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Shape coexistence in even-even superheavy nuclei

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The structures of the even-even superheavy nuclei with proton number $Z=100$–114 are systematically investigated using self-consistent relativistic mean-field theory. The calculated binding energies are in good agreement with all available experimental data. The experimental alpha decay energies and lifetimes of the newly discovered superheavy nuclei are also reasonably reproduced by the model. Large scale calculations with a quadrupole moment constraint clearly show the variation of energy with the quadrupole deformation parameter. It reliably demonstrates that there is shape coexistence in superheavy nuclei. In some cases the configuration with superdeformation may be the ground state of superheavy nuclei near $Z=114$ and $N=174$.

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For a long time it was believed that the existence of superheavy nuclei is due to their spherical shell structure. However, it is known experimentally that the heavy nuclei of the actinium series ($Z=93$–103) are well deformed. This fact strongly suggests that deformed configurations are as important as the spherical one for stability of superheavy nuclei. Bohr and Mottelson [1] also pointed out that deformation can increase the stability of the heavy nuclei. In this communication we study the ground state properties of all known even-even superheavy nuclei ($Z=100$–116) [2–7] and their neighboring nuclei. We put emphasis on the role of deformation on the structure of superheavy nuclei.

At present, although there exist some self-consistent mean-field calculations on superheavy nuclei [8–12], a systematic comparison between theoretical binding energies and experimental data is still missing due to the fast growth of this new field [2,4,5]. This comparison is needed to test the reliability of the nuclear models and is also useful in predicting unknown superheavy nuclei. The Frankfurt group suggested that one should test a model for a known nucleus $^{264}108$ before studying superheavy nuclei [13]. We extend their idea and test our model for all even-even nuclei with $Z=100$–108 where the experimental binding energy data are available. This approach can avoid the accidental agreement between model and experimental data that may occur for a single nucleus. This ensures the reliability of the systematic behavior of a model. Accordingly we first calculate the binding energies and alpha decay energies of known even-even nuclei with $Z=100$–108. Then we investigate the ground state properties of the newly discovered superheavy nuclei around $^{270}110$ [5], $^{288}114$ [3], and $^{292}116$ [4].

The theoretical results are listed in Tables I and II, where the deformed relativistic mean-field (RMF) codes in harmonic bases [10,11,14] are used. The force parameters TMA [10] and NLZ2 [9] are treated as input, and the number of bases is chosen to be $N_f=N_b=20$. The inputs for the pairing gaps are $\Delta_n=\Delta_p=11.2/\sqrt{A}$ MeV. An axial deformation is assumed in all calculations. For the details of the calculations please see the relevant publications [10,11,14,15].

In Tables I and II, the first column is for nuclei. B_{theor} is the theoretical binding energy. R_p and R_n are the root-mean-square radii for the proton- and neutron-density distributions, respectively. The symbols β_n and β_p in Tables I and II denote the quadrupole deformations of neutrons and protons, respectively. Further, the symbols Q_α(theor) and Q_α(expt) are used for the calculated alpha-decay energies and experimental data. The experimental binding energies B_{expt} are obtained from the nuclear mass table [16] and the experimental alpha decay energies can be deduced accordingly. They are listed in the last two columns for comparisons.

It is seen from Table I that the theoretical binding energies are very close to the experimental data. The average difference between the theoretical binding energy and the experimental one is approximately 2 MeV. This corresponds to a relative difference of 0.1%. The maximum difference is 3.45 MeV for $^{264}108$ and it corresponds to a relative difference of 0.2%. Considering the predicting ability of the RMF model on the binding energy of spherical nuclei ^{16}O, ^{40,48}Ca, ^{90}Zr, ^{116,124}Sn, and ^{208}Pb is approximately 0.2%, we can say the RMF model works well for the binding energy of the superheavy nuclei studied here. The theoretical alpha decay energies agree well with the experimental ones within 1 MeV. This ensures the good predicting ability of the RMF model for the alpha decay properties. Calculations show that there is a prolate deformation in the ground state of these nuclei. In order to confirm the deformation, we have carried out a constraint calculation and found that this is really the ground state of this nucleus.

Table II is the RMF results with NLZ2 force. It is seen again that the theoretical results agree well with the experimental binding energies and alpha decay energies. The precision of the force NLZ2 is as good as the force TMA. A quadrupole deformation in the ground state of these nuclei is also obtained for NLZ2. Its value is close to that of TMA force. This indicates that the RMF model is stable in this mass range. All previous discussions on Table I hold true for Table II.

When we compare Tables I and II together, we notice that the experimental binding energy is between the theoretical value with TMA and that with NLZ2. It seems that the obtained value with TMA sets the upper limit of the binding energy and the obtained value with NLZ2 sets the lower limit. This is very useful for the prediction of properties of superheavy nuclei because both obtained values with TMA and NLZ2 are very close. Therefore the theoretical results can be used for a guide of future experiments of superheavy

TABLE I. The ground-state properties of even-even superheavy nuclei with $100\leqslant Z$ and $150\leqslant N$. The TMA force is used as input in the deformed RMF calculation. The last two columns are the experimental alpha decay energy and binding energy.

Nuclei	B_{theor} (MeV)	β_n	β_p	R_n	R_p	Q_α(theor)	Q_α(expt)	B_{expt} (MeV)
^{250}Fm	1867.01	0.26	0.27	6.15	5.96	7.59	7.56±0.01	1865.48±0.01
^{252}Fm	1880.07	0.26	0.27	6.17	5.97	7.18	7.16±0.01	1878.87±0.01
^{254}Fm	1892.47	0.26	0.27	6.19	5.98	6.80	7.31±0.01	1890.93±0.01
^{256}Fm	1903.71	0.26	0.26	6.21	5.99	7.03	7.03±0.01	1902.49±0.01
^{252}No	1873.17	0.26	0.27	6.15	5.98	8.59	8.55±0.01	1871.25±0.01
^{254}No	1887.22	0.26	0.27	6.17	5.99	8.09	8.24±0.02	1885.54±0.02
^{256}No	1900.69	0.26	0.27	6.19	6.00	7.68	8.57±0.01	1898.60±0.01
^{258}No	1912.85	0.26	0.27	6.21	6.01	7.92		
^{256}Rf	1892.63	0.25	0.26	6.17	6.01	8.84	8.96±0.03	1890.59±0.03
^{258}Rf	1906.98	0.26	0.27	6.20	6.02	8.54		
^{260}Rf	1919.99	0.23	0.23	6.21	6.02	9.00		
^{262}Rf	1932.67	0.22	0.22	6.23	6.03	8.48		
^{260}Sg	1911.85	0.25	0.26	6.20	6.04	9.08	9.93±0.04	1908.96±0.04
^{262}Sg	1925.90	0.25	0.26	6.22	6.06	9.38		
^{264}Sg	1939.26	0.22	0.23	6.23	6.06	9.03		
^{266}Sg	1952.40	0.22	0.22	6.25	6.07	8.57		
^{264}Hs	1930.17	0.24	0.25	6.23	6.07	9.98	10.54±0.30	1926.72±0.30
^{266}Hs	1944.46	0.24	0.24	6.24	6.08	9.74	10.18±0.02	
^{268}Hs	1958.42	0.22	0.23	6.26	6.09	9.14		
^{270}Hs	1971.80	0.22	0.22	6.28	6.10	8.90		
^{270}110	1961.39	0.22	0.22	6.26	6.11	11.34	11.03±0.05	

TABLE II. The ground-state properties of even-even superheavy nuclei with $100\leqslant Z$ and $150\leqslant N$. The NLZ2 force is used as input in the deformed RMF calculation. The last two columns are the experimental alpha decay energy and binding energy.

Nuclei	B_{theor} (MeV)	β_n	β_p	R_n	R_p	Q_α(theor)	Q_α(expt)	B_{expt} (MeV)
^{250}Fm	1863.65	0.30	0.31	6.27	6.04	7.71	7.56±0.01	1865.48±0.01
^{252}Fm	1876.03	0.30	0.31	6.30	6.06	7.75	7.16±0.01	1878.87±0.01
^{254}Fm	1887.90	0.30	0.31	6.32	6.07	7.24	7.31±0.01	1890.93±0.01
^{256}Fm	1899.60	0.29	0.30	6.35	6.08	6.43	7.03±0.01	1902.49±0.01
^{252}No	1870.69	0.30	0.32	6.27	6.07	7.86	8.55±0.01	1871.25±0.01
^{254}No	1884.14	0.30	0.32	6.30	6.08	7.81	8.24±0.02	1885.54±0.02
^{256}No	1896.98	0.30	0.31	6.33	6.09	7.35	8.57±0.01	1898.60±0.01
^{258}No	1909.53	0.30	0.31	6.35	6.11	6.67		
^{256}Rf	1890.73	0.30	0.32	6.30	6.10	8.26	8.96±0.03	1890.59±0.03
^{258}Rf	1904.50	0.30	0.31	6.33	6.11	7.94		
^{260}Rf	1917.87	0.30	0.31	6.35	6.13	7.41		
^{262}Rf	1930.84	0.29	0.30	6.38	6.14	6.99		
^{260}Sg	1909.01	0.30	0.31	6.33	6.14	10.02	9.93±0.04	1908.96±0.04
^{262}Sg	1923.35	0.29	0.30	6.35	6.15	9.45		
^{264}Sg	1937.25	0.29	0.30	6.38	6.16	8.92		
^{266}Sg	1950.47	0.28	0.29	6.40	6.17	8.67		
^{264}Hs	1926.63	0.28	0.29	6.35	6.17	10.68	10.54±0.30	1926.72±0.30
^{266}Hs	1941.35	0.28	0.29	6.38	6.18	10.30	10.18±0.02	
^{268}Hs	1955.59	0.27	0.28	6.40	6.19	9.96		
^{270}Hs	1969.22	0.27	0.28	6.42	6.20	9.55		
^{270}110	1958.86	0.26	0.26	6.40	6.21	10.79	11.03±0.05	

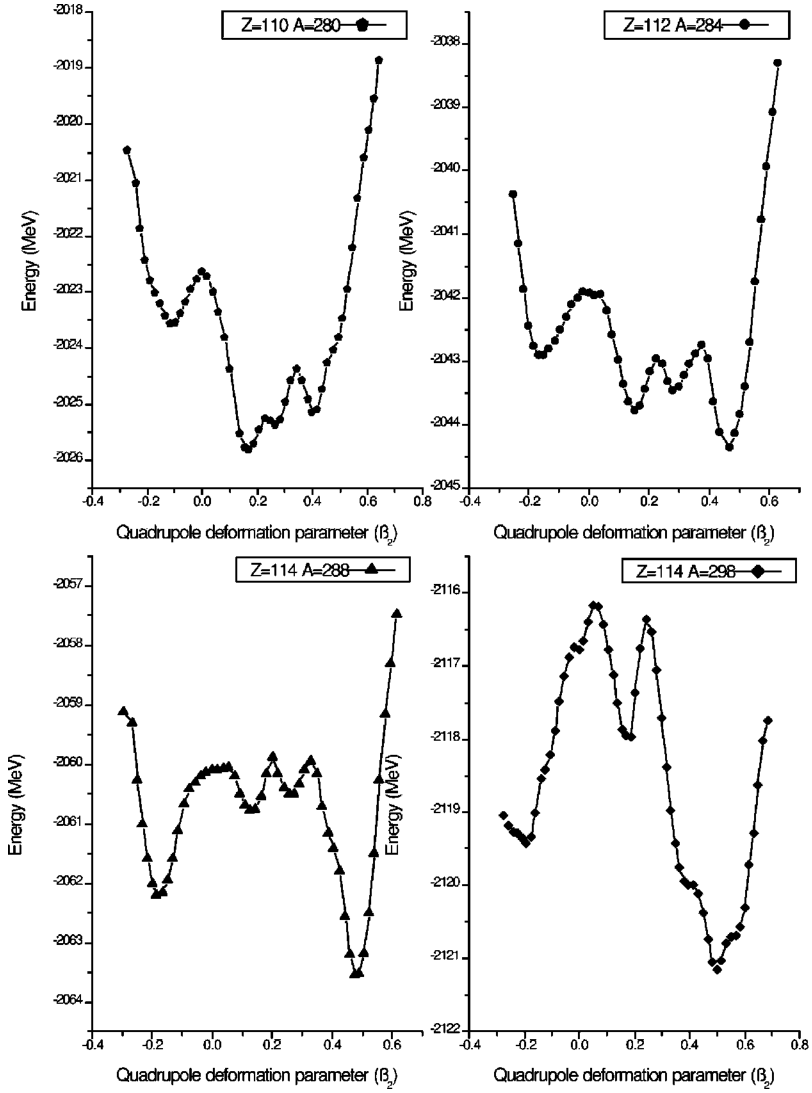

FIG. 1. The variation of the quadrupole deformation energies of nuclei $^{280}110$, $^{284}112$, $^{288}114$, and $^{298}114$ with the deformation parameter β_2. The TMA force is used.

nuclei. By the way, there are many sets of force parameters in the RMF model. The behavior of many force parameters for superheavy nuclei is similar to that of the TMA force. They also set the upper limit of the binding energy of a superheavy nucleus. Therefore TMA is a typical force for the upper limit of the total binding energy and NLZ2 is a typical force for the lower limit.

Very recently it was reported that the nucleus $^{270}110$ is produced at Darmstadt [5] and $^{270}108$ is produced at Paul Scherrer Institute [6]. The nuclei $^{288}114$ and $^{292}116$ are produced at Dubna [3,4]. The binding energy and alpha decay energy of $^{270}110$ and $^{270}108$ are given in Tables I and II, together with those of the nuclei on its alpha decay chain. The theoretical values are very close to the experimental data. On the properties of superheavy nuclei around $Z=114$, we plot their quadrupole deformation energies in Fig. 1 and list the numerical results in Tables III and IV.

At first let us focus on the lengthy constraint RMF results on the quadrupole deformation energy of $^{280}110$, $^{284}112$, $^{288}114$, and $^{298}114$ in Fig. 1. The black points are numerical results and they are connected by solid lines. This constraint calculation is carried out with a constraint on quadrupole moments in the RMF model [10,15]. It is a rather time-consuming calculation for superheavy nuclei. This kind of calculation is very scarce for superheavy nuclei as far as we know. Figure 1 is the result of the TMA force. It is seen from Fig. 1 that the curve of the quadrupole deformation energy of $^{280}110$, $^{284}112$, $^{288}114$, and $^{298}114$ is more complex than that in light nuclei. There are three or four minimums in the curve of $^{280}110$, $^{284}112$, $^{288}114$, and $^{298}114$ (the nucleus $^{298}114$ is chosen because it was considered as a spherical magic nucleus). The lowest one should correspond the ground state of a superheavy nucleus. For $^{280}110$, the ground state is a configuration with a prolate deformation $\beta_2=0.17$. The other solutions of $^{280}110$ are higher in energy. With the increase of proton number and (/or) neutron number, the solution with a superdeformation $\beta_2\approx0.5$ becomes lower in energy and can be finally the ground state of a superheavy nucleus. The valley around this superdeformed minimum is wider and deeper with the increase of proton number and (/or) neutron number. The superdeformed solution may be the ground state of $^{284}112$ and $^{288}114$. For nuclei near $Z=114$ and $N=184$, the superdeformed solution can become the ground state of superheavy nuclei because the valley

TABLE III. The binding energies, deformations, nuclear radii, alpha decay energies, and lifetimes of superheavy nuclei on the alpha decay chain of $^{292}116$. The last two columns are experimental decay energies and lifetimes. The input pairing gaps: $\Delta_p=\Delta_n=11.2\ \mathrm{MeV}/\sqrt{A}$. The TMA force is used. The excited solutions are denoted by * and **.

Nuclei	B(MeV)	β_n	β_p	R_n	R_p	Q_α	T_α	Q_α(expt)	T_α(expt)
$^{292}116$	2080.89	0.49	0.51	6.62	6.46	11.01	14.3 ms	10.71 ± 0.15	33^{+155}_{-15} ms
$^{292}116$*	2080.51	−0.21	−0.21	6.45	6.27				
$^{292}116$**	2077.73	0.25	0.26	6.48	6.30				
$^{288}114$	2063.60	0.48	0.49	6.58	6.41	9.12	876.47 s	9.84 ± 0.05	$1.9^{+3.8}_{-0.8}$ s
$^{288}114$*	2061.97	−0.18	−0.19	6.41	6.23				
$^{288}114$**	2060.67	0.26	0.27	6.45	6.27				
$^{284}112$	2044.42	0.46	0.47	6.54	6.36	9.83	1.21 s	9.17 ± 0.05	$9.8^{+18}_{-3.8}$
$^{284}112$*	2043.47	0.27	0.29	6.43	6.25				
$^{284}112$**	2042.64	−0.17	−0.17	6.38	6.19				
$^{280}110$	2025.95	0.17	0.18	6.36	6.15	10.08	0.05 s		$7.5^{+14}_{-2.9}$ s
$^{280}110$*	2025.41	0.26	0.26	6.39	6.20				
$^{280}110$**	2025.09	0.41	0.41	6.48	6.28				
$^{280}110$***	2025.30	−0.12	−0.12	6.34	6.14				

around it is very wide and deep. Therefore the nuclei at the center of superheavy islands may be superdeformed nuclei.

After we know the variation of the energy with the deformation parameter, we carry out axially deformed RMF calculations near these minimums. The properties of nuclei $^{280}110$, $^{284}112$, $^{288}114$, $^{292}116$ produced at Dubna are listed in Tables III and IV for two sets of force parameters. We show all solutions which correspond to the minimums of the energy surface in Fig. 1. The solutions with labels * and ** are the excited solutions. Table III is the RMF result with the TMA force. Similar notations to Table I are used. Because the lifetime is also measured at Dubna, we list the experimental lifetime T_α(expt) in the last column. The theoretical lifetime T_α(theor) is calculated according to the Viola-Seaborg formula [17,18]

$$\log_{10}(T_\alpha)=(aZ+b)(Q_\alpha)^{-1/2}+(cZ+d), \tag{1}$$

where T_α is given in seconds and Q_α in MeV, and Z is the proton number of the parent nucleus. This is a well-known formula and it is often used to estimate the lifetime of alpha decays by the decay energies [17,18]. The constants in this expression have been determined as $a=1.66175$, $b=-8.5166$, $c=-0.20228$, $d=-33.9069$ for even-even nuclei. These values are obtained by fitting the experimental data of middle and heavy nuclei [17–19].

It is concluded from Tables III and IV that there is shape coexistence in superheavy nuclei. In some cases the superdeformed solution can be the ground state of a nucleus. The experimental alpha decay energy and lifetime are listed in the last two columns for comparison. It is seen that theoret-

TABLE IV. The binding energies, deformations, nuclear radii, alpha decay energies, and lifetimes of superheavy nuclei on the alpha decay chain of $^{292}116$. The last two columns are experimental decay energies and lifetimes. The input pairing gaps: $\Delta_p=\Delta_n=11.2\ \mathrm{MeV}/\sqrt{A}$. The NLZ2 force is used. The excited solutions are denoted by * and **.

Nuclei	B(MeV)	β_n	β_p	R_n	R_p	Q_α	T_α	Q_α(expt)	T_α(expt)
$^{292}116$	2078.65	0.55	0.57	6.79	6.59	10.92	24.2 ms	10.71 ± 0.15	33^{+155}_{-15} ms
$^{292}116$*	2076.77	0.06	0.06	6.53	6.31				
$^{292}116$**	2076.60	−0.05	−0.05	6.53	6.30				
$^{288}114$	2060.87	0.15	0.16	6.54	6.30	9.51	50.29 s	9.84 ± 0.05	$1.9^{+3.3}_{-0.8}$ s
$^{288}114$*	2060.27	0.56	0.58	6.77	6.56				
$^{288}114$**	2057.15	−0.20	−0.20	6.55	6.33				
$^{284}112$	2042.08	0.16	0.17	6.51	6.27	9.02	373.14 s	9.17 ± 0.05	$9.8^{+18}_{-3.8}$ s
$^{284}112$*	2041.30	0.58	0.60	6.77	6.54				
$^{284}112$**	2037.76	−0.18	−0.18	6.50	6.26				
$^{280}110$	2022.80	0.18	0.19	6.49	6.25	8.81	360.86 s		$7.5^{+14}_{-2.9}$ s
$^{280}110$*	2021.66	0.56	0.58	6.72	6.49				
$^{280}110$**	2017.64	−0.18	−0.18	6.49	6.24				

ical alpha decay energies are very close to the data. The biggest difference between the theoretical value and the data is less than 1.0 MeV. We see in Table III that the calculated alpha decay energies agree well with the experimental data for the nuclei with $Z=110$–116 produced at Dubna. We calculate the corresponding lifetimes of these nuclei by using the Viola-Seaborg formula. The ratio of theoretical lifetime to experimental one is between 10^{-3} and 10^{3}. Usually the ratio between the experimental lifetime and the theoretical one is around 10^{4} or even larger. Therefore we can say that the RMF prediction on lifetime is good.

Now let us make a short discussion on the difference of force parameters in the RMF models. As we stated before, the behavior of many forces is similar to that of the TMA force. There is also shape coexistence of superheavy nuclei for NLZ2 force. However, there is a slight difference between the TMA force and NLZ2 force. The superdeformed solution sets in a little late for the NLZ2 force with the increase of the nucleon number. We list the results of NLZ2 in Table IV as an explanation of this. It is seen that the superdeformed solution becomes lower with the increase of nucleon number. This is similar to that of TMA. The alpha decay energies and lifetimes from NLZ2 are also very close to experimental data. But for $^{288}114$ the superdeformed solution with NLZ2 is still higher than the prolate solution with $\beta_2=0.17$. Finally the superdeformed solution may become the ground state of superheavy nuclei such as $^{292}116$.

It was believed that the existence of the superheavy island is due to the spherical shell closure. Here we demonstrate that there is shape coexistence in superheavy nuclei. Deformations may exist for many superheavy nuclei, even for a nucleus $^{298}114$. In view of the fact that the nuclei in the actinium series are deformed, our conclusions are compatible with present data on superheavy nuclei. Very recently Muntian, Patyk, and Sobiczewski considered that superheavy nuclei around $^{270}108$ are deformed [20]. This agrees with our conclusions on even-even nuclei of this paper and on odd nuclei [10]. Extracting information of deformation experimentally will be useful to test these views. One possible way is to investigate the rotational bands and another way is to look for the isomer of superheavy nuclei. These will shed light on deformation of superheavy nuclei.

In summary we have investigated the structure of even-even superheavy nuclei with proton number $Z=100$–116 in the RMF model. This is the first systematic comparison between the theoretical binding energies of the RMF model and available data. The calculated binding energy agrees well with the data. The biggest difference is 0.2% and this is also the precision of the RMF model for stable nuclei. The calculations also set an upper limit and a lower limit for the binding energy based on the comparison with present data. This is useful for guiding future experiments on superheavy nuclei. The RMF results show that there is shape coexistence in superheavy nuclei and deformations can appear for many superheavy nuclei. In some cases the superdeformed configuration is the ground state of superheavy nuclei, especially for nuclei around $Z=114$ and $N=174$. The RMF results are in good agreement with the experimental alpha decay energies and lifetimes. Extracting information of deformation in superheavy nuclei is very useful for the understanding of the structure of superheavy nuclei and may be also possible with present facilities.

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