Colloquium: Superheavy elements: Oganesson and beyond

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Abstract

During the last decade, six new superheavy elements were added into the seventh period of the periodic table, with the approval of their names and symbols. This milestone was followed by proclaiming 2019 the International Year of the Periodic Table of Chemical Elements by the United Nations General Assembly. According to theory, due to their large atomic numbers, the new arrivals are expected to be qualitatively and quantitatively different from lighter species. The questions pertaining to superheavy atoms and nuclei are in the forefront of research in nuclear and atomic physics, and chemistry. This Colloquium offers a broad perspective on the field and outlines future challenges.

CONTENTS

I. INTRODUCTION

In 2012 and 2016, six new synthetic elements with atomic numbers $Z = 113$ (Nh, nihonium), $Z = 114$ (Fl, flerovium), $Z = 115$ (Mc, moscovium), $Z = 116$ (Lv, livermorium), $Z = 117$ (Ts, tennessine), and $Z = 118$ (Og, oganesson) joined the periodic table (Barber

et al., 2011; Karol *et al.*, 2016a,b). They were all produced by scientists in the period 1998-2010 using heavy-ion fusion reactions. The road to their final confirmations took a dedicated experimental effort worldwide. But how significant were these recent additions? And how relevant is this to fundamental knowledge of nuclear and electronic shell structure? As we argue in this Colloquium, there are strong indications that the atoms and nuclei at the limits of mass and charge have the potential to transform and challenge our understanding of atomic and nuclear physics, and chemistry.

The science drivers of superheavy element research are aligned with the overarching questions that motivate much of nuclear and atomic science (NAS Report, 2012): How did visible matter come into being and how does it evolve? How does subatomic matter organize itself and what phenomena emerge? Are the fundamental interactions that are basic to the structure of matter fully understood? The specific questions asked in the context of superheavy elements are:

- Where do nuclei and elements come from? Can superheavy nuclei be produced in the cosmos?

- How are superheavy nuclei and atoms made and organized? Do very long-lived superheavy nuclei exist in nature?

- What are the heaviest nuclei that can exist? Where does the periodic table of elements end?

- How can superheavy nuclei and atoms be exploited to reveal the fundamental symmetries of nature? What is the interplay between strong and electromagnetic interactions as the product of the fine-structure constant and atomic number approaches one ($\alpha Z \to 1$)?

- What are the chemical and physical properties of superheavy atoms?

The term "superheavy" usually refers to transactinides – chemical elements with $Z \geq 104$ (Hoffman *et al.*, 2000; Seaborg and Loveland, 1990). All currently known superheavy nuclei are radioactive; they have been synthesized in nuclear reactions by scientists. The current superheavy territory consists of two disjoint areas. The *lower superheavy region* includes the lighter isotopes of elements $Z = 110 - 113$, which were discovered during 1994-2004 in the

so-called "cold fusion" reactions involving lead and bismuth targets irradiated by medium-mass projectiles such as nickel and zinc (Hofmann and Münzenberg, 2000; Münzenberg and Morita, 2015). The rapid drop in production cross section with Z for cold-fusion reactions (it drops down to 0.02 picobarn for nihonium) suggested that a different approach to reach even higher atomic numbers was needed. The new strategy has relied on "hot-fusion" reactions with the rare ^{48}Ca beam and actinide targets. Relatively large cross sections (in the range of picobarns) associated with those reactions have enabled the discovery of over fifty isotopes of new elements with $Z = 114-118$ during 1998-2010 (Oganessian *et al.*, 2017; Oganessian and Utyonkov, 2015a). These new isotopes form the *upper superheavy region*, which is currently not connected to the lower superheavy region via known nuclear decay chains.

Theoretically, it had been concluded by the end of the 1960s (Myers and Swiatecki, 1966; Nilsson *et al.*, 1969; Nix, 1970; Sobiczewski *et al.*, 1966), that the existence of the heaviest nuclei with $Z > 104$ was primarily determined by shell effects due to the quantum-mechanical motion of protons and neutrons inside the nucleus. These early calculations predicted the nucleus with $Z = 114, N = 184$ to be the center of an island of long-lived superheavy nuclei with lifetimes ranging from minutes to millions of years, and this is how the term "island of stability" was coined (Myers and Swiatecki, 1966; Viola and Seaborg, 1966). This suggestion stayed practically unchallenged until the late 1990s when more refined models, based on realistic effective interactions, were applied to superheavy nuclei, and revised early predictions.

The heaviest element studied chemically to date is flerovium. Its relatively long half-life, 1–2 s, enables chemical studies with several atoms/day, which marks the limit of chemistry today (Düllmann, 2017b; Türler *et al.*, 2015). The nucleus ^{294}Og, produced in Dubna (Oganessian *et al.*, 2006) with a ∼0.5 picobarn cross section, marks the current limit of nuclear charge and mass. It decays to ^{290}Lv by α-decay with a half-life of 0.58 ms (Brewer *et al.*, 2018), which is currently too short for "atom-at-a-time" chemical studies. As a result, computing its electronic and nuclear structure is the only option currently available to study such elements.

There have been a number of reviews on superheavy element research (Ćwiok *et al.*, 2005; Hofmann, 2015; Hofmann and Münzenberg, 2000; Möller and Nix, 1994; Oganessian *et al.*, 2017; Oganessian and Utyonkov, 2015a; Schädel, 2015) as well as more popular overviews (Düllmann and Block, 2018; Nazarewicz, 2018; Oganessian and Rykaczewski, 2015). The

purpose of this Colloquium is to offer a broad perspective on the field, focused on theoretical expectations.

II. THE SUPERHEAVY TERRITORY

The superheavy nuclei occupy the upper region of the table of nuclides. As shown in Fig. 1, the known superheavy nuclei lie on the left flank of the valley of beta stability. Since those are all proton-rich systems, they can in principle decay by means of electron capture (EC) or β^+ decay, see, e.g., (Heßberger *et al.*, 2016). So far, however, no weak decay modes have been observed in the upper superheavy region. The main observed decay modes are alpha decay and spontaneous fission (SF) (Oganessian *et al.*, 2017; Oganessian and Utyonkov, 2015a), and this is consistent with theoretical estimates (Ćwiok *et al.*, 1996; Heenen *et al.*, 2015; Möller *et al.*, 1997; Sheng *et al.*, 2014).

As seen in Fig. 1, the territory of superheavy isotopes is vast and primarily unexplored, except for a small proton-rich corner. The isotopic chain of Og is a case in point. According to nuclear density functional theory (DFT) (Bender *et al.*, 2003) based on realistic energy density functionals (Agbemava *et al.*, 2014; Erler *et al.*, 2012a), about 100 isotopes of Og are expected to exist, between $N \approx 170$ (proton drip line) and $N \approx 270$ (neutron drip line). The center of the β-stability valley for Og is predicted at $N \approx 192$ (Ćwiok *et al.*, 1996; Heenen *et al.*, 2015; Möller *et al.*, 1997; Sheng *et al.*, 2014). Since, as discussed later, there are currently no obvious ways to synthesize neutron-rich superheavy systems, all information about those nuclei must come from theoretical modeling that involves huge extrapolations.

As far as atomic territory is concerned, the currently known superheavy elements belong to the seventh period of the periodic table, with Og completing it (Reedijk, 2018). Og belongs to Group 18, but – as we shall discuss in Sec. VII – strong relativistic effects make it a very unusual addition to the periodic table. Can the table of nuclides and periodic table of elements be further extended in charge and mass? This question will be addressed in Sec. VIII, through various theoretical scenarios.

III. PROTON AND NEUTRON DENSITIES AND SHELL STRUCTURE

Nucleonic density distributions and their moments contain key information on bulk properties of nuclei. However, direct experimental information on proton and neutron distributions and their moments in superheavy nuclei is nonexistent because of their very short lifetimes. In this respect, experimental laser spectroscopy studies of nuclear charge radii and quadrupole moments, recently extended to $^{252-254}$No ($Z = 102$), carry great promise (Düllmann and Block, 2018; Raeder *et al.*, 2018), see also (Backe *et al.*, 2015; Ferrer *et al.*, 2017; Laatiaoui *et al.*, 2016). However, we still have a long way to go to reach higher atomic numbers in such studies. For the time being, the new data can be used to test the predictive power of current nuclear models when it comes to charge radii in the actinide nuclei. This is done for two different DFT models in Fig. 2. The results are encouraging as they show that DFT predictions in the region of very heavy nuclei are reliable.

Figure 3 shows density profiles for three Og isotopes. An intriguing feature is the depression of proton density in the nuclear interior. This effect, referred to as semi-bubble distribution, is driven in superheavy nuclei by strong Coulomb repulsion and manifests itself foremost in heavy nuclei above Pb ($Z = 82$). Speculations on such exotic nuclear structures (bubbles, tori, rings) came up rather early in connection with superheavy nuclei, see, e.g., (Davies *et al.*, 1972; Dechargé *et al.*, 1999; Dietrich and Pomorski, 1998; Wong, 1973) and (Schuetrumpf *et al.*, 2017; Staszczak *et al.*, 2017). The origin of such exotic geometries of nuclear densities is the mismatch of ranges of two opposing forces: the short-range attractive nuclear interaction and the long-range Coulomb repulsion. This competition, known as Coulomb frustration, is also known to produce a great variety of involved phases in bulk nuclear matter, coined nuclear "pasta" (Bonche and Vautherin, 1981; Fattoyev *et al.*, 2017; Pethick and Ravenhall, 1995; Sonoda *et al.*, 2008; Williams and Koonin, 1985). The situation in finite superheavy systems is more subtle. The leading mechanism to release Coulomb pressure is nuclear fission, see Sec. VI. Superheavy nuclei can be sufficiently long-lived only by virtue of extra binding through shell effects, and this puts a stringent limit on the existence of exotic geometries. The example considered in Fig. 3 is on the safe side in this respect: semi-bubbles in ^{294,326}Og represent stable configurations in spite of significant quadrupole deformations. (It is interesting to note that the charge distributions of ^{252,254}No are expected to have appreciable central depressions (Raeder *et al.*, 2018). The computed

charge radii shown in Fig. 2 take this effect into account.) For discussion of shell effects related to semi-bubble configurations, see (Afanasjev and Frauendorf, 2005).

As mentioned in the introduction, quantum shell stabilization is the basis for the existence of superheavy systems. Early studies of shell structure in superheavy nuclei used empirical shell model potentials (Mosel and Greiner, 1969; Myers and Swiatecki, 1966; Nilsson *et al.*, 1969; Nix, 1972; Sobiczewski *et al.*, 1966, 1971), see (Ćwiok *et al.*, 1996) for an overview. These studies were focused on defining new "magic shell closures" beyond ^{208}Pb. However, as it was realized later through more microscopic studies, in which the Coulomb interaction was treated self-consistently, the shell structure of superheavy nuclei differs significantly from that of lighter species.

As discussed in, e.g., (Afanasjev and Frauendorf, 2005; Agbemava *et al.*, 2015; Bender *et al.*, 2001, 1999; Berger *et al.*, 2003; Ćwiok *et al.*, 1996; Shi *et al.*, 2014b), the general pattern of single-particle energies undergoes significant changes in superheavy systems. Figure 4 shows the single-particle energies for the doubly-magic nucleus ^{132}Sn and superheavy nuclei ^{302}Og and $^{472}164$ predicted with the Skyrme-DFT models SV-min and UNEDF1. (It should be emphasized that the details of shell structure in superheavy nuclei show strong model dependence, general features are robust.) While for ^{132}Sn the magic gaps are sizable, around 4 MeV, the neutron gap $N = 184$ for ^{302}Og is about half that size. This is even more pronounced for the proton spectra where well isolated shell gaps can hardly be found. First, the level density of single-particle states is large; in fact it grows faster than expected from oscillator scaling $A^{1/3}$ (Agbemava *et al.*, 2015). Consequently, small changes in theoretical modeling can impact shell structure substantially. Second, the shell structure of superheavy nuclei is influenced by Coulomb frustration and the concept of magic shell gaps fades away. This phenomenon of shell diffusion has also been analyzed in (Jerabek *et al.*, 2018) where it was demonstrated that the nucleon localization functions of superheavy nuclei approach the Fermi-gas limit in the valence region.

As seen in Fig. 4, high-j shells tend to cluster, which results in regions of quantum stabilization. Actually, the presence of a central depression strongly affects high-j orbits due to their large single-particle radii (Afanasjev and Frauendorf, 2005; Ćwiok *et al.*, 1996; Dechargé *et al.*, 1999; Dechargé *et al.*, 2003; Pei *et al.*, 2005). The proton level scheme for ^{302}Og in Fig. 4 shows a few low-j states near the Fermi level, which inhibits strict shell closure but still maintains a low level density (due to low multiplicities), hence large

shell stabilization. On the other hand, the low-j intruders reduce the impact of the $i_{13/2}$ state to drive bubble shapes. The situation looks extremely favorable for the hypothetical superheavy nucleus $^{472}164$ where high-j states cluster around the Fermi level. Its proton density shows a well developed semi-bubble with a central density coming down to 66% of the maximum density (Schuetrumpf *et al.*, 2017).

In spite of the fact that current self-consistent nuclear models do not have spectroscopic quality when it comes to the description of known levels in heavy nuclei, most of those models predict shell-stabilized regions at $N \approx 172 - 184$ and $Z \approx 112 - 126$ (Agbemava *et al.*, 2015; Bender *et al.*, 2001, 1999; Ćwiok *et al.*, 1996; Kruppa *et al.*, 2000) as well as around $N = 258$, $N = 308$, and $N = 410$ (Afanasjev *et al.*, 2018b; Bender *et al.*, 2001; Zhang *et al.*, 2005) (see also (Denisov, 2005; Ismail *et al.*, 2016) for estimates based on empirical average potentials).

The importance of Coulomb pressure increases with increasing system size. This favors a reduction of nuclear density around the center and so may give way to exotic nuclear topologies such as bubbles or toroids. Figure 5 illustrates the competition between various configurations in the superheavy nucleus $^{780}254_{526}$ (Nazarewicz *et al.*, 2002) involving normal profiles (similar to densities of stable nuclei), bubbles which have a void at the center, and band-like toroids. In many cases, such exotic profiles are predicted to be energetically competitive. However, their stability in superheavy nuclei remains an open question. Some recent calculations suggest that many such forms are unstable against triaxial distortions and fission (Afanasjev *et al.*, 2018b; Brodziński and Skalski, 2013).

Although questions related to exotic configurations in $Z \gg 120$ systems may seem hardly relevant from the perspective of laboratory experiments, they can gain relevance in the exotic (neutron rich) atmosphere of stellar explosions or in neutron stars, where exotic forms of nuclear matter are expected (Schuetrumpf *et al.*, 2015). In any case, such massive extrapolations require models which are well tested against information from the heaviest nuclei which are experimentally accessible.

IV. COLLECTIVITY

There are numerous indications that many superheavy nuclei are deformed in their ground states. Theoretical predictions of quadrupole deformations for the transfermium nuclei sum-

marized in (Afanasjev and Abdurazakov, 2013; Heenen *et al.*, 2015) are consistent with quadrupole moment measurements recently extended to $^{252-254}$No (Raeder *et al.*, 2018) and observed large moments of inertia (Greenlees *et al.*, 2012; Herzberg and Greenlees, 2008). As discussed in Sec. V, energies of α particles emitted by superheavy nuclei are impacted by deformation effects. For instance, the measured α-decay energies have provided confirmation of the prolate-deformed subshell closure around $N = 162 - 164$ predicted by theory (Cwiok *et al.*, 1983; Möller and Nix, 1994). The transition towards spherical shapes happens around $N = 184$. In-between located is a transitional region of deformation-soft and triaxial nuclei, exhibiting rich shape isomerism (Agbemava *et al.*, 2015; Bürvenich *et al.*, 1998; Ćwiok *et al.*, 2005; Heenen *et al.*, 2015; Jachimowicz *et al.*, 2017b; Prassa *et al.*, 2012; Ren, 2002). The softness of the potential energy surface (PES) generally grows with the level density at the Fermi level, due to reduced shell effects. Consequently, as the level density increases with increasing system size, deformation softness and shape coexistence become important issues in superheavy nuclei. In addition to that rich deformation scenario, there is another type of coexistence in deformed superheavy nuclei, related to K-isomerism (David *et al.*, 2015; Jachimowicz *et al.*, 2015; Liu *et al.*, 2014; Xu *et al.*, 2004).

As a representative example, the PESs of Og isotopes are shown in Fig. 6. The upper panel of the figure shows a two-dimensional PES in the triaxial quadrupole deformation plane. There are two axial competing minima, prolate ($\gamma = 0°$) and oblate ($\gamma = 60°$) separated by a triaxial barrier. The sequence of the axial PESs in the lower panel illustrates the transition from a well deformed $^{290}\mathrm{Og}_{172}$, over the transitional $^{294}\mathrm{Og}_{176}$, to the spherical $^{302}\mathrm{Og}_{184}$. Increasing the neutron number further, the PESs again become extremely soft and the barriers become so low that these isotopes are expected to have extremely short lifetimes. While topological features of PESs are robust, the barrier heights depend sensitively on both model and parametrization. As a consequence, the predictions for fission lifetimes can differ by many orders of magnitude, see (Agbemava *et al.*, 2017; Brodziński and Skalski, 2013) and Sec. VI. The span of predictions can be reduced by establishing connections with other observables better accessible to experiment, see, e.g., (Reinhard, 2018).

Figure 7 shows the predicted energies of the low-lying 2^+ collective states. The trend confirms again what we have seen in Fig. 6. Namely, the spherical isotopes around $N \approx 184$ show larger energies while the rather soft PESs farther from $N = 184$ yield significantly lower 2^+ excitations. Note that these excitation energies are rather low as compared to the

2^+ states in lighter nuclei. For more discussion of collective excited states in superheavy nuclei, see (Baran and Staszczak, 2013; Mişicu *et al.*, 2002; Sharipov and Ermamatov, 2005; Sun *et al.*, 2008).

Ground-state reflection-asymmetric shapes characterized by octupole deformations are well known in light actinides around $Z = 90, N = 132$ (Butler and Nazarewicz, 1996). They appear as a result of the $\Delta\ell = \Delta j = 3$ coupling between the proton $0i_{13/2}$ and $1f_{7/2}$ and the neutron $0j_{15/2}$ and $1g_{9/2}$ shells. As shown in Fig. 8, the next regions of strong octupole coupling are expected around $N = 196$ ($0k_{17/2}$ and $1h_{11/2}$ neutron shells), $Z = 96$ ($0i_{13/2}$ and $1f_{7/2}$ proton shells), and $Z = 120$ ($0j_{15/2}$ and $1g_{9/2}$ proton shells) (Afanasjev *et al.*, 2018a; Agbemava and Afanasjev, 2017; Erler *et al.*, 2012b; Möller *et al.*, 2008, 1995; Warda and Egido, 2012). However, since the energies of the octupole-driving shells show considerable model dependence, boundaries and extensions of the predicted octupole deformed regions of heavy actinides and superheavy nuclei differ in detail. As discussed in Sec. III, such a situation is typical to superheavy nuclei due to the diffused shell structure (Bender *et al.*, 2001). In any case, reflection asymmetric ground-states are expected to appear in certain regions of superheavy nuclei and can potentially impact their lifetimes (Erler *et al.*, 2012b; Jachimowicz *et al.*, 2017b; Warda and Egido, 2012).

Nuclear structure observables strongly depend on the underlying shell structure. Unfortunately, current empirical shell model potentials as well as self-consistent DFT models do not produce robust, consistent explanations of the steadily-growing body of spectroscopic information on transactinides (Ackermann, 2015; Ackermann and Theisen, 2017; Gates *et al.*, 2015; Herzberg, 2016; Heßberger, 2016; Rudolph *et al.*, 2015, 2013; Theisen *et al.*, 2015). This strong model dependence can be attributed to large single-particle level density and the fact that theoretical input still lacks spectroscopic quality (Dobaczewski *et al.*, 2015; Shi *et al.*, 2014a,b).

V. α DECAY

As discussed in Sec. II, the dominant decay modes of superheavy nuclei are α decay and spontaneous fission. As a result, superheavy nuclei are often identified through α-decay chain analysis (Hofmann and Münzenberg, 2000; Oganessian *et al.*, 2006). Information on the daughter decays comes from both experimental data and theoretical calculations of

the energy of the emitted alpha particle, or Q_α values. In order to properly tune future experiments for the identification of new superheavy nuclei, theoretical predictions of Q_α values are essential.

Numerous calculations of Q_α energies for superheavy nuclei have been performed with microscopic-macroscopic and DFT methods, see, e.g., (Adamian *et al.*, 2018; Agbemava *et al.*, 2015; Bender, 2000; Ćwiok *et al.*, 2005; Ćwiok *et al.*, 1999; Erler *et al.*, 2012b; Gambhir *et al.*, 2005; Jachimowicz *et al.*, 2014; Muntian *et al.*, 2003; Tolokonnikov *et al.*, 2017; Typel and Brown, 2003; Wang *et al.*, 2015; Warda and Egido, 2012); comparisons between the results of these methods have also been carried out (Heenen *et al.*, 2015; Sobiczewski and Pomorski, 2007). Microscopic calculations of α-decay half-lives are demanding since the α-spectroscopic (or preformation) factor is difficult to compute (Id Betan and Nazarewicz, 2012). The commonly-used strategy is to estimate the barrier penetrability by adjusting a core+α potential to reproduce experimental Q_α values, and estimate the reduced widths from measured lifetimes in known nuclei. This approach has resulted in various empirical formulas (Brown, 1992; Budaca *et al.*, 2016; Chowdhury *et al.*, 2008; Dong *et al.*, 2011; Koura, 2012; Muntian *et al.*, 2003; Parkhomenko and Sobiczewski, 2005; Royer and Zhang, 2008; Santhosh and Nithya, 2018b; Viola and Seaborg, 1966) and models (Clark and Rudolph, 2018; Ward *et al.*, 2015) for the α-decay half-life.

In general, predicted Q_α values are fairly robust in the regions away from potential shell closures (Heenen *et al.*, 2015; Sobiczewski and Pomorski, 2007). This is illustrated in Fig. 9 for the α-decay chain of ^{294}Og using several Skyrme-DFT models. For Fl and Lv, the results are within the bounds of the EDFs, while the results for Og are all underestimated. Overall, we observe a reasonable consistency between theoretical predictions. The increase in Q_α up to Cn followed by a sudden drop at Fl is explained by the abrupt shape transition from prolate to oblate deformations (see Fig. 10) through the region of triaxial shapes around $N = 174$ (Ćwiok *et al.*, 2005), see Sec. IV for more discussion.

Figure 10 shows the Q_α values and regions of quadrupole deformations (prolate, oblate, spherical) of the even-even isotopes from Fm to Og predicted with the UNEDF2 model. The shape transition from oblate to spherical shapes is due to the predicted region of spherical shapes and enhanced shell-stability near $N = 184$ (Bender *et al.*, 1999; Ćwiok *et al.*, 1996; Kruppa *et al.*, 2000), see also Secs. III and IV. Also, the large gap in values between Hs and Ds is due to the deformed neutron subshell closure around $N = 164$ (Cwiok *et al.*,

1983; Möller and Nix, 1994). Given the large extrapolations in mass and charge involved, the agreement between experiment and theory is very reasonable. In the future, machine learning techniques relying on the statistical modeling of deviations between experiment and predictions (Neufcourt *et al.*, 2018) have the potential to improve the quality of theoretical extrapolations of Q_α values to unknown superheavy nuclei.

For α-decays involving odd-A, odd-odd nuclei, and isomeric states, half-lives can be significantly increased due to hindrance associated with configuration changes between parent and daughter nuclei (Ćwiok *et al.*, 1999; Xu *et al.*, 2004). Estimates of this hindrance can be found in (Clark and Rudolph, 2018; Delion *et al.*, 2007; Jachimowicz *et al.*, 2018; Ward *et al.*, 2015). In this context, experimental studies of high-K isomers in deformed superheavy nuclei (Ackermann, 2015; Asai *et al.*, 2015; David *et al.*, 2015; Hofmann *et al.*, 2001; Robinson *et al.*, 2011; Sulignano *et al.*, 2012) are of great interest.

VI. FISSION

Although α-decay is the dominant decay mode for all superheavy nuclei which have been observed through their associated α-decay chains, spontaneous fission (SF) often competes with it and terminates the chain. For example, the observed isotopes for Fl and Ts undergo SF after several α emissions (Khuyagbaatar *et al.*, 2014; Utyonkov *et al.*, 2018). Other, more neutron-rich superheavy nuclei are predicted to decay directly via SF (Afanasjev *et al.*, 2018b; Giuliani *et al.*, 2018; Staszczak *et al.*, 2013) (see Fig. 11).

Accurate modeling of nuclear fission – a quantum-mechanical process involving large-amplitude nuclear collective motion – poses enormous challenges to nuclear theory (Schunck and Robledo, 2016). To give just two examples: spontaneous fission half-lives in heavy and superheavy elements span a range of over 35 orders of magnitude (Krappe and Pomorski, 2012), while at the same time, tiny variations of a few percent of specific fission product yields can have a dramatic impact in modeling critical assemblies in nuclear reactors (Gooden *et al.*, 2016). While the fission of actinide nuclei is, at least semi-quantitatively, relatively well understood, superheavy nuclei offer specific challenges. Due to their large atomic numbers, the fissility parameter $x = E_{\text{Coul.}}/2E_{\text{surf.}}$ takes values greater than 1 in the superheavy region, inner fission barriers are generally smaller than in actinides, and outer fission barriers are expected to be low or nonexistent due to increasing Coulomb pressure. Consequently, the

familiar picture of penetration through a double-humped fission barrier (Bjørnholm and Lynn, 1980) undergoes serious revisions in the superheavy region. These revisions have an impact on fission observables such as the SF lifetimes, the distribution of fission fragments, and the characteristics of the fission spectrum (neutrons, γ, β, etc.).

Theoretical estimates of SF lifetimes for superheavy nuclei depend strongly on the computed PESs (see also Sec. IV). A considerable effort has been devoted to systematic predictions of PESs and their saddle points (fission barriers) in the superheavy region (Abusara *et al.*, 2012; Agbemava *et al.*, 2017; Bürvenich *et al.*, 2004; Bürvenich *et al.*, 1998; Erler *et al.*, 2012b; Jachimowicz *et al.*, 2015; Karatzikos *et al.*, 2010; Kowal *et al.*, 2010; Möller *et al.*, 2009; Pomorski *et al.*, 2018; Prassa *et al.*, 2012; Staszczak *et al.*, 2013), including structures of excited configurations in compound nuclei (Pei *et al.*, 2009; Sheikh *et al.*, 2009; Zhu and Pei, 2017); see also (Baran *et al.*, 2015; Heßberger, 2017; Reinhard, 2018) for recent overviews.

Spontaneous fission lifetimes of superheavy nuclei are typically calculated by estimating the tunnelling probability through the multidimensional PES (Brack *et al.*, 1972). While there have been attempts to do this within the macroscopic-microscopic approach (Brack *et al.*, 1972; Gherghescu *et al.*, 1999; Möller *et al.*, 1989; Smolańczuk *et al.*, 1995), a more microscopic description based, e.g., on nuclear DFT, provides more consistency since all of the ingredients for the calculations (PES and collective inertia tensor) are derived from a single energy functional (Baran *et al.*, 2011; Giuliani and Robledo, 2013). Such microscopic calculations of SF lifetimes have become increasingly predictive in recent years (Erler *et al.*, 2012b; Sadhukhan *et al.*, 2016; Schindzielorz *et al.*, 2009; Staszczak *et al.*, 2013; Warda and Egido, 2012). In this context, the prediction of SF lifetimes depends upon several factors, such as the nuclear zero-point energy, the number of collective coordinates considered, and nuclear pairing (Giuliani *et al.*, 2014; Reinhard, 2018; Rodrıguez-Guzmán and Robledo, 2017; Sadhukhan *et al.*, 2014; Zhao *et al.*, 2016).

Figure 11 shows a comprehensive theoretical survey of the dominant decay modes of superheavy nuclei calculated within the Skyrme-DFT framework (Staszczak *et al.*, 2013) (see also (Erler *et al.*, 2012b; Warda and Egido, 2012) for other results). A region of superheavy isotopes with very short SF lifetimes is predicted in a corridor separating the upper and lower region of superheavy nuclei. This is consistent with systematics of experimental SF lifetimes (Oganessian and Utyonkov, 2015a), which show the minimum of SF lifetimes at

^{282}Cn.

Similar to the case of α-decay discussed in Sec. V, SF lifetimes are expected to be substantially increased in many-quasiparticle states of superheavy nuclei, such as levels of odd-A nuclei or low-lying K-isomers, see (David *et al.*, 2015; Jachimowicz *et al.*, 2015; Liu *et al.*, 2014; Rodrıguez-Guzmán and Robledo, 2017; Xu *et al.*, 2004). This opens an intriguing possibility of existence of very long-lived isomers of superheavy isotopes.

An interesting, albeit yet experimentally unexplored, decay mode of superheavy nuclei is cluster radioactivity. This phenomenon, first observed in 1984 (Rose and Jones, 1984) as the emission of ^{14}C from ^{223}Ra, has since been confirmed in a number of heavy nuclei with $Z > 86$, which decay by emitting light clusters between ^{14}C and ^{34}Si, as well as in superheavy nuclei with $Z \leq 116$ (Itkis *et al.*, 2015; Kozulin *et al.*, 2014). For superheavy nuclei with $Z \geq 118$, cluster radioactivity is expected to become competitive with alpha decay and spontaneous fission (Poenaru and Gherghescu, 2018; Poenaru *et al.*, 2011, 2012, 2013, 2015; Santhosh and Nithya, 2018a; Zhang and Wang, 2018). Microscopically, cluster emission can be considered as an extremely asymmetric fission, with the heavy fragment corresponding to a nucleus in the neighborhood of the doubly-magic ^{208}Pb (Warda and Robledo, 2011). Nuclear DFT calculations (Warda and Robledo, 2011; Warda *et al.*, 2018) of nuclei with the same N/Z ratio as known cluster emitters clearly show a lowering of the cluster-decay potential energy valley with respect to the fission valley as Z increases.

The nucleus ^{294}Og is expected to be an excellent candidate for cluster radioactivity as the emitted cluster is the magic nucleus ^{86}Kr with $N = 50$, and consequently the asymmetric channel is expected to be particularly favored (see Fig. 12) (Baran *et al.*, 2015; Matheson *et al.*, 2018; Warda and Egido, 2012). The corresponding SF half-life is predicted to be $\sim$13 minutes (Staszczak *et al.*, 2013). This should be compared with the measured α-decay half-live of 580 μs (Brewer *et al.*, 2018).

VII. CHEMISTRY AND RELATIVISTIC EFFECTS

It was long assumed that electrons in valence shells responsible for chemical properties are not affected much by relativistic effects because valence electrons move rather slowly as compared to the velocity of light (Dirac, 1929; Glashow, 1993), i.e., $v_{\rm val} \ll c$ should hold for all elements in the periodic table including the latest superheavy additions. While in a

classical sense this is correct, quantum theory tells us that this simple picture is insufficient and that even "slow moving" valence electrons have a substantial electron density close to the nucleus where relativistic perturbation operators act. Low angular momentum wave functions, such as s-orbitals, are therefore directly affected by these operators, and are drawn inwards by their tails (the direct relativistic effect) resulting in an orbital contraction and stabilization. In fact, it has been known since the 1970s that relativistic perturbation operators act almost exclusively in the K-shell region (Dzuba *et al.*, 1983; Schwarz *et al.*, 1989; Sobel'Man, 1972). This indicates that relativistic effects are intertwined throughout the whole electron cloud and cannot be argued away only by energetic arguments. In the following, we will address three important relativistic effects taking place in super-heavy atoms.

The first relativistic effect is related to the $1s$ state and overall stability of the atom. Relativistic quantum theory for fermions is fundamentally based on the Dirac equation. For hydrogen-like atoms with a point-like nucleus, the discrete spectrum of the Dirac operator is given by the Sommerfeld fine-structure formula:

$$\frac{E_{nk}}{mc^2} = \left(1 + \frac{(Z\alpha)^2}{\left[n - k + \sqrt{k^2 - (Z\alpha)^2}\right]^2}\right)^{-1/2}, \tag{1}$$

where $k = j + \frac{1}{2}$. The positive- and negative-energy continuum corresponds to $E \geq mc^2$ and $E \leq -mc^2$, respectively. We immediately see that for $Z \to 1/\alpha$ the ground-state energy $E_{1,1} \to 0$. Beyond this limit, the lowest energy eigenvalue becomes imaginary (the so-called $1s$ catastrophe). That is, the $1s$ level should be viewed as a resonance embedded in the negative energy continuum. While this does not strictly hold for multi-electron systems, the screening of the nuclear charge by all electrons in an atom is not sufficient and will only slightly shift the $Z_c = 1/\alpha \approx 137$ limit. While this caused some concern in the relativistic electronic structure community more than 30 years ago, predicting that the Dirac equation fails in the superheavy element region, it was pointed out early (Pomeranchuk and Smorodinsky, 1945) that the finite size of the nucleus increases the value of critical nuclear charge at which the catastrophe occurs to $Z_c = 169$. In this case, however, for known functional forms of the nuclear charge distribution, analytical eigenvalues are no longer available (Andrae, 2000).

The second relativistic effect concerns contraction of outer shells. In addition to inter-

pretational difficulties with the Dirac equation, it initially came as a surprise that the outer ns-shells with higher principal quantum number n can undergo large relativistic contractions when compared to the inner ns-shells with low n values (Desclaux and Pyykkö, 1976; Pitzer, 1979; Pyykkö and Desclaux, 1979) thus contradicting the original orthogonality argument that the outer shells contract only because of the inner-shell contractions (Pyykkö, 1988). However, these shell effects can be rather subtle and strongly dependent on the nuclear charge Z, quantum numbers $(n\ell j)$, and shell occupancies (Autschbach *et al.*, 2002; Schwarz *et al.*, 1990).

Figure 13(a) demonstrates this nicely for the ratio $q_{n\ell j} = \langle r \rangle^{\rm R}_{n\ell j} / \langle r \rangle^{\rm NR}_{n\ell j}$ of the relativistic (R) to nonrelativistic (NR) $\langle r \rangle_{n\ell j}$ expectation values for the element Cn ($Z = 112$; [Rn]$5f^{14}6d^{10}7s^2$ configuration). The rather large $7s$ valence shell contraction (stabilization) shown in the figure makes Cn chemically more inert compared to the lighter congener Hg (Eichler *et al.*, 2008; Gaston *et al.*, 2007; Pitzer, 1975; Steenbergen *et al.*, 2017a), where relativistic effects are known to be large; they are responsible for Hg being the only elemental liquid metal at room temperature (Calvo *et al.*, 2013; Steenbergen *et al.*, 2017b). Relativistic effects are also responsible for changing the ground-state configuration of Rg ($Z = 111$) from $6d^{10}7s^1$ ($^2S_{1/2}$) to $6d^97s^2$ ($^2D_{5/2}$) and halving its atomic size, making Rg as small as copper in the same periodic group (Eliav *et al.*, 1994).

The rather large ns-shell contractions/stabilizations observed for the Group 11 and 12 elements (compared for example to the Group 1 and 2 elements) originates from the occupation of the lower-lying diffuse $(n-1)d$-shell, which does not efficiently screen the nucleus, thus increasing the effective nuclear charge $Z_{\rm eff}$ experienced by the valence ns electrons. Figure 13 clearly shows the predicted rather large valence $7s$ shell contraction in Cn compared to the $8s$ shell contraction in element $Z = 120$. Moreover, direct shell contractions (mainly the ns and $np_{1/2}$ shells) lead to additional screening of the nucleus. which lowers the effective nuclear charge $Z_{\rm eff}$ and results in an expansion/destabilization of the more diffuse higher angular momentum states such as the f, g- and $d_{5/2}$ orbitals (known as the indirect relativistic effect) (Pyykkö, 1988). The $p_{3/2}$ and $d_{3/2}$ orbitals may contract or expand depending on the nuclear charge and shell occupancy. A more detailed discussion about these subtle shell-structure effects can be found in (Autschbach *et al.*, 2002).

The third principal relativistic effect comes from the fine-structure splitting (mainly *spin-orbit coupling*) of orbitals with angular momentum $\ell > 0$ (Pyykkö, 1988). For Og^+, the

$^2P_{3/2} - {}^2P_{1/2}$ splitting is 10.1 eV at the Fock-space coupled-cluster level (Jerabek *et al.*, 2018), i.e., it is larger than most bond dissociation energies. The relativistic $7p_{3/2}$ expansion/destabilization ($q_{7p_{3/2}} = 1.052$ for neutral Og) and the large relativistic $8s$ contaction/stabilization ($q_{8s} = 0.739$ for Og in the $7p_{3/2}^3 8s^1$ configuration) lead to a positive electron affinity of 0.064 eV (with a sizeable QED correction of −0.006 eV) (Goidenko *et al.*, 2003), a novelty within Group 18 of noble gases. Spin-orbit effects make flerovium a closed shell atom ([Rn]$5f^{14}6d^{10}7s^2p_{1/2}^2$ configuration) with zero electron affinity (Borschevsky *et al.*, 2009), and chemically more inert compared to the lighter Group 14 elements (Pitzer, 1975). The large $p_{1/2}/p_{3/2}$ separation for all shells in a superheavy element is also reflected in the q_{np} values shown in Fig. 13.

A. Atomic and chemical properties of superheavy elements: experiment and theory

The chemistry of superheavy elements and the influence of relativistic effects have been reviewed in, e.g., (Pershina, 2015; Schädel, 2006, 2015; Schwerdtfeger *et al.*, 2015; Türler and Pershina, 2013). In the following, we emphasize those chemical and physical properties of the superheavy elements that are strongly influenced by relativistic shell-structure effects leading to anomalies and often unexpected features when comparison is made to their lighter congeners in the periodic table (Schwerdtfeger and Seth, 1998). So far, chemical experiments at the atom-at-a-time scale have only been carried out for transactinides up to Hs (Nagame *et al.*, 2016; Türler and Pershina, 2013) and for Cn and Fl (Eichler *et al.*, 2008, 2010; Yakushev *et al.*, 2014), which all have reasonably long-lived isotopes in the time range of seconds.

Experimental studies giving direct information about the electronic shell structure are only available up to the heaviest actinides including Fm, No, and Lr (Chhetri *et al.*, 2017, 2018; Laatiaoui *et al.*, 2016; Raeder *et al.*, 2018; Sato *et al.*, 2015; Sewtz *et al.*, 2003). However, optical lines of actinide atoms up to Es have been identified in the Visual Echelle Spectrography of the main-sequence star HD 101065 (Przybylski's star) (Gopka *et al.*, 2008). It may thus be speculated that the spectra of neutron-rich superheavy elements created in neutron star mergers or supernovae can be observed (see Sec. IX). This requires accurate theoretical predictions of atomic spectra for superheavy elements, which currently is a major challenge for open-shell many-electron systems (Sewtz *et al.*, 2003). In this context,

large isotope shifts and hyperfine structure in electronic spectra of superheavy elements are investigated in (Dzuba *et al.*, 2017), comparing different isotopes measured in the laboratory (which are neutron-poor) with those in interstellar space (which are mostly stable and neutron-rich). The reach of laser spectroscopy measurements of isotope shifts and nuclear moments in the heaviest elements corresponds to $^{252-254}$No (Raeder *et al.*, 2018). The electronic spectrum of neutral Og was computed in (Lackenby *et al.*, 2018).

Precision mass measurements of unstable atoms provide a direct measure of the nuclear and electronic binding energy. Direct mass measurements of transfermium nuclei have been carried out with the Penning trap mass spectrometer for $^{252-255}$No and ^{255,256}Lr (Block *et al.*, 2010; Ramirez *et al.*, 2012). Recently mass excesses of several transfermium nuclei were obtained by means of time-of-flight mass spectrometry (Ito *et al.*, 2018), which enabled mass determination of heavier nuclei, up to ^{261}Bh and ^{266}Mt. The mass of an atom M_A can be decomposed into $M_A = Z(m_p + m_e) + Nm_n - (B_{\rm nuc} + B_{\rm el})/c^2$, where m_p, m_e and m_n are, respectively, proton, electron, and neutron masses known to high precision, and $B_{\rm nuc}$ and $B_{\rm el}$ are the nuclear and electronic binding energies. It is to be noted that the electronic binding energy is not negligible for superheavy elements. For instance, for Og the Dirac-Coulomb Hartree-Fock calculations predict $B_{\rm el}$=1.487 MeV. At the nonrelativistic level the electronic binding energy is significantly smaller, $B_{\rm el}^{\rm NR}$= 1.260 MeV. The difference of 0.227 MeV originates mostly from the inner shells close to the nucleus (Jerabek *et al.*, 2018). Interestingly, the electron density gets smeared out due to relativistic effects, making the valence electron cloud of Og a Fermi-like gas as Fig. 14 illustrates.

Gas phase chromatographical set-ups can be easily coupled to accelerators and are ideal to study the volatility of superheavy elements (Gäggeler, 2011). Most recent adsorption studies of Cn and Fl on gold surfaces suggest that both elements bind weakly to the surface, i.e., $-\Delta H_{\rm ads}$(Au) (in kJ/mol) = 98±3 (Hg) (Soverna *et al.*, 2005), 52^{+4}_{-3} (Cn) (Eichler *et al.*, 2008), ≥48 (Fl) (Yakushev *et al.*, 2014), and 20 (Rn) (Soverna *et al.*, 2005). This is in good agreement with the latest theoretical studies (Pershina, 2018; Pershina *et al.*, 2009, 2008a,c; Rampino *et al.*, 2015). From an empirical relationship between $\Delta H_{\rm ads}$(Au) and the cohesive energy of the bulk material $E_{\rm coh}$, one estimates $E_{\rm coh}$= 38^{+10}_{-12} kJ/mol for Cn (Eichler *et al.*, 2008). This agrees with the recent incremental relativistic coupled-cluster theory (Steenbergen *et al.*, 2017a), which yields $E_{\rm coh}$= 39.6 kJ/mol. Consequently, Cn is predicted to be rather volatile (Pershina *et al.*, 2010) with an expected melting point around

that of Hg, but perhaps being still a liquid at standard conditions. For Fl only very few atoms were identified on a gold surface, and the predictions are not yet accurate enough to determine $\Delta H_{\rm ads}$(Au). Recent solid-state calculations using relativistic density functional theory predict $E_{\rm coh}$= 48.6 kJ/mol (Yakushev *et al.*, 2014), in rather good agreement with the experimental estimated value (Hermann *et al.*, 2010). Thus one might speculate that Fl is liquid at room temperature. The possibility of future adsorption experiments of Nh on an inert surface has been explored theoretically (Pershina, 2016; Pershina *et al.*, 2008b).

Relativistic effects can have a decisive influence on the stability of oxidation states. For example, the relativistic $7s$ stabilization together with the indirect relativistic $6d_{5/2}$ destabilization support efficient *sd*-mixing in chemical bonding, thus stabilizing higher oxidation states in compounds of Rg (as high as the oxidation state +5 in RgF_6^-) (Seth *et al.*, 1998a), Cn (oxidation state +4 like in CnF_4) (Seth *et al.*, 1997), and possibly also for Ds (Waber and Averill, 1974). In contrast, the strong relativistic $7s$ stabilization diminishes *sp* mixing in chemical bonding for the $7p$ block elements (known as the relativistic inert pair effect (Schwerdtfeger *et al.*, 1992)), and thus reduces the stability of high oxidation states in Nh and Fl (and possibly in Mc as well) (Schwerdtfeger and Seth, 2002; Seth *et al.*, 1998b, 1999). In contrast to XeF_6, which has been isolated and identified (Hoyer *et al.*, 2006), the large spin-orbit splitting between the $7p_{1/2}$ and $7p_{3/2}$ levels will most likely restrict the oxidation state in Og to +4. Note that spin-orbit effects change the structure of OgF_4 from the expected D_{4h} symmetry to T_d (Nash and Bursten, 1999).

B. Bulk properties of superheavy elements

Thermodynamic properties of the bulk superheavy elements from Nh to Og have been predicted empirically by extrapolation in (Bonchev and Kamenska, 1981), and for Ts and Og in (Takahashi, 2002). From these it is expected that Fl and element 119 could be either liquid or solid under normal conditions, and Og is a gas. On the other hand, based on atomic polarizability arguments (Nash and Bursten, 1999) Og is likely to be solid at room temperature. Indeed, Og is calculated to have a rather high dipole polarizability (α_d= 58.0 a.u.) as compared to the other rare gas elements, which increases dispersive interactions (Jerabek *et al.*, 2018). Methods are now available for the accurate determination of bulk properties including phase transitions for the rare gas elements (Pahl *et al.*, 2008;

Schwerdtfeger, 2016; Schwerdtfeger and Hermann, 2009). For example, density functional theory predicts solid state properties for the $6d$ metals from Lr to Rg (Gyanchandani and Sikka, 2011). According to these calculations, the next nearest neighbor distance in the solid is $R(5d) < R(6d)$ for the elements within the same group of the periodic table; hence, no evidence for strong relativistic effects are expected for this quantity in contrast to many other chemical properties (Iliaš and Pershina, 2017; Pershina, 2002; Türler and Pershina, 2013; Wang *et al.*, 2016). Recently, using parallel tempering Monte-Carlo simulations within a many-body expansion for the atomic interaction potential (Smits *et al.*, 2018), it was possible to confirm the melting temperature of $T_m = 202\,\mathrm{K}$ of ^{222}Rn originally measured in 1909 (Gray and Ramsay, 1909). Preliminary simulations suggest $T_m \approx 320\,\mathrm{K}$ for Og (Smits *et al.*, 2018). For Cn and Fl, many-body effects in the interaction potential are so important that melting simulations become prohibitively expensive (see recent successful simulations for Hg (Steenbergen *et al.*, 2017b)).

VIII. BEYOND $Z = 120$: EXTENDED PERIODIC TABLE

The first attempt to extend the periodic table beyond element 120 goes back to (Mann, 1969; Mann and Waber, 1970). Soon afterwards it was pointed out (Fricke *et al.*, 1971) that beyond element 120 the $7d_{3/2}, 8_{p1/2}, 6f_{5/2}$ and $5g_{7/2}$ shells are expected to be filled more or less simultaneously, making a clear placement in the periodic table difficult. They predicted the filling of the $5g$-shell to be complete at element 144, whereas a newer version of the periodic table proposed by Pyykkö completes the g-shell filling at element 138 (Pyykkö, 2011; Pyykkö, 2016). Clearly, accurate multi-reference configuration interaction calculations are required to determine the correct ground state of the elements beyond Z=120 (Lu *et al.*, 1971). Accurate Fock-space coupled-cluster calculations for the superheavy elements 121 and 122 (Eliav *et al.*, 2015) show that the ground states are ${}^2P_{1/2}(8s^2 8p_{1/2})$ for element 121 and $8s^2 7d_{3/2} 8p_{1/2}(J = 2)$ for element 122 (with the $8s^2 8p_{1/2}^2$ state being close in energy with ΔE=0.185 eV). Thus, according to (Eliav *et al.*, 2015), the g-shell is not occupied up to $Z = 122$. In earlier Hartree-Fock-Slater calculations, g-shell occupation starts at element 125 (Lu *et al.*, 1971; Mann, 1969; Mann and Waber, 1970). Note that for element 140 the ground-state configuration could either be $8s^2 8p^2 7d^1 6f^3 5g^{14}$ or $8s^2 8p^4 6f^1 5g^{15}$ according to (Indelicato *et al.*, 2011). Such calculations are already at the limit of available computer resources due

to the huge number of possible configurations involved. In spite of the difficulties of correctly placing superheavy elements into the periodic table, a new periodic table was obtained in (Pyykkö, 2011; Pyykkö, 2016) from average level multireference Dirac-Fock calculations with successive occupation of electronic shells as shown in Fig. 15. The anomalies to the Madelung rule (Wong, 1979) shown in the figure are due to the strong spin-orbit stabilization of the $8p_{1/2}$ and $9p_{1/2}$ shells.

Little is known about the chemistry of the elements beyond Z=120 (Fricke *et al.*, 1971). The Dirac-Coulomb DFT calculations for the hexafluorides of the elements 125-129 (Dognon and Pyykkö, 2017) suggest g-level occupations for these compounds. However, besides the relativistic expansion of the $5g$ orbitals (for 140^{2+} with a full g-shell one predicts $q_{5g_{7/2}} = 1.190$ and $q_{5g_{9/2}} = 1.394$), the g-electrons do not participate in the chemical bonding and are therefore core-like, similar to the $4f$-electrons in the lanthanide series.

A. At and beyond the critical nuclear charge

As discussed in Sec. VII, the current electronic shell structure predictions end at elements with critical nuclear charge $Z_{\rm crit} \sim 172 - 173$, where the lowest $1s$ level enters the negative energy continuum (supercritical region) as predicted by a mean-field treatment of the Dirac equation (Indelicato *et al.*, 2011; Pomeranchuk and Smorodinsky, 1945; Schwerdtfeger *et al.*, 2015), see Fig. 16. In multi-electron systems, since the nucleus becomes screened by all the electrons including those in higher $(n\ell j)$ shells, $Z_{\rm crit}$ shifts to slightly larger values. In this supercritical region, the small (lower) component of the Dirac spinor becomes appreciable as shown in Fig. 17, and the terms "small" and "large" for the two Dirac components are no longer valid. Near the critical nuclear charge, the single-particle approximation (e.g., Dirac-Coulomb-Hartree-Fock) breaks down and a proper treatment involves the full QED Lagrangian. Moreover, in strong Coulomb fields, the $Z\alpha$ expansion used to treat QED shifts for one-particle levels also breaks down (Soff *et al.*, 1982). Nonetheless, effective QED operators obtained at nuclear charges $Z \ll 137$ are usually continued into the highly nonperturbative domain (Indelicato *et al.*, 2011; Schwerdtfeger *et al.*, 2015). It was noted that QED corrections to the $1s$ level for $Z \sim 172$ are rather small compared to $2m_ec^2$ as self-energy and vacuum-polarization contributions almost cancel out in such supercritical fields (Soff *et al.*, 1982).

The extension of the periodic system into new areas has been investigated in (Greiner, 2008), who hypothesized that in the supercritical region with $Z \sim 172 - 173$, where the $1s$ state becomes a resonance embedded in the negative-energy continuum of the Dirac equation, spontaneous e^+e^- pair creation becomes possible because of vacuum fluctuations (Gershtein and Zel'dovich, 1969; Pieper and Greiner, 1969; Reinhard *et al.*, 1971). In a simple picture, an electron from the Dirac sea occupies the $1s$ state leaving a hole in the sea, which escapes as a positron while the electron's charge remains near the source. In this process, energy is conserved because the occupation of the $1s$ level frees up an energy of $> 2mc^2$. One can view this as the inverse pair annihilation, which is well described by ordinary Feynman diagrams. From the energy-time uncertainty principle one can estimate that such a process would happen on the time scale of $\sim 10^{-21}$ s. Since the $1s$ orbit is occupied by two electrons, the inverse pair annihilation can happen twice. However, once the $1s$ state becomes doubly occupied, the vacuum becomes stable due to the Pauli principle (Greiner, 2008; Müller-Nehler and Soff, 1994; Reinhardt *et al.*, 1981). We note that the e^+e^- pair creation process has never been observed in a collision of atoms with high nuclear charges (Ahmad *et al.*, 1997, 1999), and may require collision experiments with fully stripped ions. The electron-positron pair creation in low-energy collisions of heavy bare nuclei has been investigated only recently (Maltsev *et al.*, 2015).

It is currently unclear how to accurately treat single- or multi-electron systems beyond $Z_{\rm crit}$. However, there are no compelling arguments suggesting that $Z_{\rm crit}$ should determine the end of the electronic shell stability and therefore the end of the periodic table, even though Pyykkö's analysis ends at $Z_{\rm crit}$ (Pyykkö, 2011).

B. Nuclear physics and the limits of the periodic table

The existence of elements with $Z > 118$ also depends on nuclear physics. For instance, as the $1s$ density starts to accumulate around the nucleus in strong Coulomb fields (see Fig. 17), the probability of electron capture increases. One might speculate that the most difficult hurdle to the stabilization of the electronic $1s$ shell as one gets closer to $Z_{\rm crit}$, and ultimately the cause of the end of the superheavy elements, could be K-capture (Schwerdtfeger *et al.*, 2015).

Another important factor that needs to be considered is the huge difference between elec-

tronic and nuclear timescales. According the report of the *Transfermium Working Group* (Wapstra *et al.*, 1991), in order to talk about a new element, the corresponding nuclide with an atomic number Z must exist for at least 10^{-14} s, which is a reasonable estimate of the time it takes a nucleus to acquire its outer electrons, bearers of the chemical properties. Consequently, if for all isotopes of some superheavy element, including isomeric states (Heenen *et al.*, 2015; Jachimowicz *et al.*, 2017a), nuclear lifetimes are shorter than 10^{-14} s, the corresponding element does not exist. On the other hand, in order to define a nuclide, its lifetime should be longer then the single-particle time scale $T_{\mathrm{s.p.}} \approx 1.3{\cdot}10^{-22}$ s (Goldanskii, 1966; Thoennessen, 2004) that corresponds to the time scale needed to create the nuclear mean field. Consequently, there is no chemistry for nuclides with lifetimes between 10^{-14} s and 10^{-22} s.

Unfortunately, reliable predictions of lifetimes of nuclei with $Z > 118$ are currently not available, primarily due to difficulties related to the assessment of Coulomb frustration effects on fission. Indeed, since it is difficult to say at present whether the exotic topologies of nuclear density illustrated in, e.g., Fig. 5 can occur as long-lived (metastable) states, the limits of nuclear mass and charge are presently unknown (Afanasjev *et al.*, 2018b; Brodziński and Skalski, 2013). It is thus possible that the periodic table will end well before reaching Z_{crit} for purely nuclear reasons (Gambhir *et al.*, 2015).

IX. COSMIC ORIGIN OF SUPERHEAVY NUCLEI

The heavy elements of Es and Fm were discovered in 1952 in the debris from the thermonuclear explosion conducted at Eniwetok Atoll in the Pacific Ocean. The fermium nucleus was made through the capture of 17 neutrons by ^{238}U followed by subsequent beta decays (Ghiorso, 2003; Seaborg, 1959). In nature, a similar process known as the rapid neutron-capture process (or r-process) is invoked in order to explain the existence of roughly half of the nuclei heavier than iron, including all of the actinides (Burbidge *et al.*, 1957; Cameron, 1957; Cowan *et al.*, 1991). This nucleosynthesis process occurs in astrophysical scenario(s) where the timescale for neutron capture is much shorter than the timescale for beta decay (Arnould *et al.*, 2007; Qian and Wasserburg, 2007). The recent observation of the electromagnetic transient associated with the GW170807 neutron star merger (Abbott *et al.*, 2017; Pian *et al.*, 2017) confirmed that material with high opacities can be produced during such

events, suggesting neutron star mergers as primary candidate sites for hosting the r-process (Davies *et al.*, 1994; Eichler *et al.*, 1989; Lattimer and Schramm, 1974, 1976; Symbalisty and Schramm, 1982). Numerical simulations show that high neutron densities can be achieved in the dynamical ejecta of this astrophysical scenario (Bauswein *et al.*, 2013; Goriely *et al.*, 2011; Kasen *et al.*, 2017; Korobkin *et al.*, 2012; Radice *et al.*, 2016; Rosswog *et al.*, 1999; Sekiguchi *et al.*, 2015) and in the accretion disk formed after the merging of two neutron stars (Fernández *et al.*, 2018; Siegel and Metzger, 2017a,b). These high neutron densities allow the seed nuclei that are present in the environment to undergo multiple neutron captures before beta decaying, leading to the synthesis of neutron-rich nuclei (see also (Freiburghaus *et al.*, 1999; Goriely, 2015; Lippuner and Roberts, 2015; Mendoza-Temis *et al.*, 2015; Thielemann *et al.*, 2017)). The termination of the r-process path is determined by the region of the nuclear chart where fission is the dominant decay mode and where the fragments produced cycle the material to lower mass regions (Beun *et al.*, 2008; Panov *et al.*, 2005). The fundamental question of whether superheavy nuclei can be produced in nature is thus intrinsically related to determining which neutron-rich nuclei are stable against fission.

During the initial phase of the r-process, the main competing decays are neutron captures, beta decays and, for fissioning nuclei, neutron-induced fission (Martínez-Pinedo *et al.*, 2007; Panov, 2016, 2018; Panov and Thielemann, 2004). As long as neutron captures dominate over neutron-induced fission, the r-process path can proceed towards heavier and more neutron-rich regions of the nuclear chart, but as soon as it enters in a region of low fission barriers, the fragments formed in fission are cycled back (Beun *et al.*, 2008). Since the excitation energy of a nucleus after capturing a low-energy neutron is roughly given by the neutron separation energy, the competition between neutron captures and fission barriers is roughly driven by the difference between the height of the fission barrier and the neutron separation energy $B_f - S_n$ (Panov *et al.*, 2010). Several systematic calculations of the fission properties of r-process nuclei showed that close to the neutron drip line, fission barriers tend to increase with increasing neutron number, leading to positive values of $B_f - S_n$ (Giuliani *et al.*, 2018; Möller *et al.*, 2015; Petermann *et al.*, 2012). This suggests that the production of heavier nuclei could be enhanced if the r-process path proceeds closer to the neutron drip line, where neutron-induced fission is hindered. While superheavy nuclei produced in the r process are expected to be short-lived, they may impact the observed r-process abundances and electromagnetic transients produced by the radioactive decay of r-process

nuclei (kilonova) (Wanajo, 2018; Wu *et al.*, 2018; Zhu *et al.*, 2018).

Because of the competition between neutron capture, neutron-induced fission, and beta decay, the neutron number $N = 184$ may play a major role in determining the production of superheavy nuclei (Martínez-Pinedo *et al.*, 2007). Indeed, as discussed in Sec. IV, most nuclear models predict the region of increased shell stability around $N = 184$. Consequently, the neutron separation energy sharply drops for $N > 184$; this pushes the material towards nuclei with higher proton number ($Z \sim 100$), where several nuclear structure models predict nuclei with rather low fission barriers (Baran *et al.*, 2015; Erler *et al.*, 2012b; Giuliani *et al.*, 2018; Goriely, 2015; Möller *et al.*, 2015). As shown in Fig. 18, low fission barriers could prevent the production of nuclei beyond $N = 184$ due to neutron-induced fission.

In spite of the general lowering of fission barriers above $N = 184$, some r-process simulations show that for a particular combination of nuclear masses and fission barriers, nuclei with $Z \geq 104$ could be produced during the first seconds of the r-process (Petermann *et al.*, 2012). In this case, other fission channels that could prevent the formation of superheavy nuclei are beta-delayed fission and spontaneous fission (Erler *et al.*, 2012b; Korneev and Panov, 2011; Mumpower *et al.*, 2018; Panov *et al.*, 2013; Thielemann *et al.*, 1983b). The beta-delayed fission channel is powered by the large Q_β value of neutron-rich nuclei, which can populate the daughter nuclei at excitation energies close to the fission barrier (Mumpower *et al.*, 2018; Thielemann *et al.*, 1983a). Moreover, a region of vanishing fission barriers is predicted around $Z/N \approx 104/188$ where spontaneous fission becomes the dominant decay channel (Erler *et al.*, 2012b; Giuliani *et al.*, 2018). This region seems to cross the beta-decay path of superheavy nuclei produced during the r-process, thus blocking their decays towards stability.

The successful synthesis of superheavy nuclei in the laboratory revived the question of whether these nuclei can be found in nature. There have been searches for traces of superheavy elements in astrophysical data, including galactic cosmic rays, meteorites, and terrestrial ores (Donnelly *et al.*, 2012; Ter-Akopian and Dmitriev, 2015). In galactic cosmic ray studies, the most conclusive results were obtained by extracting olivine crystals from pallasite meteorites and analyzing the deposited nuclear tracks (Perelygin *et al.*, 2003a,b; Polukhina, 2012). A recent study from the OLIMPIYA experiment claimed that three tracks belonging to superheavy nuclei with charge number 119^{+10}_{-6} have been found in meteorite olivine crystals (Alekseev *et al.*, 2017), but this result has not yet been confirmed

by independent studies. In another development, the search for superheavy elements in terrestrial and extraterrestrial samples was carried out with accelerator mass spectrometry techniques (Dellinger *et al.*, 2011; Korschinek and Kutschera, 2015) but the outcome of those investigations has been negative so far. In short, in spite of numerous efforts, no definitive proof of existence of superheavy nuclei in nature has been found (Ter-Akopian and Dmitriev, 2015).

X. PERSPECTIVES AND EXPECTATIONS

There is an exciting world beyond oganesson; major expansions of the nuclear chart and periodic table are on the horizon. In the short term, the search for the new elements $Z = 119$ and 120 will be carried out in several laboratories (Düllmann, 2016, 2017a; Heßberger and Ackermann, 2017; Hofmann *et al.*, 2016; Roberto and Rykaczewski, 2018). The reactions considered involve beams of ^{44}Ca, ^{50}Ti, ^{51}V, ^{54}Cr, ^{58}Fe, and ^{64}Ni (Adamian *et al.*, 2018; Düllmann, 2016; Hofmann, 2015; Hofmann *et al.*, 2016; Li *et al.*, 2018; Liu and Bao, 2013; Nasirov *et al.*, 2011; Wang *et al.*, 2012; Zagrebaev and Greiner, 2015; Zhu *et al.*, 2014), and actinide targets (Roberto *et al.*, 2015; Roberto and Rykaczewski, 2018).

Since the lower and upper superheavy regions are still disjointed experimentally, i.e., they are not connected by known decays, the Z and A assignments of superheavy nuclei produced in hot-fusion reactions rely on indirect techniques. Another short-term goal is, therefore, to connect these two superheavy regions to provide a direct mass/charge identification. This can be achieved through, e.g., X-ray spectroscopy (Ackermann, 2015; Rudolph *et al.*, 2013) and direct mass measurements (Gates, 2016; Gregorich, 2016). Recently, the first direct measurements of the mass numbers of ^{288}Mc and ^{284}Nh were carried out at Berkeley (Gates *et al.*, 2018), confirming the previous (indirect) mass-number assignments.

The excursion towards the $N = 184$ region of longer-lived superheavies is the longer-term goal. Current experimental lifetimes are indicative of increasing stability for $Z > 110$ when adding neutrons. But to get closer to $N = 184$ is not going to be easy. To find the optimal production methods, systematic fusion reaction studies are being carried out (Hinde *et al.*, 2017; Itkis *et al.*, 2015; Khuyagbaatar *et al.*, 2018; Loveland, 2016). One proposed route involves an enriched ^{251}Cf target and ^{58}Fe beam (Rykaczewski *et al.*, 2016). Reactions using multi-nucleon transfer and radioactive neutron-rich beams are also being considered

(Karpov *et al.*, 2018; Loveland, 2007; Schädel, 2016; Zagrebaev and Greiner, 2008). Here, the challenge for theory is to develop predictive models of superheavy nuclei production, capable of guiding future experimental searches (Giardina *et al.*, 2018; Zagrebaev and Greiner, 2015).

Another major challenge will be in atomic structure calculations at the accuracy of a few wave numbers including accurate values for transition dipole moments. Here, sophisticated electron correlation frameworks including quantum electrodynamic effects are required to correctly predict the dense valence-electron spectrum of superheavy elements, required for future experimental atom-at-a-time studies (Sewtz *et al.*, 2003) in, e.g., cold traps. While such an accuracy has been already achieved for closed-shell atoms or for few-valence electron systems (Eliav *et al.*, 2015; Pašteka *et al.*, 2017; Schwerdtfeger *et al.*, 2015), and even for small closed-shell molecules with lighter atoms (Owens *et al.*, 2018, 2015), this is not yet the case for complex multi-electron, open-shell systems where a very large multi-reference and configuration-interaction space within a relativistic and QED framework is required to correctly describe both static and dynamic electron correlation effects. Such calculations will give a deep insight into the electronic shell structure with the correct predition of ground-state symmetry (configuration) for the superheavy elements beyond oganesson, and into the regime of the critical nuclear charge $Z_{\rm crit}$. The correct description of the elements beyond $Z_{\rm crit}$ involves the treatment of resonance states, which are well established for the positive energy continuum (Fossez *et al.*, 2016; Jagau *et al.*, 2015).

On the chemical side, experimental studies of Cn and Fl have illuminated the importance of relativistic effects on the properties of superheavy atoms, thus making the search for chemistry beyond the standard periodic table the major science driver. Here fully relativistic quantum calculations, including QED effects, will continue providing guidance and stimulation for future atom-at-a-time experiments. The accurate simulation of the chemistry of superheavy elements in solution, gas-phase and the bulk, or adsorbed on surfaces, with both density functional and wave-function-based methods, using relativistic pseudopotential theory including QED (Hangele *et al.*, 2012, 2013; Schwerdtfeger, 2011), will remain a major challenge for the chemistry (well) beyond the standard periodic table (Schwerdtfeger *et al.*, 2015; Türler and Pershina, 2013).

Concerning atom-at-a-time chemistry, the future will see new chemical compounds being formed for the transactinide elements up to Og and possibly beyond. For example, there are currently worldwide efforts to study the carbonyls of Sg and beyond (Even *et al.*, 2014, 2015;

Iliaš and Pershina, 2017; Malli, 2015) and many other transactinides. Another difficult task on the horizon is to synthesize more neutron-rich, longer-lived isotopes of known superheavy elements with $Z = 110 - 118$, with the goals of moving closer to $N = 184$ and enabling chemical studies. The discovery of new elements beyond Og will add the eighth period to the periodic table.

The field of superheavy element research puts nuclear and atomic theory to the test. There are strong theoretical suggestions that superheavy atoms and nuclei differ from lighter species because of their large charges and masses. The presence of large electrostatic forces gives rise to strong Coulomb frustration effects in the nuclear system and huge relativistic effects in the atomic system; both present unusual challenges for many-body theory. Will next-generation hyperfine studies help to pin-down the presence of exotic topologies? Since theories of superheavy nuclei heavily rely on extrapolations, it is essential to provide uncertainty quantification on predictions. To constrain nuclear models in the superheavy region, new high-quality data on bulk properties and spectroscopy of superheavy systems are required. High-quality experimental data have been accumulated on global properties of superheavy nuclei and their spectroscopy (Ackermann, 2015; Ackermann and Theisen, 2017; Herzberg, 2016; Heßberger, 2016; Rudolph *et al.*, 2015, 2013; Theisen *et al.*, 2015).

Whether superheavy nuclei can be produced during the r-process nucleosynthesis, and whether the observed elemental abundances contain unambiguous information on the role of superheavy elements, can only be addressed through systematic reaction network calculations. On the nuclear physics side, such calculations require a consistent set of nuclear reaction rates, binding energies, beta- and gamma-decay decay rates, fission rates, and fission fragment distributions, as well as a consistent treatment of weak interactions (Horowitz *et al.*, 2018). From an experimental point of view, further constraints will be provided by the data on neutron-rich rare isotopes from next-generation radioactive ion beam facilities. This new experimental information is expected to significantly reduce the uncertainties arising from the prediction of nuclear properties of some of the r-process nuclei (Horowitz *et al.*, 2018; Langanke and Schatz, 2013; National Research Council, 2007; Surman and Mumpower, 2018). Unfortunately, very heavy, neutron-rich nuclei that are key for our understanding of fission in the r-process are likely to remain out of experimental reach in the foreseeable future. Consequently, the progress in this area will heavily rely on high-fidelity theoretical simulations.

The long term prospects in the unexplored regions of mass and charge are fascinating. They include the exploration of the region of long-lived superheavy nuclei around $N = 184$; the bold expansion of the chart of the nuclides; pinning down the presence of voids and other exotic topologies of nucleonic densities due to Coulomb frustration; delineating the role of superheavy nuclei in nucleosynthesis; and carrying out atomic and chemistry studies in the regime governed by huge relativistic effects. The outstanding discovery potential has greatly motivated worldwide development of new facilities and novel experimental tools. New-generation, high-current stable-beam accelerators will enable new discoveries at the picobarn level. The dedicated facilities in Dubna (Dmitriev *et al.*, 2016) and RIKEN (Haba, 2016) will substantially increase the production of superheavy species for physics and chemistry. Other major players in different areas of superheavy nuclei research include GSI/FAIR in Germany (Münzenberg, 2015; Münzenberg *et al.*, 2017), ORNL (Roberto *et al.*, 2015; Roberto and Rykaczewski, 2018) and Berkeley (Gates, 2016; Gates *et al.*, 2015, 2018) in the USA, GANIL in France (Ackermann and Theisen, 2017; Theisen, 2017), and several other major laboratories worldwide (Back, 2017; Hinde *et al.*, 2017; Yang *et al.*, 2013; Zhang *et al.*, 2012)

The scientific expedition continues into the uncharted regions of atomic number and nuclear mass. It was launched the 1960s, fueled by the dream of the island of stability inhabited by very long-lived superheavy species. While this idea has been revised, present-day scientific drivers are, arguably, far more exciting. The prospects for discoveries in the interdisciplinary field of superheavy nuclei and atoms, on the intersection of nuclear physics, atomic physics, chemistry, and astrophysics, are outstanding.

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FIGURES

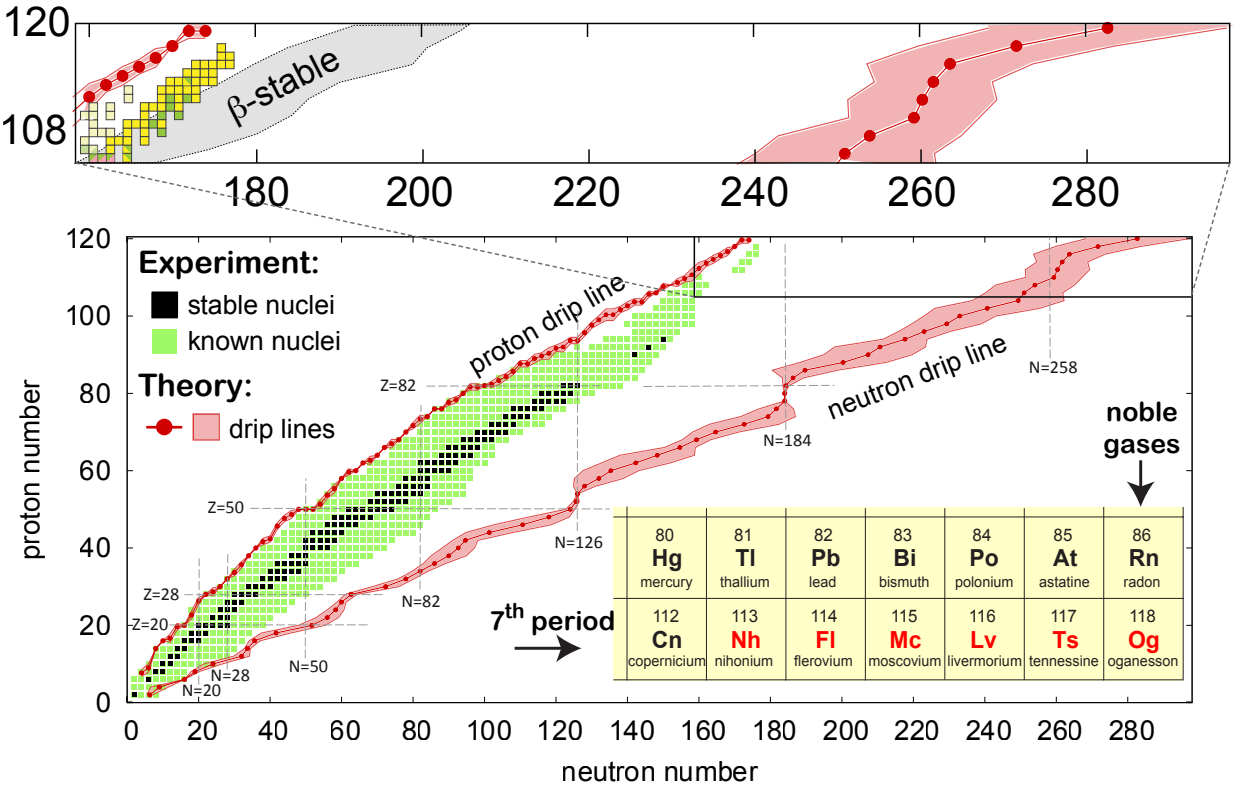


FIG. 1 Landscape of nucleon-bound nuclei in the (Z,N)-plane (adapted from (Nazarewicz, 2018)). The stable isotopes are shown as black squares and those known experimentally are marked in green. Particle drip lines predicted by theory are shown together with their uncertainties (red). The upper inset shows the details of the superheavy region ($Z > 104$ and $N > 160$). The isotopes synthesized in heavy-ion fusion reactions are indicated (Oganessian *et al.*, 2017; Oganessian and Utyonkov, 2015a) together with the anticipated valley of β-stability (Ćwiok *et al.*, 1996; Heenen *et al.*, 2015; Möller *et al.*, 1997; Sheng *et al.*, 2014). The lower inset marks the placement of the recently named six superheavy elements in the periodic table. The element oganesson completes the seventh period of the periodic table. It is the only element of Group 18 of the periodic table (noble gases), which does not naturally occur.

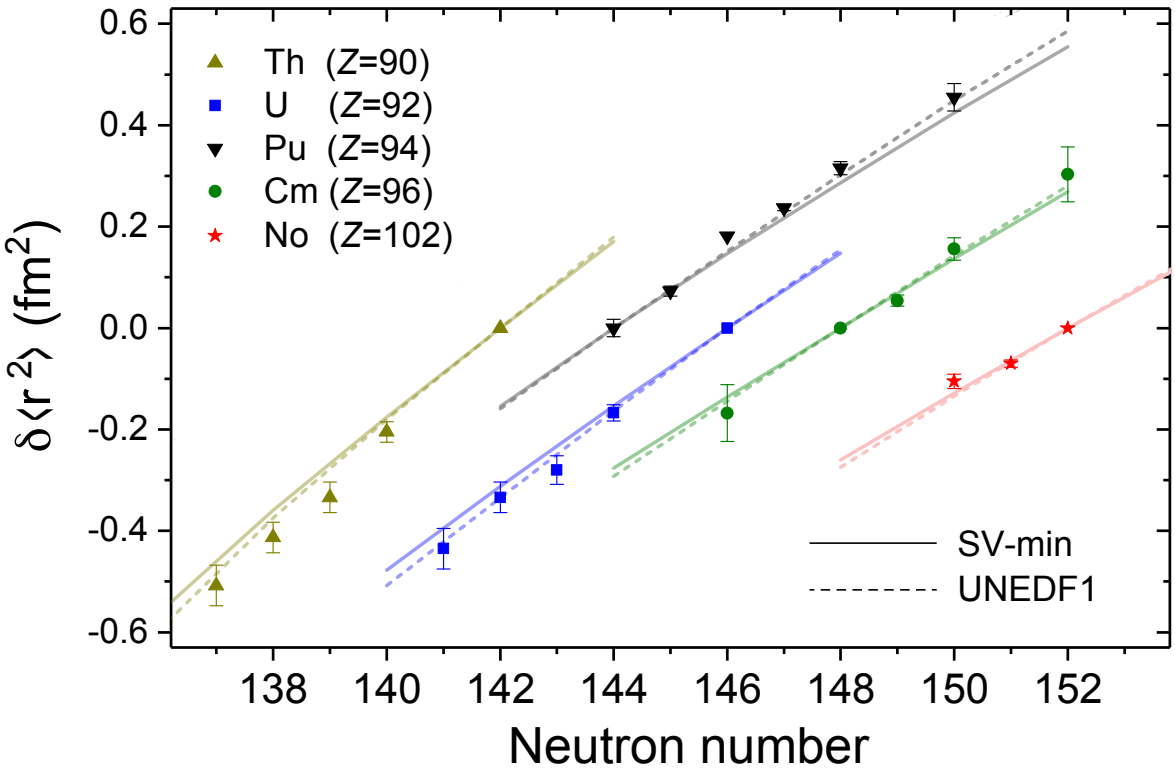


FIG. 2 Differential root mean square charge radii for Th, U, Pu, Cm, and No isotopes. The measurements (filled symbols) are compared to nuclear DFT calculations with two Skyrme-DFT models: UNEDF1 (dashed line) and SV-min (solid line). (Adapted from (Raeder *et al.*, 2018).)

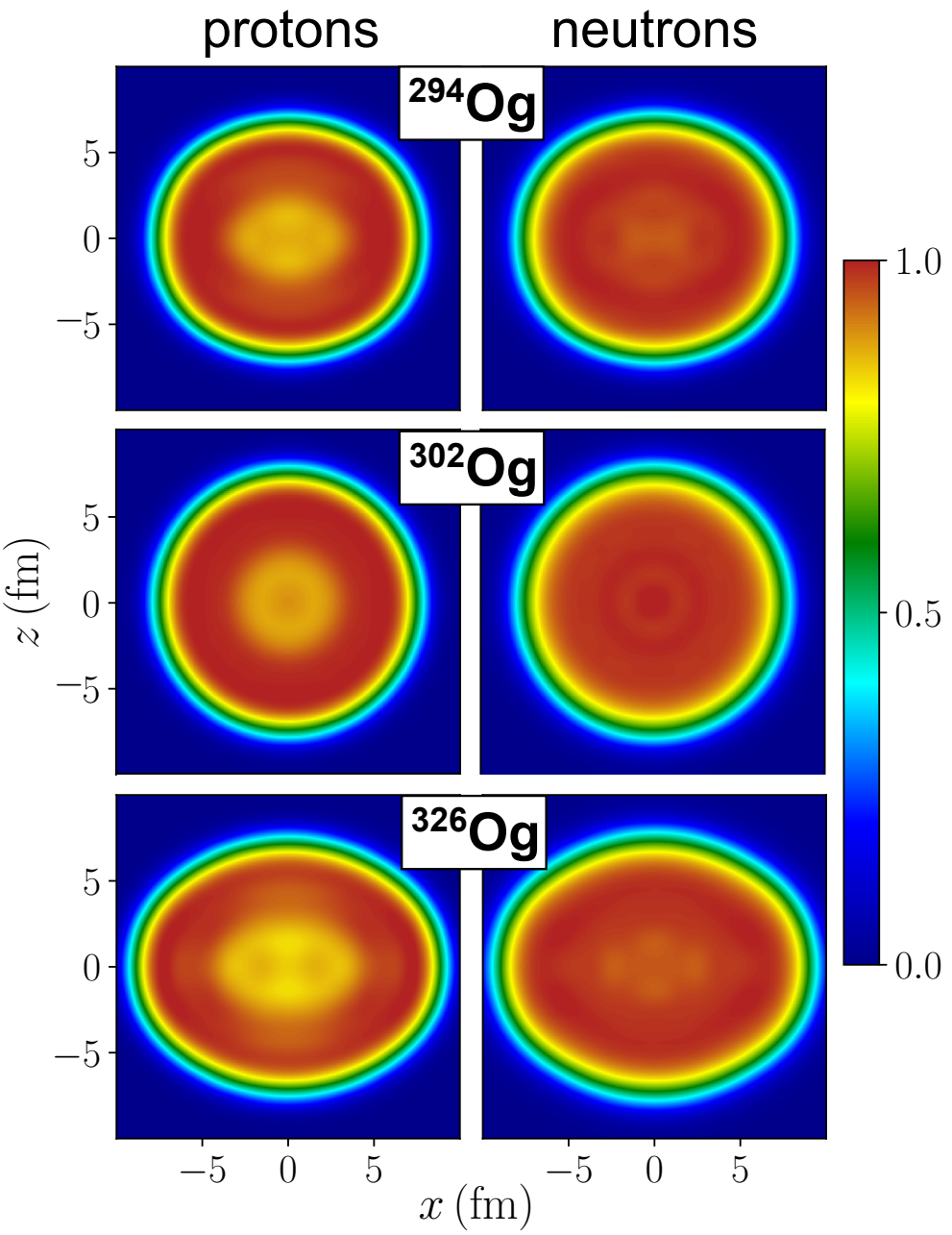


FIG. 3 Proton (left) and neutron (right) densities of ^{294}Og (top), ^{302}Og (middle), and ^{326}Og (bottom) calculated with SV-min in the (x, z) plane at $y = 0$. The densities are normalized to the maximum density. The central depression of the proton density (semi-bubble structures) is clearly seen in all three cases. (From (Schuetrumpf *et al.*, 2017).)

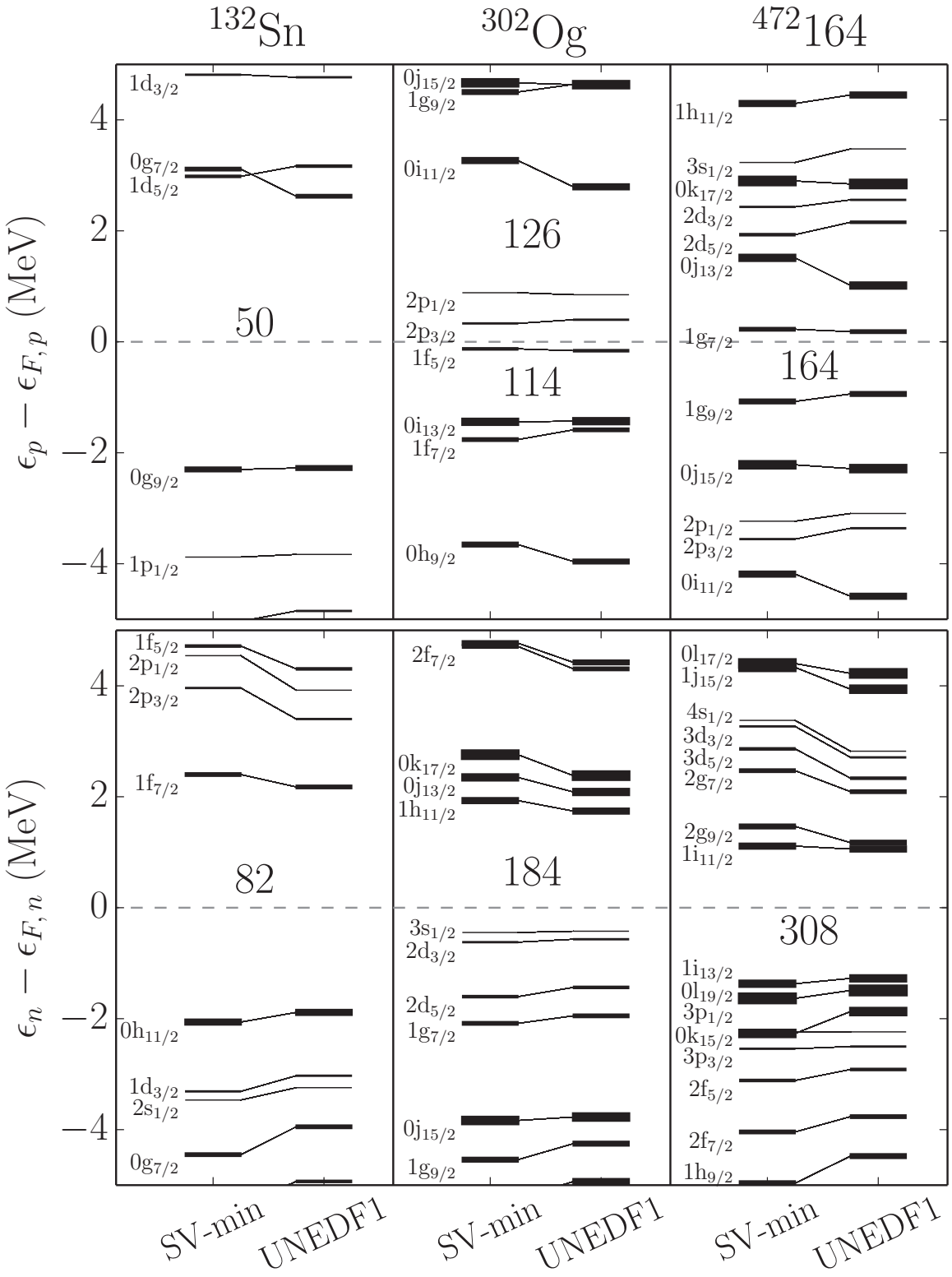

^{132}Sn
^{302}Og
^{472}164
$\epsilon_p - \epsilon_{F,p}$ (MeV)
$\epsilon_n - \epsilon_{F,n}$ (MeV)
4
2
0
−2
−4
1d$_{3/2}$
0g$_{7/2}$
1d$_{5/2}$
50
0g$_{9/2}$
1p$_{1/2}$
0j$_{15/2}$
1g$_{9/2}$
0i$_{11/2}$
126
2p$_{1/2}$
2p$_{3/2}$
1f$_{5/2}$
114
0i$_{13/2}$
1f$_{7/2}$
0h$_{9/2}$
1h$_{11/2}$
3s$_{1/2}$
0k$_{17/2}$
2d$_{3/2}$
2d$_{5/2}$
0j$_{13/2}$
1g$_{7/2}$
164
1g$_{9/2}$
0j$_{15/2}$
2p$_{1/2}$
2p$_{3/2}$
0i$_{11/2}$
1f$_{5/2}$
2p$_{1/2}$
2p$_{3/2}$
1f$_{7/2}$
82
0h$_{11/2}$
1d$_{3/2}$
2s$_{1/2}$
0g$_{7/2}$
2f$_{7/2}$
0k$_{17/2}$
0j$_{13/2}$
1h$_{11/2}$
184
3s$_{1/2}$
2d$_{3/2}$
2d$_{5/2}$
1g$_{7/2}$
0j$_{15/2}$
1g$_{9/2}$
0l$_{17/2}$
1j$_{15/2}$
4s$_{1/2}$
3d$_{3/2}$
3d$_{5/2}$
2g$_{7/2}$
2g$_{9/2}$
1i$_{11/2}$
308
1i$_{13/2}$
0l$_{19/2}$
3p$_{1/2}$
0k$_{15/2}$
3p$_{3/2}$
2f$_{5/2}$
2f$_{7/2}$
1h$_{9/2}$
SV-min
UNEDF1
SV-min
UNEDF1
SV-min
UNEDF1

FIG. 4 Proton (top) and neutron (bottom) Hartree-Fock single-particle energies relative to the Fermi level ε_F predicted with the Skyrme-DFT models SV-min and UNEDF1 for ^{132}Sn (left), ^{302}Og (middle), and ^{472}164 (right). The line thickness is proportional to the orbital's degeneracy $2j+1$ and the numbers indicate shell-model occupations. While the details of shell structure in superheavy nuclei show strong model dependence, general features are robust.

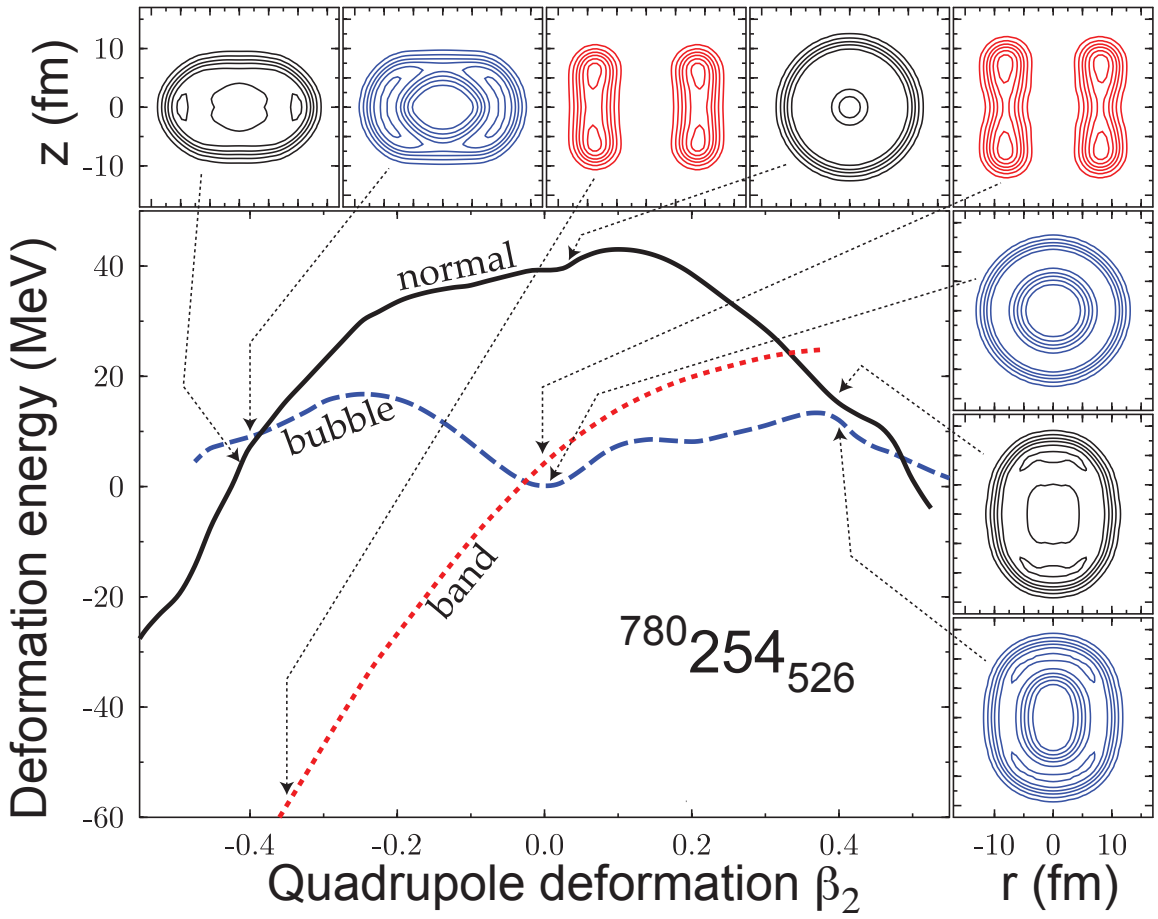
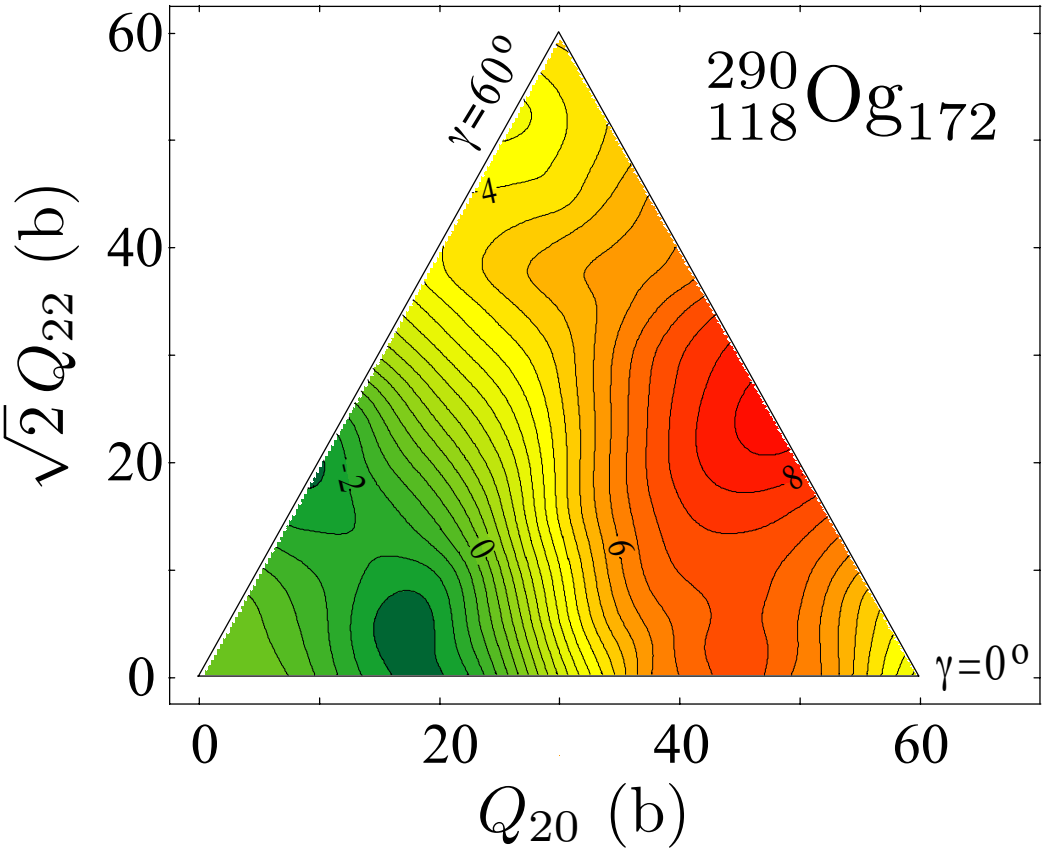


FIG. 5 Coexisting configurations associated with different density distributions calculated in the SLy6 Skyrme-DFT model for the hypothetical superheavy nucleus $^{780}254_{526}$. Three topologies are considered: normal nuclear densities similar to those found in stable nuclei, bubble nuclei distinguished by a substantial dip at the center, and band configurations out of a thin band of nuclear matter wound up to a torus. The contour plots of the total densities are given in the boxes, arrows connect the profile with the corresponding point on the energy surface, and colors help further to relate the topologies. All contours are axially symmetric (around the z axis) and the equi-density lines in the contour plots lie at 0.01, 0.03, 0.06, 0.09, 0.12, and 0.15 (nucleons/fm^3). Adapted from (Nazarewicz *et al.*, 2002).


$^{290}_{118}$Og$_{172}$
γ=60°
γ=0°
$\sqrt{2}\,Q_{22}$ (b)
Q_{20} (b)
0
20
40
60
4
2
0
6
8

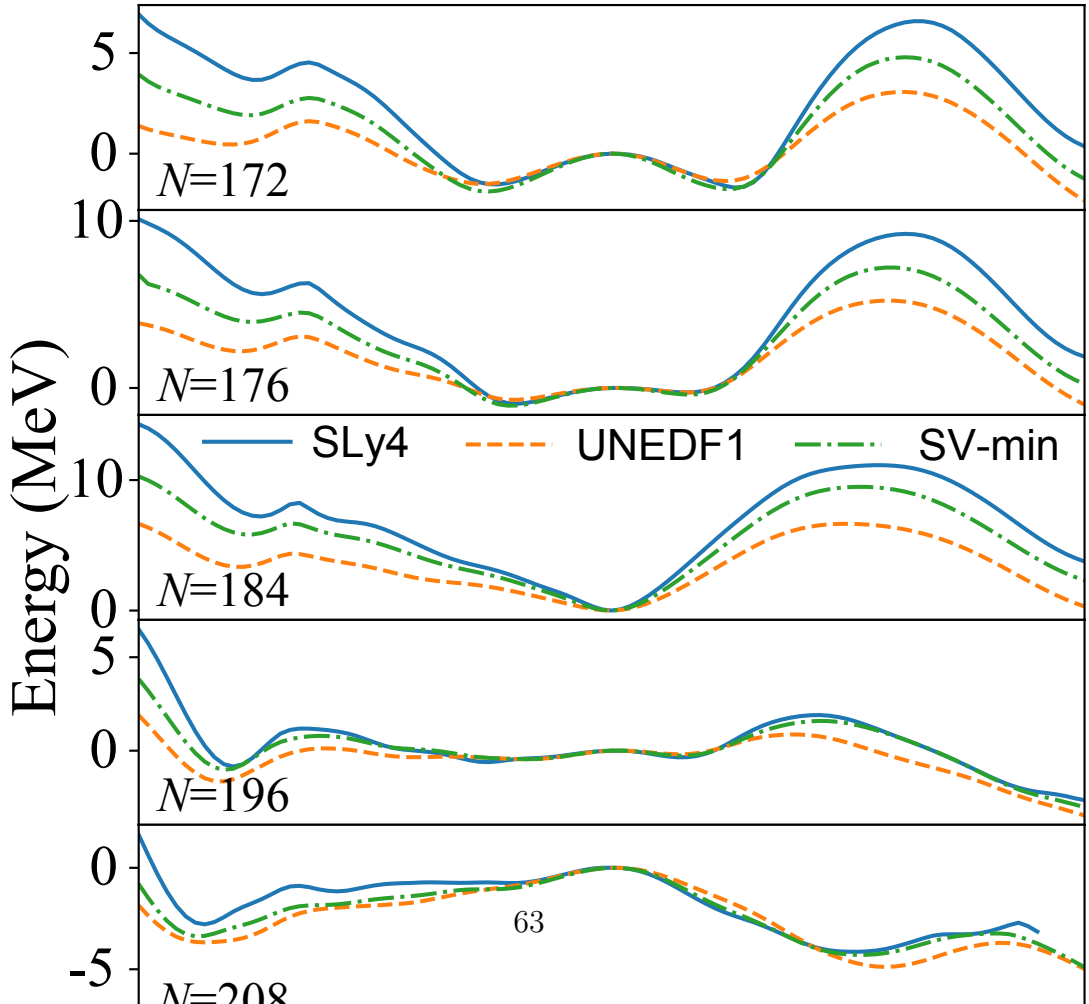

Energy (MeV)
N=172
N=176
N=184
N=196
N=208
SLy4
UNEDF1
SV-min

FIG. 6 Top: Triaxial PES in the Q_{20}-Q_{22}-plane for ^{290}Og obtained with the SLy4 Skyrme-DFT model. (Adapted from (Ćwiok *et al.*, 2005).) Bottom: Axial PESs for selected Og isotopes obtained with the Skyrme functionals SLy4, SV-min, and UNEDF1. All models predict very similar PES topology.

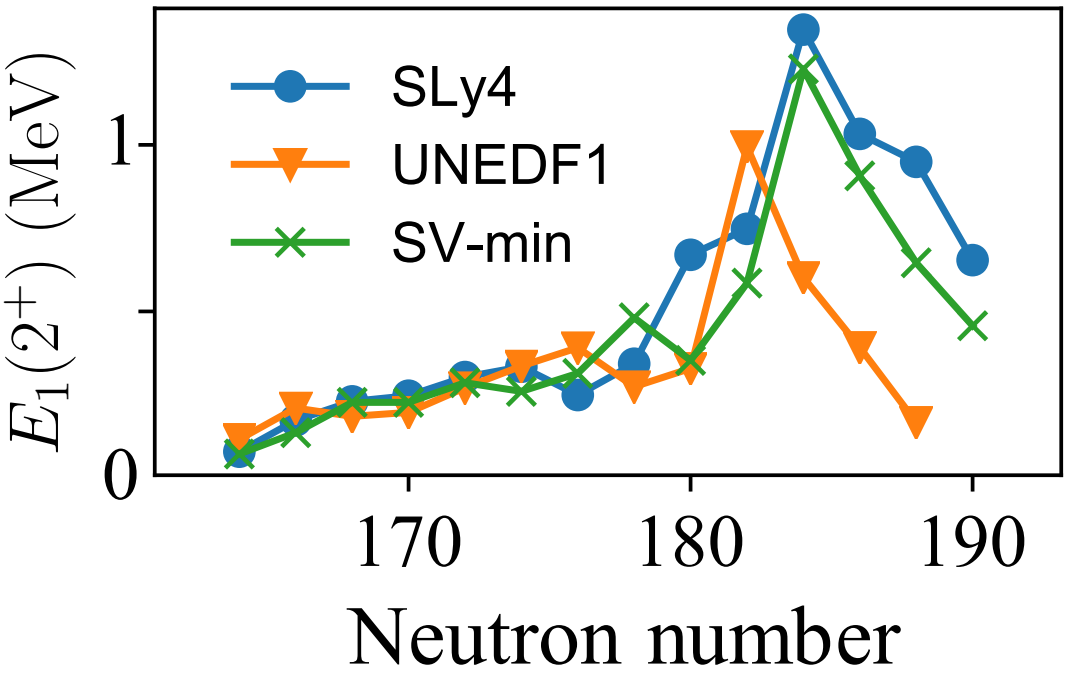


FIG. 7 Excitation energies of the 2^+ collective state computed for the three parametrizations as in Fig. 6 with the method from (Klüpfel *et al.*, 2008).

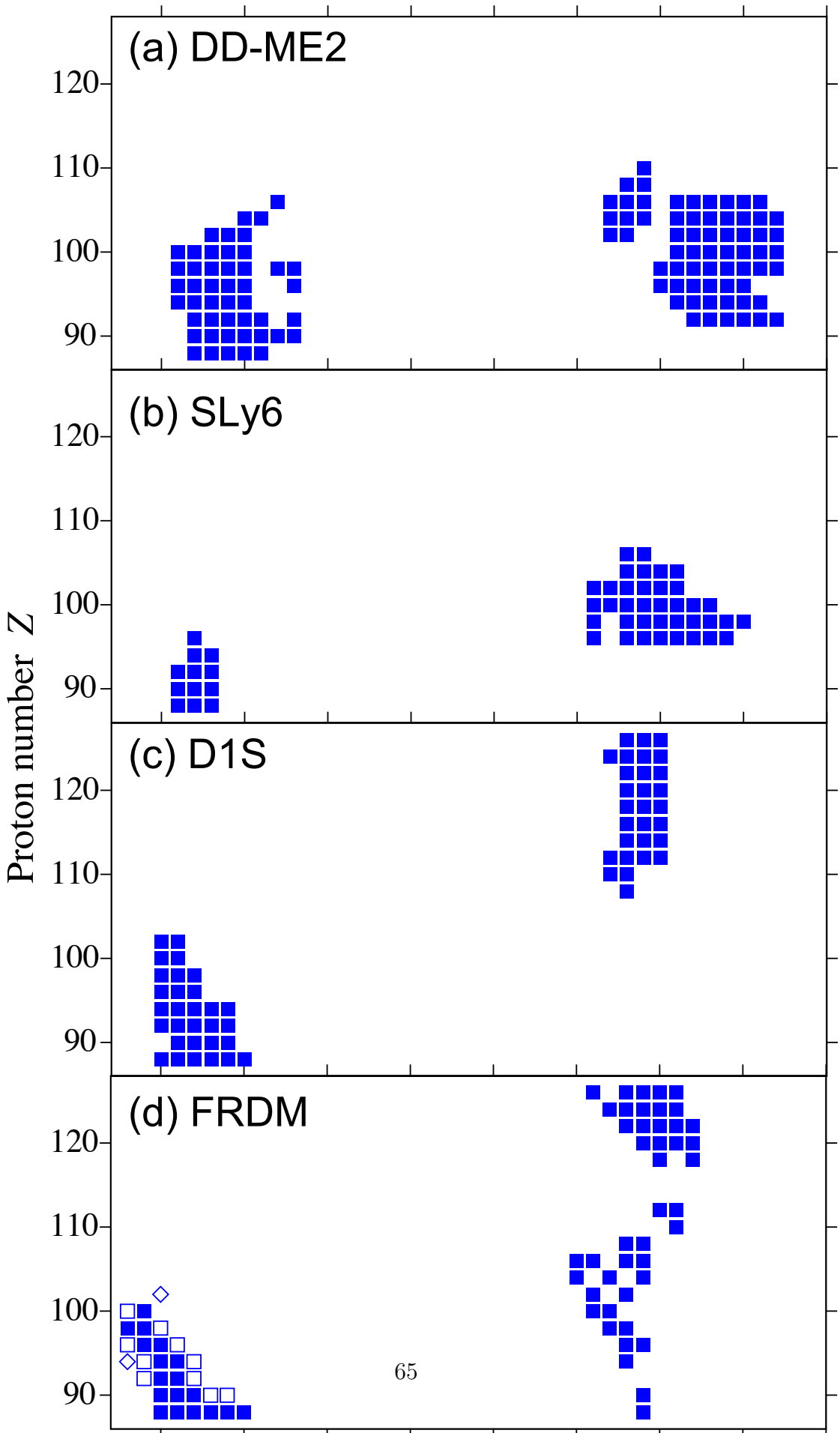

(a) DD-ME2
(b) SLy6
(c) D1S
(d) FRDM
Proton number Z
120
110
100
90

FIG. 8 Nuclei with ground-state octupole deformations predicted with different models. Adapted from (Agbemava and Afanasjev, 2017).

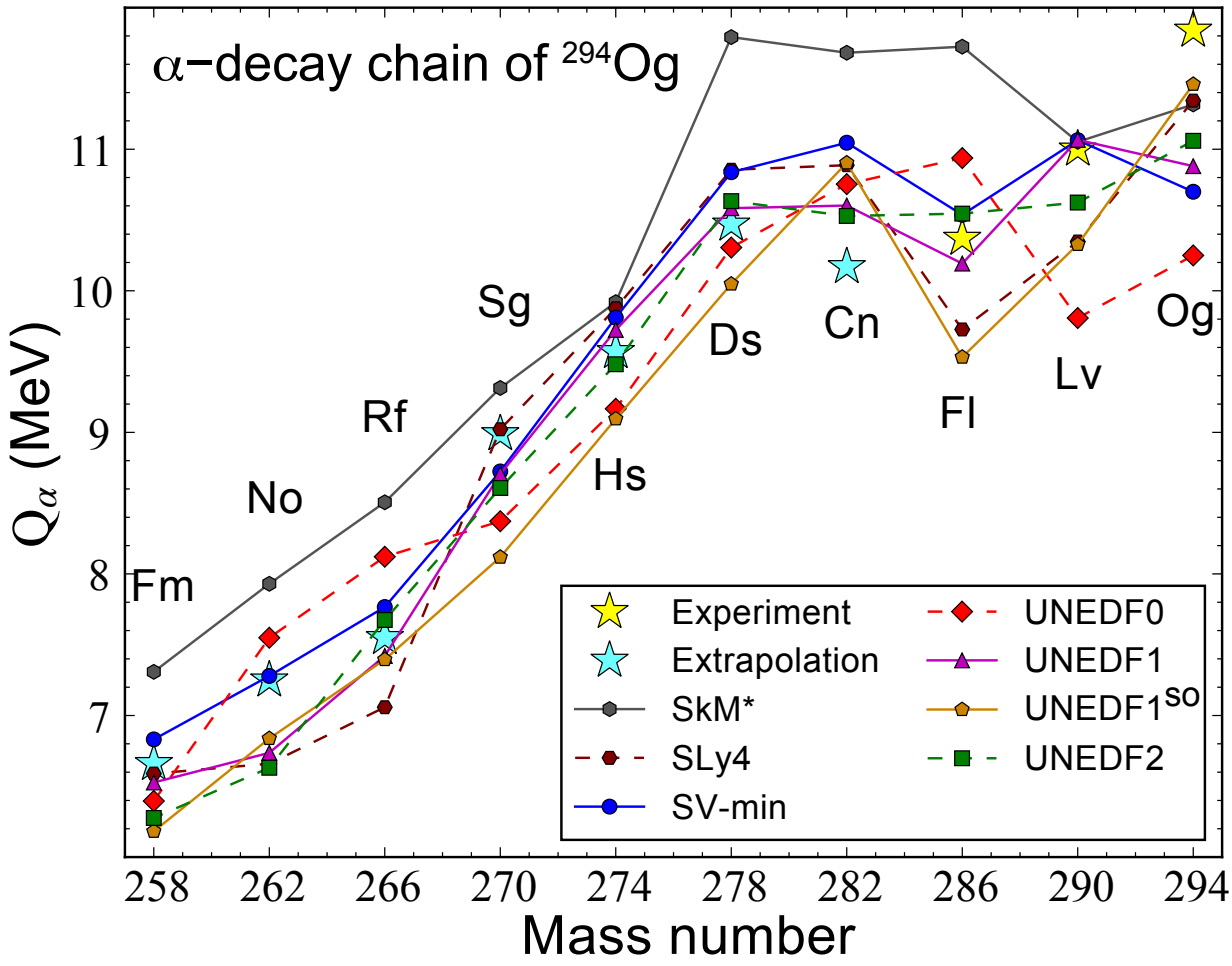


FIG. 9 Q_α values along the α-decay chain of ^{294}Og computed in nuclear DFT with different energy density functionals. Experimental and empirical extrapolated values (Wang *et al.*, 2017) are marked by stars. In ^{286}Fl, α decay competes with fission and the latter takes over in ^{282}Cn (Brewer *et al.*, 2018); hence, direct experimental information on Q_α values is not available below ^{282}Cn.

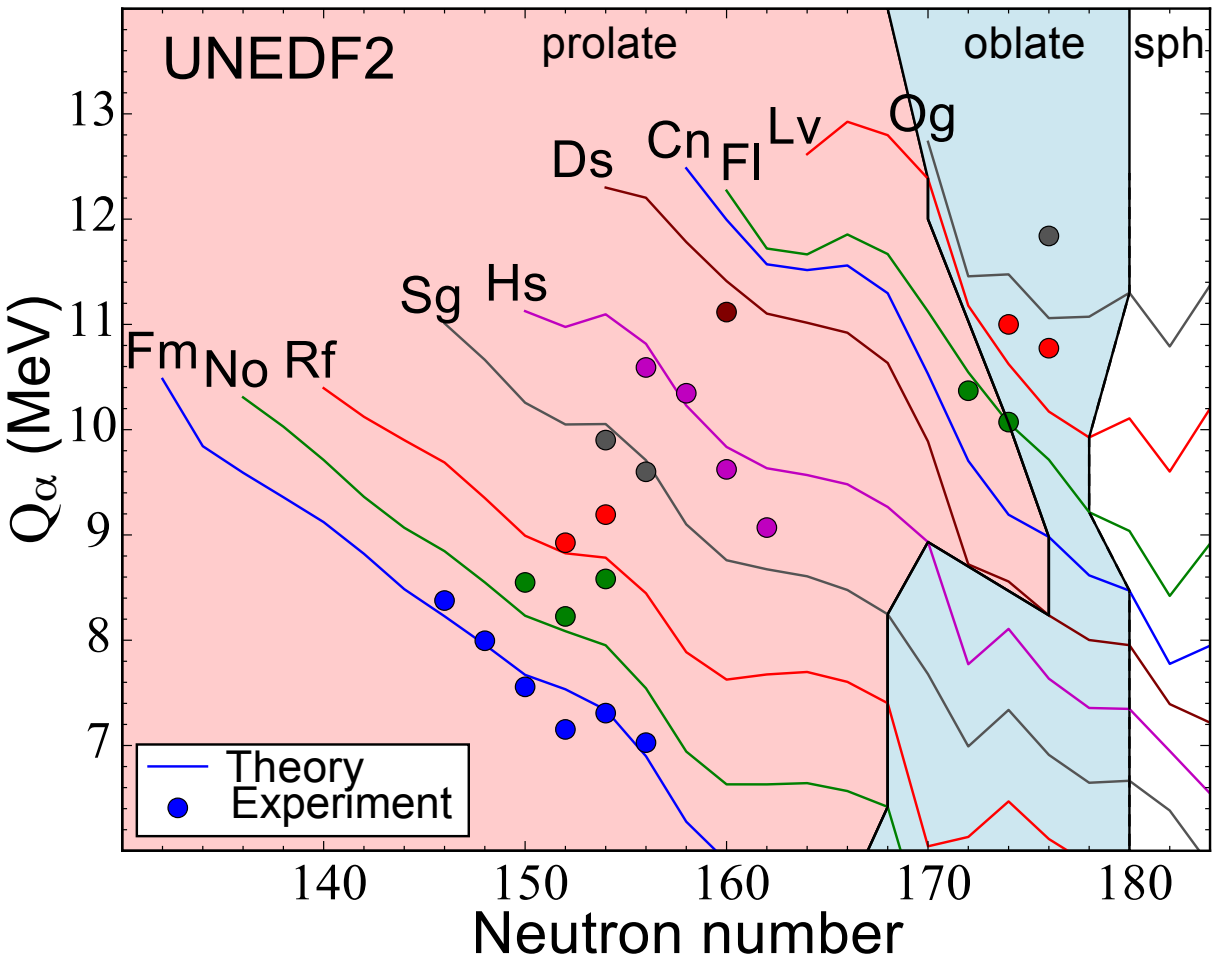


FIG. 10 Q_α values of the even-even isotopic chains from Fm to Og for the UNEDF2 Skyrme-DFT model. Regions of different shapes (prolate, oblate, spherical) are marked. Experimental values (Oganessian and Utyonkov, 2015b; Wang *et al.*, 2017) are represented by circles and match the color of the corresponding theoretical predictions (lines).

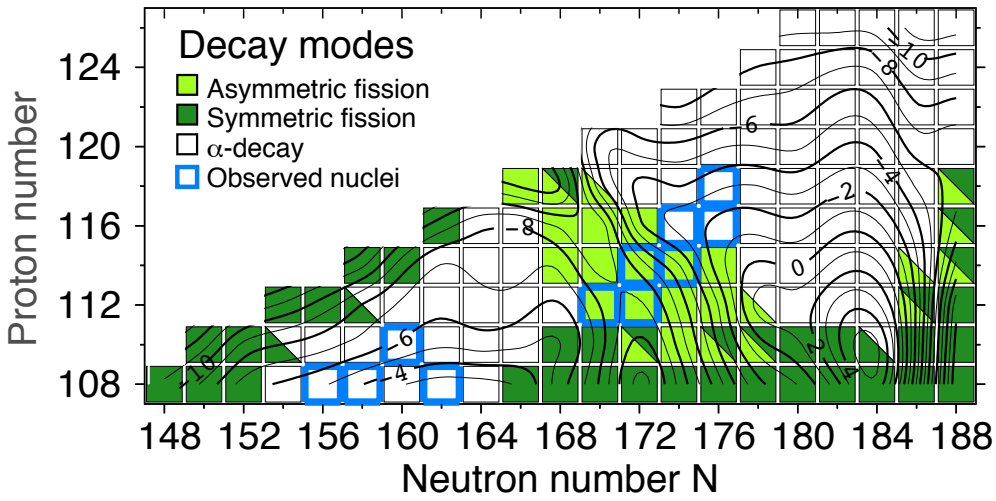


FIG. 11 Dominant decay modes for even-even superheavy elements in the range $108 \leq Z \leq 126, 148 \leq N \leq 188$ predicted with the Skyrme-DFT model SkM*. Spontaneous fission half-lives were computed using the semiclassical approximation while α-decay half-lives were estimated using the Viola-Seaborg formula (Viola and Seaborg, 1966). The contours show the predicted half-lives in logarithmic scale. Adapted from (Staszczak *et al.*, 2013).

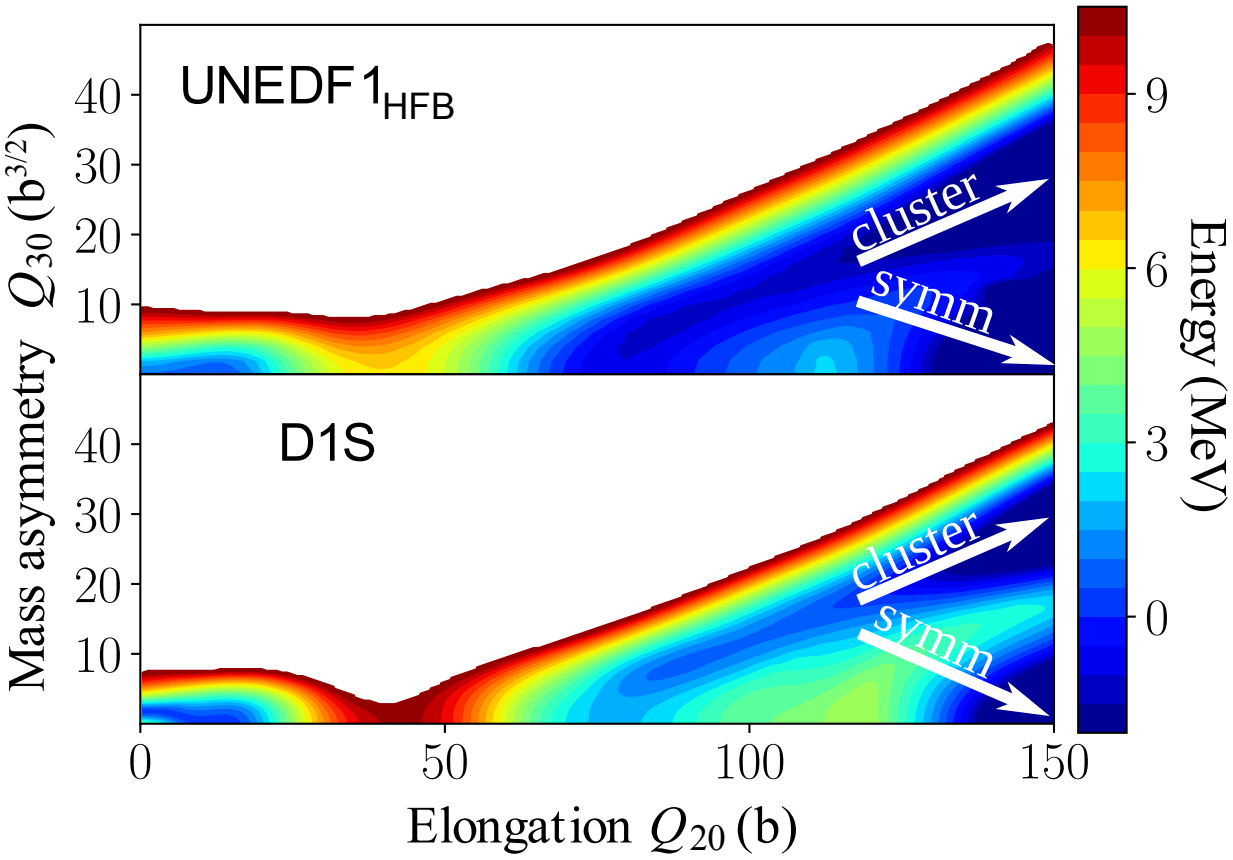


FIG. 12 Potential energy surface of ^{294}Og in the (Q_{20}, Q_{30}) coordinates calculated in nuclear DFT using the functionals UNEDF1$_{\rm HFB}$ and D1S, taken from (Matheson *et al.*, 2018). Two SF pathways are indicated: nearly-symmetric (symm) and strongly asymmetric corresponding to cluster decay (cluster).

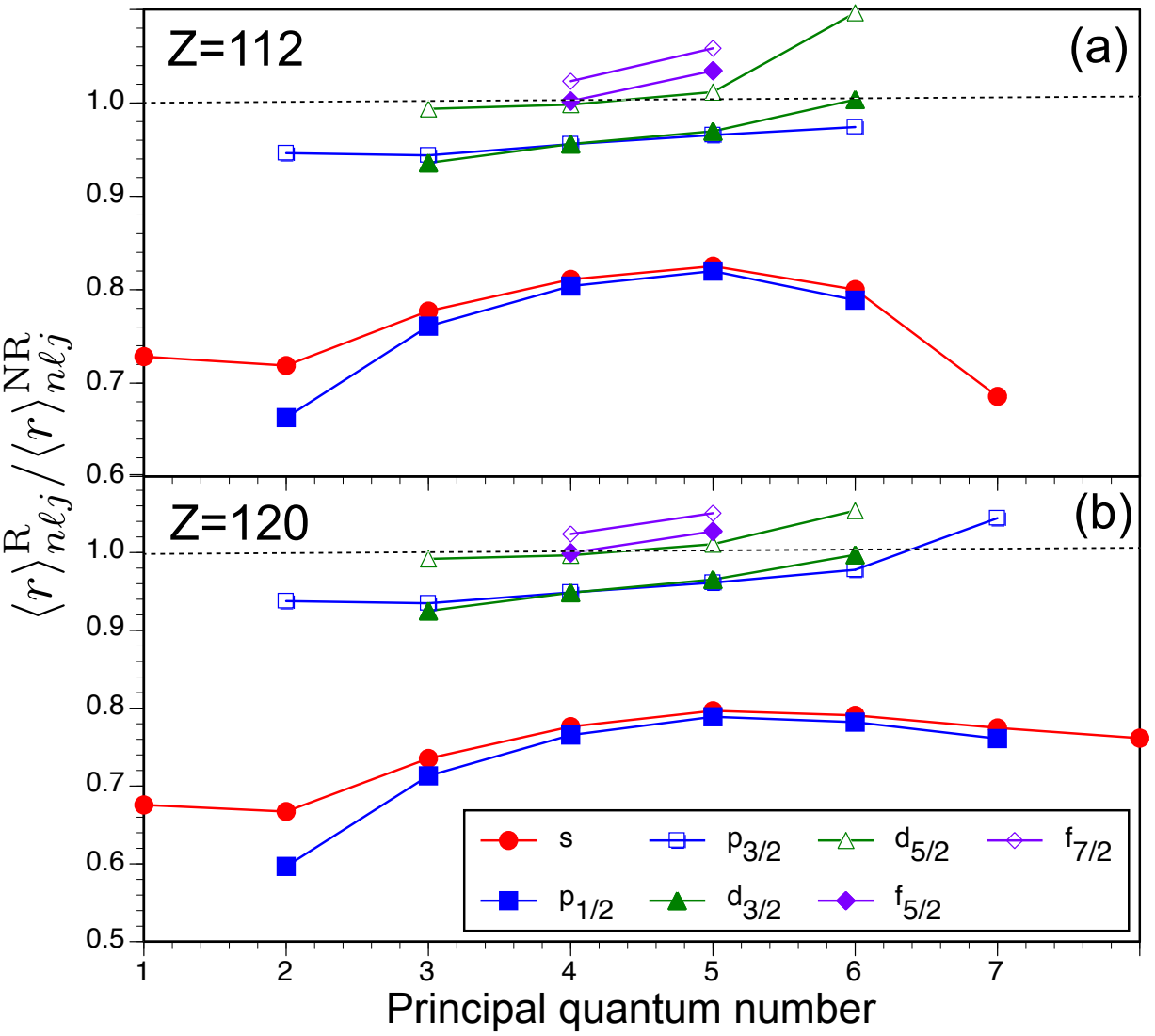


FIG. 13 Ratio of the relativistic (R) to nonrelativistic (NR) expectation values of orbital radii for different Dirac-Hartree-Fock $(n\ell j)$-orbitals in Cn ($Z = 112$, top) and $Z = 120$ (bottom).

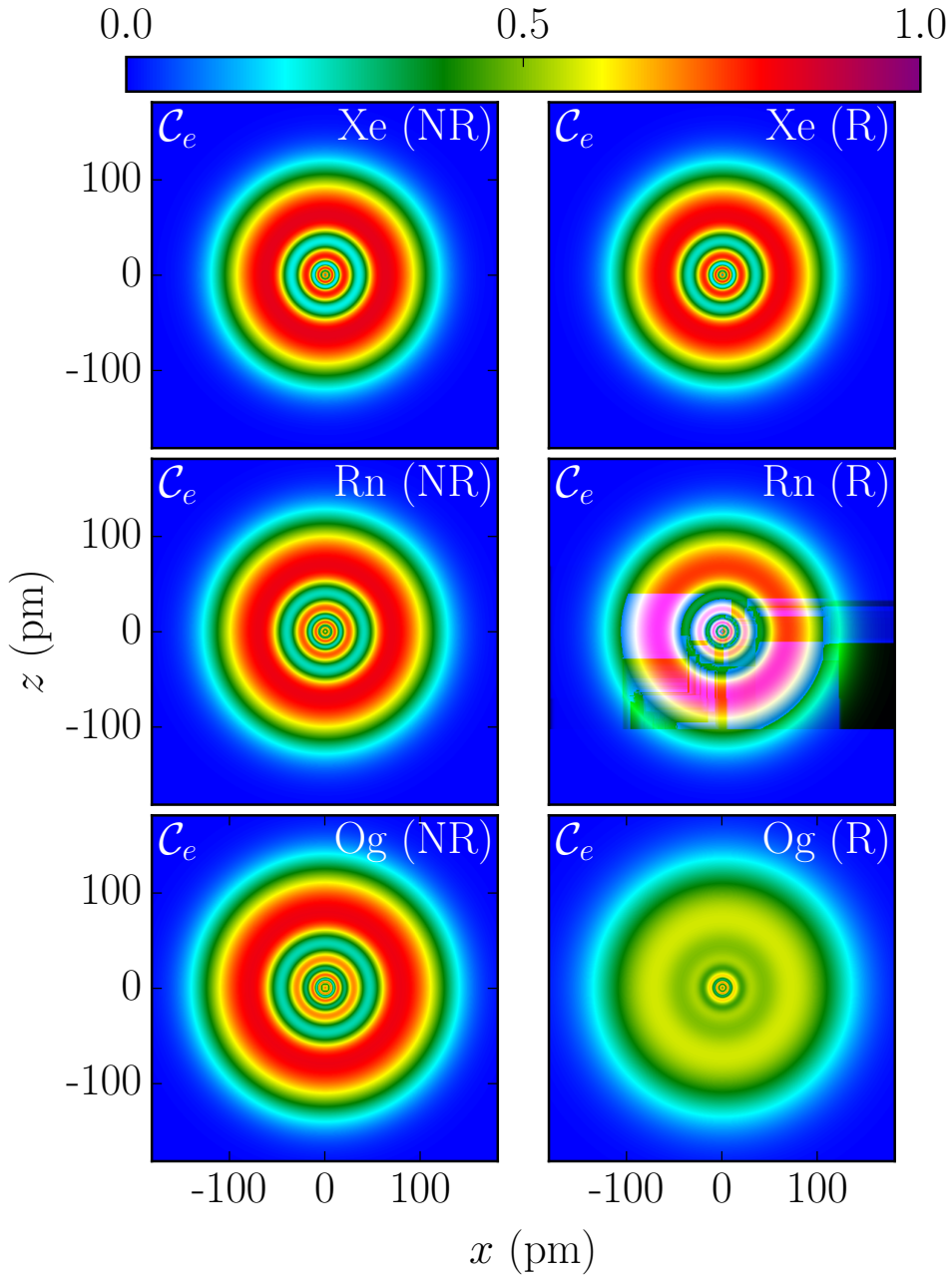


FIG. 14 Electron localization functions $\mathcal{C}_e$ from nonrelativistic (NR, left) and Dirac-Hartree-Fock calculations (R, right) for the heavy rare gas atoms Xe (top), Rn (middle), and Og (bottom). (From (Jerabek *et al.*, 2018).)

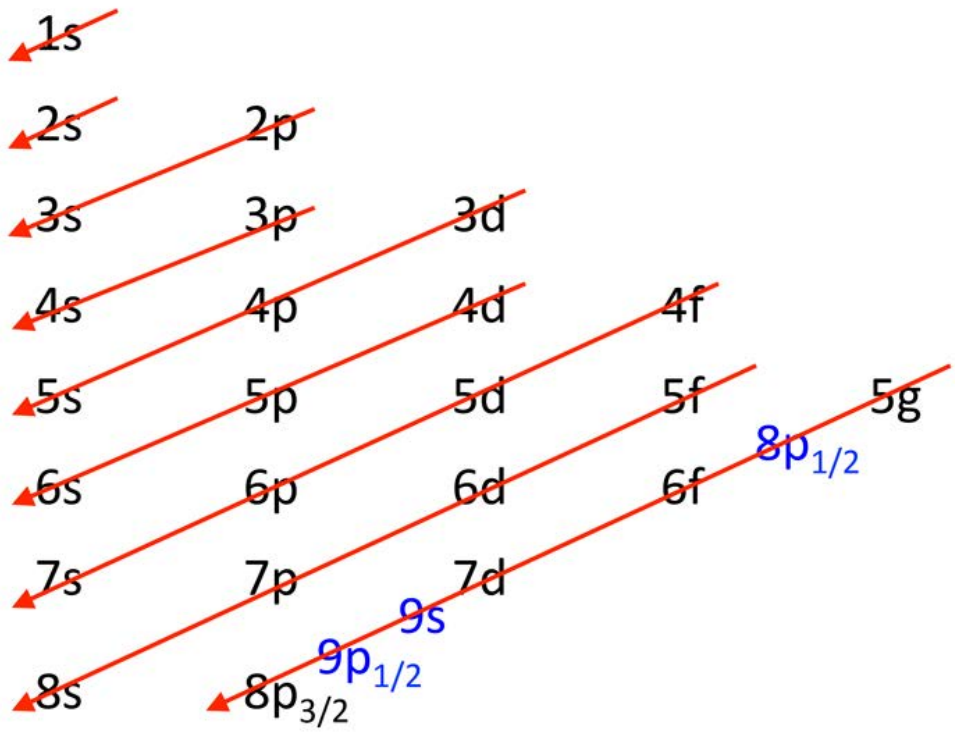


FIG. 15 Successive shell filling (according to (Pyykkö, 2011; Pyykkö, 2016)) up to the heaviest noble gas element with $Z = 172$ according to the Madelung rule. The anomalies in expected shell filling are highlighted in blue and result from strong relativistic stabilization effects of the $p_{1/2}$ shells at high atomic numbers.

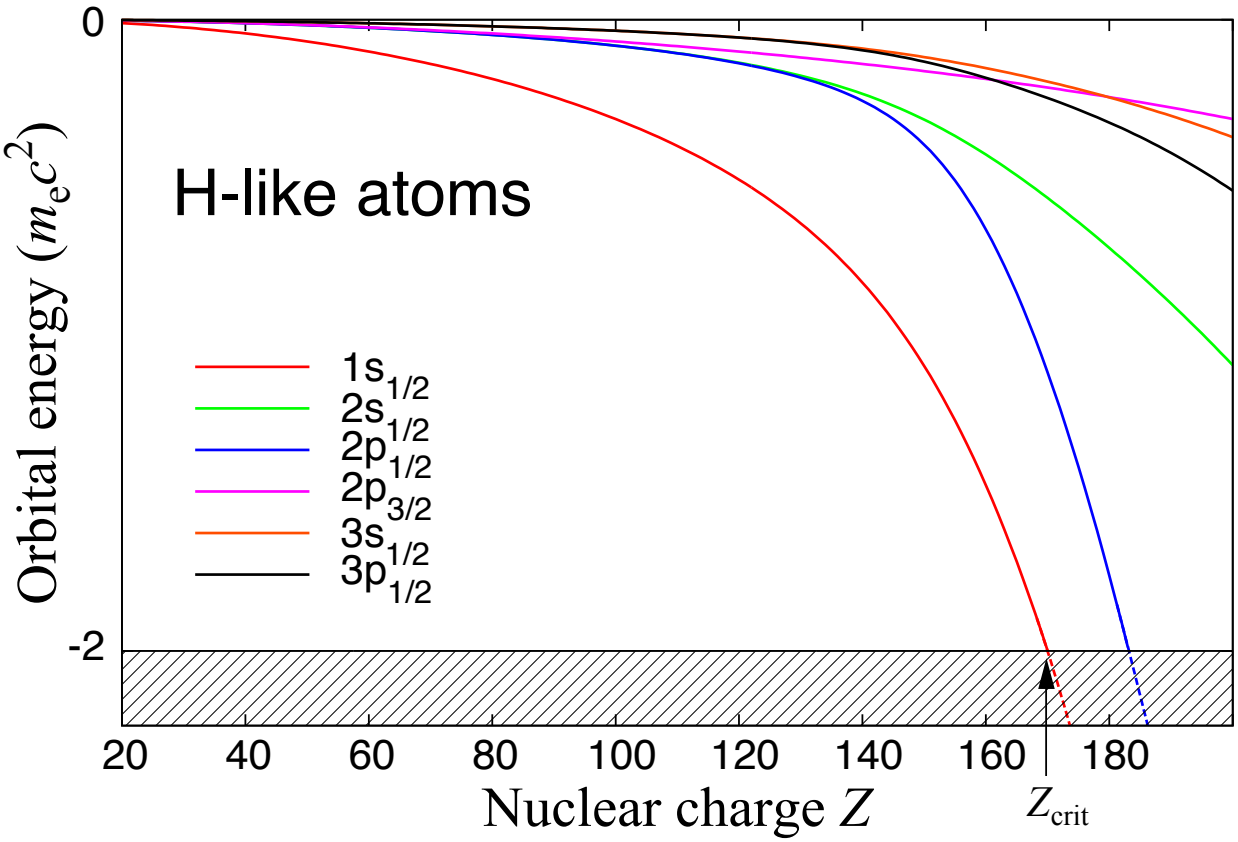


FIG. 16 Orbital energy dependence on nuclear charge Z for H-like atoms. The $1s_{1/2}$ orbit dives into the negative-energy continuum at -$2m_e c^2$ at $Z_{\rm crit}$ (positive-energy continuum set at zero energy). Extrapolations into the negative-energy continuum region are marked by dashed lines. Adapted from (Schwerdtfeger *et al.*, 2015).

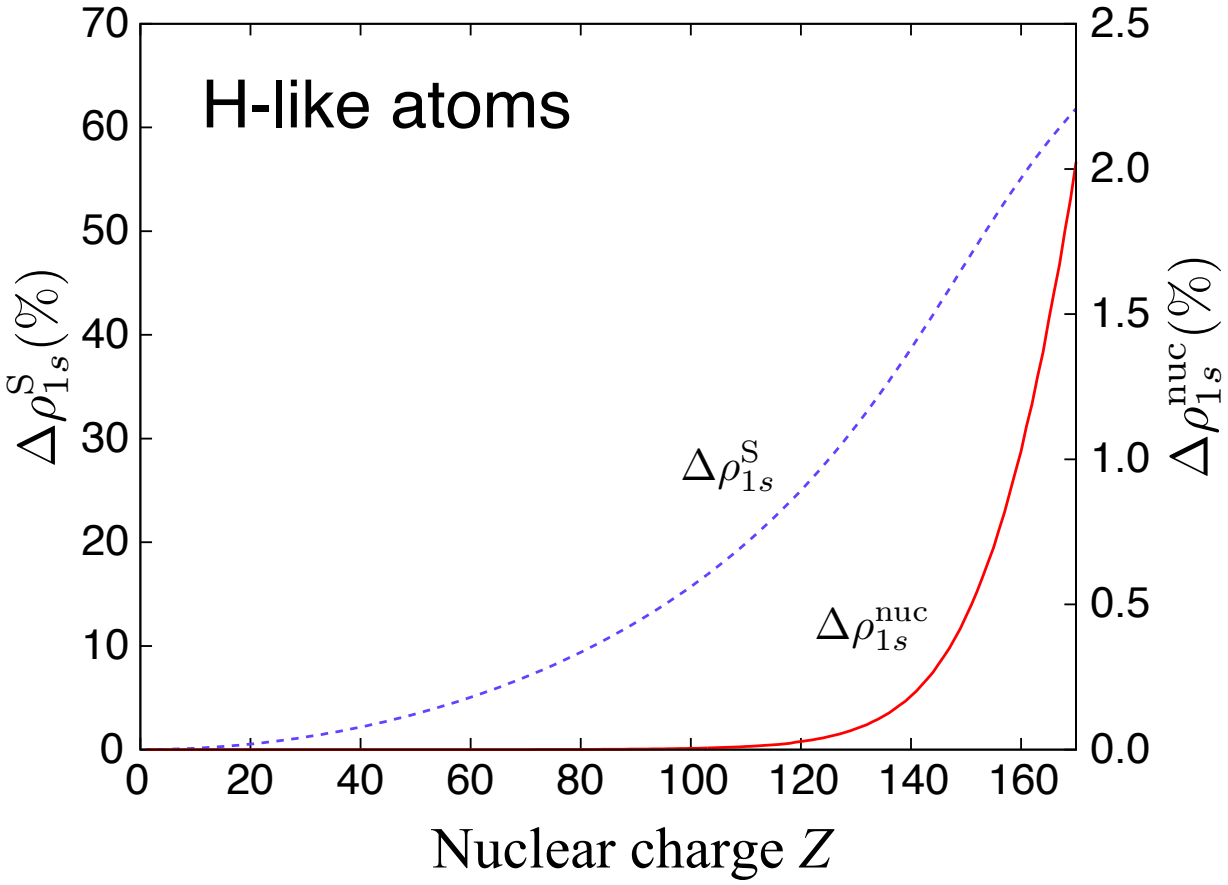


FIG. 17 The fraction of the $1s$ electron density due to the small component $\Delta\rho^{\rm S}_{1s}$ (dashed line) and the fraction of the $1s$ electron density contained within the nuclear radius $\Delta\rho^{\rm nuc}_{1s}$ (solid line) as a function of nuclear charge Z for H-like atoms. Adapted from (Schwerdtfeger *et al.*, 2015).

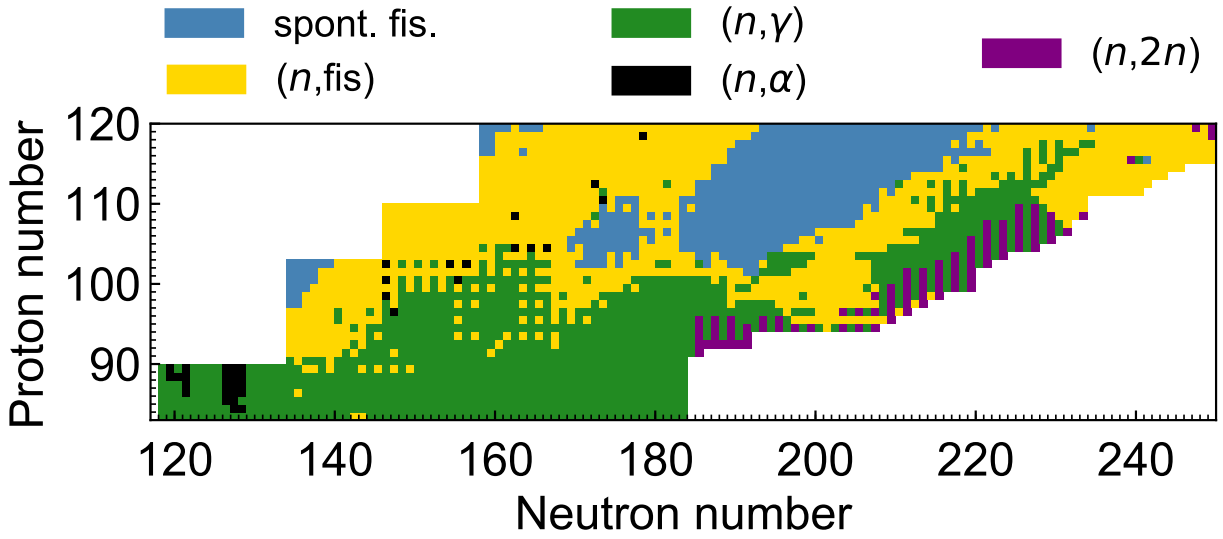


FIG. 18 Dominant decay channels as a function of proton and neutron number predicted in the BCPM-DFT model for typical conditions ($T = 0.9\,\mathrm{GK}$, $n_n = 10^{28}\,\mathrm{cm}^{-3}$) of the r process in neutron star mergers: spontaneous fission, neutron capture, neutron-induced α emission, neutron-induced fission, and neutron-induced two-neutron emission. α decay is not competitive at the astrophysical conditions assumed. Adapted from (Giuliani *et al.*, 2018).