Nuclear shapes in covariant density functionals theory: recent results

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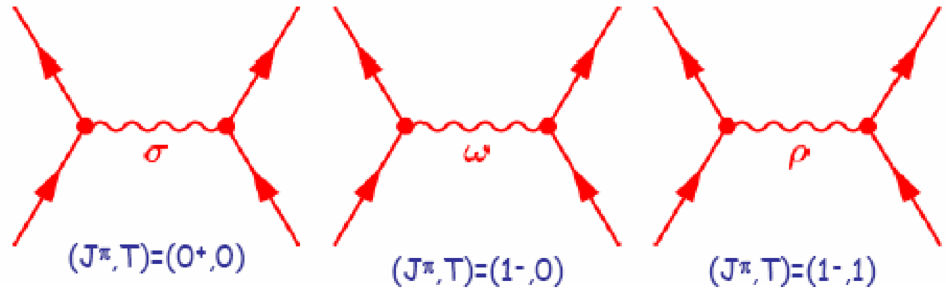
1. Motivation
2. Global analysis of octupole deformation with an assessment of theoretical uncertainties.
3. The competition of oblate and spherical deformations in superheavy nuclei
4. Extreme deformations and clusterization in the A~40 N~Z nuclei
5. Conclusions

In collaboration with

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

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

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

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**

Motivation: few words about global studies and assesment of theoretical uncertainties

Global performance

Ground state observables: S.E.Agbemava, AA, D.Ray and P.Ring, PRC **89**, 054320 (2014), AA and S. Abgemava PRC 93, 054310 (2016)

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

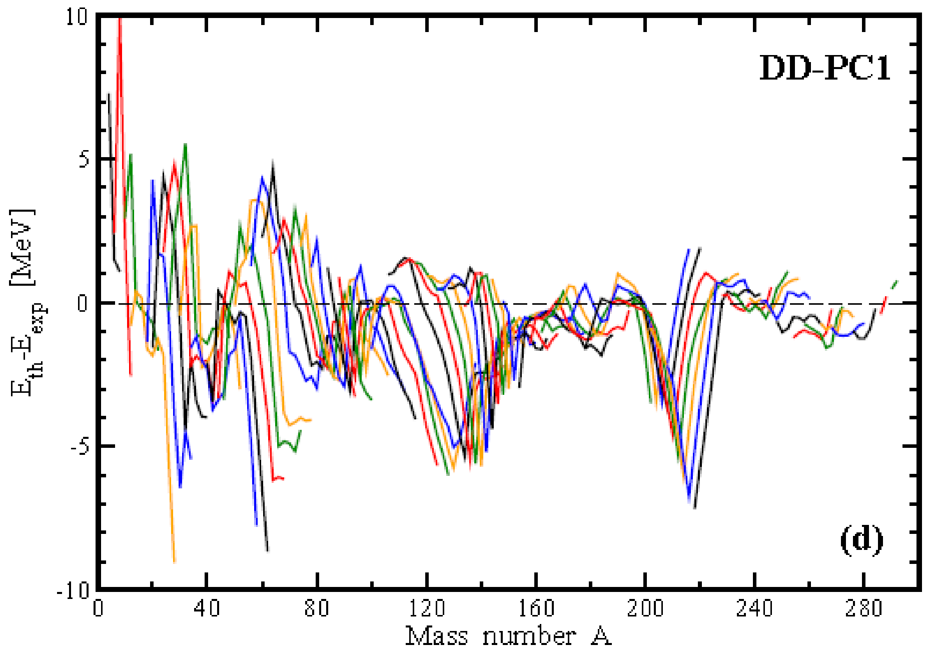
Systematic studies in local regions (mostly actinides)

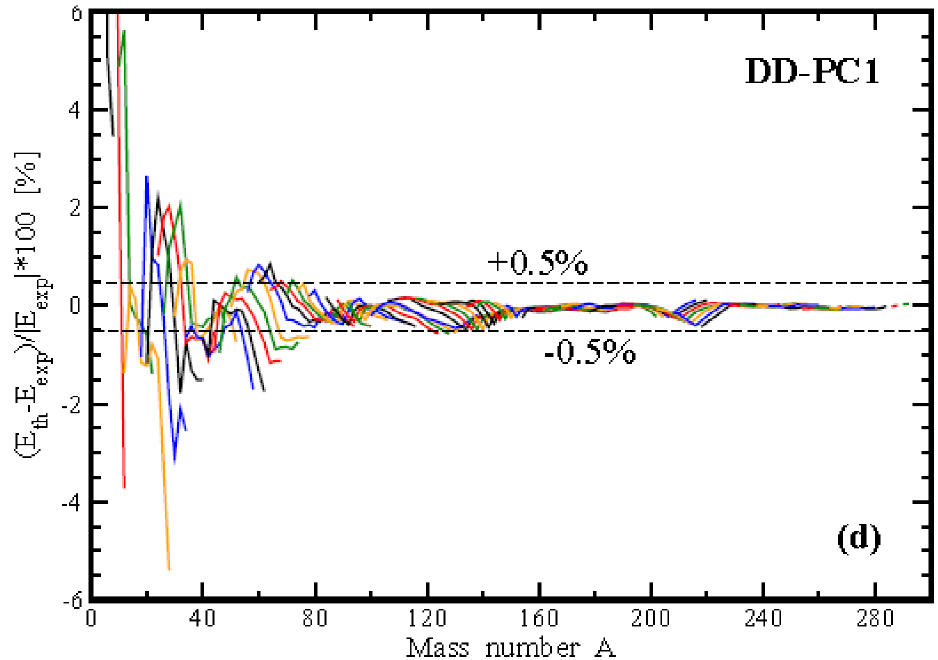
Accuracy of the description of deformed one-quasiparticle states
AA and S.Shawaqfeh, PLB 706 (2011) 177

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)

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

Systematic errors in the RHB description of masses





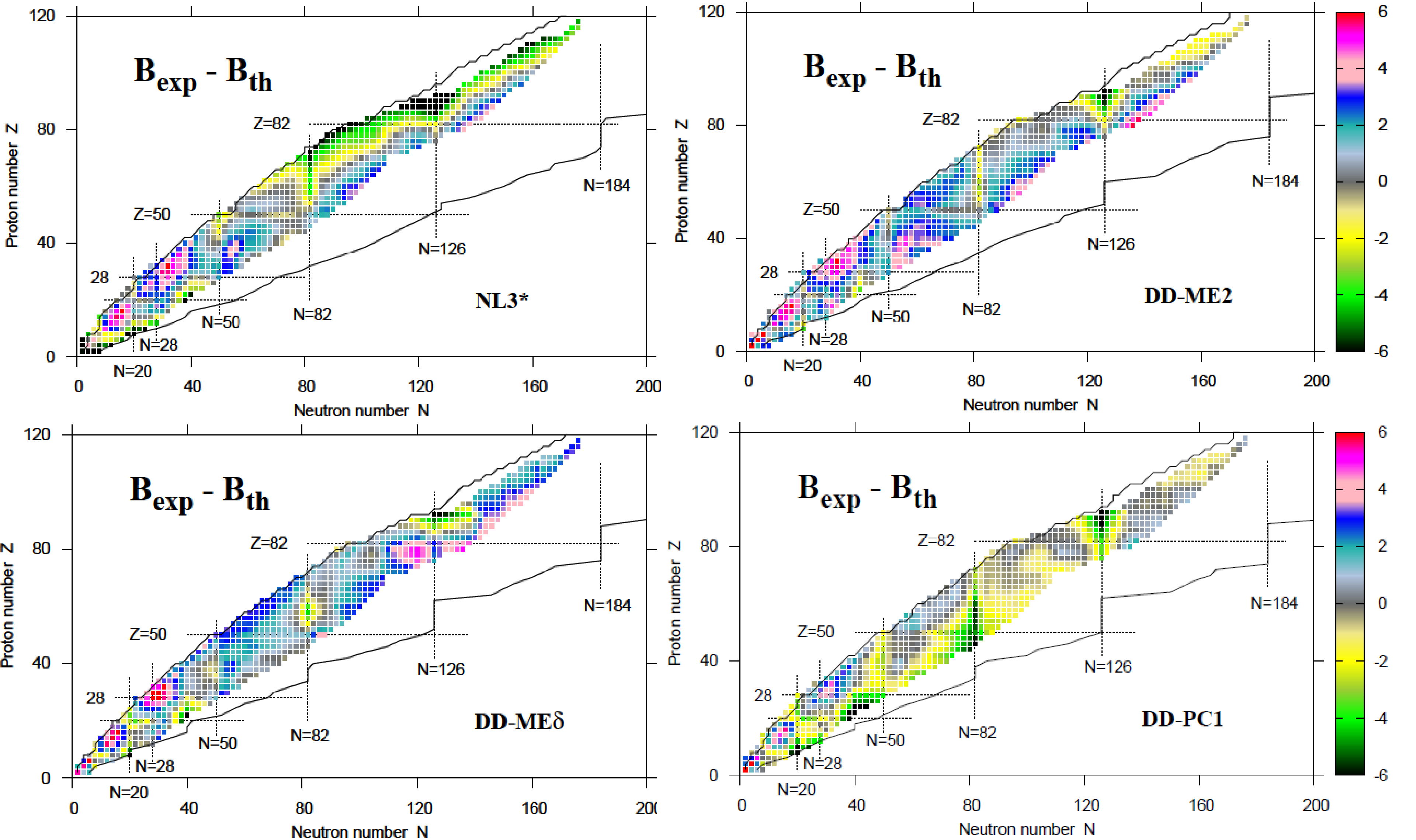
EDF	measured	measured+estimated		
	$\Delta E_{\rm rms}$	$\Delta E_{\rm rms}$	$\Delta(S_{2n})_{\rm rms}$	$\Delta(S_{2p})_{\rm rms}$
NL3*	2.96	3.00	1.23	1.29
DD-ME2	2.39	2.45	1.05	0.95
DD-MEδ	2.29	2.40	1.09	1.09
DD-PC1	2.01	2.15	1.16	1.03

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

Uncertainties in radii

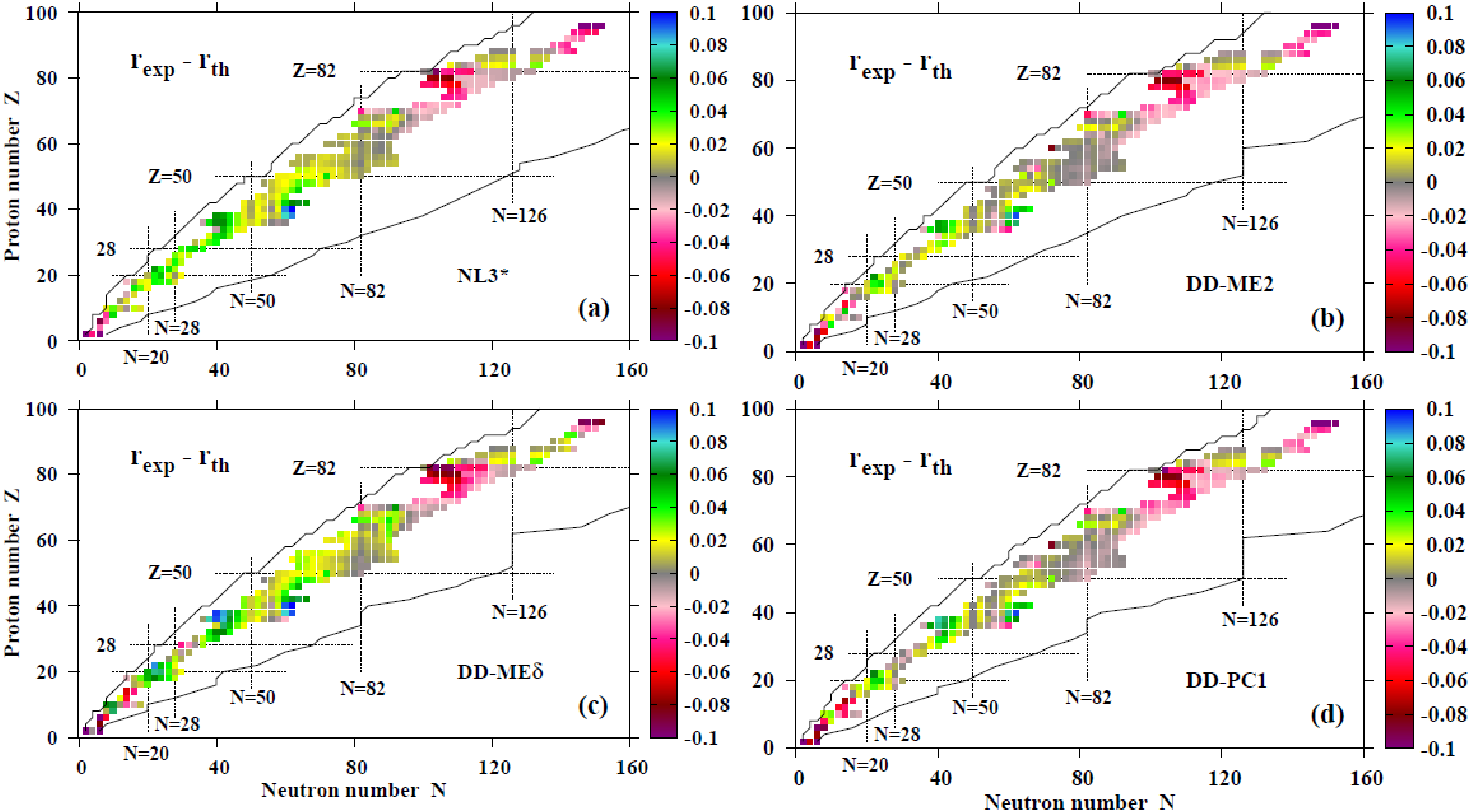
CEDF	Δr_{ch}^{rms} [fm]
NL3*	0.0283
DD-ME2	0.0230
DD-MEd	0.0329
DD-PC1	0.0253

Masses: the deviations between theory and experiment



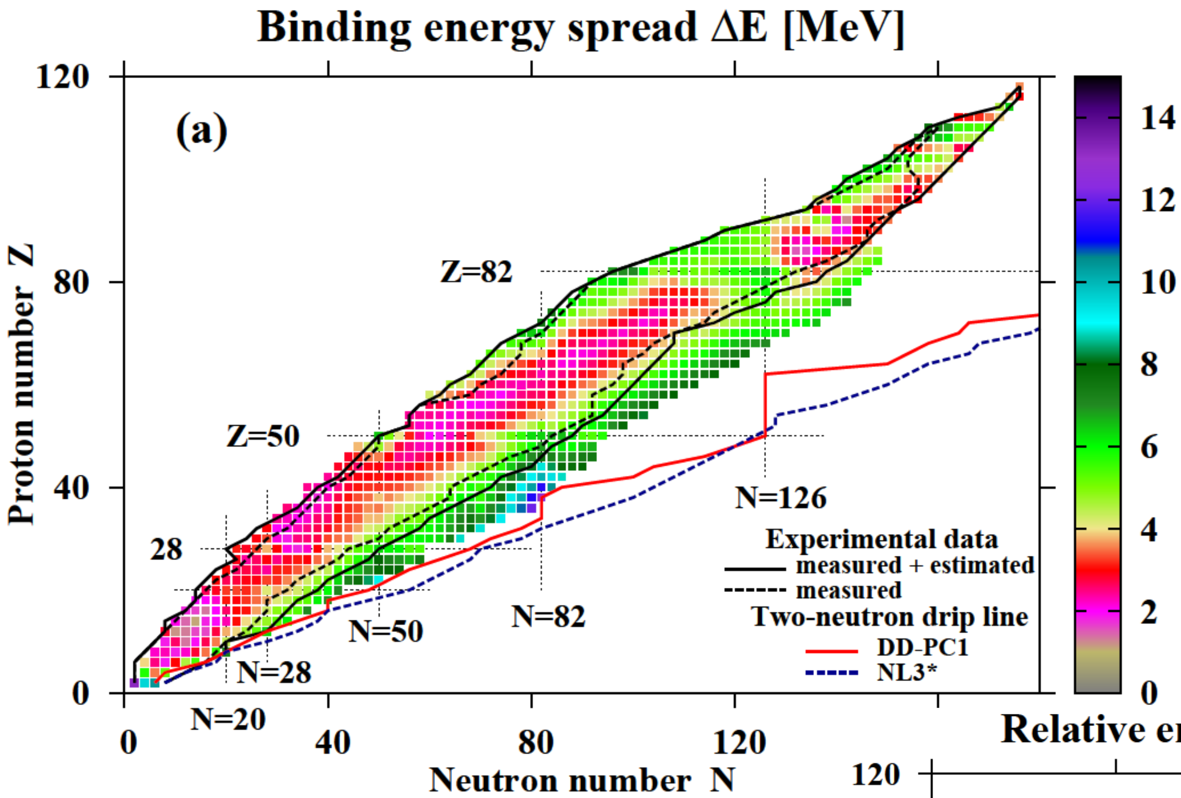
The residuals are non-statistical in nature → the difficulty in the estimation of systematic errors in unknown regions

Systematic errors in the description of charge radii



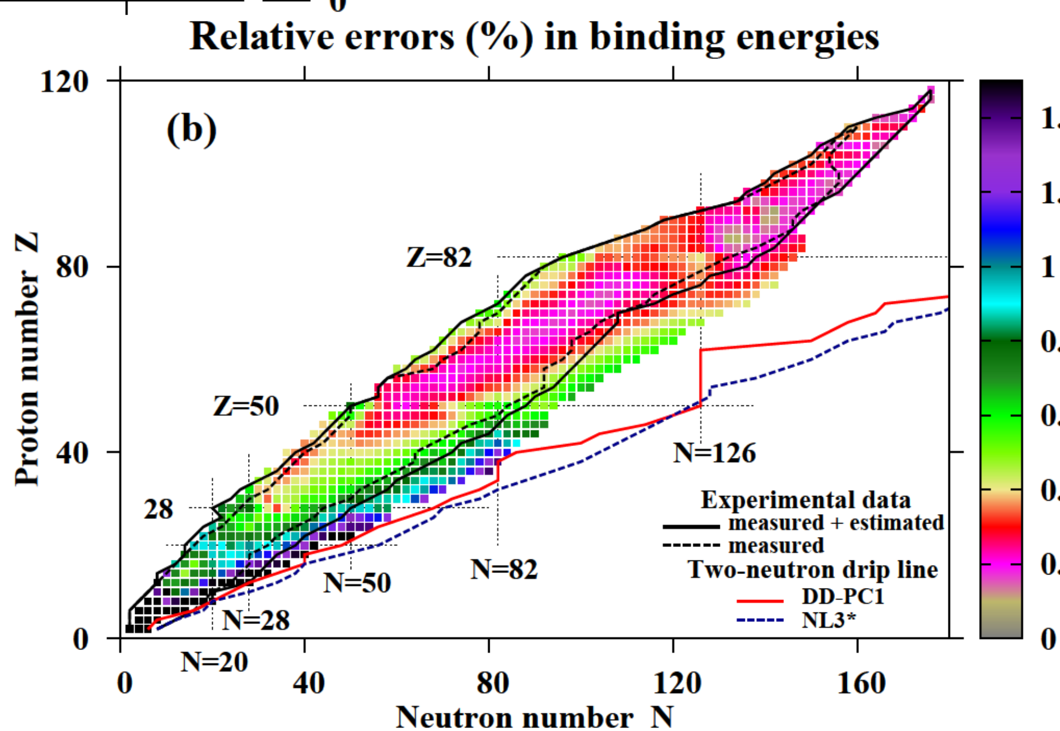
Charge radii – rather well described in all functionals

- very little difference between CEDFs



Propagation of theoretical uncertainties in masses with isospin

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



Impact of mass measurements at FRIB:

some improvement of isovector properties of EDFs,

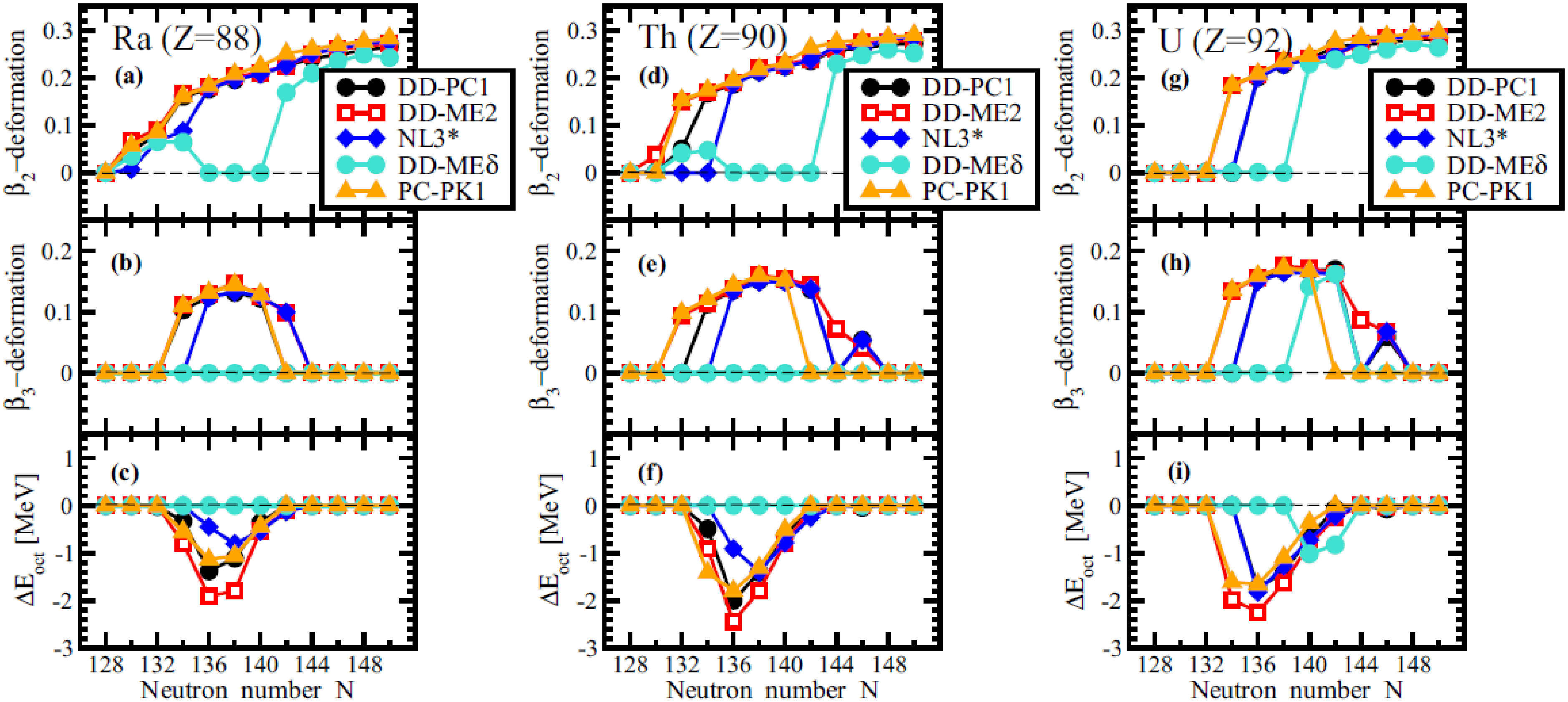
some reduction (not elimination) of theoretical uncertainties in mass predictions of neutron-rich nuclei

Global analysis of octupole deformation with an assessment of theoretical uncertainties.

according to S. Agbemava, AA and P. Ring, PRC 93, 044304 (2015)

RHB calculations with separable pairing

Octupole deformation in Ra-Th-U isotopes and related theoretical uncertainties in predictions



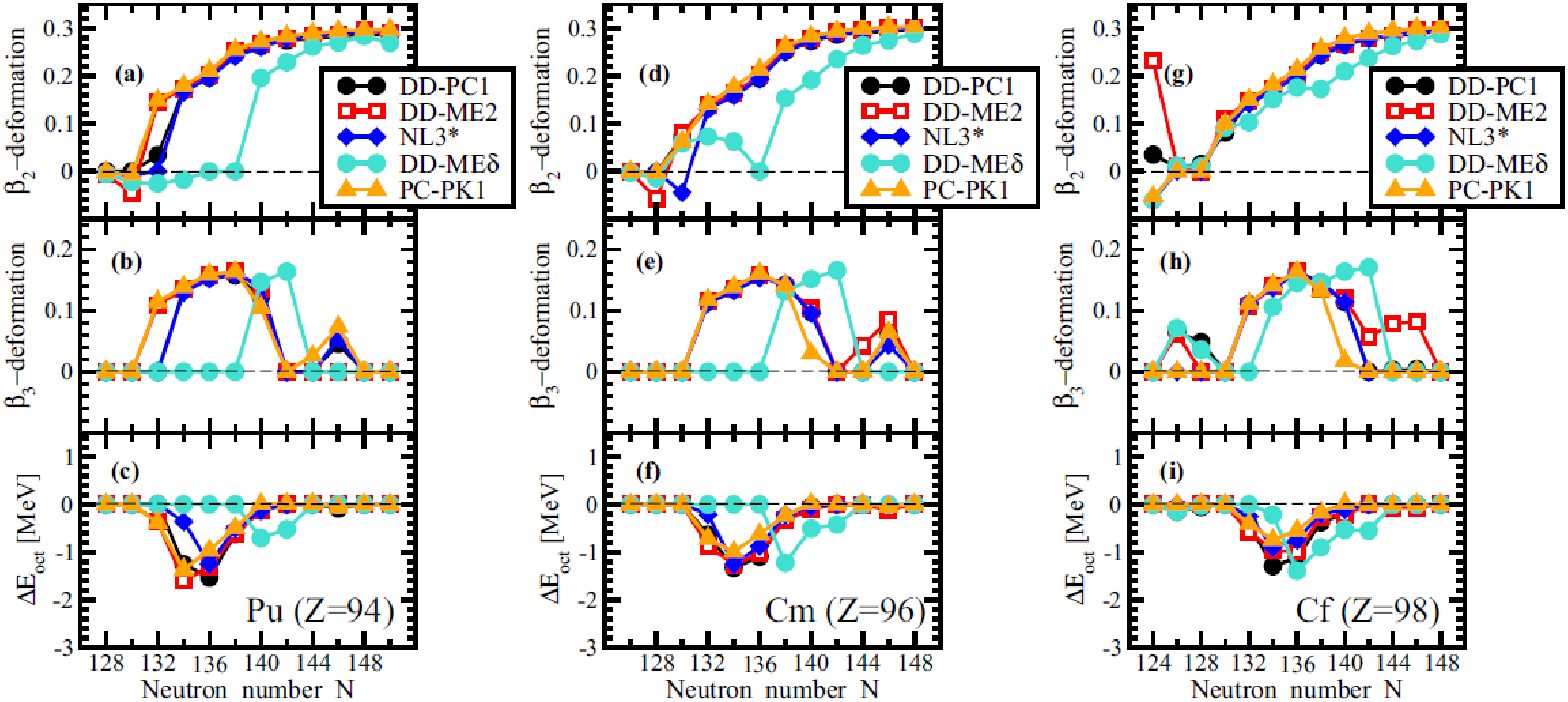
$$\Delta E_{\rm oct} = E^{\rm oct}(\beta_2,\beta_3) - E^{\rm quad}(\beta_2',\beta_3'=0)$$

$|\Delta E_{\rm oct}|$ - the gain of binding due to octupole deformation

- indicator of stability of the octupole deformed shapes (small – octupole soft, large – static octupole deformation)

The maximum gain in binding due to octupole deformation takes place at N~136 in the Ra, Th and U isotopes which agrees with experimental data.

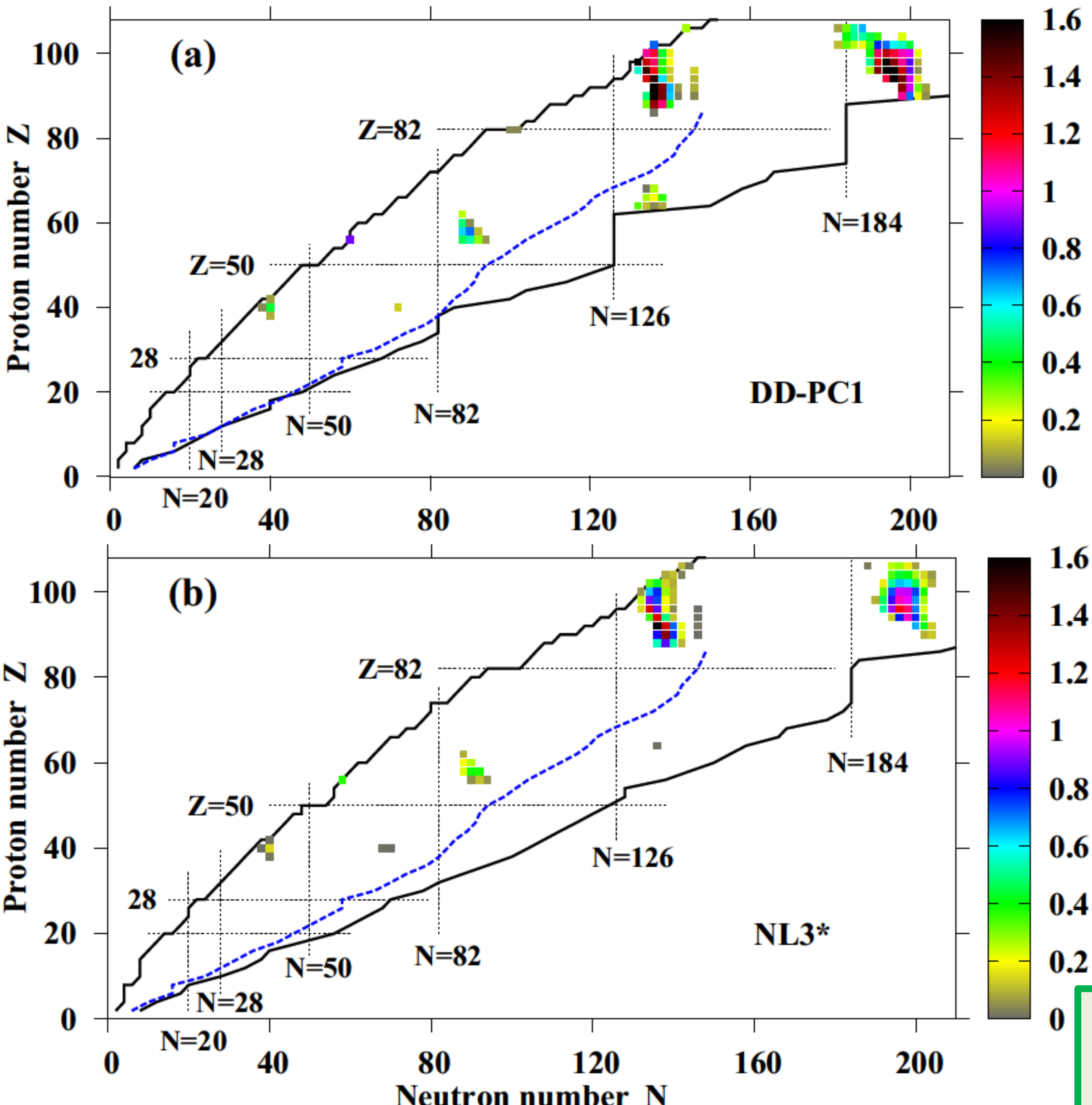
Octupole deformation in Pu-Cm-Cf isotopes and related theoretical uncertainties in predictions



There are no experimental data on octupole deformed Pu, Cm and Cf isotopes

The RHB calculations predict the weakening of the stabilization of octupole deformation with increasing Z

Global search for octupole deformed nuclei

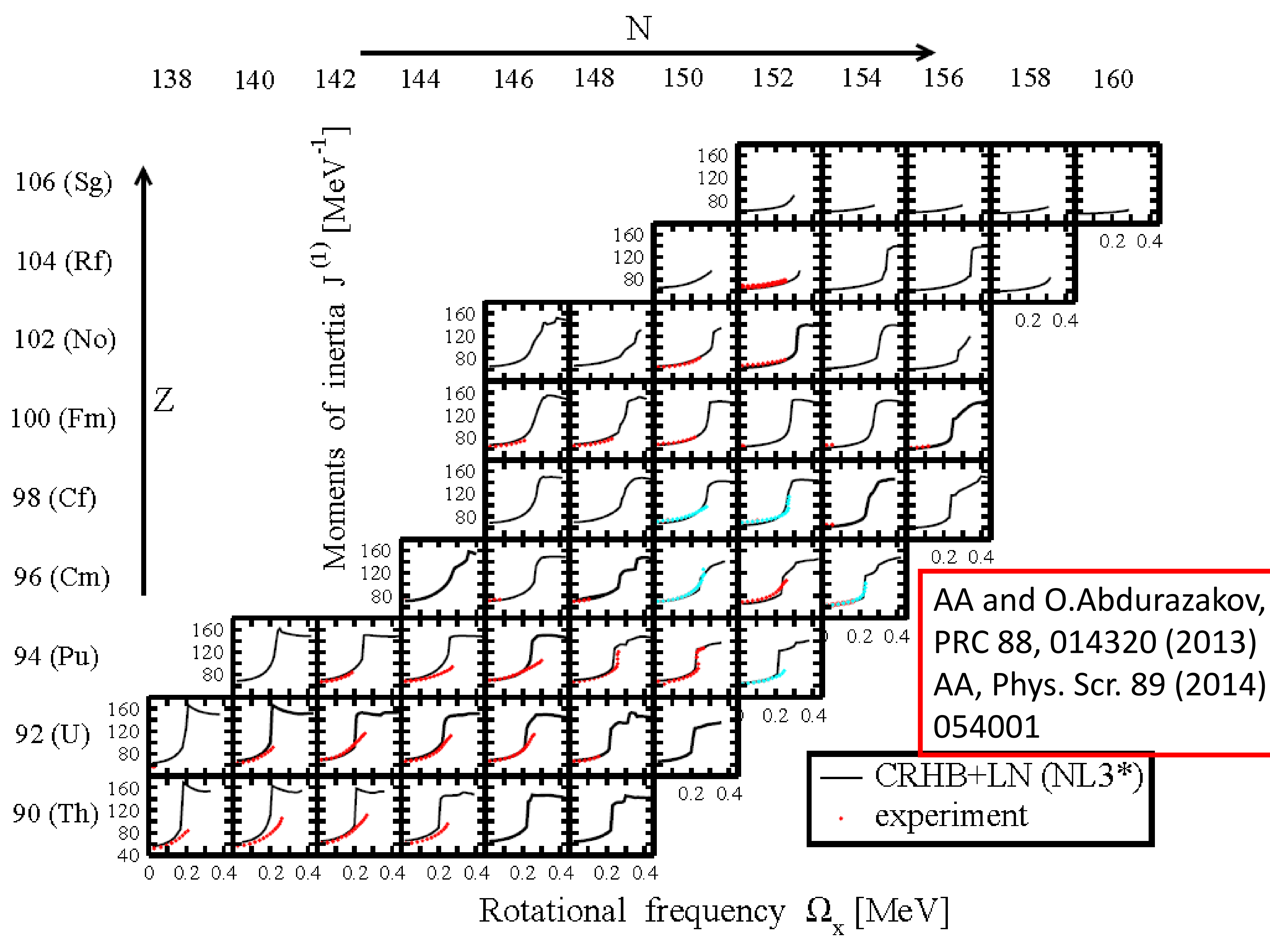


Colormap shows the gain in binding due to octupole deformation.

A new region of octupole deformation, centered around $Z \sim 98$, $N \sim 196$, has been predicted for the first time.

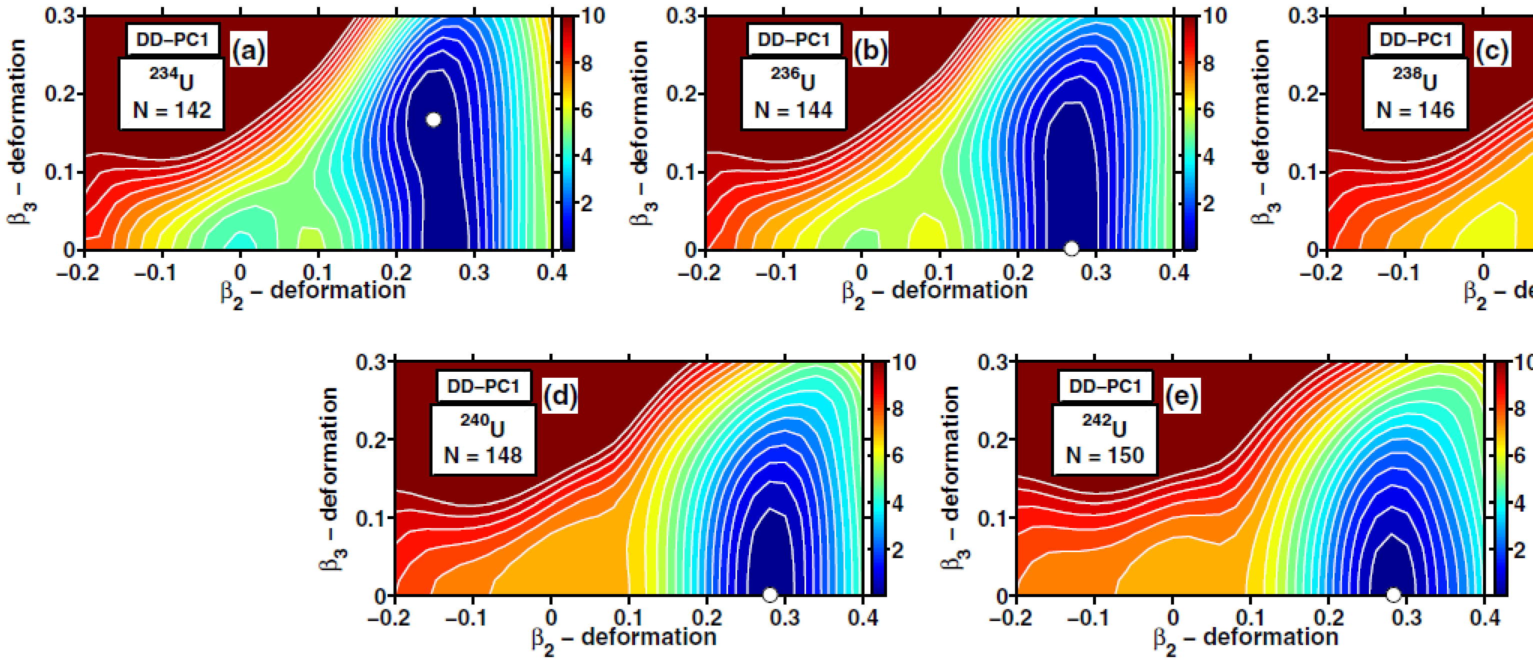
the interaction of the $2h_{11/2}$ and $1k_{17/2}$ neutron orbitals and of the $1i_{13/2}$ and $2f_{7/2}$ proton orbitals is responsible for it

Will impact fission recycling in neutron star mergers



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]
Rotational frequency Ωx [MeV]
CRHB+LN (NL3*)
experiment
AA and O.Abdurazakov, PRC 88, 014320 (2013)
AA, Phys. Scr. 89 (2014) 054001

How to understand these features?



1. PES of the $N \leq 146$ actinides are soft in octupole deformation. Thus, at low spin these nuclei are in octupole vibrational regime in which the CRHB+LN calculations with no octupole deformation describe well the moments of inertia. However, the transition to static octupole deformation (not taken into account in the calculations) takes at higher spin; it leads to a delay of alignment.

2. PES of the $N \geq 148$ actinides are stiff in octupole deformation. → no transition to static octupole deformation at high spin and good description in the CRHB+LN calculations.

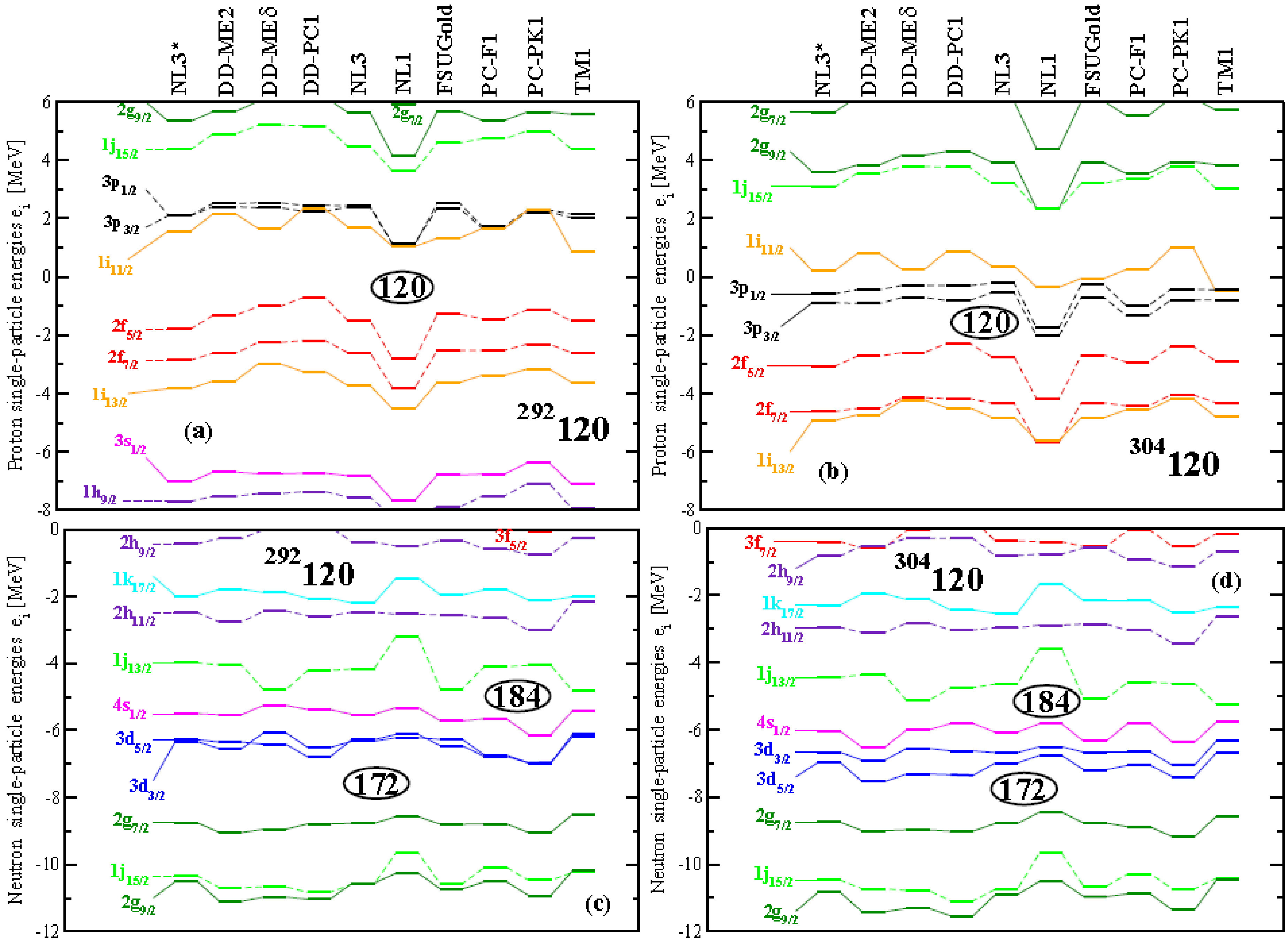
The competition of oblate and spherical deformations in superheavy nuclei

according to S.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

RHB calculations with separable pairing

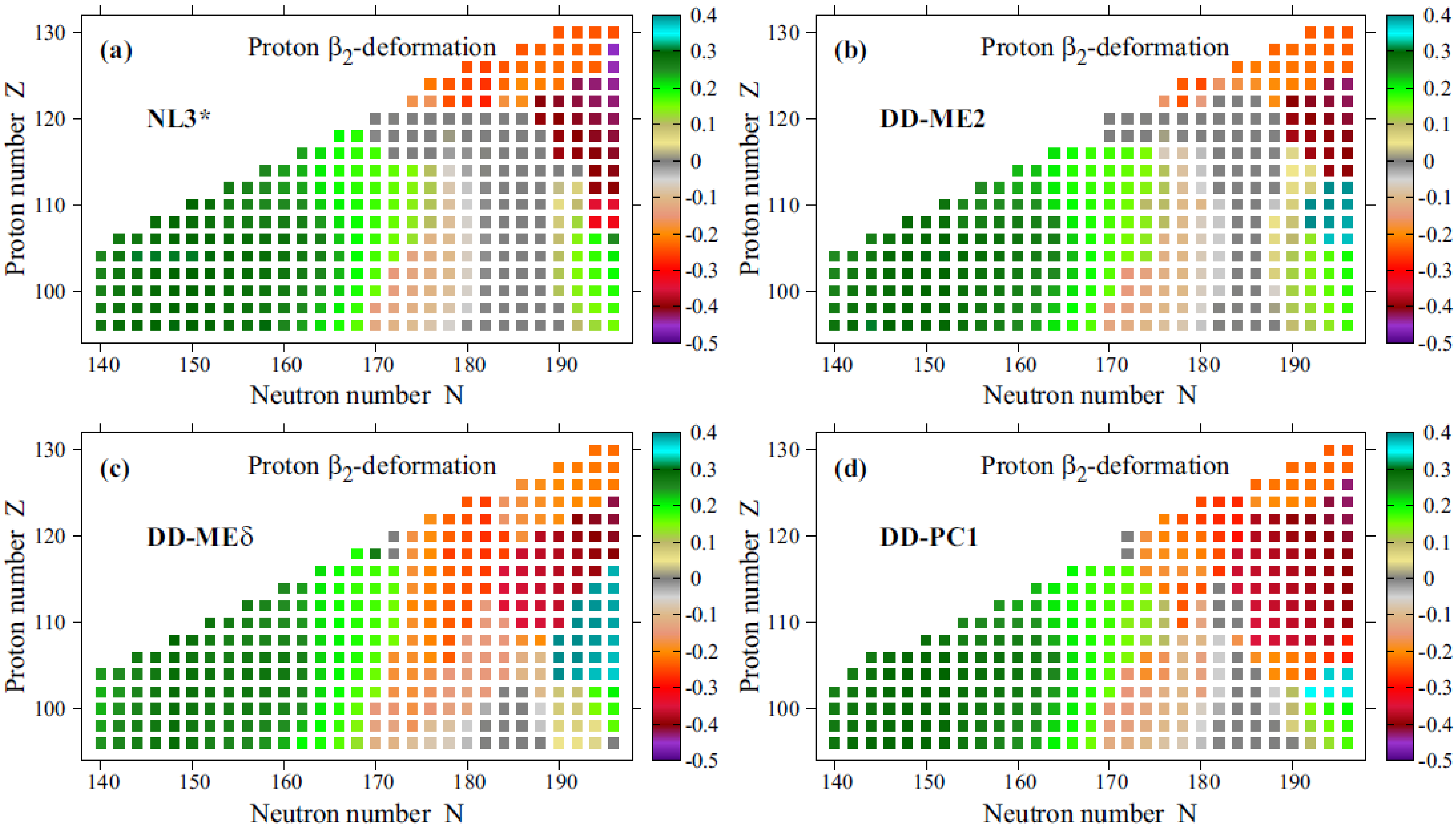


NL3*
DD-ME2
DD-MEδ
DD-PC1
NL3
NL1
FSUGold
PC-F1
PC-PK1
TM1
Proton single-particle energies e_i [MeV]
Neutron single-particle energies e_i [MeV]
(a)
(b)
(c)
(d)
$^{292}120$
$^{304}120$
120
184
172
$2g_{9/2}$
$2g_{7/2}$
$1j_{15/2}$
$3p_{1/2}$
$3p_{3/2}$
$1i_{11/2}$
$2f_{5/2}$
$2f_{7/2}$
$1i_{13/2}$
$3s_{1/2}$
$1h_{9/2}$
$2h_{9/2}$
$3f_{5/2}$
$3f_{7/2}$
$1k_{17/2}$
$2h_{11/2}$
$1j_{13/2}$
$4s_{1/2}$
$3d_{5/2}$
$3d_{3/2}$

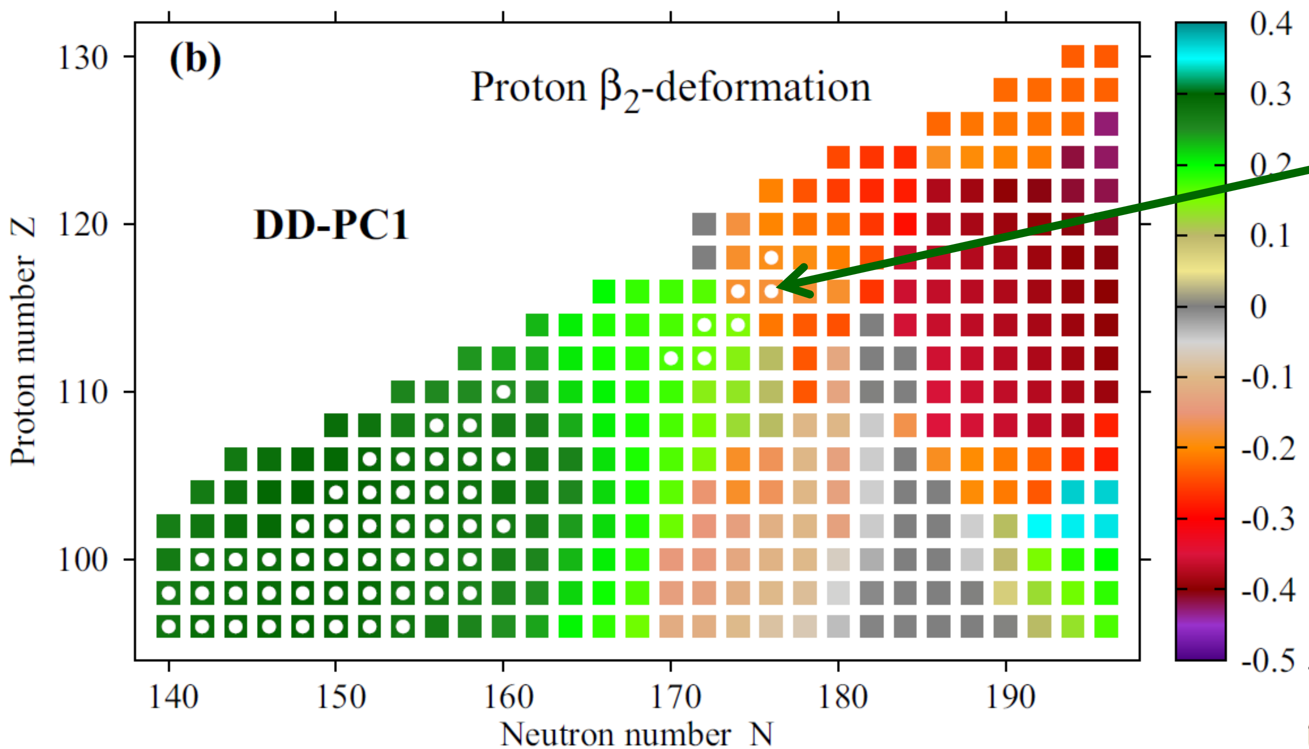
Deformation effects on shell structure

→ Very important – deformed results differ substantially from spherical ones

Unusual feature: oblate shapes above the spherical shell closures

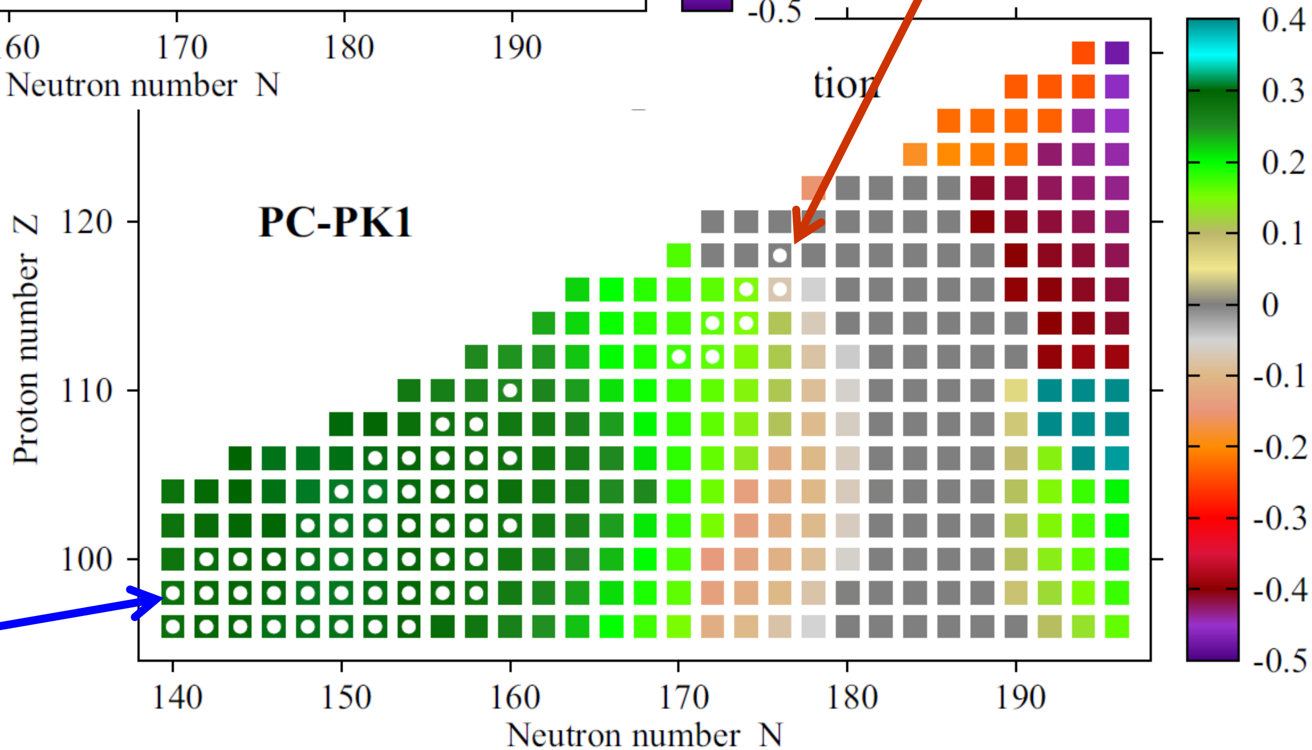


Results for PC-PK1 are very similar to the ones with NL3*



DD-PC1: Experimental Z=116, 118 nuclei are oblate

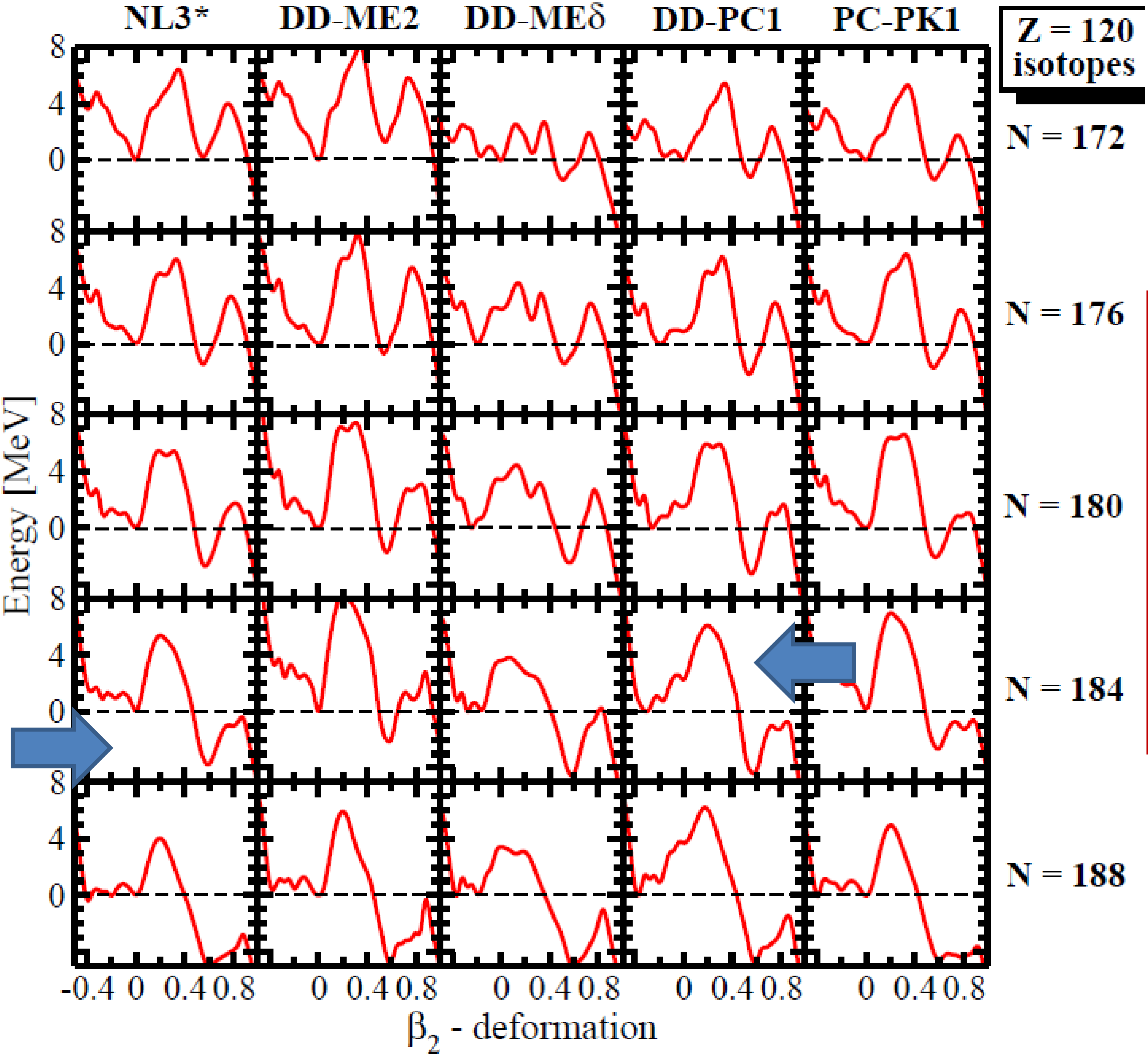
PC-PK1: Experimental Z=118 nucleus is spherical



Other experimental SHE are prolate

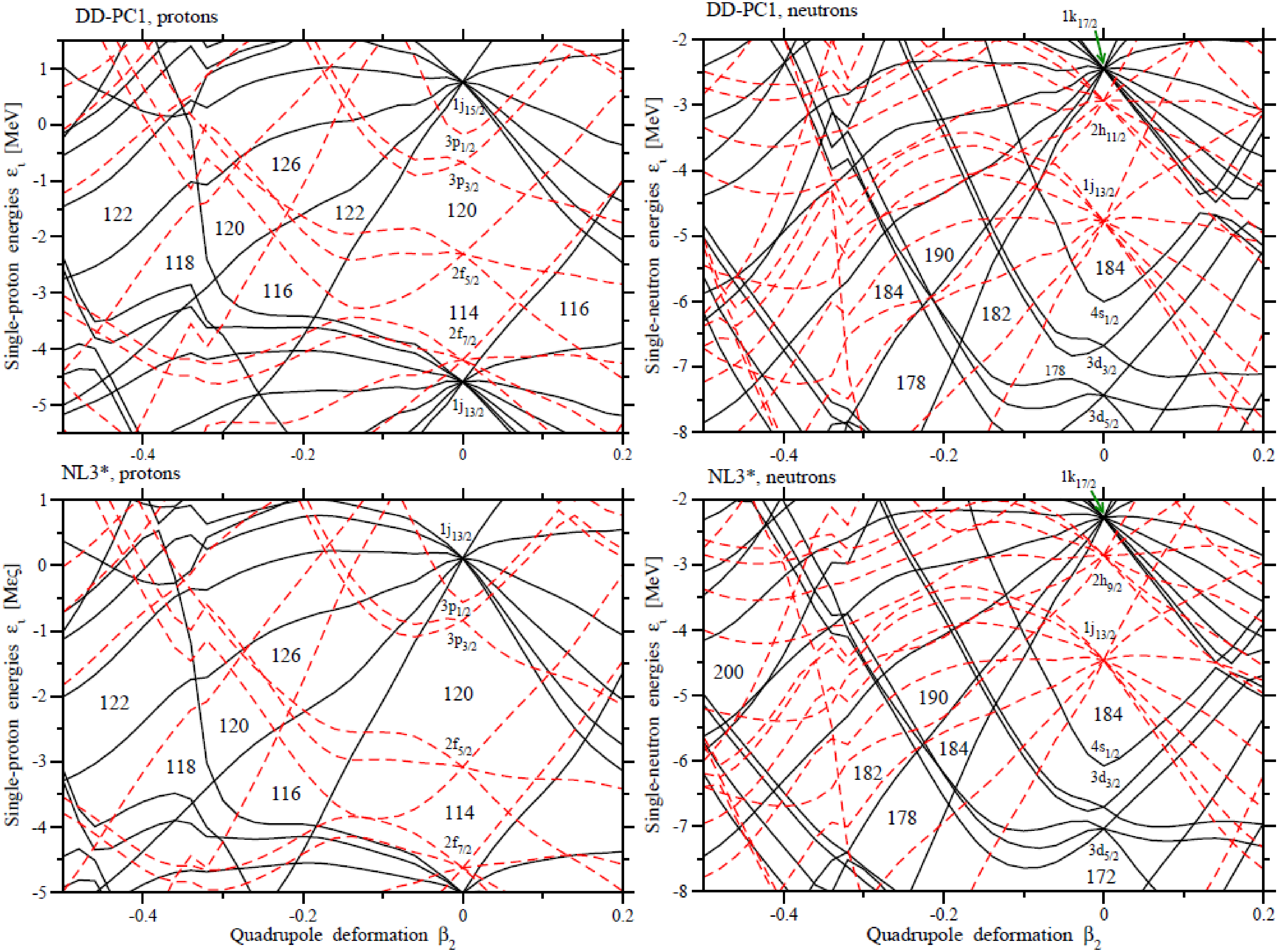
Open circles – experimentally observed nuclei

S.Agbemava, AA, T. Nakatsukasa, P. Ring ,PRC 92, 054310 (2015)



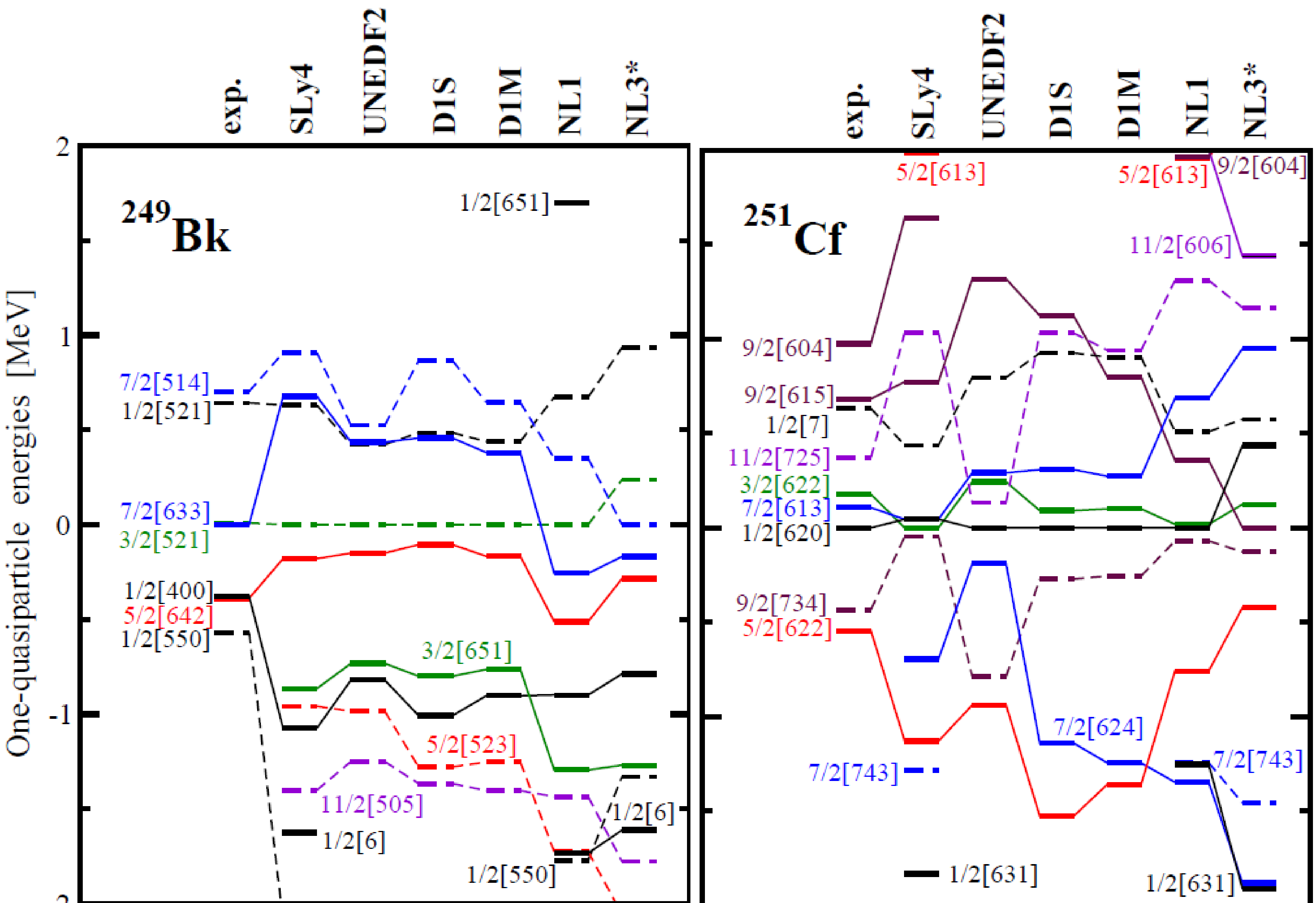
Potential energy surfaces in axially symmetric RHB calculations with separable pairing

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



S.Agbemava, AA, T. Nakatsukasa, P. Ring ,PRC 92, 054310 (2015)

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



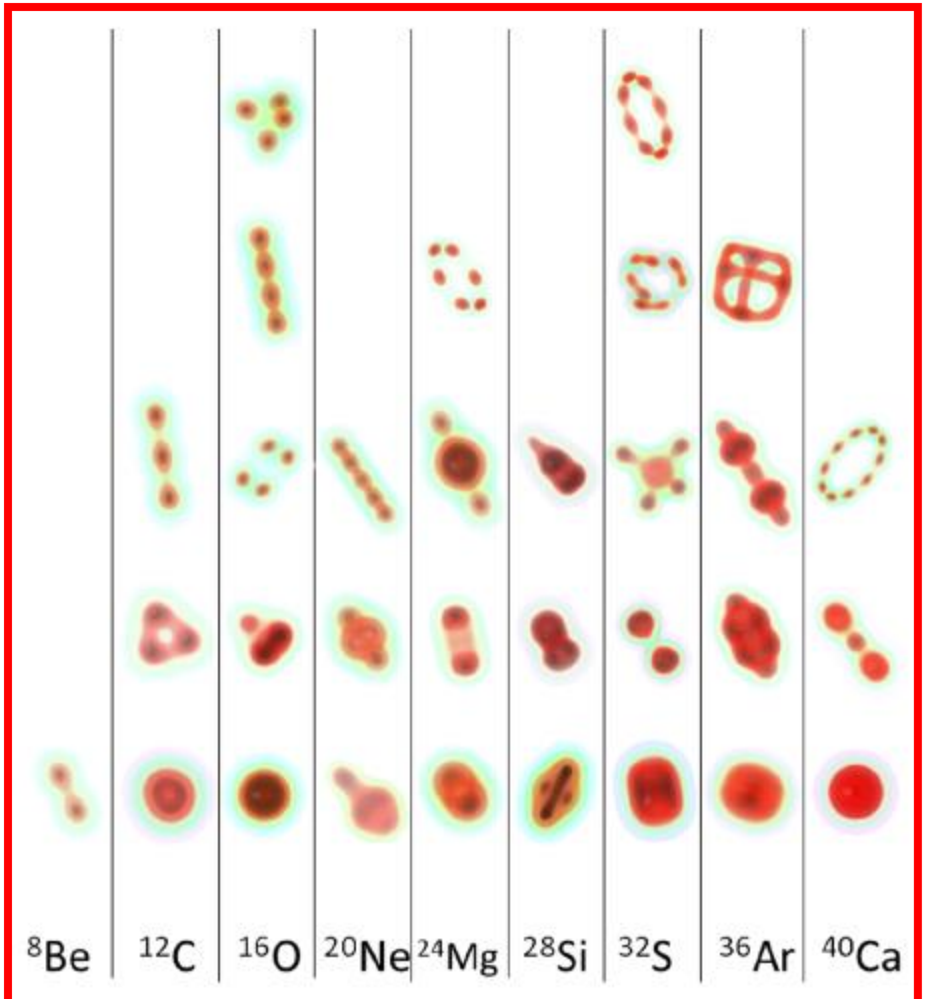
J.Dobaczewski, AA, M.Bender, L.M.Robledo, Yue Shi, NPA 944 (2015) 388

Extreme deformations and clusterization in the A~40 N~Z nuclei

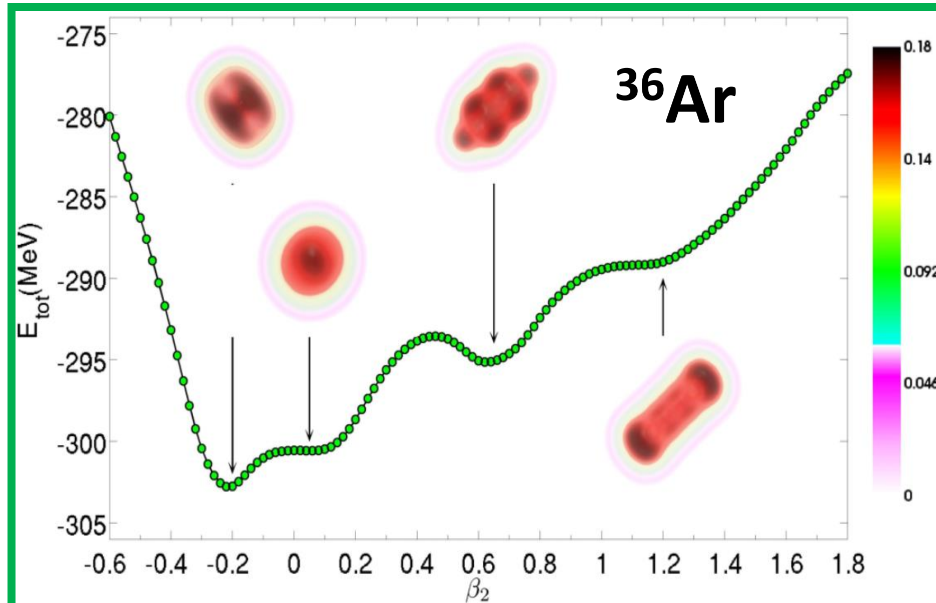
according to D. Ray and AA, PRC 94, 014310 (2016)

CRMF calculations with no pairing

Density functional studies of cluster states in nuclei



From J.P. Ebran et al, PRC 90, 054329 (2014)

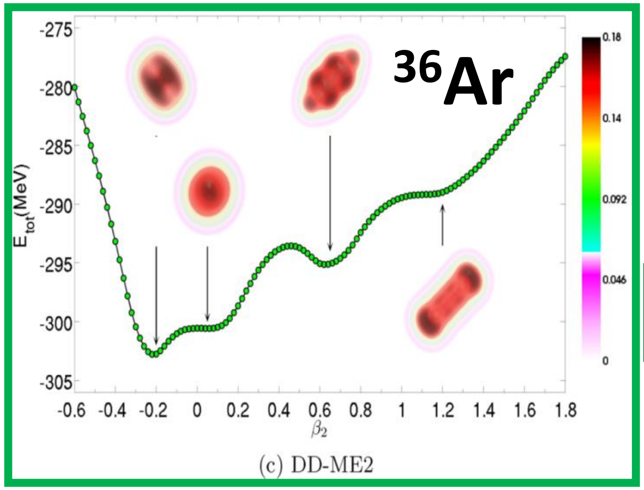


(c) DD-ME2

Relativistic functionals (as compared with non-relativistic ones) predict much more pronounced cluster structures
J.P.Ebran et al, Nature 487, 341 (2012)

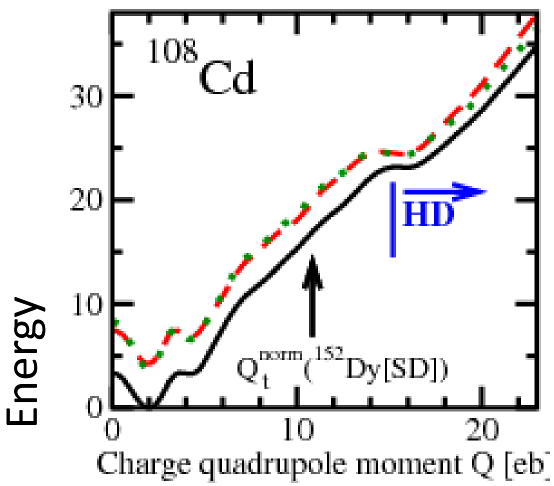
How to observe these states in experiment?

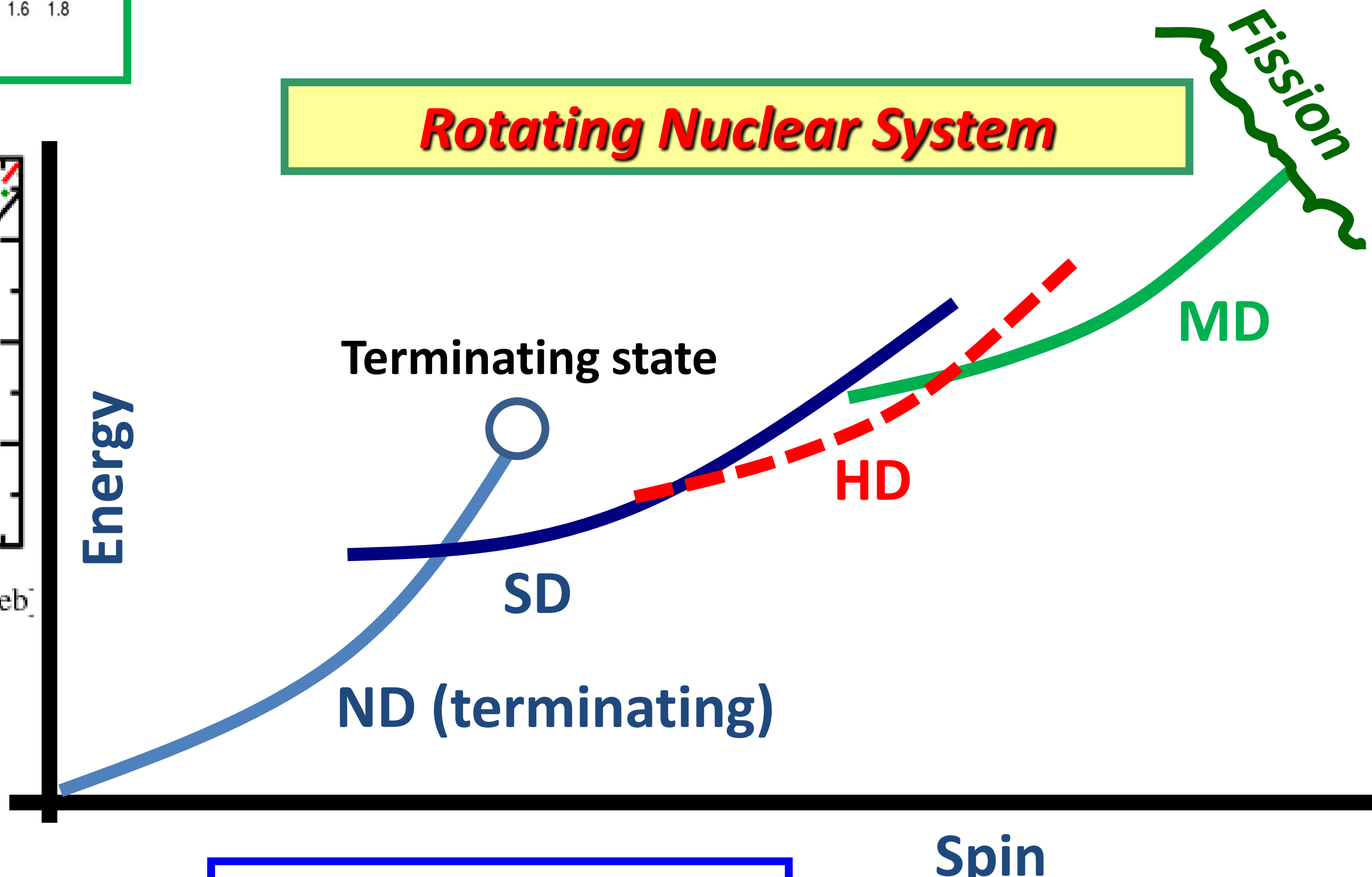
How to observe the extreme deformation and clusterization?



I=0 system

Rotating Nuclear System





Yrast= lowest in energy

What is important for observation of extremely deformed structures at high spin?

1. Such structures have to be yrast (lowest in energy at given spin) or near-yrast at the spins where the feeding takes place. Otherwise, lower deformed configurations will be fed with much higher intensity.

2. Highest spins observed in experiment in even-even nuclei of the mass region of interest is I=16 (SD bands in ^{36}Ar and ^{40}Ca and ND band in ^{48}Cr)

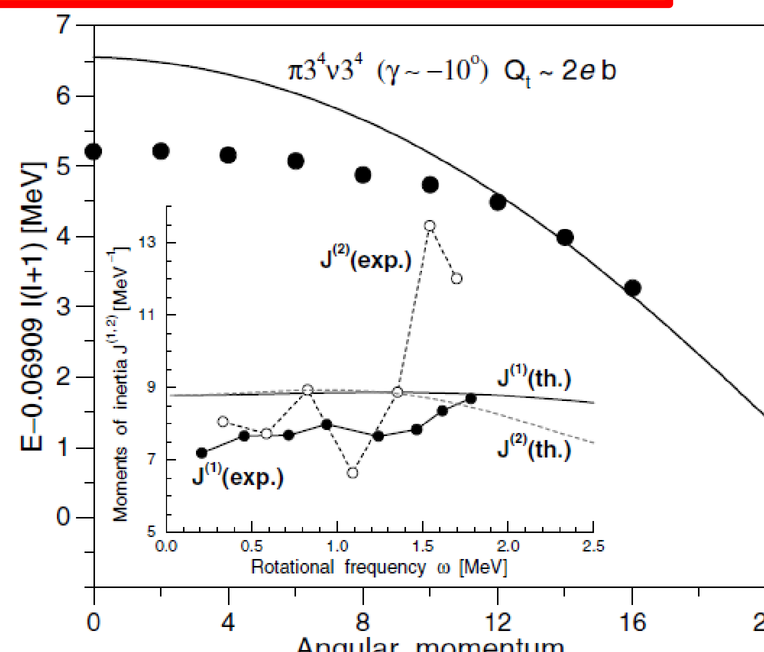
Neglect of pairing in the CRMF calculations

Quenching of pairing at high spin in deformed structures due to

- Coriolis antipairing effect
- large shell gaps
- blocking effect.

Typically above I~ 10 in the mass region of interest

Pairing is very weak near the termination of rotational bands



E. Ideguchi et al, PRL 87, 222501 (2001)

Configuration labelling

Pairing correlations are neglected → intrinsic structure of the configurations Can be described by means of the dominant single-particle components of the intruder/hyperintruder/megaintruder states occupied.

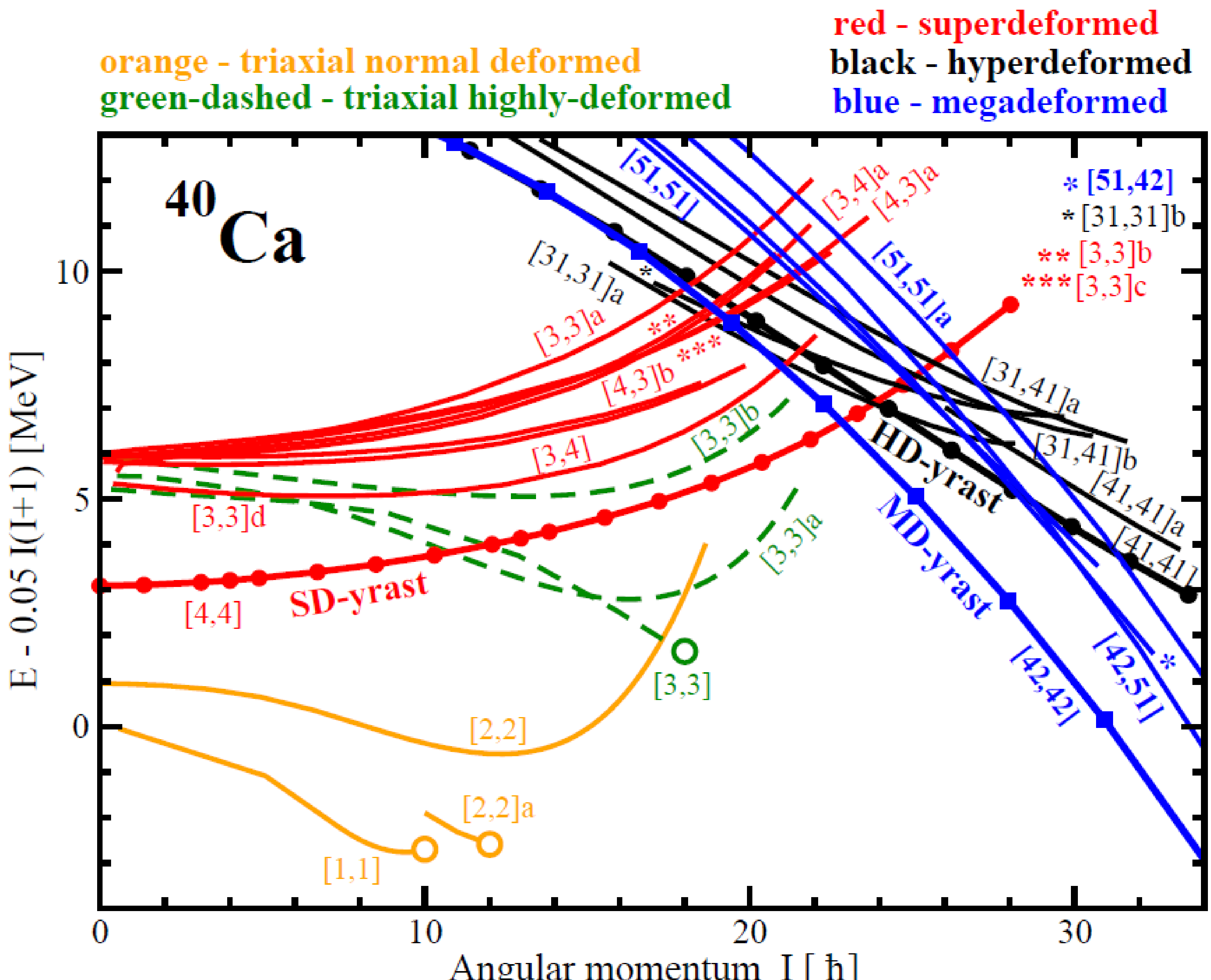
Shorthand notation $[n_1(n_2)(n_3),p_1(p_2)(p_3)]$

n_1 (p_1) - # of neutrons (protons) in the intruder N=3 orbitals

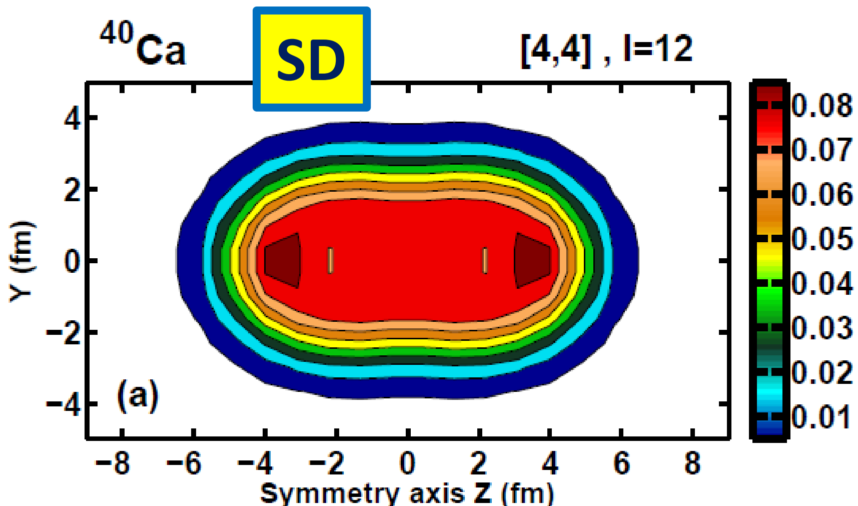
n_2 (p_2) - # of neutrons (protons) in the hyperintruder N=4 orbitals

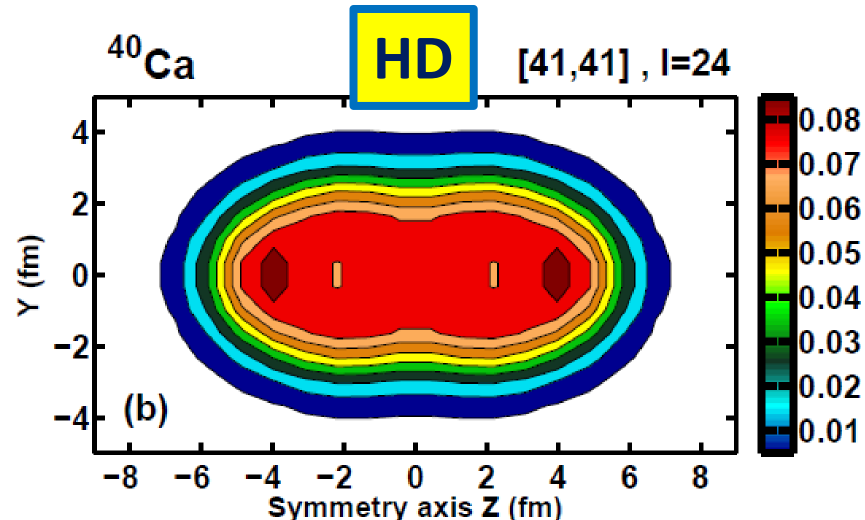
n_3 (p_3) - # of neutrons (protons) in the megaintruder N=5 orbitals

High-spin structure of the ^{40}Ca nucleus



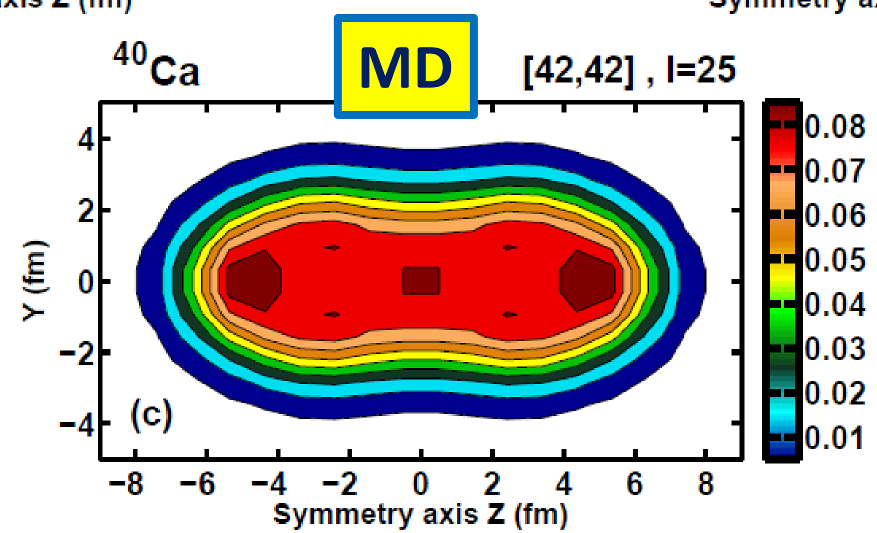
Density distribution: enhancement of clusterization with deformation



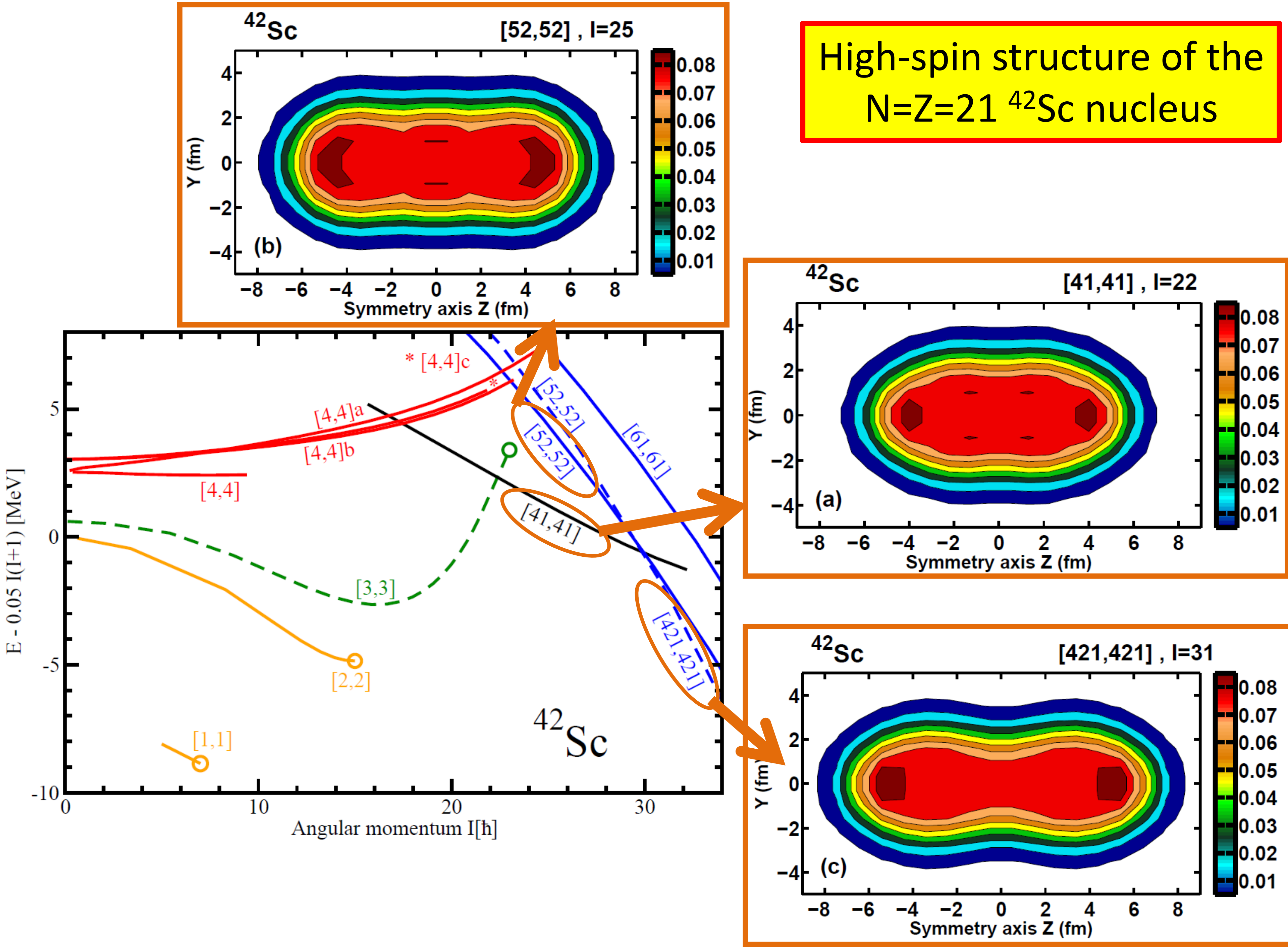


$^{20}Ne+^{20}Ne$?

$^{12}C+^{16}O+^{12}C$?

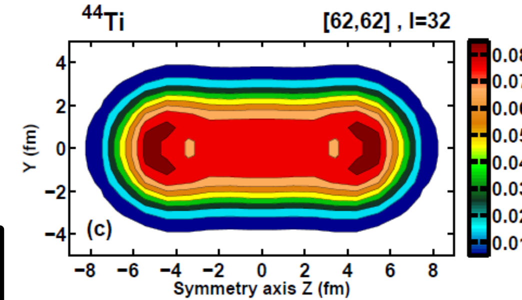


High-spin structure of the N=Z=21 ^{42}Sc nucleus



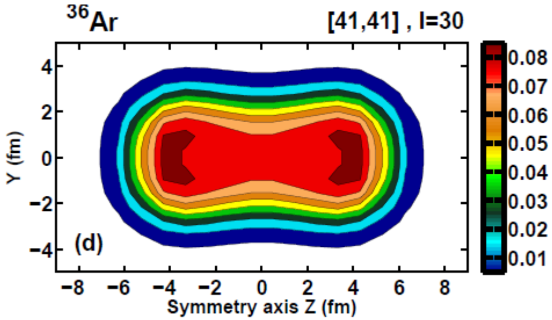
Systematics of interesting configurations

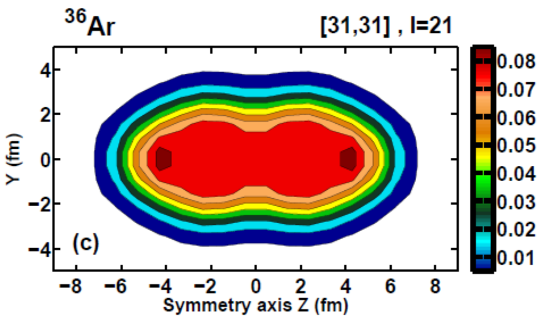
Rod-shape structures

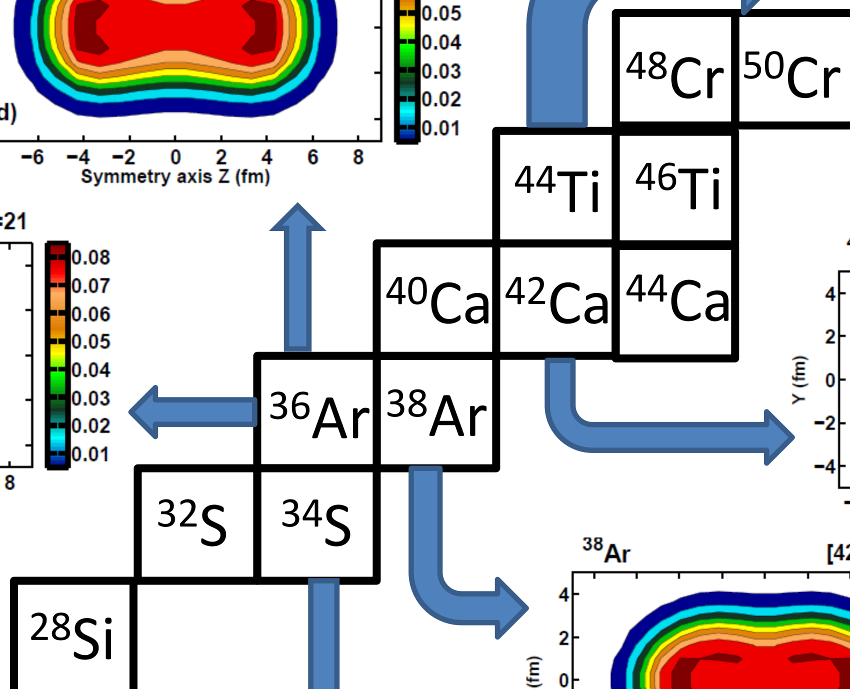


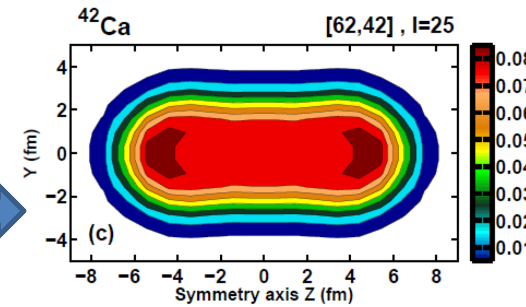
$^{16}O+^{12}C+^{16}O$?

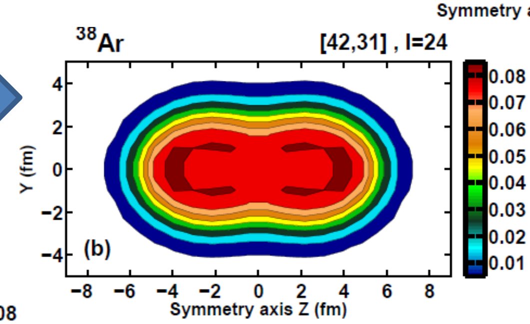
Nuclear molecules



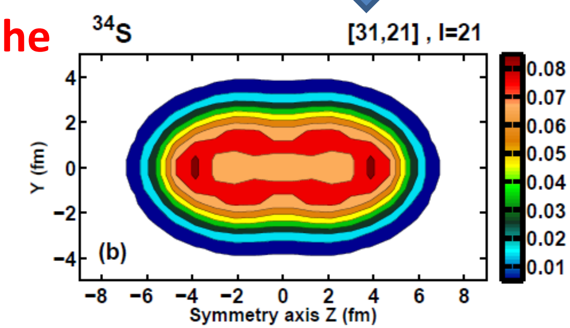






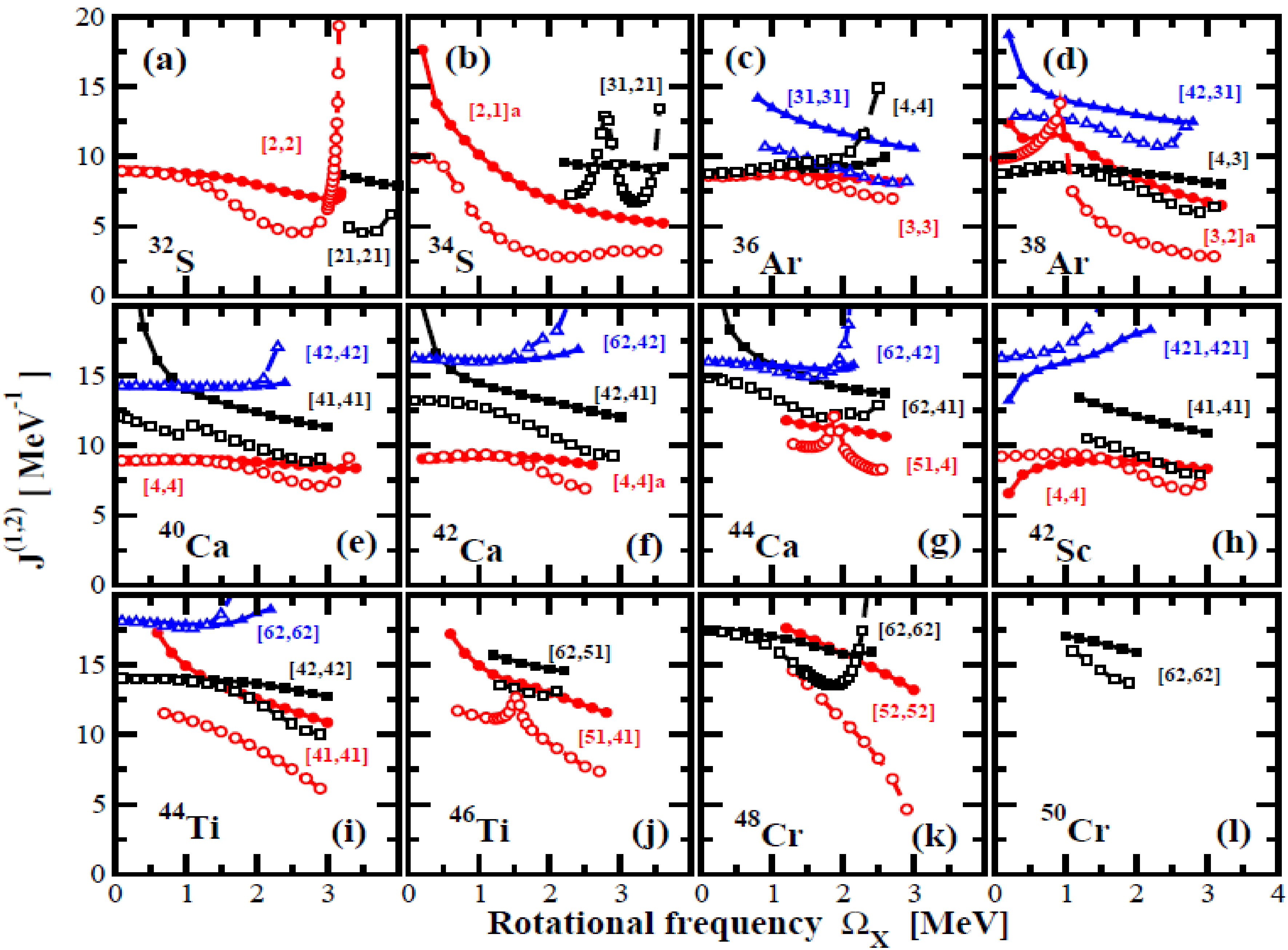


^{36}Ar – the best candidate for observation of HD and MD since the transition to these shapes takes place at I=18



$^{16}O+^{16}O+2n$?

Kinematic and dynamic moments of inertia



Conclusions

1. Systematic and global investigation of octupole deformed even-even nuclei with an estimate of theoretical uncertainties has been performed for the first time. A new region of octupole deformation, centered around $Z \sim 98$, $N \sim 196$, has been predicted for the first time.

1. Systematic investigation of SHE with an assessment of theoretical uncertainties.
OOPS #1: N=172 shell gap is no longer "magic" in CDFT
OOPS #2: N=184 shell gap is more important
OOPS #3. Z=120 nuclei are not necessary spherical (they may be oblate)

3. Extremely deformed structures inevitably become yrast with increasing spin in the nuclei under study. This is because normal and highly-deformed configurations forming the yrast line at low and medium spins have limited angular momentum content. The nuclei most favored for the observation of extremely deformed structures are located in the vicinity of ^{36}Ar and ^{40}Ca.

4. The N = Z nuclei are better candidates for the observation of extremely deformed structures as compared with the nuclei which have an excess of neutrons over protons since the transition to extremely deformed structures takes place at lower spins.