Investigation of octupole effects in superheavy nuclei with improved potential-energy-surface calculations

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It has been found that high-order deformation (e.g. β_6) can have important effects on the structures of superheavy nuclei. In the present work, we investigate octupole deformation effects on superheavy nuclei with an improved potential-energy-surface (PES) calculation by including reflection-asymmetric deformations in a space of $(\beta_2, \beta_3, \beta_4, \beta_5)$. The calculations give various deformations including highly deformed ($\beta_2 \approx 0.4$) and superdeformed ($\beta_2 \approx 0.7$) shapes. The octupole-deformation degree of freedom mainly affects the fission barrier beyond the second minimum of PES.

octupole correlation, Woods-Saxon potential, potential energy surface, Lipkin-Nogami approach, energy curves

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Experimentally, octupole correlation manifests itself in atomic nuclei usually with enhanced $E1$ transitions connecting interleaved positive and negative-parity bands, which is similar to the rotational bands observed in reflection-asymmetric molecules [1]. Such correlation originates from the coupling of a pair of single-particle orbitals close to the Fermi Surface and having $\Delta N = 1$, $\Delta l = 3$ and $\Delta j = 3$. Favorable N or Z numbers for the occurrence of octupole correlations include 34 ($g_{9/2} \otimes p_{3/2}$ coupling), 56 ($h_{11/2} \otimes d_{5/2}$ coupling), 88 ($i_{13/2} \otimes f_{7/2}$ coupling), 134 ($j_{15/2} \otimes g_{9/2}$ coupling) [1] (These numbers locate just above the closed shells, implying weak quadrupole deformations). The octupole interaction can be so strong that there exist nuclei having static reflection-asymmetric deformation, such as ^{224}Ra [1]. In addition, it has been found that rotation can stabilize octupole deformation [2–4].

There have been many examples of the coexistence of normal, super- and hyper-deformation in nuclei [5]. Octupole correlations are also expected to occur in superdeformed (SD) nuclei. Calculations suggest that the

superdeformed minima are soft with respect to octupole deformations in $A \sim 40$, $A \sim 150$ and $A \sim 190$ mass regions [6–8]. This is because the single-particle spectrum at superdeformations favors octupole excitations due to the presence of intruder states [2]. Experiments have identified some octupole-vibrational states and strong $E1$ transitions which are expected to connect these vibrational levels to the lowest SD band [7–10].

With the development of the radioactive beam facility, heavy-ion accelerator and highly-effective detector systems [11, 12], great progress has been made recently in nuclear physics including the synthesis of superheavy nuclei [13–15]. The deformations of superheavy nuclei are interesting. Superdeformed prolate [16–18] and superdeformed oblate [19] shapes have been predicted. In our previous works [20, 21], we discussed the β_6 effects in superheavy nuclei [20] and the β_3 effects on high-K states at the second well of actinide nuclei [21]. In the present paper, using an improved potential-energy-surface (PES) with the inclusion of reflection-asymmetric β_3 and β_5 deformations, we systematically calculate $^{248-264}\text{No}$, $^{254-268}\text{Rf}$, $^{258-272}\text{Sg}$, $^{264-276}\text{Hs}$, $^{268-278}\text{Ds}$ and $^{278-284}\text{Cn}$ isotopes. These nuclei have already been synthe-

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sized experimentally (<http://www.nndc.bnl.gov/chart/>).

1 The model

The PES method applied here is based on macroscopic-microscopic model [22]. The total potential energy, which is calculated as a function of shape, proton number Z , and neutron number N , is the sum of a macroscopic term and a microscopic term representing the shell correction [22, 23]. The macroscopic term changes smoothly as a function of particle number and deformation. The microscopic term can have rapid fluctuation with changing deformation and particle number. The total energy $E_{\text{total}}(Z, N, \hat{\beta})$ of a nucleus (Z, N) at the deformation $\hat{\beta}$ can be written as [22, 24]

$$E_{\text{total}}(Z, N, \hat{\beta}) = E_{\text{mac}}(Z, N, \hat{\beta}) + \delta E_{\text{shell}}(Z, N, \hat{\beta}), \quad (1)$$

where E_{mac} and δE_{shell} are for the macroscopic and microscopic energies, respectively. The macroscopic energy is obtained from the standard liquid-drop model [25]. The single-particle levels is derived from the axially deformed Woods-Saxon potential with the set of universal parameters [26]. The pairing correlation is treated using the Lipkin-Nogami (LN) approach [27, 28] in which the particle number is conserved approximately and thus the spurious pairing phase transition encountered in the usual BCS calculation can be avoided. The monopole pairing strength G is determined by the average gap method [29, 30]. After solving the LN equations in a sufficiently large space of Woods-Saxon single-particle states, the LN pairing energy can be given by [22, 24]

$$E_{\text{LN}} = \sum_k 2v_k^2 e_k - \frac{\Delta^2}{G} - G \sum_k v_k^4 + G \frac{N}{2} - 4\lambda_2 \sum_k u_k^2 v_k^2, \quad (2)$$

where v_k^2 , e_k , Δ and λ_2 represent the occupation probabilities, single-particle energies, pairing gap and number-fluctuation constant, respectively. The shell correction energy is then calculated by $\delta E_{\text{shell}} = E_{\text{LN}} - \tilde{E}_{\text{Strut}}$, where $\tilde{E}_{\text{Strut}}$ is obtained by the Strutinsky method [31, 32] with a smoothing range $\gamma = 1.20\hbar\omega_0$ ($\hbar\omega_0 = 41/A^{1/3}$ MeV), and a correction polynomial of order $p = 6$. The pairing-deformation self-consistent PES is obtained in the multi-dimensional deformation space $(\beta_2, \beta_3, \beta_4, \beta_5)$ and the nuclear equilibrium deformation is determined by minimizing the PES.

2 Calculations and discussions

Our calculations with nonaxial deformation show that the nuclei which we investigated have $\gamma \approx 0^\circ$ at both the normal deformed and superdeformed minima. Therefore, we restrict ourselves to axially symmetric shapes and perform the numerical calculations on a four-dimensional lattice of β_2 , β_3 , β_4 and β_5 . The β_2 , β_3 , β_4 and β_5 deformations vary as independent shape parameters, which differs from previous calculations where β_5 was obtained by an approximation [33].

We calculate (13, 13, 7, 7) points for $(\beta_2, \beta_3, \beta_4, \beta_5)$ deformations, respectively. Then the numerical calculated energies are interpolated using cubic spline function between the lattice points. Therefore, the effects of different shape degrees of freedom on nuclear structure can be investigated by means of the multi-dimensional PES.

We have investigated the octupole effects of 42 superheavy nuclei ranging from ^{248}No to ^{284}Cn which have already been synthesized. As an example, the PES for ^{250}No is shown in Figures 1 and 2 for 2D and 3D plots, respectively. From the two figures, it is seen that there are two deep minima: one at normal deformation with $\beta_2 \approx 0.2$ and another at superdeformation with $\beta_2 \approx 0.7$. The quadrupole deformation values corresponding to the two deep minima are in good agreement with other calculations by Möller et al. [24] and Ren et al. [16]. Compared with the superdeformed states in $A \sim 40$, $A \sim 150$ and $A \sim 190$ mass regions [6–8] where they are relatively soft against octupole deformation, the PES of ^{250}No is stiff against β_3 deformation. In addition, our calculations predict a shallow octupole minimum at $\beta_2 \approx 1.15$ and $\beta_3 \approx 0.25$. The existence of this minimum could affect the fission

Figure 1 Calculated ground-state potential energy surface for the nucleus ^{250}No . The energy difference between neighboring contours is 500 keV. At each given (β_2, β_3) point, the PES has been minimized with respect to the deformation parameters of β_4 and β_5 . The PES is reflection-symmetric about $\beta_3 = 0$.

Figure 2 Calculated 3D ground-state potential energy surface for the nucleus ^{250}No , as a function of β_2 and β_3 . At each given (β_2, β_3) point, the PES has been minimized with respect to the β_4 and β_5 deformation parameters.

Figure 3 Comparison of calculated energy curves with (black curves) and without (red curves) octupole correlations for even-even $102 \leq Z \leq 112$ superheavy isotopes as the function of quadrupole deformation β_2 . At each given β_2 point, the PES has been minimized with respect to the deformation parameters of β_3 , β_4 and β_5 . For a better display of comparison, we shift the curves without octupole deformation by +5 MeV.

trajectory of the superheavy nucleus, similar to the situation in ^{240}Pu [34].

To investigate shape evolutions and octupole effects in the superheavy region, we systematically plot the potential energy curves as the function of β_2 for all the calculated nuclei in Figure 3. The β_2 deformations of the first minima (at normal deformation) and its evolution agree with the calculations by Möller et al. [24]. In the lower-left part of Figure 3, one can see that some light No, Rf and Sg nuclei have superdeformed minima with energies close to those of the normal deformed minima. This is consistent with the prediction by Ren et al. [16]. These nuclei could be the good candidates for studying superdeformations in superheavy nuclei. With increasing neutron number N and/or proton number Z , the superdeformed minima at $\beta_2 \approx 0.7$ become shallow and disappear finally. It is noted that octupole effects on both normal-deformed and superdeformed minima are weak. However, it can be seen that the octupole correlation pulls energy curves down in the region beyond superdeformed minima as compared with those calculated without reflection-asymmetric deformations. This is consistent with the calculation for the nucleus $^{292}118$ by Muntian et al. [35]. The octupole effect can be strong enough to produce the octupole minimum in nucleus such as ^{250}No (see Figure 1). Figure 3 also shows that highly-deformed $\beta_2 \approx 0.4$ minima develop in heavier Ds and Cn isotopes.

3 Conclusions

In conclusion, octupole correlation properties for even-even

nuclei with $102 \leq Z \leq 112$ have been investigated using an improved PES method with the inclusion of reflection-asymmetric deformations. The calculated PESs show superdeformations at $\beta_2 \approx 0.7$ for light No, Rf, and Sg nuclei, and highly deformed minima at $\beta_2 \approx 0.4$ for heavier Ds and Cn isotopes. Octupole effect is significant in light No and Rf isotopes after the second minima.

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