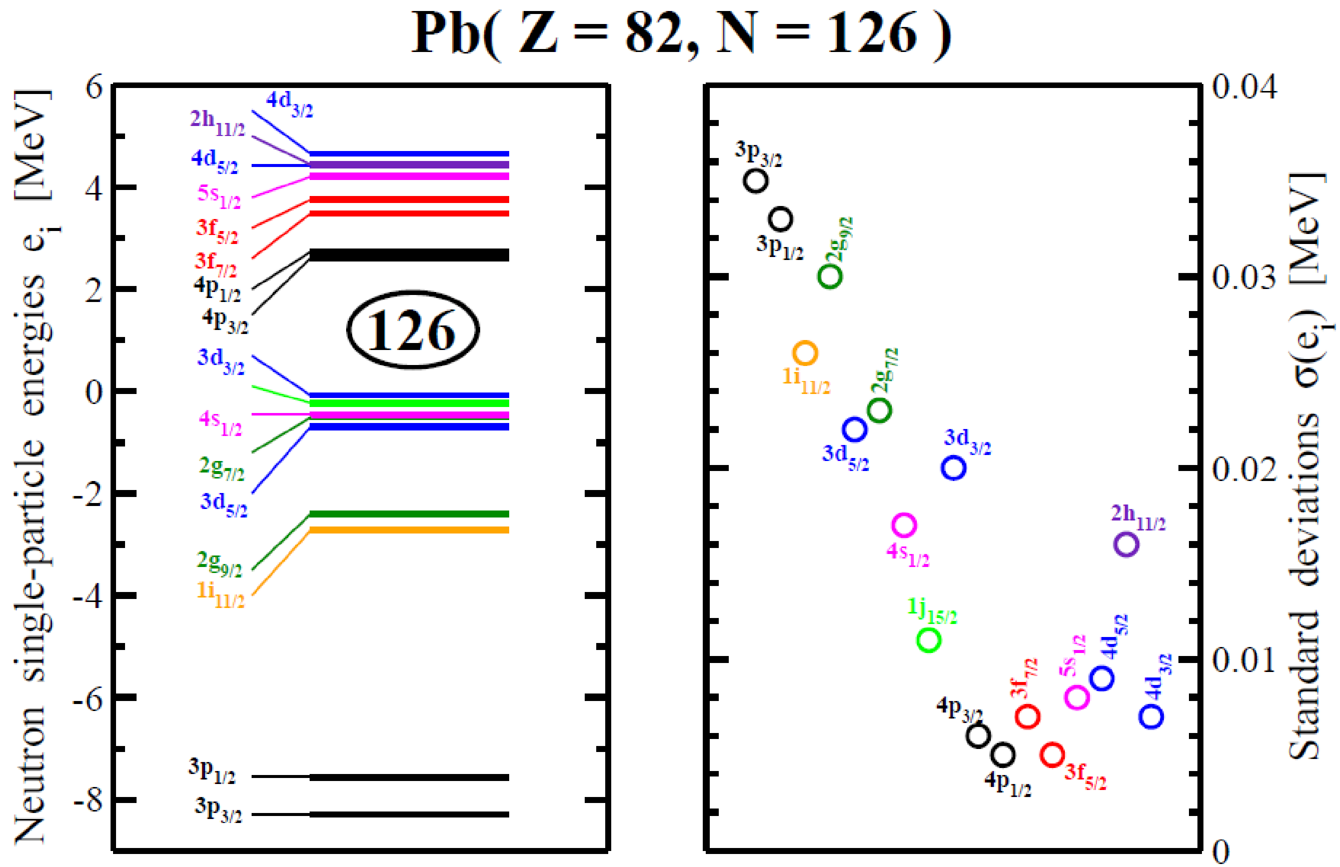
Weak dependence on the parametrization in groups A-C

Skyrme ED functionals: less localized in the parameter space

TABLE V. Parameters (t, x) of UNEDF0 and UNEDF1.

Parameters	UNEDF0	UNEDF1	Units
t_0	−1883.68781034	−2078.32802326	$\mathrm{MeV \cdot fm^3}$
t_1	277.50021224	239.40081204	$\mathrm{MeV \cdot fm^5}$
t_2	608.43090559	1575.11954190	$\mathrm{MeV \cdot fm^5}$
t_3	13901.94834463	14263.64624708	$\mathrm{MeV \cdot fm^{3+3\gamma}}$
x_0	0.00974375	0.05375692	—
x_1	−1.77784395	−5.07723238	—
x_2	−1.67699035	−1.36650561	—
x_3	−0.38079041	−0.16249117	—
b_4	125.16100000	38.36807206	$\mathrm{MeV \cdot fm^5}$
b'_4	−91.2604000	71.31652223	$\mathrm{MeV \cdot fm^5}$
γ	0.32195599	0.27001801	—

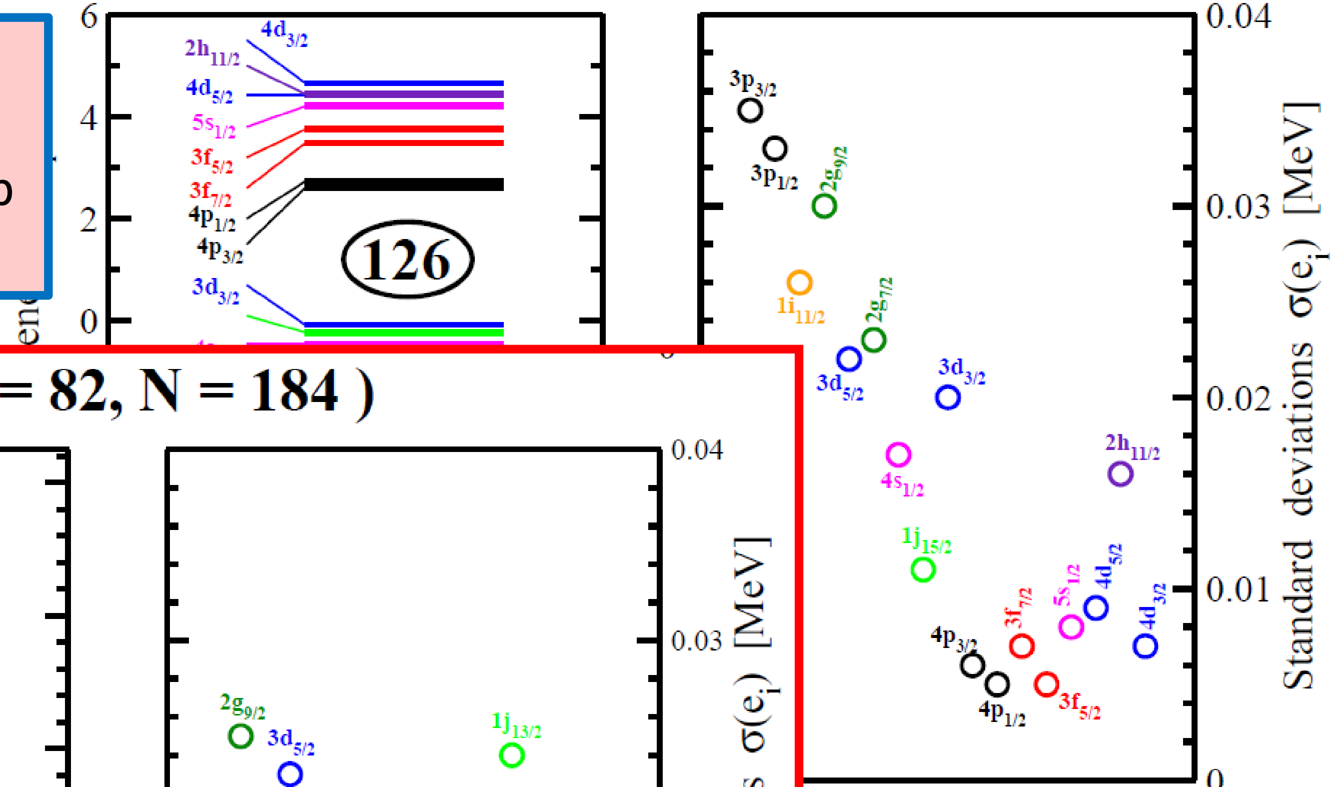
Statistical errors in the single-particle energies



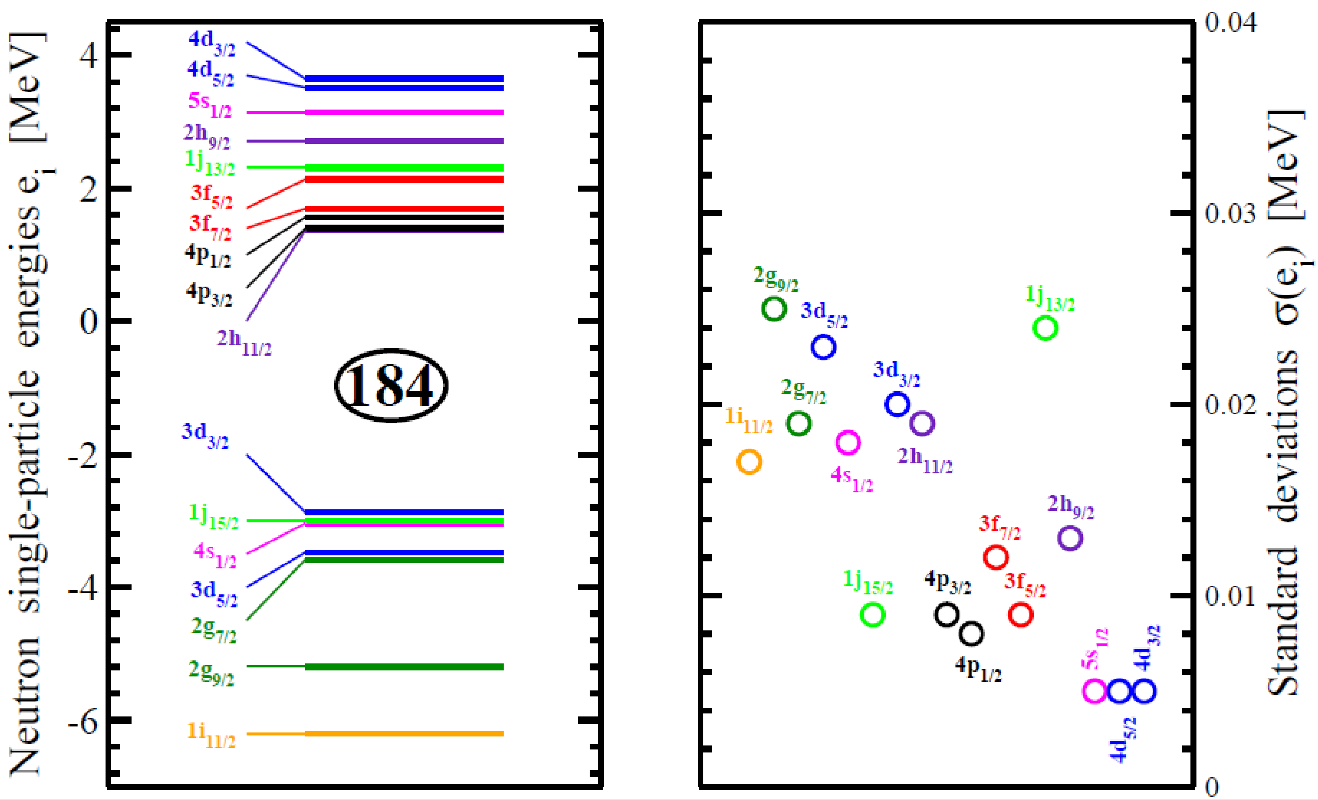
Statistical errors in the single-particle energies

They are small and somewhat decrease on going to neutron-drip line

Pb(Z = 82, N = 126)



Pb(Z = 82, N = 184)



Average standard deviation for the single-particle energies is 0.196 [proton] (0.179 [neutron]) MeV in Skyrme UNEDF0, Gao et al, PRC 87, 034324 (2013)

Systematic errors

Errors versus uncertainties:

systematic errors – well defined for the regions where experimental data exist [remember "error is a deviation from true value" (webster)]

theoretical uncertainties - not well defined for the regions beyond experimentally known

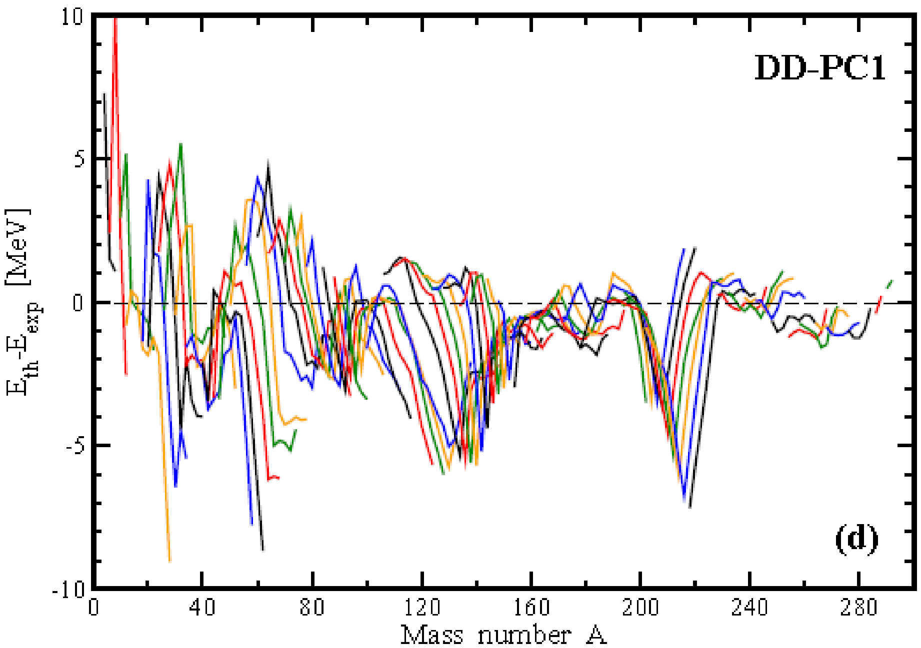
A. based on the set of the models which does not form statistical ensemble
B. biases of the models are not known
C. biases of the fitting protocols

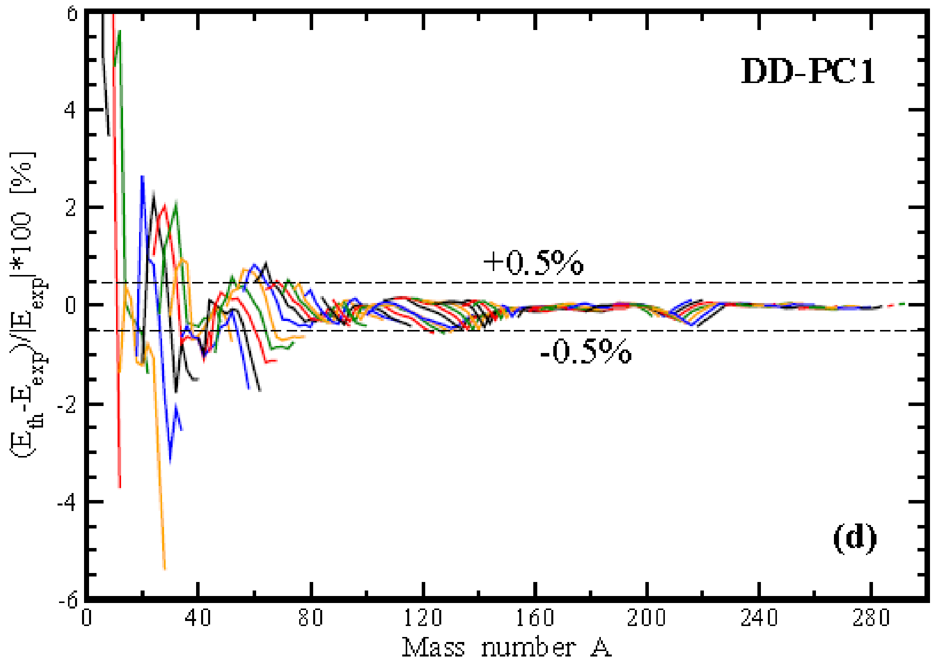
Theoretical uncertainties are defined by the **spread** (the difference between maximum and minimum values of physical observable obtained with employed set of CEDF's).

$$\Delta O(Z,N) = |O_{\max}(Z,N) - O_{\min}(Z,N)|$$

NL3*, DD-ME2, DD-MEδ, DD-PC1 [also PC-PK1 in superheavy nuclei]

Systematic errors in the description of masses





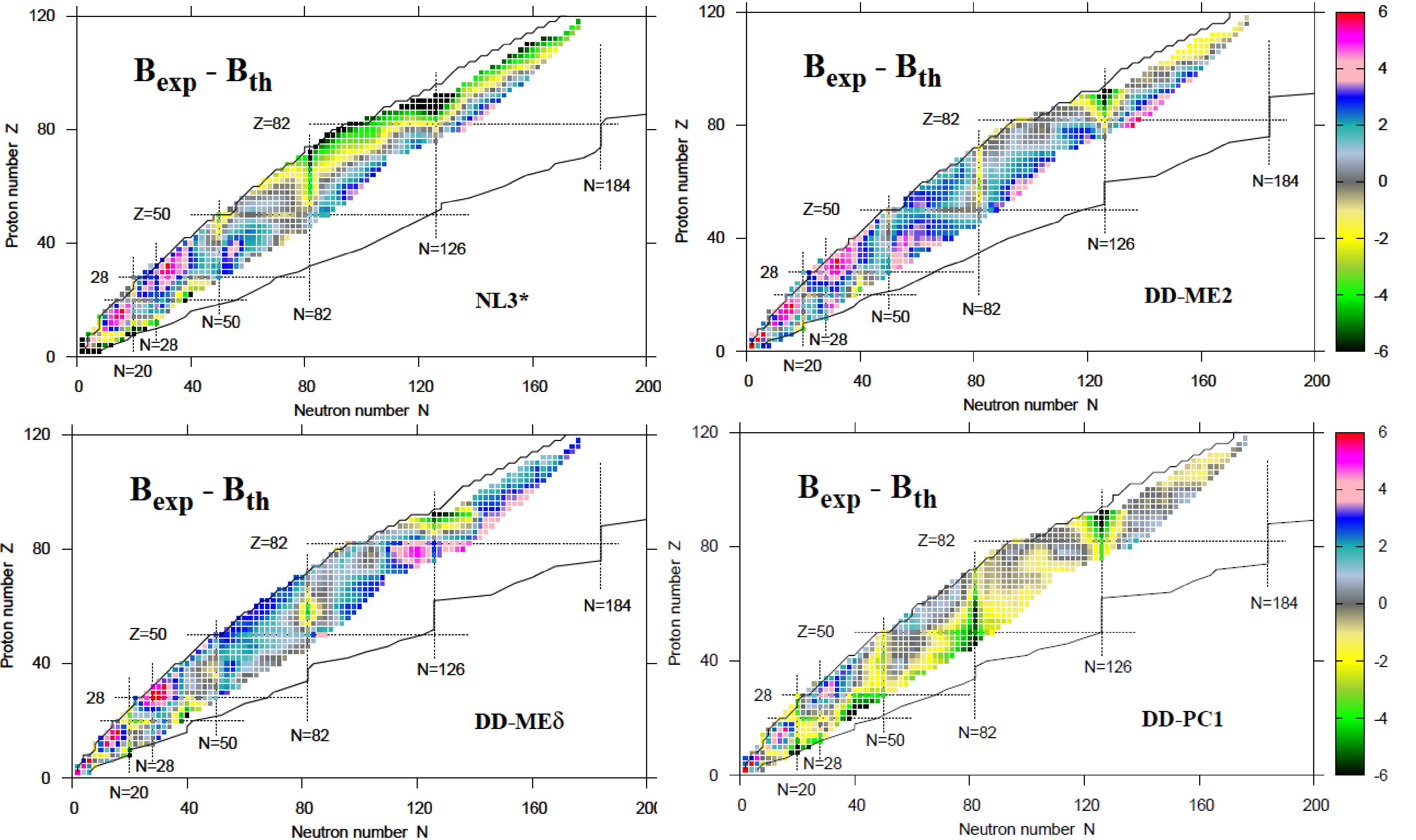
EDF	measured	measured+estimated		
	$\Delta E_{\rm rms}$	$\Delta E_{\rm rms}$	$\Delta(S_{2n})_{\rm rms}$	$\Delta(S_{2p})_{\rm rms}$
NL3*	2.96	3.00	1.23	1.29
DD-ME2	2.39	2.45	1.05	0.95
DD-MEδ	2.29	2.40	1.09	1.09
DD-PC1	2.01	2.15	1.16	1.03

S. Agbemava, AA, D, Ray, P.Ring, PRC **89**, 054320 (2014)
includes complete DD-PC1 mass table as supplement

Uncertainties in radii

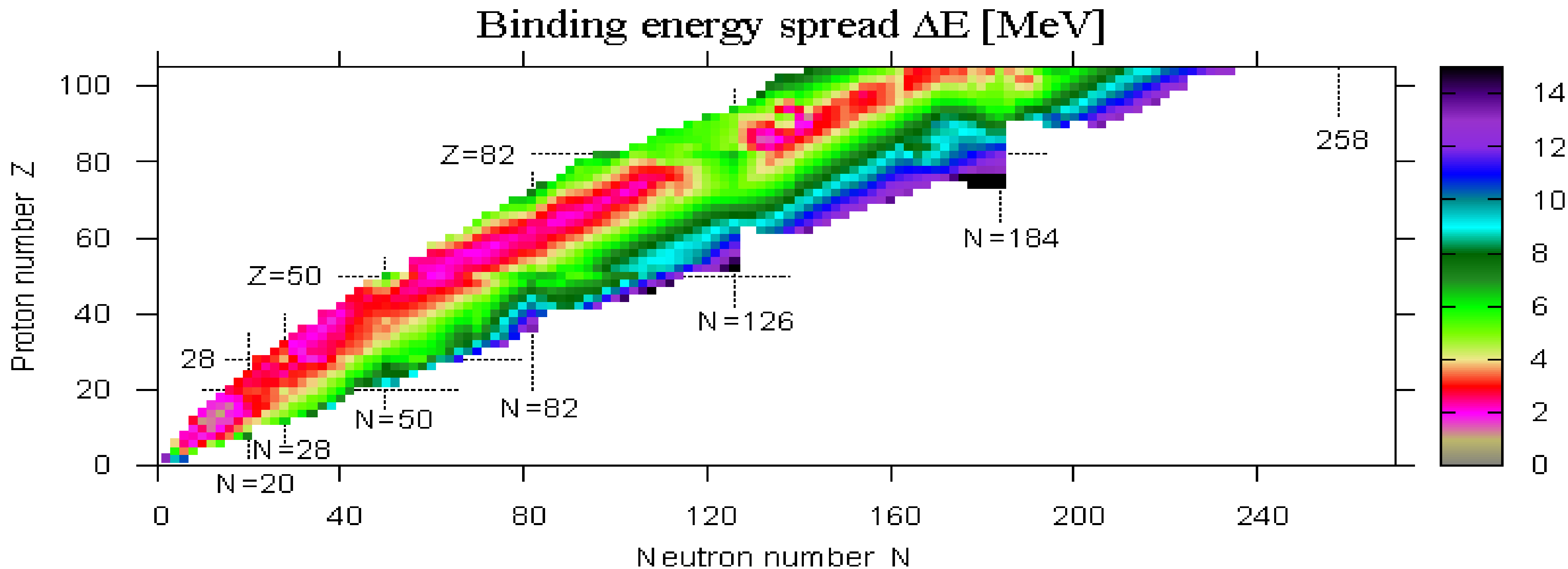
CEDF	Δr_{ch}^{rms} [fm]
NL3*	0.0283
DD-ME2	0.0230
DD-MEd	0.0329
DD-PC1	0.0253

Masses: the deviations between theory and experiment



The residuals are non-statistical in nature → the difficulty in the estimation of systematic errors in unknown regions

Propagation of theoretical uncertainties in masses with isospin

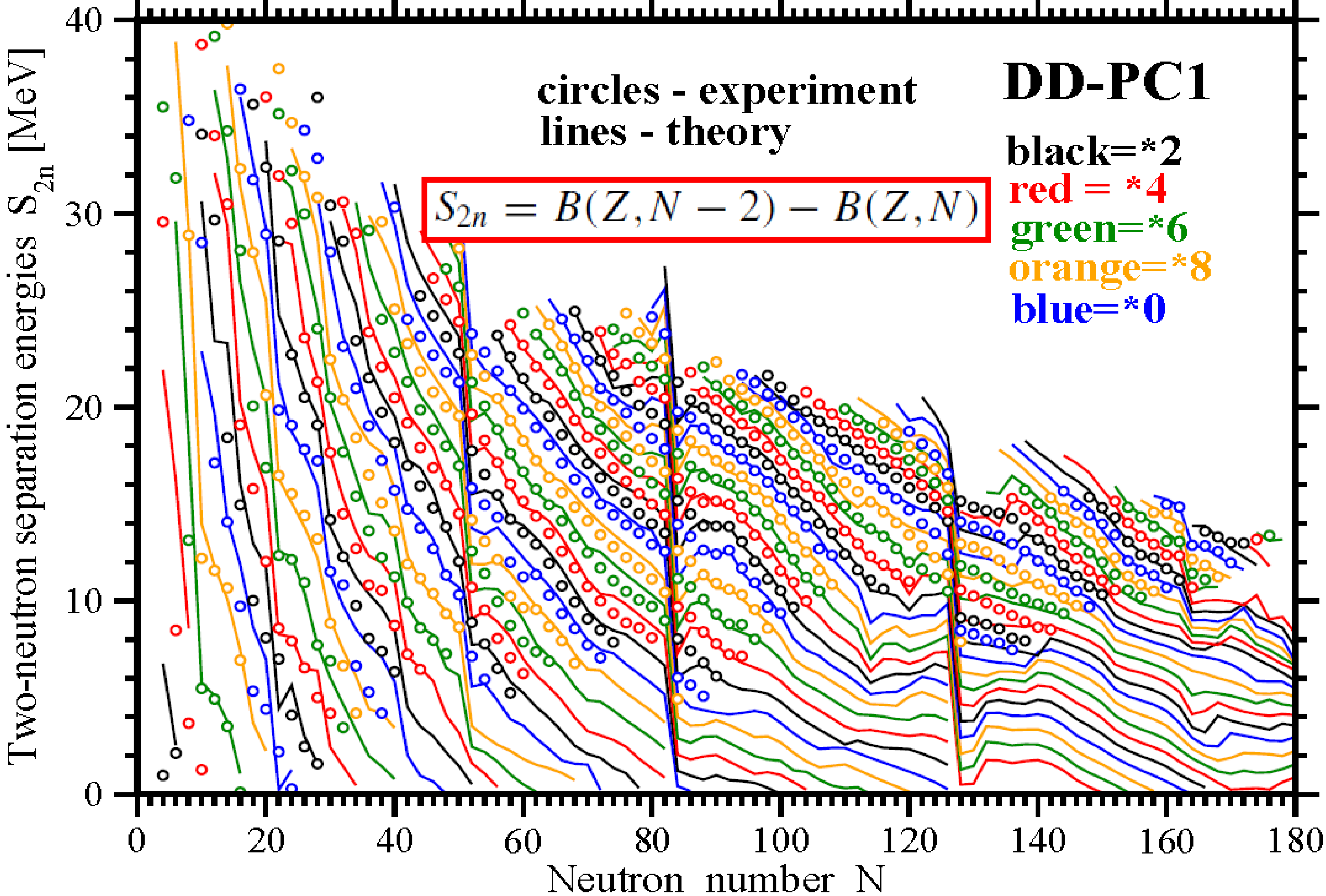


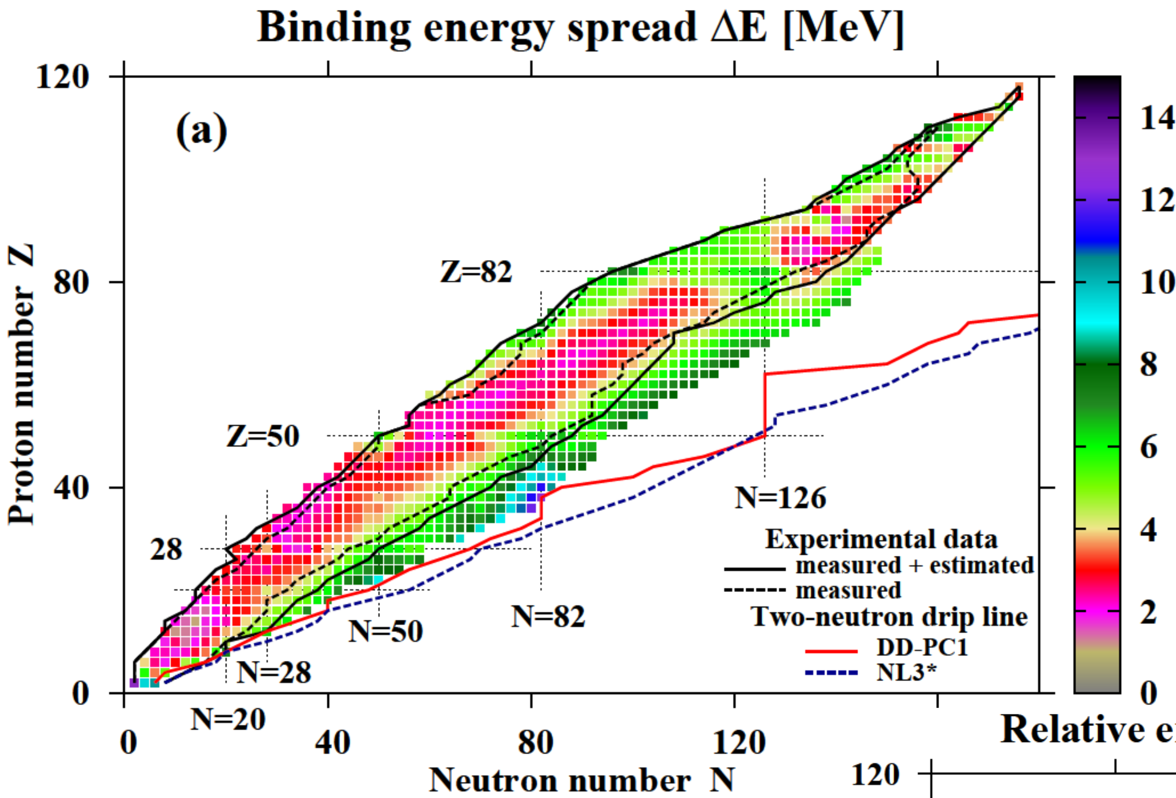
The spreads are relatively smooth functions of proton and neutron numbers

How to reduce theoretical uncertainties in mass predictions of neutron-rich nuclei:

- more mass measurements in neutron-rich nuclei (FRIB, RIKEN, …) ?
- improve nuclear matter properties of EDFs ?

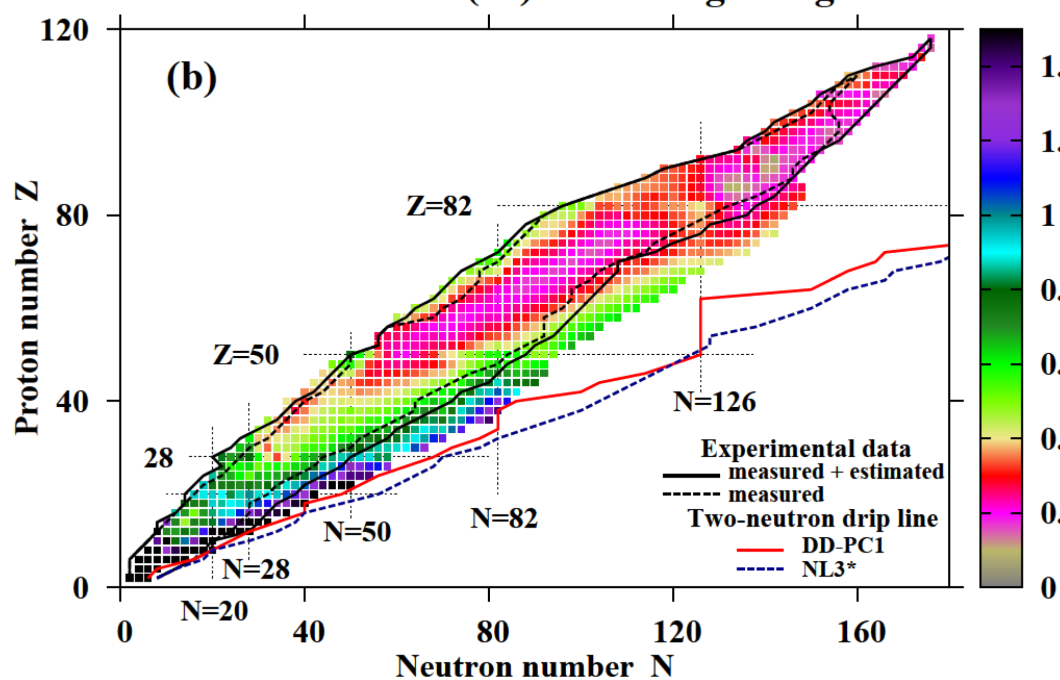
Two-particle separation energies – derivative of binding energies as a function of particle number





Propagation of theoretical uncertainties in masses with isospin

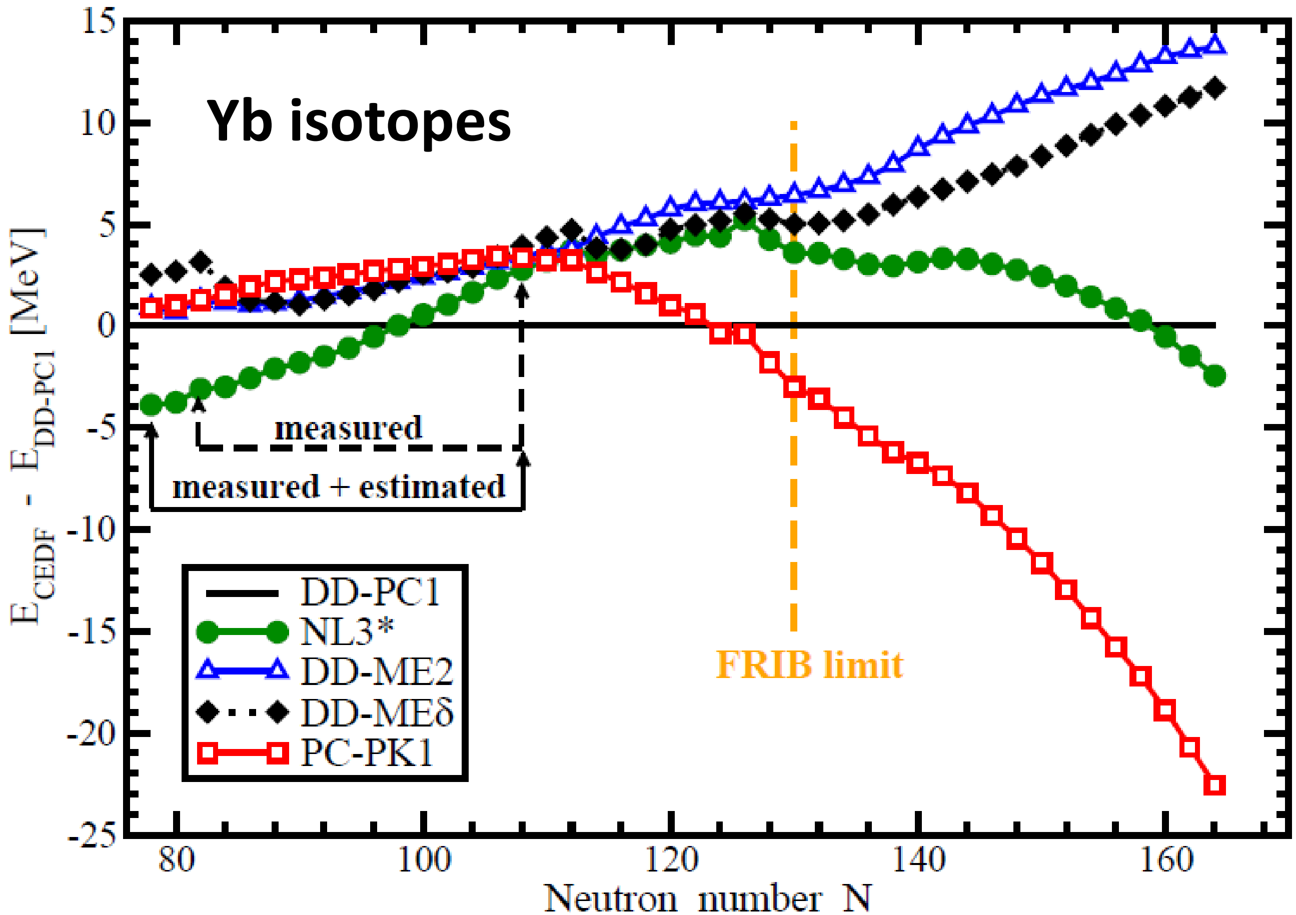
AA and S. Agbemava, 93, 054310 (2016)



Impact of mass measurements at FRIB:

some improvement of isovector properties of EDFs,
some reduction (not elimination) of theoretical uncertainties in mass predictions of neutron-rich nuclei

What will happen if we will add PC-PK1 CEDF ?



AA and S. Agbemava, 93, 054310 (2016)

Impact of mass measurements at FRIB:
some improvement of isovector properties of EDFs,
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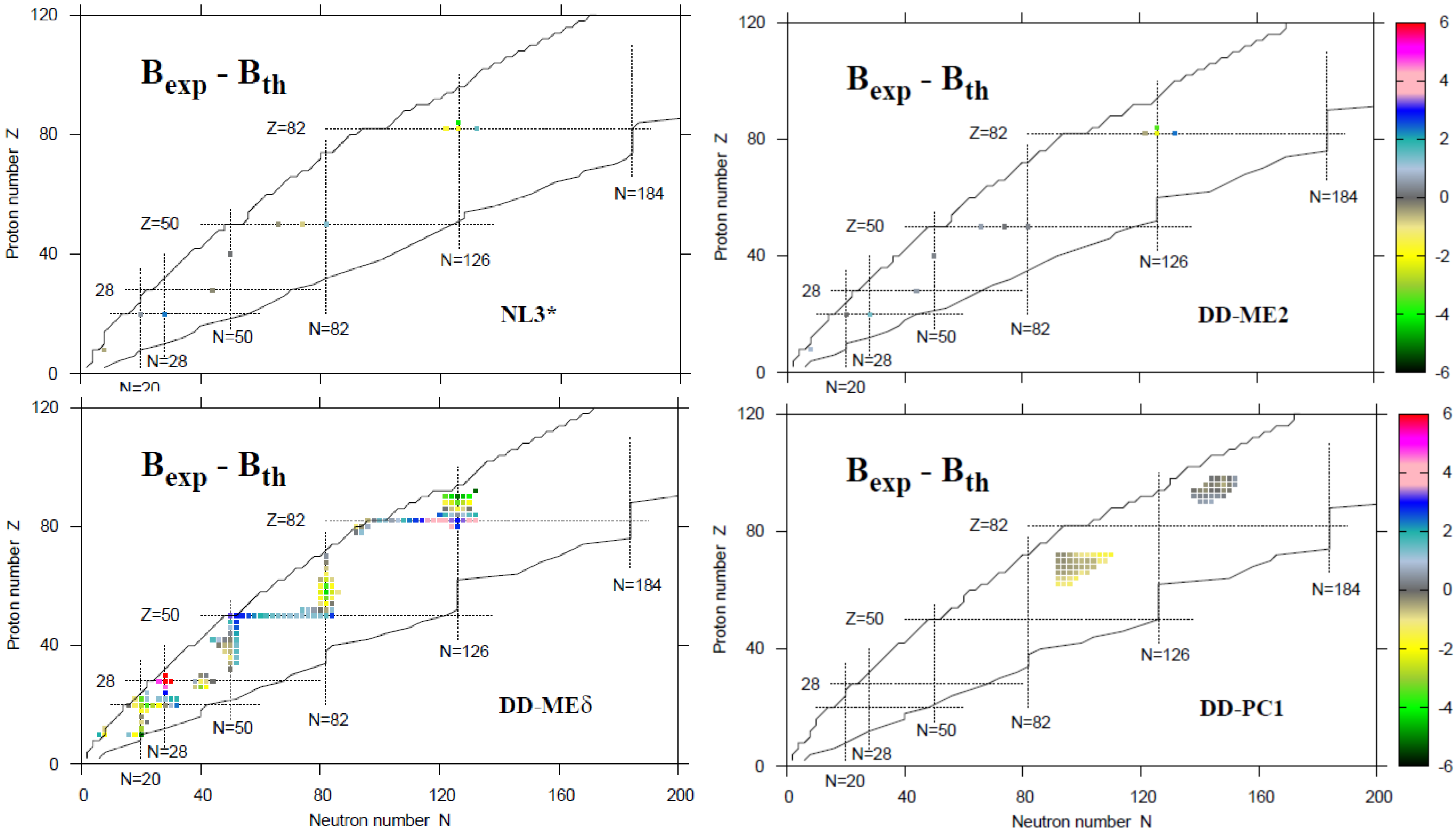


NL3* - G.A. Lalazissis et al PLB 671 (2009) 36 - **7 parameters**

DD-ME2 - G. A. Lalazissis, et al, PRC **71**, 024312 (2005) – **10 parameters**

DD-PC1 - T. Niksic et al, PRC **78**, 034318 (2008) – **10 parameters**

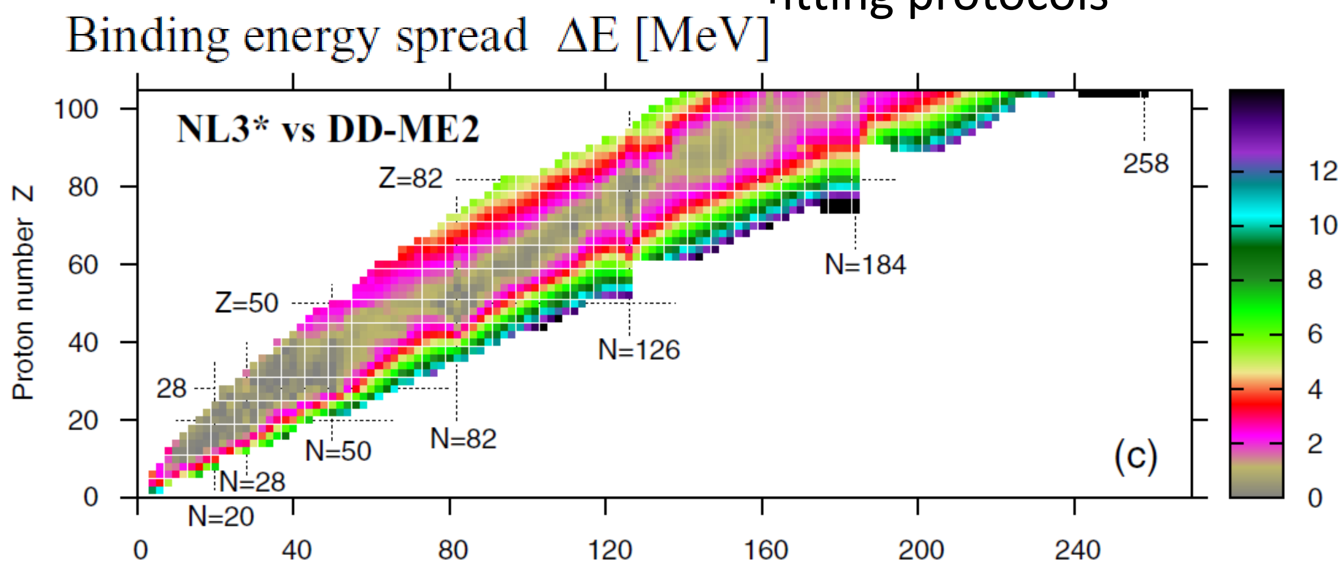
DD-Meδ - X. Roca-Maza et al, PRC **84**, 054309 (2011) – **14 parameters**

only 4 parameters are fitted to finite nuclei,

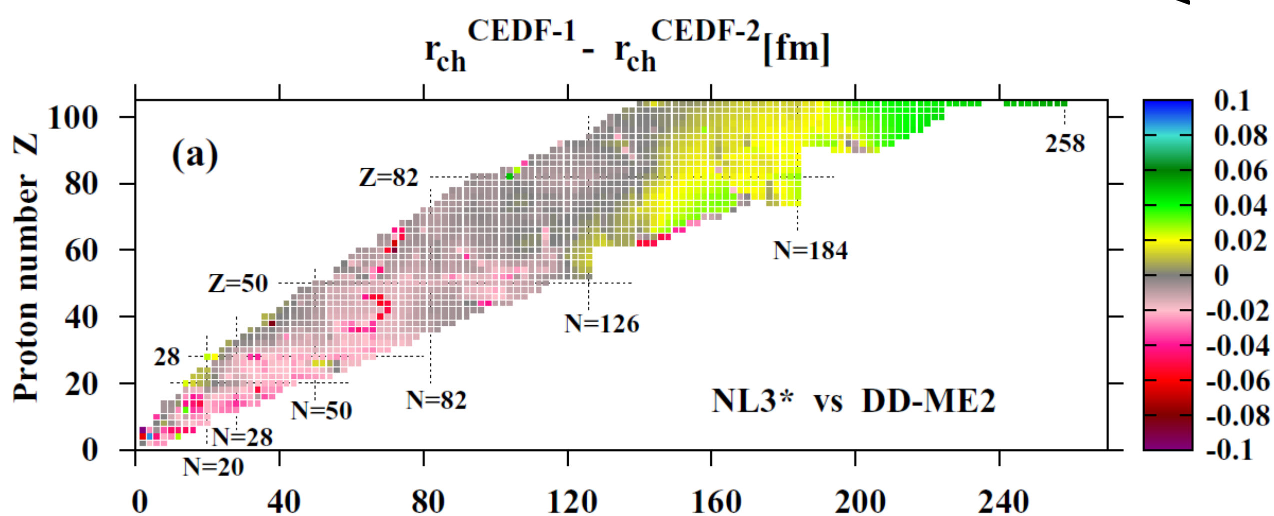
others - to Bruckner calculations of nuclear matter

The difficulties to separate the impact of different physical assumptions and the details of the fitting protocol

The only exception is the pair of the NL3* and DD-ME2 functionals which has identical fitting protocols



AA and S. Agbemava, 93, 054310 (2016)



Nuclear matter properties: could they better constraint EDF and reduce mass uncertainties towards neutron drip line?

CEDF	ρ_0 [fm^{-3}]	E/A [MeV]	K_0 [MeV]	J [MeV]	L_0 [MeV]	m^*/m
1	2	3	4	5	6	7
NL3* [18]	0.150	-16.31	258	**38.68**	**122.6**	0.67
DD-ME2 [19]	0.152	-16.14	251	32.40	49.4	0.66
DD-MEδ [21]	0.152	-16.12	219	32.35	52.9	0.61
DD-PC1 [20, 23]	0.152	-16.06	230	33.00	68.4	0.66
PC-PK1 [23]	0.154	-16.12	238	**35.6**	**113**	0.65
SET2a	~ 0.15	~ -16	190-270	25-35	25-115	
SET2b	~ 0.15	~ -16	190-270	30-35	30-80	

Nuclear matter constraints SET2a and SET2b from
M. Dutra et al, PRC 90, 055203 (2014)

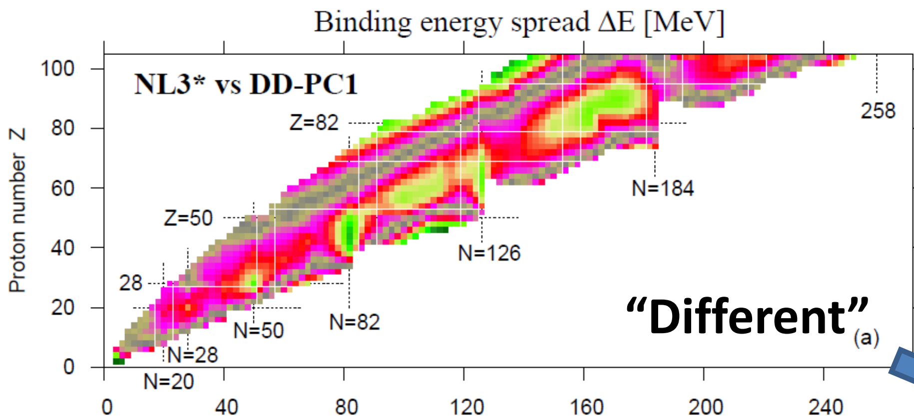
263 CEDFs are analysed: FSUGold and DD-MEδ satisfy SET2b

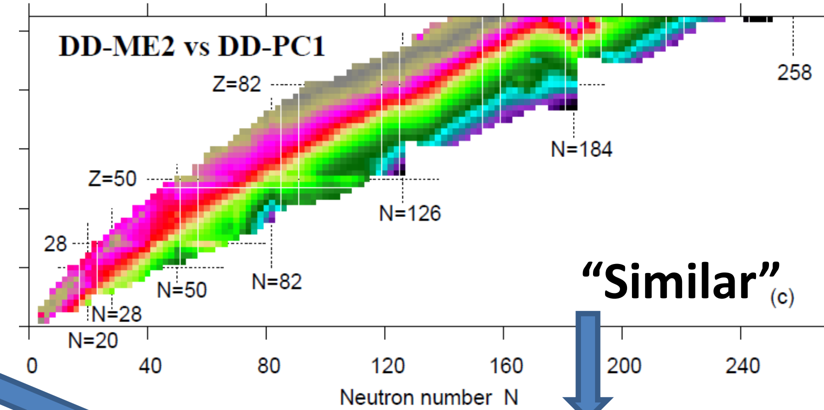
However:

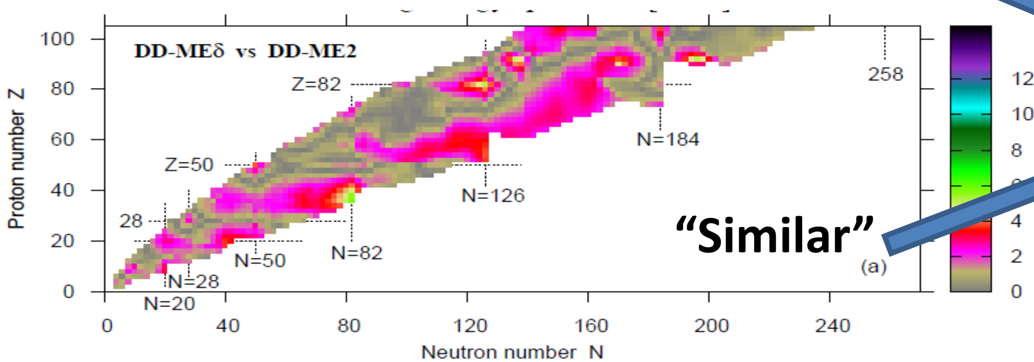
FSUGold provides worst description of masses among CEDFs

DD-MEδ misses octupole deformed region in actinides and gives too low fission barriers in SHE

Nuclear matter properties and propagation of the mass uncertainties towards neutron drip line





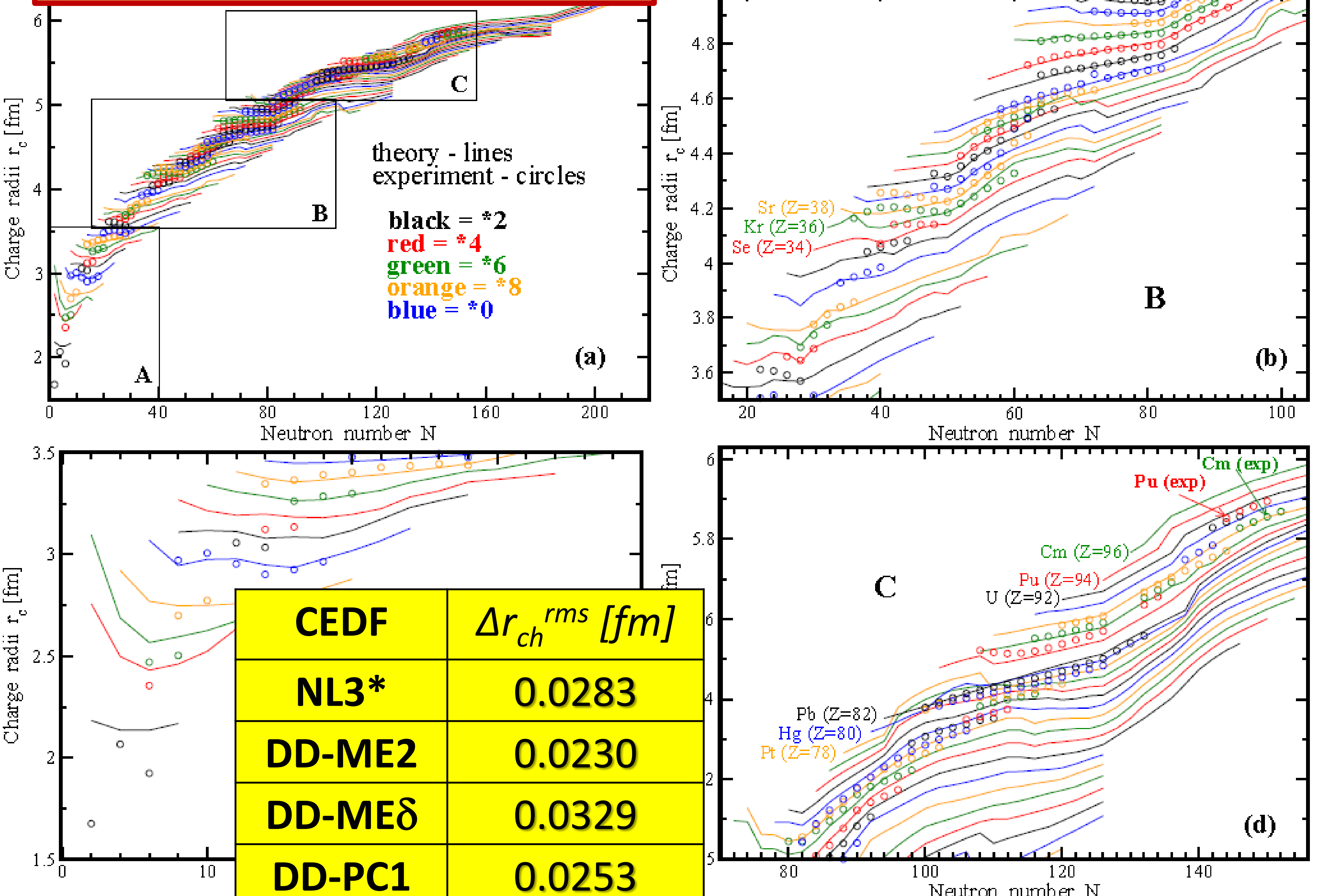


nuclear matter properties

NMP do not allow to reduce the uncertainties towards neutron drip line

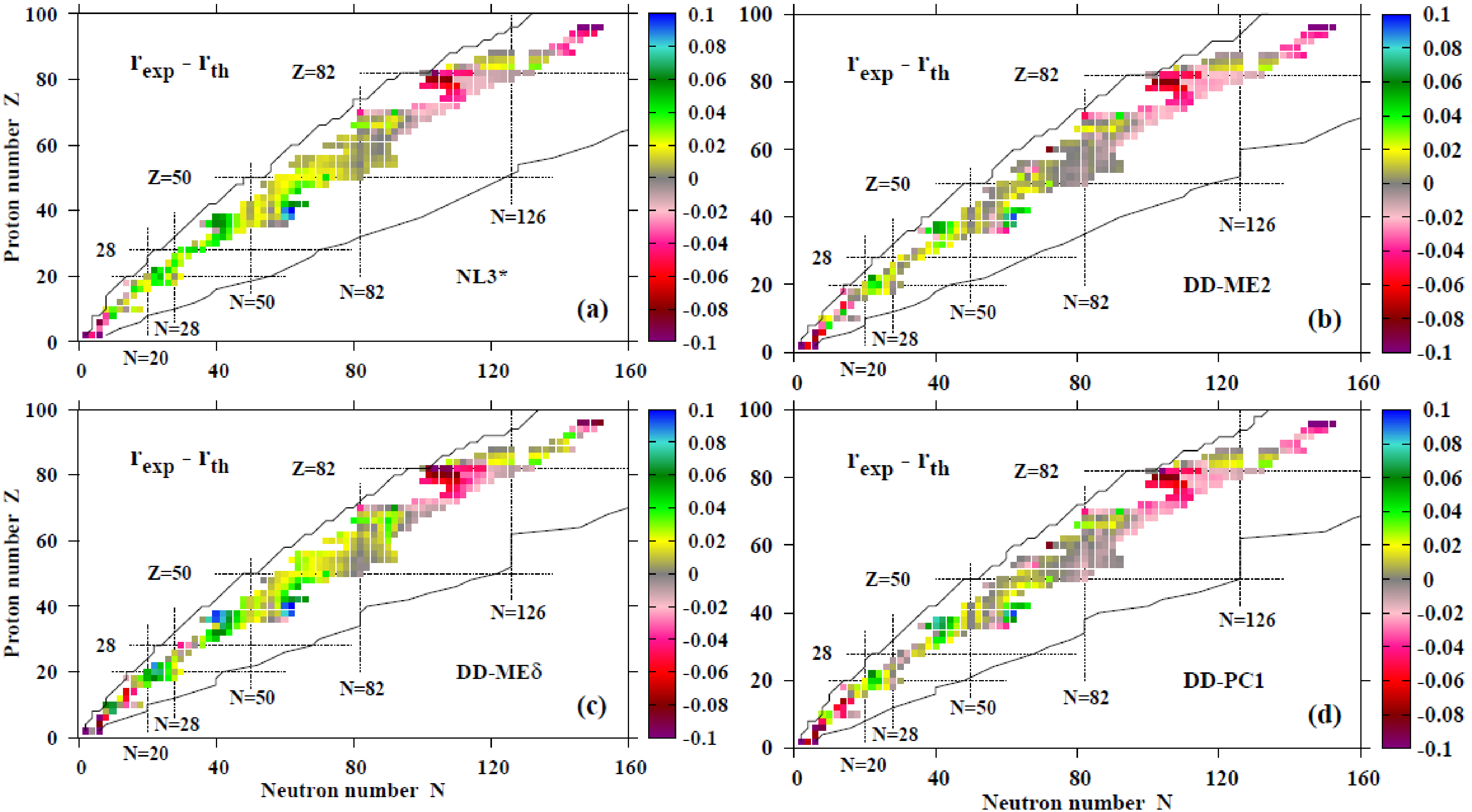
CEDF	ρ_0 [fm^{-3}]	E/A [MeV]	K_∞ [MeV]	J [MeV]	L [MeV]	m^*/m	ΔE_{rms} [MeV]
1	2	3	4	5	6	7	8
NL3* [4]	0.150	-16.31	258	**38.68**	**122.6**	0.67	2.96
DD-ME2 [5]	0.152	-16.14	251	32.40	49.4	0.66	2.39
DD-MEδ [10]	0.152	-16.12	219	32.35	52.9	0.61	2.29
DD-PC1 [11, 12]	0.152	-16.06	230	33.00	68.4	0.66	2.01
PC-PK1 [12]	0.154	-16.12	238	**35.6**	**113**	0.65	2.58

Theoretical errors in charge radii

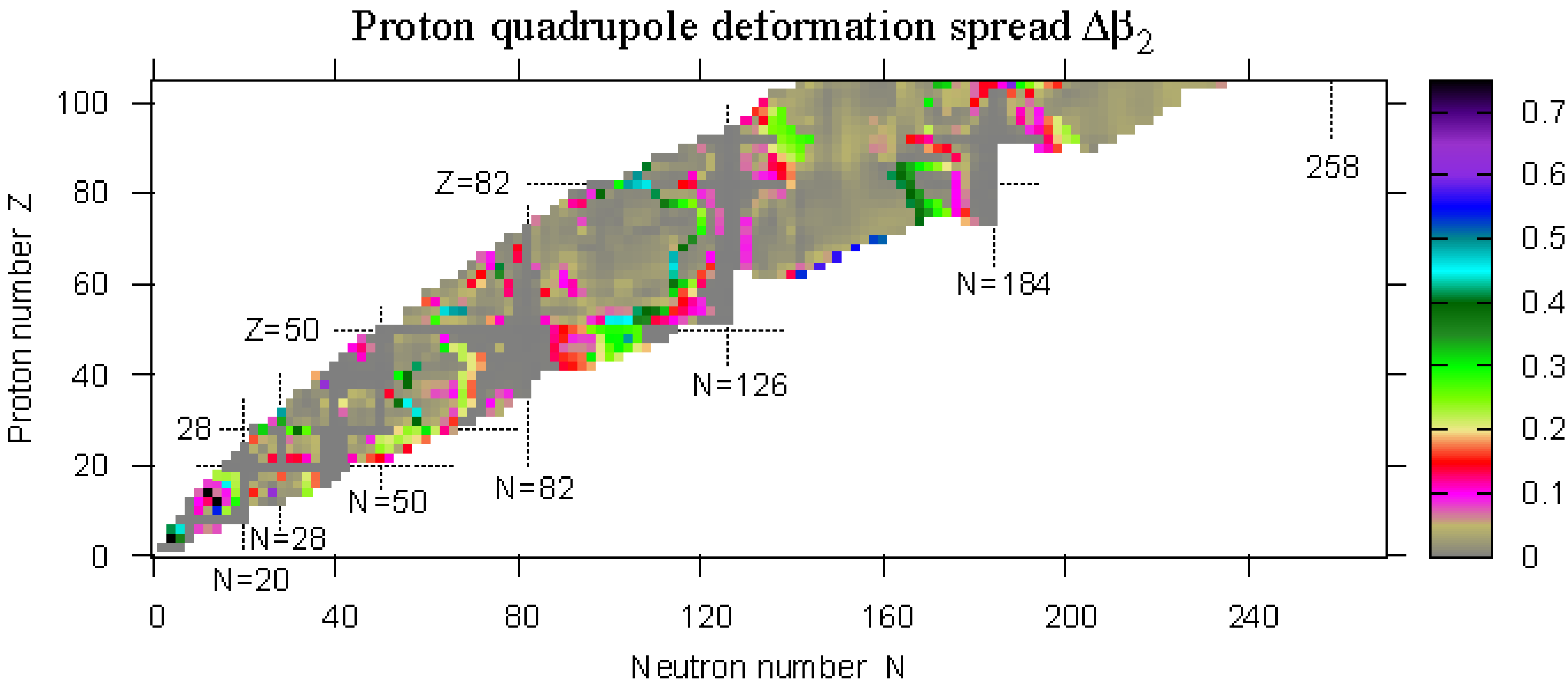


CEDF	Δr_{ch}^{rms} [fm]
NL3*	0.0283
DD-ME2	0.0230
DD-MEδ	0.0329
DD-PC1	0.0253

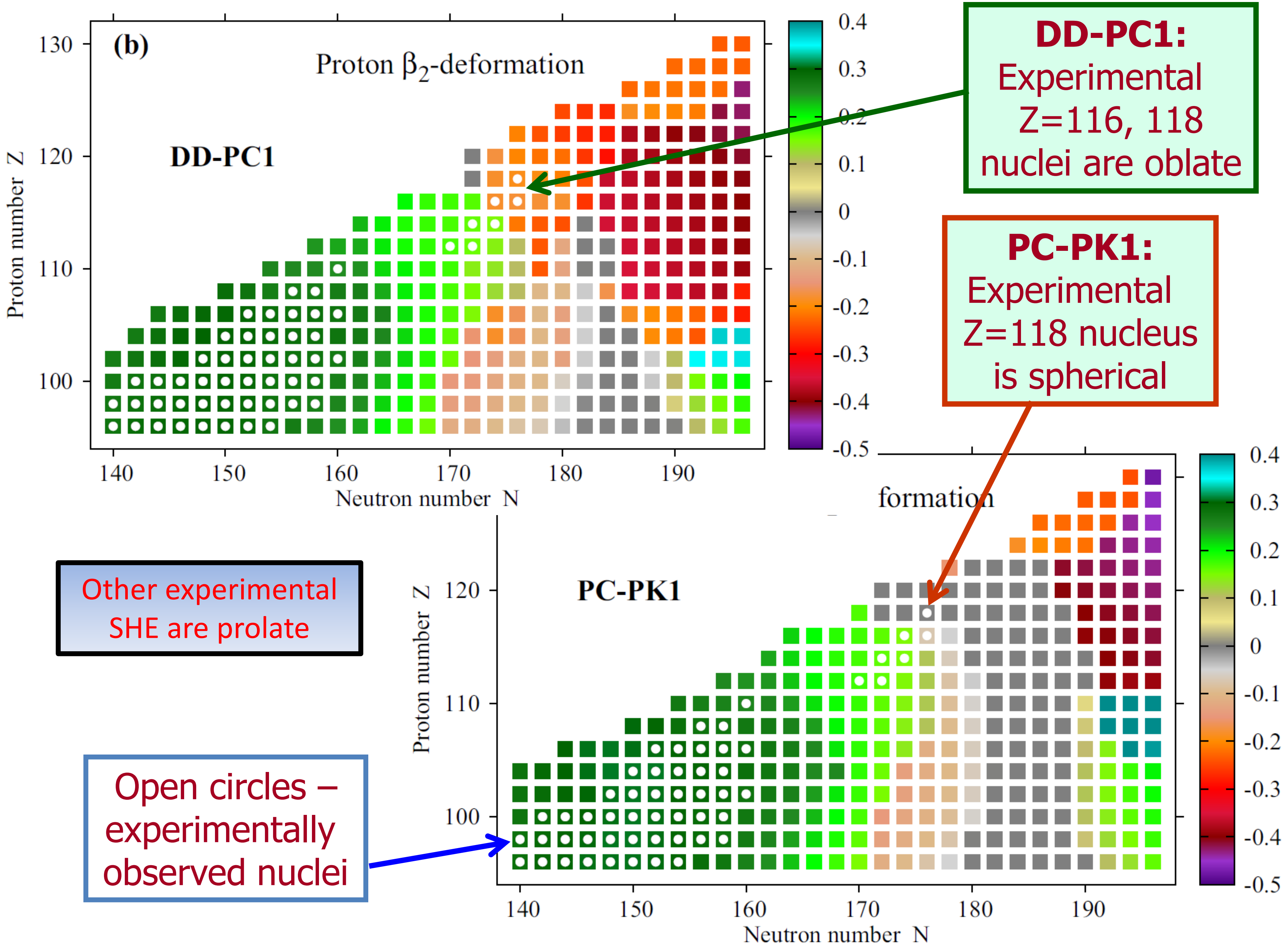
Systematic errors in the description of charge radii



Charge radii – rather well described in all functionals
- very little difference between CEDFs

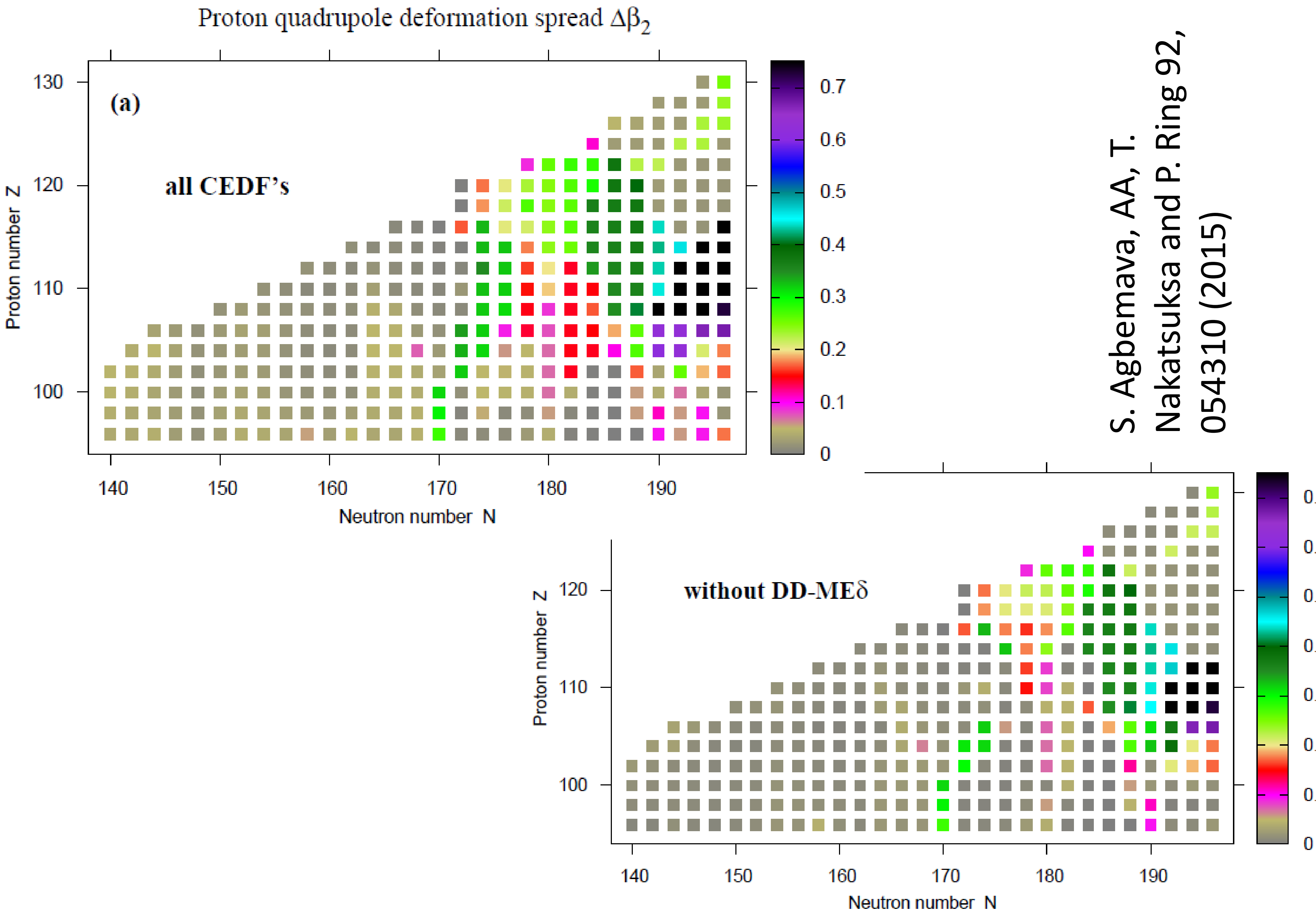


Theoretical uncertainties are most pronounced for transitional nuclei (due to soft potential energy surfaces) and in the regions of transition between prolate and oblate shapes. Details depend of the description of single-particle states

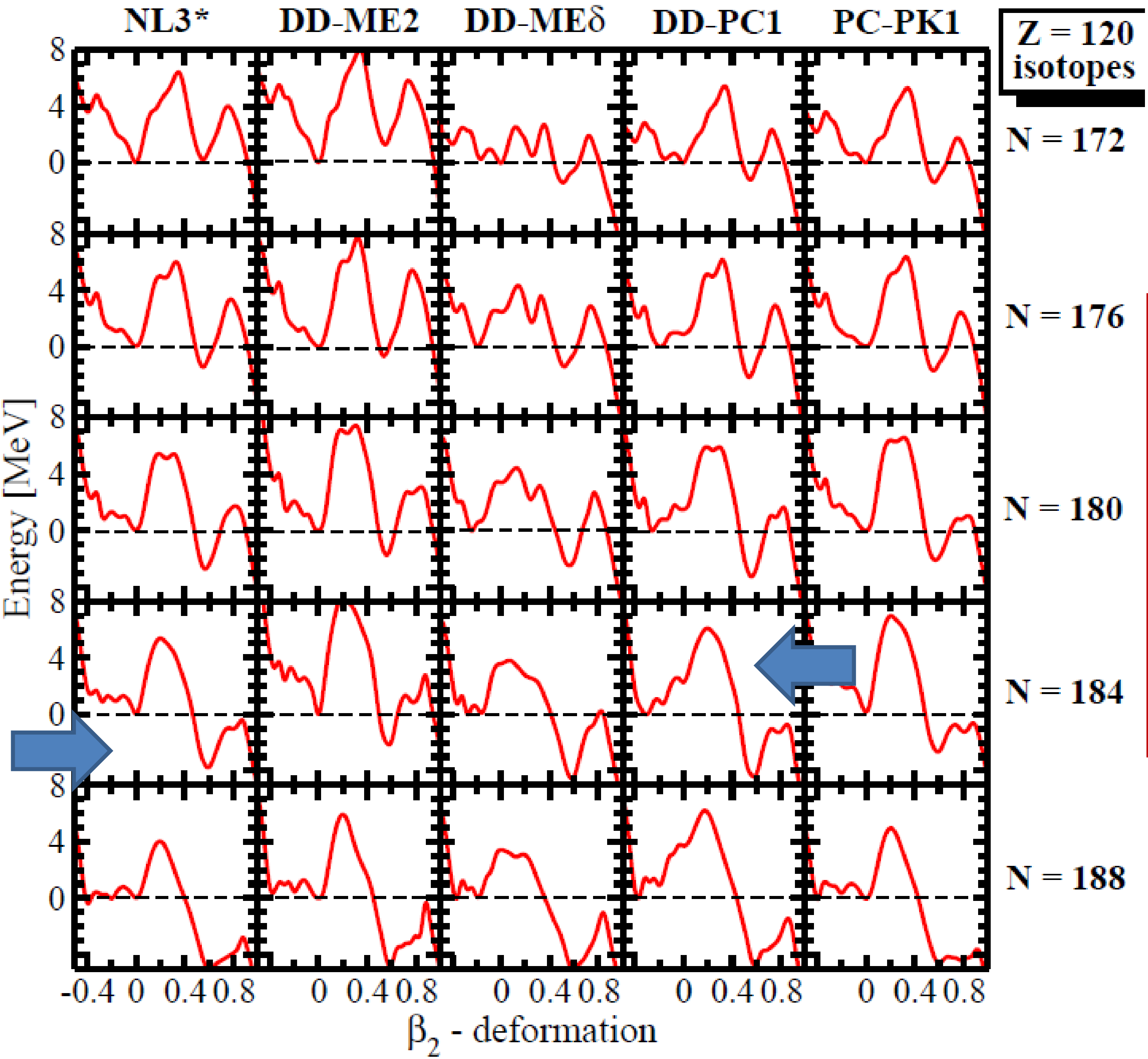


(b)
Proton β2-deformation
DD-PC1
Proton number Z
Neutron number N
130
120
110
100
140
150
160
170
180
190
0.4
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
-0.4
-0.5
DD-PC1:
Experimental Z=116, 118 nuclei are oblate
PC-PK1:
Experimental Z=118 nucleus is spherical
formation
PC-PK1
Other experimental SHE are prolate
Open circles – experimentally observed nuclei

The spreads (theoretical uncertainties) in the deformations

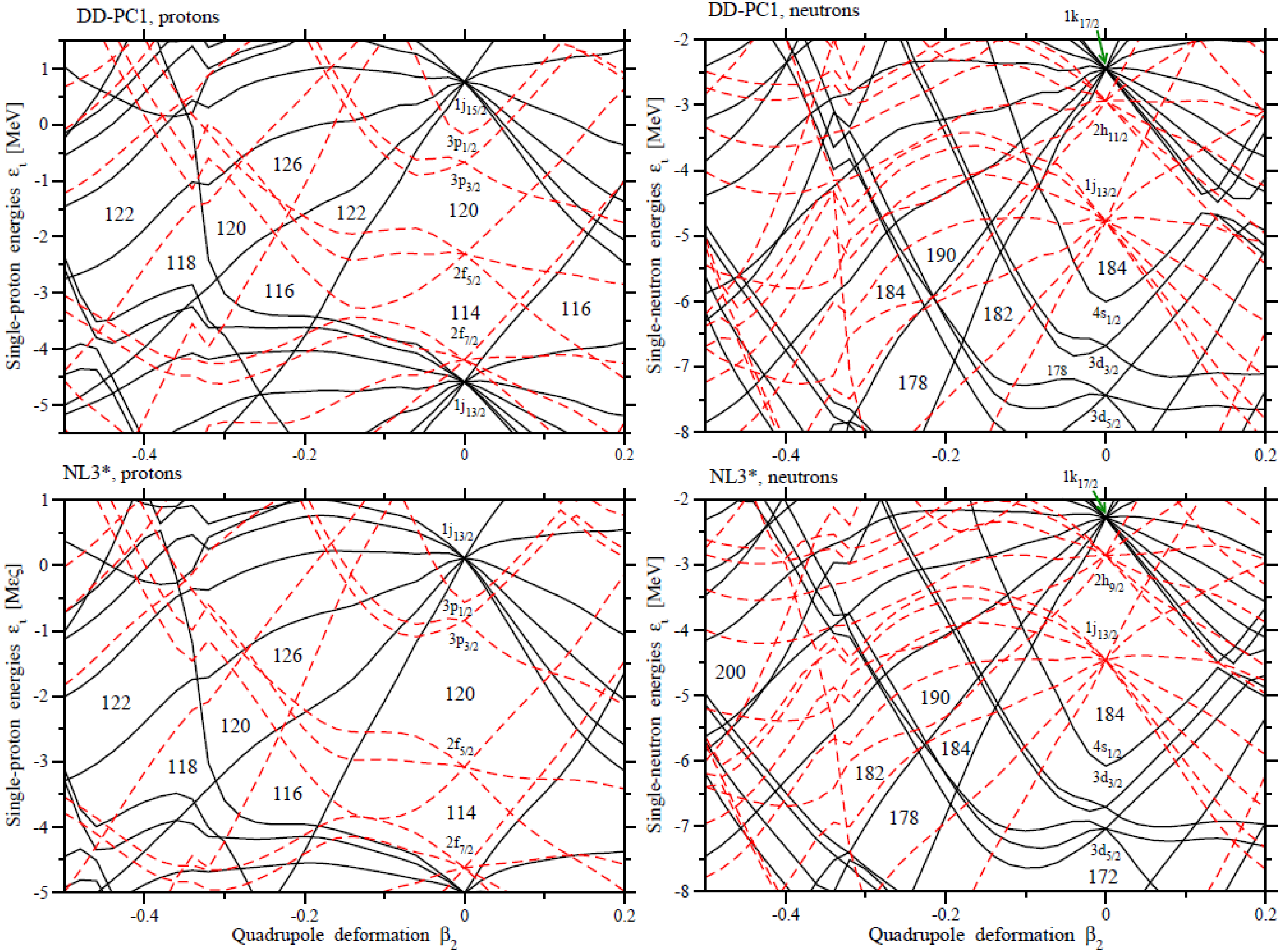


S. Agbemava, AA, T. Nakatsuksa and P. Ring 92, 054310 (2015)



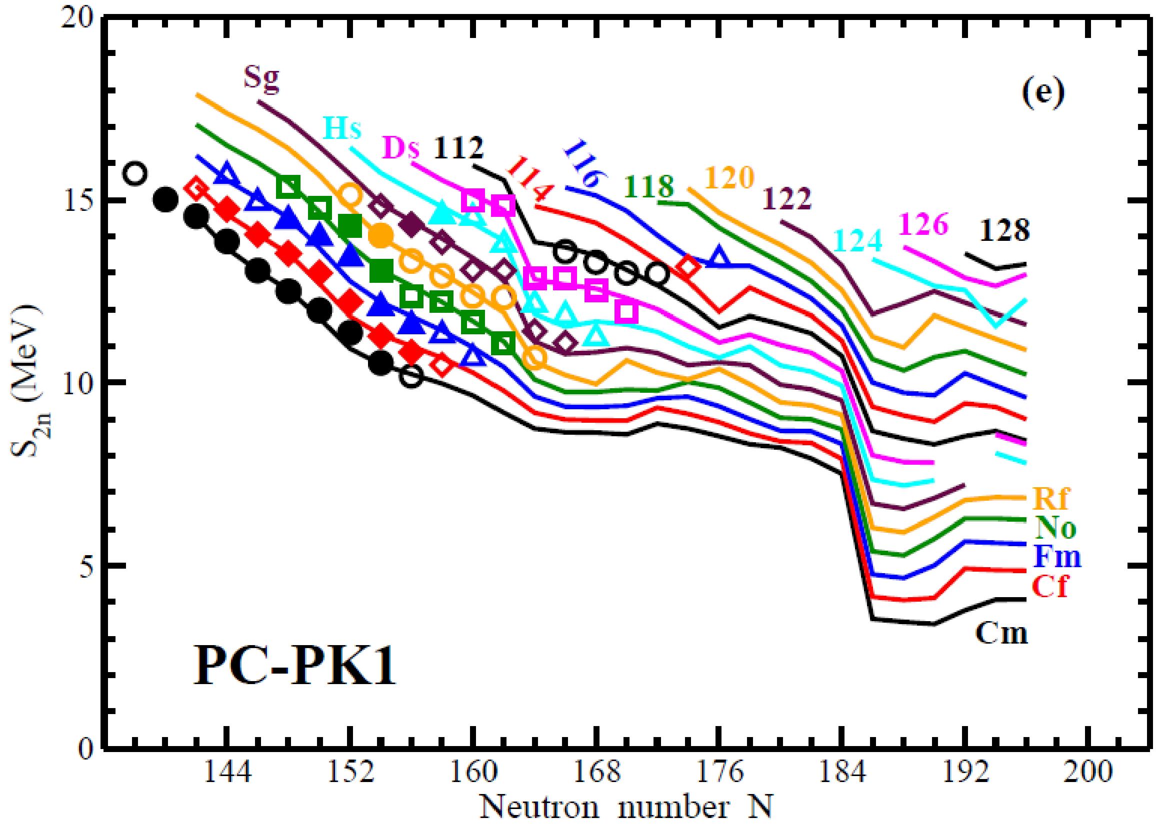
Potential energy surfaces in axially symmetric RHB calculations with separable pairing

The source of oblate shapes – the low density of s-p states



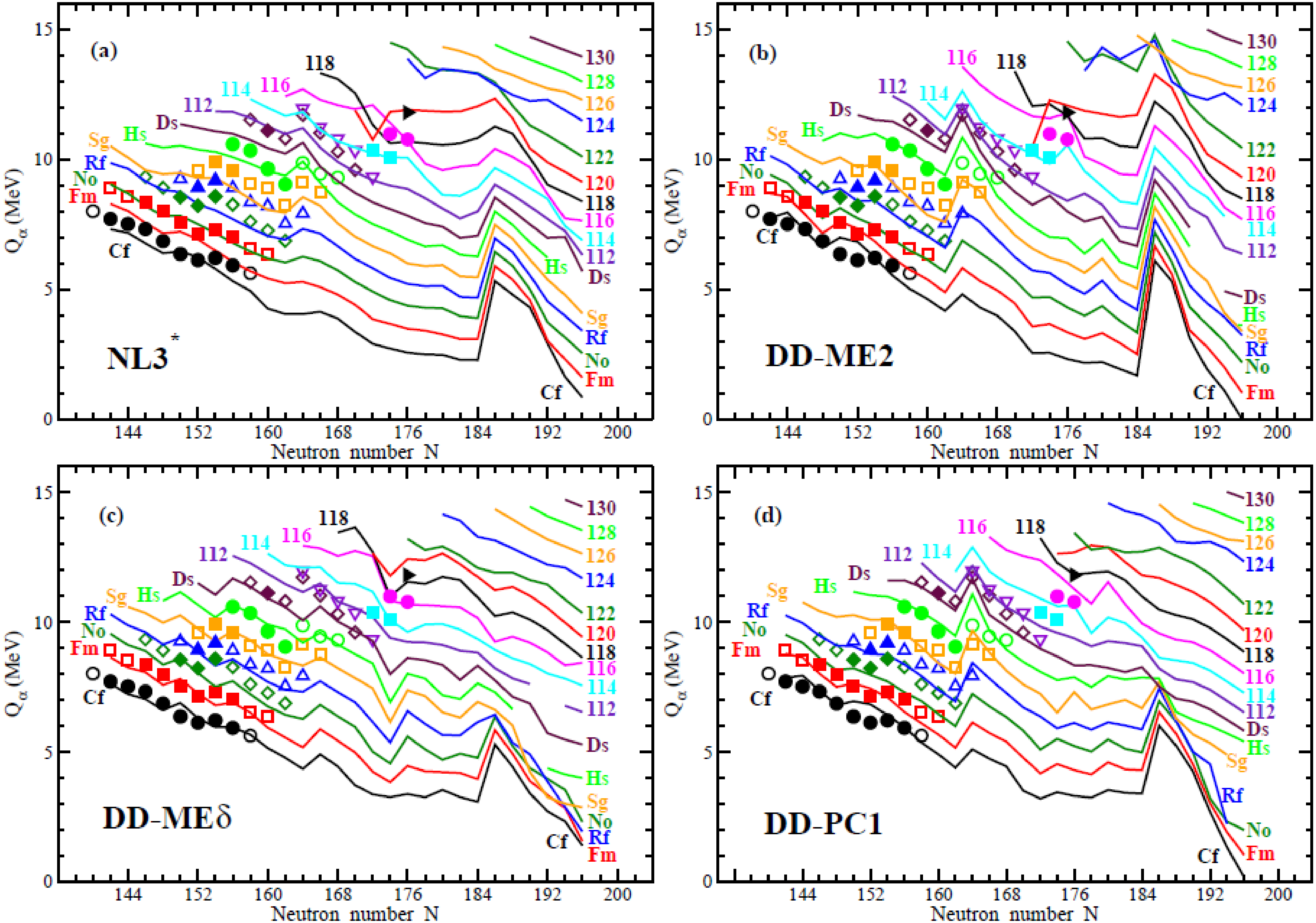
Accuracy of the description of experimental data in Z>94 nuclei

CEDF	ΔE_{rms} [MeV]	$\Delta(S_{2n})_{rms}$ [MeV]	$\Delta(S_{2p})_{rms}$ [MeV]	$\Delta(Q_\alpha)_{rms}$ [MeV]
1	2	3	4	5
NL3*	3.02/3.39	0.71/0.68	1.33/1.34	0.68/0.75
DD-ME2	1.39/1.40	0.45/0.54	0.85/0.90	0.51/0.65
DD-MEδ	2.52/2.45	0.60/0.51	0.45/0.48	0.39/0.51
DD-PC1	**0.59/0.74**	0.30/0.32	0.41/0.42	0.36/0.47
PC-PK1	2.82/2.63	**0.25/0.23**	**0.36/0.33**	**0.32/0.38**



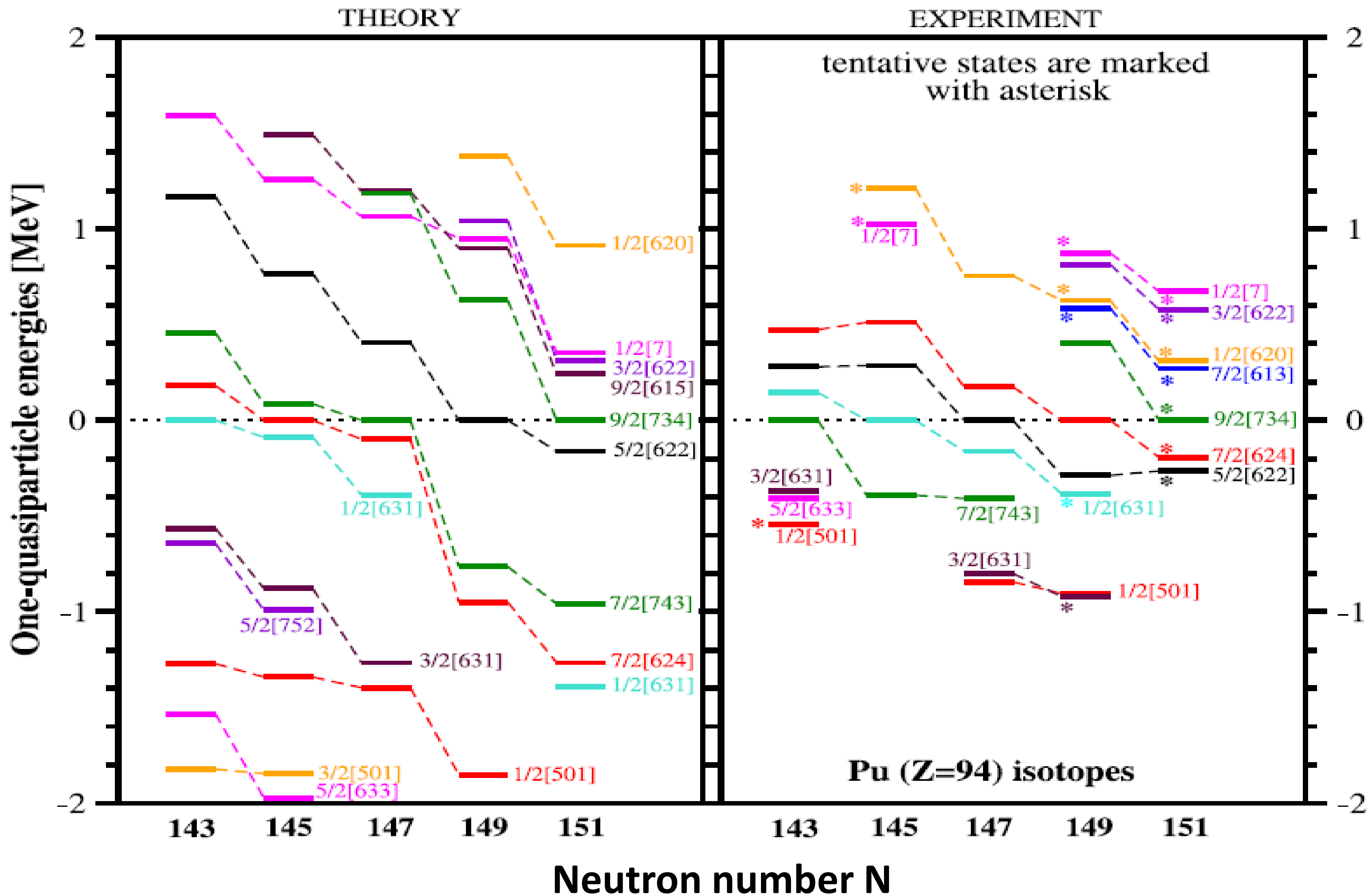
With exception of the DD-MEδ, the deformed N=162 gap is well reproduced in all CEDF's

The Q_α-values

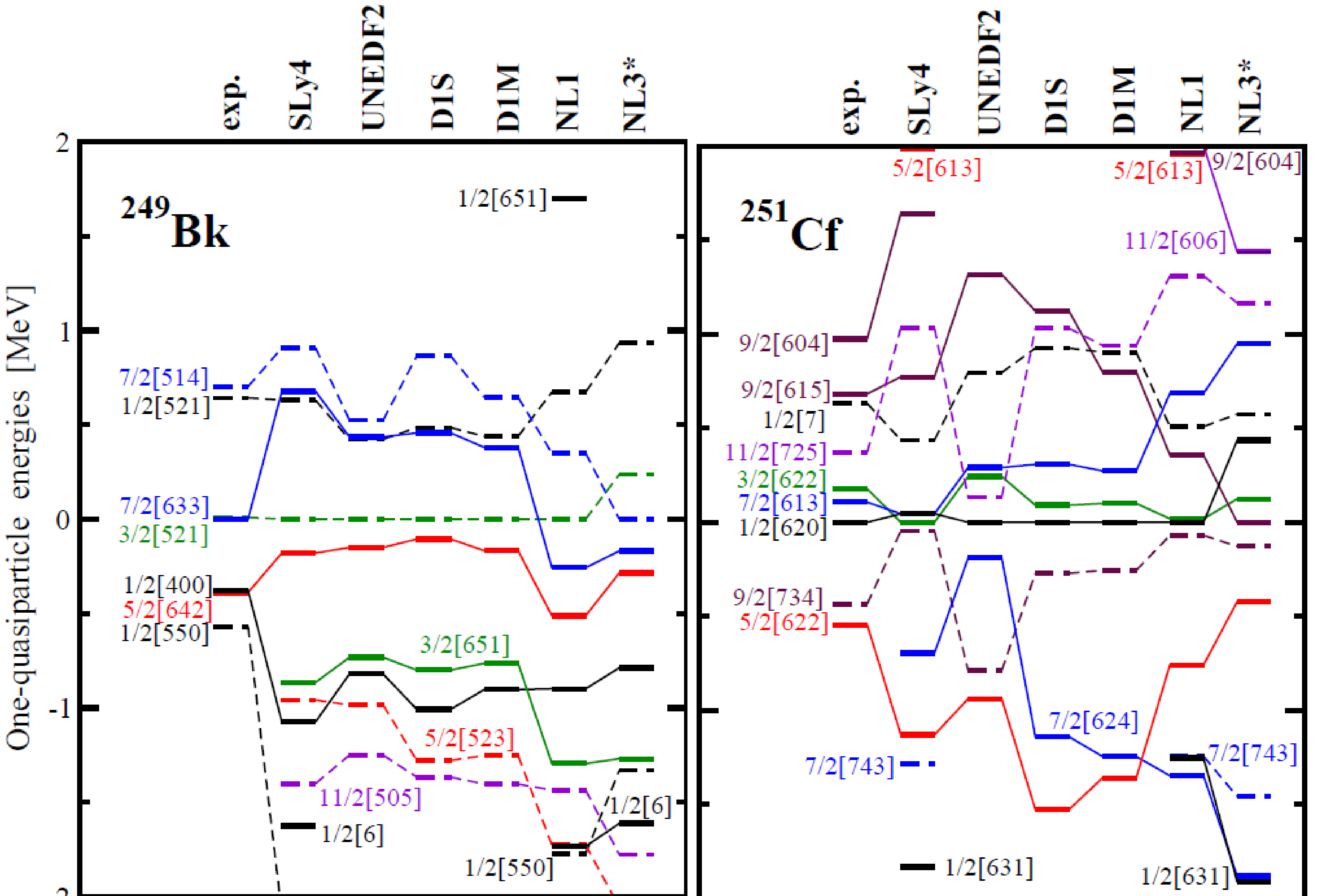


Systematics of one-quasiparticle states in actinides: the CRHB study

Triaxial CRHB; fully self-consistent blocking, time-odd mean fields included, NL3*, Gogny D1S pairing, AA and S.Shawaqfeh, PLB 706 (2011) 177

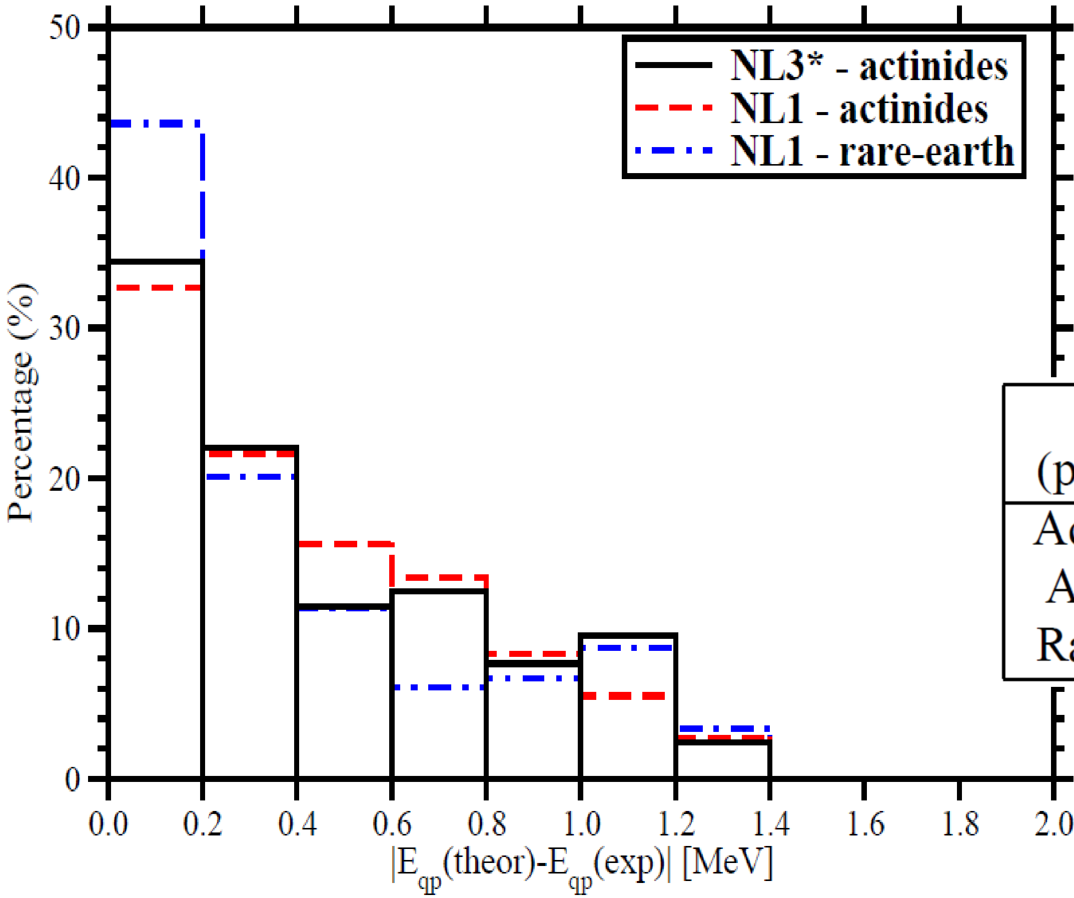


Deformed one-quasiparticle states: covariant and non-relativistic DFT description versus experiment



J.Dobaczewski, AA, et al, NPA, in press

Statistical distribution of deviations of the energies of one-quasiparticle states from experiment



The description of deformed states at DFT level is better than spherical ones by a factor 2-3 (and by a factor ~1(neutron) and ~2 (proton) as compared with spherical PVC calculations)

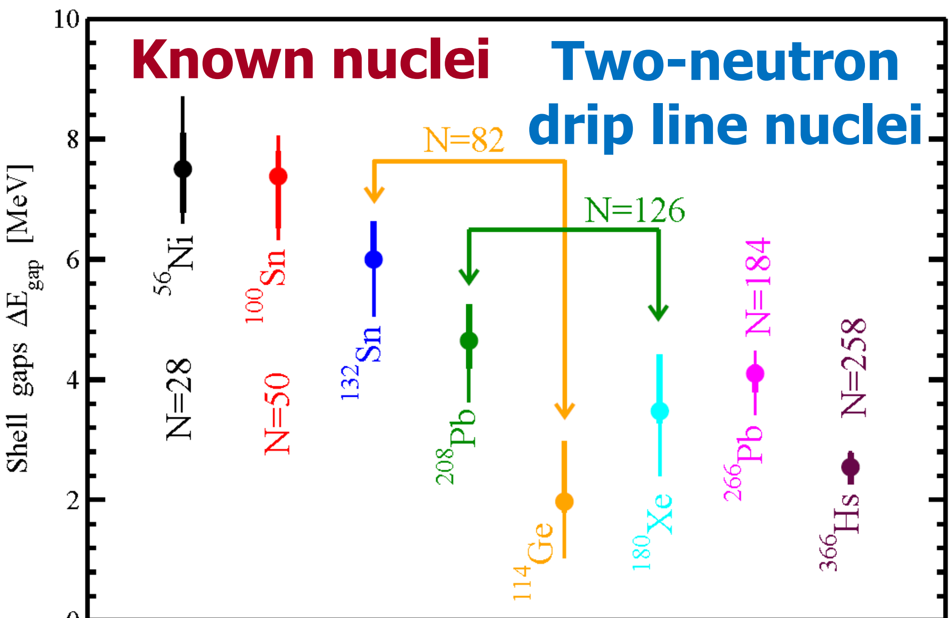
Region (parametrization)	calculated states (#)	compared states (#)
Actinides (NL3*)	415	209
Actinides (NL1)	444	217
Rare-earth (NL1)	360	149

Triaxial CRHB; fully self-consistent blocking, time-odd mean fields included, NL3*, Gogny D1S pairing, AA and S.Shawaqfeh, PLB 706 (2011) 177

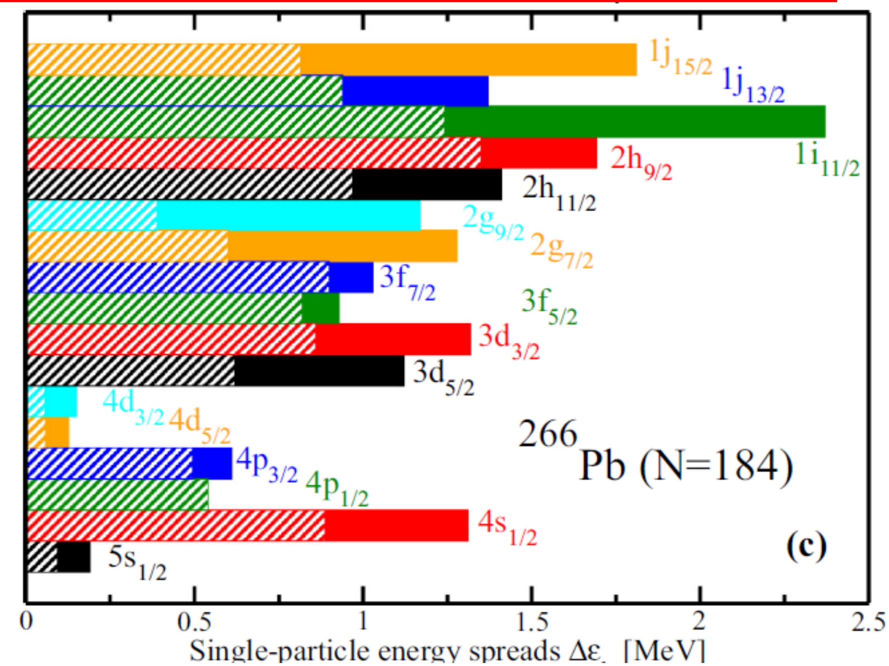
Two sources of deviations:

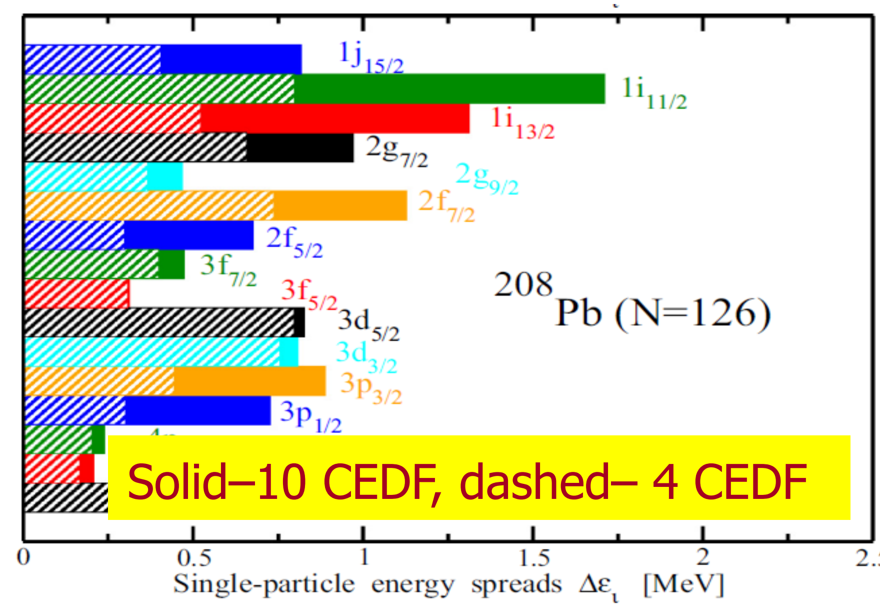
1. Low effective mass (stretching of the energy scale)
2. Wrong relative energies of the states

Systematic uncertainties in single-particle energies



Thin lines – 10 CEDF, thick – 4 CEDF

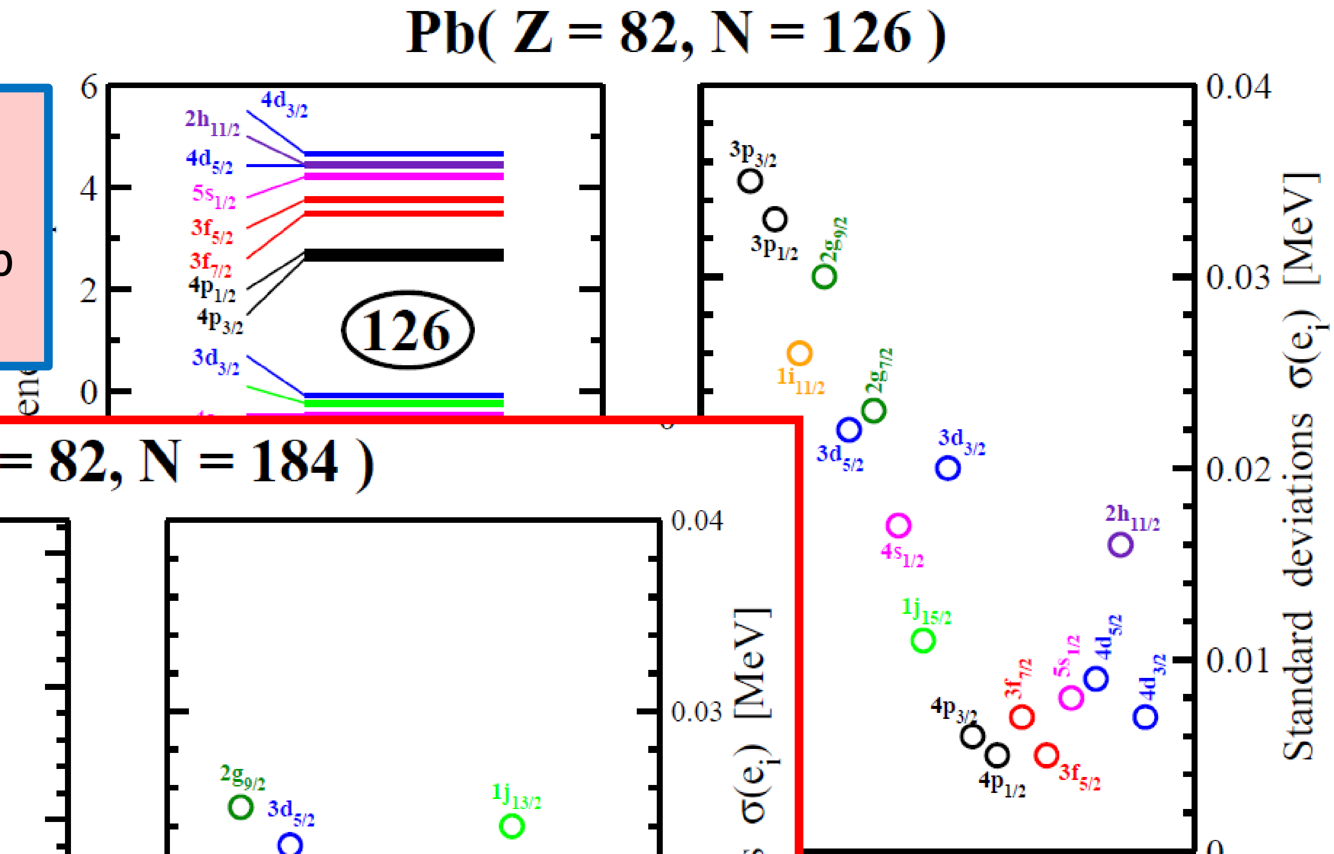


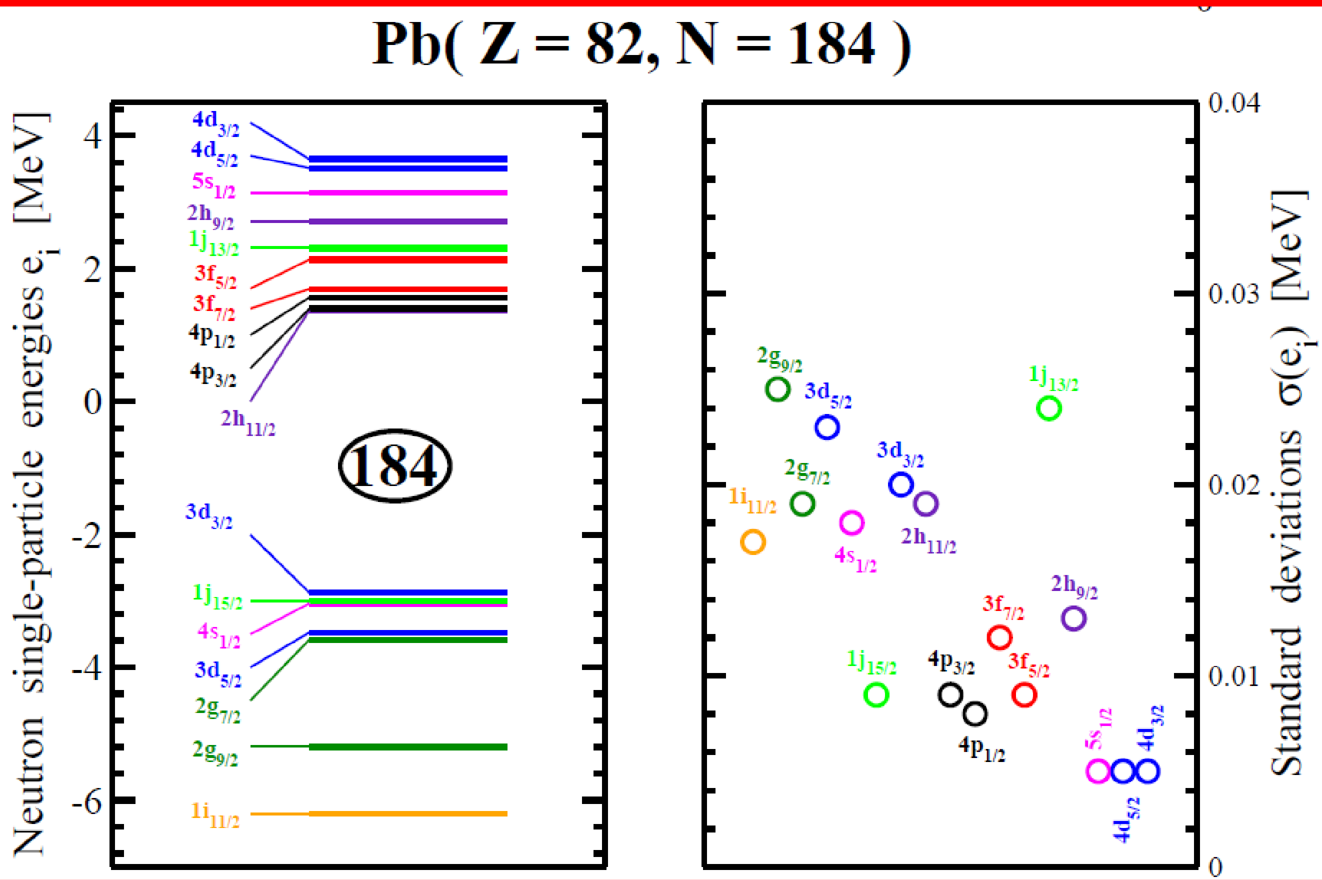


Solid–10 CEDF, dashed– 4 CEDF

Statistical errors in the single-particle energies

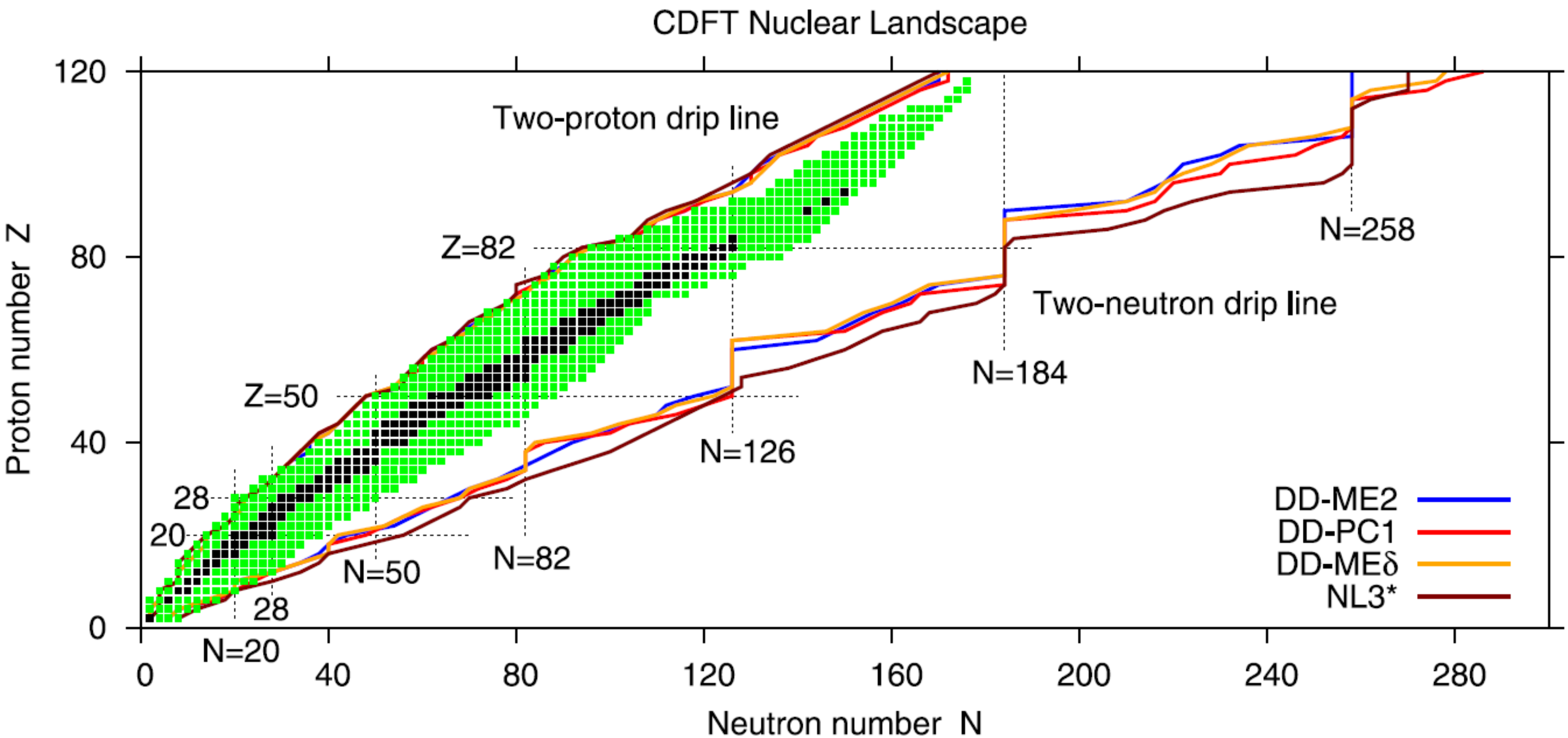
They are small and somewhat decrease on going to neutron-drip line





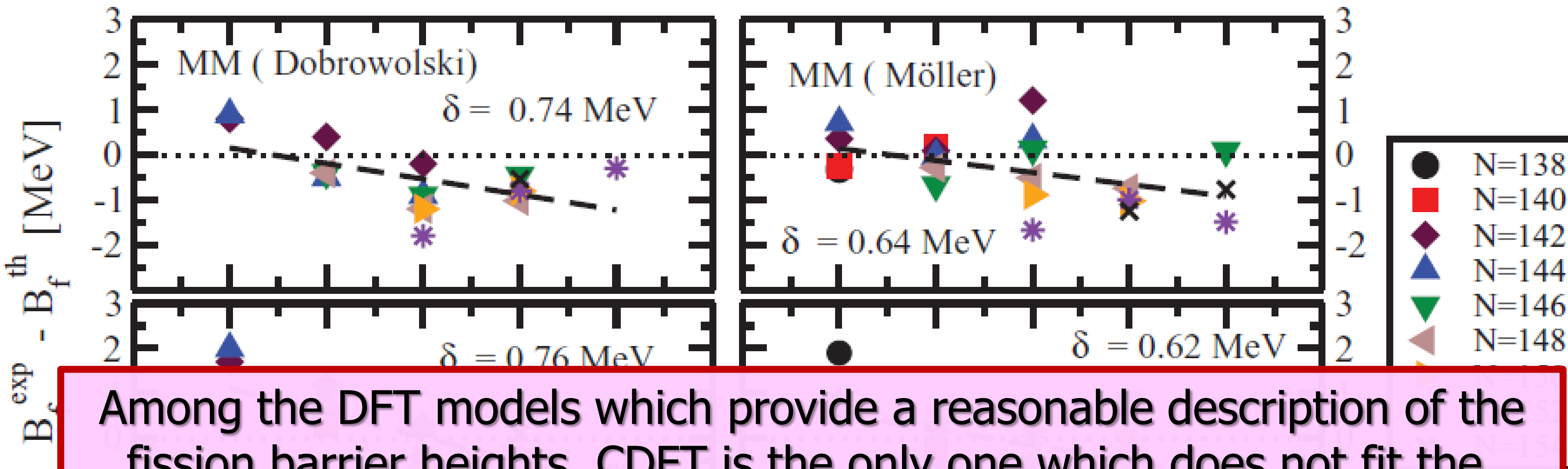
Average standard deviation for the single-particle energies is 0.196 [proton] (0.179 [neutron]) MeV in Skyrme UNEDF0, Gao et al, PRC 87, 034324 (2013)

The differences in the prediction of two-neutron drip line are mostly due to uncertainties in the position of the single-particle states



AA, S. Agbemava, D. Ray and P. Ring, PLB 726, 680 (2013)

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

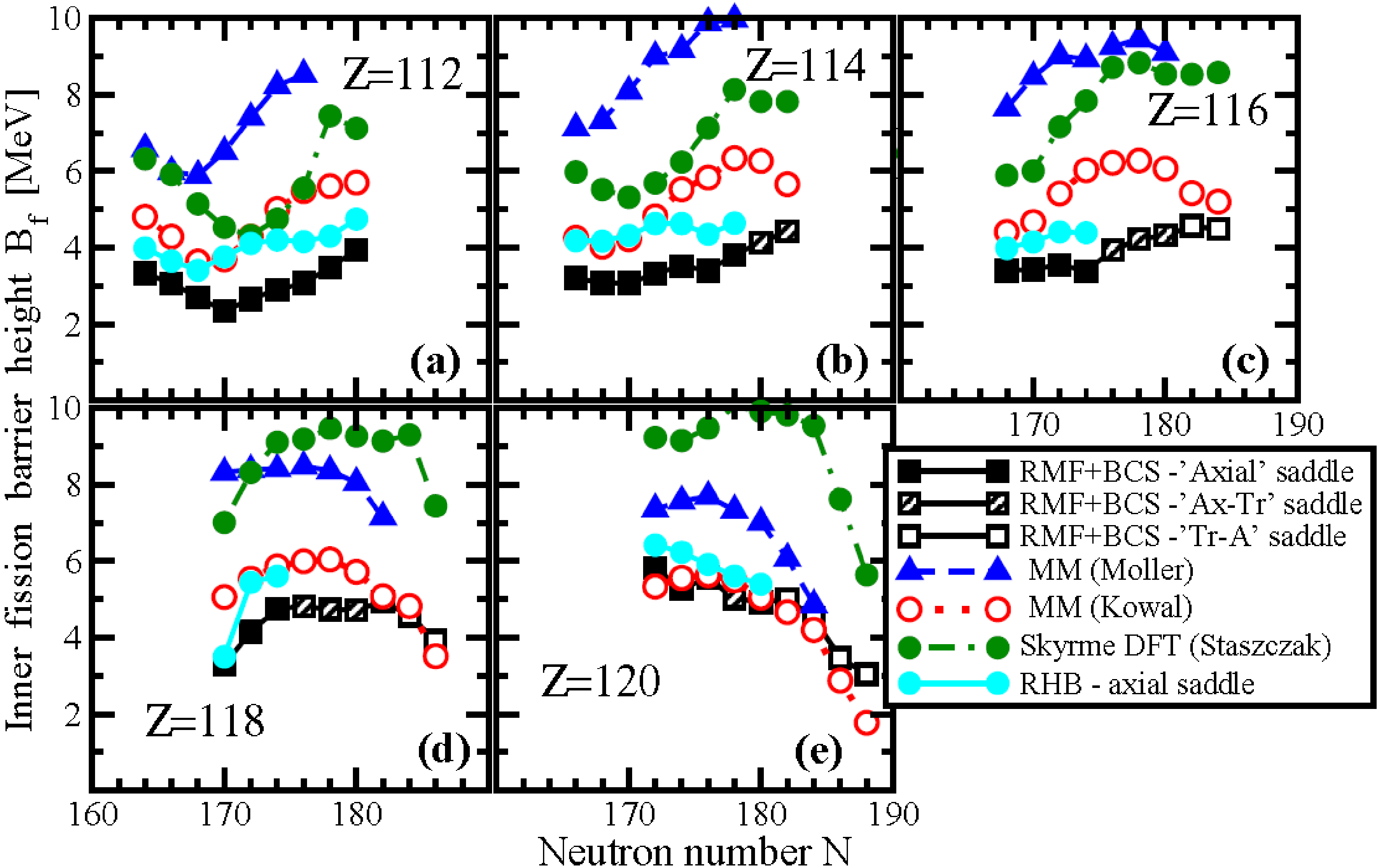


Among the DFT models which provide a reasonable description of the fission barrier heights, CDFT is the only one which does not fit the parameters to the inner fission barriers of actinides or their fission isomers.
Note also that liquid drop parameters of many mic+mac calculations are fitted to experimental fission barriers.

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)

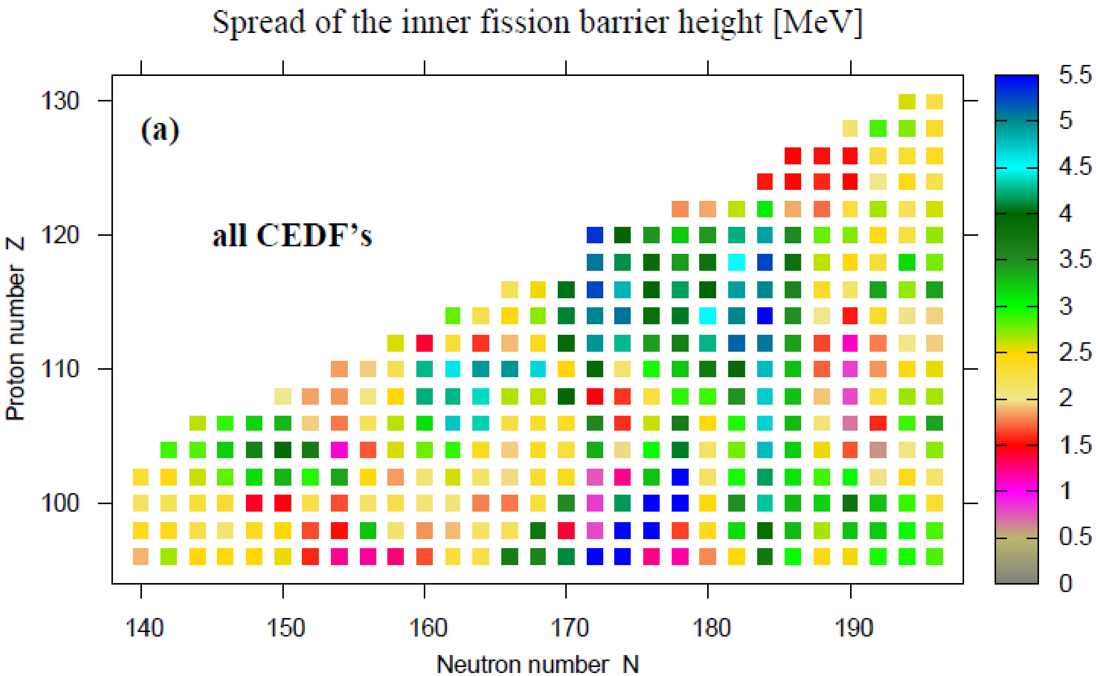
The heights of inner fission barriers in superheavy nuclei



AA, S. Agbemava, Acta Physica Polonica, 46, 405 (2015)

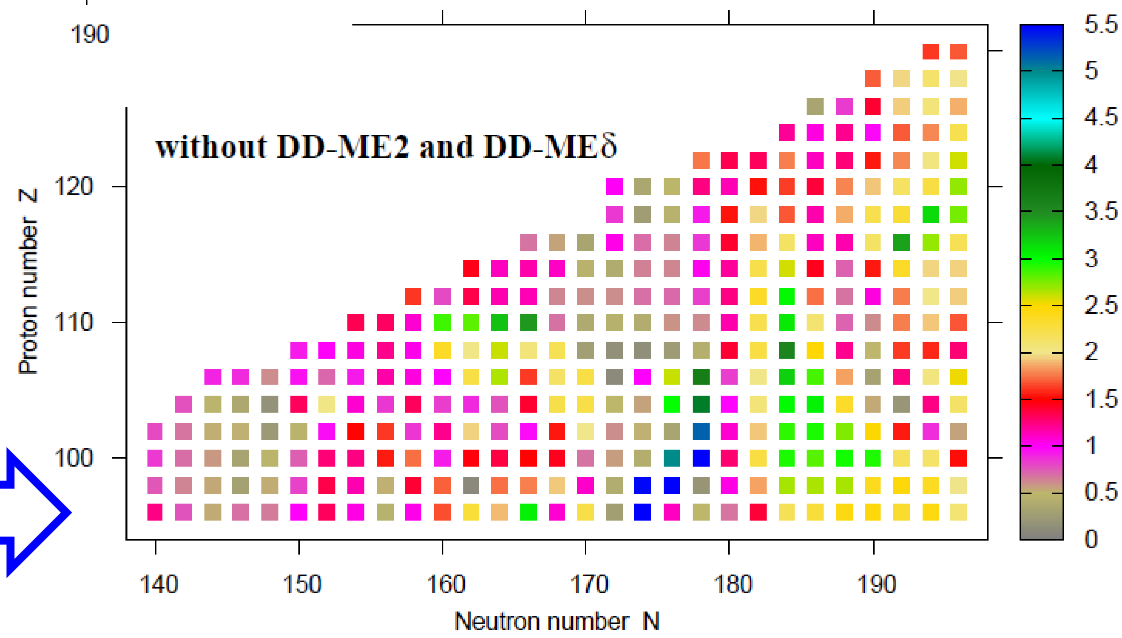
A. Staszczak et al, PRC 87, 024320 (2013) – Skyrme SkM*
M. Kowal et al, PRC 82, 014303 (2010) – WS pot. + Yukawa exponent. model
P. Moller et al, PRC 79, 064304 (2009) – folded Yukawa pot. + FRDM model

The spreads (theoretical uncertainties) in the heights of inner fission barriers in superheavy nuclei



Axial RHB calculations

Benchmarking of fission barriers in actinides (done for NL3*, DD-PC1 and PC-PK1) reduces theoretical uncertainties and makes the description of fission barriers more predictive



Conclusions:

1. Different nuclear phenomena are reasonably well described in the CDFT framework. This, in a sense, create a problem to discriminate the approaches.

2. At present stage, we can also estimate theoretical uncertainties and their propagation beyond the known region of nuclei. However, this is to a degree subjective. Note that systematic uncertainties are substantially larger than statistical errors.

3. Many theoretical uncertainties emerge from inaccuracies in the description of the single-particle states. At present, this is a real bottleneck of the DFT models (both relativistic and non-relativistic ones).

Conclusions:

4. Note that different phenomena/observables or regions of nuclear chart are differently affected by the uncertainties in the single-particle energies.

5. Theoretical uncertainties for some physical observables contain a regular [smooth] component (which is reasonably well described) and chaotic component (where the model becomes unpredictable). **How to treat such a situation with statistical methods and what we can learn from that?**

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Global performance

Ground state observables: S.E.Agbemava, AA, D.Ray and P.Ring, PRC **89**, 054320 (2014) (37 pages)
includes as a supplement to the manuscript
complete mass, deformation and radii table for even-even nuclei with Z<104 obtained with DD-PC1

Neutron drip lines and sources of their uncertainties:
PLB 726, 680 (2013), PRC **89**, 054320 (2014) , PRC 91, 014324 (2015)

Superheavy nuclei reexamined
AA. S.E.Agbemava, Acta Physica Polonica, 46, 405 (2015)
S.E.Agbemava, AA, T. Nakatsukasa, P. Ring, PRC 92, 054310 (2015)
includes as a supplement to the manuscript
complete mass, deformation and radii table for even-even nuclei with 106<Z<130 obtained with DD-PC1 and PC-PK1

Global performance

Octupole deformation in even-even nuclei

S. Agbemava and AA, PRC 93, 044304 (2013)

New region of octupole deformation is predicted

Systematic studies in local regions (mostly actinides)

Accuracy of the description of deformed one-quasiparticle states

AA and S.Shawaqfeh, PLB 706 (2011) 177

Fission barriers in actinides and SHE

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

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

and to be published

Pairing and rotational properties of even-even of odd-mass actinides

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

AA, Phys. Scr. 89 (2014) 054001