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Improved Bethe–Weizsäcker Formalism With Core–Surface Parameterization and Deformation for Z > 103 Nuclei

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ABSTRACT

Evaluation of nuclear masses is important not only for studies of nuclear structure but also for the synthesis of superheavy nuclei (SHN), fission processes, and astrophysical studies. However, experimental data in the superheavy region are scarce. Accurate theoretical mass models therefore play a crucial role in extrapolating nuclear masses not only beyond Z=118 but also toward the neutron and proton drip-line regions. In this study, a modified Bethe-Weizsäcker (MBW) binding energy formula for the superheavy region is proposed. The formula is based on a new description of a nuclear structure consisting of two regions: a dense nuclear core, assumed to contain equal number of protons and neutrons (2Z), and a nuclear surface composed of excess neutrons (N-Z). The surface and the Coulomb terms have been parameterized to account for the two regions, in addition to incorporating a modified shell-correction term and a deformation term. The calculated binding energies for 188 nuclei with $Z > 103$, obtained using the modified Bethe-Weizsäcker (MBW) formula, are compared with experimental data from the AME 2020 mass table, predictions from FRDM 2012, and values obtained from the original Bethe-Weizsäcker formula. The modified formula yields a root-mean-square (RMS) deviation of 3.5 keV per nucleon, demonstrating excellent agreement with the experimental data. The proposed MBW formula is therefore well suited for extrapolating nuclear masses of superheavy nuclei that are likely to exist in the predicted island of stability.

Keywords: Binding energy, Superheavy nuclei, Liquid drop model, Nuclear core, Nuclear surface.

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1. INTRODUCTION

The liquid drop model (LDM) is a macroscopic model that describes the nucleus as an incompressible liquid drop with extremely high density. First formulated by Carl Friedrich von Weizsäcker in 1935, the model provides a framework for calculating various ground-state nuclear properties, including nuclear masses, nuclear shapes, stability, and binding energies through the well-known Bethe-Weizsäcker mass formula. The Bethe-Weizsäcker mass formula is given by [1];

$$M(A,Z) = Zm_p + Nm_n$$
$$-\left[a_v A - a_s A^{\frac{2}{3}} - a_c Z(Z-1)A^{-\frac{1}{3}} - a_a \frac{(A-2Z)^2}{A} + \delta a_p A^{-\frac{3}{4}} + \eta\right] \quad (1)$$

A combination of the coefficients a_i that provide a good approximation to the observed binding energies is as follows:

Volume term: $a_v = 15.5\ Mev$, Surface term: $a_s = 16.8\ Mev$, Coulomb term: $a_c = 0.72\ Mev$, Asymmetry term: $a_a = 23\ Mev$, Pairing term: $a_p = 34\ Mev$, and Shell term: $\eta = 1 \rightarrow 3Mev$.

However, the model does not explain the appearance of magic numbers of protons and neutrons, nor does it account for the extra binding energy and enhanced stability associated with these nucleon numbers. The model also does not consider the internal structure of the nucleus. Furthermore, it does not accurately describe the binding energies of light and superheavy nuclei. These limitations in describing heavy and superheavy nuclei have led to the development of modified versions of the liquid drop model, which incorporate additional microscopic terms to account for shell effects and other nuclear interactions.

Among the most successful modified versions of the liquid drop model are the Lublin-Strasbourg Drop (LSD) [2] and the Modified Surface Diffuseness (MSD) model proposed by Moretto *et al.* in 2012 [3]. Both of these modern models reproduce not only nuclear masses but also fission-barrier heights with a remarkable accuracy in the heavy and superheavy regions. Besides the classical liquid drop model (LDM) and its modified macroscopic-microscopic versions, tremendous progress has been made in the development of models and formulas for calculating nuclear masses and binding energies. These include mean-field models, fully microscopic models, and several *ab initio* methods, and phenomenological formulas. Mean-field and Density Functional Theory (DFF) models, coupled with rapid advances in information technology, have achieved a remarkable success in the calculation of nuclear masses, charge radii, separation energies, fission-barrier heights, and other properties of atomic nuclei. Other highly accurate and robust nuclear mass models include the Duflo-Zuker (DZ) model [4] and the more recently developed Weizsäcker-Skyrme (WS) model.

Nuclear binding energy is the minimum energy that is required to disassemble the nucleus of an atom into its constituent particles, namely protons and neutrons [5]. Equivalently, it is the energy that holds the nucleons together within the nucleus. The binding energy is always positive because energy is supplied to overcome the nuclear force and separate the nucleons from one another. Nuclear masses and binding energies play a crucial role in evaluation of shell closures as well as the limits of nuclear existence. Consequently, precise direct measurements of nuclei far from the beta-stability line are of critical importance for understanding the origin of nearly half of the heavy nuclei in the nuclear landscape. In addition, the evaluation of binding energies for finite nuclei is essential for understanding the synthesis of super heavy elements through nuclear fusion and fission processes [6].

The superheavy elements are those with atomic numbers Z=103-118, with Oganesson (Z=118) being the most recently synthesized element. Superheavy elements occupy the seventh period of the periodic table. They comprise a new series of 6d transition elements followed by the 7p elements (Z=113-118). Superheavy elements (SHE) are also commonly defined as the chemical elements whose atomic nuclei have a vanishing fission barrier in the liquid drop model.

Light nuclei typically contain equal numbers of protons and neutrons. As nuclei become heavier, more neutrons than protons are required to maintain nuclear stability. Consequently, nuclei with $Z > 20$, contain more neutrons than protons. In this model, equal number of protons and neutrons (2Z) are confined within the nuclear core, while the excess neutrons (N-Z) are assumed to occupy the larger region surrounding the core, referred to as neutron skin. Lead, for example, has 82 protons and 126 neutrons, giving a total of 208 nucleons. Of these, 164 nucleons (82 protons and 82 neutrons) are confined within the nuclear core, while the remaining 44 excess neutrons are distributed near the nuclear surface, forming the neutron skin. It is believed that the combination of low neutron separation energy and the short-range nature of the nuclear force allows the excess neutrons to occupy the region surrounding the nuclear core. The Modified Bethe-Weizsäcker mass formula derives its modification from the recent discovery of the neutron skin in neutron-rich nuclei, heavy, and superheavy nuclei [7].

The skin depth is generally defined as the difference between the radii at which the nuclear density decreases from 90% to 10% of its maximum value. The Wood-Saxon model of nuclear density distribution can be used to determine neutron skin thickness. The parametric form proposed by Wood and Saxon [8] is,

$$\rho_{N(r)} = \frac{p_0}{1+\exp(\frac{r-R_N}{t})} \tag{2}$$

where *t* is the diffuseness parameter (or skin depth), which characterizes the thickness of the nuclear surface layer over which the density falls from 90% to 10% of its maximum value.

Experimentally, several techniques have been employed to study the neutron skin, including elastic scattering experiments, hadronic probes, and parity-violating electron scattering. A recent study conducted by scientists at the Thomas Jefferson National Accelerator Facility in the United States reported a highly accurate measurement of the neutron skin thickness of the lead nucleus [9]. The experimental results revealed that a neutron skin has a thickness of 0.28 fm for lead. This study, which employed parity-violating electron scattering, is expected to facilitate even more precise measurements of neutron skin thickness in future investigations.

2. THEORETICAL FORMALISM

In this study, Bethe-Weizsäcker mass formula is modified for the superheavy nuclear region. In particular, the surface and Coulomb terms have been reformulated in light of the recently proposed nuclear structure model, which suggests the existence of a dense inner core surrounded by a less dense nuclear region. Since superheavy nuclei are stabilized by quantal shell effects, a shell correction term proposed by Dieprink and Van Isacker is adopted with a slight modification to its parameters. Additionally, a deformation term has been included because most superheavy nuclei are deformed in their ground state [10]. The manner in which excess neutrons are distributed within the nucleus is crucial for understanding nuclear structure and may significantly influence the nuclear binding energy. In this modification, the following assumptions are made.

First, as discussed above, the nuclear core consists of equal numbers of protons and neutrons, while the excess neutrons occupy the region near the nuclear surface. Second, the Coulomb repulsion among the protons is assumed to be confined within the nuclear core. Finally, the nuclear force is assumed to be charge independent, particularly near the nuclear surfaces.

The Volume Term

The volume term represents the attractive interaction between a nucleon in the nuclear core and its surrounding neighboring nucleons. Since the nuclear force is short-ranged, a nucleon interacts only with its nearest neighbors; beyond these, the attractive interaction becomes negligible. Consequently, the volume energy is assumed to be directly proportional to the total number of nucleons, or the mass number, (A). In the original Bethe-Weizsäcker mass formula, the volume term is written as;

$$\text{Volume energy} = a_v A \tag{3}$$

where a_v is the volume energy coefficient.

In the present model, the nuclear structure is parametrized into two regions; the nuclear core, containing 2Z nucleons, and the neutron skin, containing the excess neutrons (N-Z). Although the nucleus is treated as consisting of these two regions, the total nuclear volume remains unchanged. Consequently, the mathematical form of the volume term is retained, while the volume energy coefficient is slightly adjusted to $a_v = 15.99\ MeV$ through fitting with experimental binding-energy data.

Modification of the Surface Term

The surface term is derived from the analogy between the atomic nucleus and a liquid drop. Nucleons located deep within the nucleus are surrounded by neighboring nucleons in all directions, resulting in no net force acting on them. In contrast, nucleons at or near the surface have fewer neighboring nucleons and therefore experience an inward net attractive force. This imbalance gives rise to an effect analogous to surface tension, known as surface energy. As the nuclear surface area increases, the fraction of nucleons located on the surface also increases, reducing the average binding energy per nucleon. Consequently, the surface energy contributes negatively to the total binding energy. Thus, increase in the surface area leads to a decrease in binding energy.

In the original liquid drop model (LDM), the surface term is given by;

$$\text{Surface energy} = a_s A^{2/3} \tag{4}$$

where a_s is the surface energy coefficient, approximately equal to $a_s = 16.8\ MeV$ and A is the mass number. The above expression assumes uniform distribution of nucleons throughout the nucleus. However, in the present model, the nucleus is considered to consist of two distinct regions: A dense nuclear core containing 2Z nucleons and an outer neutron skin containing excess neutrons (N-Z). To account for this two-region structure, two surface contributions are considered: the surface of the nuclear core and the outer surface of the neutron skin. The modified surface term is therefore written as;

$$a_s\left[(2Z)^{2/3} + I(A)^{2/3}\right] \tag{5}$$

where $I = \frac{N-Z}{A}$

The first term represents the reduction in binding energy associated with the surface of the dense nuclear core, whereas the second term accounts for the reduction in binding energy arising from the surface of the neutron skin (skin energy). This modified surface term explicitly incorporates the effect of neutron skin formation and is therefore better suited for describing heavy and superheavy nuclei, where excess neutrons occupy the nuclear surface. The surface energy coefficient was adjusted to $a_s = 16.97\ MeV$ through fitting to experimental binding-energy data. This value remains within accepted range of surface energy coefficients reported in literature.

The Asymmetry Energy Term

The asymmetry energy term accounts for the reduction in nuclear binding energy arising from the imbalance between the numbers of protons and neutrons in the nucleus. This reduction occurs because the binding energy is maximized when the number of protons and neutrons are approximately equal, particularly for light nuclei. In the original Bethe-Weizsäcker mass formula, the asymmetry term is expressed as;

$$a_a \frac{(A-2Z)^2}{A} \tag{6}$$

where a_a is the asymmetry energy coefficient.

Since the present model assumes that the nucleus consists of a dense inner core surrounded by a neutron skin, but does not alter the overall neutron-proton imbalance, the mathematical form of the asymmetry term remains unchanged. However, the asymmetry energy coefficient has been slightly adjusted to $a_a = 20.22\ MeV$ through fitting to experimental binding-energy data.

Modification of the Coulomb Energy Term

The Coulomb energy term arises from the electrostatic repulsion between protons within the nucleus and is therefore proportional to the number of protons (Z). This contribution reduces the nuclear binding energy because the repulsive Coulomb force acts against the attractive nuclear force, thereby decreasing the stability of the nucleus.

In the original semi-empirical mass formula given by Equation (1), the Coulomb term is written as;

$$\text{Coulomb energy} = a_c \frac{Z(Z-1)}{A^{1/3}} \tag{7}$$

where a_c is the Coulomb energy coefficient.

In the present model, the nuclear core is assumed to consist of equal number of protons and neutrons (2Z), while the excess neutrons occupy the neutron skin. Since the Coulomb interaction acts only between protons, it is assumed to be effectively confined within the nuclear core. Consequently, the characteristic nuclear radius governing the Coulomb interaction is taken to be proportional to $(2Z)^{1/3}$ rather than $(A)^{1/3}$ as assumed in the original Bethe-Weizsäcker mass formula. Accordingly, Equation (7) is modified to;

$$a_c \frac{Z(Z-1)}{(2Z)^{1/3}} \tag{8}$$

Equation (8), adapted from the modified Coulomb interaction proposed in Refs. [11, 12], reflects the assumption that the Coulomb interaction is effectively confined to the dense nuclear core containing equal number of protons and neutrons. Consequently, the denominator is modified from $(A)^{1/3}$ to $(2Z)^{1/3}$, thereby emphasizing the proton-driven electrostatic repulsion that plays a dominant role in determining the stability of superheavy nuclei. The fitted value of the Coulomb energy coefficient used in the present work is $a_c = 0.7095\ MeV$.

Shell Effects

Superheavy nuclei are stabilized by quantal shell effects [13]. Numerous methods for incorporating shell corrections into nuclear mass models have been proposed in literature. Shell corrections for superheavy nuclei (SHN) are of great importance not only for the synthesis of new superheavy elements but also for predicting the location of the so-called island of stability. In the present model, a simplified shell correction term proposed in Ref. [14] is adopted with a slight modifications to its parameters. The shell correction depends on the valence protons and neutrons relative to the nearest magic shells and is expressed as;

$$B_{shell}(N_p, N_n) = a_1 G_{max} + a_2 G_{max}^2 \tag{9}$$

where $$G_{max} = \frac{N_p + N_n}{2} \tag{10}$$

The first term in Equation (9) represent the linear contribution arising from valence nucleon interactions, whereas the second term is a quadratic contribution that accounts for shell saturation effects. The fitted values of the parameters $a_1 = 0.44$ and $a_2 = -0.034$.Here, N_p and N_n denote the number of valence protons and valence neutrons relative to the nearest magic proton and neutron shells, respectively. The reference magic numbers adopted in this work are Z=114 and N=184.

Deformation Energy Term

The deformation energy is defined as the difference in energy of a nucleus between its spherical and its equilibrium shape [15]. It represents the energy gained by a nucleus as a result of deformation. Superheavy nuclei ($Z > 103$) generally exhibit either prolate or oblate shapes, with the quadrupole (β_2) and hexadecapole (β_4)deformation parameters playing a crucial role in determining their stability. A common and effective approach for incorporating these shape degrees of freedom is to include a deformation term proportional to the squares of quadrupole and hexadecapole deformation parameters [16]. The deformation parameter values used in the present work were obtained from the FRDM 2012 calculations [17].

$$E_{def} = \alpha[(\beta_2)^2 + (\beta_4)^2] \tag{11}$$

where the fitted deformation coefficient is $\alpha = -0.5$

Taking into account the modified surface, Coulomb, and asymmetry terms, together with the shell correction and deformation energy terms, the Modified Bethe-Weizsäcker binding energy formula is written as;

$$B(A,Z) = a_v A - a_s[(2Z)^{\frac{2}{3}} + I(A)^{\frac{2}{3}}] - a_c \frac{Z(Z-1)}{(2z)^{\frac{1}{3}}} - a_a \frac{(A-2Z)^2}{A} \pm \delta a_p A^{-\frac{1}{2}} + B_{shell}(N_p, N_n) + E_{def}$$

(12)

3. RESULTS AND DISCUSSION

The Modified Bethe–Weizsäcker (BW) formula derived in Equation (12) was used to calculate the binding energies of all superheavy nuclei Z=103 to Z=118 across all their isotopic chains. The calculated binding energies were analyzed graphically and compared with predictions from Finite Range Droplet Model (FRDM), the original Liquid Drop Model (OLDM), and available experimental data, as shown in Figure 1.

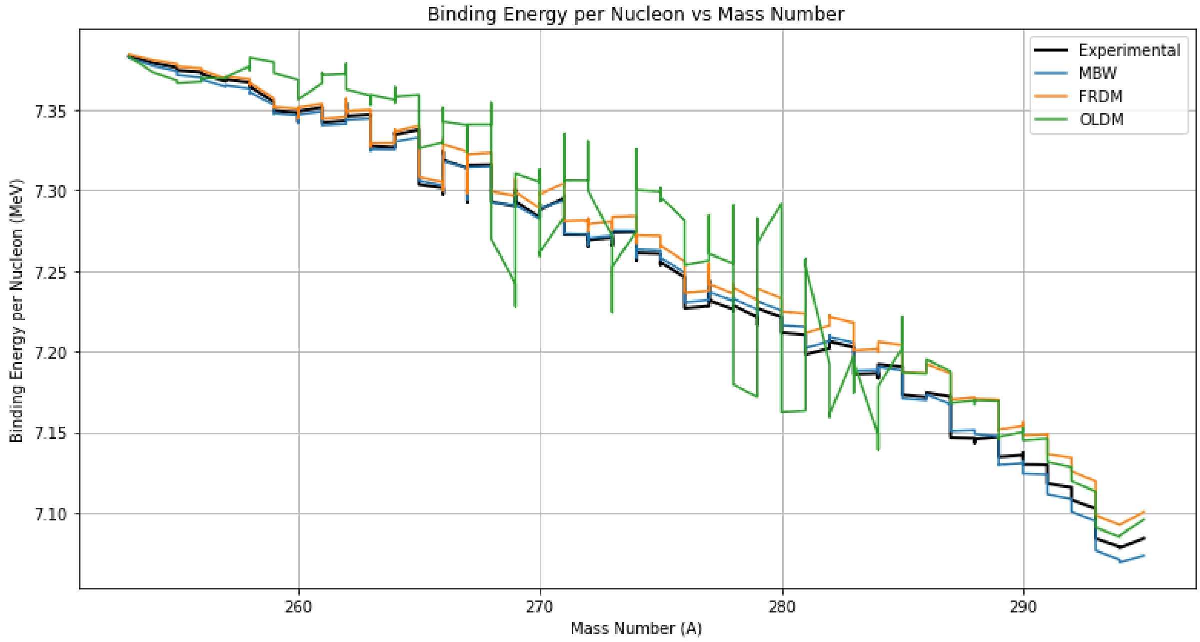

Figure 1. Binding energy per nucleon as a function of mass number for superheavy nuclei. The results obtained using the modified Bethe–Weizsäcker model (MBW) are compared with the FRDM, the original Liquid Drop Model (OLDM), and the available experimental data for Z=104–118.

Figure 1 shows that the binding energies obtained from the modified BW formula are in close agreement with experimental data. The MBW model reproduces the experimental values particularly well for nuclei with atomic numbers Z=104-115, demonstrating a significant improvement over the original liquid drop model. As the atomic number increases beyond Z=115, however, the deviations between the MBW predictions and the experimental values become progressively larger. The largest discrepancies are observed for nuclei with Z=117 and Z=118, where the increasing Coulomb repulsion and stronger shell effects make the description of these nuclei more challenging. A similar trend is observed for FRDM predictions, although the deviations are generally larger than those of the MBW model, particularly as Z approaches 118. In contrast, the original liquid drop model exhibits considerably larger deviations throughout the superheavy region because it does not incorporate microscopic corrections, such as shell and pairing effects, which play a crucial role in determining the stability of superheavy nuclei.

Furthermore, Figure 1 indicates that the binding energy per nucleon generally decreases with increasing mass number throughout the superheavy region. This trend reflects the growing influence of Coulomb repulsion among the increasing number of protons, which progressively counteracts the attractive strong nuclear force. As a result, the overall binding energy of the nucleus weakens, reducing its stability and increasing its susceptibility to radioactive decay through alpha emission and spontaneous fission. The observed trend is consistent with both theoretical predictions and experimental observations for superheavy nuclei, where the competition between nuclear attraction and Coulomb repulsion governs the limits of nuclear stability

To evaluate the predictive accuracy of the modified Bethe–Weizsäcker (MBW) formula derived in this work, the root-mean-square (RMS) deviations of the MBW, the Finite Range Droplet Model (FRDM 2012), and the original Liquid Drop Model (OLDM) were calculated with respect to the available experimental binding-energy data. The results are presented graphically in Figure 2.

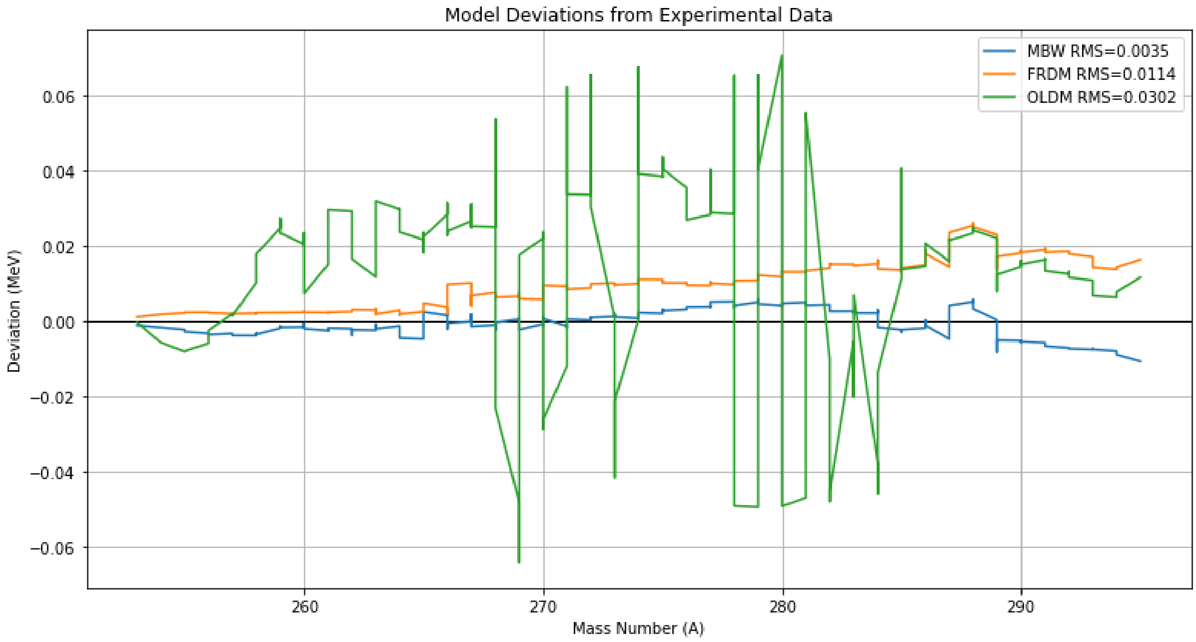

Figure 2. RMS deviations of the modified Bethe–Weizsäcker model (MBW), FRDM 2012, and the original Liquid Drop Model (OLDM) relative to the experimental binding-energy data [18].

The statistical analysis shows that the MBW model yields an RMS deviation of 3.5 keV per nucleon, compared with 11.4 keV per nucleon for the FRDM 2012 and 30.2 keV per nucleon for the original Liquid Drop Model. These results were obtained using the available experimental data for 188 superheavy nuclei with $Z \geq 104$. The significantly lower RMS deviation of the MBW model demonstrates its improved agreement with experimental measurements and indicates that the modifications introduced into the Bethe–Weizsäcker formula substantially enhance its predictive accuracy for superheavy nuclei.

The superior performance of the MBW model suggests that it provides a more reliable description of the binding energies of superheavy nuclei than both the FRDM 2012 and the original Liquid Drop Model. Consequently, the proposed formula offers a promising framework for estimating the binding energies of experimentally inaccessible or yet-to-be-synthesized superheavy nuclei. In addition, the improved agreement with experimental data enhances its usefulness in studies of nuclear structure, including investigations of shell effects, nuclear stability, the interplay between Coulomb and strong nuclear forces, and the location of the predicted island of stability in the superheavy region.

4. CONCLUSIONS

Currently, there is limited experimental reach in nuclei in the dripline and super heavy regions. The confirmed validity of the modified BW shows it can therefore be used not only to extrapolate into these unknown regions but also for the search of the location of island of stability.

A modified Bethe–Weizsäcker (MBW) mass formula has been developed for the superheavy nuclear region. The macroscopic component of the model is based on the traditional liquid drop formula with six adjustable parameters. However, the surface and Coulomb energy terms have been reformulated to account for a revised description of the nuclear structure, consisting of a dense nuclear core with equal numbers of protons and neutrons, surrounded by a less dense region containing the excess neutrons. Furthermore, two microscopic corrections namely shell correction term and a deformation correction term have been incorporated with appropriately optimized parameters to improve the predictive capability of the model.

The modified formula was validated by comparing its binding-energy predictions with the available experimental data for superheavy nuclei. The model achieved a significantly lower root-mean-square (RMS) deviation than both the FRDM 2012 and the original Liquid Drop Model, demonstrating its improved accuracy in describing the binding energies of superheavy nuclei.

Because experimental data remain scarce near the neutron drip line and in the superheavy region, reliable theoretical models are essential for guiding future investigations. The excellent agreement between the MBW predictions and the available experimental data suggests that the proposed formula provides a reliable framework for estimating the properties of experimentally inaccessible nuclei. Consequently, it may serve as a useful tool for predicting the binding energies of unknown superheavy nuclei, exploring the limits of nuclear stability, and guiding the search for the predicted island of stability.

In super heavy nuclei, the neutron skin region contains excess neutrons (N-Z), and these neutrons surround the central neutron- proton(N=Z) core. The interaction between the core and the excess neutrons is a strong nuclear force that works against the powerful internal Coulomb force that is repulsive. This interaction creates a stabilizing average potential (V_o) that governs the kinematics and the binding of the skin neutrons [19]. Values of V_o can be calculated for different SHN, and a binding energy formula can be developed to determine which SHN could be part of the "island of stability." Our future research will concentrate on these ideas.

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