Production cross sections of superheavy elements: insights from the dinuclear system model with high-quality microscopic nuclear masses

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Abstract

To accurately predict the synthesis cross sections of unknown superheavy elements and identify the optimal projectile-target combinations and evaporation channels at specific bombarding energies, we incorporate high-quality microscopic nuclear masses (HQMNM) into the dinuclear system (DNS) model for calculations; these masses are obtained from a Skyrme energy-density-functional fit to measured α-decay energies [Phys. Lett. B 851 (2024) 138578]. Because the DNS model is highly sensitive to Q-values, binding energy, shell correction energy, pairing energy, and separation energy, adopting precise nuclear masses is essential. Calculations for hot-fusion reactions reproduce existing experimental data and surpass the accuracy achieved with the finite-range droplet model (FRDM12).

A benchmark calculation for the hot-fusion reaction ^{48}Ca + ^{243}{Am} $\rightarrow$ ^{291}Mc* was performed to quantify the influence of the HQMNM on capture, fusion, and evaporation probabilities. Based on this reference, systematic calculations within the DNS model incorporating the HQMNM are extended to other hot-fusion systems and compared with available experimental excitation functions, demonstrating the model' s superior predictive power.

We further systematically evaluate all viable projectile–target combinations for synthesizing elements 119 and 120. Predicted evaporation residue cross sections, optimal excitation energies, and favored decay channels are presented, including ($^{\{50\}\mathrm{Ti}(}${249}Bk,3n)^{296}119) with (*{ER} = 5.16 fb) at (E^{}{CN} = 36 MeV), and ($^{\{50\}Ti(}${249}Cf,3n)^{296}120) with (* {ER} = 4.35 fb) at (E^{}{CN} = 34 MeV). These results offer quantitative guidance for future experiments.

Full Text

Preamble

Production Cross Sections of Superheavy Elements: Insights from the Dinuclear System Model with High-Quality Microscopic Nuclear Masses

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To accurately predict the synthesis cross sections of unknown superheavy elements and identify optimal projectile-target combinations and evaporation channels at specific bombarding energies, we incorporate high-quality microscopic nuclear masses (HQMNM) into the dinuclear system (DNS) model for our calculations. These masses are obtained from a Skyrme energy-density-functional fit to measured α-decay energies [Phys. Lett. B 851 (2024) 138578]. Because the DNS model is highly sensitive to Q-values, binding energy, shell correction energy, pairing energy, and separation energy, adopting precise nuclear masses is essential. Calculations for hot-fusion reactions reproduce existing experimental data and surpass the accuracy achieved with the finite-range droplet model (FRDM12). A benchmark calculation for the hot-fusion reaction 48Ca + 243Am $\rightarrow$ 291Mc$*$ was performed to quantify the influence of HQMNM on capture, fusion, and evaporation probabilities. Based on this reference, systematic calculations within the DNS model incorporating HQMNM are extended to other hot-fusion systems and compared with available experimental excitation functions, demonstrating the model's superior predictive power. We further systematically evaluate all viable projectile-target combinations for synthesizing elements 119 and 120. Predicted evaporation residue cross sections, optimal excitation energies, and favored decay channels are presented, including 50Ti(249Bk, 3n)296119 with σER = 5.16 fb at E$*$CN = 34 MeV and 50Ti(249Cf, 3n)296120 with σER = 4.35 fb at E$*$CN = 36 MeV. These results offer quantitative guidance for future experiments.

Keywords: dinuclear system model; superheavy nuclei; nuclear mass; synthesis cross section; potential energy surface

Introduction

The synthesis of superheavy elements (SHEs) with atomic numbers 119 and 120 represents a major frontier in modern nuclear physics [1–3]. Creating these elements is pivotal for initiating the eighth period of the periodic table and expanding the nuclear chart. The synthesis of superheavy nuclei (SHN) contributes to understanding the limits of nuclear existence and the properties of nuclear and atomic structures under extreme Coulomb force conditions, thereby validating existing theoretical models. Additionally, the fission of superheavy nuclei is crucial for astrophysical research on the rapid neutron-capture process (r-process) [4, 5].

The predominant experimental method for synthesizing SHN is fusion-evaporation reactions. Over the past few decades, significant progress has been achieved, with experiments employing cold or hot fusion reactions to create elements from 104 to 118 [6–12]. To synthesize unknown SHEs, China, Russia, Japan, Germany, and the USA have constructed or upgraded heavy-ion accelerators and spectrometer facilities, including CAFE2 and SHANS2 in Lanzhou, China [13]; DGFRS in Dubna, Russia [14]; GAERIS at RIKEN, Japan [15]; superSHIP at GSI, Germany [16]; and the 88-Inch Cyclotron at LBNL, USA [17]. Each country has also formulated plans for SHE synthesis.

The synthesis of SHEs is challenging due to limitations in projectile-target materials and extremely low synthesis cross sections, resulting in long experimental timelines and high costs. Therefore, it is essential to systematically calculate the excitation functions of evaporation residue cross sections for superheavy nuclei synthesis using theoretical models before conducting experiments. This provides experimentalists with optimal projectile-target combinations, the most suitable beam energies, and synthesis cross sections for reference.

Various theoretical models are available for studying the synthesis mechanism of superheavy nuclei, including the time-dependent Hartree-Fock (TDHF) model [18–20], improved quantum molecular dynamics models (ImQMD) [21–23], multidimensional Langevin equations [24, 25], and the DNS model [26–30]. This work employs the DNS model to predict the synthesis cross sections of new superheavy elements. The DNS model offers a clear physical picture that closely resembles the actual process of heavy-ion collisions and can self-consistently account for important factors such as dynamic energy dissipation, nucleon transfer, fission, quasi-fission, shell effects, pairing effects, and dynamic deformation [27, 31–37]. However, DNS model calculations are highly dependent on basic nuclear data, including nuclear masses, deformations, shell and pairing corrections, interaction potentials, Coulomb barriers, and fission barriers. This paper primarily investigates the dependence of DNS model results on nuclear masses.

Within the DNS framework, the Q-values, binding energies, and neutron separation energies derived from nuclear masses directly influence calculations of capture cross sections, fusion probabilities, and survival probabilities. Nuclear masses encompass a wealth of information about the nucleus, including symmetry energy, pairing corrections, shell corrections, and deformation energy, all of which affect the accuracy of superheavy element predictions. Moreover, different nuclear mass models provide somewhat different mass data tables, especially for unknown nuclei. Our previous work discussed the impact of nuclear masses on fusion probability calculations [38]. This paper focuses on using high-quality microscopic nuclear masses (HQMNM) [39, 40] to predict the synthesis cross sections of new superheavy elements within the DNS model and compares the results with those from four other nuclear mass models [38]: FRDM12 [41], WS4 [42], KUTY [43], and HFB02 [44].

The structure of this article is as follows: Section II provides a concise overview of the DNS model. Section III presents the computational findings and discussions. Finally, Section IV summarizes the key conclusions.

II. Model Description

Based on the DNS model, the evaporation residue cross section for SHE can be expressed as

$$\sigma_{ER}(E_{c.m.}) = \frac{2\mu}{E_{c.m.}} \sum_{J=0}^{J_{max}} (2J+1) T(E_{c.m.}, J) \times P_{CN}(E_{c.m.}, J) W_{sur}(E_{c.m.}, J).$$

Here, $T(E_{c.m.}, J)$ is the penetration probability—the probability of the colliding system overcoming the Coulomb barrier [26]. $P_{CN}(E_{c.m.}, J)$ is the fusion probability [45, 46]. $W_{sur}(E_{c.m.}, J)$ is the survival probability of the highly excited compound nucleus, which survives by evaporating light particles against fission.

The penetration probability $T(E_{c.m.}, J)$ is derived using the Hill-Wheeler formula [47] with a barrier distribution function, written as

$$T(E_{c.m.}, J) = \int f(B) dB \frac{1}{1 + \exp\left[\frac{2\pi(B + E_{rot}(J) - E_{c.m.})}{\hbar\omega(J)}\right]}.$$

Here $\hbar\omega(J)$ is the width of the parabolic barrier at $R_B(J)$. The normalization constant is $\int f(B) dB = 1$. The Coulomb barrier distribution is taken as an asymmetric Gaussian formula [49, 50]. The nucleus-nucleus potential is calculated by the double-folding method [45, 46, 51]. The Coulomb potential is evaluated using Wong' s formula [52].

In the fusion stage, the formation probabilities of fragments $P(Z_1, N_1, E_1)$ are estimated by solving a set of master equations [45, 53, 54]:

$$\frac{dP(Z_1, N_1, E_1, t)}{dt} = \sum_{Z_1', N_1'} W_{Z_1, N_1; Z_1', N_1'}(t) \times \left[d_{Z_1', N_1'} P(Z_1', N_1', E_1', t) - d_{Z_1, N_1} P(Z_1, N_1, E_1, t) \right].$$

Here, $W_{Z_1,N_1;Z'_1,N'_1}$ is the mean transition probability from the channel (Z_1, N_1, E_1) to (Z'_1, N'_1, E'_1), and d_{Z_1,N_1} denotes the microscopic dimension corresponding to the macroscopic state (Z_1, N_1, E_1). The summation runs over all possible proton and neutron numbers accessible to the fragment (Z'_1, N'_1); within the model, however, only one-nucleon transfer is allowed at a time, so the allowed values are restricted to $Z'_1 = Z_1 \pm 1$ and $N'_1 = N_1 \pm 1$. The E_1 is the local excitation energy ε^*_1 of fragment A_1, generated by energy dissipation from the relative motion [55]. The sticking time is derived by the parametrization method of the classical deflection function [56].

The potential energy surface (PES) of the DNS is derived by

$$U_{dr}(\{\alpha\}, J) = B_1 + B_2 - B_{CN} + V_{CN}(\alpha) + E_{rot}(J).$$

Here, $\{\alpha\}$ stands for $\{r, \beta_1, \beta_2, \theta_1, \theta_2\}$, which represent the surface distance, quadrupole deformation, and collision orientations of the colliding partners, respectively. B_i $(i = 1, 2)$ and B_{CN} are the negative binding energies of the fragment A_i and the compound nucleus A_{CN}, respectively, which are taken from nuclear mass tables [39, 57]. $E_{rot}(J)$ is the rotational energy of the compound nucleus.

The DNS model posits that all fragments capable of surpassing the Businaro-Gallone (BG) point can undergo fusion. Hence, the fusion probability can be written as

$$P_{CN}(E_{c.m.}, J) = \sum_{Z=0}^{Z_{BG}} \sum_{N=0}^{N_{BG}} P(Z, N, E', \tau_{int}(B_{in}, J)).$$

Here Z_{BG} and N_{BG} are the proton and neutron numbers at the BG point. B_{in} is the potential energy at the potential pocket bottom. $\tau_{int}(B_{in}, J)$ is the sticking time with given angular momentum J and Coulomb barrier B_{in}.

The excited compound nucleus would be de-excited by evaporating γ-rays, neutrons, protons, α-particles, etc., against fission. The survival probability of the evaporation channels with x neutrons, y protons, and z α-particles is evaluated by a statistical evaporation model based on Weisskopf' s evaporation theory, expressed as [53, 54, 58, 59]:

$$W_{sur}(E^*_{CN}, x, y, z, J) = P(E^*_{CN}, J) \prod_i \frac{\Gamma_n(E^*_i, J)}{\Gamma_{tot}(E^*_i, J)} \times \prod_j \frac{\Gamma_p(E^*_j, J)}{\Gamma_{tot}(E^*_j, J)} \times \prod_k \frac{\Gamma_\alpha(E^*_k, J)}{\Gamma_{tot}(E^*_k, J)},$$

where E^*_{CN} and J are the excitation energy and spin of the compound nucleus, respectively. The total width Γ_{tot} is the sum of partial widths for particle emission, γ-ray emission, and fission. $P(E^*_{CN}, J)$ is the realization probability of evaporation channels. The $\Gamma_n(E_i^*, J)$, $\Gamma_p(E_j^*, J)$, and $\Gamma_\alpha(E_k^*, J)$ are the decay widths for neutrons, protons, and α-particles, respectively, which are evaluated using the single-particle level density [60]. The fission width $\Gamma_f(E^*, J)$ is calculated using the Bohr-Wheeler formula [45, 46, 61].

The J-dependent fission barrier incorporates both macroscopic and microscopic contributions:

$$B_f(E^*, J) = B_f^{LD}(E^* = 0, J)\exp(-E^*/E_D) + B_M - \Delta E_{rot}(J),$$

where the macroscopic component B_f^{LD} derives from the liquid-drop model [62]. Microscopic shell correction energies were adopted from [41], with shell-damping energy $E_D = 5.48A^{1/3}/(1 + 1.3A^{-1/3})$ MeV. $\Delta E_{rot}(J)$ is the difference between the ground-state rotational energy and the saddle-point rotational energy of the compound nucleus in a spin-J state. Angular-momentum effects during survival are also reflected in the level density when collective motion is taken into account, which is applied in the calculation of the decay width $\Gamma(E^*, J)$.

III. Results and Discussions

presents the Q-values and Bass potential energies for reactions synthesizing elements 110 to 120, based on three nuclear mass models: HQMNM, FRDM12, and WS4. The differences provided by the various mass tables are within 3 MeV.

[Figure 1: see original paper] compares the mass excess and neutron separation energies from HQMNM and FRDM12. Panel (a) shows the mass excess for superheavy nuclei (SHN) with atomic numbers 110 to 120, represented by discrete points and lines. The hollow black squares, red circles, green upward triangles, blue downward triangles, cyan diamonds, magenta left triangles, dark yellow right triangles, dark blue hexagons, purple stars, burgundy pentagons, and olive crosses (with solid lines of the same color) represent isotopes of elements 110 to 120, respectively. Panels (b) through (f) display the separation energies for 1n to 5n channels, respectively. The red and black solid lines represent the isotopic masses of elements 120 and 119 from the FRDM12 mass table, while the solid red squares and black dots represent the isotopic masses of elements 120 and 119 from the HQMNM mass table, respectively. Panel (a) shows that the excess mass provided by HQMNM is generally greater than that of FRDM12. There are significant differences in separation energies between the two mass tables, with odd-neutron separation energies exhibiting a pronounced odd-even effect. Comparing the excess masses of superheavy isotopes from the two tables reveals that in the neutron-rich region, HQMNM provides larger separation energies, while in the proton-rich region, FRDM12 provides larger separation energies. These differences in separation energies will be reflected in the survival probabilities of superheavy nuclei, while differences in the absolute values of excess mass will manifest in the fusion probabilities.

presents predictions of maximum production cross sections for SHEs via HQMNM, compared with other nuclear mass models (FRDM12, WS4, KUTY, and HFB02), based on the dinuclear system model. The table lists the peak cross sections and corresponding optimal excitation energies for various reactions.

[Figure 2: see original paper] illustrates the neutron separation energies of 291Mc based on three mass tables (HQMNM, FRDM12, and WS4), along with the corresponding survival probabilities calculated using the statistical model. The black solid lines represent results based on FRDM12, the blue dotted lines indicate results based on WS4, and the red dashed lines represent results based on HQMNM. Panel (a) shows that the neutron separation energies for 291Mc are ordered from largest to smallest as FRDM12, WS4, and HQMNM. Neutron separation energy quantifies the energy required to remove a neutron from the compound nucleus; larger separation energy makes neutron evaporation less probable and consequently increases survival probability. Panel (b) shows the 1n–5n evaporation survival probabilities for excited 291Mc$*$, ordered according to the mass predictions of HQMNM, WS4, and FRDM12.

Although the capture probability itself is independent of the nuclear mass model, the choice of mass table shifts the calculated Q-value, thereby translating the excitation-energy distribution of the capture cross section along the energy axis, as illustrated in Figure 3: see original paper. The Q-values from the three mass tables FRDM12, HQMNM, and WS4 are -164.98 MeV, -165.97 MeV, and -168.23 MeV, respectively. The capture cross section distributions, from left to right, are based on calculations using FRDM12, HQMNM, and WS4. In [Figure 3: see original paper], the black solid line, red dashed line, and blue dotted line represent results based on FRDM12, HQMNM, and WS4, respectively. Differences in binding energy among the mass tables affect the calculation of the potential energy surface, resulting in different inner fusion barriers. For the reaction 48Ca + 243Am $\rightarrow$ 291Mc$*$, the inner fusion barriers are 9.53 MeV with FRDM12, 9.53 MeV with HQMNM, and 10.41 MeV with WS4. Consequently, the fusion probability distributions obtained with FRDM12 and HQMNM almost coincide in Figure 3: see original paper, whereas the WS4 result is visibly lower. Note that the HQMNM table provides only partial mass data for superheavy nuclei (Z = 110–120); masses outside this range are taken from experiment or FRDM12. Ultimately, combining the data from the three stages yields the excitation function of the evaporation residue cross section, whose 2n–5n channel excitation functions are shown in Figure 3: see original paper-(f) and compared with experimental data. The calculated results based on the three mass tables are in good agreement with experimental data, each differing within an order of magnitude. Among them, the results based on HQMNM are slightly larger than those based on the other two mass tables, due to its larger survival probability.

[Figure 3: see original paper] provides a detailed discussion of the impact that different nuclear mass tables have on the calculations of capture, fusion, and survival for the specific hot-fusion reaction system 48Ca + 243Am $\rightarrow$ 291Mc$*$.

To further validate the performance of the mass tables, we systematically calculated the evaporation residue cross sections for nine hot-fusion reactions (48Ca + 238U, 237Np, 242,244Pu, 243Am, 245,248Cm, 249Bk, 249Cf) based on five mass tables (HQMNM, FRDM12, WS4, KUTY, HFB02) and compared them with experimental data. lists the peak values of the calculated evaporation residue cross sections and the corresponding experimental values. To highlight the impact of the mass model, [Figure 4: see original paper] displays the calculated evaporation-residue excitation functions using only FRDM12 (solid lines) and HQMNM (dashed lines). Overall, the calculations agree well with experiment, with HQMNM-based results providing a slightly closer match than those obtained with FRDM12. The relative heights of the excitation functions predicted by FRDM12 and HQMNM shift as the excitation energy changes. The HQMNM curve reproduces the measured data more accurately, reflecting the fact that this mass table is directly constrained by experimental α-decay energies and therefore provides more reliable absolute and relative values.

Guided by the five mass tables that best reproduce the available data, we have evaluated the evaporation-residue (ER) cross sections for ten reactions aimed at synthesizing elements 119 and 120: 50Cr + 249Bk, 51V + 248Cm, 54Cr + 243Am, 55Mn + 244Pu, 58Fe + 237Np, 50Ti + 249Cf, 51V + 249Bk, 54Cr + 248Cm, 55Mn + 243Am, and 58Fe + 244Pu. The corresponding peak ER cross sections are collected in , and the excitation functions obtained with HQMNM and FRDM12 are compared in [Figure 5: see original paper]. In [Figure 5: see original paper], line color distinguishes the neutron-evaporation channels (xn), while line style denotes the mass table employed.

For element-119 synthesis, the HQMNM-based peak cross sections span 3.07–23.7 fb across the five reaction systems considered. However, the predicted 23.7 fb cross section for the 58Fe(237Np,3n)292119 channel is unreliable. For the 58Fe + 237Np system, the HQMNM cross sections exceed the FRDM12 values by roughly one order of magnitude. This discrepancy arises because the HQMNM neutron-separation energy is lower, which increases the survival probability. The underlying cause is that the relevant nuclei lie outside the region where HQMNM masses are experimentally constrained. Our calculations identify the most promising reactions for producing element 119 via the 3n channel: 54Cr + 243Am → 294119 with σER = 4.64 fb at E∗CN = 34 MeV; 50Ti + 249Bk → 296119 with σER = 5.16 fb at E∗CN = 36 MeV; 55Mn + 248Cm → 296119 with σER = 3.63 fb at E∗CN = 36 MeV; and 55Mn + 244Pu → 296119 with σER = 3.07 fb at E∗CN = 36 MeV. All four predicted cross sections lie within a factor of two of one another.

For element-120 synthesis, the peak distribution range of the five reaction systems based on HQMNM is from 0.09 to 4.35 fb. The synthesis cross sections vary considerably across different projectile-target combinations. Based on the cross-section values, the reaction systems are recommended in descending order as follows: 50Ti(249Cf,3n)296120 with σER = 4.35 fb at E∗CN = 34 MeV; 55Mn(243Am,3n)295120 with σER = 2.19 fb at

E∗CN = 34 MeV; 51V(249Bk,3n)297120 with σER = 1.78 fb at E∗CN = 36 MeV; 58Fe(244Pu,3n)299120 with σER = 0.17 fb at E∗CN = 34 MeV; and 54Cr(248Cm,3n)299120 with σER = 0.09 fb at E∗CN = 34 MeV.

IV. Conclusions

To accurately predict the synthesis cross sections of superheavy elements 119 and 120, identify optimal projectile-target combinations, and determine optimal collision energies, we have employed the DNS model incorporating the HQMNM nuclear mass table and compared results with four additional nuclear-mass models. Separate analyses of the capture, fusion, and survival stages reveal that: (1) The capture cross section itself is insensitive to the mass table; only the excitation energy assigned to a given capture cross section shifts. (2) The mass model changes the potential-energy surface, thereby altering fusion probabilities. (3) Most critically, even modest variations in calculated neutron-separation energy among mass tables translate into large differences in survival probability.

By accounting for the influence of nuclear masses on capture, fusion, and survival, we can predict their combined effect on the evaporation-residue cross section. Using the HQMNM mass table, we evaluated nine hot-fusion reactions and found significantly better agreement with experiment than obtained with four alternative mass models. Building on this success, we employed the same nuclear mass table to compute cross sections for ten prospective reactions leading to elements 119 and 120. The resulting peak cross sections and corresponding excitation energies are collected in . The most favorable two paths to element 119 are 54Cr + 243Am → 294119 and 50Ti + 249Bk → 296119, with maxima of \$ \$3n = 4.64 fb at E∗CN = 34 MeV and \$ \$3n = 5.16 fb at E∗CN = 36 MeV, respectively. The most favorable path to element 120 is 50Ti(249Cf,3n)296120 with σER = 4.35 fb at E∗CN = 34 MeV. We hope these results will guide experimental efforts aimed at synthesizing superheavy elements.

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