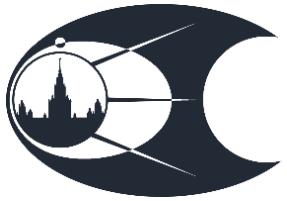

LXX International conference
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Nuclear physics technologies"

PHENOMENOLOGICAL APPROACH TO EXTRAPOLATION OF NUCLEAR BINDING ENERGIES IN THE TRANSFERMIUM REGION

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Map of superheavy elements (SHE)

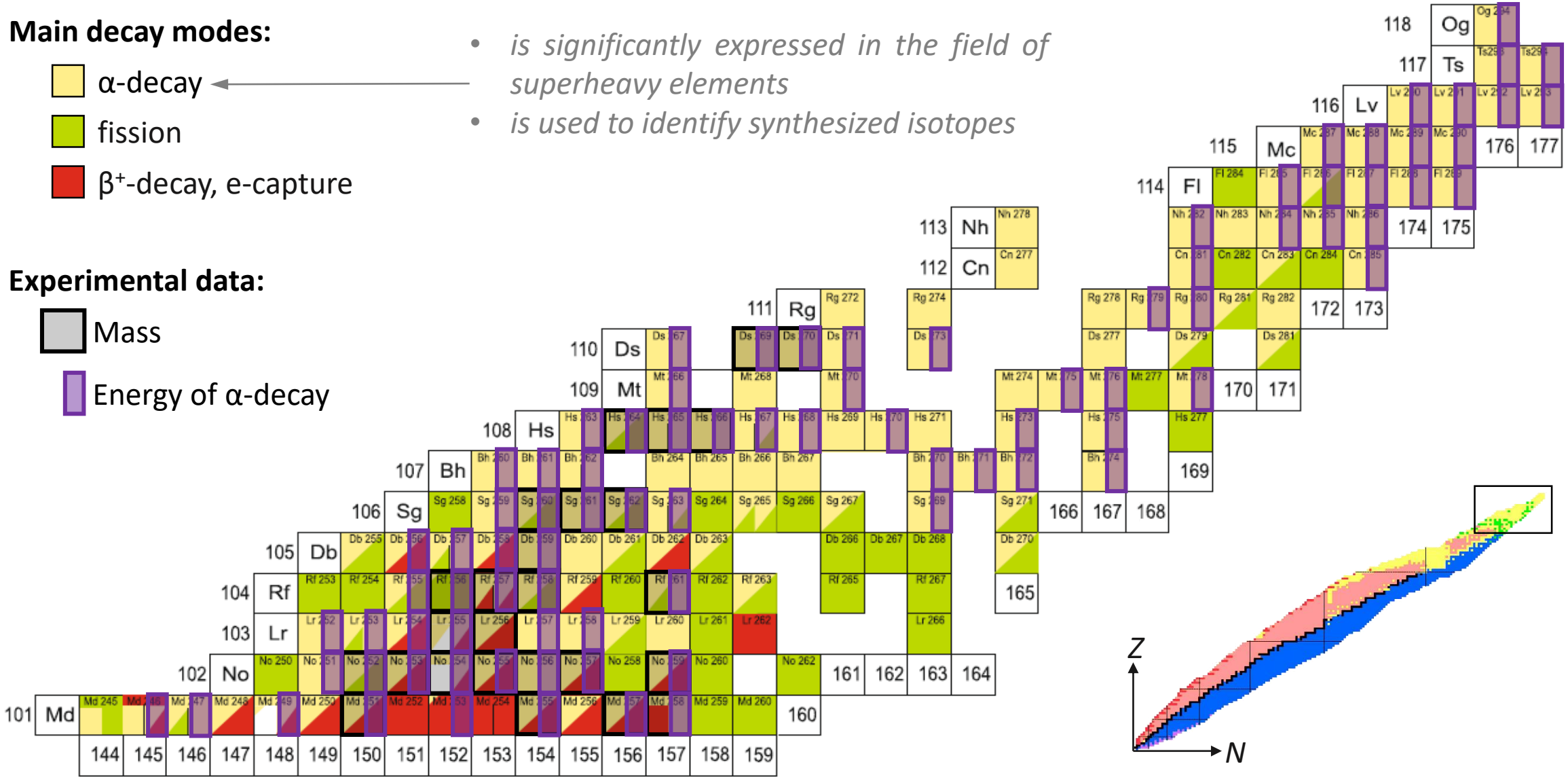
Main decay modes:

- α-decay
- fission
- β^+-decay, e-capture

Experimental data:

- Mass
- Energy of α-decay

- *is significantly expressed in the field of superheavy elements*
- *is used to identify synthesized isotopes*



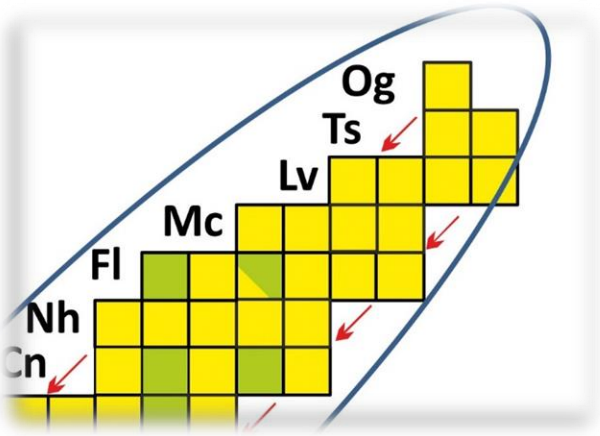
Actuality and objectives

Actuality:

- Binding energy *B* is the basic characteristic of the nucleus. Its dependence on *Z*, *N* is known, but the **residual interaction** is not fully understood. The residual interaction is associated with **nucleon correlations** and manifests itself in the effects of **nucleon pairing** and the **even-odd straggering** of the *B(Z, N)* surface.
- Calculation of the binding energy, reaction energies and mass characteristics reflecting pairing and even-odd effects requires the development of accurate computational methods with acceptable labor intensity. One of them is a method of **local mass relations**. **Machine learning algorithms** can also be applied for such calculations.
- For many isotopes of **superheavy elements (SHE)**, the **binding energies** in the ground state are not yet known. One of the main SHE decay channels is α-emitting. Estimates of the characteristics of **α-decay** are important for the registration of SHE.

Objectives:

- **Studying mass relations** reflecting proton-neutron correlations and finding mass relations with regular behavior.
- Carrying out **calculation of mass characteristics** in SHE region:
  - Binding energy
  - α-decay energy
  - α-decay half-life
- Examining the **possibility of using machine learning** algorithms for calculating of SHE mass characteristics.



Residual *np*-interaction

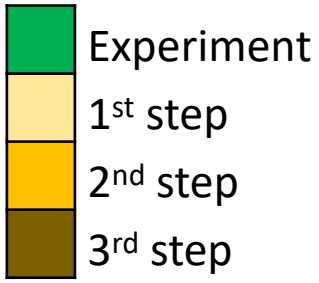
- The *B(Z, N)* surface is considered continuous and therefore the connecting of the masses of neighbouring nuclides into algebraic relations is justified and makes it possible to predict the masses of some isotopes based on others.
- We need to choose the relationships that have the smoothest behavior and insignificantly undergo shell effects. One suitable relation is a ***relation for residual proton-neutron interaction*** $\boldsymbol{\Delta_{np}}$, connecting 4 neighboring isotopes.

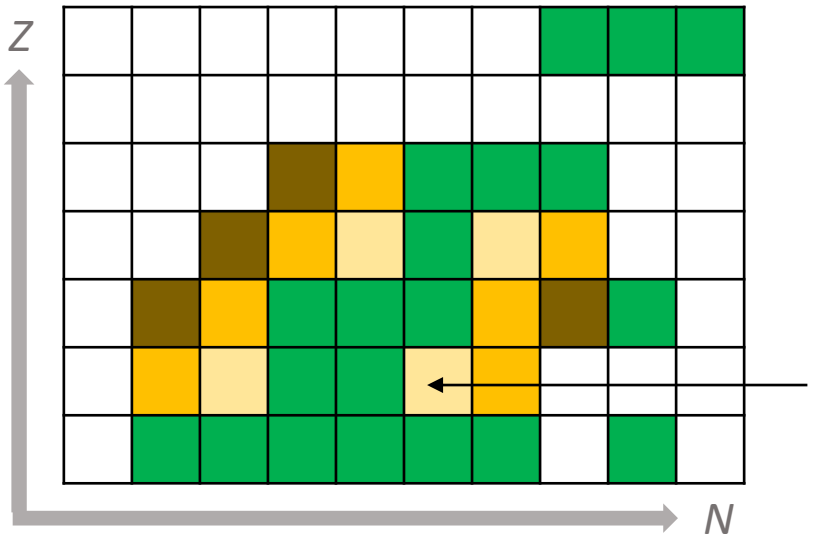
Mass relations for estimating np-correlations:

$$\Delta_{np}(Z,N) = \left[S_p(Z,N) - S_p(Z,N-1)\right] = \left[B(Z,N) - B(Z,N-1)\right] - \left[B(Z-1,N) - B(Z-1,N-1)\right]$$

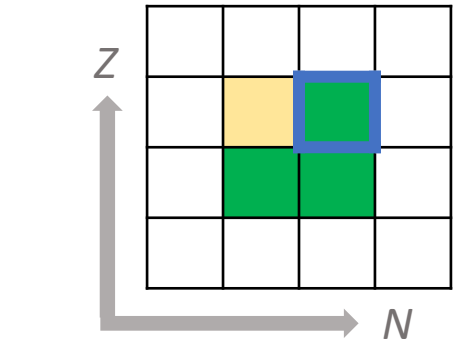
Predicted binding energy B (1 of 4 possible formulas):

$$B_{pred}(Z,N-1) = B(Z,N) - B(Z-1,N) + B(Z-1,N-1) - \Delta_{np}^{cal}(Z,N)$$





The binding energy of such nucleus can be expressed from 2 ways => predictions should be averaged



Δ_{np} is calculated for this nuclide

Predicted B

Area on the NZ-diagram with 4 nuclei included in the formula.

Approximation

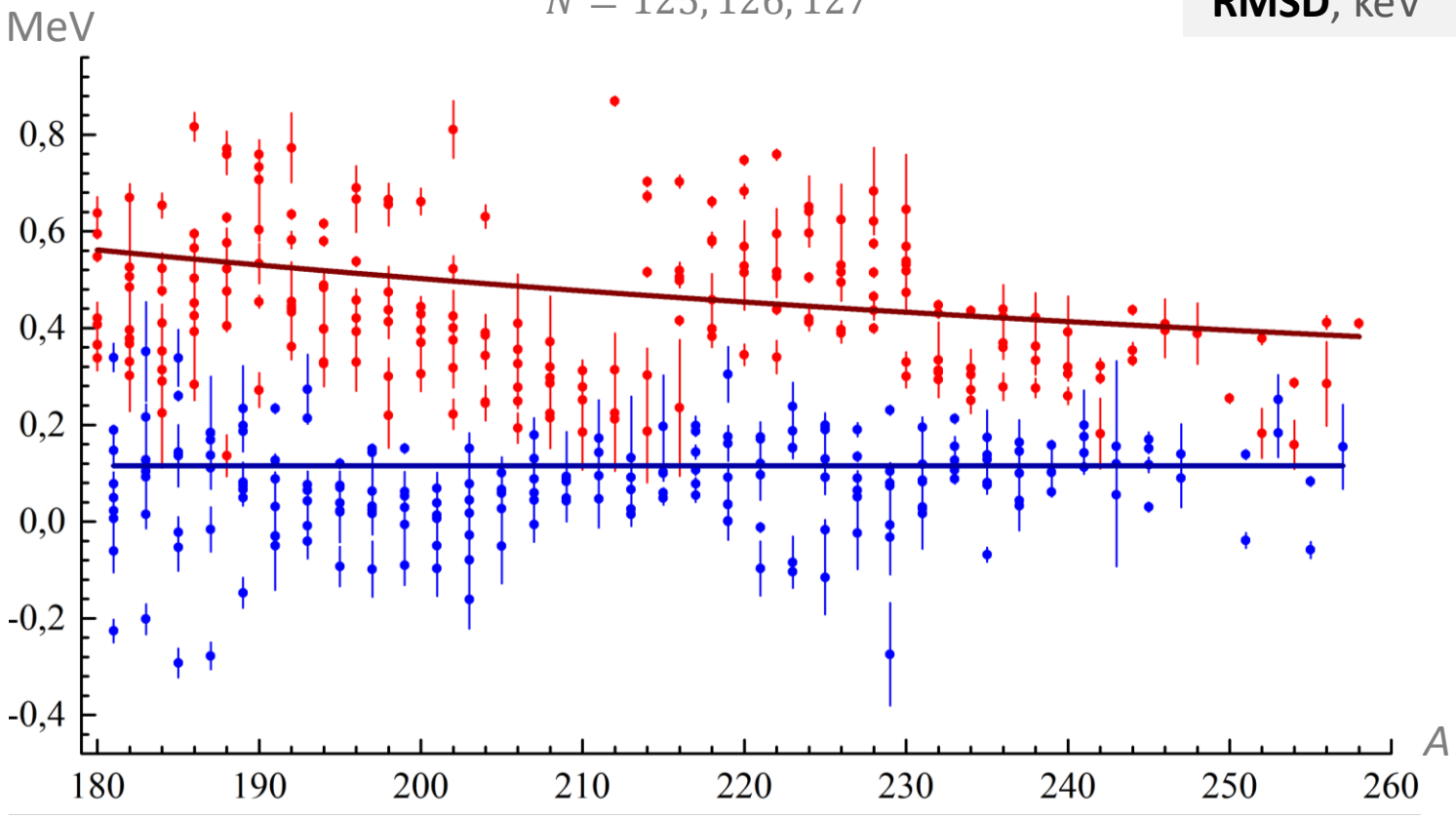
$$\Delta_{np}^{cal}(A) = C_1 + C_2 \cdot A^{\gamma}$$

Approximation area: $A \geq 180$ (heavy isotopes)

Exceptions: $Z = 81, 82, 83$

$N = 125, 126, 127$

	A even	A odd
C_1, MeV	$-0{,}031 \pm 0{,}083$	$0{,}116 \pm 0{,}005$
C_2, MeV	$106{,}599 \pm 16{,}646$	–
γ	–1	–
RMSD, keV	**153**	**111**



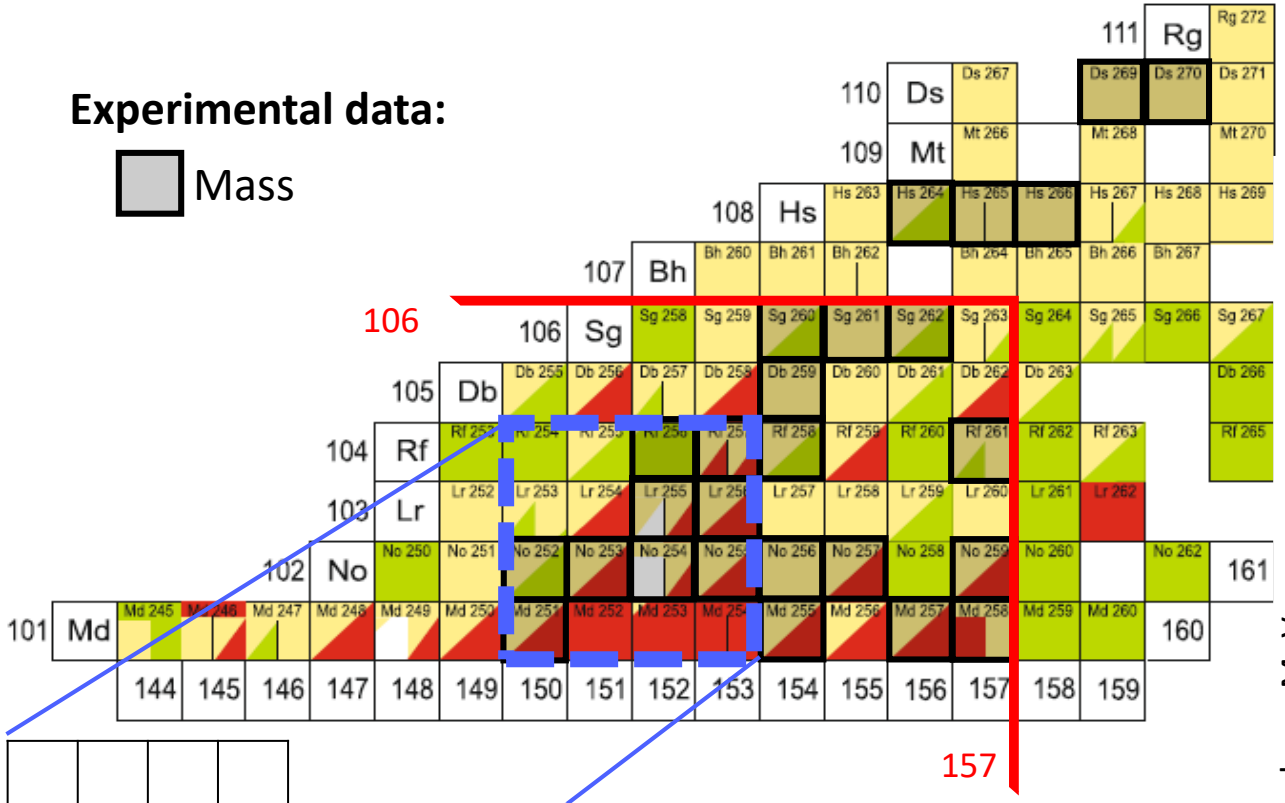
- Δ_{np} experimental (AME2016)
- $\Delta_{np}^{cal}(A)$

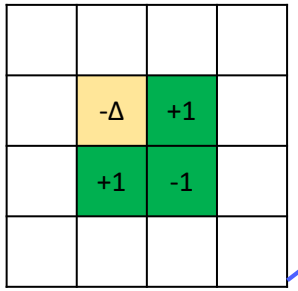
Source of experimental data:
[**Wang M., Audi G., Kondev F.G.et al.**// Chin. Phys. C 2016. 41. 030003.]

Calculation example

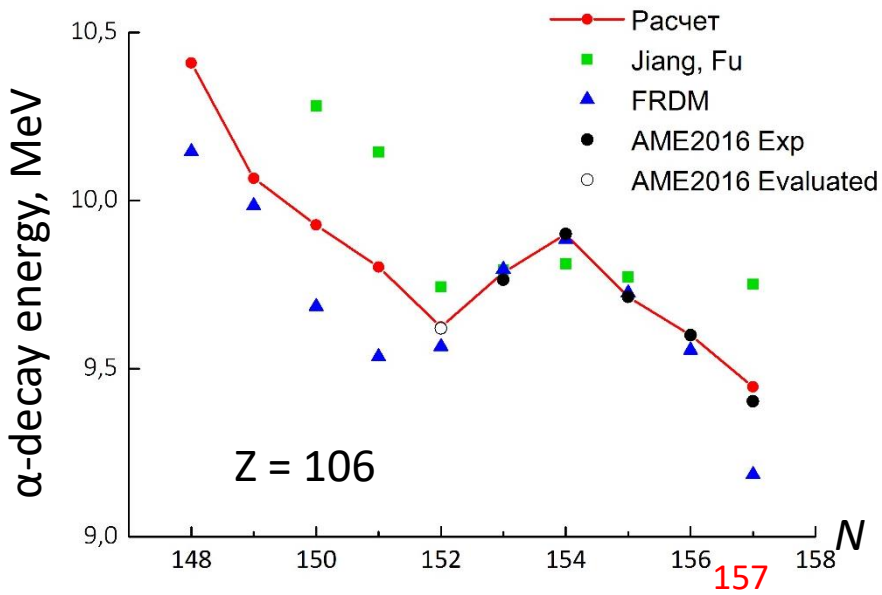
Experimental data:

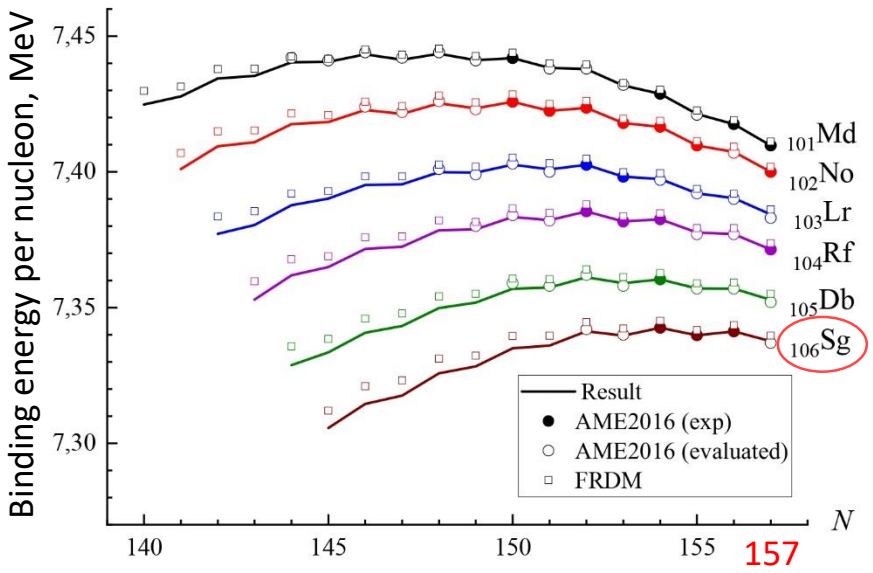
Mass





«Square» formula connecting 4 nuclei does not allow to advance beyond $^{263}_{106}Sg$. So we need other mass relations to go beyond the 106th element.





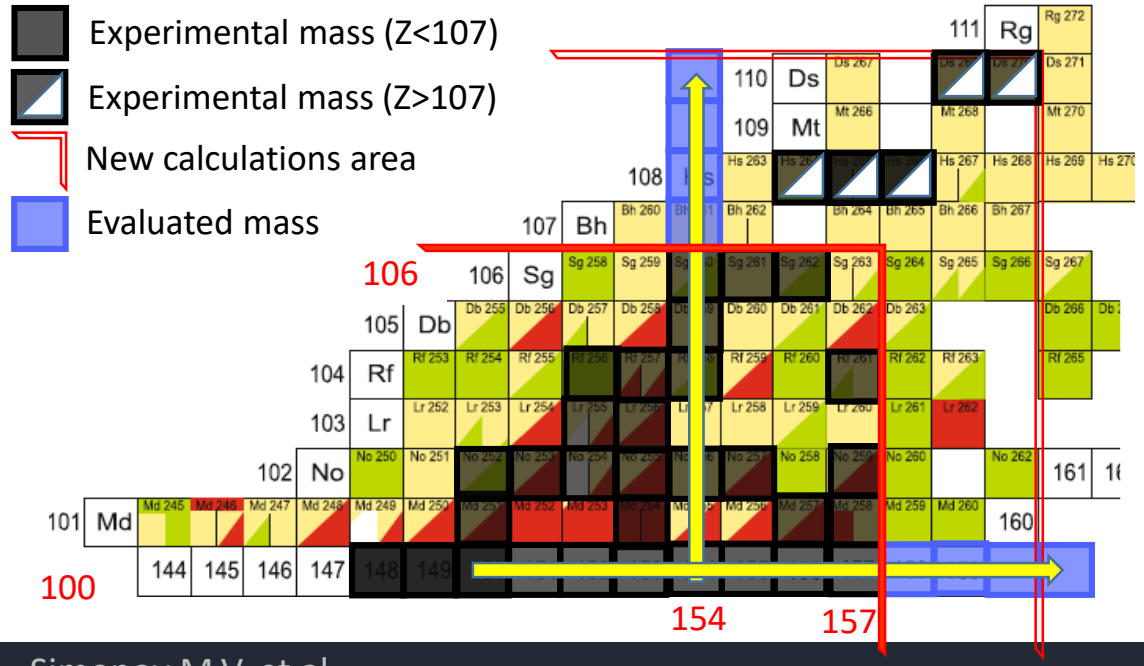
[*FRDM:* **P. Möller et al.** // At. Data and Nucl. Data Tabl. 2016. Vol. 109–110, p. 1-204.]
[**H. Jiang, G. J. Fu et al.** // Phys. Rev. 2012. C 85, 054303.]

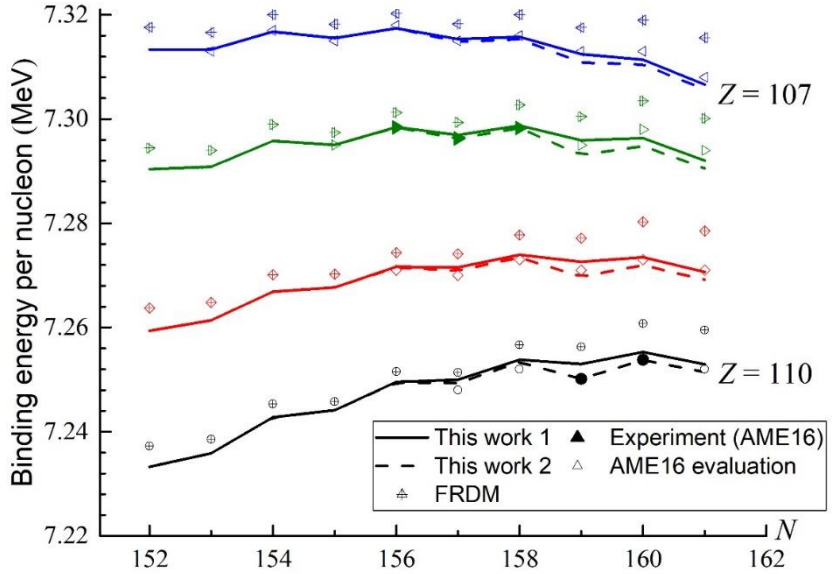
Predictions for 107-110 elements using separation energy

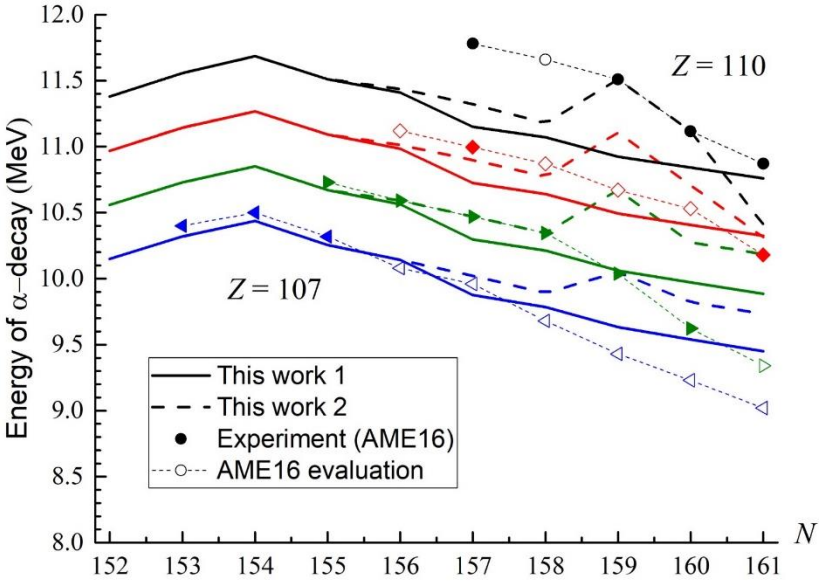
Energy of two protons/neutrons separation:

$$S_{pp}(Z,N) = B(Z,N) - B(Z-2,N),$$
$$S_{nn}(Z,N) = B(Z,N) - B(Z,N-2)$$

1. We approximated 2 lines with sufficient amount of data: $S_{pp}(N=154)\ and\ S_{nn}(Z=100)$ and got 8 evaluated masses (see down diagram).
2. We used formula for Δ_{np} (see 3 previous slides) to calculate binding and α-decay energies for 107-110th.







We had two ways for calculation:
1) not considering experimental mass Z>107
2) considering experimental mass Z>107.

Small discrepancies for evaluation of binding energy can lead to large discrepancies for α-decay energy.

Calculations without experimental masses for Z > 107 (***this work 1***) are more preferable: they do not give any special phenomena for alpha decay (see plots on the right for N = 159, also compare estimations and experimental data for Z = 110).

Predictions for 107-110 elements using energy of α-decay

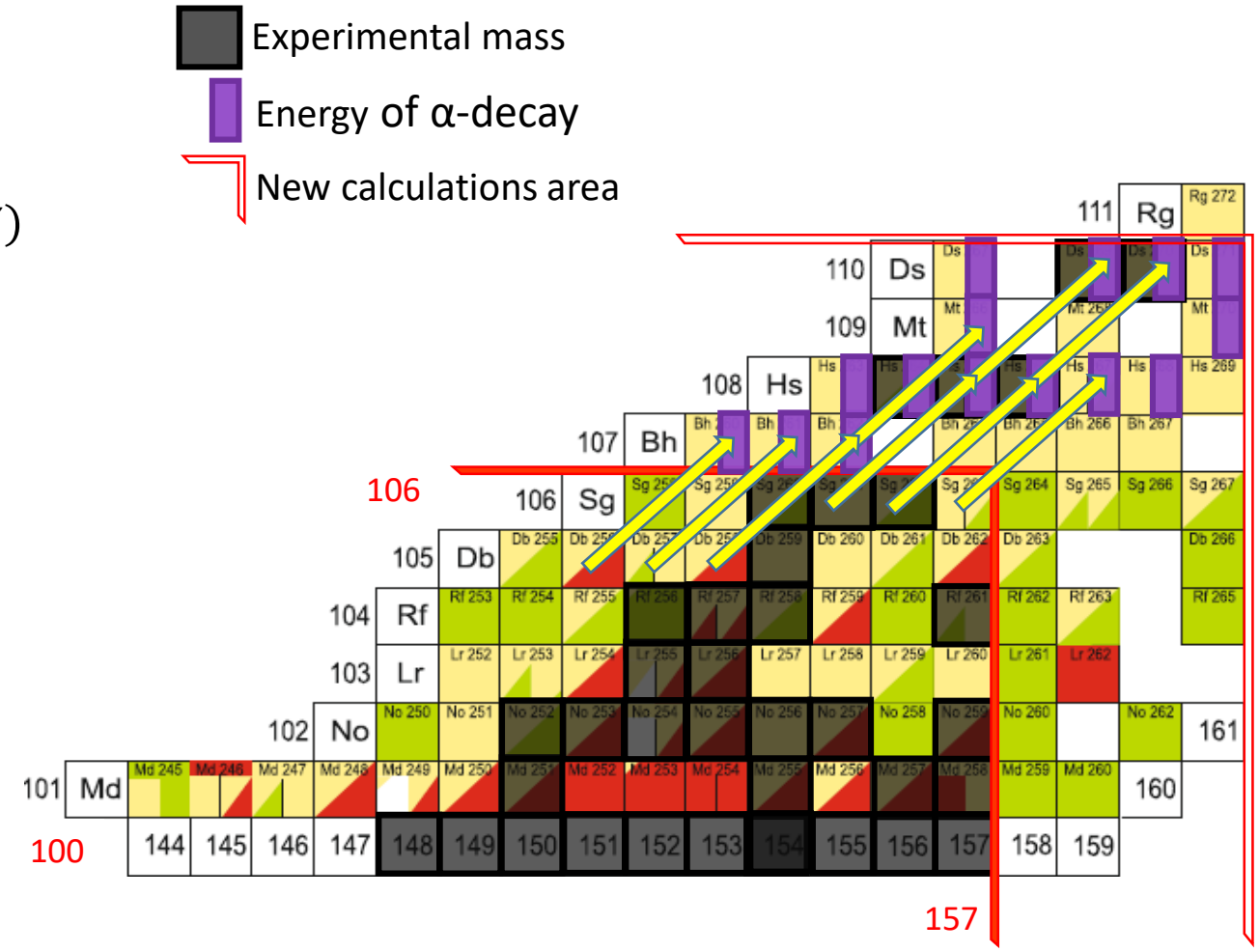
Energy of α-decay:

$$Q_\alpha(N,Z) = B(N-2,Z-2) + B(2,2) - B(N,Z),$$

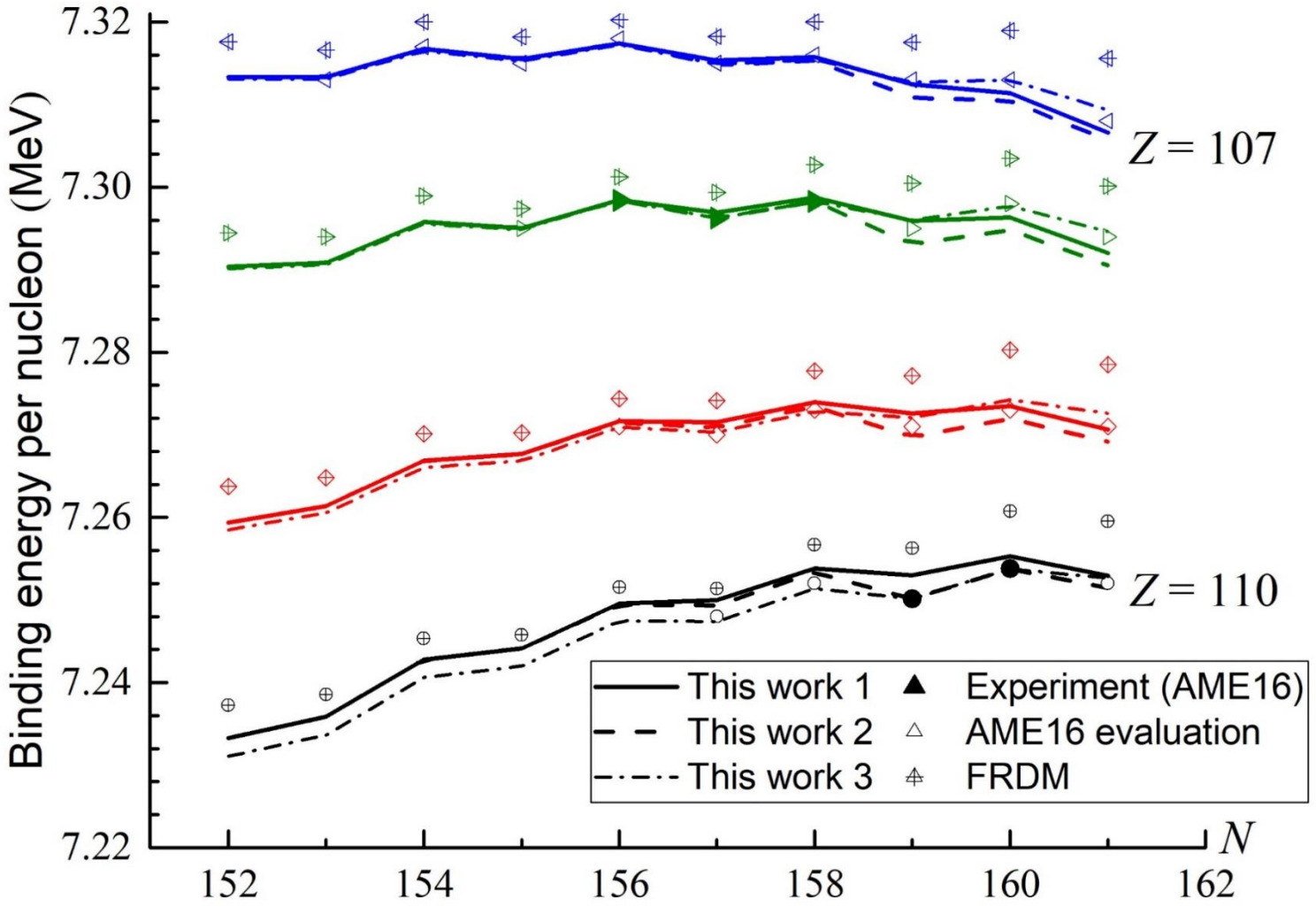
Predicted binding energy B:

$$B_{pred}(N,Z) = B(N-2,Z-2) + B(2,2) - Q_\alpha(N,Z)$$

1. We used available experimental values of α-decay energy and got 12 evaluated masses (see right diagram).
2. Then we used formula for Δ_{np} to calculate binding and α-decay energies for 107-110th elements. This method gives the best result for α-decay and therefore was used to further evaluate the half-life.



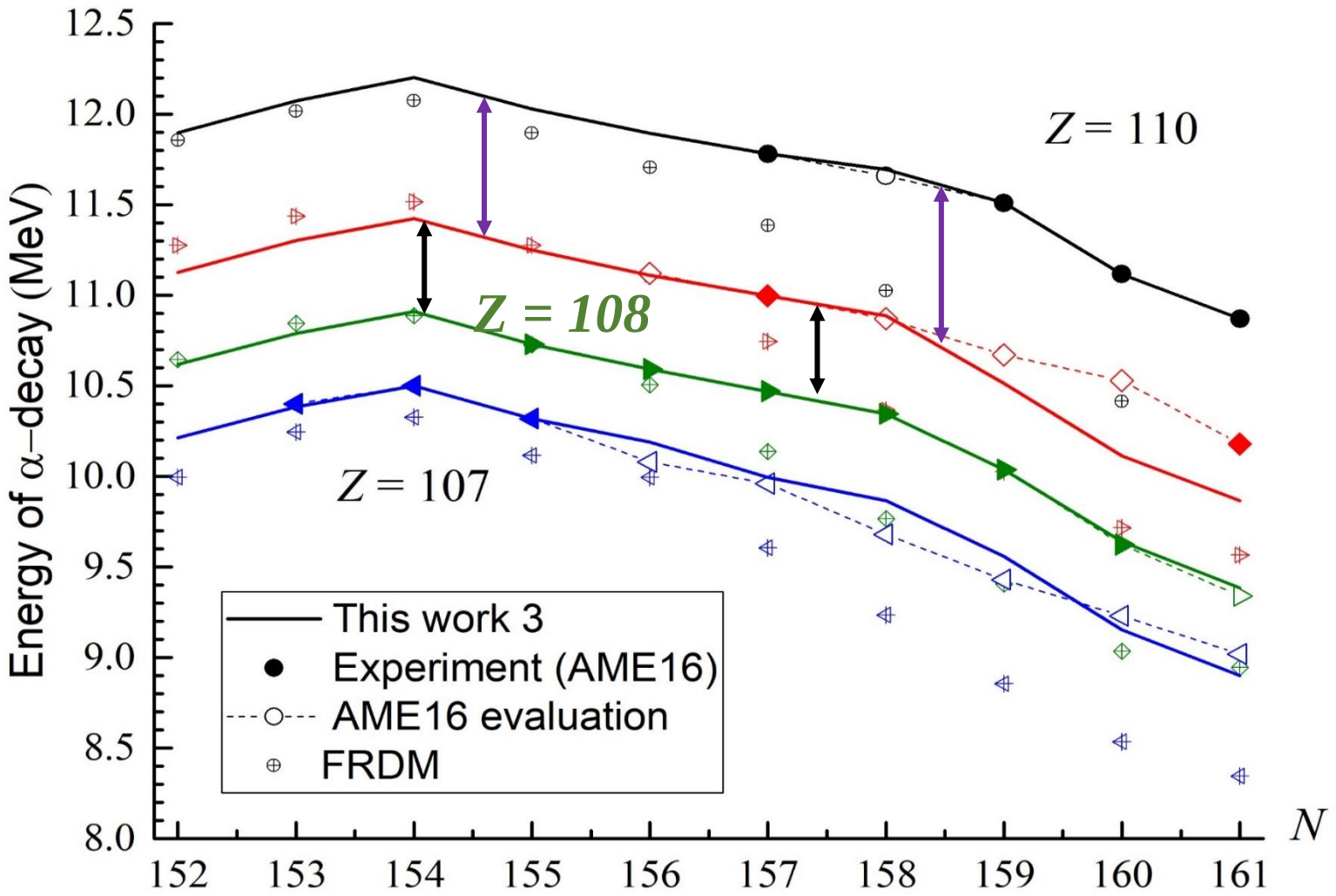
Predictions for 107-110 elements. Binding energy



This picture shows that *the local mass relations method* gives much more accurate predictions for binding energies than the global FRDM model.

Evaluations gained by the 3rd way noticeably different from ones gained by the 1st and 2nd ways (from separation energies), especially for isotopic line of the 110st element.

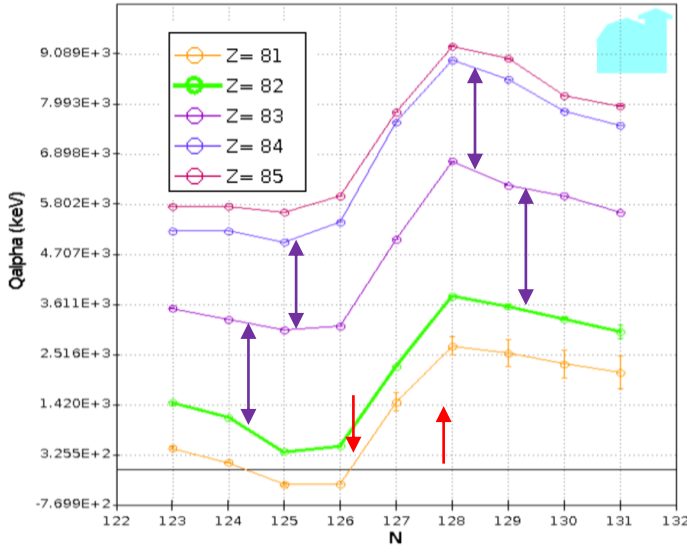
Predictions for 107-110 elements. Energy of α-decay



Some conclusions about the shell structure of superheavy elements may be done.

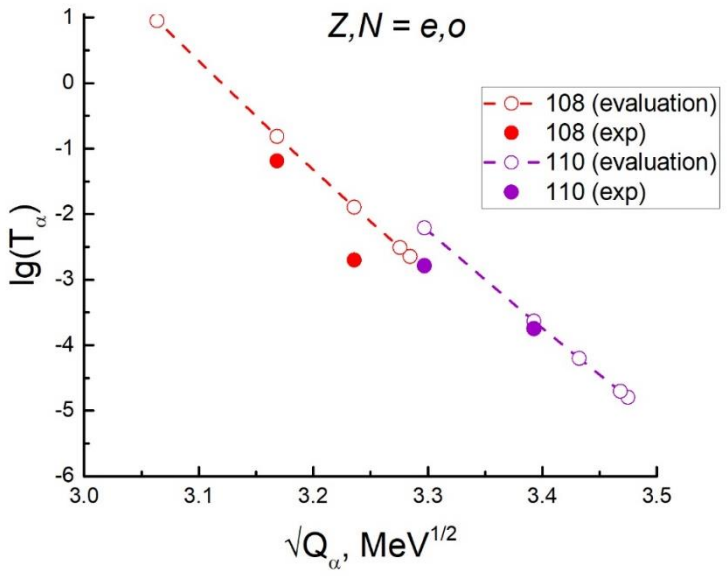
An increase in the gap between the isolines may indicate magic number Z = 108.

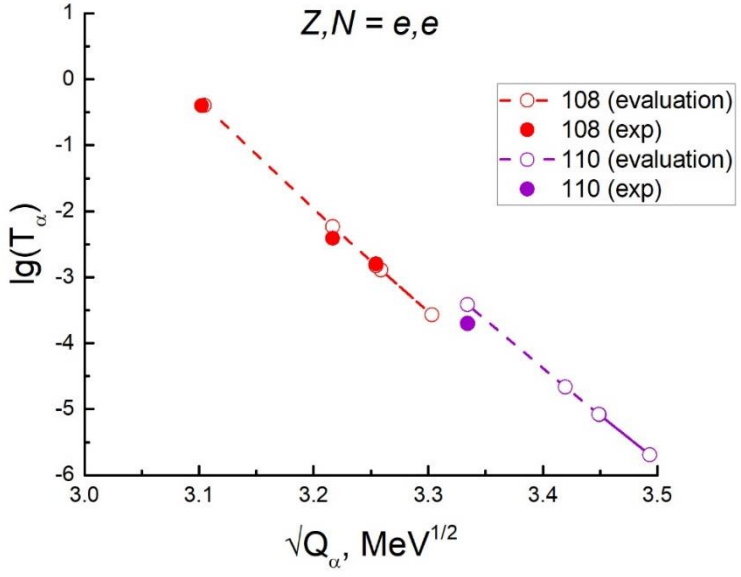
The local peak on N = 154 suggests that N = 152 is magic (look down for comparison graph).

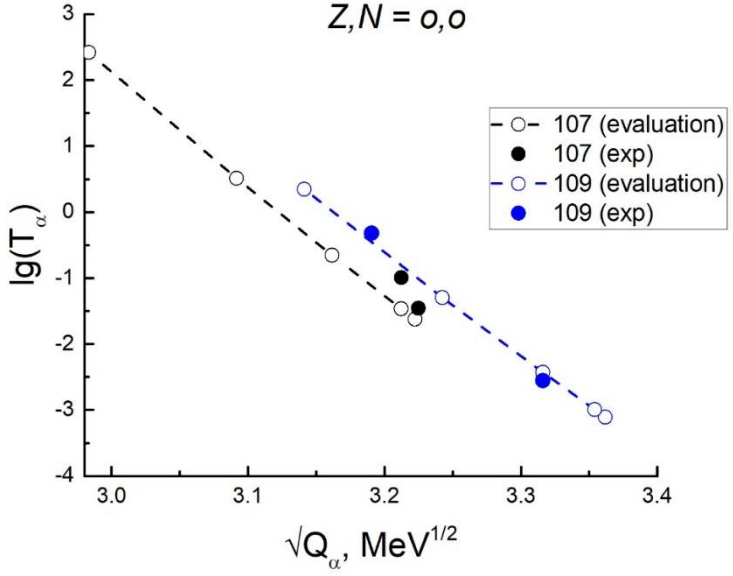


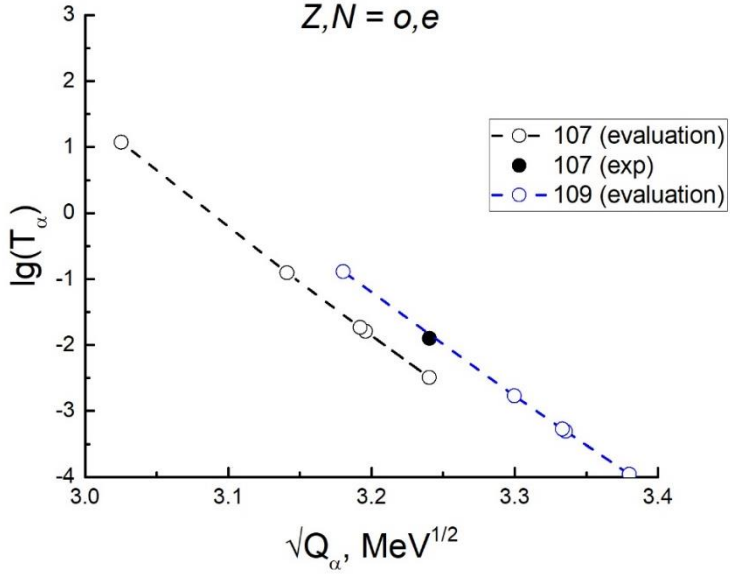
From NNDC base NuDat 2.8

Predictions for 107-110 elements. α-decay half-life









Using Viola-Seaborg's formula we obtain estimations for α-decay half-lives.

The prediction accuracy is about *one order of magnitude* for half-lives.

A small amount of experimental data is associated with a small cross section for SHE isotope production.

Viola-Seaborg's formula:

$$lgT_\alpha = \frac{(cZ+d)}{\sqrt{Q}} + (fZ+e) + h_{log}$$

[**V. E. Viola, G. T. Seaborg et al**. // Nucl. Chem. 28, 741 (1966)]

Parametrization taken from: [**A. Parkhomenko, A. Sobiczewski** // Acta Phys. Polonica B. vol. 36 № 10 (2005)]

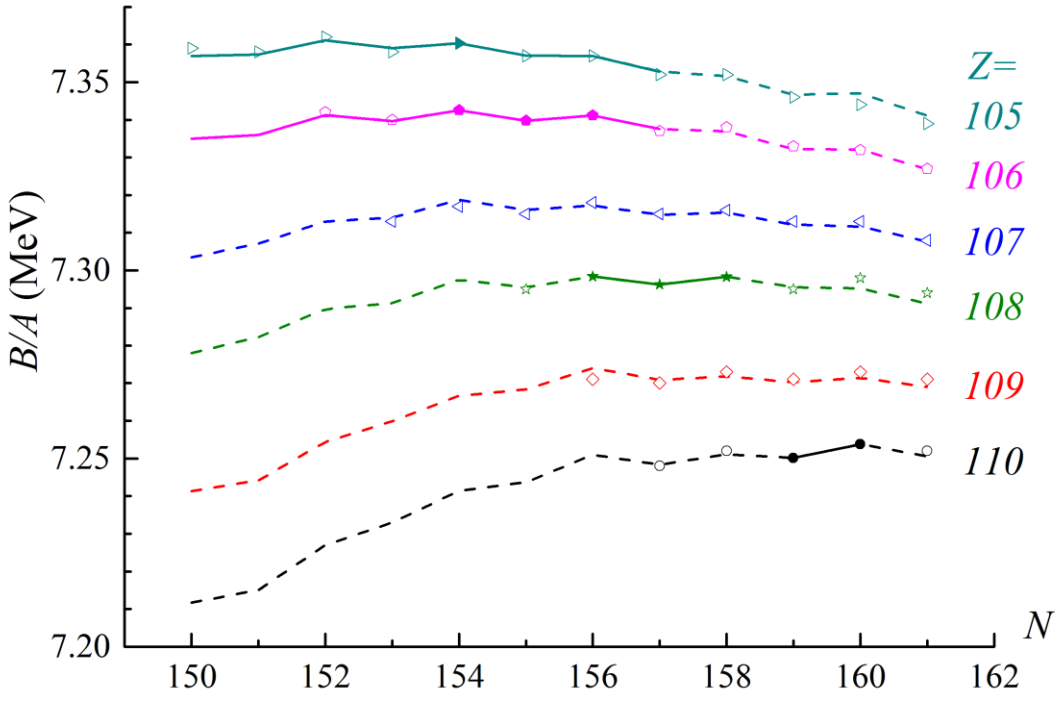
Predictions for SHE. Machine learning (ML)

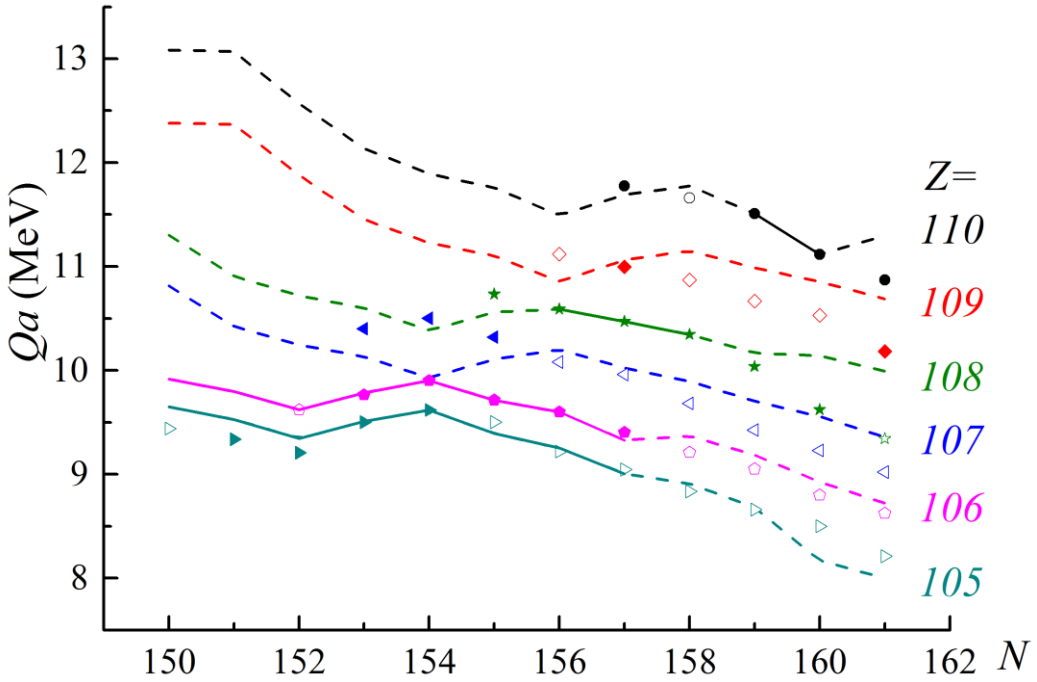
Machine learning + Local mass relations = Expanding of learning dataset → Predictions

Algorithm: support vector regression (SVR) from the Scikit-learn (Python) library.

Methodics:

- Binding energy per nucleon B/A(N, Z) prediction based on the B/A of nuclei (N – 2, Z – 2) and (N – 4, Z – 4).
- *Input array:* AME16 (experiment) + results of estimates by Δ_{np} (up to Z = 106 and N = 157, number of steps = 15)
- *Training* on the entire array of nuclei (N, Z > 10).
- *Result.* 2 runs were performed: 1) 3911 training array rows → 97 predicted, 2) 4008 rows → 90 predicted





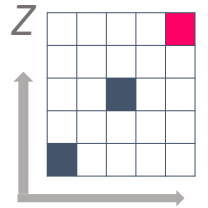


Diagram of neighbors

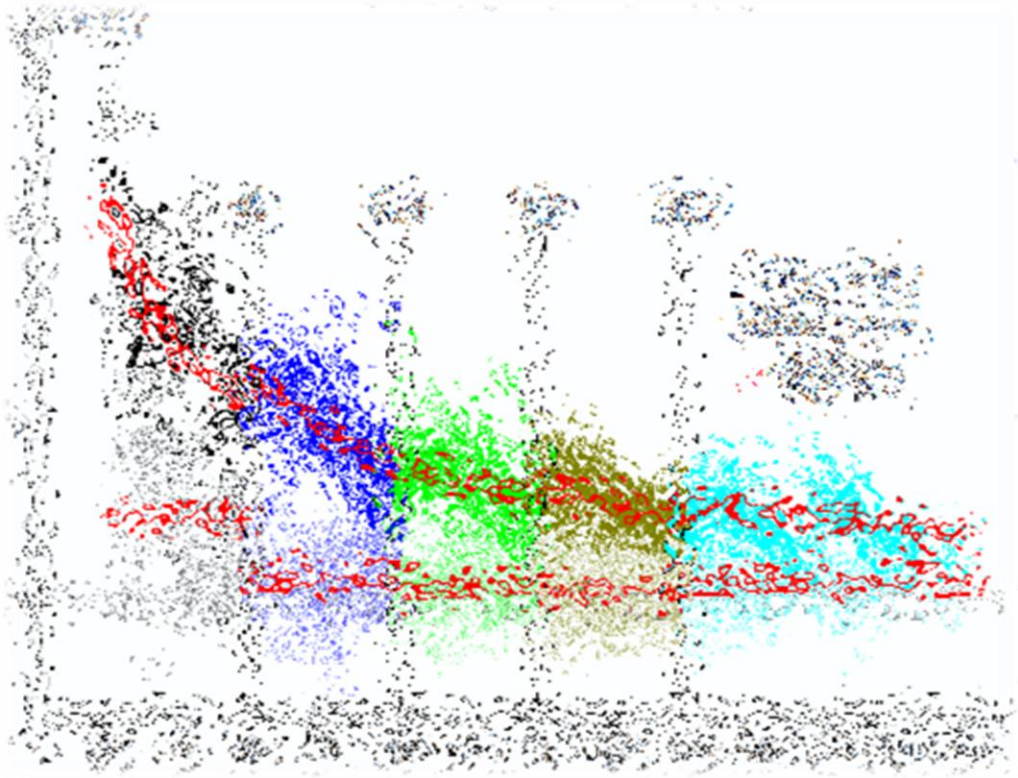
— Result by Δ_{np}
- - Result by ML
● Experiment (AME16)
○ AME16 evaluation

Results

1. Using approximation of the expression for *np*-correlations, separation energies and experimental energy of α-decay, the binding energies of the nuclei were calculated for transfermium isotopes with $Z = 107 - 110$ and $N = 152 - 161$. Comparison of calculated and experimental data showed sufficient reliability of the method.

2. Based on the obtained binding energies, the α-decay energy and half-life are calculated for superheavy nuclei with $Z = 107 - 110$. Comparison of the results obtained with the experiment (where possible) and the results of other works demonstrates sufficient acceptability of this method.

3. Machine learning algorithms combined with the method of local mass relations makes it possible to obtain predictions for mass characteristics for superheavy elements, however, the prediction accuracy is not yet satisfactory. Further development of this method is supposed.



Thank you for your attention!

Abstract

- *Background:* Nowadays all the elements up to 118^{th} are known due to success of experimental nuclear physics in new heavy element synthesis, however, not all the masses of new nuclides have been measured.
- *Method:* the phenomenological approach based on **local mass relations** is implemented to predict masses of unknown isotopes. This approach is characterized by mathematical simplicity and accuracy, especially when it is concerned with mass relations for residual proton-neutron interaction.
- *Results:* In the region of heavy and **superheavy elements** the behavior of various mass relations associated with nucleon correlations is considered. *Estimations of nuclides' masses and α-decay energy values (half-lives) for elements with Z=107-110 are gained by approximation of these mass relations.* The results are compared with **machine-learning based calculations** and also calculations using other approaches.
- *Conclusion:* mass relations can be successfully applied for evaluation of isotopes' mass characteristics in case isotopes are located near known ones.

Isotope map: experimental data and an example of calculations