Structure of Superheavy Nuclei Along Element 115 Decay Chains

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A recent high-resolution α, X-ray, and γ-ray coincidence-spectroscopy experiment offered first glimpse of excitation schemes of isotopes along α-decay chains of Z = 115. To understand these observations and to make predictions about shell structure of superheavy nuclei below 288,115, we employ two complementary mean-field models: self-consistent Skyrme Energy Density Functional approach and the macroscopic-microscopic Nilsson model. We discuss the spectroscopic information carried by the new data. In particular, candidates for the experimentally observed E1 transitions in 276Mt are proposed. We find that the presence and nature of low-energy E1 transitions in well-deformed nuclei around Z = 110, N = 168 strongly depends on the strength of the spin-orbit coupling; hence, it provides an excellent constraint on theoretical models of superheavy nuclei. To clarify competing theoretical scenarios, an experimental search for E1 transitions in odd-A systems 275, 277Mt, 275Hs, and 277Ds is strongly recommended.

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Introduction.—Superheavy nuclei at the limit of nuclear mass and atomic number pose a formidable challenge to both experiment and theory. The low cross sections for production of these nuclei, in the picobarn range or less, offer limited structural information. Moreover, the α-decay chains of nuclei synthesized in experiments using the 48Ca beam with actinide targets terminate by spontaneous fission before reaching the known region of the nuclear chart. This poses a problem with the unambiguous identification of the new isotopes, and more direct techniques to determine Z and A must be employed. Theoretical predictions of the shell structure of superheavy nuclei are also difficult, as the interplay between the electrostatic repulsion and nuclear attraction, combined with a very high density of single-particle (s.p.) states, make the results of calculations extremely sensitive to model details.

In a recent experimental study, unique structural information on low-lying states in superheavy nuclei below 288,115 has been obtained. Of particular interest is the finding that some of the measured transitions in the nucleus assigned to be 276Mt have E1 character, thus suggesting opposite parities of the connected states. The new data offer an exciting opportunity to constraint theoretical models in this region for the first time. Indeed, previous self-consistent studies have shown that the number of opposite-parity s.p. orbitals around the Fermi level is fairly limited, and this is consistent with the Nilsson model analysis of Ref. 9.

Because of the above-mentioned sensitivity to model details, robust predictions in this region are difficult to make as one is dealing with large extrapolations. To this end, when aiming at the spectroscopic quality of predictions, it is advisable to use a model that performs well in the neighboring region where experimental information is more abundant. Furthermore, since the quadrupole deformations of α-decay daughters of 288,115 are expected to increase gradually with decreasing Z and A along the α-decay chain, shape polarization is going to play a role when determining the energies of low-lying states.

In this work, we study the low-lying states in the superheavy nuclei below 288,115, using the locally-optimized self-consistent Skyrme Energy Density Functional (SEDF) and Nilsson-Strutinsky (NS) frameworks. To assess systematic errors, we also carry out calculations using a globally-optimized SEDF model.

Models.—The SEDF approach is a variant of nuclear density functional theory, which offers a global, self-consistent description of nuclear properties across the nuclear landscape. The recent self-consistent study of Ref. 15 offers a locally optimized SEDF parameterization that meets our local-extrapolability requirements: it reproduces one-quasiparticle (1-q.p.) states in 251Cf and 249Bk (the two heaviest systems where 1-q.p. energies are experimentally well known), predicts crucial deformed shell gaps at N = 152 and Z = 100, and describes rotational bands in Fm, No, and Rf isotopes. The parameter set of Ref. 21 that performs well for heavy nuclei and large deformations. We shall also...
use UNEDF1 in this study. The calculations follow closely Ref. [15]. The Skyrme Hartree-Fock-Bogolyubov (SHFB) equations were solved using the symmetry-unrestricted solver HFODD (v2.52) [29] by expanding 1-q.p. wave functions in 680 deformed harmonic-oscillator (HO) basis states. To compute 1-q.p. excitations in odd-A nuclei, we blocked relevant orbits around the Fermi level as described in Ref. [23]. The strengths of the pairing force for neutrons and protons were adjusted to the odd-even mass staggering in $^{251}$Cf and $^{248}$Bk and the kinematic moment of inertia of $^{252}$No. The SEDF results are compared with those of the Nilsson-Strutinsky (NS) approach of Ref. [24] with the modified harmonic oscillator (MO) potential shown in Fig. 2.

Results.—We first discuss properties of the even-even nuclei belonging to the $\alpha$-decay chain of $^{296}$120. Their ground states form q.p. vacua for neighboring odd-A and odd-odd systems. The calculated quadrupole moments are shown in Fig. 2. Both SEDF models predict a similar smooth increase of quadrupole deformation along the $\alpha$-chain. In the NS calculations, $^{296}$120 is nearly spherical, $^{292}$118 and $^{288}$Lv are very weakly deformed, $^{284}$Fl and $^{286}$Cn are spherical, and the shapes of the lightest daughters have deformations close to those predicted by SEDF. These results suggest that a direct comparison between SEDF and NS models is most meaningful for $Z < 112$.

![FIG. 1. (Color online) Quadrupole moments $Q_2$ of even-even nuclei forming the $\alpha$-decay chain $^{296}$120 $\rightarrow \cdots \rightarrow ^{264}$Rf, calculated with UNEDF1SO and UNEDF1 SEDF models and the NS approach.](image1)

It is instructive to begin the discussion from the Nilsson s.p. diagram of the MO potential shown in Fig. 2. The main features of this diagram, such as the appearance of spherical shell gaps at $Z = 114$ and $N = 184$, have remained unchanged since the late 1960s [29, 30]. The deformed shell structure of nuclei at the end of the $\alpha$-decay chain of $^{296}$120 (or $^{288}$115) is relatively simple: both in neutrons and protons there appears one unique-parity, high-$\Omega$ Nilsson state ($\nu[716]_{13/2}$ and $\pi[615]_{11/2}$) surrounded by levels of opposite parity, such as neutron ([613]_{5/2}, [611]_{3/2}), ([606]_{11/2}, [604]_{9/2}) and proton ([503]_{7/2}, [505]_{9/2}), ([510]_{1/2}, [512]_{3/2}) pseudo-spin doublets, respectively.

The spherical shell structure in superheavy nuclei strongly depends on the spin-orbit splitting, which governs the size of the $Z = 114$ gap (cf. Table 4 of Ref. [10] and discussion therein). Also, the coupling between Coulomb interaction and nuclear interaction is expected to impact the predictions. To consider both effects, we studied s.p. canonical states obtained with UNEDF1SO and UNEDF1 SEDF models, which differ in the spin-orbit sector and treat the electrostatic energy self-consistently.

The s.p. energies of UNEDF1SO along the $\alpha$-decay chain of $^{296}$120 are depicted in Fig. 3. The s.p. neutron spec-
FIG. 3. (Color online) Single-neutron (top) and single-proton (bottom) canonical energies of UNEDF1SO for nuclei along the α-decay chain of 296120 as in Fig. 1. The orbits are labelled by the standard asymptotic Nilsson numbers corresponding to the dominant components of the SHFB canonical wave functions. The positive/negative parity levels are marked by solid/dashed lines. The Fermi levels are indicated by thick dotted lines.

The spectrum is dominated by deformed gaps at $N = 152$ and 162, and a large spherical shell gap at $N = 184$. In the deformed region $160 \leq N \leq 168$, the Nilsson states close to the Fermi level are primarily $N_{osc} = 6$ levels and one unusual-parity, high-$\Omega$ intruder level $\nu[716]13/2$ originating from the spherical $1j_{15/2}$ shell. The structure of the proton Nilsson diagram in Fig. 3 is dominated by deformed gaps at $Z = 100$, 102, and 108, and a weak spherical subshell closure at $Z = 114$. The unusual-parity, high-\(\Omega\) intruder level $\pi[615]11/2$ originating from the spherical $1i_{13/2}$ shell is surrounded by several $N_{osc} = 5$ Nilsson orbitals.

The general pattern of s.p. states predicted by UNEDF1SO is not that far from that in Fig. 2 of the MO potential. However, there are differences in the spherical shell structure, which will impact detailed predictions for deformed superheavy nuclei belonging to $Z = 115$ α-decay chains. In particular, MO predicts larger spherical shell gaps at $Z = 114$, $N = 148$, and $N = 178$. In UNEDF1SO, the splitting between the $1j_{15/2}$ and $1i_{11/2}$
spherical neutron shells is very small. This results in an upward shift of the \([606]11/2, [604]9/2\) doublet.

In the case of UNEDF1 the unique-parity \(\nu 1j_{15/2}\) and \(\pi 13/2\) shells are shifted up by a few hundred keV, which results in a significant reduction of spherical \(N = 164\) and \(Z = 114\) shell closures \(15\). The change in the spin-orbit potential also impacts positions of deformed levels (see Fig. SM 1 in Supplemental Material \(31\)). In particular, the deformed neutron gap at \(N = 152\) is reduced, and that at \(N = 162\) opens up. In the proton sector, the deformed Nilsson state \([615]11/2\) appears just below the significantly increased \(Z = 116\) gap, close to the \([505]9/2\) and \([510]1/2\) levels. The second proton intruder state \([624]9/2\) shows up just below the deformed proton gap at \(Z = 108\).

Although s.p. energies are not experimental observables, those around the Fermi level carry information about the low-lying q.p. configurations in neighboring odd-\(A\) and odd-odd nuclei. To get more insights, we computed the energies of 1-q.p. excitations for odd-\(Z\), even-\(N\) superheavy nuclei that form the \(\alpha\)-decay chains \(287\text{Lv} \rightarrow \cdots \rightarrow 277\text{Ds} \) predicted with UNEDF1\(^{SO}\) (upper sequence) and UNEDF1 (lower sequence). \(Q_\alpha\) values for g.s. \(\rightarrow\) g.s. transitions are marked. The binding energy differences between different nuclei are shifted arbitrarily, whereas the excitation energies within a given nucleus are shown to scale.

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![Diagram](https://example.com/diagram.png)

**FIG. 4.** (Color online) 1-q.p. spectra for nuclei forming the \(\alpha\)-decay chain \(287\text{Lv} \rightarrow \cdots \rightarrow 277\text{Ds} \) predicted with UNEDF1\(^{SO}\) (upper sequence) and UNEDF1 (lower sequence). \(Q_\alpha\) values for g.s. \(\rightarrow\) g.s. transitions are marked. The binding energy differences between different nuclei are shifted arbitrarily, whereas the excitation energies within a given nucleus are shown to scale.

**FIG. 5.** (Color online) Similar as in Fig. 4 but for the \(\alpha\)-decay chain \(293\text{Fl} \rightarrow \cdots \rightarrow 277\text{Mt} \).

Let us look into the structure of \(276\text{Mt}\) in some detail. The structural information relevant to this nucleus, predicted by SEDF, is contained in the 1-q.p. spectra of its odd-\(A\) neighbors shown in Table 1. \(275\text{Mt}, 279\text{Hs},\) and \(277\text{Ds}\). As seen in tables in Supplemental Material \(31\), all low-lying 1-q.p. states in these nuclei correspond to very similar quadrupole mass deformation of \(\beta_2 \approx 0.22\), which facilitates comparison with the Nilsson diagram of Fig. 3. The lowest 1-q.p. proton states are the unique-parity \([615]11/2\) and \(N_{\text{osc}} = 5\) excitations \([512]3/2, [521]1/2, [510]1/2,\) and \([512]5/2\). The 1-q.p. neutron structure corresponds to the \([716]13/2\) intruder and \(N_{\text{osc}} = 6\) \([611]3/2, [613]5/2, [611]1/2,\) and
TABLE I. 1-q.p. excitation energies for the odd-\(A\) neighbors of \(^{279}\text{Mt}_{167}\) calculated with \textsc{unedf1} and \textsc{unedf1SO} parameters. The intrinsic configurations are labelled as in Fig. 5.

| Nucleus   | Config. | \(E_x\) (MeV) | Config. | \(E_x\) (MeV) |
|-----------|---------|---------------|---------|---------------|
| \(^{275}\text{Mt}_{166}\) | [512]3/2 | 0 | [615]11/2 | 0 |
|          | [615]11/2 | 0.159 | [615]11/2 | 0.243 |
|          | [505]9/2 | 0.167 | [521]1/2 | 0.402 |
|          | [510]1/2 | 0.173 | [515]2/2 | 0.500 |
|          | [624]9/2 | 0.318 | [510]1/2 | 0.512 |
| \(^{275}\text{Mt}_{168}\) | [512]3/2 | 0 | [615]11/2 | 0 |
|          | [615]11/2 | 0.131 | [521]1/2 | 0.174 |
|          | [505]9/2 | 0.136 | [515]2/2 | 0.260 |
|          | [512]5/2 | 0.182 | [510]1/2 | 0.480 |
|          | [624]9/2 | 0.300 | [515]2/2 | 0.532 |
| \(^{275}\text{Hs}_{167}\) | [512]3/2 | 0 | [613]5/2 | 0 |
|          | [611]3/2 | 0.067 | [613]5/2 | 0.016 |
|          | [611]1/2 | 0.104 | [611]1/2 | 0.117 |
|          | [716]13/2 | 0.173 | [604]9/2 | 0.235 |
|          | [604]9/2 | 0.242 | [716]13/2 | 0.479 |
| \(^{277}\text{Dy}_{167}\) | [611]3/2 | 0 | [613]3/2 | 0 |
|          | [613]5/2 | 0.035 | [613]5/2 | 0.046 |
|          | [611]1/2 | 0.090 | [611]1/2 | 0.107 |
|          | [716]13/2 | 0.157 | [604]9/2 | 0.335 |
|          | [604]9/2 | 0.227 | [716]13/2 | 0.564 |

[604]9/2 Nilsson orbits. The most significant difference between the two SEDF models is the appearance of the \([505]9/2\) 1-q.p. proton excitation low in energy in \textsc{unedf1}. According to the MO model of Fig. 2, the lowest 1-q.p. proton excitations are the \([615]11/2\), \([521]1/2\), and \([505]9/2\) Nilsson orbits, while the lowest neutron states are: \([606]11/2\), \([604]9/2\), \([611]3/2\), \([613]5/2\), and \([716]13/2\).

As noted in [9], there is a very limited choice of q.p. configurations that could generate the observed \(E1\) transitions in \(^{276}\text{Mt}\). If one insists on a strict conservation of the \(\Omega\) quantum number for protons and neutrons, low-energy \(E1\) transitions are predicted by \textsc{unedf1SO}. Formally, one can construct states that can be connected by an \(\Delta \Omega = 0, \pm 1\), parity changing operator, e.g., \(\pi [615]11/2 \otimes \nu [613]5/2\)\(3+\) and \(\pi [521]1/2 \otimes \nu [613]5/2\)\(2-\), but a significant Coriolis coupling would be required to produce a measurable \(E1\) rate. The situation is fairly straightforward with \textsc{unedf1}. Here, the stretched \(E1\) transition \(\pi [505]9/2 \rightarrow \pi [615]11/2\) can explain the data, with the neutron spectator orbital being \([611]3/2\) or \([613]5/2\) or \([611]1/2\). The NS approach predicts two scenarios: the proton \(\pi [615]11/2 \rightarrow \pi [505]9/2\) transition as in \textsc{unedf1} and the neutron \(\nu [716]13/2 \rightarrow \nu [606]11/2\) transition. According to 2-q.p.-plus-rotor calculations [32], both scenarios are equally likely.

To analyse the case of \(^{272}\text{Bh}\), we have calculated the [2-q.p. spectra of \(^{271}\text{Bh}\), \(^{273}\text{Hs}\), and \(^{274}\text{Sg}\) (see Supplemental Material [31] for the corresponding tables). In this case, there are quite a few candidates for low-energy \(E2\) and \(M1\) transitions that were seen experimentally.

The calculated \(Q_\alpha\) values depend, of course, on the structure of parent and daughter states [17] (see Figs. 4 and 5). The agreement with the measured values for the heaviest elements is usually better than 1 MeV. This is consistent with other calculations [14, 33–35].

**Conclusions.**—In summary, we studied shell structure of superheavy nuclei within the self-consistent SHFB approach and macroscopic-microscopic NS model. Detailed predictions have been made for the quasi-proton and quasi-neutron structures of nuclei belonging to the \(\alpha\)-decay chains of \(^{287}\text{Hs}\), \(^{289}\text{Lv}\), and \(^{293}\text{Hg}\). The \textsc{unedf1} and \textsc{unedf1SO} SEDF models differ in the strength of the spin-orbit term, and this impacts detailed predictions for the deformed nuclei around \(Z = 110\) and \(N = 168\). The recent observation of low-energy \(E1\) transitions in \(^{276}\text{Mt}\) [9] provides a stringent constraint on theoretical models. Indeed, the recently proposed \textsc{unedf1SO} parametrization that performs well in the transfermium region does not offer a simple explanation of the \(E1\) data, whereas the global \textsc{unedf1} parametrization explains the data in terms of the proton \(\pi [505]9/2 \rightarrow \pi [615]11/2\) transition. The MO models suggest two competing scenarios: a proton transition similar to that of \textsc{unedf1}, and an alternative neutron \(\nu [716]13/2 \rightarrow \nu [606]11/2\) \(E1\) transition. To confirm or disprove these scenarios, theory strongly recommends a search for \(E1\) transitions in neighboring odd-\(A\) systems \(^{275,277}\text{Mt}\), \(^{275}\text{Hs}\), and \(^{277}\text{Ds}\). Experimentally, this calls for high-resolution \(\alpha\)-photon coincidence spectroscopy of decay chains starting from \(^{293}\text{Hg}\), \(^{287,289}\text{Lv}\), or \(^{285,287}\text{Fl}\), respectively. However, these systems are either hampered by relatively low production cross-sections or large spontaneous fission branches on the way to the nuclei of structural interest [19]. A solution to this spectroscopic puzzle will have far-reaching consequences for our understanding of shell structure in superheavy nuclei, and the strength of the spin-orbit splitting in particular.

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