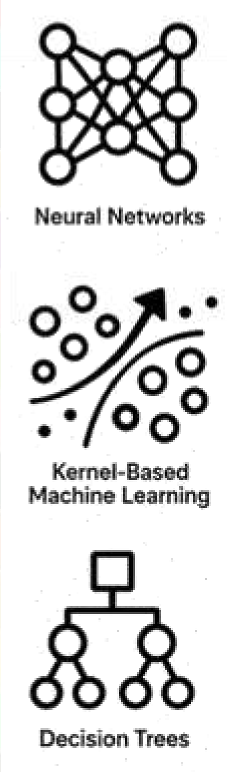
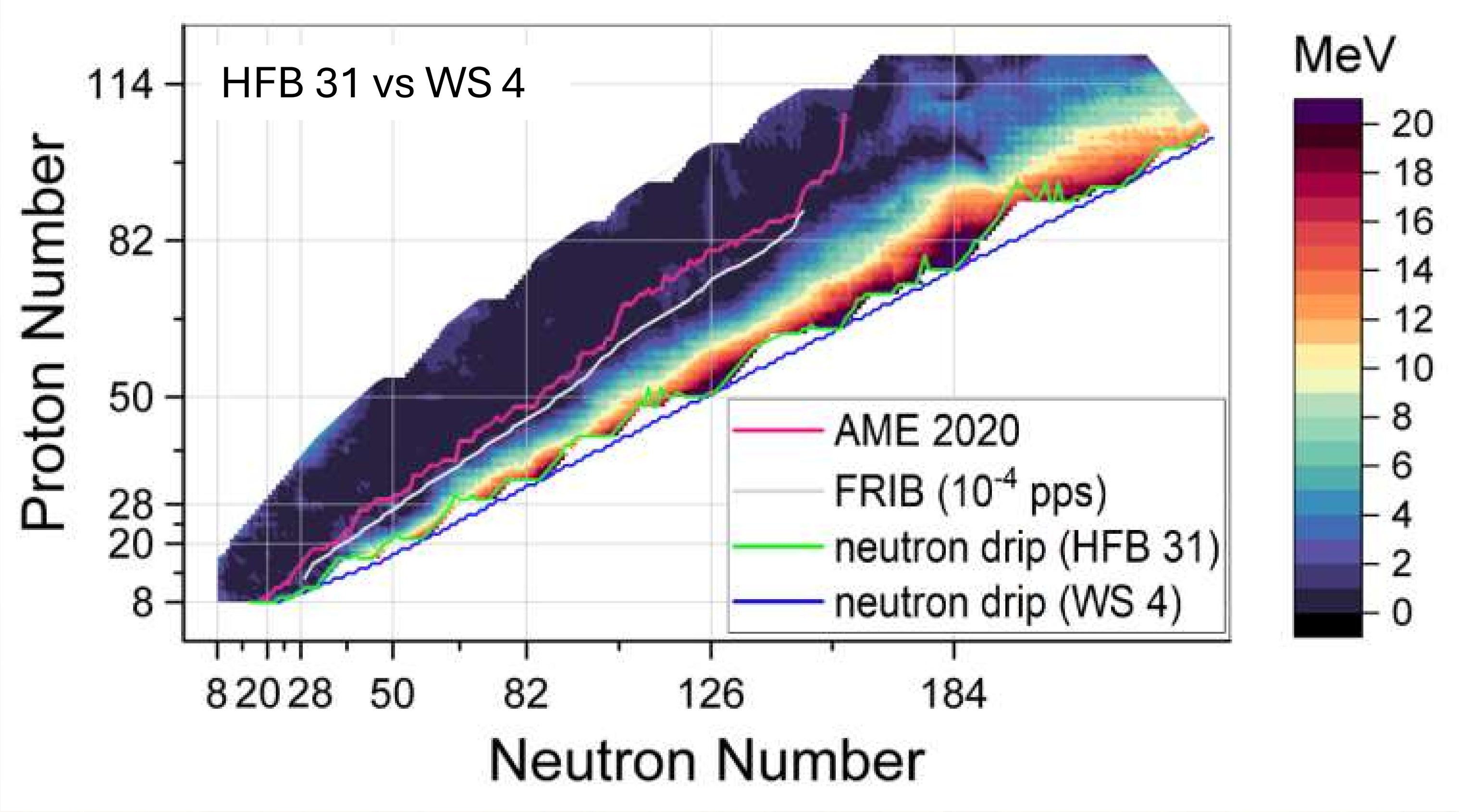


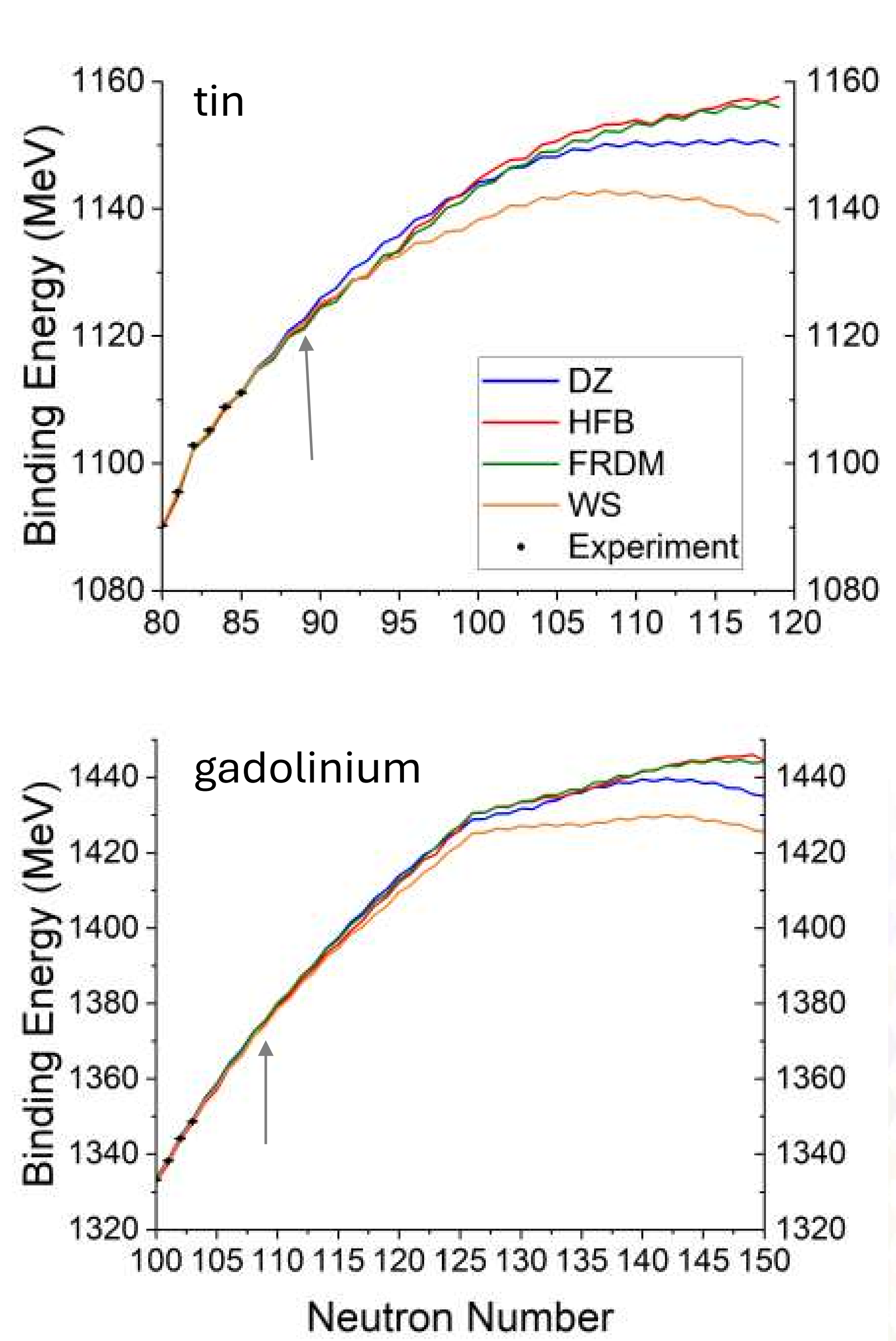
Machine Learning Based Determinations of Binding Energies

Ian Bentley

Nuclear Masses in Astrophysics for the Next 25 Years Workshop

Problem statement: the best models differ





Machine learning approaches

Neural Networks

- Fully Connected Neural Networks (FCNN)
- Convolutional Neural Networks
- Recurrent Neural Networks
- Trained Models (e.g., TabNet)

Phys. Rev. C **97**, 014306 (2018) by R. Utama et al.
Phys. Rev. C **106**, 014305 (2022) by A. E. Lovell et al.
Phys. Rev. C **109**, 034318 (2024) by Lin-Xing Zeng et al.
Phys. Rev. C **111**, 014325 (2025) by Yanhua Lu et al.

Kernel Based Approaches

- Gaussian Process Regression (GPR)
- Support Vector Machines (SVM)

Phys. Rev. C **109**, 064322 (2024) by Esra Yüksel et al.

Tree Based Approaches

- Decision Trees
- Boosted Trees

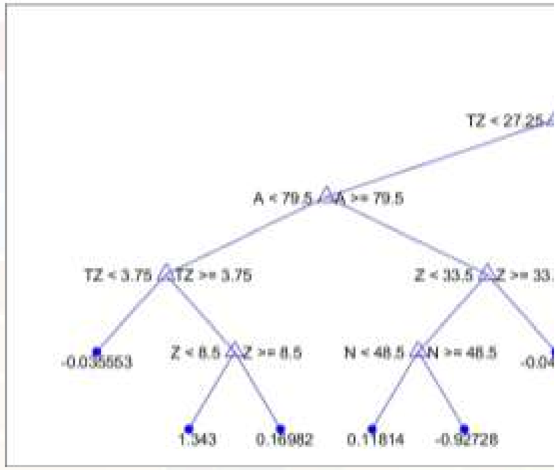
Phys. Rev. C **111**, 034305 (2025) by I. Bentley et al.
Phys. Rev. C **112**, 014324 (2025) by I. Bentley et al.

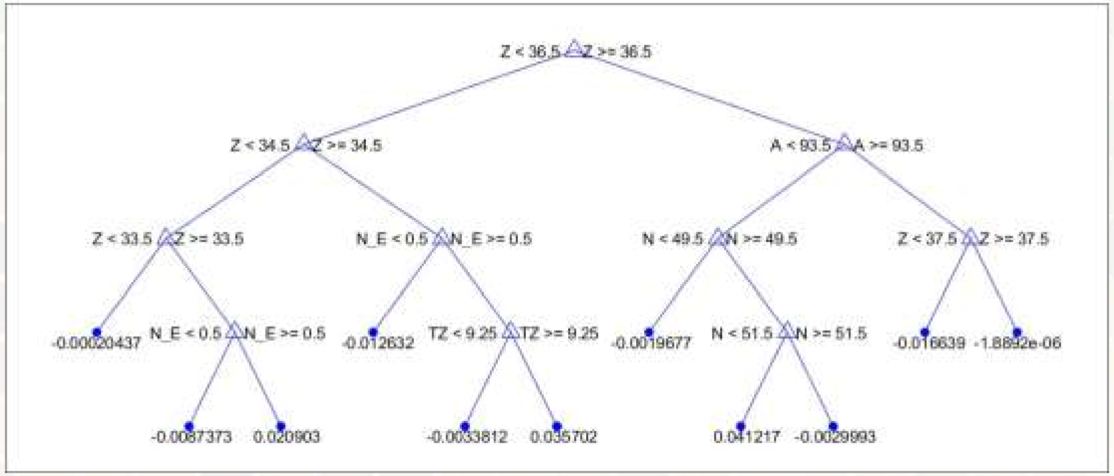
Polynomial or Piecewise Regression

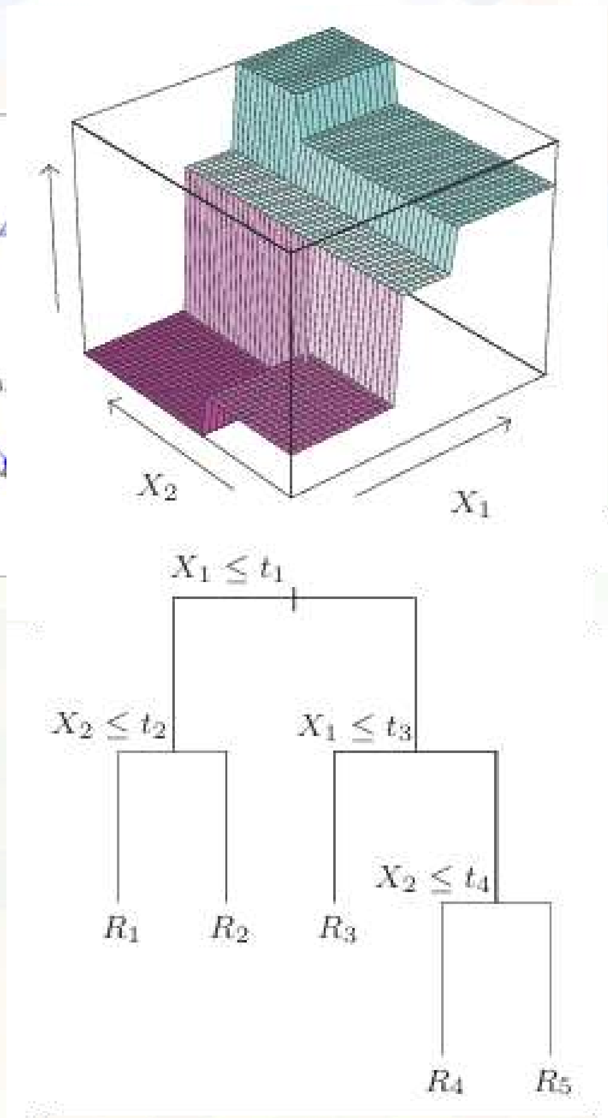
Least Squares Boosted Ensemble of Trees (LSBET)

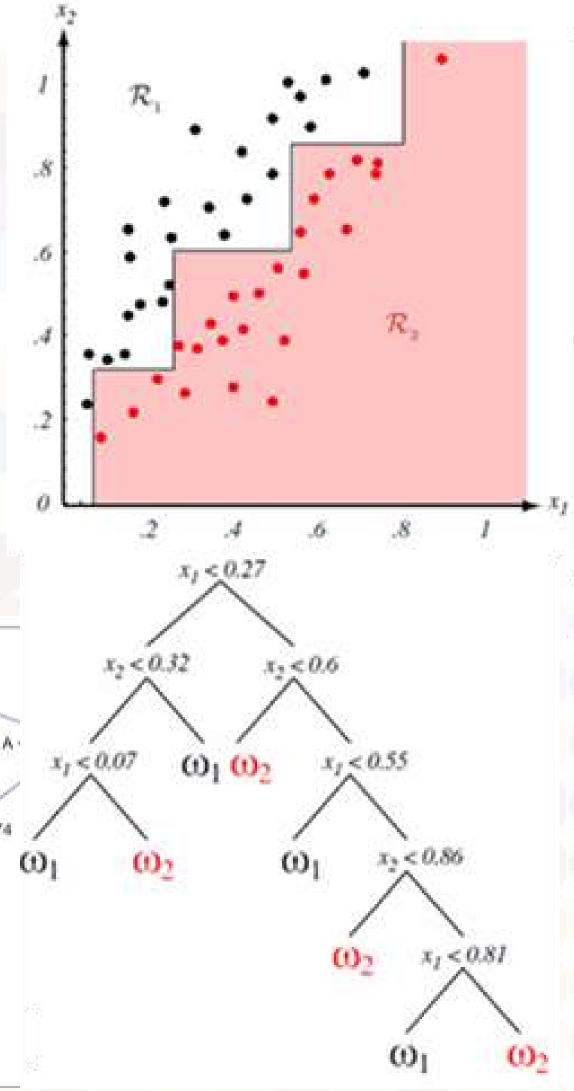
[The Elements of Statistical Learning](#) (2nd Ed.) Hastie, et al.

https://people.eecs.berkeley.edu/~jrs/189s19/lec/16.pdf









Parameters used in Phys. Rev. C **106**, 014305 (2022) and Phys. Rev. C **109**, 064322 (2024)

- Many of the models use physical features which can be as simple as:
  - N,
  - Z, and
  - A.
- Or features motivate by semi empirical arguments:
  - $A^{2/3}$,
  - $(N-Z)/A$,
  - $(N-Z)^2/A$, and
  - $Z(Z-1)/A^{1/3}$.
- Valence particle parameters:
  - $v_N = N - N_{min}$,
  - $v_Z = Z - Z_{min}$, and
  - $P = v_N v_Z/(v_N + v_Z)$.
- Other shell considerations
  - N_{shell}, and
  - Z_{shell}.
- And even-odd staggering
  - $N_E = 1$ if N is even, 0 if N is odd, and
  - $Z_E = 1$ if Z is even, 0 if Z is odd.

Insights from varying dropout in ML training

Setting up the dropout seed tests

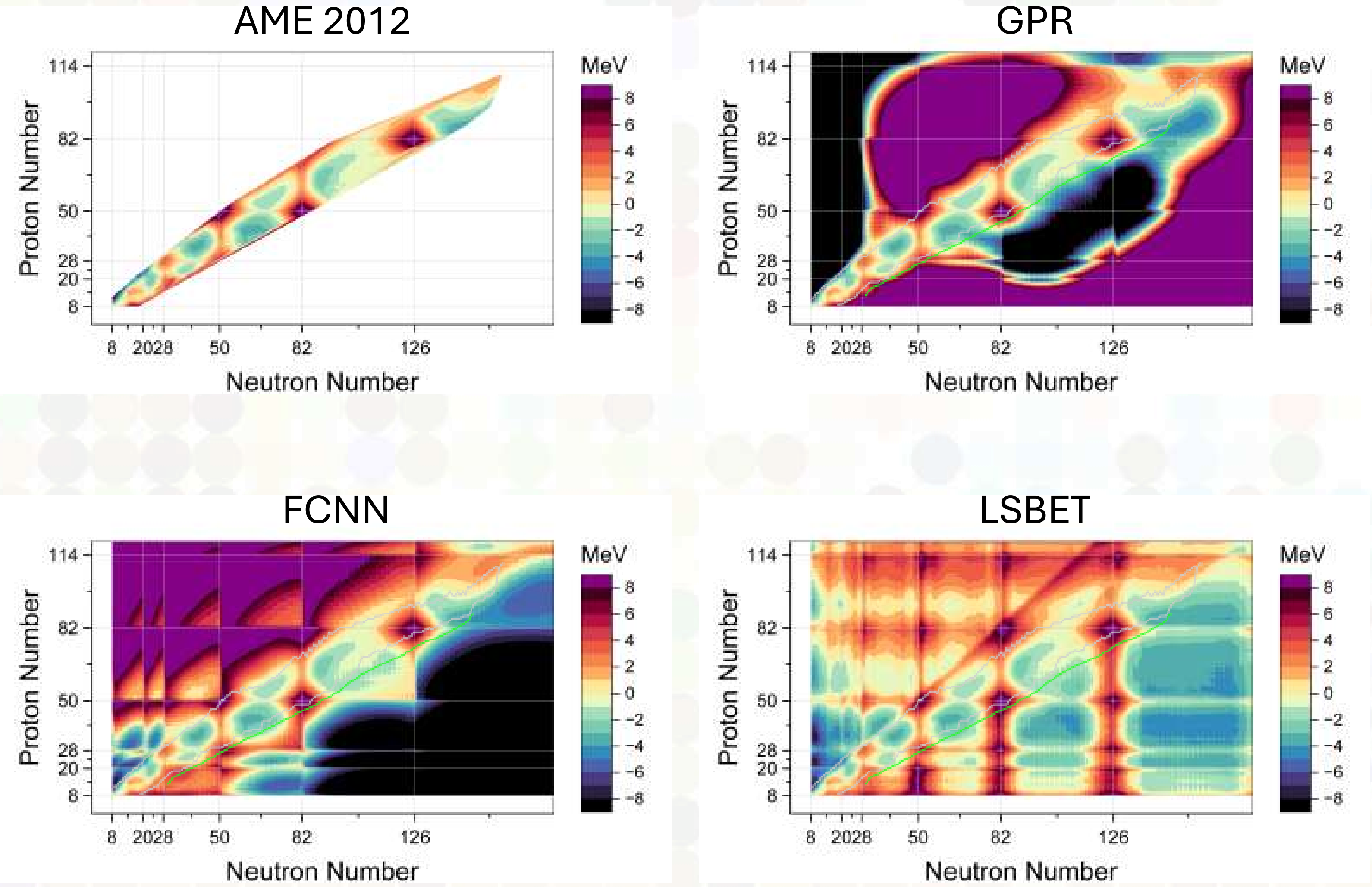
$$\nu = \frac{2N - N_{max} - N_{min}}{N_{max} - N_{min}} \qquad \zeta = \frac{2Z - Z_{max} - Z_{min}}{Z_{max} - Z_{min}}$$

- We will model binding energies three ways: using a simple liquid drop, using a successful historic model, using a successful contemporary model.
- This test will use the 10 physical features (N, Z, A, T_Z, ν, ζ, N_{sub}, Z_{sub}, N_E, and Z_E) for all models.
- These variables are all defined by the number of neutrons and protons.
- A five-fold cross validation will be used and approximately 20% of the data is reserved for the test set.
- We have run 50 different seeds with about 1/7 dropout for three machine learning approaches:
    - GPR with an Isotropic Matern 5/2 function and a linear basis function.
    - FCNN two hidden layers with 200 nodes each and Tanh as the activation function.
    - LSBET with LSBoost as the Ensemble method and 3000 learners.
- The results for the top half (best 25) of these models based on performance compared to AME 2012 will be discussed.

$$\Delta B_{model}(N,Z) = B_{expt.}(N,Z) - B_{model}(N,Z)$$

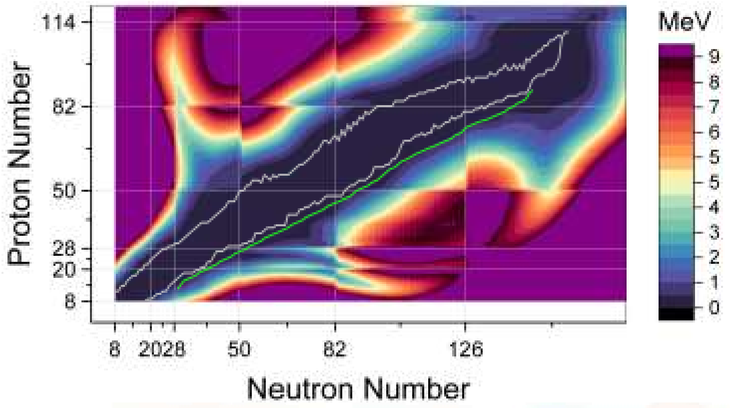
$$B_{LD5} = (a_v A + a_s A^{2/3})(1 + \kappa T_Z(T_Z+1)A^{-2}) + (a_c Z(Z-1) + \Delta)A^{-1/3})$$

ML Model Mean Values: ΔB_{LD5}

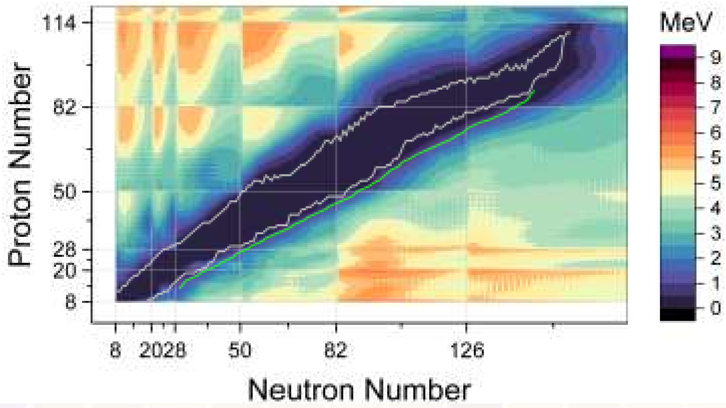


ML Model Standard Deviation Values: ΔB_{LD5}

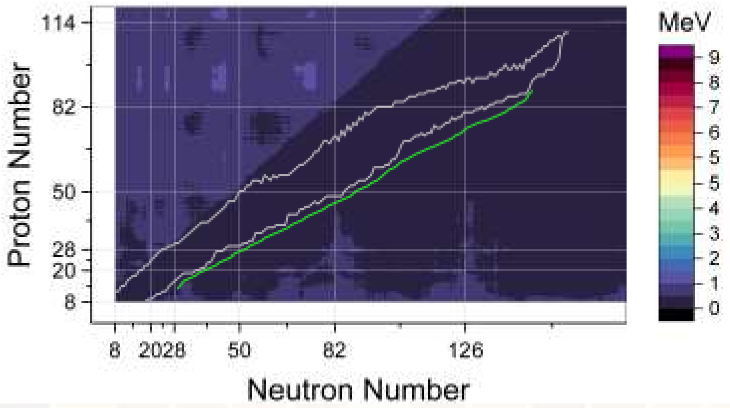
GPR



FCNN



LSBET



Garvey Kelson relations

$$\begin{aligned} &M(N+2, Z-2) - M(N,Z) \\ &+M(N, Z-1) - M(N+1, Z-2) \\ &+M(N+1, Z) - M(N+2, Z-1) \approx 0, \end{aligned}$$

for $N \geq Z$, and

$$\begin{aligned} &M(N-2, Z+2) - M(N,Z) \\ &+M(N-1, Z) - M(N-2, Z+1) \\ &+M(N, Z+1) - M(N-1, Z+2) \approx 0, \end{aligned}$$

for $N < Z$.

Please note that Garvey Kelson relations aren't always zero.

Near $N = Z$ they are sensitive to the Wigner cusp.

REVIEWS OF

MODERN PHYSICS

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Set of Nuclear-Mass Relations and a Resultant Mass Table*

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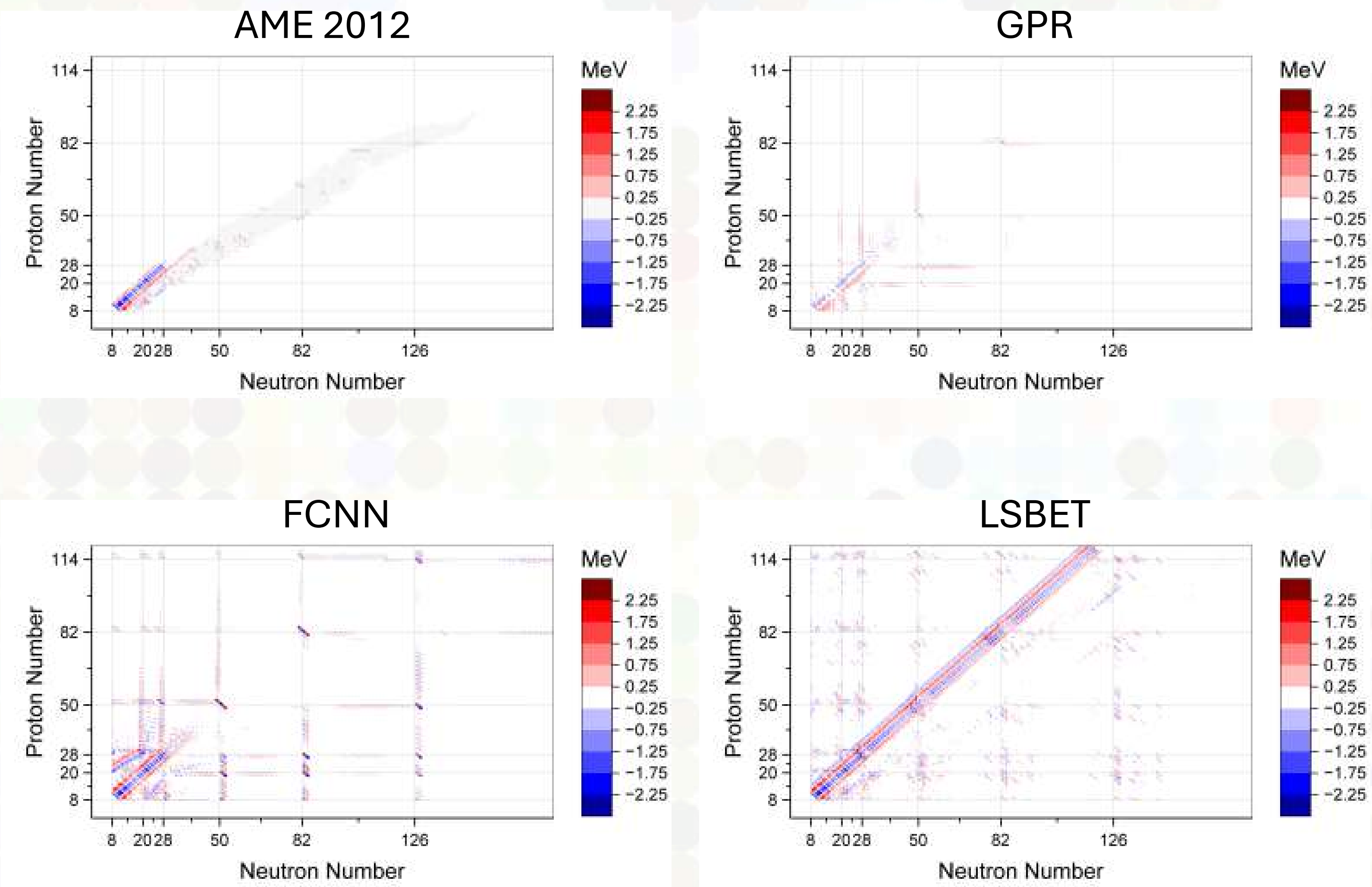
Two new independent mass relations are derived and are shown to be consistent with several existing nuclear models. The most general functional dependence on proton number, neutron number, and mass number (or isospin value) of masses which satisfy these relations exactly is discussed, and a procedure for determining the values of these functions which give a best least-squares fit to the body of known masses is developed. The functions which give the best over-all fit are listed together with the resulting theoretical mass table which shows the discrepancies to known masses and the theoretical values for proton, neutron, and alpha-particle decay energies.

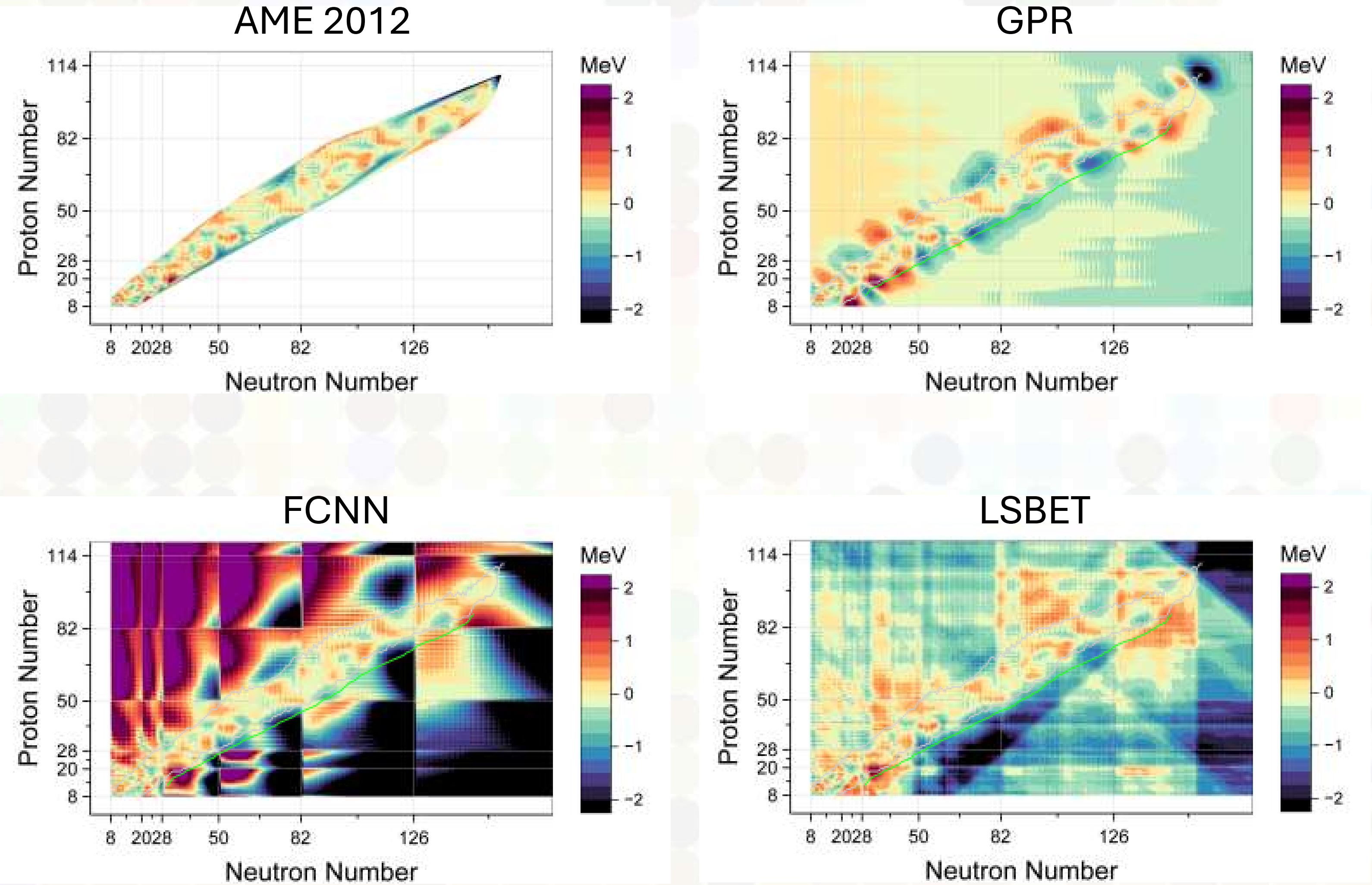
TABLE I. The deviations from zero encountered when Eq. (1) is employed for $N=Z$. When isotopic inversion occurs (lowest $T=0$ level lies above lowest $T=1$ level) in a self-conjugate odd–odd nucleus, the energy of the lowest $T=0$ state is employed rather than the energy of the ground state. Note the systematic deviations from zero encountered when $N=Z$ equals an odd number.

	Deviations (MeV)	
$N+Z$	N even	N odd
16	0.01	
18		−1.9±0.3
20	0.34	
22		−2.05±0.03
24	−0.23	
26		−1.9±0.3
28	0.19	
30		−2.1±0.3
32	0.08	
34		−0.93±0.3
36	0.22	
38		−0.89±0.3
40	0.04	
42		−0.86
44	0.48	
46		−0.53
48	0.07	
50		−1.06
52	0.10	
54		−0.49
56	0.00	

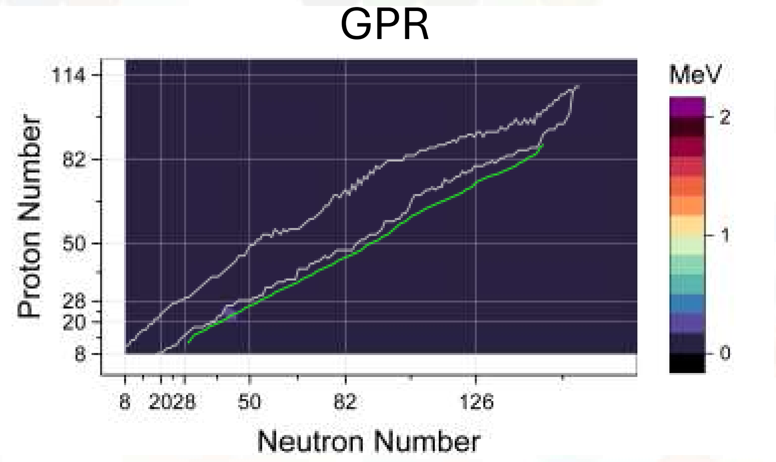
Garvey Kelson Relations: $B_{LD5} + \Delta B_{LD5}$

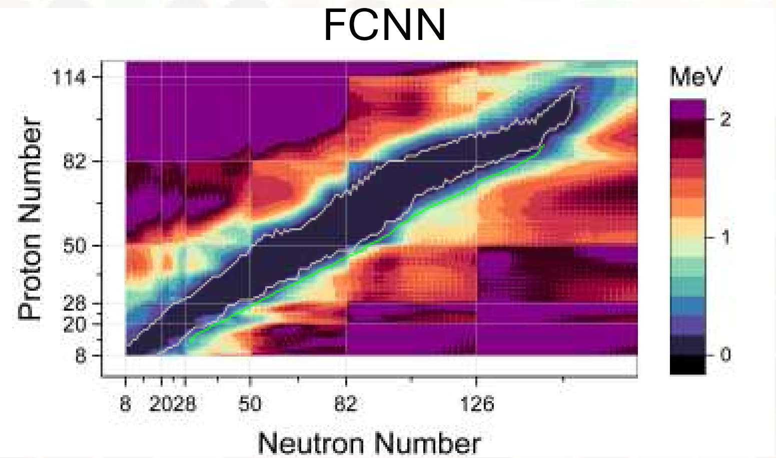


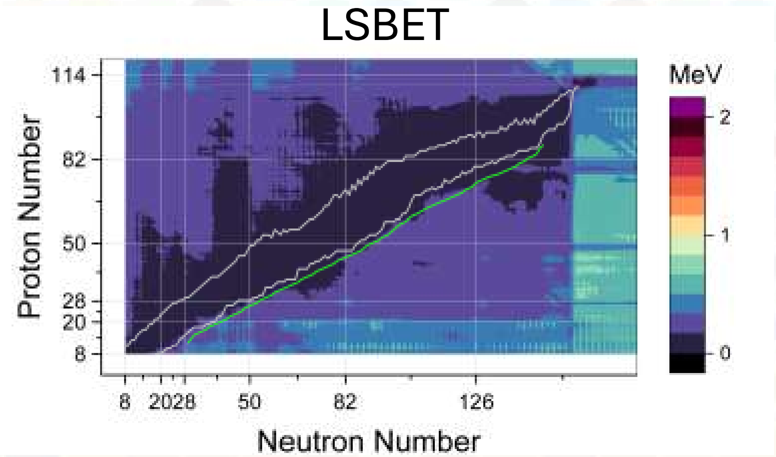
ML Model Mean Values: ΔB_{DZ}



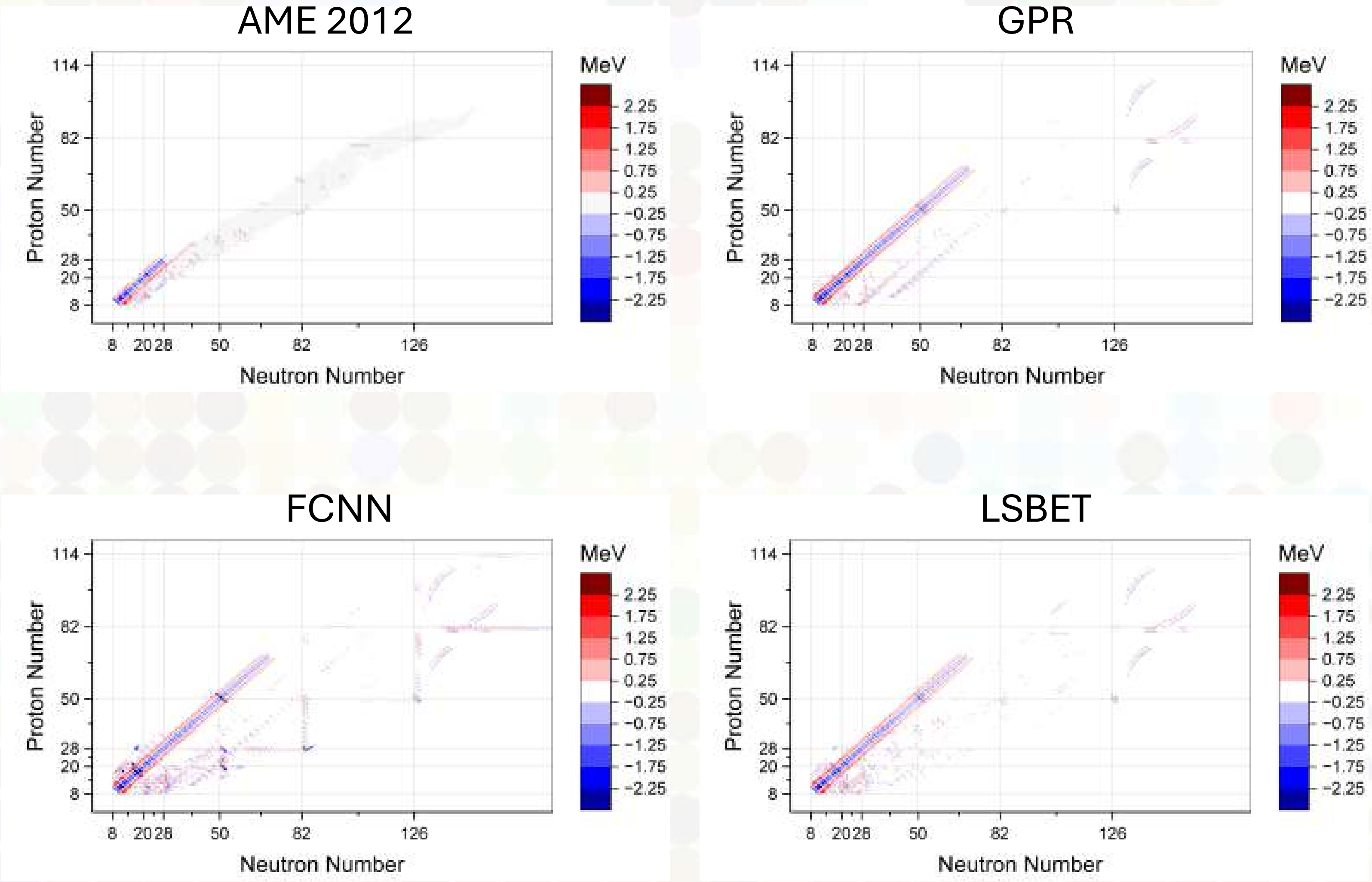
ML Model Standard Deviation Values: ΔB_{DZ}



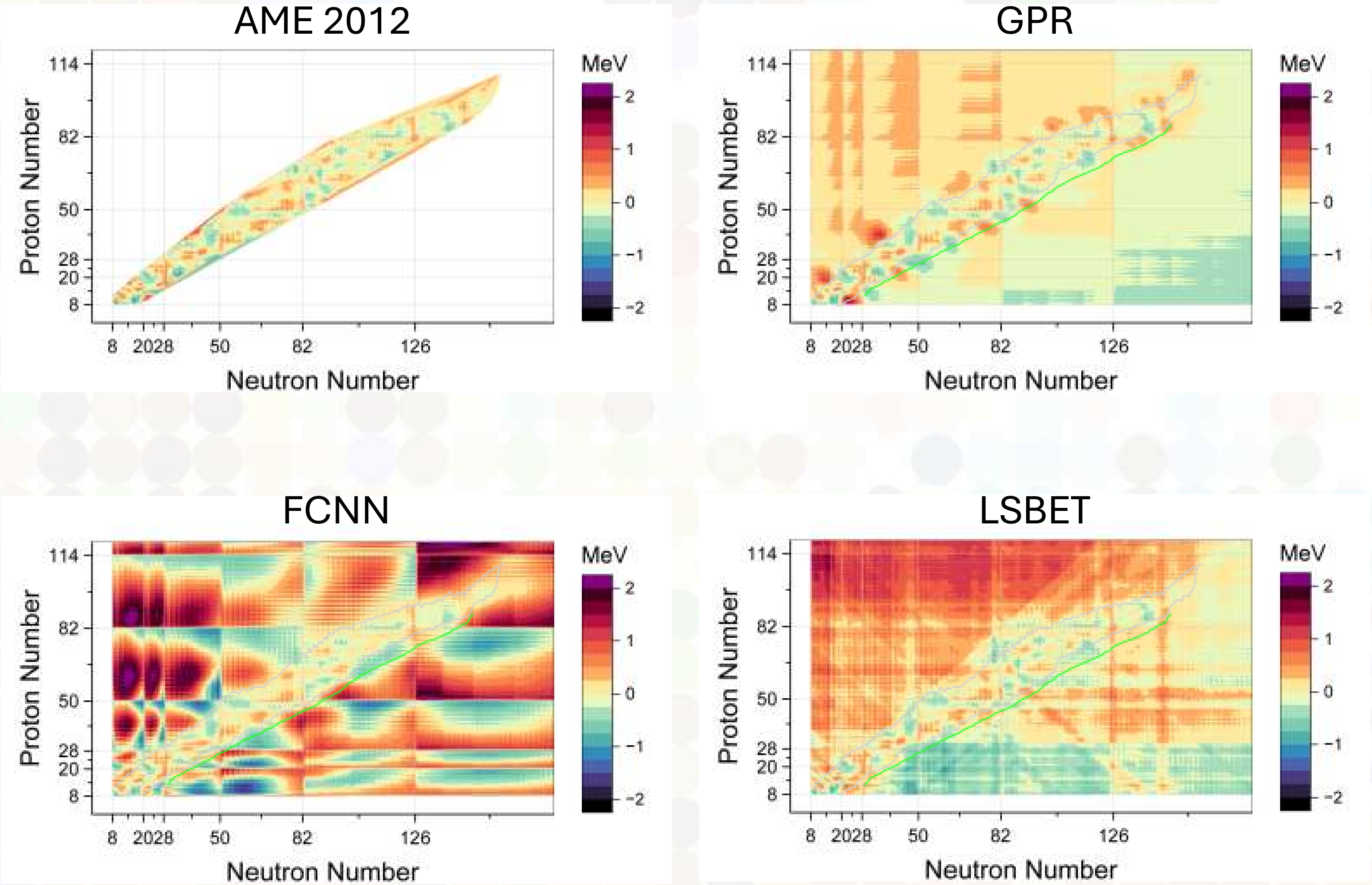




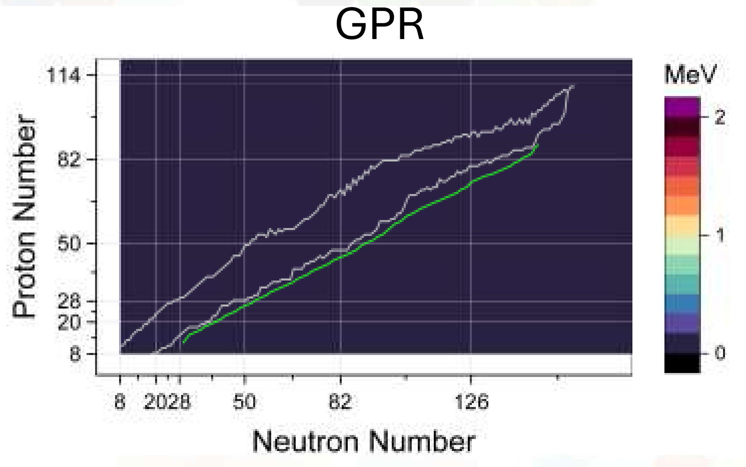
Garvey Kelson Relations: $B_{DZ} + \Delta B_{DZ}$

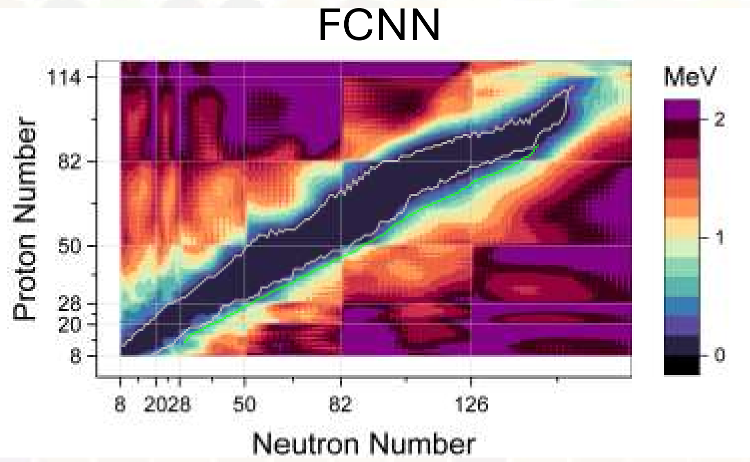


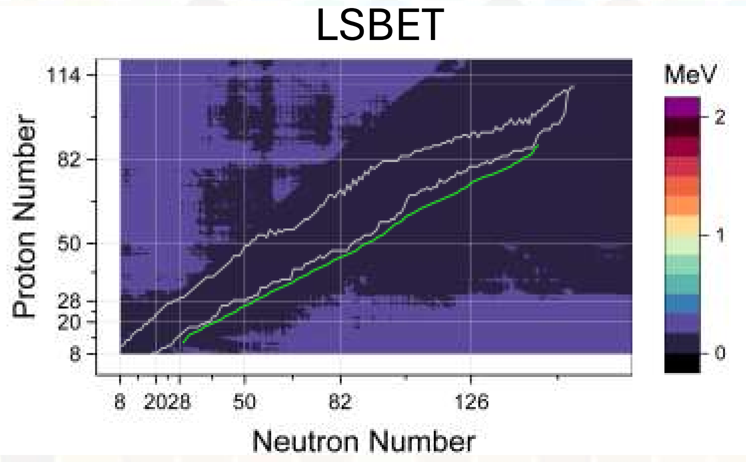
ML Model Mean Values: ΔB_{WS}



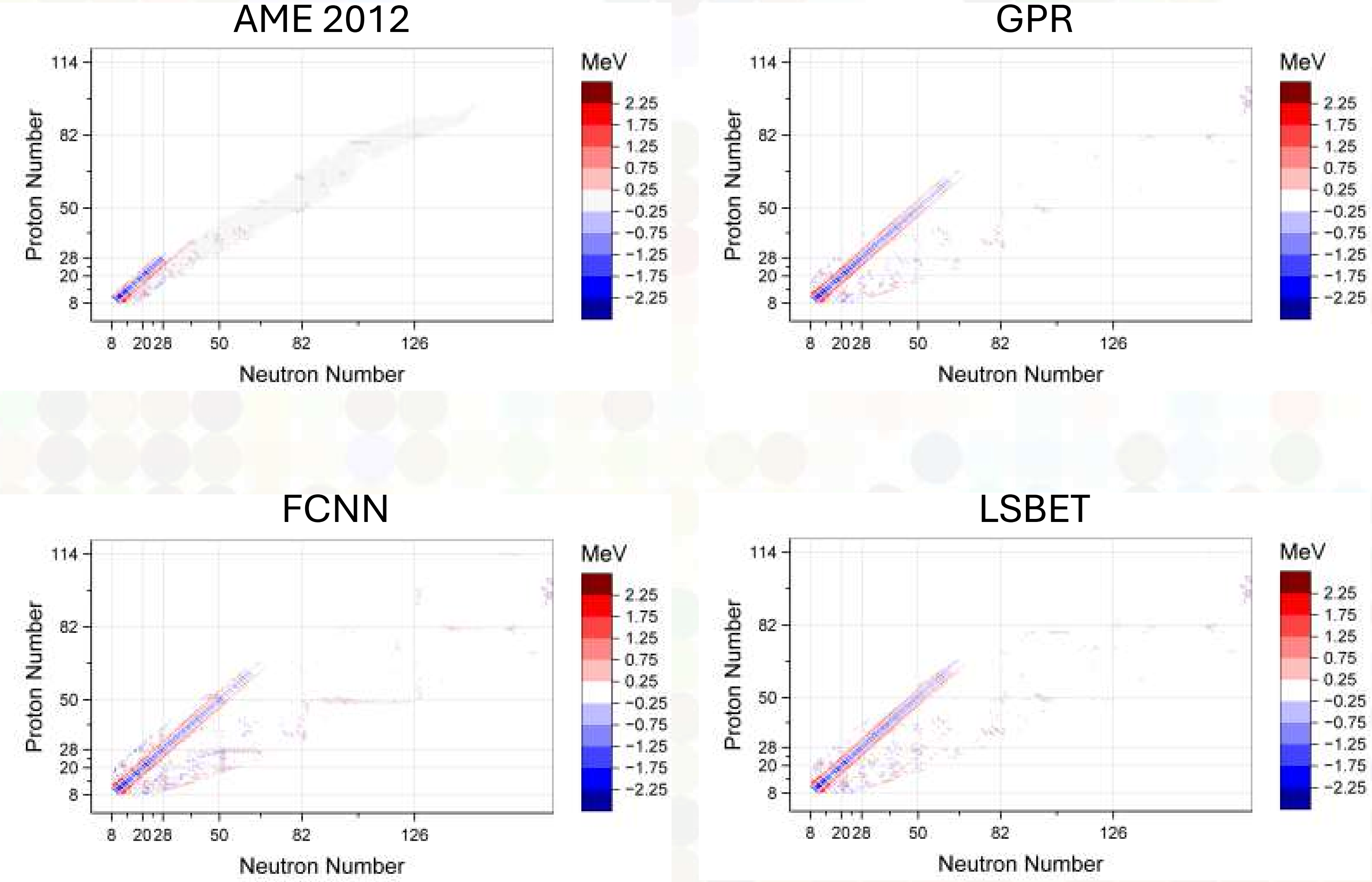
ML Model Standard Deviation Values: ΔB_{WS}





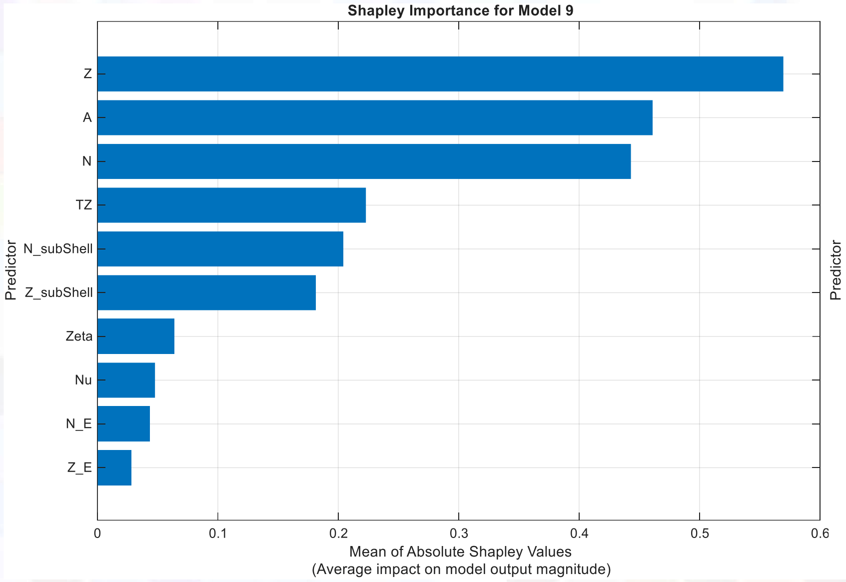


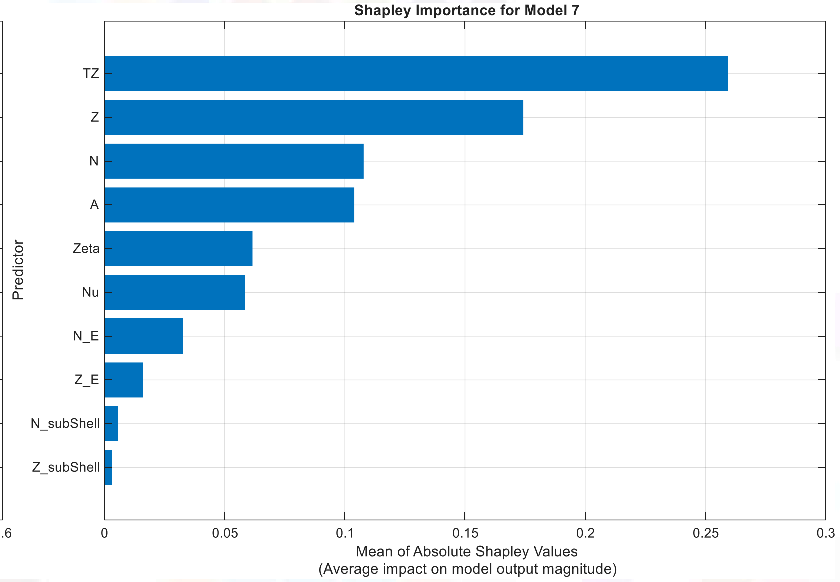
Garvey Kelson Relations: $B_{WS} + \Delta B_{WS}$



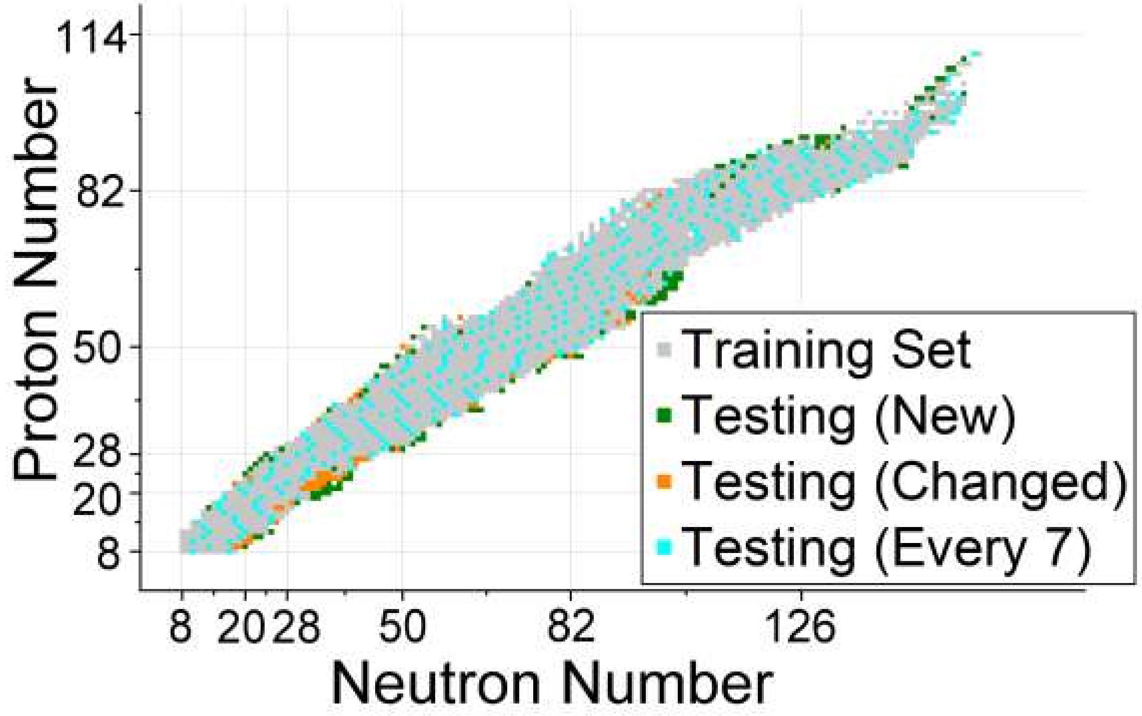
Four Model Tree Ensemble

Model development approach





1. We model binding energy residuals:
$$\Delta B = B_{expt.} - B_{model}.$$
2. We train using about a dozen physical features (including shape parameters from models).
3. We use an initial analysis of Shapley values to test the impact of excluding the less impactful features.
4. We use an independent training set from AME 2012, and test set from AME 2020.
5. We cast a wide net by testing multiple ML approaches.



Physical features used in the best LSBET models

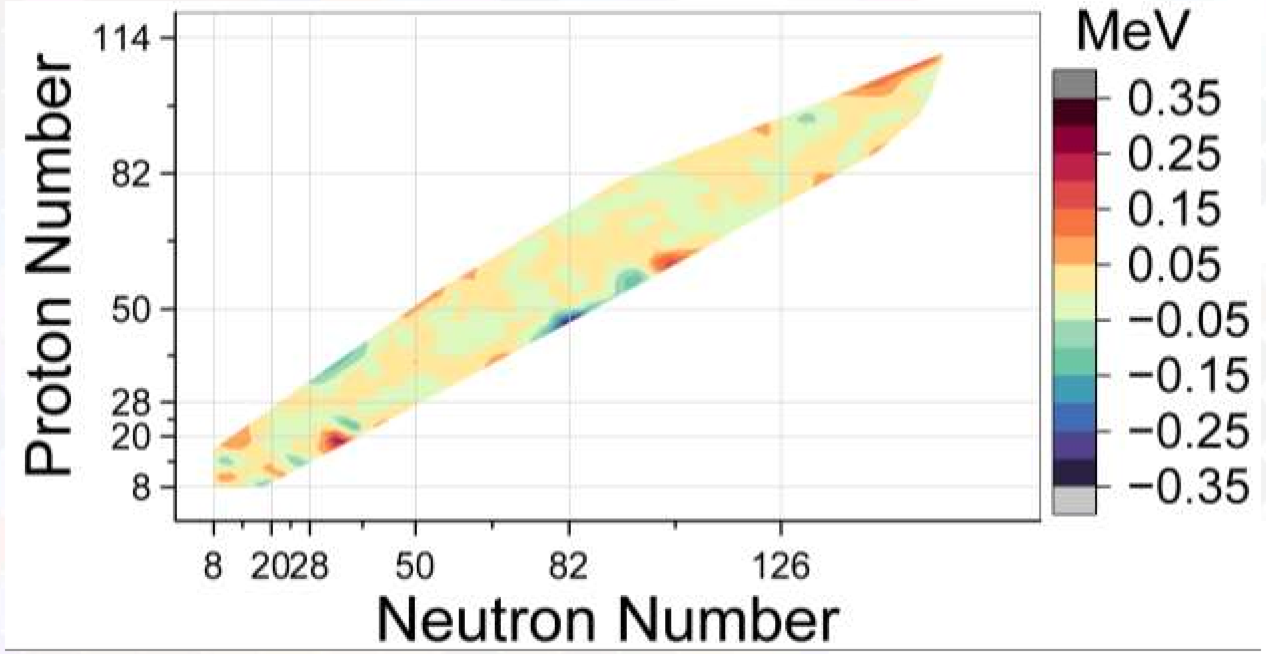
Model	Number of Features	Physical Features
LD5LSBET	8	$N, Z, A, T_Z, N_S, Z_E, N_E, Z_S$
LD6LSBET	6	Z, N, T_Z, A, N_S, Z_S
DZLSBET	8	$T_Z, Z, A, N, N_E, Z_E, Z_S, N_S$
FRDMLSBET	11	$\nu, T_Z, Z, N, A, \beta_2, \zeta, Z_S, N_E, Z_E, N_S$
HFBLSBET	11	$\nu, \zeta, Z, N, \beta_2, T_Z, R_C, A, \beta_4, Z_E, N_E$
WSLSBET	11	$Z, T_Z, N, \beta_2, A, \zeta, \nu, Z_E, N_E, Z_S, N_S$
WSpLSBET	9	$T_Z, N_E, Z_E, \beta_2, \nu, Z, N, A, \zeta$

Features Not Included
-2 (shell)
-4 (shell, eo)
-2 (shell)
-3 (deformation)
-2 (subshell)
-2 (deformation)
-4 (subshell, deformation)

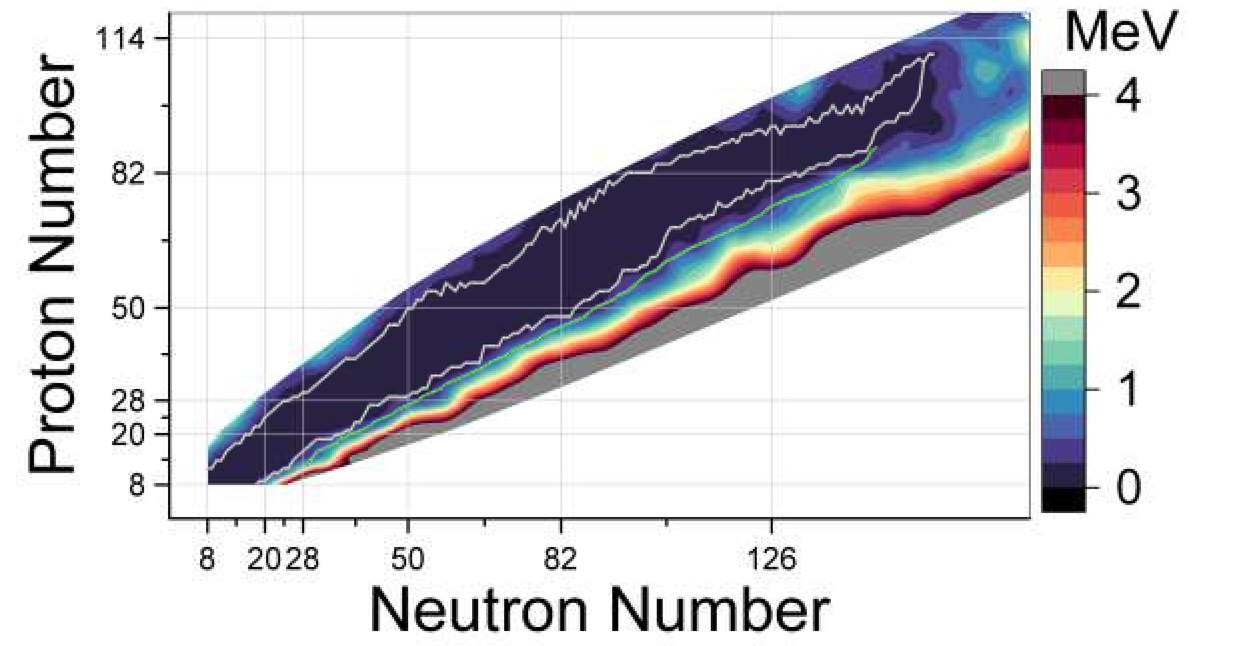
Comparison metrics for the LSBET models and creating the Four Model Tree Ensemble (FMTE)

	Model Name	$\sigma_{12Train}$ (MeV)	$\overline{AE}_{12Train}$ (MeV)	σ_{12} (MeV)	$\overline{AE}_{12}$ (MeV)	σ_{20Test} (MeV)	$\overline{AE}_{20Test}$ (MeV)	σ_{20} (MeV)	$\overline{AE}_{20}$ (MeV)
	WS4+	0.168	0.131	0.170	0.132	0.253	0.178	0.189	0.141
	LD5LSBET	0.018	0.014	0.117	0.043	0.317	0.208	0.145	0.055
	LD6LSBET	0.018	0.013	0.114	0.041	0.328	0.193	0.150	0.051
42.1%	DZLSBET	0.017	0.013	0.084	0.034	0.199	0.130	0.092	0.039
5.8%	FRDMLSBET	0.017	0.013	0.101	0.037	0.266	0.164	0.122	0.046
3.2%	HFBLSBET	0.055	0.042	0.148	0.072	0.378	0.247	0.179	0.085
48.9%	WSLSBET	0.021	0.016	0.094	0.038	0.181	0.128	0.085	0.041
	WSpLSBET	0.023	0.017	0.059	0.031	0.189	0.119	0.088	0.039
	FMTE	0.015	0.012	0.081	0.031	0.164	0.112	0.076	0.034

ΔB FMTE compared to AME 2020



The weighted standard deviation for FMTE

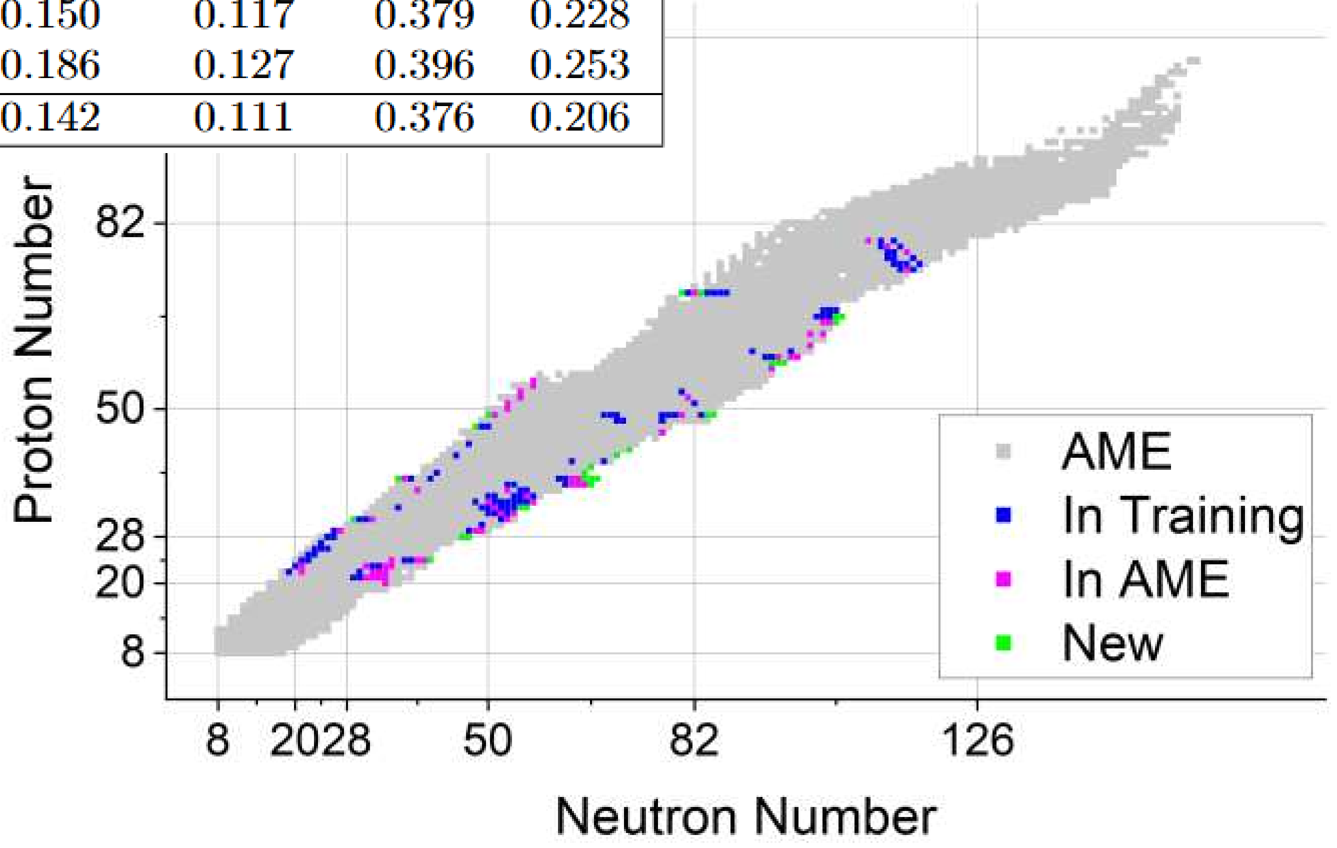


Model Name	σ_{Recent} (MeV)	$\overline{AE}_{Recent}$ (MeV)	$\sigma_{inTrain}$ (MeV)	$\overline{AE}_{inTrain}$ (MeV)	σ_{inAME} (MeV)	$\overline{AE}_{inAME}$ (MeV)	σ_{New} (MeV)	$\overline{AE}_{New}$ (MeV)
DZ28	0.570	0.398	0.411	0.315	0.693	0.486	0.674	0.449
FRDM2012	0.836	0.631	0.724	0.558	0.945	0.701	0.743	0.549
HFB31	0.647	0.484	0.578	0.423	0.668	0.497	0.801	0.614
WS4	0.341	0.267	0.299	0.243	0.318	0.259	0.488	0.360
WS4+	0.267	0.186	0.196	0.156	0.241	0.178	0.445	0.295
DZLSBET	0.207	0.115	0.058	0.038	0.206	0.157	0.417	0.258
FRDMLSBET	0.246	0.133	0.060	0.040	0.300	0.199	0.420	0.261
HFBLSBET	0.371	0.209	0.077	0.057	0.362	0.281	0.761	0.533
WSLSBET	0.180	0.099	0.060	0.041	0.150	0.117	0.379	0.228
WSpLSBET	0.193	0.102	0.060	0.040	0.186	0.127	0.396	0.253
FMTE	0.175	0.090	0.058	0.038	0.142	0.111	0.376	0.206

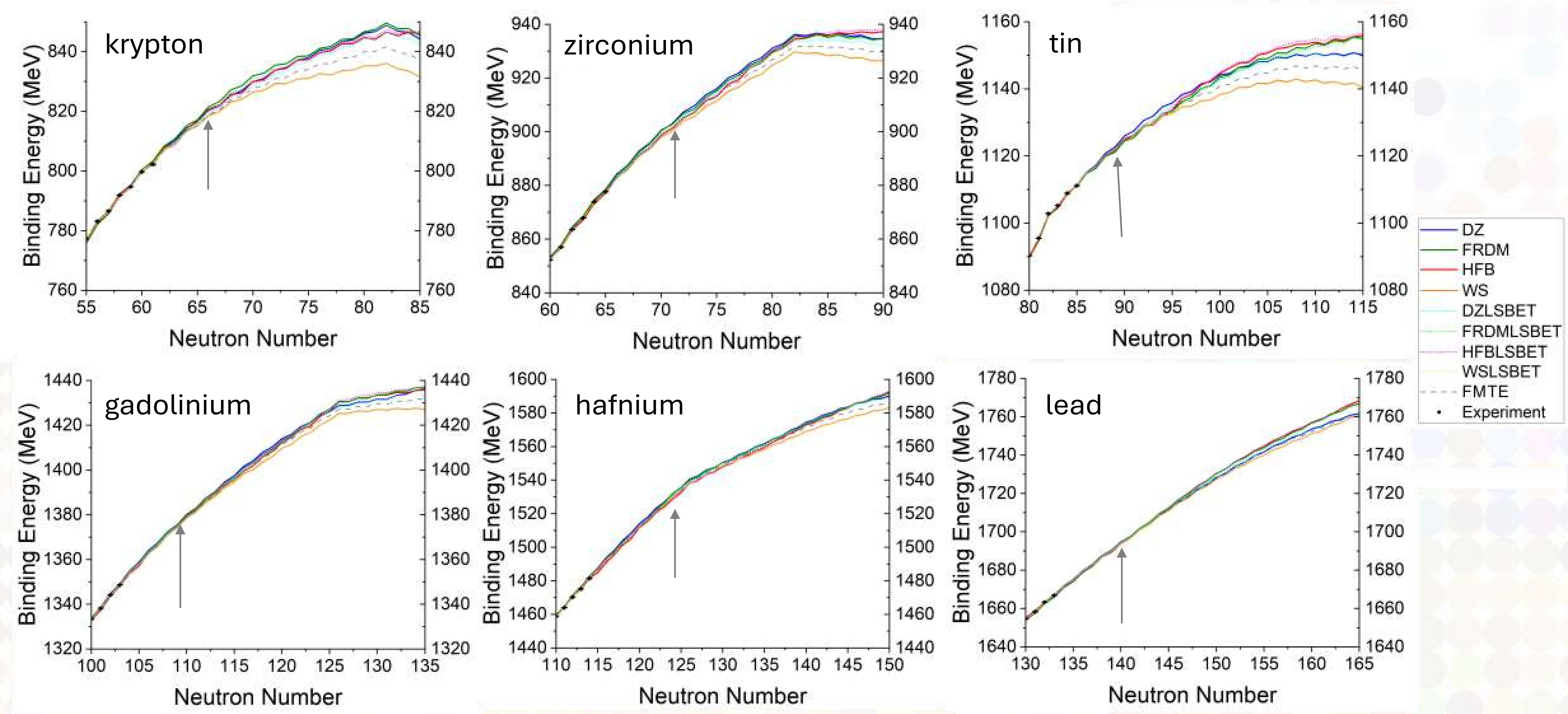
FMTE: new measurements

We have conducted a survey of 25 articles post AME 2020, with 207 new mass measurements to compare with.

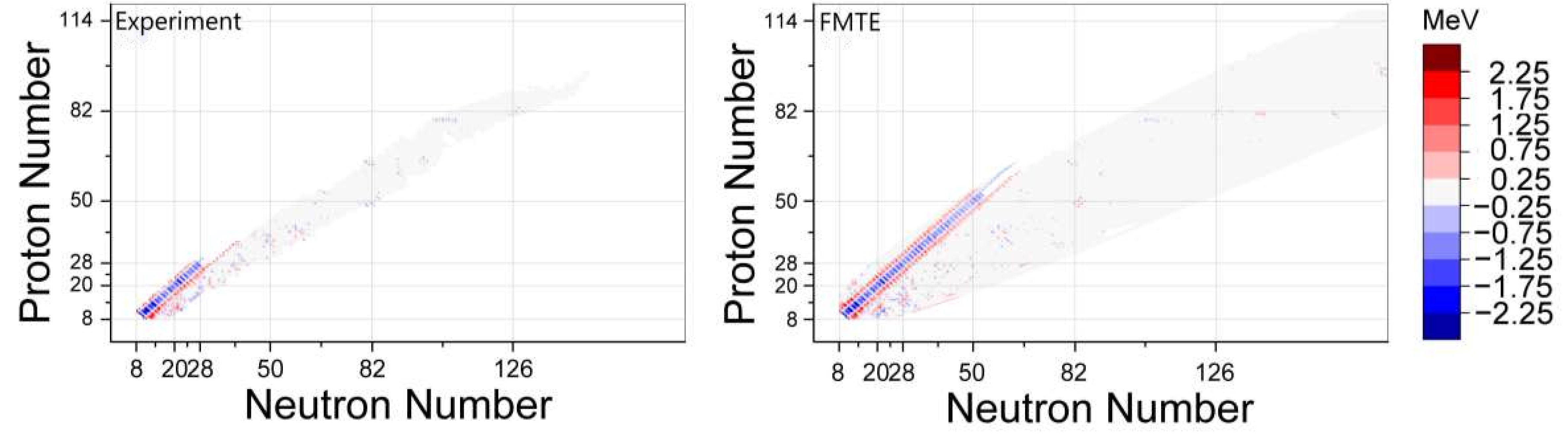
Of the 207, 106 are for isotopes in the training set, 68 for isotopes in either AME 2012 or AME 2020, and 33 for isotopes not previously tabulated.



FMTE: neutron rich extrapolations



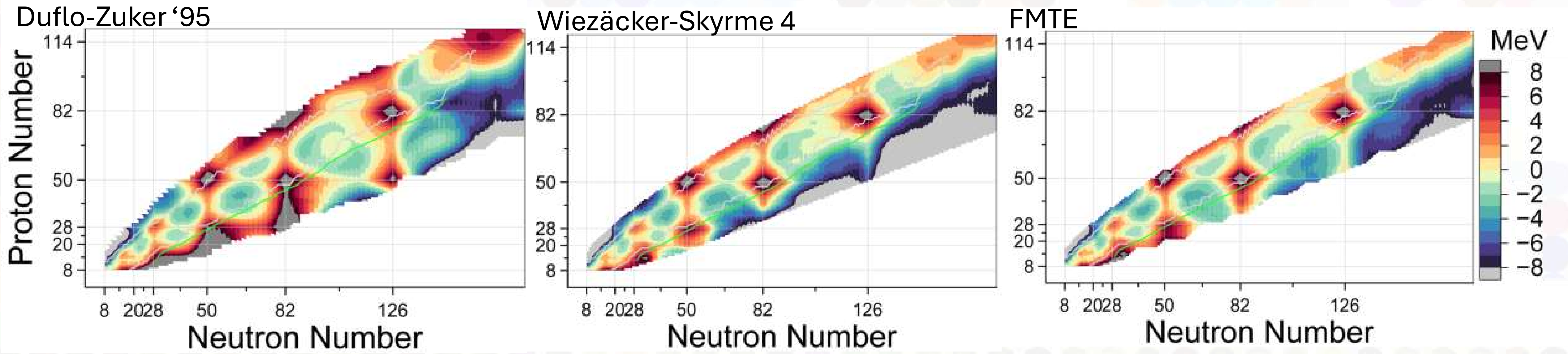
FMTE: Garvey Kelson relations



Liquid drop feasibility check of the FMTE

$$\Delta B_{model}(N,Z) = B_{expt.}(N,Z) - B_{model}(N,Z)$$

$$B_{LD5} = (a_v A + a_s A^{2/3})(1 + \kappa T_Z(T_Z+1)A^{-2}) + (a_c Z(Z-1) + \Delta)A^{-1/3}$$



Summary of FMTE

- For our approach of fitting binding energy residuals, trained on a (partially) random subset of AME 2012, the LSBET approach is superior.
- LSBET is superior because it: performs well regarding the statistical metrics, the extrapolations are on scale, the standard deviations between comparable seeds is small, the GK relations are reasonable, they require fewer physical features, they can be ensembled, and they will not overfit because of too many learners.
- The four best of these approaches were combined to make the Four Model Tree Ensemble (FMTE).
- For Experimentalists, the FMTE model reproduces the AME 2020, better than the other models compared (σ =76 keV, vs σ = 189-606 keV) and is the best on completely new masses (σ =376 keV, vs σ = 445-801 keV).
- For Astrophysics, the FMTE serves as an informed weighted average of four of the best mass models which are frequently used.

Conclusion the future of ML and mass models

- All of those who make models need to continue to
  - check for statistical reliability (to determine where the how far the model extrapolations are statistically valid),
  - use for GK relations or something comparable,
  - compare with new mass measurements, and
  - make the results from the table available (www.researchgate.net Search: FMTE search type=dataset).
- Tree based models might be the worst possible chose.
- Ensembled tree based models might be the best.
- Incorporating GK relations, a semiempirical checks, and other physics into the loss function.

Thank you!