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An improved α-decay energy formula for heavy and superheavy nuclei[*]

Song Luo (骆松)[1], Xiao Pan (潘霄)[1], Jian-Jun Dong (董建军)[2,], Xi-Jun Wu (吴喜军)[3,**], Biao He (何彪)[4] and Xiao-Hua Li (李小华)[1,5,6,**]**

[1] School of Nuclear Science and Technology, University of South China, Hengyang 421001, China
[2] School of Primary Education, HengYang Preschool Education College, Hengyang 421001, China
[3] School of Math and Physics, University of South China, Hengyang 421001, China
[4] School of Physics and Electronics, Central South University, Changsha 410083, China
[5] Cooperative Innovation Center for Nuclear Fuel Cycle Technology & Equipment, University of South China, Hengyang 421001, China
[6] Key Laboratory of Low Dimensional Quantum Structures and Quantum Control, Hunan Normal University, Changsha 410081, China

E-mail: 765024370@qq.com, wuxijun1980@yahoo.cn and lixiaohuaphysics@126.com

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Abstract

Based on the liquid-drop model and using the first derivative of the normalized Gaussian function to consider the shell correction, a simple α-decay energy formula is proposed for heavy and superheavy nuclei. The values of corresponding adjustable parameters are obtained by fitting α-decay energies of 209 nuclei ranging from $Z = 90$ to $Z = 118$ with $N \geqslant 140$. The calculated results are in good agreement with the experimental data. The average and standard deviations between the experimental data and theoretical results are 0.141 and 0.190 MeV, respectively. For comparison, the reliable formulae proposed by Dong T K *et al* (2010, *Phys. Rev. C* **82**, 034 320), Dong J M *et al* (2010, *Phys. Rev. C* **81**, 064 309) and the WS3+ nuclear mass model proposed by Wang N *et al* (2011, *Phys. Rev. C* **84**, 051 303) are also used. The results indicate that our improved 7-parameter formula is superior to these empirical formulae and is largely consistent with the WS3+ nuclear mass model. In addition, we extend this formula to predict the α-decay energies for nuclei with $Z = 117$, 118, 119 and 120. The predicted results of these formulae are basically consistent.

Supplementary material for this article is available online

Keywords: α-decay energy, heavy and superheavy nuclei, shell correction

(Some figures may appear in colour only in the online journal)

1. Introduction

The synthesis of superheavy nuclei(SHN) has always been a hot topic in nuclear physics. Many studies have been done on the decay properties of superheavy nuclei, which provides valuable guidance for experiments. In the experiments, elements 107–112 have been synthesized in cold-fusion reactions [1, 2]. While elements 113–118 have been successfully synthesized in hot-fusion reactions [3–8]. Moreover, the syntheses of new elements 119 and 120 are also in progress [9, 10]. For SHN, α decay is one of the dominant decay modes, which can be used as a powerful tool to identify new elements or new isotopes by detecting the α decay chains [11–17]. Furthermore, the study on α decay can provide valuable nuclear structure information, such as ground-state

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[**] Author to whom any correspondence should be addressed.

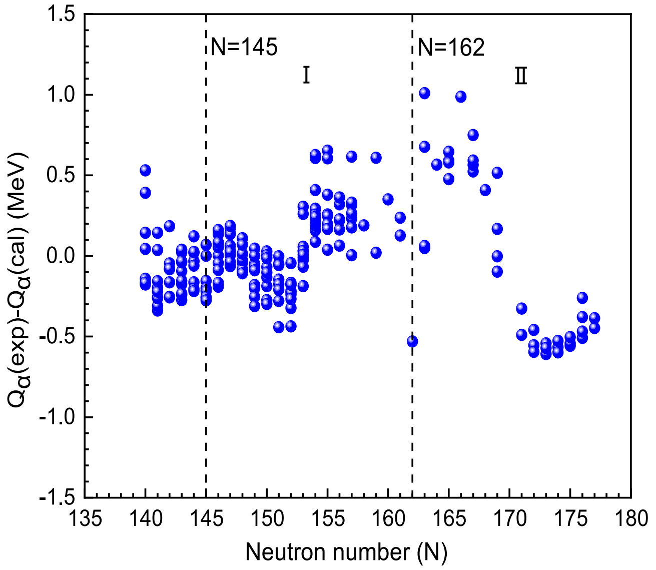

Figure 1. The deviations between experimental α-decay energies and calculated ones by using equation (5) for 209 nuclei.

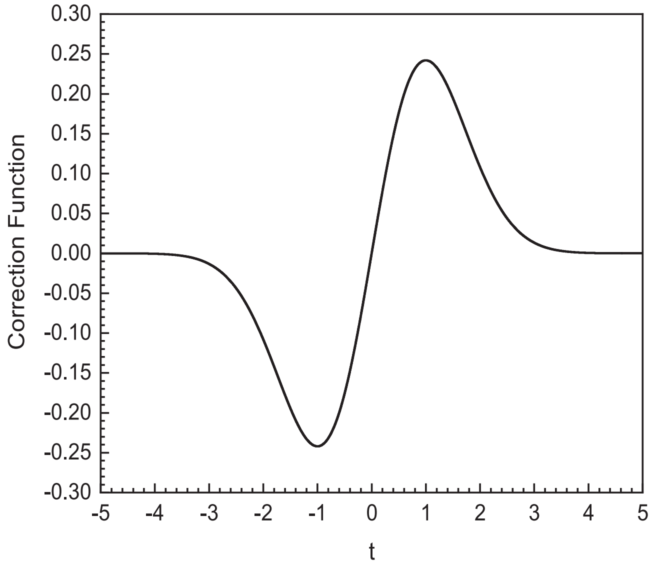

Figure 2. The shape of the first derivative of the normalized Gaussian function.

energies, half-lives, nuclear spins, shell effects, nuclear deformation and so on [18–24].

α decay was first observed as an unknown radioactive phenomenon by Becquerel in 1896 and further explained as a process in which the parent nucleus emits a ^{4}He particle by Rutherford and Geiger in 1908 [25]. Subsequently, it was successfully explained by Gamow [26] and by Condon and Gurney [27] as a quantum tunneling effect. Since then, many phenomenological and/or macroscopic-microscopic models have been proposed to study this process, such as the generalized liquid drop model [28, 29], the density-dependent M3Y effective interaction [30, 31], the cluster model [32, 33], the coupled channel approach [34, 35], the two-potential approach [36, 37], etc. Meanwhile, a lot of empirical formulae have also been proposed to calculate α-decay half-lives, which are in good agreement with experimental data [38–48]. More importantly, these works are often used to predict α-decay half-lives of unknown superheavy nuclei to aid in experimental design.

It is well known that α-decay half-life is extremely sensitive to the decay energy Q_α. For instance, an uncertainty of 1 MeV in α-decay energy results in an uncertainty of α-decay half-life ranging from 10^3 to 10^5 times in the heavy and superheavy regions [49]. However, it is still a challenge to accurately predict the values of α-decay energy for superheavy nuclei, which brings great difficulties to design experiments for the synthesis of new elements 119 and 120. Meanwhile, in recent years, many experimental data have been accurately measured and/or added in the heavy and superheavy regions. Whether there is a more accurate formula to calculate α-decay energy with fewer parameters or not seems to be a worthwhile attempt. For this purpose, based on the liquid-drop model, we put forward an improved formula to evaluate α-decay energy for heavy and superheavy nuclei. The calculated results are in good agreement with the experimental data. The corresponding average and standard deviation of 209 nuclei are 0.141 and 0.190MeV, respectively. Moreover, we generalize this formula to predict the α-decay energies for nuclei with $Z = 117$, 118, 119 and 120. For comparison, the reliable formulae proposed by Dong J M *et al* (DZ formula) [50], Dong T K *et al* (DR formula) [51] and WS3+ nuclear mass model proposed by Wang N *et al* (WS3+) [52] are also used. The corresponding predictions of these formulae are basically consistent.

This article is organized as follows. In section 2, the theoretical framework is briefly described. The detailed results and discussion are presented in section 3. Finally, a succinct summary is given in section 4.

2. Theoretical framework

Based on the liquid-drop model, the standard Bethe-Weizsäcker formula of nuclear binding energy is expressed as

$$\begin{aligned} B(Z, A) &= B_v + B_s + B_c + B_a + B_p \\ &= a_v A - a_s A^{2/3} - a_c Z^2 A^{-1/3} \\ &\quad - a_a \left(\frac{A}{2} - Z\right)^2 A^{-1} + B_p, \end{aligned} \tag{1}$$

where B_v, B_s, B_c, B_a and B_p are the volume, surface, Coulomb, symmetry and pairing energy, respectively. A and Z are the mass and proton numbers of the nucleus, respectively.

The α-decay energy is related to the parent and daughter nuclei by the relation

$$Q_\alpha = B_\alpha + B(Z-2, A-4) - B(Z, A) = B_\alpha + \Delta B, \tag{2}$$

where B_α, $B(Z-2, A-4)$ and $B(Z, A)$ are the binding energy of the α particle, daughter nucleus and parent nucleus, respectively. If the change in binding energy is smooth as

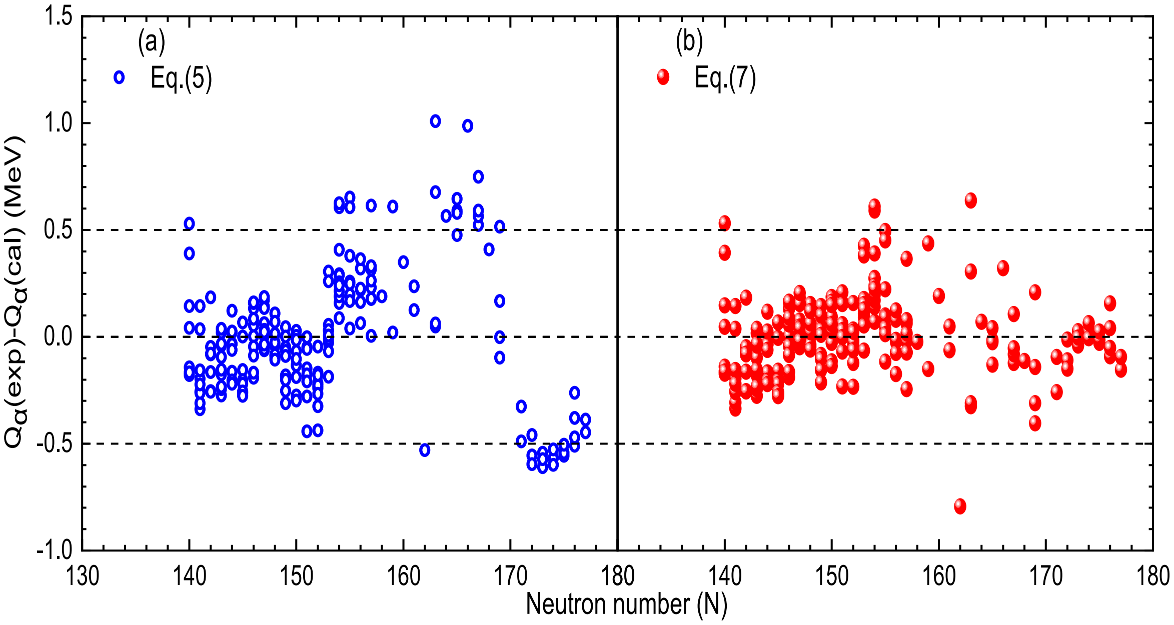

Figure 3. The deviations between experimental α-decay energies and calculated ones for 209 nuclei. (a) for calculations by using equation (5) denoted as the blue circle, (b) for calculations by using equation (7) denoted as the red ball.

Z and A, ΔB can be approximated as

$$\Delta B \approx \frac{\partial B}{\partial Z}\Delta Z + \frac{\partial B}{\partial A}\Delta A, \tag{3}$$

with $\Delta Z = -2$ and $\Delta A = -4$. Combining equations (2) and (3), we obtain the α-decay energy formula without considering shell correction. It can be given as

$$\begin{aligned} Q_\alpha &= B_\alpha + B(Z-2, A-4) - B(Z, A) \\ &= B_\alpha - 4a_v + \frac{8}{3}a_s A^{-1/3} + \Delta B_p \\ &\quad + 4a_c\frac{Z}{A^{1/3}}\left(1-\frac{Z}{3A}\right) - a_a\left(\frac{N-Z}{A}\right)^2 \\ &= a_1 + a_2 A^{-1/3} + \Delta B_p \\ &\quad + a_3\frac{Z}{A^{1/3}}\left(1-\frac{Z}{3A}\right) + a_4\left(\frac{N-Z}{A}\right)^2. \end{aligned} \tag{4}$$

In the above equation, the second term i.e. $a_2A^{-1/3}$ denoted the contribution of surface energy to α-decay energy can be incorporated into the constant term since this term approaches a small constant with the mass number A of the parent nucleus increasing or decreasing, especially for SHN. Meanwhile, the third term i.e. ΔB_p denoted the contribution of the paring energy to α-decay energy, can be ignored since the number of nucleons for the parent and daughter nuclei are even or odd at the same time in the α decay process. Consequently, the symmetry energy and Coulomb energy became the main contributions to α-decay energy. After the above discussion, the α-decay energy Q_α can be written as

$$Q_\alpha = a_1 + a_2\frac{Z}{A^{1/3}}\left(1-\frac{Z}{3A}\right) + a_3\left(\frac{N-Z}{A}\right)^2, \tag{5}$$

which is basically consistent with the DZ formula for α-decay energies of heavy and superheavy nuclei without considering shell correction [50].

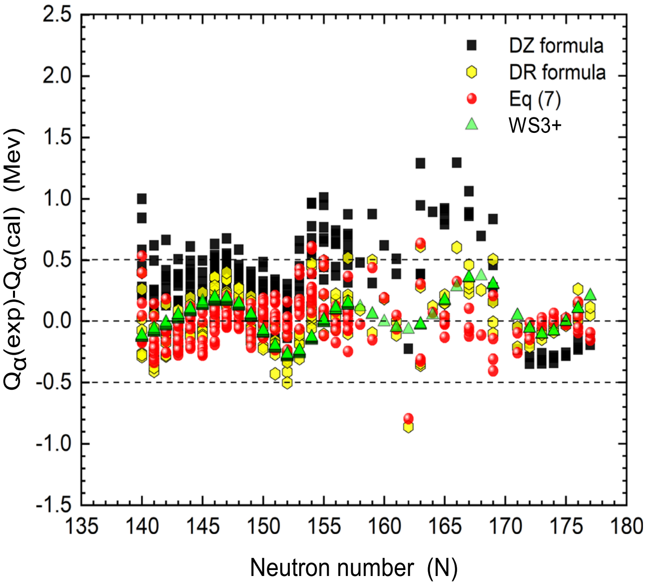

Figure 4. The deviations between experimental α-decay energies and calculated ones for 209 nuclei. The black square, yellow hexagon, red ball, and green triangle denote the deviations calculated by the DZ formula, DR formula, equation (7), and WS3+, respectively.

It is well-known that the standard Bethe-Weizsäcker formula completely depends on the liquid-drop model, which only reflects the average trend of energy change. However, when the nucleon number is close to the region near the shell, both binding energy and α-decay energy change abruptly [53, 54]. This difference can lead to large deviations between experimental data and theoretical results. Therefore, it is necessary to quantify the deviations

Table 1. Calculations of α-decay energies (in MeV) for 209 nuclei. Q_α^{cal}, Q_α^{DZ}, Q_α^{DR} and $Q_\alpha^{\mathrm{WS3+}}$ denote the calculated ones by using equation (7), DZ formula, DR formula and WS3+, respectively. The experimental α-decay energies Q_α^{exp} for 209 nuclei are taken from the latest evaluated nuclear properties table NUBASE2020 [61].

Nuclei	Q_α^{exp}	Q_α^{cal}	Q_α^{DZ}	Q_α^{DR}	$Q_\alpha^{\mathrm{WS3+}}$	Nuclei	Q_α^{exp}	Q_α^{cal}	Q_α^{DZ}	Q_α^{DR}	$Q_\alpha^{\mathrm{WS3+}}$
^{230}Th	4.770	4.238	3.771	4.374	4.786	^{236}Np	5.010	5.286	4.848	5.259	5.104
^{231}Th	4.213	4.069	3.595	4.162	4.342	^{237}Np	4.957	5.123	4.678	5.037	5.003
^{232}Th	4.082	3.899	3.418	3.941	3.969	^{238}Np	4.691	4.957	4.508	4.820	4.838
^{233}Th	3.745	3.727	3.240	3.712	3.799	^{239}Np	4.597	4.786	4.337	4.617	4.563
^{234}Th	3.672	3.555	3.062	3.481	3.699	^{240}Np	4.557	4.605	4.165	4.436	4.569
^{235}Th	3.376	3.381	2.882	3.255	3.457	^{241}Np	4.360	4.407	3.992	4.283	4.251
^{233}Th	3.333	3.201	2.702	3.043	3.133	^{242}Np	4.100	4.188	3.818	4.160	4.231
^{237}Th	3.196	3.012	2.521	2.853	3.103	^{234}Pu	6.310	6.263	5.859	6.383	6.368
^{231}Pa	5.150	4.756	4.306	4.889	5.071	^{235}Pu	5.951	6.106	5.696	6.184	6.030
^{232}Pa	4.627	4.590	4.133	4.680	4.665	^{236}Pu	5.867	5.948	5.532	5.975	5.755
^{233}Pa	4.375	4.423	3.959	4.461	4.273	^{237}Pu	5.748	5.789	5.367	5.759	5.773
^{234}Pa	4.076	4.255	3.785	4.236	4.178	^{238}Pu	5.593	5.629	5.201	5.540	5.514
^{235}Pa	4.101	4.086	3.609	4.008	4.062	^{239}Pu	5.245	5.466	5.033	5.326	5.318
^{236}Pa	3.755	3.914	3.433	3.785	3.835	^{240}Pu	5.256	5.298	4.865	5.125	5.138
^{237}Pa	3.795	3.738	3.255	3.575	3.685	^{241}Pu	5.140	5.121	4.696	4.947	5.135
^{238}Pa	3.628	3.551	3.077	3.389	3.381	^{242}Pu	4.984	4.925	4.526	4.798	4.954
^{232}U	5.414	5.267	4.832	5.395	5.340	^{243}Pu	4.757	4.709	4.355	4.678	4.850
^{233}U	4.909	5.104	4.663	5.189	4.965	^{244}Pu	4.666	4.480	4.184	4.581	4.640
^{234}U	4.858	4.940	4.492	4.974	4.661	^{235}Am	6.576	6.749	6.361	6.866	6.824
^{235}U	4.678	4.775	4.320	4.752	4.629	^{236}Am	6.260	6.596	6.201	6.669	6.506
^{236}U	4.573	4.608	4.148	4.527	4.476	^{238}Am	6.040	6.285	5.878	6.251	6.049
^{237}U	4.234	4.440	3.975	4.307	4.239	^{239}Am	5.922	6.128	5.715	6.035	6.036
^{238}U	4.270	4.266	3.800	4.100	4.022	^{240}Am	5.710	5.968	5.551	5.824	5.800
^{239}U	4.130	4.082	3.625	3.916	3.906	^{241}Am	5.638	5.803	5.385	5.626	5.692
^{240}U	4.035	3.882	3.449	3.761	3.811	^{242}Am	5.588	5.628	5.219	5.451	5.536
^{233}Np	5.630	5.769	5.350	5.893	5.696	^{243}Am	5.439	5.436	5.052	5.305	5.471
^{234}Np	5.356	5.609	5.184	5.690	5.481	^{244}Am	5.138	5.222	4.884	5.187	5.168
^{235}Np	5.194	5.448	5.016	5.478	5.185	^{245}Am	5.160	4.995	4.716	5.093	5.137
^{236}Cm	7.067	7.228	6.854	7.341	7.167	^{252}Cf	6.217	6.046	5.615	6.198	6.175
^{237}Cm	6.770	7.077	6.698	7.148	6.918	^{253}Cf	6.126	6.025	5.451	6.039	6.116
^{238}Cm	6.670	6.926	6.540	6.945	6.589	^{254}Cf	5.927	5.949	5.286	5.860	5.952
^{239}Cm	6.540	6.773	6.381	6.735	6.502	^{240}Es	8.260	8.479	8.142	8.538	8.340
^{240}Cm	6.398	6.619	6.221	6.522	6.493	^{241}Es	8.259	8.337	7.994	8.345	7.992
^{241}Cm	6.185	6.462	6.060	6.314	6.192	^{242}Es	8.160	8.193	7.844	8.144	8.006
^{242}Cm	6.216	6.300	5.898	6.120	6.260	^{243}Es	8.072	8.047	7.693	7.941	8.201
^{243}Cm	6.169	6.128	5.735	5.947	6.128	^{245}Es	7.909	7.746	7.389	7.556	7.883
^{244}Cm	5.902	5.938	5.571	5.804	5.840	^{247}Es	7.464	7.402	7.079	7.257	7.490
^{245}Cm	5.624	5.727	5.405	5.689	5.688	^{251}Es	6.597	6.634	6.448	6.918	6.685
^{246}Cm	5.475	5.503	5.240	5.598	5.437	^{252}Es	6.738	6.561	6.288	6.820	6.640
^{247}Cm	5.354	5.294	5.073	5.517	5.302	^{253}Es	6.739	6.543	6.127	6.692	6.753
^{248}Cm	5.162	5.138	4.905	5.431	5.191	^{254}Es	6.617	6.524	5.966	6.535	6.670
^{249}Cm	5.148	5.057	4.737	5.325	5.186	^{255}Es	6.436	6.450	5.803	6.359	6.484
^{250}Cm	5.170	5.031	4.568	5.189	5.103	^{243}Fm	8.690	8.652	8.317	8.600	8.512
^{243}Bk	6.874	6.789	6.402	6.606	6.782	^{246}Fm	8.379	8.214	7.871	8.021	8.411
^{244}Bk	6.779	6.620	6.242	6.436	6.663	^{247}Fm	8.258	8.053	7.720	7.860	8.222
^{245}Bk	6.455	6.433	6.081	6.296	6.392	^{248}Fm	7.995	7.875	7.567	7.728	8.008
^{246}Bk	6.070	6.225	5.919	6.184	6.111	^{249}Fm	7.709	7.675	7.414	7.625	7.826
^{247}Bk	5.890	6.004	5.756	6.095	5.916	^{250}Fm	7.557	7.463	7.260	7.545	7.580
^{248}Bk	5.830	5.798	5.592	6.017	5.803	^{251}Fm	7.425	7.264	7.104	7.475	7.313
^{249}Bk	5.521	5.644	5.427	5.934	5.656	^{252}Fm	7.154	7.119	6.948	7.400	7.195
^{239}Cf	7.760	8.019	7.668	8.082	7.862	^{253}Fm	7.198	7.048	6.791	7.304	7.183
^{240}Cf	7.711	7.874	7.516	7.886	7.592	^{254}Fm	7.308	7.032	6.632	7.179	7.320
^{242}Cf	7.517	7.578	7.210	7.475	7.619	^{255}Fm	7.240	7.017	6.473	7.025	7.139
^{244}Cf	7.329	7.271	6.899	7.084	7.446	^{256}Fm	7.025	6.945	6.314	6.851	7.050
^{245}Cf	7.258	7.105	6.742	6.918	7.279	^{257}Fm	6.864	6.801	6.153	6.674	6.751
^{246}Cf	6.862	6.921	6.584	6.780	6.950	^{244}Md	8.950	9.104	8.783	9.049	9.180
^{247}Cf	6.503	6.716	6.425	6.671	6.713	^{246}Md	8.890	8.822	8.493	8.658	9.237

Table 1. (Continued.)

Nuclei	Q_α^{exp}	Q_α^{cal}	Q_α^{DZ}	Q_α^{DR}	$Q_\alpha^{\mathrm{WS3+}}$	Nuclei	Q_α^{exp}	Q_α^{cal}	Q_α^{DZ}	Q_α^{DR}	$Q_\alpha^{\mathrm{WS3+}}$
^{248}Cf	6.361	6.497	6.265	6.586	6.529	^{247}Md	8.764	8.675	8.346	8.478	9.066
^{249}Cf	6.293	6.294	6.103	6.510	6.293	^{248}Md	8.500	8.517	8.197	8.321	8.840
^{250}Cf	6.128	6.143	5.942	6.430	6.217	^{250}Md	8.155	8.145	7.898	8.091	8.391
^{251}Cf	6.177	6.067	5.779	6.329	6.196	^{251}Md	7.963	7.935	7.746	8.014	8.161
^{253}Md	7.573	7.597	7.440	7.875	7.803	^{269}Sg	8.580	8.904	8.196	8.938	8.378
^{255}Md	7.906	7.515	7.130	7.659	7.886	^{260}Bh	10.400	10.272	10.112	10.509	10.328
^{257}Md	7.557	7.433	6.817	7.336	7.566	^{261}Bh	10.500	10.274	9.973	10.402	10.279
^{258}Md	7.271	7.291	6.659	7.162	7.223	^{262}Bh	10.319	10.277	9.833	10.266	10.261
^{251}No	8.752	8.608	8.374	8.551	8.929	^{270}Bh	9.060	9.370	8.677	9.402	8.680
^{252}No	8.549	8.400	8.226	8.476	8.611	^{271}Bh	9.420	9.350	8.528	9.299	9.061
^{253}No	8.415	8.207	8.076	8.412	8.445	^{272}Bh	9.300	9.315	8.379	9.151	9.106
^{254}No	8.226	8.067	7.925	8.343	8.332	^{274}Bh	8.940	9.062	8.079	8.711	8.780
^{255}No	8.428	8.002	7.774	8.252	8.422	^{263}Hs	10.730	10.717	10.287	10.705	10.966
^{256}No	8.582	7.991	7.621	8.133	8.610	^{264}Hs	10.591	10.666	10.148	10.551	10.626
^{257}No	8.477	7.981	7.467	7.983	8.375	^{265}Hs	10.470	10.542	10.009	10.395	10.561
^{259}No	7.854	7.775	7.158	7.643	7.784	^{266}Hs	10.346	10.369	9.868	10.252	10.326
^{252}Lr	9.164	9.064	8.844	9.004	9.165	^{267}Hs	10.038	10.189	9.726	10.135	10.026
^{253}Lr	8.918	8.859	8.698	8.932	8.870	^{270}Hs	9.070	9.863	9.296	9.929	9.184
^{254}Lr	8.822	8.669	8.552	8.871	8.672	^{273}Hs	9.650	9.780	8.858	9.614	9.614
^{255}Lr	8.556	8.532	8.404	8.804	8.664	^{275}Hs	9.450	9.531	8.562	9.178	9.297
^{256}Lr	8.850	8.469	8.255	8.716	8.777	^{266}Mt	10.996	10.981	10.461	10.832	11.216
^{257}Lr	9.070	8.461	8.105	8.599	8.850	^{275}Mt	10.480	10.158	9.186	9.878	10.246
^{258}Lr	8.904	8.453	7.954	8.453	8.765	^{276}Mt	10.100	9.994	9.040	9.639	9.962
^{255}Rf	9.055	9.124	9.020	9.323	8.941	^{278}Mt	9.580	9.372	8.745	9.076	9.495
^{256}Rf	8.926	8.989	8.875	9.259	8.960	^{267}Ds	11.780	11.415	10.908	11.263	11.765
^{257}Rf	9.083	8.929	8.729	9.174	9.094	^{269}Ds	11.510	11.072	10.636	11.014	11.316
^{258}Rf	9.196	8.924	8.582	9.059	9.241	^{270}Ds	11.117	10.926	10.499	10.933	10.880
^{261}Rf	8.650	8.723	8.134	8.585	8.632	^{271}Ds	10.870	10.822	10.360	10.874	10.720
^{256}Db	9.340	9.572	9.482	9.769	9.312	^{273}Ds	11.370	10.732	10.081	10.758	10.726
^{257}Db	9.206	9.440	9.340	9.707	9.338	^{272}Rg	11.197	11.259	10.811	11.310	11.182
^{258}Db	9.437	9.383	9.197	9.625	9.440	^{274}Rg	11.480	11.175	10.536	11.198	11.289
^{259}Db	9.620	9.380	9.052	9.513	9.451	^{278}Rg	10.850	10.903	9.976	10.544	11.096
^{259}Sg	9.765	9.830	9.658	10.070	9.751	^{279}Rg	10.530	10.643	9.834	10.276	10.663
^{260}Sg	9.901	9.830	9.516	9.961	9.940	^{280}Rg	10.149	10.290	9.691	9.990	10.193
^{261}Sg	9.714	9.830	9.373	9.822	9.651	^{277}Cn	11.620	11.579	10.713	11.406	11.953
^{262}Sg	9.600	9.774	9.229	9.664	9.650	^{281}Cn	10.430	10.740	10.155	10.439	10.493
^{263}Sg	9.400	9.645	9.084	9.502	9.180	^{278}Nh	11.990	12.015	11.161	11.840	12.287
^{282}Nh	10.780	11.184	10.613	10.882	10.961	^{288}Mc	10.650	10.653	10.969	10.756	10.227
^{284}Nh	10.280	10.374	10.334	10.329	10.124	^{289}Mc	10.490	10.497	10.831	10.577	10.096
^{285}Nh	10.010	10.023	10.193	10.084	9.787	^{290}Mc	10.410	10.424	10.692	10.427	10.093
^{286}Nh	9.790	9.763	10.052	9.870	9.436	^{290}Lv	11.000	10.936	11.283	11.015	10.878
^{285}Fl	10.560	10.818	10.791	10.771	10.323	^{291}Lv	10.890	10.865	11.147	10.866	10.885
^{286}Fl	10.360	10.469	10.652	10.528	9.944	^{292}Lv	10.791	10.842	11.010	10.740	10.917
^{287}Fl	10.170	10.211	10.513	10.316	9.626	^{293}Lv	10.680	10.834	10.872	10.629	10.563
^{288}Fl	10.076	10.053	10.373	10.135	9.472	^{293}117	11.320	11.280	11.461	11.176	11.370
^{289}Fl	9.950	9.978	10.233	9.982	9.427	^{294}117	11.180	11.274	11.325	11.067	11.157
^{290}Fl	9.860	9.951	10.091	9.851	9.361	^{294}118	11.870	11.713	11.906	11.608	11.974
^{287}Mc	10.760	10.909	11.106	10.967	10.373						

caused by the shell effect and introduce shell correction. However, it is a tricky issue to deal with the shell effect. In 1960, Strutinsky [55] treated the shell effect as the deviation between the nonuniform level density and a uniform one and further added this deviation to the liquid-drop model. Based on this method, the macroscopic-microscopic models [49, 56] are developed to study the properties of superheavy nuclei and achieve great success, which proves the shell effect can be considered separately. Subsequently, Ren *et al.* use analytical formulae to consider shell correction and further calculate the binding energy and α- decay energy [51, 53, 54], which also obtain satisfactory results.

Table 2. The standard and average deviation (in MeV) between experimental α-decay energies and calculated ones denote as $\sqrt{\sigma^2}$ and $\overline{\sigma}$, respectively. * denotes the number of parameters is uncertain, the current one comes from the WS3 model [60].

Cases	$\sqrt{\sigma^2_{\mathrm{DZ}}}$	$\sqrt{\sigma^2_{\mathrm{DR}}}$	$\sqrt{\sigma^2_{\mathrm{Ours}}}$	$\sqrt{\sigma^2_{\mathrm{WS3+}}}$
209	0.482	0.223	0.190	0.167
Cases	$\overline{\sigma}_{\mathrm{DZ}}$	$\overline{\sigma}_{\mathrm{DR}}$	$\overline{\sigma}_{\mathrm{Ours}}$	$\overline{\sigma}_{\mathrm{WS3+}}$
209	0.416	0.177	0.141	0.121
Parameters	5	8	7	16^*

Using the same method, we systematically calculate 209 α-decay energies and plot the deviations between the experimental data and calculated ones by using equation (5) in figure 1. From this figure, especially in regions I and II, one can see that the deviations have an obvious symmetry with different amplitudes similar to the sine function, which is largely due to the shell effect. Whether similar analytical formulae can be used to better express shell correction for different regions attracts our interest. After many attempts, the shell correction is expressed by the first derivative of the normalized Gaussian function, which can be written as

$$f(t) = \frac{1}{\sqrt{2\pi}} t \exp\left[-\frac{1}{2}t^2\right]. \tag{6}$$

Combining equations (5) and (6), we obtain the final formula of α-decay energy. It can be expressed as

$$\begin{aligned} Q_\alpha = {} & a_1 + a_2\frac{Z}{A^{1/3}}\left(1-\frac{Z}{3A}\right) + a_3\left(\frac{N-Z}{A}\right)^2 \\ & + a_4\left(\frac{N-N_0}{a_5}\right)\exp\left[-\frac{1}{2}\left(\frac{N-N_0}{a_5}\right)^2\right] \\ & + a_6\left(\frac{N-N_1}{a_7}\right)\exp\left[-\frac{1}{2}\left(\frac{N-N_1}{a_7}\right)^2\right]. \end{aligned} \tag{7}$$

In this formula, N_0 and N_1 represent the center point corresponding to the correction function in regions I and II, respectively. The position of N_0 and N_1, properties of the correction function and detailed calculations will be shown in the next section.

3. Results and discussion

Based on the liquid-drop model, considering the shell correction, we put forward an improved formula to evaluate α-decay energy for heavy and superheavy nuclei. In this formula, the shell correction is described by the first derivative of the normalized Gaussian function. In order to exhibit more details of this function, the shape of this function is plotted in figure 2. One can see that the shape of this function is similar to the deviations between experimental data and calculated ones in figure 1. Meanwhile, this function is also localized, which does not have an influence on other nuclei. Based on the properties of this function, it is critical to find the center of this function, that is, the position of the neutron number corresponding to $t = 0$ in these two regions. Based on equation (7), we use the least square method to fit 209 experimental α decay energies and obtain $N_0 = 154$ and $N_1 = 170$ as the matched center point corresponding to this correction function in the region I and II, respectively. Meanwhile, the corresponding values of parameters are as follows

$$\begin{cases} a_1 = -26.3930 \\ a_2 = 2.7500 \\ a_3 = -95.1273 \\ a_4 = 0.3753 \\ a_5 = 2.5528 \\ a_6 = -1.0495 \\ a_7 = 3.7382. \end{cases}$$

For these parameters, a_5 and a_7 are dimensionless, and other parameters are in MeV. The a_2 and a_3 are the coefficients of Coulomb energy and symmetry energy, respectively. Where a_4 and a_6 are the amplitudes of the correction function, their values depend on the extent of deviations caused by the shell effects. From figure 1, it can be seen that the wave crest and valley of the deviations in region II are exactly opposite to the correction function, which is the reason why a_6 is negative.

For a more intuitive comparison of the results with or without introducing shell correction, the deviations between experimental α-decay energy and calculated ones by using equations (5) and (7) are plotted in figure 3. From this figure, one can see that there is a marked improvement by introducing shell correction. Noticeably, the shell effects are complex for nuclei with $N \geqslant 170$ and the experimental data can hardly be reproduced. While the calculated results by using equation (7) can reproduce the experimental α-decay energy within 0.1 MeV for most nuclei in this region. More importantly, it is well known that the shell effects will be strong and the deviations between experimental α-decay energies and predicted ones will be very large when the experimental synthesis approaches the next neutron magic number. This region is still far from the neutron magic number $N = 184$ predicted by the macroscopic-microscopic model and Skyrme-Hartree–Fock model [49, 56, 57]. Therefore, it is feasible to give a reliable prediction for nuclei with $170 \leqslant N \leqslant 180$.

The detailed calculations of 209 α-decay energies are shown in table 1. In this table, the first two columns denote the parent nuclei of α decay and corresponding values of decay energy Q_α, respectively. The last four columns denote the calculated results by using equation (7), the DR formula, the DZ formula, and WS3+, respectively. From this table, it can be found that the value of α-decay energy in the isotope chains decreases gradually with the increase of the number of neutrons, which is consistent with the conclusion of the quantum tunneling effect. The lower the decay energy, the more difficult it is for the α particle to penetrate the barrier from the parent nuclei and therefore the more stable nucleus they are, which also indicates that superheavy nuclei should be neutron-rich [50]. Meanwhile, from the results calculated by using equation (7), it can be seen that the calculated results

Table 3. Predictions of α-decay energies (in MeV) for nuclei with $Z = 117$, 118, 119, and 120. Q_α^{cal}, Q_α^{DZ}, Q_α^{DR} and $Q_\alpha^{\text{WS3+}}$ denote the corresponding predictions by using equation (7), DZ formula, DR formula, and WS3+, respectively.

Z	A	Q_α^{cal}	Q_α^{DZ}	Q_α^{DR}	$Q_\alpha^{\text{WS3+}}$	Z	A	Q_α^{cal}	Q_α^{DZ}	Q_α^{DR}	$Q_\alpha^{\text{WS3+}}$
117	289	11.773	11.996	11.828	11.790	119	295	12.140	12.347	12.034	12.570
117	291	11.370	11.730	11.447	11.460	119	297	12.123	12.083	11.833	12.300
117	295	11.255	11.188	10.967	11.120	119	299	12.016	11.816	11.643	12.730
117	297	11.140	10.914	10.769	11.540	119	301	11.816	11.547	11.434	12.370
117	299	10.932	10.636	10.553	11.390	120	292	13.031	13.292	13.082	13.310
117	301	10.679	10.357	10.309	11.540	120	293	12.786	13.165	12.883	13.240
118	290	12.197	12.433	12.251	12.410	120	294	12.641	13.038	12.714	13.070
118	291	11.948	12.303	12.047	12.220	120	295	12.577	12.910	12.574	13.100
118	292	11.799	12.171	11.875	12.010	120	296	12.563	12.782	12.455	13.190
118	293	11.731	12.039	11.730	12.020	120	297	12.562	12.652	12.353	13.020
118	295	11.708	11.773	11.501	11.700	120	298	12.550	12.522	12.258	12.900
118	296	11.692	11.638	11.402	11.560	120	299	12.512	12.391	12.166	13.185
119	291	12.617	12.865	12.669	12.870	120	300	12.446	12.259	12.072	13.287
119	293	12.222	12.607	12.297	12.510						

can reproduce the experimental α-decay energies within 0.3 MeV for most nuclei. After careful analysis of the nuclei with large deviations, we divide them into two categories. The first category mainly includes ^{255}Md, ^{255}No, ^{256}No, ^{257}No, ^{257}Lr and ^{258}Lr. These nuclei are mainly concentrated in the region near the proton number $Z = 102$ and the neutron number $N = 154$, which we believe is determined by the complex shell effects around $Z = 100$ and $N = 152$. It should be pointed out that this situation also occurs in the calculated results of the binding energy for heavy and superheavy nuclei [53, 54]. The second category mainly includes ^{270}Hs, ^{267}Ds, ^{269}Ds and ^{273}Ds, the ^{270}Hs has been predicted to be a deformed doubly magic nucleus by the macroscopic-microscopic models [49, 56] and this is supported by experiments [58, 59]. For these nuclei, their proton numbers are near $Z = 108$ or the neutron numbers are around $N = 162$. These factors may result in large deviations. Since the shell effect is a complex mechanism, there is no ideal approach to deal with this effect at present. In this work, the shell effect is considered by introducing analytic formula, which is an approximate method. Following this approach, the shell effect can not be completely described by analytical formulae bur what can be done is to search for a more appropriate analytical formula to minimize this approximate difference as much as possible. After the above discussion, it is reasonable to have a few nuclei with large deviations among 209 nuclei.

The $\overline{\sigma}$ and $\sqrt{\sigma^2}$ represent the average and standard deviation between experimental data and calculated ones. In this work, they are defined as follows

$$\overline{\sigma} = \sum_{i=1}^{209} |Q_\alpha^i \exp - Q_\alpha^i \text{cal}|/209, \tag{8}$$

$$\sqrt{\sigma^2} = \left[\sum_{i=1}^{209} (Q_\alpha^i \exp - Q_\alpha^i \text{cal})^2 / 209 \right]^{\frac{1}{2}}. \tag{9}$$

Using equations (8) and (9), we calculate the average and standard deviation between experimental data and calculated ones by using the DZ formula, DR formula, WS3+, and equation (7), respectively. The detailed calculated results are listed in table 2. From this table, it can be seen that our formula achieves satisfactory results with only seven parameters. In addition, the differences between experimental data and calculated ones for 209 nuclei by using these formulae and equation (7) are plotted in figure 4. One can see that compared with the DZ formula and DR formula, our improved 7-parameter formula can reproduce experimental data better.

Finally, as an application, we extend this formula to predict the α-decay energies for nuclei with $Z = 117$, 118, 119 and 120. For comparison, the reliable DZ formula, DR formula, and WS3+ are also used. The corresponding predictions are listed in table 3. In this table, the first two columns denote the proton and mass number of the parent nucleus, respectively. The last four columns denote the α-decay energies predicted by using equation (7), DR formula, DZ formula, and WS3+, respectively. From this table, it can be seen that the predicted results of these formulae are basically consistent, which can provide useful information for experiments of synthesising new elements and isotopes.

4. Summary

In this work, we put forward an improved formula to systematically calculate the α-decay energy based on the liquid-drop model. The calculated results are in good agreement with the experimental data. The corresponding average and standard deviation are 0.141 and 0.190 MeV, respectively. The α-decay energy calculated by our improved formula is found to be in better agreement with experimental data compared with the DZ formula and DR formula. Meanwhile, the results calculated by our improved formula are largely consistent with the WS3+ nuclear mass model. Finally, we extend this formula to predict the α-decay energies for nuclei with $Z = 117$, 118, 119, and 120. The predicted results of these formulae are basically consistent with each other. More importantly, this formula can be used as an independent tool to quantify the α-decay energy of unknown nuclei and further test theoretical predictions of other methods and/or models. It is hoped that this work will be the basis for better experimental design in the future.

ORCID iDs

Xiao-Hua Li (李小华) https://orcid.org/0000-0002-3399-6057

References

[1] Hofmann S and Münzenberg G 2000 The discovery of the heaviest elements *Rev. Mod. Phys.* **72** 733

[2] Oganessian Y T and Rykaczewski K P 2015 A beachhead on the island of stability *Phys. Today* **68** 32

[3] Oganessian Y T *et al* 2007 Synthesis of the isotope ^{282}113 in the ^{237}Np+^{48}Ca fusion reaction *Phys. Rev.* C **76** 011601

[4] Oganessian Y T 2007 Heaviest nuclei from ^{48}Ca-induced reactions *J. Phys.* G **34** R165

[5] Hofmann S *et al* 2012 The reaction ^{48}Ca+^{248}Cm $\rightarrow$ $^{296}116^{*}$ studied at the GSI-SHIP *Eur. Phys. J.* A **48** 62

[6] Ellison P A *et al* 2010 New superheavy elements isotopes: ^{242}Pu(^{48}Ca,5n)^{285}114 *Phys. Rev. Lett.* **105** 182701

[7] Oganessian Y T *et al* 2006 Synthesis of the isotopes of elements 118 and 116 in the ^{249}Cf and ^{245}Cm+^{48}Ca fusion reactions *Phys. Rev.* C **74** 044602

[8] Oganessian Y T *et al* 2010 Synthesis of a new element with atomic number Z = 117 *Phys. Rev. Lett.* **104** 142502

[9] Hofmann S *et al* 2016 Review of even element super-heavy nuclei and search for elements 120 *Eur. Phys. J.* A **52** 180

[10] Oganessian Y T, Utyonkov V K, Lobanov Y V *et al* 2009 Attempt to produce element 120 in the ^{244}Pu+^{58}Fe reaction *Phys. Rev.* C **79** 024603

[11] Hamilton J H, Hofmann S and Oganessian Y T 2015 The importance of closed shell structures in the synthesis of super heavy elements *J. Phys.: Conf. Ser.* **580** 012019

[12] Oganessian Y T *et al* 2000 Synthesis of superheavy nuclei in the ^{48}Ca+^{244}Pu reaction: ^{288}114 *Phys. Rev.* C **62** 041604

[13] Dvorak J *et al* 2008 Observation of the 3n Evaporation Channel in the Complete Hot-Fusion Reaction ^{26}Mg+^{248}Cm Leading to the New Superheavy Nuclide ^{271}Hs *Phys. Rev. Lett.* **100** 132503

[14] Gan Z G *et al* 2004 New isotope ^{265}Bh *Eur. Phys. J.* A **20** 385

[15] Oganessian Y T *et al* 2004 Experiments on the synthesis of element 115 in the reaction ^{243}Am(^{48}Ca,xn)$^{291-x}$115 *Phys. Rev.* C **69** 021601(R)

[16] Ellison P A *et al* 2010 New superheavy element isotopes: ^{242}Pu(^{48}Ca,5n)^{285}114 *Phys. Rev. Lett.* **105** 182701

[17] Oganessian Y T 2011 Synthesis of the heaviest elements in ^{48}Ca-induced reactions *Radiochim. Acta* **99** 429

[18] Ren Z Z and Xu G O 1987 Reduced alpha transfer rates in a schematic model *Phys. Rev.* C **36** 456

[19] Xu C and Ren Z Z 2007 α transitions to coexisting 0^{+} states in Pb and Po isotopes *Phys. Rev.* C **75** 044301

[20] Audi G, Bersillon O and Wapstra A H 2003 The NUBASE evaluation of nuclear and decay properties *Nucl. Phys.* A **729** 3

[21] Seweryniak D *et al* 2006 α decay of ^{105}Te *Phys. Rev.* C **73** 061301(R)

[22] Hodgson P E and Betak E 2003 Cluster emission, transfer and capture in nuclear reactions *Phys. Rep.* **374** 1

[23] Horiuchi H 1991 Microscopic study of clustering phenomena in nuclei *Nucl. Phys.* A **522** 257

[24] Leppänen A P *et al* 2007 α decay studies of the nuclides ^{218}U and ^{219}U *Phys. Rev.* C **75** 054307

[25] Rutherfold E and Geiger H 1908 The charge and nature of the α-particle *Proc. R. Soc. London* A **81** 162

[26] Gamow G 1928 Zur quantentheorie des atomkernes *Z. Phys.* **51** 204

[27] Condon E U and Gurney R W 1928 Wave mechanics and radioactive disintegration *Nature (London)* **122** 439

[28] Dong J M *et al* 2010 Alpha-decay for heavy nuclei in the ground and isomeric states *Nucl. Phys.* A **832** 198

[29] Royer G and Zhang H F 2008 Recent α decay half-lives and analytic expression predictions including superheavy nuclei *Phys. Rev.* C **77** 037602

[30] Chowdhury P R, Samanta C and Basu D N 2006 α decay half-lives of new superheavy elements *Phys. Rev.* C **73** 014612

[31] Bhattacharya M and Gangopadhyay G 2008 α-decay lifetime in superheavy nuclei with A < 282 *Phys. Rev.* C **77** 047302

[32] Xu C and Ren Z Z 2004 α decay of nuclei in extreme cases *Phys. Rev.* C **69** 024614

[33] Ni D and Ren Z Z 2009 Exotic α decays around the N = 126 magic shell *Phys. Rev.* C **80** 014314

[34] Delion D S, Peltonen S and Suhonen J 2006 *Phys. Rev.* C **73** 014305

[35] Peltonen S, Delion D S and Suhonen J 2007 Folding description of the fine structure of α decay to 2^{+} vibrational and transitional states *Phys. Rev.* C **75** 054301

[36] Sun X D, Guo P and Li X H 2016 Systematic study of α decay half-lives for even-even nuclei within a two-potential approach *Phys. Rev.* C **93** 034316

[37] Deng J G *et al* 2018 α decay properties of ^{296}Og within the two-potential approach *Chin. Phys.* C **42** 044102

[38] Hatsukawa Y, Nakahara H and Hoffman D C 1990 Systematics of alpha decay half-lives *Phys. Rev.* C **42** 674

[39] Ni D *et al* 2008 Unified formula of half-lives for α decay and cluster radioactivity *Phys. Rev.* C **78** 044310

[40] Liu H M *et al* 2020 Systematic study of the α decay preformation factors of the nuclei around the Z = 82, N = 126 shell closures within the generalized liquid drop model *Chin. Phys.* C **44** 094106

[41] Sobiczewski A, Patyk Z and Cwiok S 1989 Deformed superheavy nuclei *Phys. Lett.* B **224** 1

[42] Xu Y Y *et al* 2022 An improved formula for the favored α decay half-lives *Eur. Phys. J.* A **58** 16

[43] Viola V E and Seaborg G T 1966 Nuclear systematics of the heavy elements-II Lifetimes for alpha, beta and spontaneous fission decay *J. Inorg. Nucl. Chem.* **28** 741

[44] Zou Y T *et al* 2021 Systematic studies on α decay half-lives of neptunium isotopes *Phys. Scr.* **96** 075301

[45] Royer G 2000 Alpha emission and spontaneous fission through quasi-molecular shapes *J. Phys.* G **26** 1149

[46] Brown B A 1992 Simple relation for alpha decay half-lives *Phys. Rev.* C **46** 811

[47] Qi C, Xu F R and Wyss R 2009 Universal decay law in charged-particle emission and exotic cluster radioactivity *Phys. Rev. Lett.* **103** 072501

[48] Xu Y Y *et al* 2022 Systematic study on α-decay half-lives of uranium isotopes with a screened electrostatic barrier *Chin. Phys.* C **46** 114103

[49] Möller P, Nix J R and Kratz K L 1997 Nuclear properties for astrophysical and radioactive-ion-beam applications *At. Data and Nucl. Data Tables* **66** 131

[50] Dong J M, Zuo W and Peng B 2010 α-decay half-lives and Q_{α} values of superheavy nuclei *Phys. Rev.* C **81** 064309

[51] Dong T K and Ren Z Z 2010 α-decay energy formula for superheavy nuclei based on the liquid-drop model *Phys. Rev.* C **82** 034320

[52] Wang N and Liu M 2011 Nuclear mass predictions with a radial basis function approach *Phys. Rev.* C **84** 051303(R)

[53] Dong T K and Ren Z Z 2005 New model of binding energies of heavy nuclei with $Z < 90$ *Phys. Rev.* C **72** 064331

[54] Dong T K and Ren Z Z 2008 Improved version of a binding energy formula for heavy and superheavy nuclei with $Z \geqslant 90$ and $N \geqslant 140$ *Phys. Rev.* C **77** 064310

[55] Strutinsky V M 1967 Shell effects in nuclear masses and deformation energies *Nucl. Phy.* A **95** 420

[56] Möller P, Nix J R and Swiatecki W J 1995 Nuclear ground-state masses and deformations *At. Data and Nucl. Data Tables* **59** 185

[57] Kruppa A T, Bender M and Cwiok S 2000 Shell corrections of superheavy nuclei in self-consistent calculations *Phys. Rev.* C **61** 034313

[58] Lazarev Yu A *et al* 1996 α decay of $^{273}110$: shell closure at $N = 162$ *Phys. Rev.* C **54** 620

[59] Dvorak J *et al* 2006 Doubly magic nucleus $^{270}_{108}\mathrm{Hs}_{162}$ *Phys. Rev. Lett.* **97** 242501

[60] Liu M *et al* 2011 Further improvements on a global nuclear mass model *Phys. Rev.* C **84** 014333

[61] Wang M *et al* 2021 The AME 2020 atomic mass evaluation (II). Tables, graphs and references* *Chin. Phys.* C **45** 030003