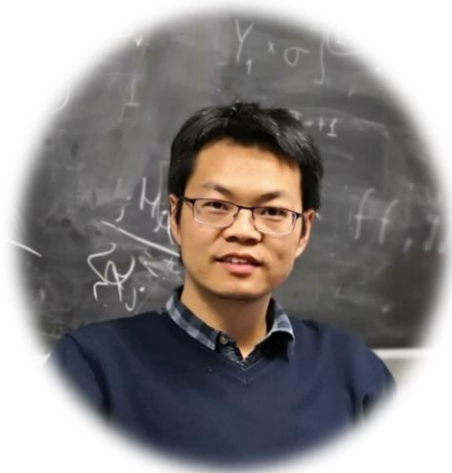




The 7th workshop on nuclear mass table with DRHBc theory @2024.07.01-07.04, Gangneung, Korea

Nuclear mass predictions within convolutional neural network

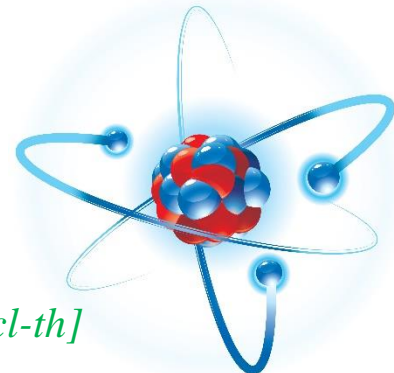


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Yanhua Lu, Tianshuai Shang, Pengxiang Du, Jian Li, Haozhao Liang and Zhongming Niu, arXiv:2404.14948 [nucl-th]



Current status of nuclear mass research

❑ Mass (or binding energy): basic physical quantity, plays a crucial role in understanding the nuclear structure and studying the astrophysical nucleosynthesis.

❑ Experiment: accurate measurement; AME2020 evaluate and recommends the masses of 3557 nuclei.

M. Wang, W. Huang, F. G. Kondev, G. Audi, and S. Naimi. Chinese Phys. C 45, 030003(2021)

❑ Theory: global model and local relation model

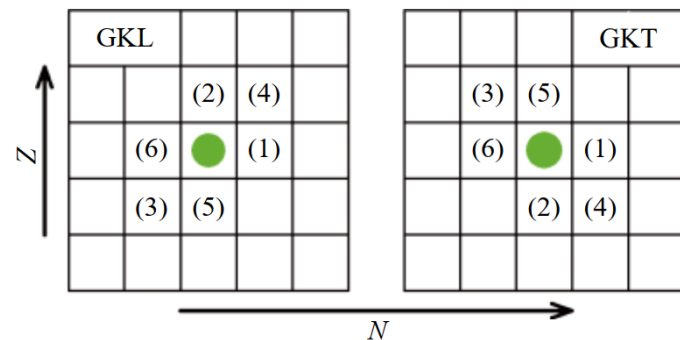
✓ Global mass models: BW2, KTUY, FRDM12, WS4, HFB-31, DZ28, etc., about 0.3 MeV (WS4).

N. Wang, M. Liu, X.Z. Wu, J. Meng, Phys. Lett. B 734 (2014) 215.

the nuclear mass table in relativistic density functional theory: **RCHB** ⇒ **DRHBc**

At. Data Nucl. Data Tables 121–122 (2018) 1–215; At. Data Nucl. Data Tables 144 (2022) 101488; At. Data Nucl. Data Tables 158 (2024) 101661

✓ Local relation model: Garvey-Kelson local mass relation (GK relation), or the neutron-proton interaction (0.2 MeV)

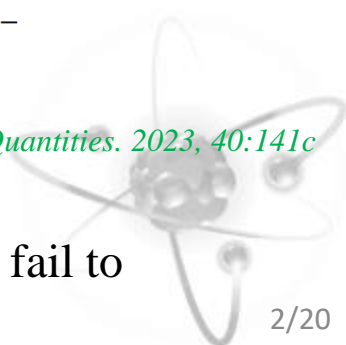


Jiang H, Fu G J, Sun B, et al. Phys Rev C, 2012, 85: 054303.

$$D_L(N, Z) = M(N+1, Z) + M(N, Z+1) + M(N-1, Z-1) - M(N+1, Z+1) - M(N, Z-1) - M(N-1, Z) \approx 0,$$

$$D_T(N, Z) = M(N+1, Z) + M(N, Z-1) + M(N-1, Z+1) - M(N+1, Z-1) - M(N, Z+1) - M(N-1, Z) \approx 0.$$

Bao Man, Jiang Hui, Zhao Yumin. Systematic Study on Nuclear Mass and Related Physical Quantities. 2023, 40:141c



Although the predictive accuracy of nuclear mass models has improved significantly, theoretical models still fail to meet the research needs of nuclear structure and celestial nucleosynthesis.



Machine learning



game of go



computer vision



translation



autonomous car



voice recognition

Machine learning in nuclear physics

- **(D)NN**: (Deep) Neural Network
- **BNN**: Bayesian Neural Network
- **CNN**: Convolutional Neural Network
- **MDN**: Mixture Density Network
- **(B)GP**: (Bayesian) Gaussian Processes
- **CGP**: Constrained Gaussian Processes
- **DT**: Decision Tree
- **NBP**: Naive Bayesian Probability Classifier
- **SVM**: Support Vector Machines
- **RBF**: Radial Basis Function
- **KRR**: Kernel Ridge Regression
- **CLEAN**: CLEAN Image Reconstruction
- ...





Recent progress about machine learning

Chinese Physics C Vol. 45, No. 12 (2021) 124107

Magnetic moment predictions of odd- A nuclei with the Bayesian neural network approach*

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物理学报 *Acta Phys. Sin.* Vol. 72, No. 15 (2023) 152101

Prediction of ground-state spin in odd- A nuclei within decision tree*

Wen Hu-Feng^{1)##} Shang Tian-Shuai^{1)##} Li Jian^{1)†} Niu Zhong-Ming²⁾

Yang Dong^{1)‡} Xue Yong-He¹⁾ Li Xiang¹⁾ Huang Xiao-Long³⁾

Nuclear Science and Techniques (2022) 33:153
<https://doi.org/10.1007/s41365-022-01140-9>



Prediction of nuclear charge density distribution with feedback neural network

Tian-Shuai Shang¹ · Jian Li¹ · Zhong-Ming Niu²

Received: 15 September 2022 / Revised: 30 October 2022 / Accepted: 3 November 2022
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Abstract

Nuclear charge density distribution plays an important role in both nuclear and atomic physics, for which the two-parameter Fermi (2pF) model has been widely applied as one of the most frequently used models. Currently, the feedforward neural network has been employed to study the available 2pF model parameters for 86 nuclei, and the accuracy and precision of the parameter-learning effect are improved by introducing $A^{1/3}$ into the input parameter of the neural network. Furthermore, the average result of multiple predictions is more reliable than the best result of a single prediction and there is no significant difference between the average result of the density and parameter values for the average charge density distribution. In addition, the 2pF parameters of 284 (near) stable nuclei are predicted in this study, which provides a reference for the experiment.

PHYSICAL REVIEW C **109**, 044325 (2024)

Inference of parameters for the back-shifted Fermi gas model using a feedforward neural network

Peng-Xiang Du , Tian-Shuai Shang , Kun-Peng Geng, and Jian Li
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(Received 12 January 2024; accepted 25 March 2024; published 24 April 2024)

The back-shifted Fermi gas model is widely employed for calculating nuclear level density (NLD) as it can effectively reproduce experimental data by adjusting parameters. However, selecting parameters for nuclei lacking experimental data poses a challenge. In this study, a feedforward neural network (FNN) was utilized to learn the level density parameters at neutron separation energy $a(S_n)$ and the energy shift Δ for 289 nuclei. Simulations were performed for 2000 nuclei, and the results showed that the FNN, using the training data, can

PHYSICAL REVIEW C
covering nuclear physics

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Global prediction of nuclear charge density distributions using a deep neural network

Tian Shuai Shang, Hui Hui Xie, Jian Li, and Haozhao Liang
Phys. Rev. C **110**, 014308 – Published 2 July 2024



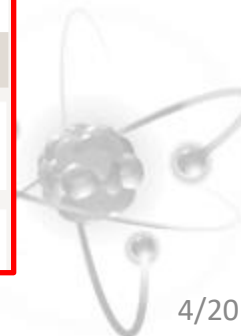
Article References No Citing Articles Supplemental Material PDF HTML Export Citation



ABSTRACT

A deep neural network (DNN) has been developed to generate the distributions of nuclear charge density, utilizing the training data from the relativistic density functional theory and incorporating available experimental charge radii of 1014 nuclei into the loss function. The DNN achieved a root-mean-square deviation of 0.0193 fm for charge radii on its validation set. Furthermore, the DNN can improve the description in both the tail and central regions of the charge density, enhancing agreement

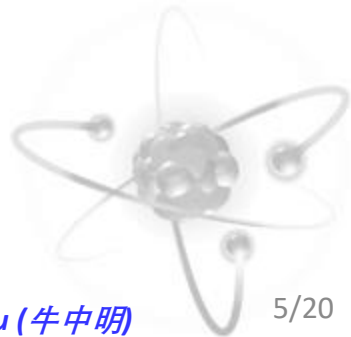
Issue
Vol. 110, Iss. 1 — July 2024





Machine learning in nuclear mass predictions

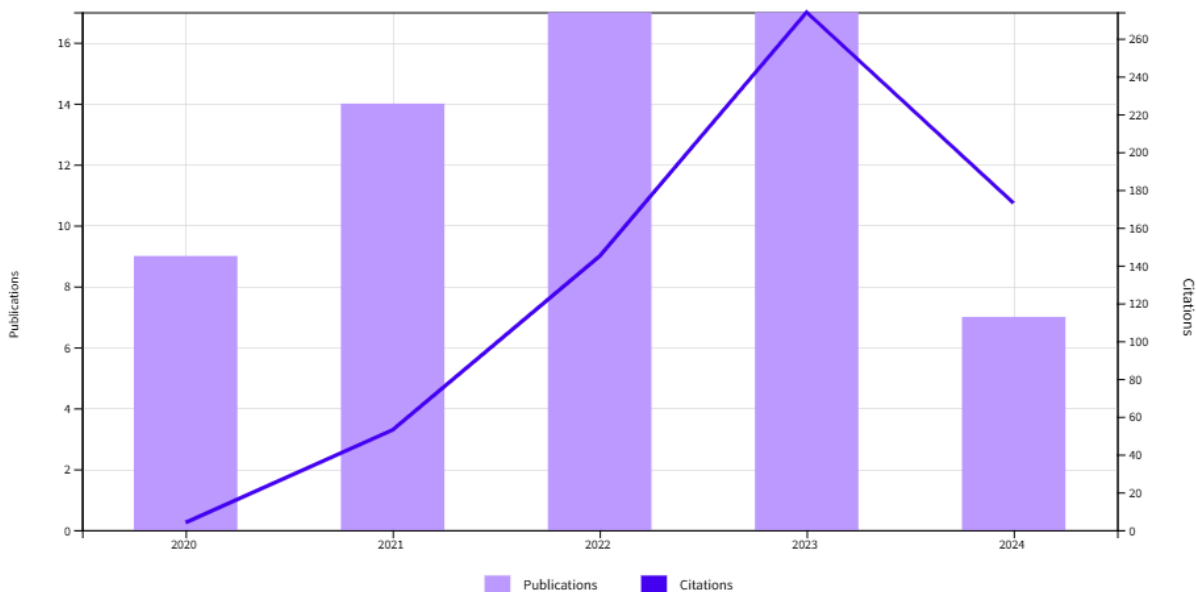
- ★ **ANN:** Gazula1992NPA, Athanassopoulos2004NPA, Bayram2014ANE, Zhang2017JPG, Ming2022NST, Yuksel2021IJMPE, Li2022PRC, Zeng2024PRC
- ★ **BNN:** Utama2016PRC, Niu2018PLB, Niu2019PRC, Niu2022PRCL, Rodriguez2019EPL, Rodriguez2019JPG
- ★ **CNN:** Yang2023PRC **DNN:** ChenPRC2022, To-Chung-Yiu2024CPC
- ★ **LightGBM:** Gao2021NST
- ★ **KRR:** Wu2020PRC, Wu2021PLB, Du2023CPC, Wu2022PLB, Wu2024PRC, Wu2023Front. Phys.
- ★ **NBP:** Liu2021PRC **PUN:** Babette-DellenPLB2024
- ★ **RBF:** Wang2011PRC, Niu2013, 2016PRC, 2018SciB
- ★ **BGP:** Neufcourt2018, 2020PRC, Neufcourt2019PRL
- ★ **SVM:** Clark2006IJMPB
- ★ **CLEAN:** Morales2010PRC **MDN:** A. E. Lovell2022PRC **PIML:** Mumpower2022PRC
- ★



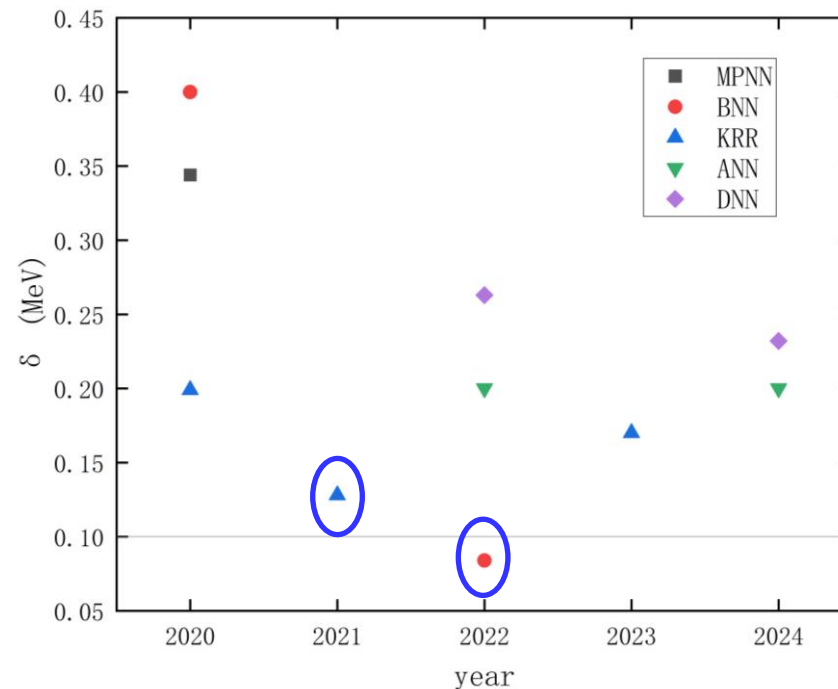


Machine learning in nuclear mass predictions

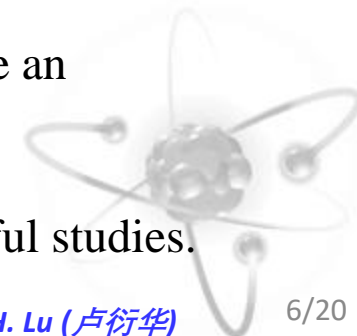
Publications/citations per year



Precision of prediction



- ✓ Although there are many studies using machine learning to predict nuclear masses, most of them achieve an accuracy of only around 200 keV.
- ✓ To overcome this bottleneck, it is necessary to consider more physics, as demonstrated by some successful studies.





Nuclear mass predictions with Kernel Ridge regression



Precision on experimentally known nuclei

- KRR: 199 keV

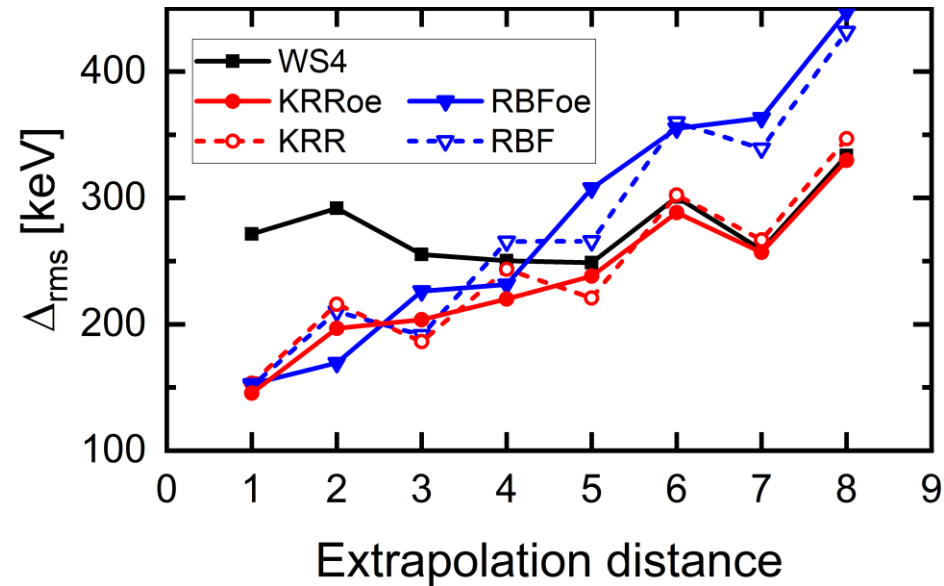
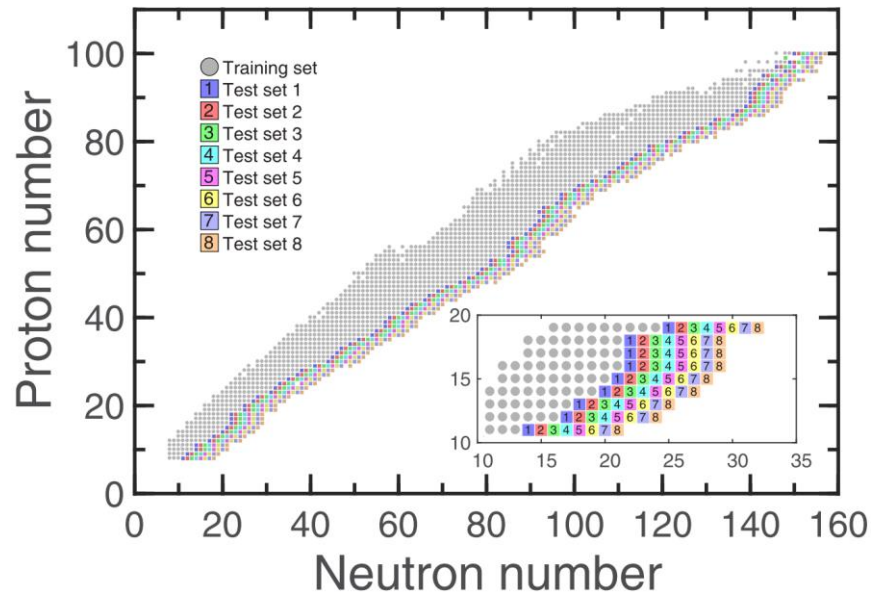
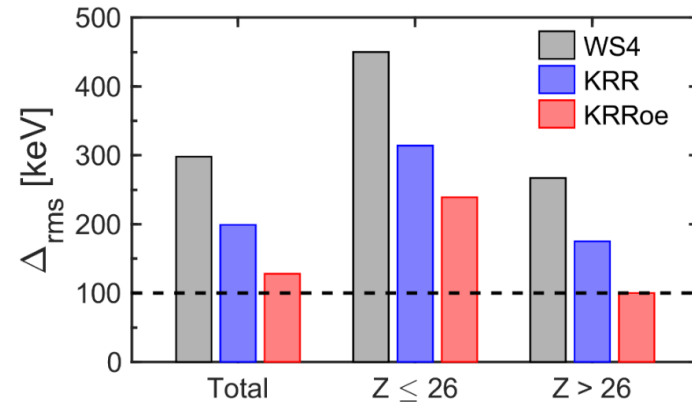
X. H. Wu and P. W. Zhao, *Phys. Phys. C* 101, 051301 (R) (2020)

- KRRoe: 128 keV

X. H. Wu, L. H. Guo, and Zhao, *Phys. Lett. B* 819, 136387 (2021)



Extrapolation performance

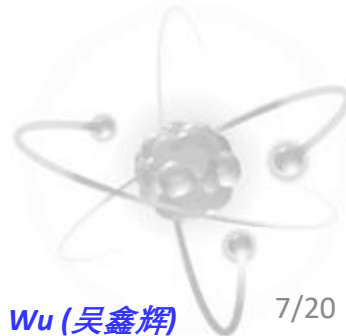


- Avoid worsening mass predictions at large extrapolation distance.

Du, Guo, Wu, and Zhang, *Chin. Phys. C* 47, 074108 (2023)

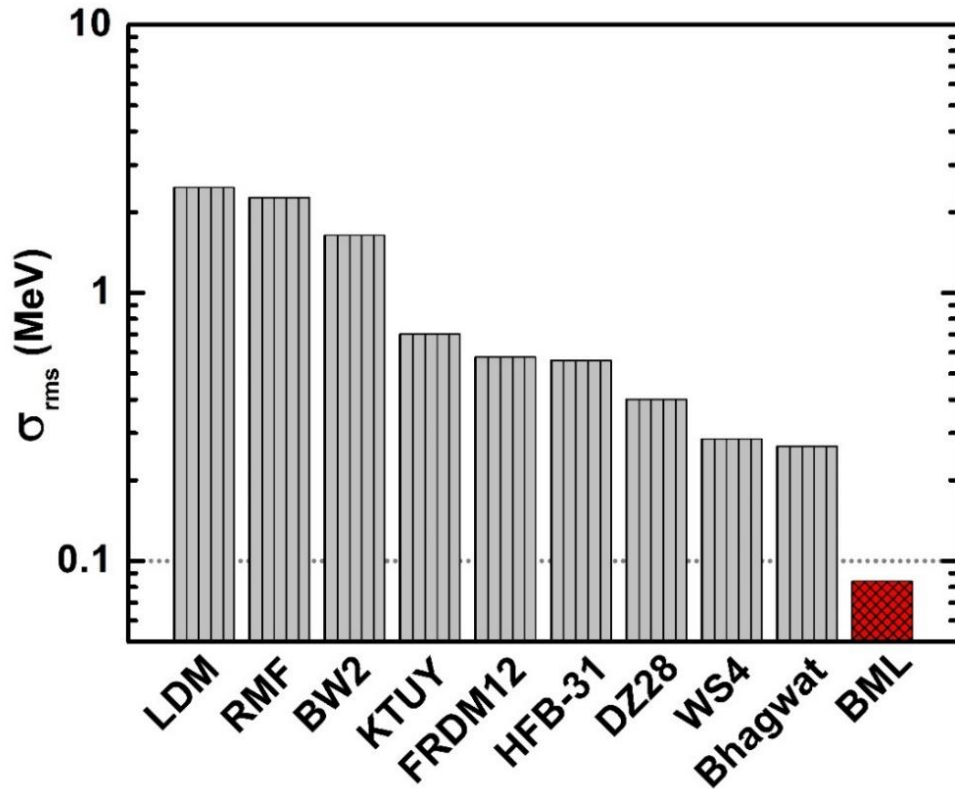
Wu, Lu, and Zhao, *Phys. Lett. B*, 834, 137394 (2022)

Wu, Pan, Zhang, and Hu, *Phys. Rev. C*, 109, 024310 (2024)





Bayesian Machine Learning (BML) mass model



Model	M	S_n	S_{2n}	S_p	S_{2p}	S_D	Q_β
FRDM12	0.576	0.340	0.442	0.341	0.420	0.411	0.450
HFB-31	0.559	0.451	0.456	0.489	0.496	0.566	0.557
WS4	0.285	0.254	0.261	0.261	0.300	0.324	0.327
BML	0.084	0.078	0.105	0.083	0.111	0.096	0.099

★ A nuclear mass model with accuracy smaller than 100 keV in the known region is constructed.

★ Its accuracies to S_x and Q_x are at least about 3 times higher than other mass models.

Z.M. Niu and H.Z. Liang, PRC 106, L021303 (2022)





Motivation

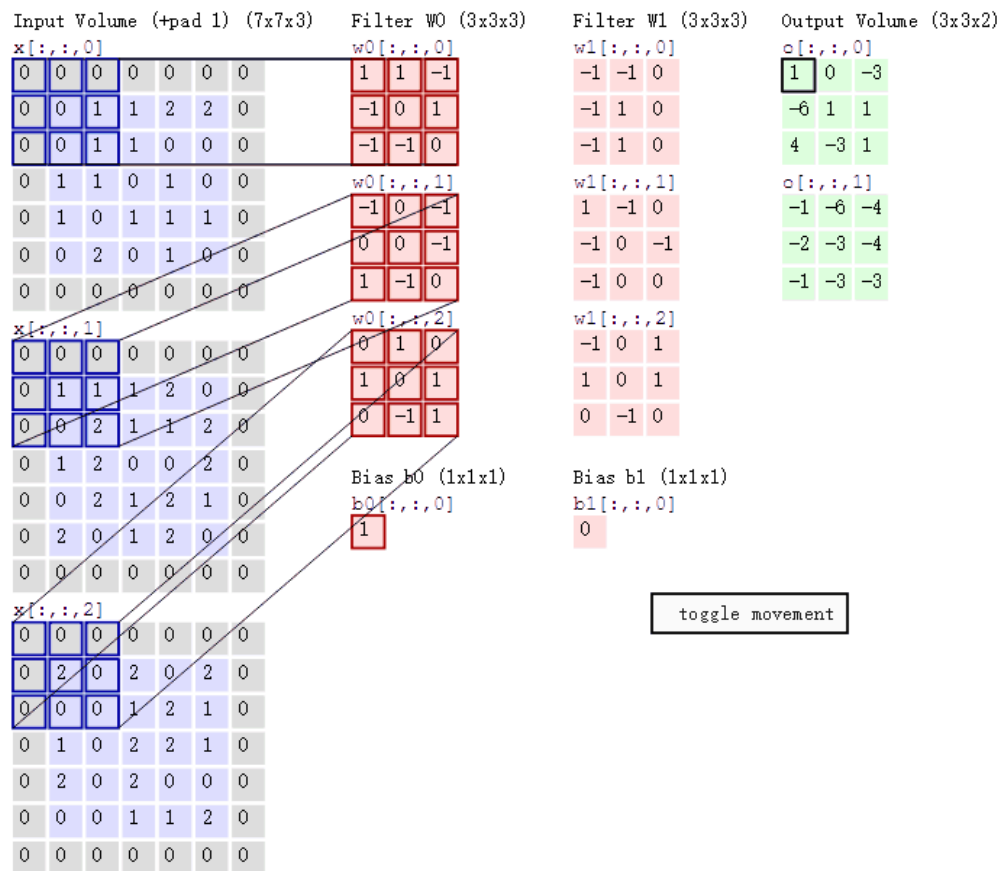
- ✓ **Most machine learning-related work only considers global theoretical models and does not effectively extract the local physical relationships of nuclear mass.**
- ✓ **In this work, a global-local model based on convolutional neural network (CNN) is developed for the first time. By gradually introducing more physical factors, the learning accuracy is further improved, and the accuracy of 0.070 MeV is obtained.**



» CNN: convolutional neural network

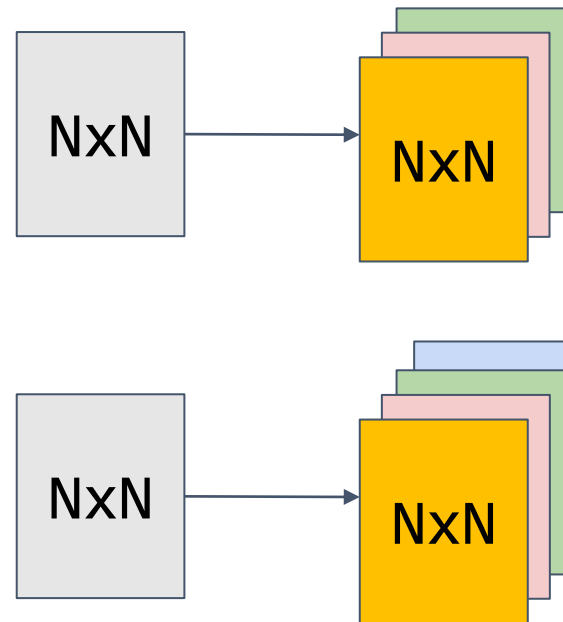
Convolutional neural networks (CNN) are neural networks that have at least one convolutional layer. Convolutional networks are one of the most widely used basic neural network architectures. The convolution layer is a network layer that uses convolution operations instead of ordinary matrix multiplication operations.

The **blue box** refers to a data window. The **red box** is the convolution kernel (filter), and the final **green square** is the result of the convolution (the data in the data window is multiplied and summed element by element)



Model framework and numerical details

^{54}Zn	^{55}Zn	^{56}Zn	^{57}Zn	^{58}Zn
^{53}Cu	^{54}Cu	^{55}Cu	^{56}Cu	^{57}Cu
^{52}Ni	^{53}Ni	^{54}Ni	^{55}Ni	^{56}Ni
^{51}Co	^{52}Co	^{53}Co	^{54}Co	^{55}Co
^{50}Fe	^{51}Fe	^{52}Fe	^{53}Fe	^{54}Fe



CNN-I3

Input: **3**(channels)*5*5
Channels: Z, N, the binding energy of nearby nuclei.

CNN-I4

Input: **4**(channels)*5*5
Channels: Z, N, the binding energy of nearby nuclei, **pairing δ**

$$\delta = [(-1)^N + (-1)^Z]/2$$

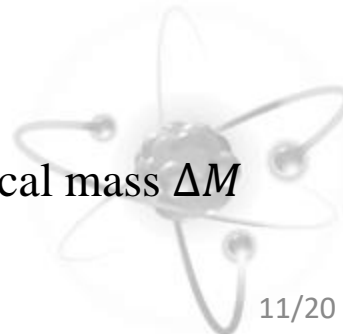
- ✓ The size of the convolution kernel is set as 3×3 with a stride of 1. The two dimensional convolution formula is stated as

$$O(u, v) = \sum_i \sum_j g(i, j)h(u - i, v - j)$$

- ✓ Activation function: ReLU(Rectified Linear Unit) ✓ Difference between experimental mass and theoretical mass ΔM

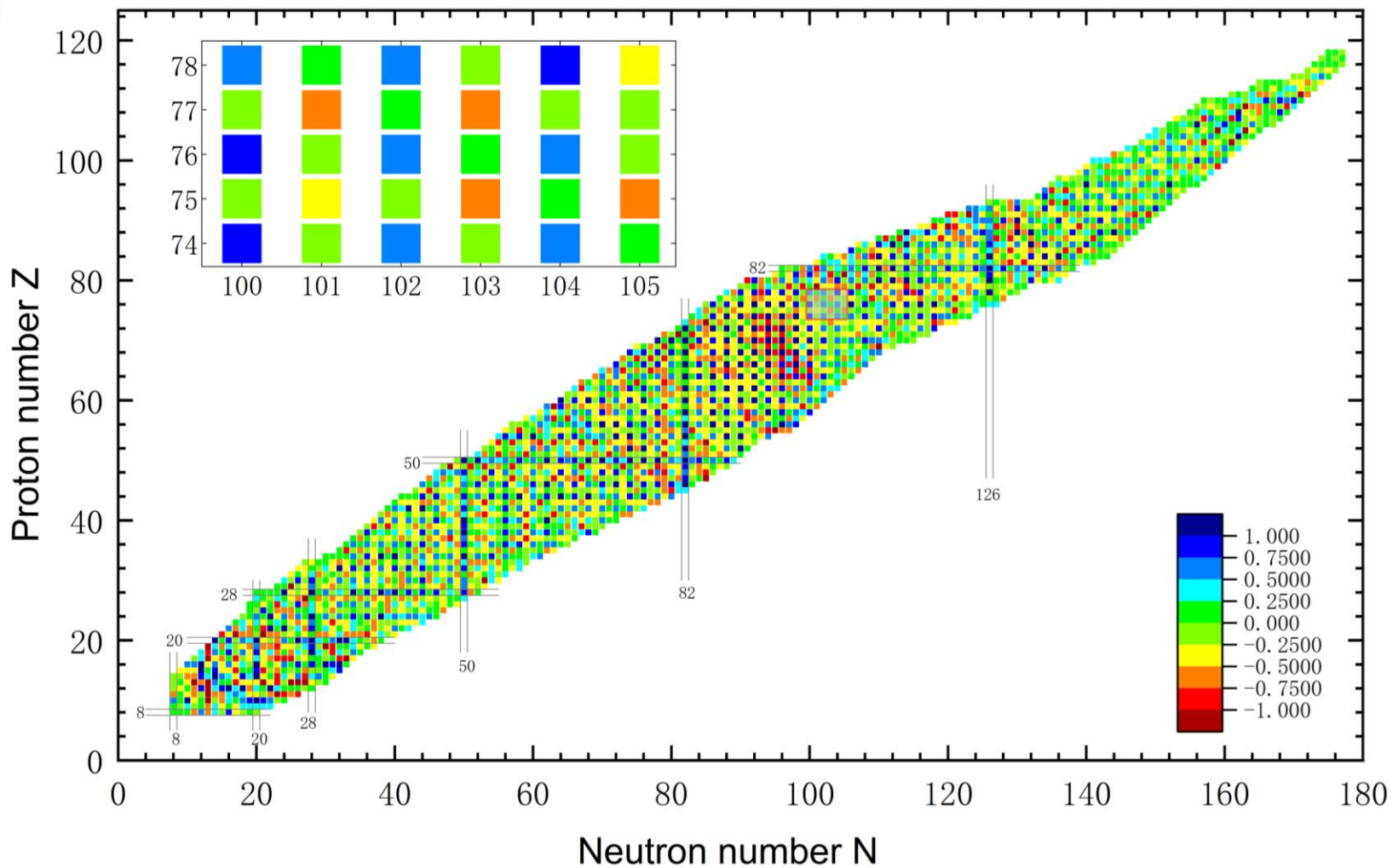
$$\text{ReLU}(x) = \begin{cases} x & x \geq 0 \\ 0 & x < 0 \end{cases} = \max(0, x)$$

$$\Delta M = M_{exp.} - M_{th.}$$





Directly learning mass **CNN-I3**: Z、N、 neighbor mass

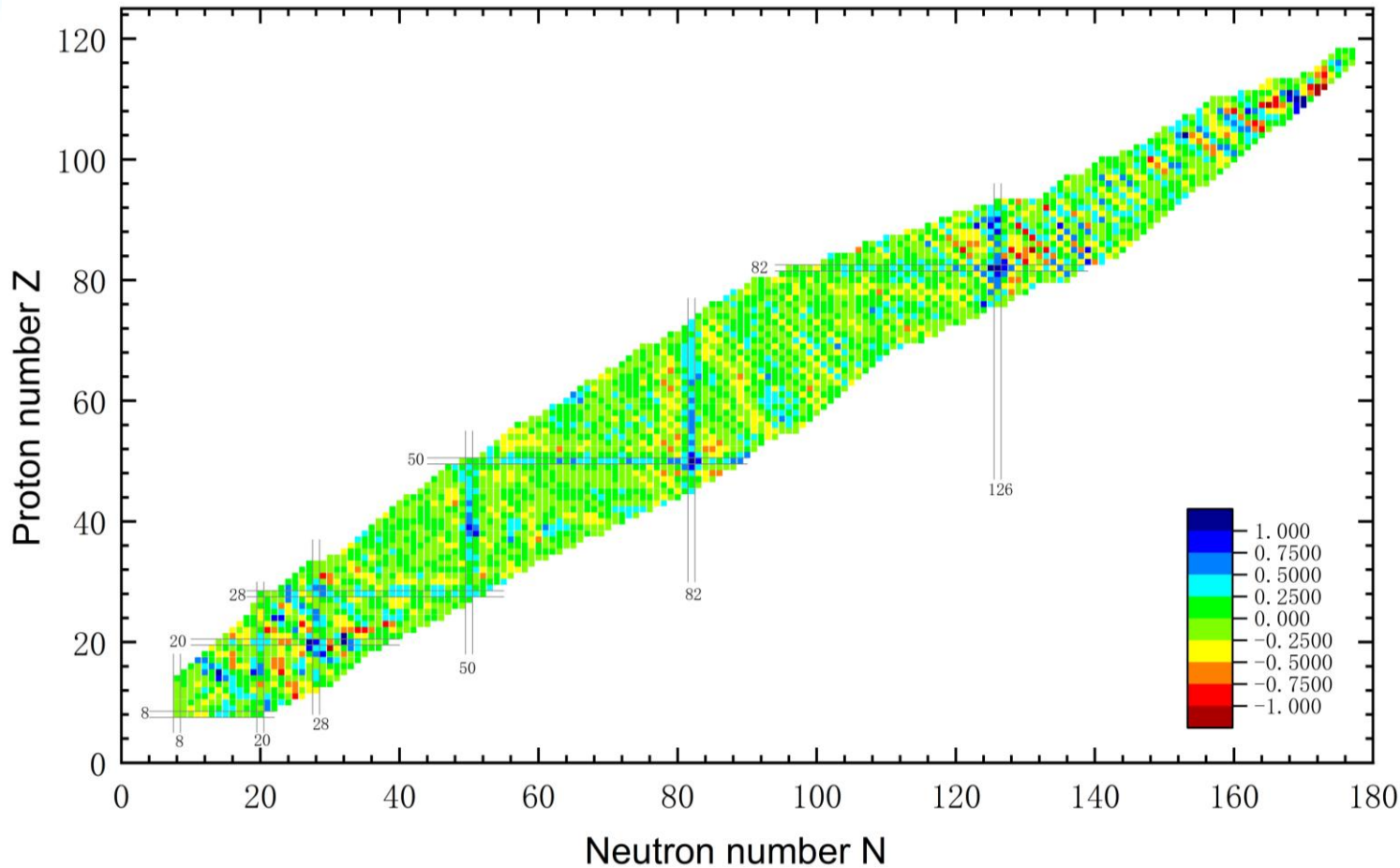


- ✓ Difference between experimental mass (AME2016) and CNN-I3 model prediction, overall RMSE: 0.535 MeV;
- ✓ The results demonstrate a distinct **odd-even staggering**.



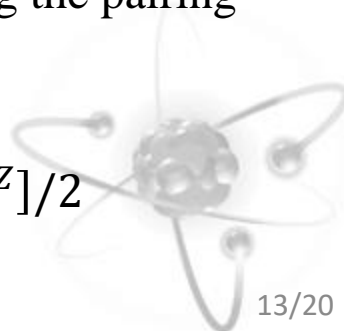


Directly learning mass **CNN-I4**: Z, N, neighbor mass, pairing



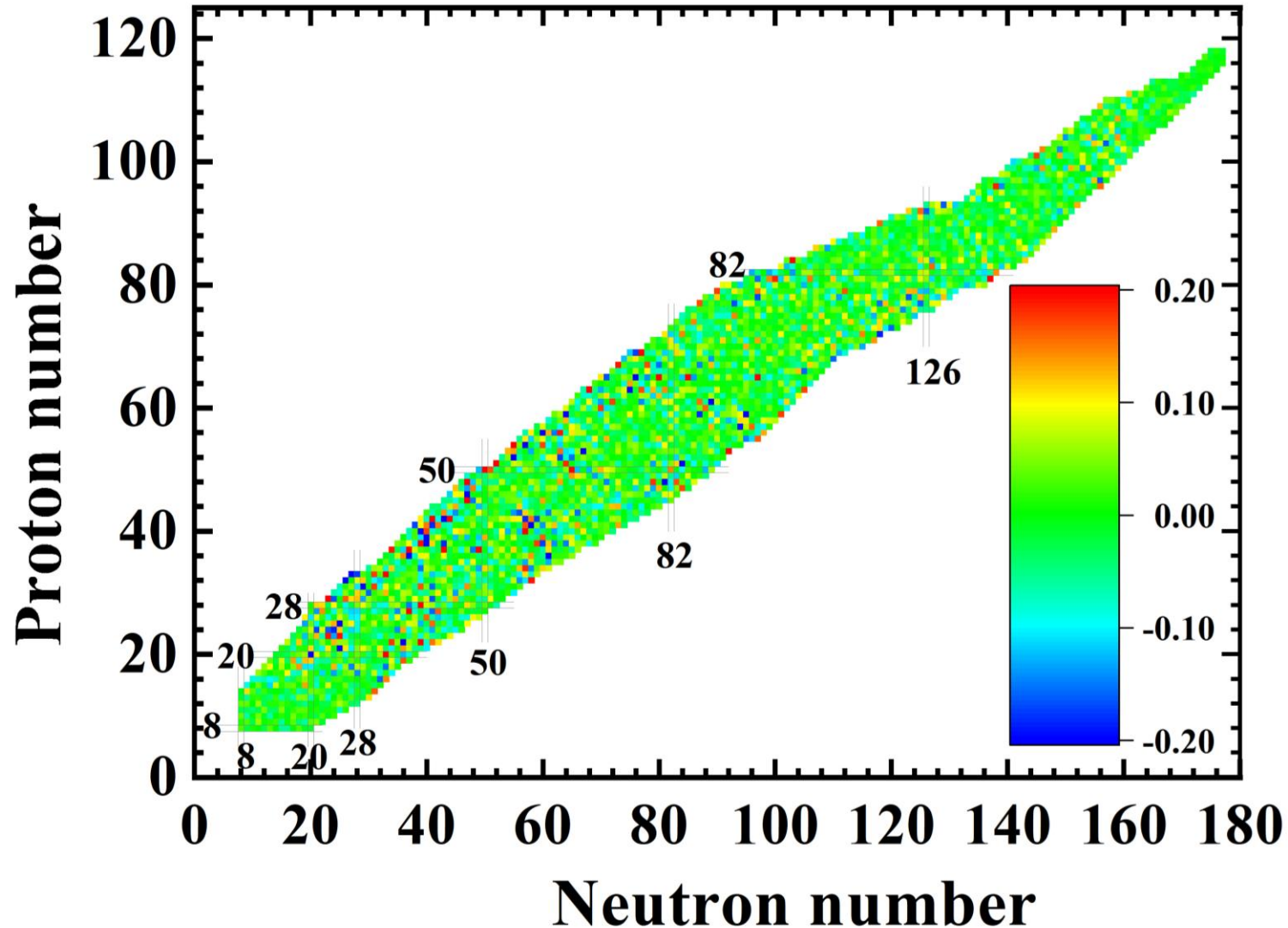
- ✓ Difference between experimental mass (AME2016) and CNN-I4 predictions, overall RMS: 0.291MeV
- ✓ The overall learning effect has been significantly improved and prominent odd-even staggering observed in the results of the CNN-I3 model almost disappears, after considering the pairing effect in the input

$$\delta = [(-1)^N + (-1)^Z]/2$$





The mass prediction for **CNN-WS4**: Z、 N、 neighbor mass、 paring

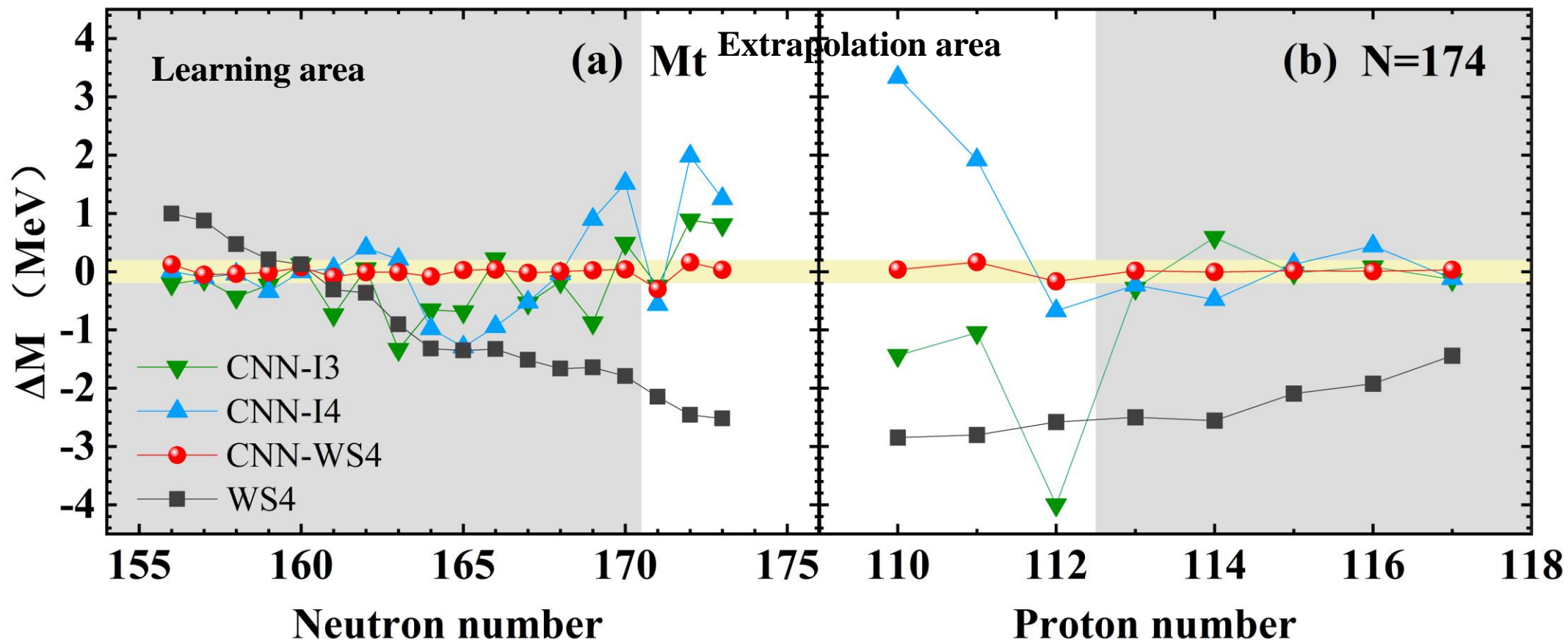


- ✓ The WS4 nuclear mass model is incorporated into the convolutional neural network, resulting in a significant improvement in overall predicting ability.
- ✓ The RMSE within the known experimental data range decreased to 0.070 MeV: very high accuracy achieved so far in theoretical models for predicting nuclear masses, and proves the validity of the CNN-WS4 approach, which combines the global theoretical model with methods capable of extracting local features to predict nuclear mass.





Z=109 and N=174 chain: learning and extrapolation performance

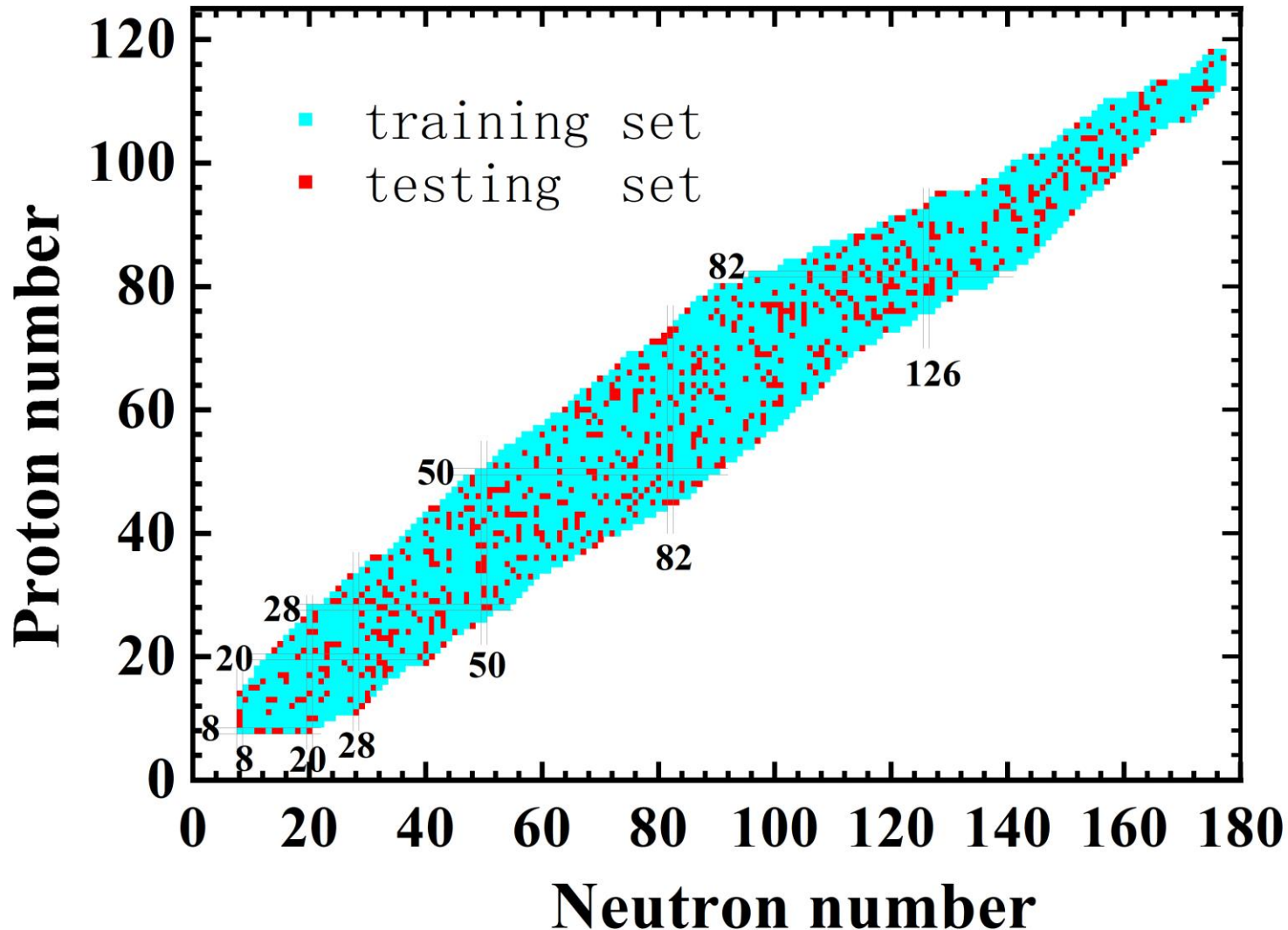


- ✓ Extrapolation: overall RMSE is 0.211MeV (newly emerged nuclei from AME2020).
- ✓ Z=109: 0.994 MeV to -2.519 MeV; N=174: systematic deviation \Rightarrow Considering more physical factors, especially considering physical models, both extrapolation and learning have achieved good results.





AME2020: the training and test sets by 8:2



- ✓ The 3456 nuclei in AME2020 are divided according to the ratio of training set and testing set 8:2. The RMSE for the training set is 0.095 MeV and the RMSE for the test set is 0.171 MeV.
- ✓ This result further demonstrates the robustness of the CNN-WS4 model.



» Summary and prospect

Summary:

- A machine learning method based on **convolutional neural network** is used to learn the nuclear mass for the first time.
- Considering the **local relation**, the features of the surrounding nuclei are extracted more carefully, and the accuracy reaches **0.07 MeV**.
- Gradually introducing **more physical factors enhances the interpretability** of the neural network. The more physical factors are considered, the higher the accuracy can be achieved.

prospect:

- Network input level: Consider shell effect
- Network output level: do not only rely on the WS4 mass model, but also introduce more physical models





Thanks!

