High- K isomers in neutron-rich zirconium isotopes

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(Received 17 January 2012; published 24 February 2012)

The neutron-rich zirconium isotopes are a key testing ground for nuclear models due to their sensitivity to shape changes, and because they cross the r -process path of explosive nucleosynthesis. Furthermore, recent experimental data have revealed a high-spin isomer in ^{108}Zr . Here we report the results of configuration-constrained potential-energy-surface calculations of ground states and high- K states in $^{104-110}\text{Zr}$, restricted to quadrupole and hexadecapole shapes. These calculations enable the existing isomer data to be understood, and predictions are made for ^{110}Zr .

DOI: [10.1103/PhysRevC.85.027307](https://doi.org/10.1103/PhysRevC.85.027307)

PACS number(s): 21.10.-k, 21.60.-n, 27.60.+j

The zirconium ($Z = 40$) isotopes are well known [1] for their variety of shapes, with considerable sensitivity to the neutron number, which is at least partly a consequence of the $Z = 40$ subshell gap in single-particle energies. On the neutron-rich side of stability, the shape sensitivity extends into the landscape of rapid-neutron-capture, r -process nucleosynthesis relevant to supernova detonations, giving an added incentive to understand the nuclear structure. In the past decade there have been many theoretical studies related to this theme (see for example Refs. [2–9]), but only Xu *et al.* [2], albeit with a more phenomenological approach, have given detailed predictions of isomeric states in the neutron-rich even-even zirconium isotopes. Now, with the success of the RIKEN RIBF accelerator complex, major experimental advances have been possible, extending knowledge of these isotopes [10,11]. One of the notable nuclear structure features was the discovery [11] of an isomer in ^{108}Zr , but not in ^{106}Zr or ^{104}Zr . The isomer in ^{108}Zr was tentatively interpreted as being due a tetrahedral shape, which has been predicted to be most favored in ^{110}Zr [12], though the excited-state structure of that isotope has not yet itself been studied experimentally. In the present work, we extend the earlier configuration-constrained potential-energy-surface (PES) calculations for this region [2], now focused on even-even $^{104-110}\text{Zr}$. We consider the quadrupole (β_2 and γ) and hexadecapole (β_4) deformations as the relevant degrees of freedom, and show that the existing data can be understood on this basis. We also predict the low-lying two-quasiparticle structure of ^{110}Zr .

The configuration-constrained PES model [13] has been widely used in various mass regions, including the superheavy [14,15] and drip-line [16] regions, to calculate the energies and shapes of high- K states, where K is the projection of the angular momentum on the nuclear axis of symmetry. High- K states at low excitation energy are often associated with isomerism, due to the K -forbidden nature of their decays

[17]. In the model, single-particle levels are obtained from the Woods-Saxon potential with the set of universal parameters [18]. For the pairing correlations, particle-number projection is approximated by the Lipkin-Nogami technique [19], with the pairing strength determined by the average-gap method [20]. The total energy of a nucleus consists of a macroscopic part that is obtained with the standard liquid-drop model [21] and a microscopic part which is calculated by the Strutinsky approach [22]. In the configuration-constrained calculations, it is necessary to block adiabatically the unpaired nucleon orbits that specify a given configuration [13]. This has been achieved by calculating and identifying the average Nilsson quantum numbers for each orbit involved in the configuration. Such PESs can show the shape changes due to the polarization of unpaired nucleons.

Considering the shape transitions in the zirconium region [1,2], it is apparent that the shape of an excited state can differ significantly from that of its ground state. This is most evident in the calculations [2] through the prediction of oblate high- K states with prolate ground states, and vice versa. Therefore, a configuration-constrained approach is needed for the calculation of excited-state energies. The results of the present work are given in Table I for $^{104-110}\text{Zr}$. For each even-even isotope, the ground-state shapes are specified, together with the energies and shapes of the four lowest-energy two-quasineutron configurations. The quoted K^π values correspond to the maximum- K couplings, i.e., $K = \Omega_1 + \Omega_2$. The calculated two-quasiproton states are consistently above 2 MeV and their energies change little with neutron number. Therefore, they are not likely to form isomeric states. Nevertheless, as examples, we show specific energies and shapes for the three lowest two-quasiproton states calculated for ^{108}Zr . It can be seen in Table I that all the β -deformation values are similar, mostly with $\beta_2 \approx 0.35$ and $\beta_4 \approx -0.02$. The emphasis of the following discussion will be on the K^π value, the γ deformation, and the lowest two-quasiparticle excitation energy for each isotope.

For ^{104}Zr , the lowest-energy two-quasiparticle state is at 1.45 MeV, with $K^\pi = 5^-$. At first sight, this seems to be a

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TABLE I. Calculated configurations, shapes, and energies of low-lying states in $^{104-110}\text{Zr}$.

Nuclide	K^π	Configuration	β_2	γ°	β_4	E (MeV)
^{110}Zr	0^+	vacuum	0.347	0.0	-0.04	0.0
	6^-	$\nu \frac{5}{2}^+ [402] \otimes \frac{7}{2}^- [523]$	0.325	0.0	-0.04	1.586
	8^+	$\nu \frac{9}{2}^- [514] \otimes \frac{7}{2}^- [523]$	0.336	0.1	-0.05	2.471
	4^-	$\nu \frac{1}{2}^+ [411] \otimes \frac{7}{2}^- [523]$	0.366	3.6	-0.02	2.073
	3^+	$\nu \frac{1}{2}^+ [411] \otimes \frac{5}{2}^+ [402]$	0.337	6.0	-0.03	2.162
^{108}Zr	0^+	vacuum	0.353	1.0	-0.03	0.0
	4^-	$\nu \frac{7}{2}^- [523] \otimes \frac{1}{2}^+ [411]$	0.357	1.5	-0.03	1.414
	6^+	$\nu \frac{7}{2}^- [523] \otimes \frac{5}{2}^- [532]$	0.333	0.0	-0.04	1.997
	3^+	$\nu \frac{5}{2}^+ [402] \otimes \frac{1}{2}^+ [411]$	0.327	5.6	-0.02	2.165
	5^-	$\nu \frac{5}{2}^+ [402] \otimes \frac{5}{2}^- [532]$	0.309	0.1	-0.03	2.561
	4^-	$\pi \frac{3}{2}^- [301] \otimes \frac{5}{2}^+ [422]$	0.322	0.0	-0.03	2.326
	5^-	$\pi \frac{5}{2}^- [303] \otimes \frac{5}{2}^+ [422]$	0.313	1.2	-0.02	2.726
	3^-	$\pi \frac{3}{2}^- [301] \otimes \frac{3}{2}^+ [431]$	0.307	0.3	-0.03	3.421
	0^+	vacuum	0.347	1.0	-0.02	0.0
^{106}Zr	3^-	$\nu \frac{1}{2}^+ [411] \otimes \frac{5}{2}^- [532]$	0.339	0.0	-0.02	1.705
	4^-	$\nu \frac{1}{2}^+ [411] \otimes \frac{7}{2}^- [523]$	0.354	0.7	-0.02	1.884
	6^+	$\nu \frac{7}{2}^- [523] \otimes \frac{5}{2}^- [532]$	0.350	1.0	-0.02	2.020
	5^-	$\nu \frac{5}{2}^- [532] \otimes \frac{5}{2}^+ [413]$	0.344	0.2	-0.02	1.796
	0^+	vacuum	0.350	0.0	-0.00	0.0
^{104}Zr	5^-	$\nu \frac{5}{2}^- [532] \otimes \frac{5}{2}^+ [413]$	0.351	6.8	-0.00	1.450
	3^+	$\nu \frac{5}{2}^+ [413] \otimes \frac{1}{2}^+ [411]$	0.343	0.5	-0.01	1.945
	3^-	$\nu \frac{5}{2}^- [532] \otimes \frac{1}{2}^+ [411]$	0.346	0.4	-0.00	1.603
	4^-	$\nu \frac{5}{2}^+ [413] \otimes \frac{3}{2}^- [541]$	0.329	5.2	-0.01	2.446

good isomer candidate, on account of its low energy and high K value. However, there is a significant degree of triaxiality, with $\gamma = 7^\circ$. Since the K quantum number depends on axial symmetry for its conservation, this triaxiality would lead to K mixing and, potentially, the loss of K isomerism. Furthermore, the PES (see Fig. 1) shows very little energy variation in the γ direction, i.e., the PES is very “ γ soft,” supporting the suggested loss of K isomerism. Therefore, these calculations are consistent with the absence of an observed isomer in ^{104}Zr [11].

For ^{106}Zr , the lowest-energy two-quasiparticle state is at 1.71 MeV, with $K^\pi = 3^-$. This is higher in energy and lower in spin than that found for ^{104}Zr , and, even though the shape is axially symmetric, the lack of observed isomerism [11] is consistent with the calculations. It should also be noted that, in our previous work [2], an *oblate* $K^\pi = 5^-$ state was calculated at 2.7 MeV in ^{106}Zr , but that energy may be too high for isomer formation.

For ^{108}Zr , the lowest-energy two-quasiparticle state is at 1.41 MeV, with $K^\pi = 4^-$. In this case the energy is low enough and the spin is high enough so that isomerism can be expected, consistent with what has been observed [11]. However, the

FIG. 1. Calculated potential energy surfaces for the lowest-energy two-quasiparticle states in (a) ^{104}Zr , (b) ^{108}Zr , and (c) ^{110}Zr , as a function of quadrupole deformation parameters β_2 and γ , with each value minimized with respect to β_4 . The energy interval between contours is 200 keV. Quasiparticle configurations, K^π values, and excitation energies are given in Table I.

K^π value has not been determined experimentally, and this will form an important future test of our calculations. The value of $\gamma = 2^\circ$ is associated with a somewhat γ -soft PES, as shown in Fig. 1, which could lead to a reduced half-life compared to examples with better axial symmetry. This issue needs further study, but goes beyond the scope of the present work. It is notable, however, that another nuclide in the same mass region, ^{100}Sr , has a $K^\pi = 4^-$ isomer at 1.62 MeV, with a half-life of 82 ns [23], which is not too different from the 620 ns measured for ^{108}Zr [11].

For ^{110}Zr , the lowest-energy two-quasiparticle state is at 1.59 MeV, with $K^\pi = 6^-$. This state has axial symmetry and the γ softness is less than that found for ^{104}Zr and ^{108}Zr , as shown in Fig. 1. This state is likely to be isomeric. It was already predicted in our earlier work [2]. We note, however, that the $\frac{5}{2}^+ [402] \otimes \frac{7}{2}^- [523]$, $K^\pi = 6^-$ configuration has parallel intrinsic-spin coupling, which is energetically unfavoured according to the Gallagher rules [24], and the final $K^\pi = 6^-$ energy could be ≈ 0.2 MeV higher than the 1.59 MeV given in Table I. On that assumption, it remains the lowest-energy two-quasiparticle excitation, apart from its favored $K^\pi = 1^-$ ($K = \Omega_1 - \Omega_2$) partner, and isomerism can be expected.

Although the present results can, at this stage, only be compared qualitatively with existing experimental results, it is hoped that future experiments will provide energies and K^π values, through both isomer and β -decay studies, that will allow the testing of our quantitative predictions.

In summary, detailed results have been shown from configuration-constrained PES calculations, using the $(\beta_2, \gamma, \beta_4)$ deformation space, for two-quasiparticle states in even-even $^{104-110}\text{Zr}$. A qualitative understanding is obtained for isomerism in ^{108}Zr , and its absence in $^{104,106}\text{Zr}$, without any consideration of tetrahedral shapes. A full understanding of K isomerism in the neutron-rich zirconium isotopes requires additional experimental data that can identify two-quasiparticle energies and K^π values, for comparison with the calculations.

We thank the UK STFC, AWE plc, and the Natural Science Foundation of China (Grants No. 10735010 and No. 10975006) for financial support.

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