Global improvement of covariant energy density functionals: mass tables and nuclear shapes

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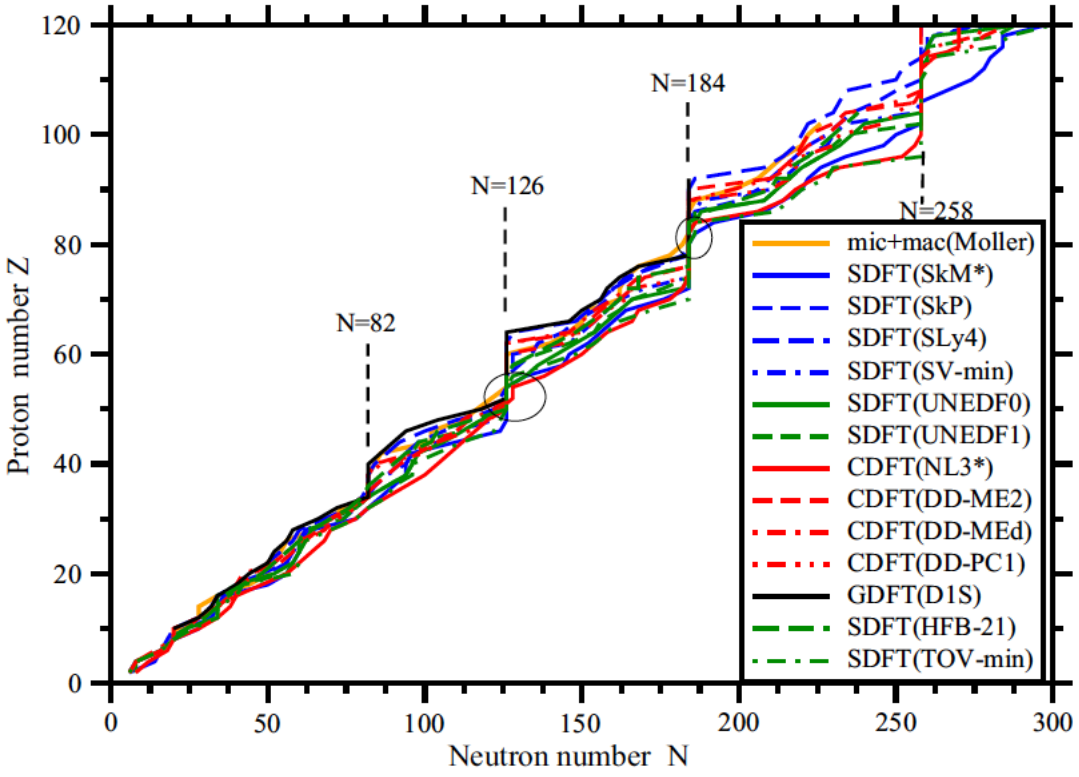
1. **Motivation:**
2. **Improving the energy density functionals on a global scale**
3. **Conclusions**

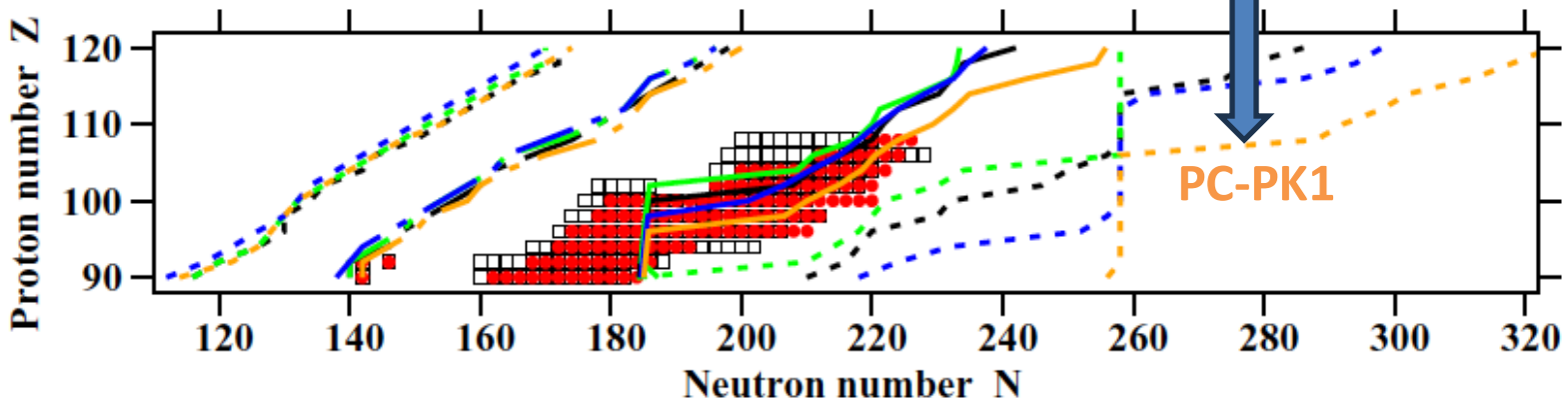
In collaboration with A.Taninah, S.Teeti, U.Perera and B.Osei (Missisippi State University), V.A.Dzuba and V.V.Flambaum (Univ. New South Wales,Australia)

Challenges: reduction of theoretical uncertainties in the binding energies, deformations and size of nuclear landscape

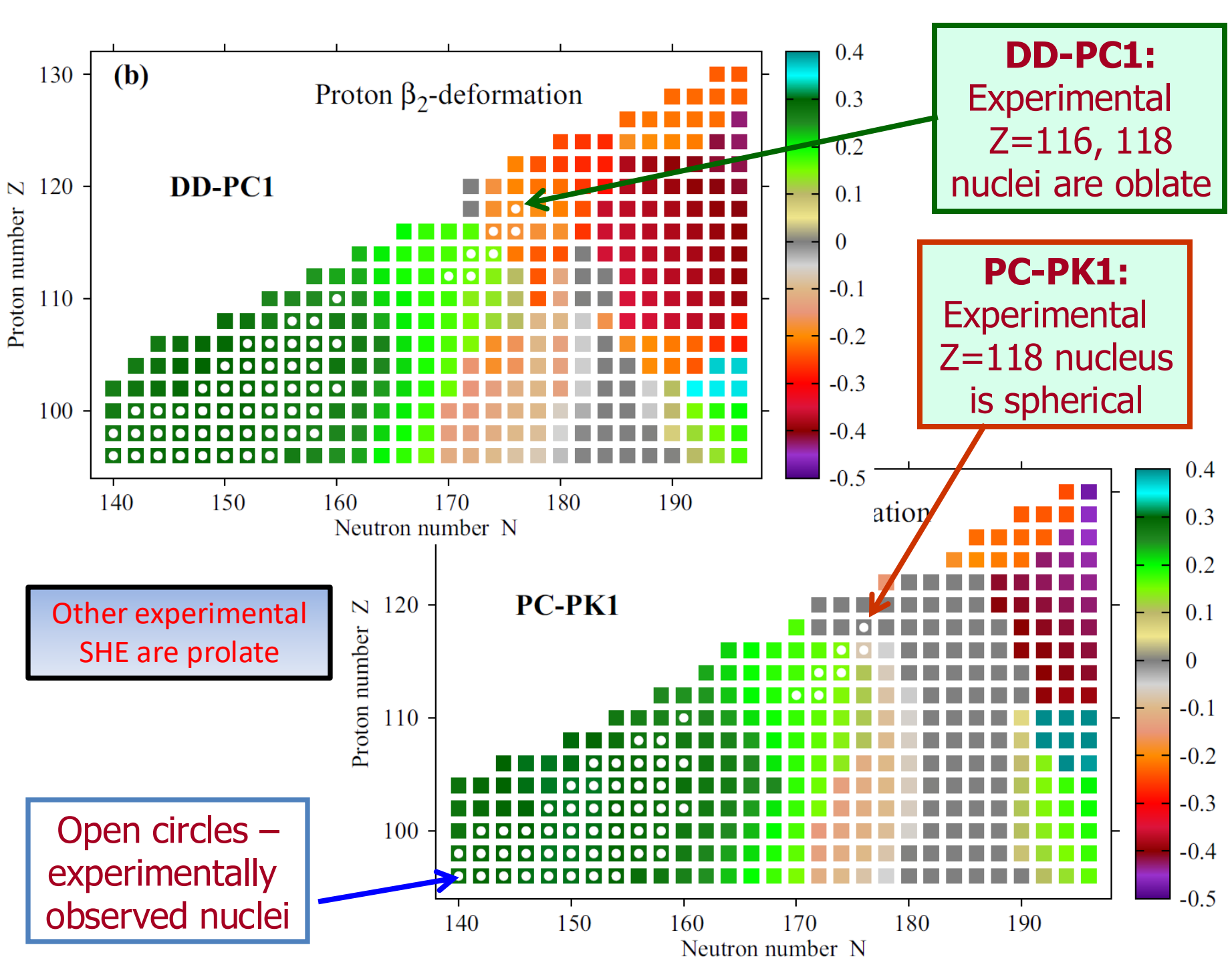
S.E.Agbemava et al, PRC 89, 054320 (2014)



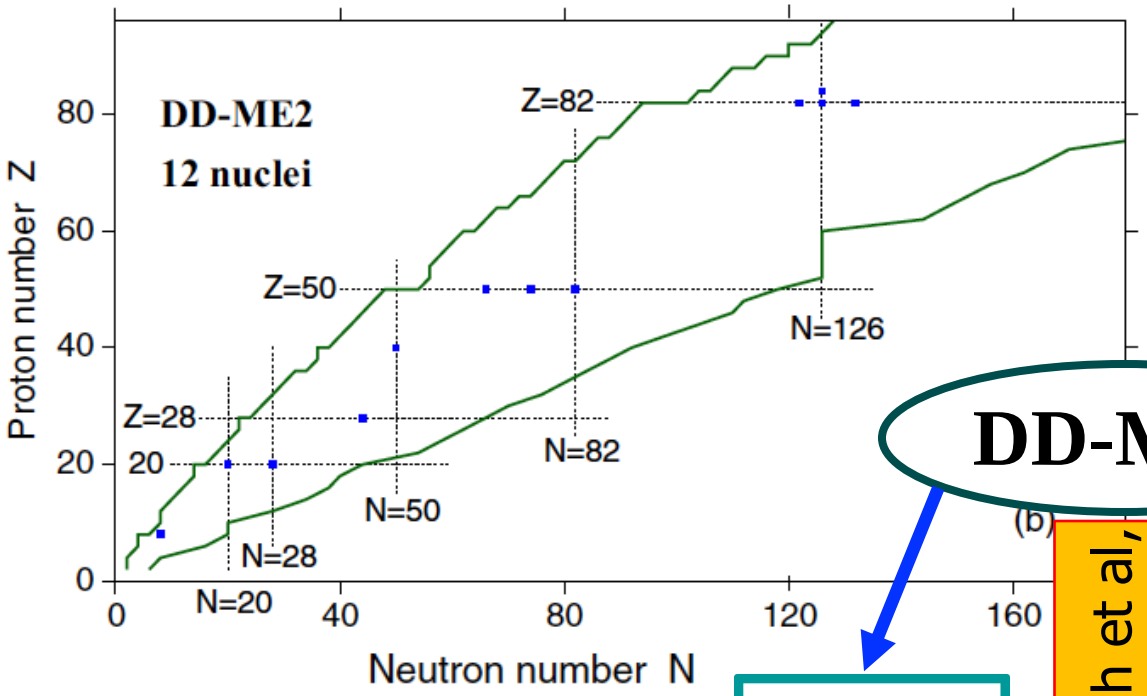
The PC-PK1 functional is outlier:
it predicts around 1000 extra nuclei located between proton and neutron drip lines as compared with other functionals.



A.Taninah et al, PRC 102, 054330 (2020)


(b)
Proton β_2-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
PC-PK1
Other experimental
SHE are prolate
Open circles –
experimentally
observed nuclei
A.Agbemava et al, PRC 92, 054310 (2015)

The need to include the information on deformed nuclei



DD-ME2

$\chi^2 = 39$

Performance for the **12 spherical nuclei**

$\chi^2 = 24$

Refit A. Taninah et al, PLB 800, 135065 (2020)

ΔE_{rms}= 2.45 MeV

Global performance

ΔE_{rms}= 2.89 MeV

DD-MEX

Relativistic Hartree-Bogoliubov (RHB) framework

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

The separable version of the finite range Brink-Booker part of the Gogny D1S force is used in the particle-particle channel

$$V(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_1', \boldsymbol{r}_2') = \\ = -f\, G\delta(\boldsymbol{R}-\boldsymbol{R'})P(r)P(r')\frac{1}{2}(1-P^\sigma)$$

$$f_\pi = 1.877(N+Z)^{-0.1072}$$ Proton pairing = mass dependent

$$f_\nu = 1.208e^{-0.674\frac{|N-Z|}{N+Z}}$$ Neutron pairing = isospin dependent

S. Teeti and AA, PRC 103, 034310 (2021)

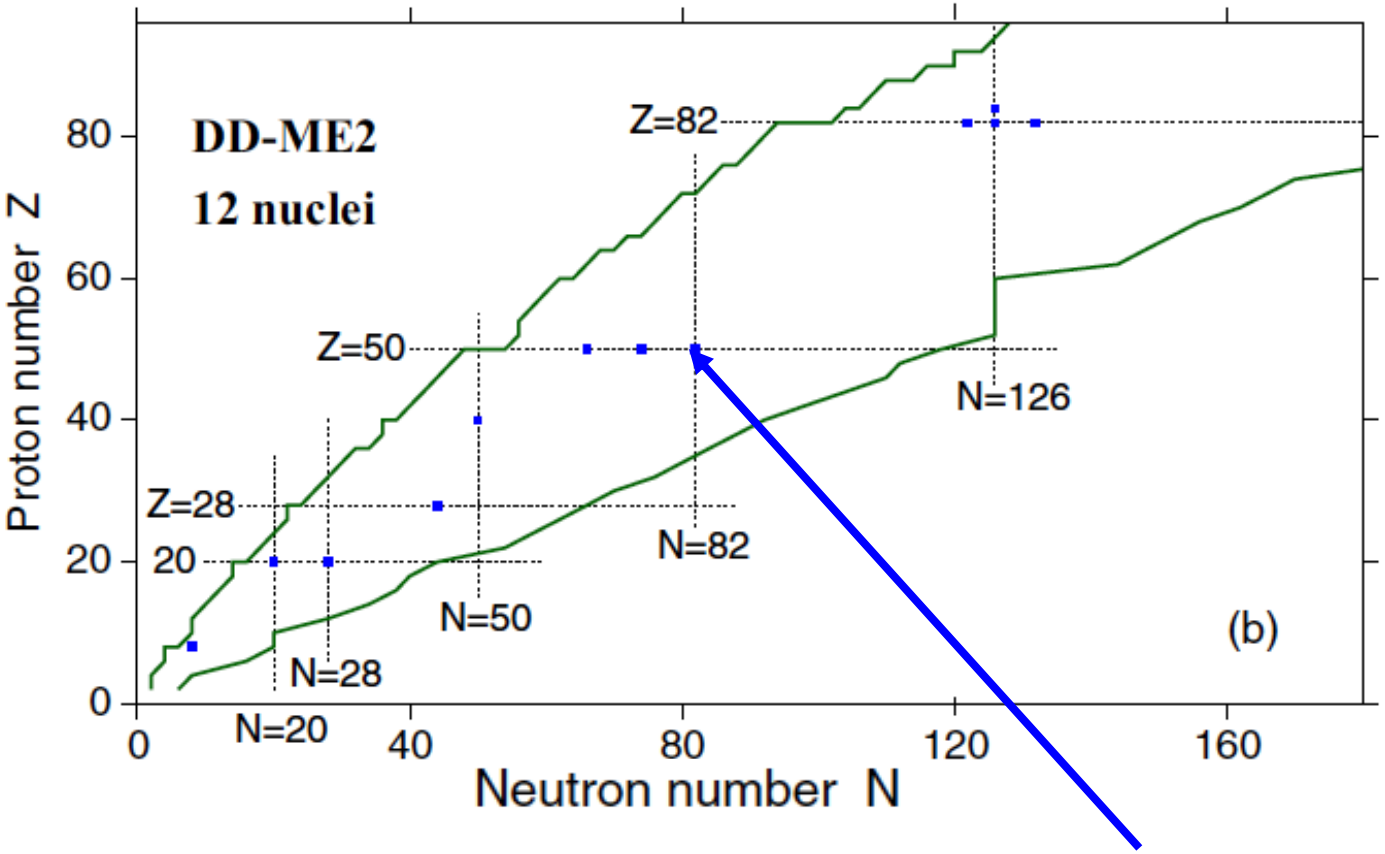
Y – class of the functionals: N_F=20 and N_B=20

Z – class of the functionals:

- infinite basis correction to binding energies in fermionic and bosonic sectors of CDFT
- total electron binding energies are accounted in definition of experimental nuclear binding energies

Anchor based method of optimization (ABOA) of EDFs

A.Taninah and AA, PRC 107, L041301 (2023)



Anchor spherical nuclei

PROs: 1. fast convergence due to pairing collapse in at least one subsystem
2. no numerical instabilities

Physical observables in anchor nuclei: masses, charge radii

Basic idea of ABOA: correct the experimental data in anchor spherical nuclei by the information on the differences between theory and experiment on a global scale

1. Define the functional $\mathrm{EDF}_i\ (i=0)$ by fit to anchor spherical nuclei

2. Make global calculations with EDF_i Masses of 882 even-even nuclei

3. Introduce correction function $E_{corr}(Z,N) = \alpha_i(N-Z) + \beta_i(N+Z) + \gamma_i$

and define its optimum parameters α_ι, β_ι and γ_ι which minimize the difference between $E_{pseudo}(Z,N) = E_{EDF_i}(Z,N) + E_{corr}(Z,N)$

and experiment $\Delta E_{rms} = \sqrt{\frac{\sum_{i=1}^{n}(E_{pseudo}(Z,N) - E_{exp}(Z,N))}{n}}$

using all even-even nuclei for which experimental data exist

4. Redefine the energies of anchor spherical nuclei

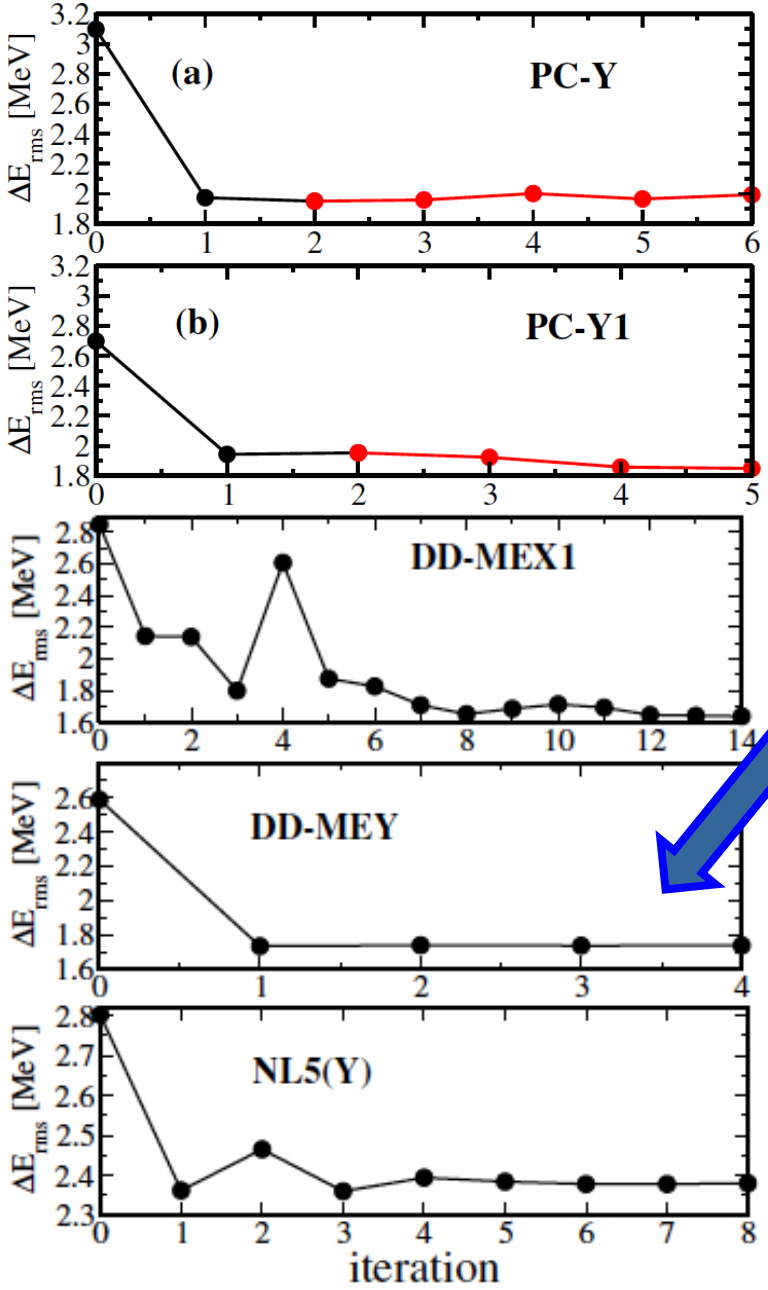
$$E_{exp}^{pseudo}(Z,N) = E_{exp}(Z,N) + E_{corr}(Z,N)$$

and define new functional EDF_{i+1} by fit to these new energies

5. Make global calculations with EDF_{i+1}

If further improvement is needed, repeat steps 3-5.

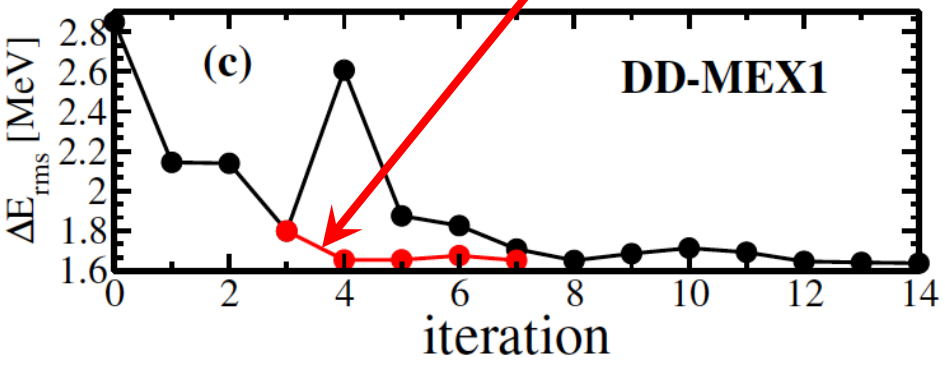
How fast is convergence in ABOA



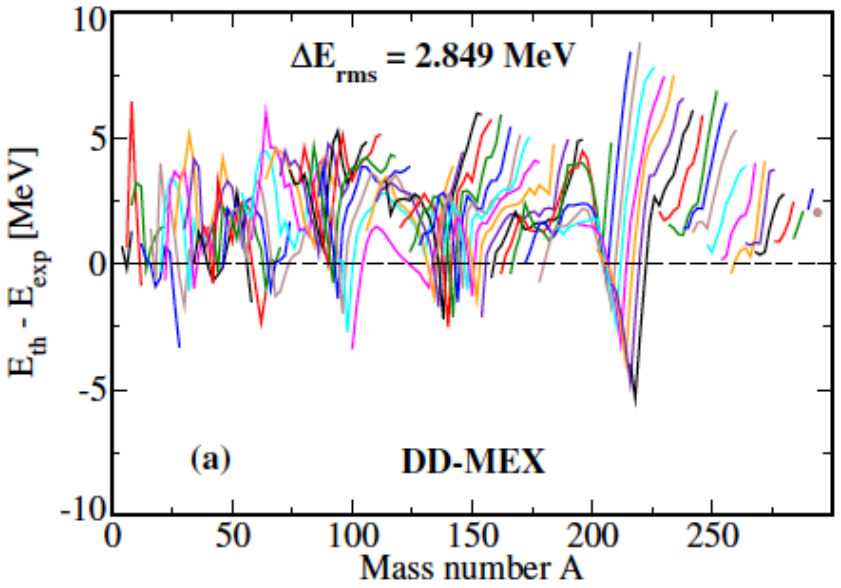
A.Taninah and AA,
PRC 107, L041301 (2023)

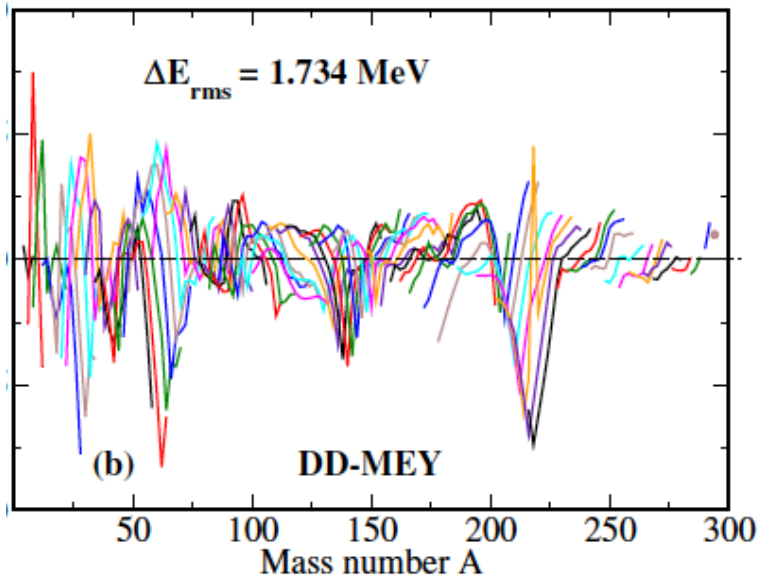
iteration i	ΔE_{rms} [MeV]	α_i	β_i	γ_i
0	2.589	0.074	-0.019	-0.97
1	1.734	0.003	-0.001	0.10
2	1.739	0.003	0.000	-0.03
3	1.737	0.002	0.000	0.01
4	1.738	-0.001	0.000	0.01

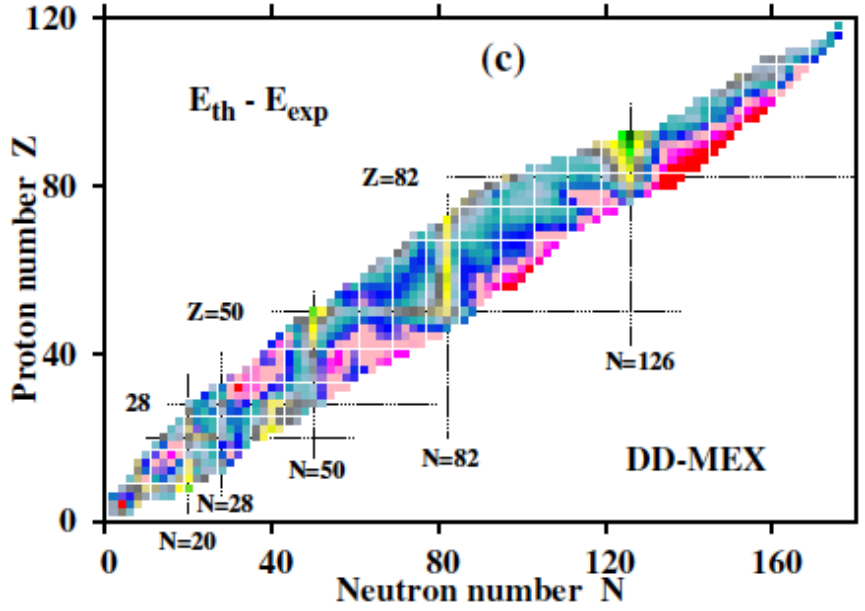
$$E^{mod}_{corr}(Z,N) = \frac{\alpha_i}{2}(N-Z) + \frac{\beta_i}{2}(N+Z) + \frac{\gamma_i}{2}$$

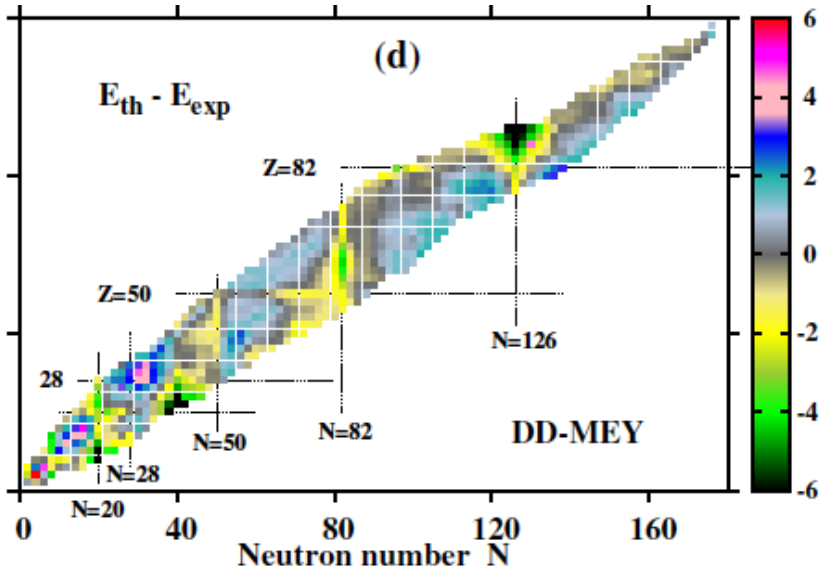


Example of the application of anchor based method of optimization to DD-ME* functionals









A.Taninah and AA, PRC 107, L041301 (2023)

How to obtain binding energies corresponding to infinite basis in basis set expansion method?

$$\psi_i(\vec{r}, s, t) = \begin{pmatrix} f_i(\vec{r}, s, t) \\ i g_i(\vec{r}, s, t) \end{pmatrix}$$

Fermionic basis

$$f_i(\vec{r}, s, t) = \sum_{\alpha}^{\alpha_{\max}} f_{\alpha}^{(i)} \Phi_{\alpha}(\vec{r}, s) \chi_{t_i}(t)$$

$$g_i(\vec{r}, s, t) = \sum_{\tilde{\alpha}}^{\tilde{\alpha}_{\max}} f_{\tilde{\alpha}}^{(i)} \Phi_{\tilde{\alpha}}(\vec{r}, s) \chi_{t_i}(t)$$

Fermionic basis is truncated at N_F for large components of the Dirac spinor and at N_F+1 for small components

$$|\alpha\rangle = |n_z n_r \Lambda s\rangle \text{ and } |\tilde{\alpha}\rangle = |\tilde{n}_z \tilde{n}_r \tilde{\Lambda} \tilde{s}\rangle$$

$$\Phi_{\alpha}(\vec{r}, s) = \varphi_{n_z}(z, b_z) \varphi_{n_r}^{\Lambda}(r_{\perp}, b_{\perp}) \frac{e^{i\Lambda\phi}}{\sqrt{2\pi}} \chi(s)$$

Bosonic (mesonic) basis

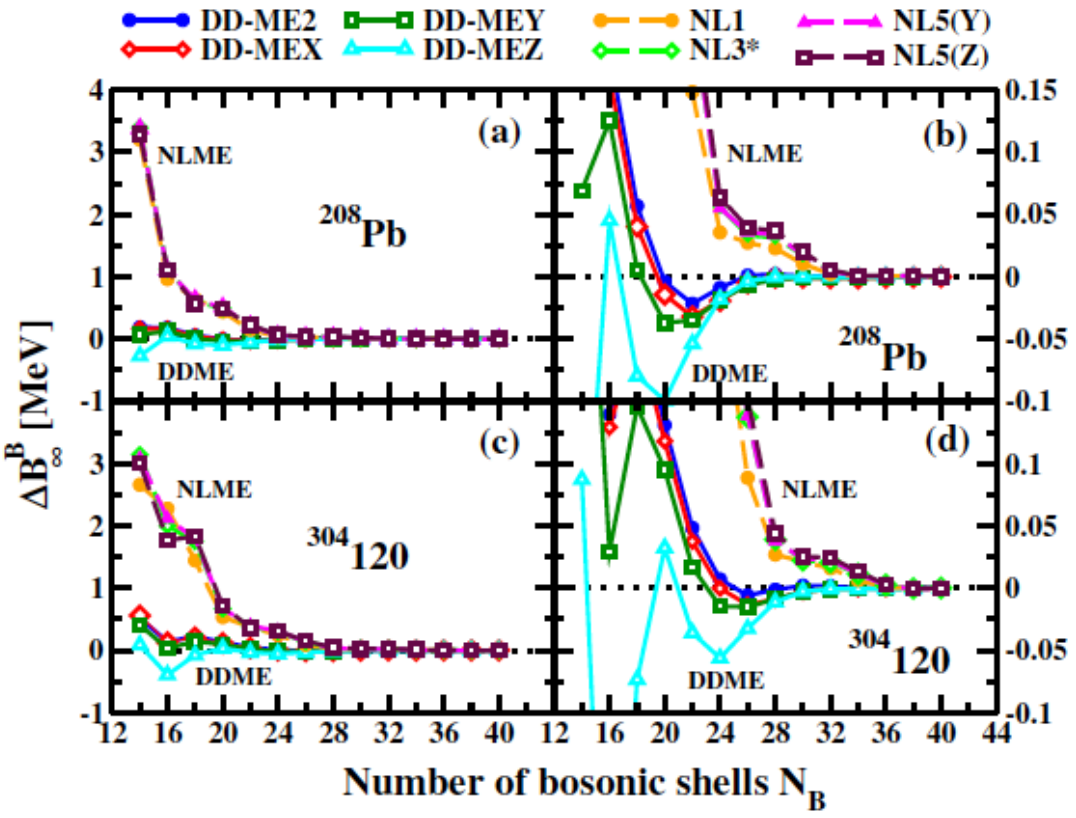
$$\phi(z, r_{\perp}) = \sum_{n_z n_r}^{N_B} \phi_{n_z n_r} \varphi_{n_z}(z, b_z) \varphi_{n_r}^{0}(r_{\perp}, b_{\perp})$$

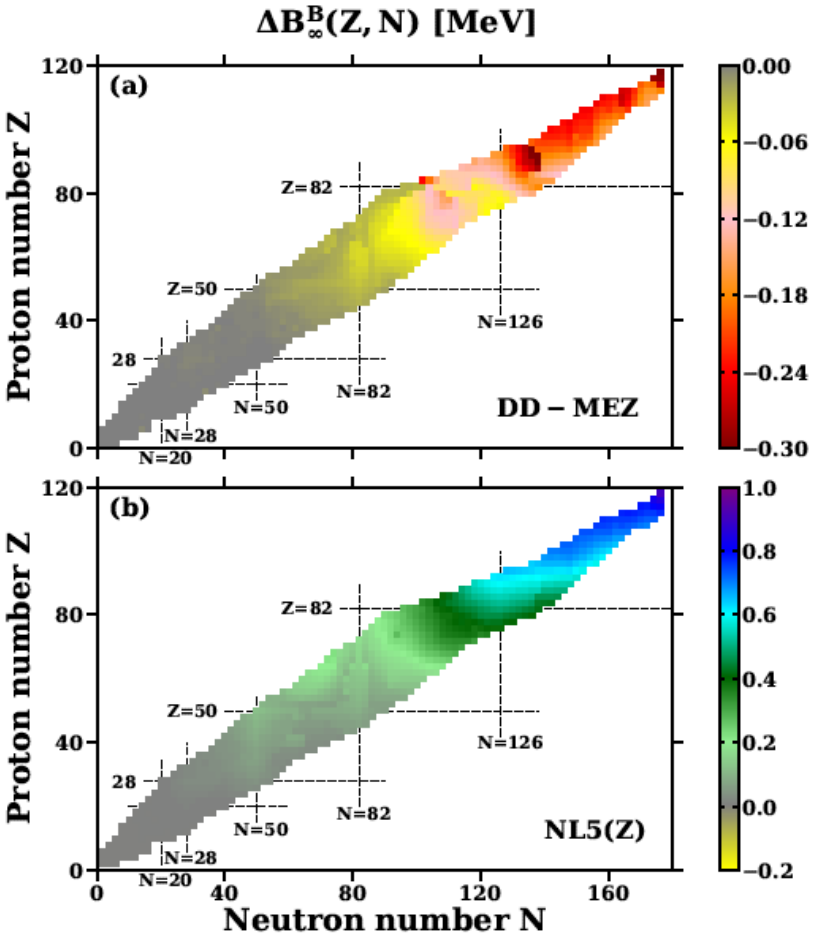
Bosonic basis is truncated at N_B

How to obtain binding energies corresponding to infinite basis in basis set expansion method?

Easy part – bosonic basis.

$$\Delta B^{B}_{\infty}(Z,N) = B(N_B = \infty)(Z,N) - B(N_B)(Z,N)$$





Bosonic basis with N_B=40 corresponds (within a few keV) to infinite bosonic basis

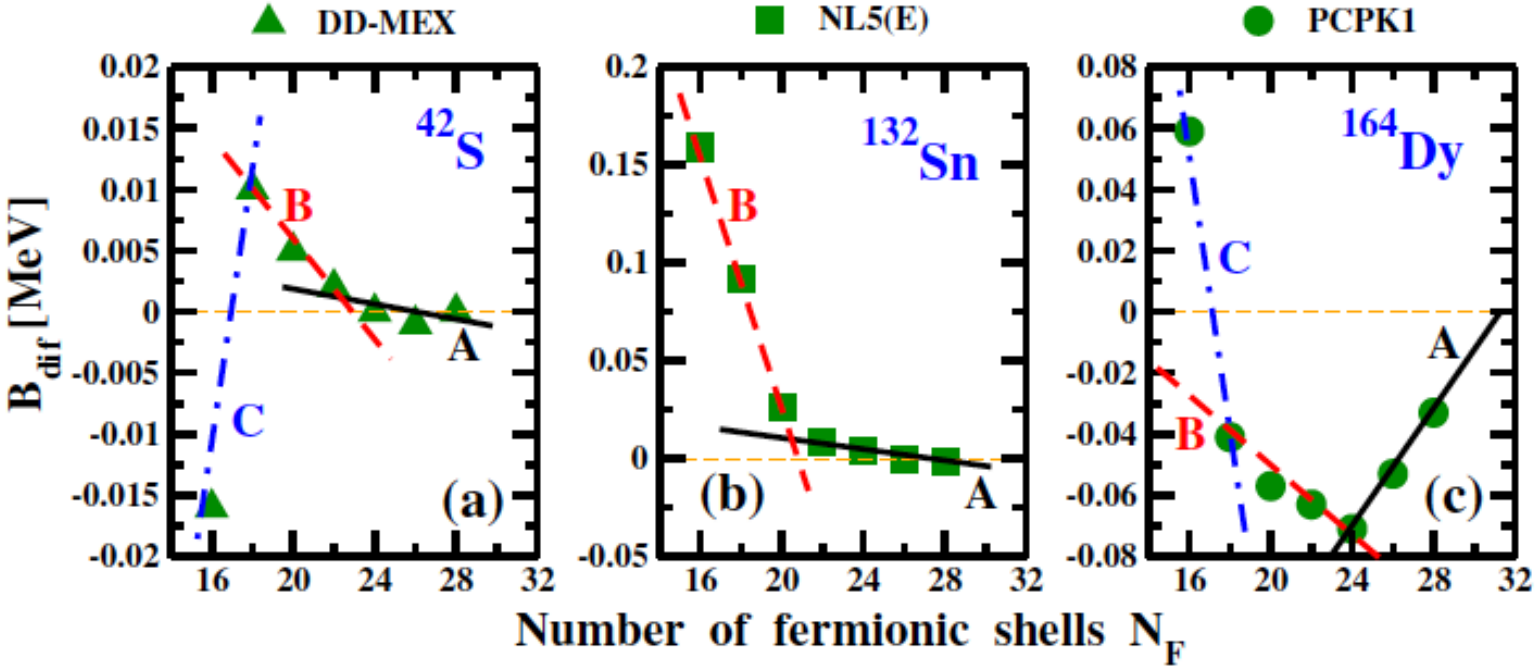
How to obtain binding energies corresponding to infinite basis in basis set expansion method?

Difficult part – fermionic basis.

Define asymptotic binding energies

$$\Delta B^{F}_{\infty}(Z,N) = B(N_F = \infty)(Z,N) - B(N_F = 20)(Z,N)$$

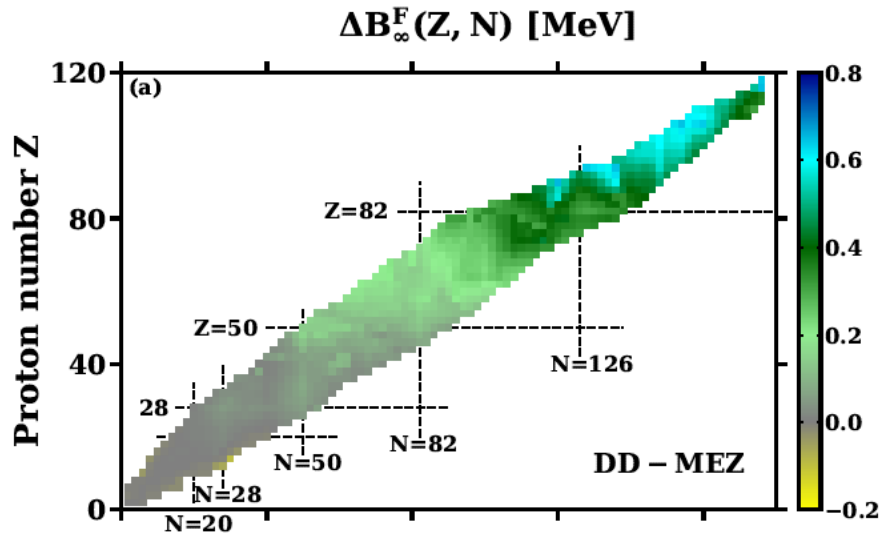
$$B_{dif}(N_F) = B(N_F + 2) - B(N_F)$$



Precise definition of asymptotic binding energies requires the calculations with N_F=20, 22, 24, 26, 28 and 30.

How to obtain binding energies corresponding to infinite basis in basis set expansion method?

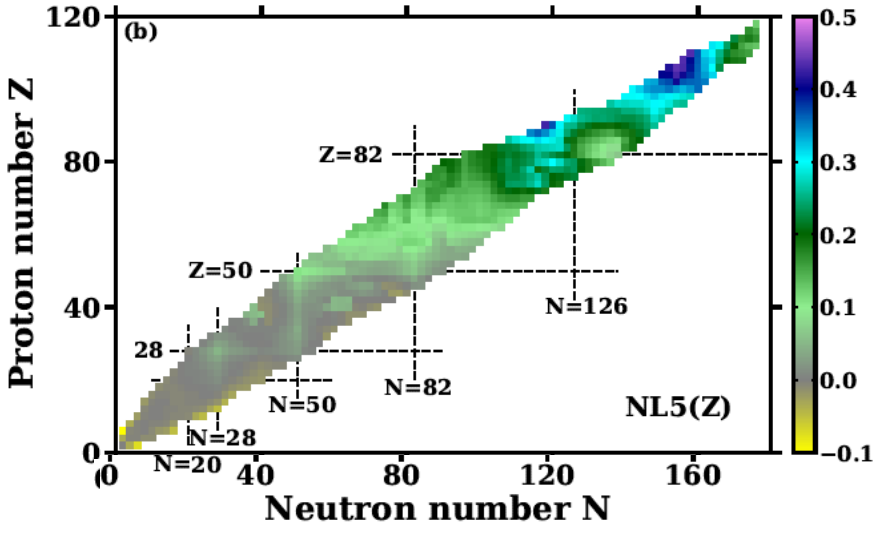
Difficult part – fermionic basis.

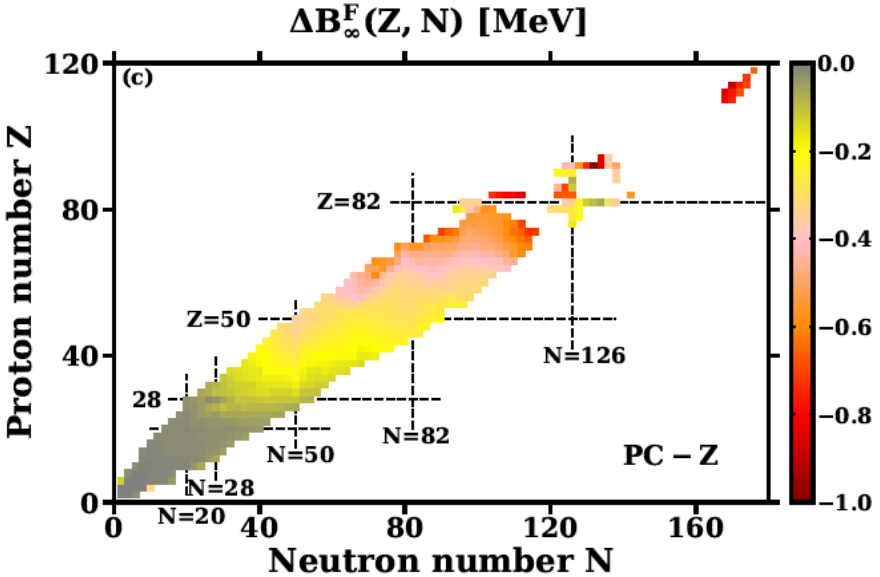


Requires 2-3 rounds of ABOA until desired accuracy ε is achieved and condition

$$|\Delta B(Z,N)| = |\Delta B^F_\infty(Z,N)[\mathrm{PC}(\mathrm{round_i})] - \Delta B^F_\infty(Z,N)[\mathrm{PC}(\mathrm{round_{(i+1)}})]| < \varepsilon$$

is satisfied





The inclusion of total electron binding energies

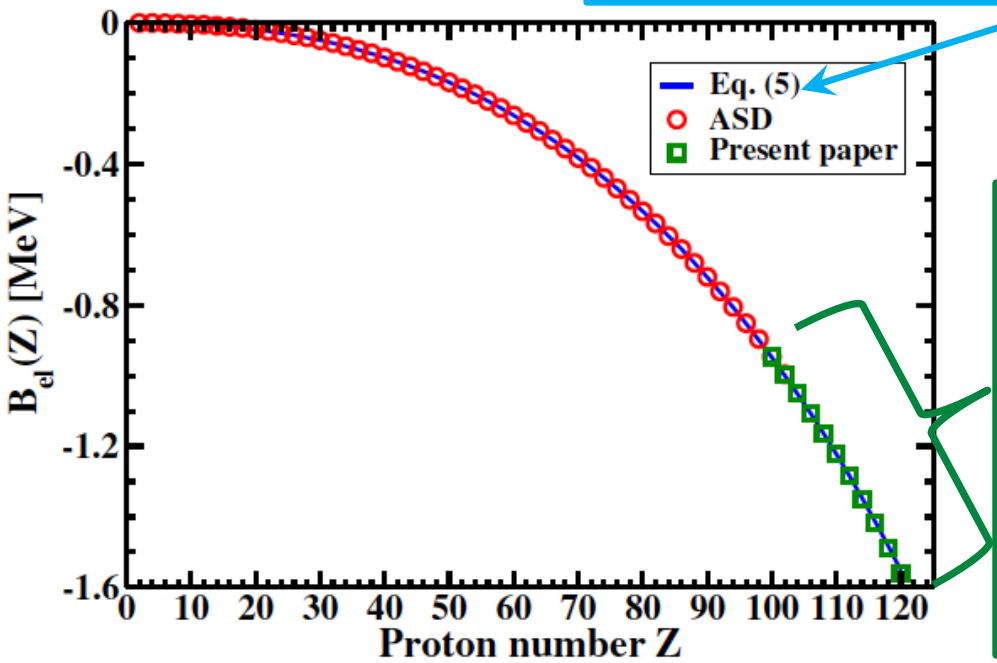
$$B(Z,N) = B^{AME}(Z,N) + ZB_{el}(Z=1) - B_{el}(Z)$$

ignored in fitting protocols of very many functionals

^{208}Pb (binding energies)

	B [MeV]	B/A [MeV/nucleon]
Atomic (AME)	-1636.4302	-7.867
Nuclear	-1635.863	-7.865

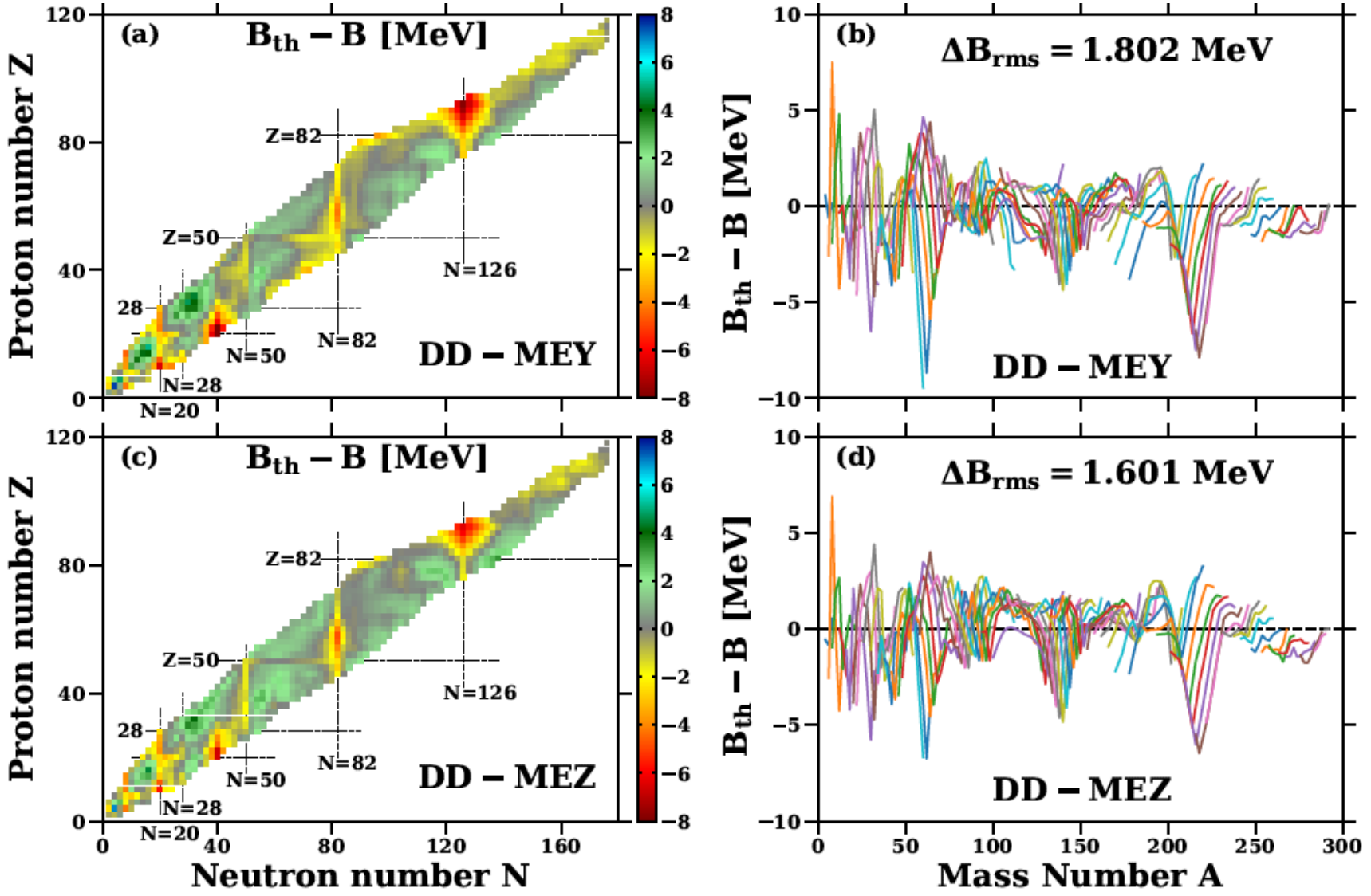
$$B_{el}(Z) = -14.4381 Z^{2.39} - 1.55468 \times 10^{-6} Z^{5.35} \text{ eV}$$



New calculations of total electron binding energies within improved atomic Relativistic Hartree-Fock framework with proper assessment of theoretical uncertainties which are extremely low (by V.Dzuba and V.Flambaum)

B. Osei et al, submitted to PRC

The consequences for the accuracy of description of experimental nuclear binding energies



B. Osei et al, submitted to PRC

Rms errors with respect of AME2020

Modifications for the functionals and nuclear matter properties (NMPs)

Parameter	DD-MEY	DD-MEZ	$ratio_i$
m_σ [MeV]	551.321796	558.605889	1.013
g_σ	10.411867	10.602029	1.018
g_ω	12.803298	12.881123	1.006
g_ρ	3.692170	3.514796	0.952
b_σ	2.059712	2.667539	1.295
c_σ	3.210289	4.070271	1.268
c_ω	3.025356	4.352258	1.439
a_ρ	0.532267	0.649431	1.220

Define central potential

Define explicit density dependence of meson-nucleon interaction

Empirical SET2b constraints on NMPs, PRC 90, 055203 (2014)

$K_0 = 190$–270 MeV

$J = 30$–35 MeV

$L_0 = 30 - 80$ MeV

	DD-MEY	DD-MEZ	$ratio_j$
E/A [MeV]	-16.1	-16.0	0.994
ρ_0 [fm^{-3}]	0.153	0.150	0.980
K_0 [MeV]	265.8	286.6	1.078
J [MeV]	32.8	31.3	0.954
L_0 [MeV]	51.8	44.1	0.851

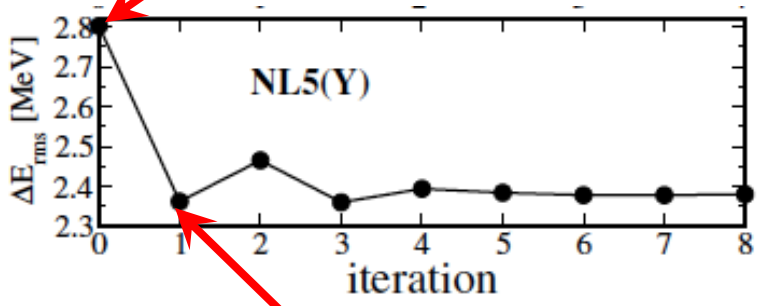
NMPs most sensitive to the variation of the parameters

Allocated calculational time of different approaches

1. Minimization of the functional to the set of 12 spherical nuclei
   ~ 20000 CPU-hours

2. **Anchor based optimization approach**

0-th iteration = ~ 33000 CPU-hours



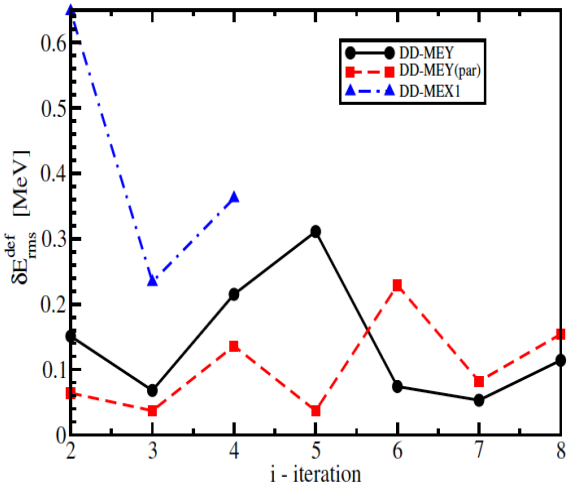
3 iterations = ~ 80000 CPU-hours

8 iterations = ~ 158000 CPU-hours

n-th iteration = ~ 15600 CPU-hours

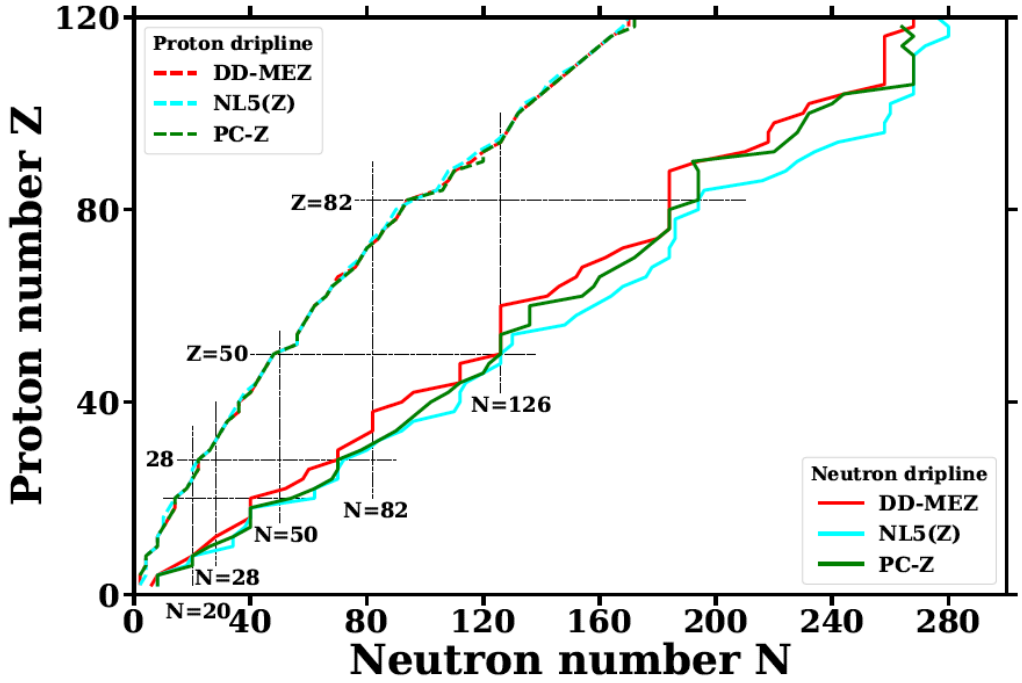
3. **Reduced global approach (RGA):**
   optimization for set of spherical nuclei the binding energies of which are corrected by deformation energies

855 even-even nuclei: one iteration
~ 427000 CPU-hours



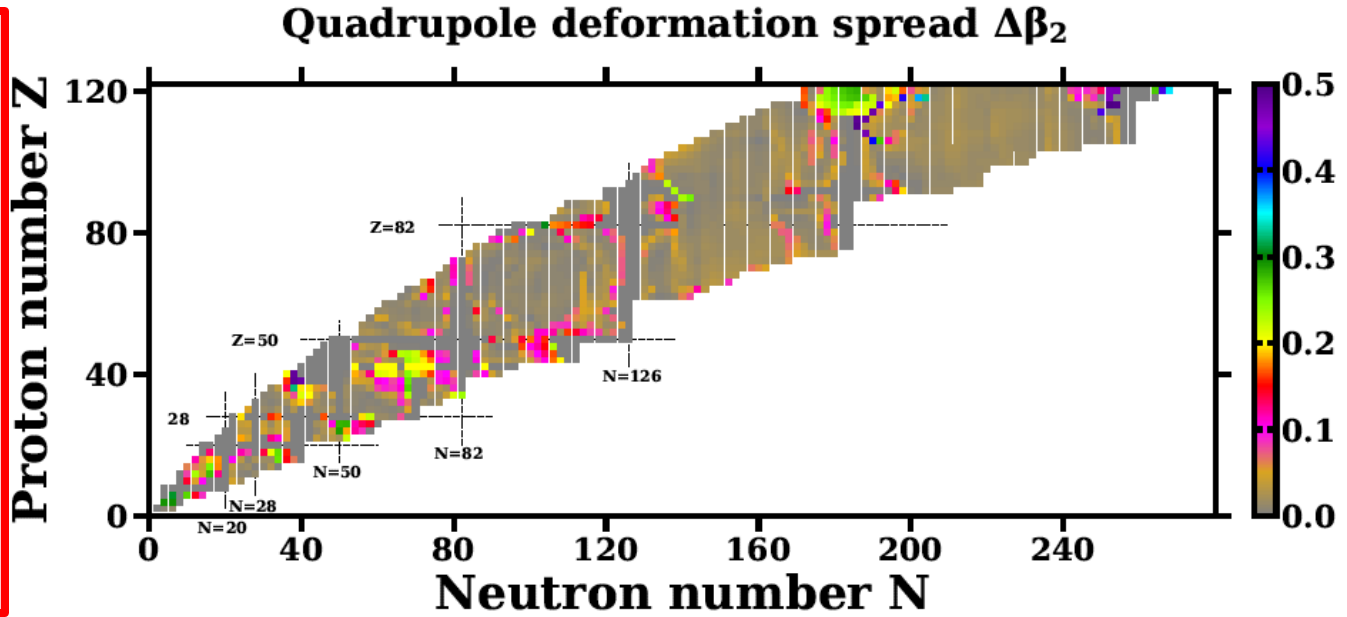
A. Taninah et al, PRC 109, 024321 (2024)

Some preliminary results



The results for position of the neutron-drip line obtained by PC-Z are close to those of DD-MEZ. Thus, the overprediction of the number of neutron-rich nuclei (by ~ 1000) in PC-PK1 as compared with other functionals does not exist in PC-Z.

Reliable prediction of the deformations of superheavy nuclei in the vicinity of the Z~120, N~184 is still an issue.
Open questions about form and the range of the functionals.



Conclusions

1. New anchor based optimization approach (ABOA) has been suggested for improving of energy density functionals. It leads to a substantial improvement of the global description of binding energies at acceptable computational cost which is more than by order of magnitude lower than for alternative methods.

2. For the first time, different functionals representing three classes of CEDFs are fitted:
- with accounting of infinite basis corrections to binding energies in fermionic and bosonic sectors of CDFT
- with direct accounting of total electron binding energies

in transformation of experimental atomic binding energies into nuclear ones.

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