

HNPS Advances in Nuclear Physics

Vol 15 (2006)

HNPS2006



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doi: [10.12681/hnps.2608](https://doi.org/10.12681/hnps.2608)

To cite this article:

Athanasopoulos, S., Mavrommatis, E., Gernoth, K. A., & Clark, J. W. (2020). Proton drip line evaluation by complementing the Finite Range Droplet Model with neural networks. *HNPS Advances in Nuclear Physics*, 15, 258–261. <https://doi.org/10.12681/hnps.2608>

Proton drip line evaluation by complementing the Finite Range Droplet Model with neural networks

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We evaluate the location of the proton drip line in the regions $31 \leq Z \leq 49$ and $73 \leq Z \leq 91$ based on the one- and two-proton separation energies predicted by our latest Hybrid Mass Model. The latter is constructed by complementing the mass-excess values ΔM predicted by the Finite Range Droplet Model (FRDM) of Möller et al. with a neural network model trained to predict the differences $\Delta M^{\text{exp}} - \Delta M^{\text{FRDM}}$ between these values and the experimental mass-excess values published in the 2003 Atomic Mass Evaluation AME03.

1. Introduction

The precise location of the proton drip line is of great current interest in connection with experimental studies of nuclei far from stability conducted at heavy-ion and radioactive ion-beam facilities, as well as for astrophysical problems such as nucleosynthesis and supernova explosions. More specifically, prediction of the proton drip line in the region $31 \leq Z \leq 49$ is important in nucleosynthesis because it determines a possible path of the rapid proton capture process [1]. On the other hand, studies in the region $73 \leq Z \leq 91$ are helpful in planning experiments on proton radioactivity [2]. Global models of the proton separation energies are mainly derived from the available global models of atomic mass. Atomic mass models range from those with high theoretical input that take explicit account of known physical properties in terms of a relatively small number of fitting parameters, to models that are shaped mostly by the data and have a correspondingly larger number of adjustable parameters. A prominent example of the former class is the Finite Range Droplet Model (FRDM) of Möller et al. [3]. At the other end of the spectrum one finds artificial neural network models, which, in their purest form, would make predictions for new measurements of $\Delta M(Z, N)$ based on the data with which

*This research has been supported in part by the U. S. National Science Foundation under Grant No. PHY-0140316 and by the University of Athens under Grant No. 70/4/3309. We thank J. Rayford Nix for suggesting the hybrid strategy explored here.

they are trained, and *only* that information. Through several phases of development, these systems have attained demonstrable predictive power, with significant prospects for further improvement [4,5].

In this work, we present results from a recently proposed synthesis [6] of the two approaches – theoretical/phenomenological as represented by the FRDM, and statistical as represented by multilayer feedforward neural networks. Under training by example, a neural network is constructed that estimates the *differences* $\Delta M^{\text{exp}} - \Delta M^{\text{FRDM}}$ between the experimental and FRDM values of the nuclidic mass excess ΔM . Thus, the neural network serves to model the residual effects *not* captured by the FRDM. This hybrid strategy is pursued with the aim of determining whether the corrections to a state-of-the-art global semi-microscopic model stem from a large number of small effects that may fluctuate strongly with Z and N , *defying* systematic quantification, or instead can be attributed in substantial part to *regularities* of nuclear structure not yet embodied in macroscopic/microscopic models. Combining the ΔM values predicted by the FRDM with the differences estimated by the neural network, we obtain a hybrid global mass model that displays, on average, improved predictive performance for the systematics of atomic masses and related nuclear properties. From the one- and two-proton separation energies evaluated using the masses of the hybrid model, we make predictions for the proton drip line. These predictions are compared with the theoretical values obtained with the FRDM and with the relativistic Hartree-Bogoliubov model of Ref. [7] and also with the available experimental data published in the 2003 Atomic Mass Evaluation [8].

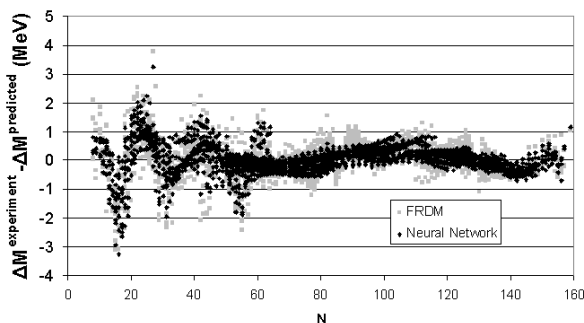


Figure 1. Mass-excess differences between experiment and the FRDM for the data sets $AML \cup AMV$ are compared with the corresponding differences predicted by the neural network.

2. Hybrid Mass Model

We briefly describe the methodology applied in building our latest version of the Hybrid Mass Model. (For further details, we refer to the development of the model denoted HM2 in Ref. [6]). In order to create a global mass model with enhanced extrapolation capabilities, we train candidate multilayer network systems using the *entire* database of 2149 ($Z, N \geq 8$) nuclei having experimental mass-excess assignments in the most recent atomic mass evaluation (AME03) of Audi et al. [8]. Thus, we depart from earlier practice in *not* reserving a portion of the experimental database for testing predictive performance. The

four input units of the neural network serve to encode the atomic number Z , the neutron number N , and their respective parities (even or odd). A single output unit encodes the target quantity, i.e., the mass-excess difference $\Delta M^{\text{exp}} - \Delta M^{\text{FRDM}}$. The 2149 nuclei are divided randomly into two data sets of 1693 (AML) and 456 (AMV) nuclei, comprising respectively the *learning* and *validation* sets for neural-network modeling. Performance on the learning set serves as the criterion for progressive adjustment of the network parameters, while performance on the validation set is used to decide when to terminate training, fixing the parameters of the final network. Several novel training techniques have been applied to optimize network performance [6]. The ability of the neural network to model the difference $\Delta M^{\text{exp}} - \Delta M^{\text{FRDM}}$ is illustrated in Fig. 1. Viewed over the entire database $\text{AML} \cup \text{AMV}$ in the $Z - N$ plane, the deviations of the FRDM evaluation from experiment are substantially reproduced by the neural network model.

To generate estimated mass-excess values for nuclides of specified Z and N within the Hybrid Mass Model HM2, we add the mass-excess value given by the Finite-Range Droplet Model to the network estimate of the FRDM error for the given Z and N . As documented more fully in Ref. [6], the HM2 model demonstrates improved overall accuracy on the existing experimental database and improved simulated predictive performance on estimated (i.e., non-experimental) masses in the AME03 tabulation. In Table 1, we compare the errors of the HM2 model for the mass excess and for the derived one- and two-proton separation energies, as measured by the root-mean-square error σ_{rms} over the database relative to experiment, with the corresponding errors of the FRDM and two other recently constructed neural-network models. Although our latest neural network model, trained for direct prediction of the mass excess, exhibits overall rms performance comparable to that of the hybrid HM2 model, it shows inferior generalization capabilities. For that reason – as argued more fully in Ref. [6] – we consider HM2 to be the preferred global mass model among those considered.

Table 1

Root-mean-square error σ_{rms} (MeV) in estimation of mass excess and one- and two proton separation energies. For each of these quantities, the number of experimental data points is given in parentheses.

Model	ΔM (2149)	$S(p)$ (1968)	$S(2p)$ (1836)
FRDM [3]	0.66	0.40	0.49
Neural network mass model [5]	0.64	0.53	0.61
Neural network mass model (latest version)	0.41	0.36	0.40
Hybrid Mass Model - HM2 [6]	0.37	0.37	0.40

2.1. Proton Drip Line

The proton drip line is usually defined by the last nuclide per isotone chain for which both one- and two-proton separation energies are positive, although as Z increases, deviation from this definition is to be expected because of the Coulomb barrier. In Fig. 2 we compare predicted proton drip lines in the regions $31 \leq Z \leq 49$ and $73 \leq Z \leq 91$ for the HM2 model, the FRDM, and the relativistic Hartree-Bogoliubov model of Ref. [7]. Differences between the proton drip lines predicted by the HM2 model and the FRDM are

minor, yet suggestive of subtle systematics. In contrast to the HM2 model, the FRDM predicts ^{61}Ga and ^{178}Au nuclides to be unstable, whereas AME03 projects stability. Similarly, in the region $31 \leq Z \leq 49$, the FRDM also makes erroneous predictions for ^{64}As and ^{76}Y , according to the latest experimental data [9]. The relativistic Hartree-Bogoliubov model exhibits significant deviations from the FRDM and HM2 models for the even- Z nuclei in the region $31 \leq Z \leq 49$.

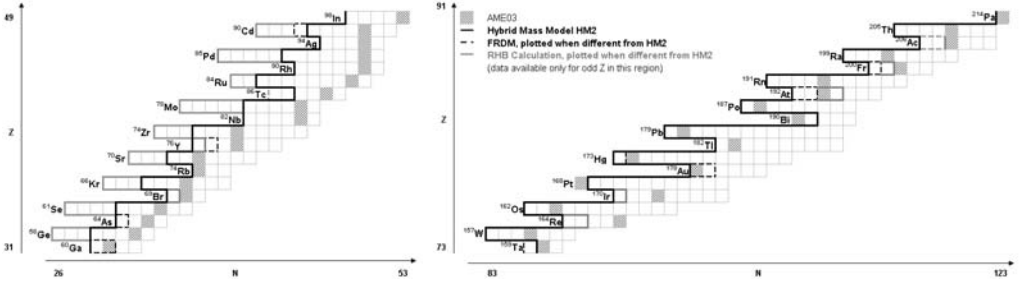


Figure 2. Proton drip line in the regions $31 \leq Z \leq 49$ and $73 \leq Z \leq 91$, as predicted from the HM2 model, is compared with predictions of the FRDM [3] and the relativistic Hartree-Bogoliubov model [7]. The last nucleus in each isotope chain having positive one- and two-proton separation energies according to AME03 is also indicated.

3. Conclusions

The work presented here demonstrates that macroscopic/microscopic and statistical models can complement one another in accurate prediction of atomic masses and related quantities far from stability. A hybrid model that combines the two approaches outperforms either and yields results that can provide valuable input to nuclear astrophysics.

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