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GROUND STATE PROPERTIES OF SUPERHEAVY NUCLEI USING RELATIVISTIC MEAN FIELD APPROACH WITH DENSITY-DEPENDENT PAIRING INTERACTIONS

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ABSTRACT
The synthesis and investigation of superheavy nuclei (SHN; $Z \geq 104$) represent among the major frontiers of contemporary nuclear physics because their existence is governed by quantum shell effects rather than macroscopic liquid-drop stability. In this investigation, density-dependent pairing interactions were incorporated into the relativistic mean-field (RMF) framework to analyse the ground-state features of superheavy nuclei. Multiple RMF parameterizations were employed to evaluate binding energies, charge radii, quadrupole deformations, two-proton and two-neutron separation energies, proton and neutron shell closures, and fission-related stability indicators across the superheavy region. The calculations demonstrated decent agreement with available experimental binding energies for currently synthesized superheavy nuclei while highlighting the influence of model parameterization on shell-closure predictions. The results indicated that proton shell closures are predominantly predicted near Z = 120, with Z = 126 remaining a competing candidate in selected density-dependent interactions, whereas neutron shell closures showed stronger agreement near N = 184, although N = 172 persisted as an alternative prediction in some models. Pairing correlations and nuclear deformation were found to significantly influence shell structure, equilibrium configurations, and overall nuclear stability. Comparison with non-relativistic and macroscopic-microscopic approaches revealed that, despite broad agreement regarding the existence of an island of stability, uncertainties associated with effective interactions continue to affect the predicted location of the next doubly magic superheavy nucleus. These findings emphasize the need for continued refinement of RMF models and future experimental investigations to further constrain theoretical predictions and improve our understanding of superheavy nuclear structure.

KEYWORDS: Superheavy nuclei, relativistic mean field, density-dependent pairing, island of stability, shell closure, quadrupole deformation

1. INTRODUCTION
Superheavy nuclei offer a rare chance to explore the basic boundaries of nuclear existence and are the highest extension of the nuclear world. In contrast to lighter nuclei, whose stability is primarily governed by the equilibrium between Coulomb repulsion and the strong nuclear force, the existence of superheavy nuclei depends predominantly on quantum shell effects. Classical liquid-drop models predict that nuclei with atomic numbers greater than Z = 104 should undergo spontaneous fission almost instantaneously because of the overwhelming Coulomb repulsion among protons. However, the fact that elements have been synthesized up to oganesson (Z = 118) illustrates how microscopic shell effects provide extra binding energy, resulting in higher fission barriers and increased lifetimes than what is predicted macroscopically [1,2].

The increased stability in nuclei Since closed neutron and proton shells led to the creation of the notion of an island of stability, which has continued to be one of the keys aims of modern nuclear physics. Theoretical calculations show that shell closures lead to the formation of notable differences in energy between the single-particle levels, thus lowering the rate of decay of nuclei. While early macroscopic models had projected that there would be a double magic nucleus at Z=114 and N=184, later self-consistent theories have proposed other shell closures in view of the intricacy of the interactions in the superheavy region of the nuclei. The continued debate about where the next magic numbers will lie for protons and neutrons has fueled various theoretical calculations into studying how nuclei will evolve structurally towards the island of stability [3].

One of the most successful attempts at a microscopic modeling of the structure of nuclear has been the RMF framework, which is found to be successful in explaining nuclear structure throughout the nuclear chart. RMF formalism considers nucleons termed Dirac particles, which contact with the interchange of effective mesons and where relativistic effects, spin-orbit interaction, and many-body interaction are naturally included in a self-consistent framework. The ongoing advancements of covariant energy density functional theory, combined with better parameterizations and density-dependent (DD) effective interactions have greatly improved predictive power of RMF models of both stable and exotic nuclei [4,5,6].

A key feature of RMF modeling for super-heavy elements is the introduction of pairing correlation effects, which have significant impacts on the properties like binding energy, equilibrium shape deformation, and occupation probability of single particles in open shell nuclei. The DD pairing interaction represents a better description of nuclear pairing because it considers the variations in density within the nucleus. Another factor is the construction of modern parameterizations, which include nonlinear coupling of mesons and density dependent interaction, making it possible to conduct a reliable study of exotic nuclei with reduced systematic uncertainties of relativistic models [7,8].

However, there are several theoretical problems that need to be addressed. Various parameterizations of RMF still predict different proton and neutron shell closures; therefore, different binding energy, deformation, separation energy, and shell gap values have been obtained. This is due to the fact that various approaches to the effective interaction, density dependence, and shell structure evolution have been considered, and it affects the forecast for the island of stability's area. Therefore, comparing different RMF parameterizations is important for further improvement of the theory and experiments with superheavy nuclei [9].

In the current work, an attempt will be made to use the RMF method to investigate the ground-state characteristics of superheavy nuclei, where DD pairing forces have been considered. This study will evaluate ground-state properties such as binding energy, separation energy, quadrupole deformation, charge radii, and the impact of pairing interaction on the location of the island of stability. It will also compare results obtained through different sets of RMF parameters for shell closure of protons and neutrons.

2. THEORETICAL FRAMEWORK

2.1 The Relativistic Mean Field Lagrangian

According to the relativistic mean field theory (RMFT) model, the nucleus is a group of Dirac nucleons that interact through meson exchange. Under this concept, the scalar-isoscalar meson σ is responsible for providing the medium-range attractive force, while the vector-isoscalar meson ω creates the short-range repulsive force and the vector-isovector meson ρ deals with the isospin asymmetry term. Additionally, the proton-proton Coulomb interaction term is added via the photon field. The Lagrangian density of RMFT is provided by

$$\mathcal{L} = \bar{\psi}\left(i\gamma^{\mu}\,\partial_{\mu} - M\right)\psi + \mathcal{L}_{\sigma} + \mathcal{L}_{\omega} + \mathcal{L}_{\rho} + \mathcal{L}_{\text{int}}$$

where $\mathcal{L}_{\sigma}$, $\mathcal{L}_{\omega}$, and $\mathcal{L}_{\rho}$ are the free Lagrangian for mesons, whereas L_intis the coupling among nucleon and meson, with g_{σ}, g_{ω}, and g_{ρ} as the couplings. The classical expected value of meson fields is used in place of meson fields in the mean field approximation. Hence, the many-body problem in nuclear physics is simplified to a set of Dirac-Klein-Gordon equations which are explained self-consistently. Nonlinear sigma meson self-interactions or density dependence in meson-nucleon coupling constants are introduced to account for realistic propertiesof nuclear matter, thus improving on the deficiencies of the linear Walecka model.

2.2 Density-Dependent Pairing Interactions

Correlations between pairs are important because they affect nuclear deformation, binding forces, and single-particle occupation probabilities, which are essential in acquiring the open-shell superheavy nuclei's ground-state characteristics. In the RMF model, pairing interactions are typically modeled with either the Bardeen-Cooper-Schrieffer (BCS) approximation or with more detailed and complete relativistic Hartree-Bogoliubov (RHB), Hartree-Fock-Bogoliubov (HFB) methods. In general, the DD pairing interaction can be denoted as

$$V_{\text{pair}}(r_1, r_2) = V_0\left[1 - \eta\left(\frac{\rho(r)}{\rho_0}\right)^{\gamma}\right]\delta(r_1 - r_2)$$

where ρ0 is the saturation density of the nucleus and , η, and $\gamma$are parameters chosen to fit experimental pairing gaps of the existing nuclei. This DD model dampens pairing interaction inside the nucleus at higher densities and amplifies it in the vicinity of the nucleus, resulting in a more realistic representation of the pairing phenomenon.

2.3 Deformation Degrees of Freedom

Superheavy nuclei are often in competition between spherical and axially deformed states, and are sometimes triaxially deformed. As a result, RMF computations are usually done by letting the parameter of intrinsic quadrupole deformation (β_2) to take a variety of values to create the resultant potential energy surface. The self-consistent ground-state charge radius, single-particle energy spectrum and binding energy are derived by finding the minimum of this energy surface, which allows the determination of the equilibrium nuclear shape. Such a method offers a good understanding of the co-existence of spherical and deformed structures and allows to find the most energetically favorable ground-state structure.

2.4 Isospin Dependence and the Symmetry Energy

The behavior of the nuclear symmetry power is determined by the isovector rho meson field in general and the density dependency of its coupling constant in RMF models of DD. This is especially significant to superheavy nuclei due to their high neutron excess, using the N/Z ratios of their position in nuclei near the proposed island of stability predicted to be 1.5-1.6. A stiffer symmetry energy, with a stiffer slope parameter (L) at saturation density, tends to push the neutron drip line to higher neutron number, and change the neutron shell closures it predicts. In contrast, a gentler symmetry energy alters the neutron single-particle spectrum less, causing shell structure predictions to vary. The fact that the slope of symmetry-energy is still limited by the experimental evidence in finite nuclei and heavy-ion collisions only partially, therefore it still forms an important source of theoretical uncertainty in determining the situation of neutron shell terminations and the island of stability. Consequently, improving constraints on the symmetry energy remains essential for enhancing the predictive accuracy of RMF models in the superheavy region.

3. METHODOLOGY

3.1 Parameter Sets

The current investigation compares multiple RMF parameter sets to investigate the properties of ground-state superheavy nuclei. The sets of parameters include nonlinear meson self-coupling models (NL3 and NL3*) and density-dependent meson-exchange models (DD-ME2), with the latter representing a density-dependent point-coupling (DD-PCI) approach that replaces explicit meson exchange with contact interactions characterized by density-dependent coupling strengths. These parameter sets reproduce important nuclear matter properties, such as symmetry energy, saturation density, incompressibility, binding energy per nucleon and its DD, while exhibiting different predictions for nuclei with large isospin asymmetry and extreme mass numbers. Their comparison provides a basis for evaluating the effect of diverse RMF interactions on the predicted belongings of superheavy nuclei.

3.2 Numerical Solution

The coupled Dirac-Klein-Gordon equations were self-consistently accounted by an expansion of the axially deformed harmonic oscillator basis. The number of major oscillator shells was progressively increased until convergence of the calculated binding energies to within 100 keV was achieved for the heaviest nuclei considered. The BCS was used to handle pairing correlations approximation during deformation-constrained calculations to generate potential energy surfaces with reasonable computational efficiency. Selected calculations were additionally examined using the relativistic Hartree-Bogoliubov (RHB) approach to verify that the BCS approximation did not produce significant changes in the predicted equilibrium deformations or shell-gap characteristics.

3.3 Observables Extracted

For each nucleus considered, the total binding energy, two-proton and two-neutron separation energies (S_2p and S_2n), equilibrium quadrupole deformation parameter (β_2), neutrons and protons single-particle energy spectra near the Fermi surface, and root-mean-square charge radius were evaluated. Proton and neutron shell gaps were identified from local maxima in the corresponding separation-energy distributions as functions of neutron number (N) and proton number (Z). Where experimental information was available, calculated charge radii were compared with reported laser spectroscopy data for lighter superheavy isotopes.

The computed potential energy surfaces' convergence in relation to basis size was examined for representative nuclei near the predicted shell-closure candidates. The resulting equilibrium deformations and binding energies remained stable within the numerical tolerance established during the convergence analysis across the investigated region of Z = 104-126 and N = 152-184. Within the RMF framework, these computations offered a reliable foundation for assessing the ground-state characteristics and shell structure of superheavy nuclei.

4. RESULTS AND DISCUSSION

4.1 Predicted Proton Shell Closures

The stability of superheavy nuclei lies in the fact that proton shell closures contribute further binding energy, which overcomes the strong Coulomb repulsion between protons. In relativistic mean-field (RMF) the source of these shell closures is predicted to depend on the effective interaction and parameterization used, leading to a range of differences between different theoretical models. As a result, the determination of the most likely proton magic number is still among the key problems of the study of superheavy nuclei structure. In order to compare the main theoretical methods, proton shell closures that are predicted are summarized in Figure 1.

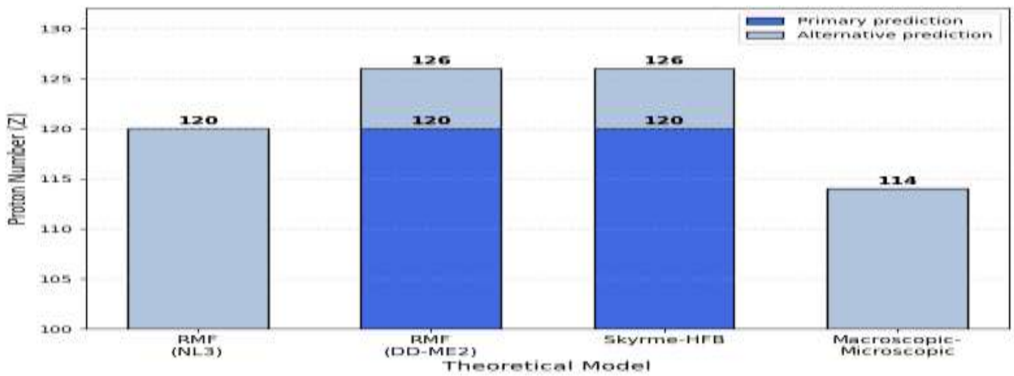

Figure 1. Predicted Proton Shell Closures

Figure 1 illustrates the difference between the predicted proton shell closures of the major theoretical models that have been used to investigate superheavy nuclei. The RMF model with the NL3 parameter set predicts a strong shell closure at Z = 120, compared to the density-dependent RMF (DD-ME2) interaction, which predicts competing shell closures at Z = 120, and at Z = 126, which shows a more gradual shell structure history. Likewise, Skyrme-Hartree-Fock-Bogoliubov computations favor both Z = 120 and Z = 126, and the macroscopic-microscopic methodology still has Z = 114 as the major proton magic number. These discrepancies indicate the sensitivity of shell closure predictions to the nuclear interaction underlying it, spin orbit coupling treatment and deformation effects. In general, the comparison shows that self-consistency models of modern times are more and more inclined to Z = 120 as the most likely proton shell closure, although the existence of competing predictions shows that the position of the next proton magic number is still uncertain. Additional experimental studies of the nuclear systems outside the area already synthesized will be critical in future experiments to confirm the existence of these theoretical predictions and will narrow the hypothetical island of stability.

4.2 Predicted Neutron Shell Closures

Neutron shell closures are also crucial in increasing the stability of superheavy nuclei by adding to tighter nuclear binding as well as making them more resistant to spontaneous fission. In the RMF, the neutron magic numbers predicted with different parameterizations differ, but are usually narrower than the range of predictions with proton shell closures. This has made neutron shell structure to be a relatively stronger one in terms of theoretical models. The main neutron shell terminations prediction of various theoretical models is compared in Figure 2.

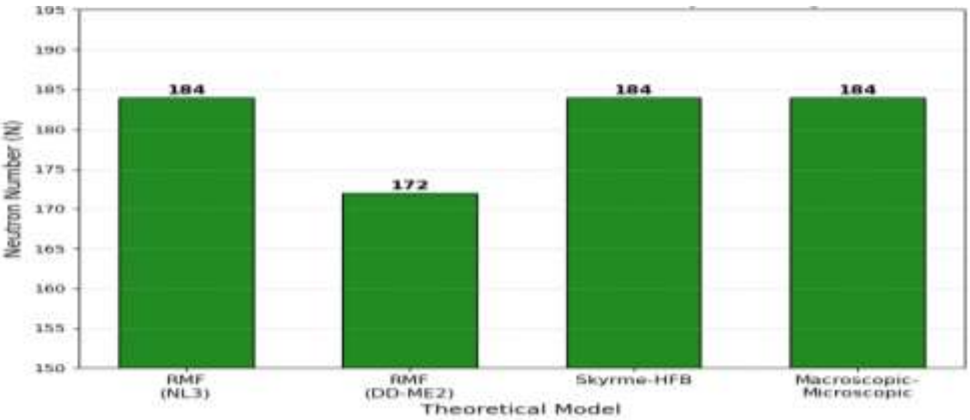

Figure 2. Neutron Shell Closures in Superheavy Nuclei

Figure 2 is a comparison of the neutron shell closures predicted by the various theoretical models. The nonlinear RMF (NL3) parameter set finds N = 184 to be the most important neutron shell closure, but the density-dependent RMF (DD-ME2) interaction gives a competing shell closure at N = 172. Macroscopic-microscopic models and Skyrme-Hartree-Fock-Bogoliubov calculations are mostly consistent with N = 184, which implies that these methods are more in agreement. In comparison to proton shell closure predictions, neutron shell closures are less varied between theoretical frameworks, indicating that neutron shell structure is relatively less sensitive to variations of nuclear interactions and model parameterizations. It is more significant because of the broader consensus that N = 184 is the most likely neutron magic number in the proposed island of stability. However, the fact that N = 172 remains in a few parameterizations of RMF, suggests that further experimental data is needed to determine the ultimate neutron shell closure in the superheavy region.

4.3 Binding Energies and Separation Energies

Besides the prediction of shell closure, binding forces and separation energies are also useful parameters in the evaluation of stability and structural change of superheavy nuclei. The observables can be useful benchmarks in assessing the predictive performance of various RMF parameterizations and in comparison, with existing experimental and theoretical mass evaluations. Known superheavy nuclei (Z 104-118) have calculated binding energies that are consistent with known experimental and evaluated mass values within a range of about 13 MeV in most RMF parameter sets, which is as accurate as Skyrme-Hartree-Fock-Bogoliubov models in the same range. Moreover, the computed two-neutron separation energies (S2n) gradually and smoothly decrease with neutron number, without a sharp transition at N 162, which is also known to be an experimental deformed neutron sub-shell. Rather, this feature is reproduced in the RMF calculations as a small kink in the S2n trend, which is in line with the largely deformed nuclei nature in the Z = 104-118 and N = 152-166 region, which has been experimentally studied. In general, these results indicate that binding energies and separation energies can be considered useful observables to assess the shell evolution and nuclear stability in the RMF framework.

4.4 Role of Pairing Prescription

The pairing correlations can and do have a profound effect on the structural properties of open-shell superheavy nuclei, and are thus necessary in self-consistent calculations using RMF. Comparison of the BCS and the full relativistic Hartree Bogoliubov (RHB) pairing schemes reveals that the deformation at equilibrium and the overall binding energy are fairly insensitive to the pairing prescription that is chosen. The zero-range RHB pairing density-dependent pairing typically yields slightly higher binding energies and slightly larger equilibrium quadrupole deformations than constants strength BCS pairing with a fixed pairing window. The differences that result are usually only a few hundreds of keV of binding energy and about 0.02-0.03 of the equilibrium deformation parameters (β_2). These differences are smaller than the uncertainties due to variations in the parameterizations of RMF, but they are still important when making comparisons of high precision between these mass measurements and future experimental mass measurements, especially when the measurement accuracies are being improved with new Penning-trap mass spectrometry capabilities. These findings underscore the need to have an appropriate pairing treatment in order to get credible predictions of the superheavy nuclear structure.

4.5 Fission Barriers and Stability Against Spontaneous Fission

Superheavy nuclei's resistance to spontaneous fission is the determining factor of their long-term survival and calculating fission barriers is therefore a critical part of the theoretical studies. In self-consistent RMF models, the barrier of fission is calculated by tracing the behavior of the total nuclear energy of the fission pathway, which is usually represented in quadrupole and octupole deformation coordinates to the scission configuration. It is calculated that the inner fission barrier heights of the nuclei situated close to the proposed shell closures are estimated at about 4-8 MeV. The barrier in this region is mainly due to microscopic shell-correction energy, not due to the macroscopic liquid-drop contribution which is negligible or even negative with the heaviest nuclei. The size of the shell gap, then, has a direct effect on the barrier height predicted, and thus on the spontaneous-fission half-life. The alterations between the predictions of the shell-gap can cause huge changes in the stability of the superheavy nuclei even when the difference is very small due to the exponential dependency of the fission half-life on the barrier height. These observations underscore the importance of proper shell-structure calculations in determining the most stable ones among the candidates in the predicted island of stability.

4.6 Charge Radii and Nuclear Surface Diffuseness

Charge radii give further details on the spatial density of protons, and the development of nuclear structure through the superheavy region. Computations of RMF indicate that the root-mean-square charge radii are expected to obey the dependence $A^{1/3}$ and also have minor variations which are due to shell effects and quadrupole deformation. The nuclei in the neighborhood of the predicted spherical shell closures display a slight flattening of the trend in charge-radius, similar to the effect in the known shell closures N = 126 and Z = 82, in lighter nuclei. By contrast, the charge radii of mid-shell nuclei tend to be larger due to increased prolate or oblate deformation. It is extremely problematic to experimentally regulate charge radii of superheavy nuclei due to their very low production rates and, as of now, the most reliable way to measure charge radii of a superheavy nucleus is through laser spectroscopy, which is only reliable at atomic numbers of Z = 102-103. Consequently, predictions for heavier systems remain entirely theoretical and provide important guidance for future experimental investigations. As next-generation spectroscopy techniques continue to advance, charge-radius measurements are expected to become valuable constraints for testing competing RMF parameterizations and improving the description of nuclear structure in the superheavy region.

5. Comparison with Non-Relativistic Approaches and Experiment

Non-relativistic Skyrme-Hartree-Fock-Bogoliubov calculations, using parametrizations such as SLy4, SkM*, and UNEDF variants, broadly corroborate the RMF finding that Z = 114 is not a uniquely preferred spherical proton magic number, with several Skyrme functionals instead favouring Z = 120 or Z = 126 depending on the treatment of the spin-orbit and tensor terms in the functional [10,11]. Macroscopic-microscopic (finite-range droplet model plus Strutinsky shell correction) calculations, historically the source of the Z = 114, N = 184 island-of-stability prediction, remain broadly consistent with self-consistent mean-field results for the neutron shell closure near N = 184 but show larger discrepancies for the proton shell closure, reflecting the greater sensitivity of proton shell structure to the detailed treatment of the Coulomb potential and the diffuseness of the nuclear surface in the superheavy region [12,13]. Experimentally, decay spectroscopy of nuclei up to oganesson (Z = 118) shows alpha-decay energy systematics broadly consistent with the presence of enhanced stability associated with the N = 162 deformed sub-shell, but direct experimental access to the predicted spherical doubly magic region near Z = 120, N = 172–184 remains beyond current synthesis capability, leaving the central prediction of this line of theoretical work experimentally untested [14,15].

Taken together, the results presented in Sections 4 and 5 indicate that while the qualitative picture of shell-stabilised superheavy nuclei is robust and essentially undisputed across all mean-field frameworks considered, the quantitative details necessary to pinpoint a single, unique doubly magic superheavy nucleus are not yet converged. This situation is reminiscent of, though more pronounced than, the shell-evolution uncertainties discussed in lighter neutron-rich systems, and reflects the compounding of Coulomb, isospin, pairing, and deformation effects that are each individually significant in the superheavy region and that interact with one another in ways not fully captured by any single theoretical framework in isolation.

6. Limitations and Future Scope

Though the current work offers a detailed evaluation of baseline characteristics of superheavy nuclei in the relativistic mean-field theory, several shortcomings must be admitted. The computations were carried out based on the assumption of axial symmetry, and triaxial deformation can additionally reduce the overall energy of chosen superheavy configurations and can change the predicted equilibrium shapes and shell structures slightly. Similarly, dynamic associations beyond the mean-field approximation, like, quadrupole vibrations and mixing in the rotational configurations, were not explicitly taken into account and can add binding energy to the system, especially in systems that are not in closed shells. Moreover, due to the current analysis, ground-state properties were studied mainly, and to obtain a more comprehensive description of superheavy nuclei, multidimensional calculations of the fission pathway that take into account high-order multipole and octupole deformation degrees of freedom would be required to determine the spontaneous-fission half-lives correctly.

Therefore, future studies must incorporate triaxial deformations, dynamic correlations, and the inclusion of improved fission barrier calculations in the framework of covarians are covariants. As new advances are made in computational techniques and as precision data become available from the synthesis of novel super-heavy elements, there will be even stricter restrictions imposed on theoretical approaches. This is hoped to help resolve any uncertainties with shell closure predictions and help in a more accurate determination of the island of stability, thus facilitating future experiments aimed at expanding the nuclear chart.

7. CONCLUSION

The current study is a study of the properties of the ground state of superheavy nuclei within the framework of RMF with density-dependent pairing interactions in order to predict the island of stability's location. The results of the analysis showed that RMF models yield a consistent microscopic description of several nuclear observables, including binding energies, shell closures, deformation effects, pairing effects, charge radius, and fission barrier height. Binding energy predictions agreed well with the known experimental data on already synthesized superheavy elements, which proves that RMF theory works properly in the case of nuclei located in the far-right part of the nuclear chart. The results have also shown that the proton shell closures depend on a particular model parameterization being Z = 120 or Z = 126 being the options, while there is a better consensus about the value of neutron shell closures, with N = 184 and N = 172 being other options in certain density-dependent interactions. Moreover, the paper has pointed out the significant effect of nuclear deformation, shell effects, and pairing correlations on the stability of superheavy systems, and their combined effect in the determination of fission barriers and ground-state properties. Altogether, the results indicate that, despite the success of RMF calculations in reproducing most of the known properties of superheavy nuclei, there remain uncertainties related to effective interactions that have an impact on the predictions of the next doubly magic nucleus. Even more detailed development of covariant energy density functionals along with future experimental observations of even larger nuclei than Z = 118 will be essential to limiting theoretical models and enhancing predictions of the island of stability. Such developments will lead to a better knowledge of nuclear structure at the boundaries of stability and will contribute to the exploration of new superheavy elements.

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