Letter

Simple corrections in theoretical models of atomic masses and nuclear charge radii

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We study the systematic deviations of the theoretical results (the Hartree-Fock-Bogoliubov, the relativistic mean field, the Duflo-Zuker, and Weizsäker-Skyrme models) and experimental values of atomic masses, one-nucleon separation energies, and nuclear charge radii. Strong correlations of these deviations, which has not been discerned hitherto, are highlighted, and are applied to improve the agreement of theoretical models with experimental experimental data. Substantial refinements of the consistency between theoretical models and experimental databases are achieved with additionally *only one parameter* which reflects the correlation reported in this Letter. The root mean square deviation values of these theoretical models in comparison with experimental databases are about 100–300 keV for atomic masses, 120–350 keV for one-nucleon separation energies, and 0.008–0.017 fm for nuclear charge radii, for nuclei with proton number Z larger than 28.

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Atomic masses (or equivalently binding energies) and nuclear charge radii are fundamental quantities of atomic nuclei, and are important in both traditional nuclear physics and nuclear astrophysics. There have been tremendous theoretical efforts to address these issues [1], and here we mention the Duflo-Zuker (DZ) model [2], the Skyrme-Hartree-Fock Bogoliubov (SHFB) theory [3], the relativistic mean field (RMF) model [4], the WS4 models [5], and the finite-range droplet model (FRDM)[6], and so on. There are also local and regional mass formulas [7], such as the Garvey-Kelson (G-K) mass relations [8,9], the neutron-proton interaction relation [10], and mass formulas between mirror nuclei [11].

In recent years, a few statistical approaches, including the radial basis functions (RBF) [12–15] and Bayesian neural networks (BNN) [16,17] were used to reduce the root-mean-squared deviations (RMSD) of theoretical atomic masses and charge radii from experimental data. Although these statistical approaches are interesting and potentially useful, there are actually numerous parameters to be optimized. It is therefore interesting to investigate whether or not substantial improvements of agreement between theoretical calculated results and experimental data are possible, with *very simple* modifications.

There have been a number of efforts towards simple corrections on theoretical results of atomic mass and/or related quantities in the last decade. It was reported [18] that there are clearly odd-even staggerings of symmetry energy extracted from experimental data, which reveals systematic deviations of theoretical models from the AME databases. In Refs. [19,20], simple corrections were considered to compensate the systematic deviations of theoretical models in comparison with experimental data. However, improvements therein are small, with typically 10–20 keV for atomic masses. Very recently it was shown [21] that correlations of deviations between neutron-proton interactions given by empirical formulas and those extracted from experimental data for given nucleus and its specific neighboring nucleus, in major shells to the northwest of the doubly closed ^{208}Pb nucleus, are very strong, and are very useful to improve the agreement between theoretical results (e.g., atomic masses, Q_α, proton separation energy) with experimental database, for nuclei with proton number Z larger than 28.

The purpose of this Letter is to report that substantial improvements can be realized with considering specific correlation of deviations between calculated quantities and experimental databases with *only one parameter* related to the correlation. Our approach is exemplified by a number of popular theoretical models (here the HFB, the RMF, the DZ, and the WS4 + RBF, the relativistic continuum Hartree-Bogoliubov (RCHB), and the WS* models), for atomic masses, one-nucleon separation energies, and nuclear charge radii. We begin our discussion by denoting the deviation between theoretically calculated atomic mass and experimental result for given nucleus with neutron number N and proton number Z, using $D_M(N,Z)$, defined as follows:

$$D_M(N,Z) = M^{\rm exp}(N,Z) - M^{\rm th}(N,Z), \tag{1}$$

where $M^{\rm exp}(N,Z)$ corresponds to experimental value, and $M^{\rm th}(N,Z)$ corresponds to theoretical result. Similarly, we denote deviation between theoretical results and experimental data, by using $D_{S_n}(N,Z)$ for one-neutron separation energy, $D_{S_p}(N,Z)$ for one-proton separation energy, and $D_R(N,Z)$ for nuclear charge radius.

In the first row of Fig. 1, we plot $D_M(N,Z)$ versus $D_M(N-2,Z)$ for neutron-rich nuclei, and $D_M(N,Z)$ versus $D_M(N+$

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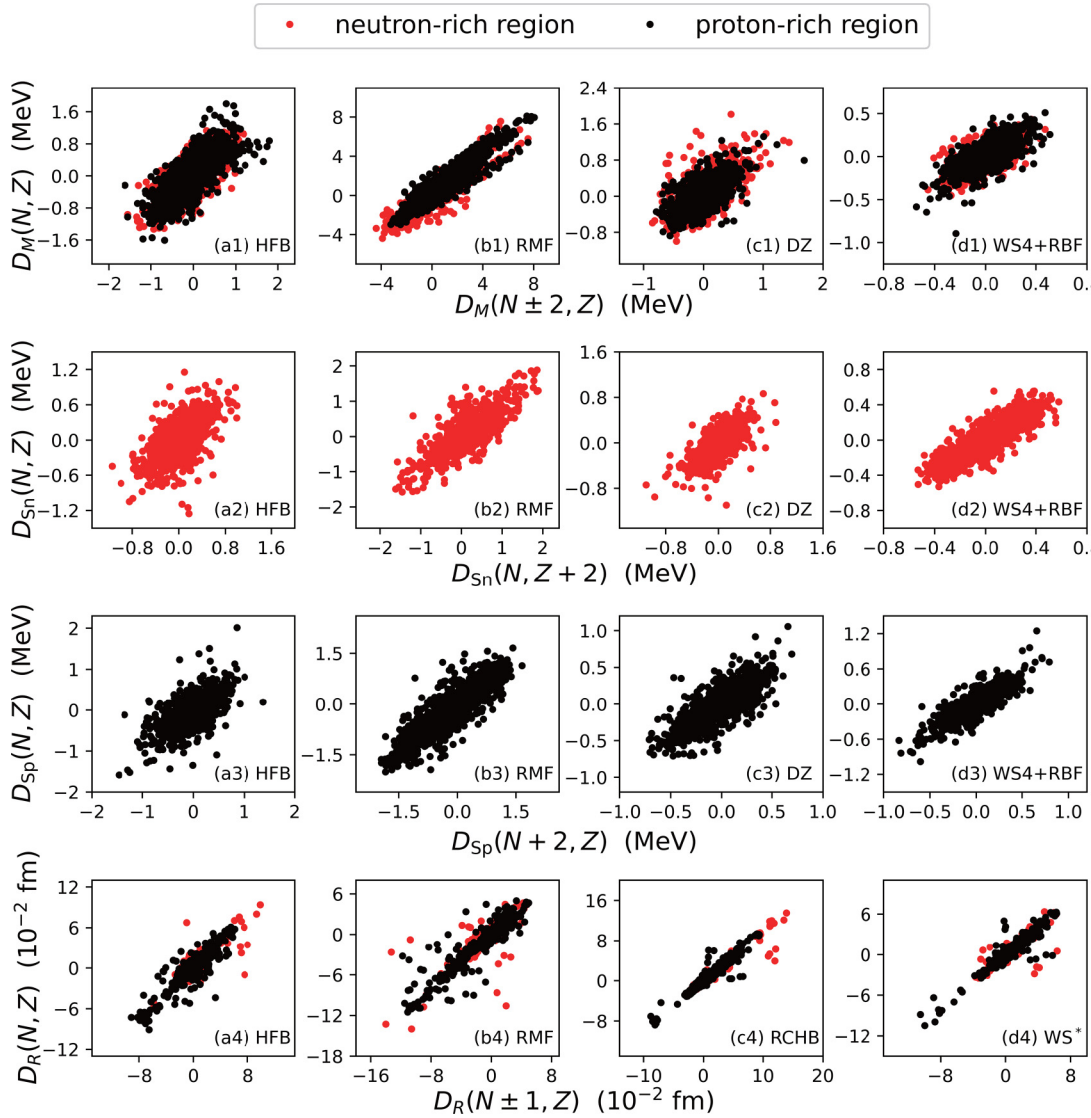

FIG. 1. Correlations between $D_X(N,Z)$ and $D_X(N',Z')$ of Eq. (2). Results of neutron-rich nuclei are plotted in red and those of proton-rich are in black. (a1)–(d1): X corresponds to atomic mass, and $Z'=Z$, $N'=N-2$ for neutron-rich nuclei, and $N'=N+2$ for proton-rich nuclei. (a2)–(d2): X corresponds to one-neutron separation energies of neutron-rich nuclei, $Z'=Z$, $N'=N-2$. (a3)–(d3): X corresponds to one-proton separation energies of proton-rich nuclei, $Z'=Z$, $N'=N+2$. In the first three rows, we exemplify the correlations by using four models, the HFB31 [3], DZ [2], RMF [22], WS4 + RBF [5]. (a4)–(d4): X corresponds to nuclear charge radii, $Z'=Z$, $N'=N-1$ ($Z'=Z$, $N'=N+1$) for neutron-rich (proton-rich) nuclei. Because there are not theoretical databases of nuclear charge radii for the DZ and the WS4 + RBF models, we take the RCHB [23] and the WS* [24] models instead. In this Letter we restrict our discussions to nuclei with proton numbers $Z>28$.

$2,Z$) for proton rich nuclei. Similarly, in the second row and third rows of Fig. 1, we plot $D_{S_p}(N,Z)$ versus $D_{S_p}(N+2,Z)$ and $D_{S_n}(N,Z)$ versus $D_{S_n}(N,Z+2)$; in the fourth row, we plot $D_R(N,Z)$ versus $D_R(N-1,Z)$ for neutron-rich nuclei and $D_R(N+1,Z)$ versus $D_R(N,Z)$ for proton-rich nuclei. One sees that for all these quantities (atomic masses, one-nucleon separation energies, and nuclear charge radii), our plots of four popular models (the HFB, the RMF, the Duflo-Zuker, and the WS4 + RBF models here) exhibit strong and linear correlations. We therefore assume that

$$D_X(N,Z)=\lambda D_X(N',Z'), \tag{2}$$

where X denotes M, S_n, S_p, and R for atomic mass, one-neutron separation energy, one-proton separation energy, and nuclear charge radius, λ is the optimized coefficient. $N'=N-2$ ($N+2$) and $Z'=Z$ for D_M with neutron-rich (proton-rich) nuclei, $N'=N+2$ and $Z'=Z$ for for D_{S_p}, $N'=N$ and $Z'=Z+2$ for D_{S_n}, and $N'=N-1$ ($N+1$) and $Z'=Z$ for D_R with neutron-rich (proton-rich) nuclei.

In Table I we present the Pearson correlation coefficient, the optimal value of λ of Eq. (2), for atomic masses, separation energies, and nuclear charge radii. One sees that the linear correlation Pearson coefficient is typically 0.6 to 0.9, which corresponds to strong correlation.

TABLE I. Summary of correlations between $D_X(N,Z)$ and $D_X(N',Z')$ of the same theoretical models in Fig. 1. X corresponds to atomic masses M, one-nucleon separation energies S_n and S_p, nuclear charge radii R. λ_X corresponds to the optimal linear coefficient in Eq. (2), and r_X is the corresponding Pearson coefficient. σ_X and $\sigma_X^{\rm pred}$ correspond to the RMSD of theoretical models for physical quantity X with respect to experimental database, without and with the corrections introduced in this paper, respectively. The RMSD values for atomic masses and one-nucleon separation energies are in unit of keV, and those for nuclear charge radii are in unit of fm.

model	type	λ_M	r_M	σ_M	$\sigma_M^{\rm pred}$	λ_S	r_S	σ_S	$\sigma_S^{\rm pred}$	λ_R	r_R	σ_R	$\sigma_R^{\rm pred}$
HFB31	N	0.76	0.74	464	318	0.63	0.60	342	275	0.91	0.88	0.023	0.012
	P			497	331	0.72	0.67	372	276			0.026	0.012
DZ	N	0.78	0.67	400	305	0.75	0.70	260	186				
	P			313	226	0.85	0.78	248	155				
RMF	N	0.97	0.93	1840	843	0.78	0.81	592	342	0.91	0.88	0.026	0.017
	P			2535	737	0.92	0.89	789	346			0.038	0.014
WS4+RBF	N	0.75	0.75	150	104	0.84	0.84	229	123				
	P			155	101	0.91	0.86	236	121				
RCHB	N									1.02	0.96	0.040	0.011
	P											0.033	0.008
WS*	N									0.94	0.91	0.018	0.010
	P											0.023	0.008

We improve theoretical results of these physical quantities by considering these correlations. Let us denote quantities of our calculated results of quantity X [i.e., with consideration the correlations exhibited in Eq. (2)] with "pred" superscript, and the results of X given by theoretical models (such as the HFB31 model and others adopted in this paper) with "th" superscript. From Eq. (2), we readily have

$$X^{\rm pred}(N,Z) = X^{\rm th}(N,Z) + \lambda D_X(N',Z').$$

Specifically, we have

$$M^{\rm pred}(N,Z) = M^{\rm th}(N,Z) + \lambda_M D_M(N-2,Z) \tag{3}$$

for neutron-rich nuclei, and

$$M^{\rm pred}(N,Z) = M^{\rm th}(N,Z) + \lambda_M D_M(N+2,Z) \tag{4}$$

for proton-rich nuclei. Similarly, we have

$$S_n^{\rm pred}(N,Z) = S_n^{\rm th}(N,Z) + \lambda_S D_{S_n}(N,Z+2) \tag{5}$$

for neutron-rich nuclei, and

$$S_p^{\rm pred}(N,Z) = S_p^{\rm th}(N,Z) + \lambda_S D_{S_p}(N+2,Z) \tag{6}$$

for proton-rich nuclei; and

$$R^{\rm pred}(N,Z) = R^{\rm th}(N,Z) + \lambda_R D_R(N-1,Z) \tag{7}$$

for neutron-rich nuclei, and

$$R^{\rm pred}(N,Z) = R^{\rm th}(N,Z) + \lambda_R D_R(N+1,Z) \tag{8}$$

for proton rich nuclei. We evaluate the RMSD deviations of such calculated results from corresponding experimental results, and denote the RMSD values without and with these corrections of the above formulas by using σ and $\sigma^{\rm pred}$, respectively. Such σ and $\sigma^{\rm pred}$ are tabulated in Table I, where one sees clearly the substantial improvements with considering the correlation of Eq. (2). We note that for the new databases after our correction in Table I, the Pearson correlation coefficient between $D(N\pm2,Z)$ and $D(N,Z)$ becomes -0.03, 0.15, 0.23, and -0.10 for the HFB, DZ, RMF, and WS4 + RBF models, respectively. It is noted that the correlation is said to be strong, medium, weak, and null, respectively, if the Pearson coefficient is 0.6–0.8, 0.4–0.6, 0.2–0.4, 0.0–0.2, respectively. This means that either the correlation does not exist or is very weak, after our corrections. In successive extrapolation process, for those whose experimental data are not accessible and thus relevant D_M are unknown, we take corresponding $\lambda D_M^{(1)}$ as the surrogates of D_M, where $D_M^{(1)}$ is the D_M used in the one-step-earlier extrapolation. We take the AME2012 database [26] and the WS4 + RBF database [5] to investigate how many successive extrapolations are practically useful if D_M is not available. We define $\Delta\sigma(k) = \sigma - \sigma^{\rm pred}(k)$, where σ is the theoretical RMSD of a given quantity calculated in Ref. [5] in comparison with experimental database of Ref. [25], and $\sigma^{\rm pred}(k)$ is the RMSD value of the same quantity predicted based on Ref. [5] but with corrections introduced in this paper, in the kth step extrapolation. $\Delta\sigma(k)$ represents the magnitude of our correction: $\Delta\sigma_M(k)$ correspond to mass, $\Delta\sigma_{S_n}(k)$ and $\Delta\sigma_{S_n}(k)$ correspond to one-neutron and one-proton separation energy, respectively, and $\Delta\sigma_R(k)$ corresponds to nuclear charge radius. Without details we note that, according to our numerical experiments, $\Delta\sigma(k)$ decreases with k, and $\Delta\sigma(k)$ is very small for M, $\Delta\sigma_{S_n}$, and $\Delta\sigma_{S_p}$ with $k \geqslant 8$; for nuclear charge radius, the correction of proton-rich nuclei is below 0.005 fm for with $k \geqslant 10$, and that of neutron-rich nuclei is negligible for $k \geqslant 8$. Such pattern is also seen in the Pearson correlation coefficients r of D values: according to our numerical experiments, the values of r for masses and one-nucleon separation energies decrease from $\sim$0.8 to $\sim$0.5 when k increases from 2 to 6, in contrast to the r value for nuclear charge radius, for which r is reduced to $\sim$0.5 for $k \geqslant 10$. This sets the applicability of the correction introduced in this paper.

Now let us investigate the predictive power of extrapolation by using our approach. This is exemplified by numerical experiments of extrapolations from the AME2012 database [26] to the AME2020 database [25] for atomic masses and one-nucleon separation energies, and from the CR2013 database

TABLE II. The RMSD values of extrapolated results with the corrections introduced in this Letter (denoted by $\sigma_X^{\rm extra}$) and without the corrections (denoted by σ_X). Here, types "P" and "N" means proton-rich and neutron-rich cases, respectively. We exclude a very few "anomalies" of Hg isotopes which involve of the shape coexistence when we evaluate $\sigma_R^{\rm extra}$ or those of which the number k of successive extrapolations is larger than ten for nuclear charge radii. The RMSD values for Atomic masses and one-nucleon separation energies are in unit of keV, and those for nuclear charge radii are in unit of fm.

model	type	σ_M	$\sigma_M^{\rm extra}$	σ_S	$\sigma_S^{\rm extra}$	σ_R	$\sigma_R^{\rm extra}$
HFB31	N	601	465	516	476	0.021	0.016
HFB31	P	689	594	453	404	0.034	0.024
DZ	N	730	459	255	179		
DZ	P	419	306	268	204		
RMF	N	1189	646	419	214	0.018	0.014
RMF	P	5245	1256	984	350	0.025	0.014
WS4+RBF	N	230	163	221	149		
WS4+RBF	P	260	220	283	224		
RCHB	N					0.020	0.017
RCHB	P					0.030	0.010
WS*	N					0.010	0.009
WS*	P					0.017	0.010

[27] to the CR2021 database [28] for nuclear charge radii. Our predicted atomic mass is obtained by using Eq. (3) or (4), depending on the nucleus neutron-rich or proton-rich. Corresponding to Eqs. (3) and (4), the statistical uncertainty of our predicted atomic mass, denoted by d_M equals

$$d_M^{\rm pred}(N,Z) = \sqrt{(\sigma^{\rm pred})^2 + \lambda^2 d_{\rm exp}^2(N-2,Z)} \qquad (9)$$

for neutron-rich nuclei, and

$$d_M^{\rm pred}(N,Z) = \sqrt{(\sigma^{\rm pred})^2 + \lambda^2 d_{\rm exp}^2(N+2,Z)}, \qquad (10)$$

for proton-rich nuclei. Here, $\sigma_M^{\rm pred}$ is the RMSD of predicted results with the correlation correction, and λ is the optimal correlation coefficient in Eq. (2); $d_{\rm exp}(N-2,Z)$ and $d_{\rm exp}(N+2,Z)$ are uncertainties of experimental data of $M(N-2,Z)$ and $M(N+2,Z)$ in the AME2012 database [26]. The statistical uncertainties of one-nucleon separation energies and nuclear charge radii, d_S and d_R, are obtained in the same way.

A comparison between our extrapolated results (those not accessible in an earlier database, namely, here the AME2012 for atomic masses and one-nucleon separation energies, or the CR2013 database, but accessible in the latest database, namely, the AME2020 or the CR2021 database) by using Eqs. (3)–(8), with respect to latest experimental data, is summarized in Fig. 2. We tabulate the RMSD of these extrapolated results, denoted by $\sigma_X^{\rm extra}$ in Table II, with a comparison of the RMSD for the same set of nuclei without the correction in this paper, denoted by σ_X. From Fig. 2 and Table II, one sees immediately that the extrapolated results with the corrections introduced in this Letter are superior to those without these corrections.

It is interesting to discuss the mechanism of our correction, as the improvement in this paper is empirical. One plausible reason for this correction is related to the treatment of pairing effect in Ref. [5] (and other theoretical models taken in this paper) might be not very sound, as the odd-even effect of deviations between the theoretical database of Ref. [26] and the AME2020 database is clearly seen [19], where an empirical and global correction was assumed with the improvement of the agreement between theoretical results and experimental data very modest (only ∼12 keV for atomic masses, and ∼30 keV for one-nucleon separation energies). In this paper the correction magnitude with local correlation is superior ($\Delta\sigma \sim 50$ keV for atomic masses, and ∼100 keV for one-nucleon-separation energies, refer to Table I) for the WS4 + BRF model; the magnitude of improvement is even larger for the RMF model, for which the improvement of atomic masses is about 1 MeV, and 250 keV for one-nucleon separation energies.

The predictive power of our simple correction encourages us to present refined results of earlier models. Here, we start from the WS4 + RBF model for atomic mass and one-nucleon separation energy, and the WS* model for nuclear charge radii. Our predicted results are presented as a supplemental material of this Letter [29], where the steps of our successive extrapolations are within $k \leqslant 6$ for atomic masses and one-nucleon separation energies, and $k \leqslant 9$ for nuclear charge radii.

To summarize, in this Letter we report an interesting correlation of deviations between theoretical models and experimental databases, defined by $D_X(N,Z) = X^{\rm exp}(N,Z) - X^{\rm th}(N,Z)$, where $X(N,Z)$ corresponds to atomic mass, one-nucleon separation energy, or nuclear charge radii. Consideration such correlations with *only one parameter* is found to improve substantially the consistency between theoretical calculations and experimental databases. Therefore the correction reported in this Letter is very suggestive to future studies for varieties of theoretical models.

The predictive power of our corrections is demonstrated by numerical experiments of extrapolation from earlier databases to the latest databases. For the WS4 + RBF model, the RMSD value of atomic masses with considering the correction in this

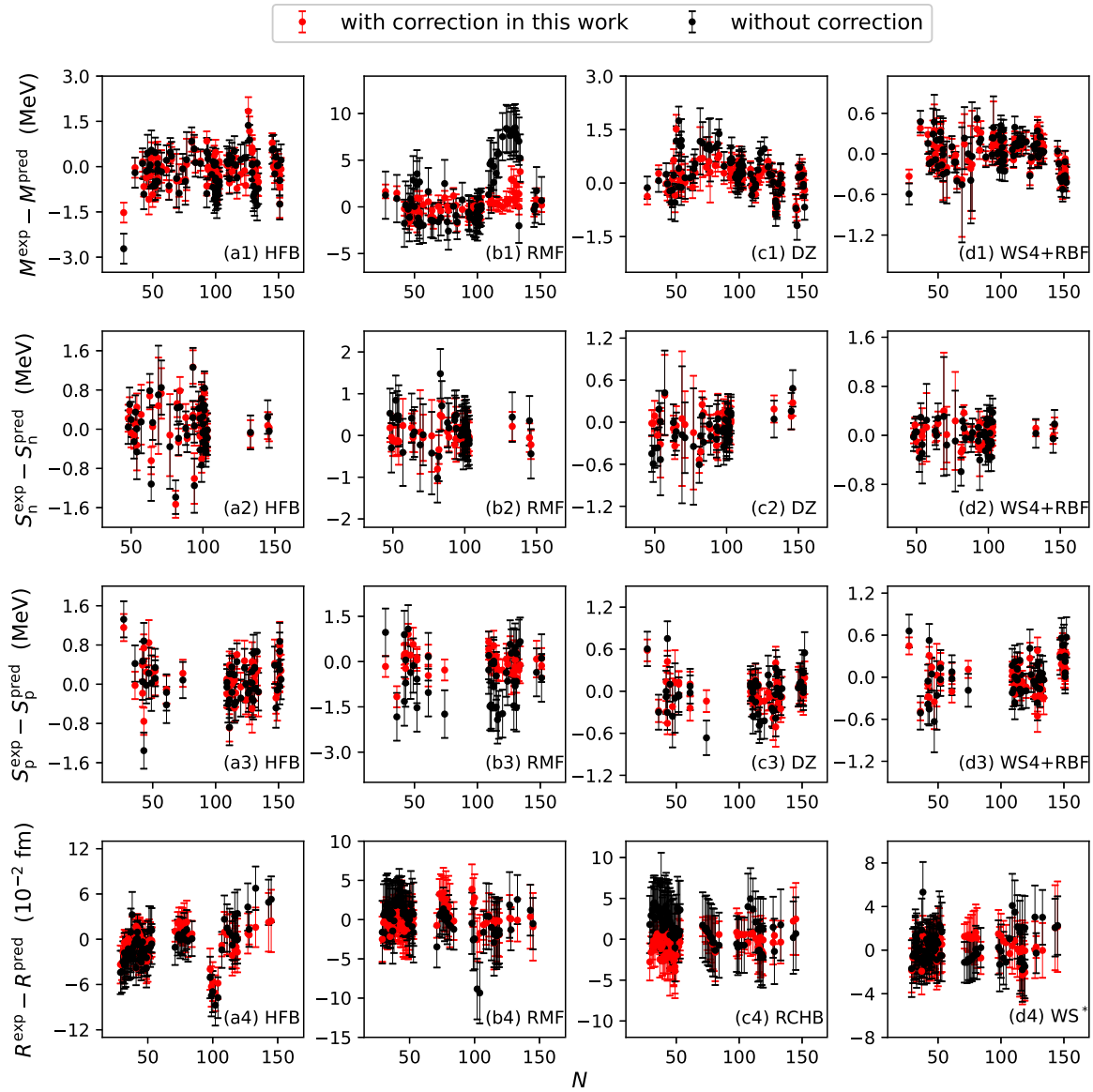

FIG. 2. Comparison of our predicted atomic masses and one-nucleon separation energies (which are not accessible in the AME2012 database [26] but available in the AME2020 database [25]), and nuclear charge radii (which are not accessible in the CR2013 database [27] but available in the latest 2021 version [28]), with latest databases, i.e., Refs. [25] and [28], versus neutron number N. Results with the corrections introduced in this Letter are plotted in red and those without the corrections are in black. For nuclear charge radii, we exclude a very few "anomalies" of Hg isotopes which involve of the shape coexistence.

Letter is reduced to about 100 keV; for the WS* model, the RMSD value of nuclear charge radii is reduced to 0.008–0.010 fm (if a very few anomalies for Hg isotopes are excluded). We enclose our predicted results of atomic masses and one-nucleon separation energies based on the WS4 + RBF model and the AME2020 database [25], and nuclear charge radii based on the WS* model and the latest version of nuclear charge radii [28], as the Supplemental Material [29] of this Letter.

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[29] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevC.106.L061304 for predicted mass excesses, one-nucleon separation energies, nuclear charge radii, which are experimentally unaccessible in the latest version of atomic masses and nuclear charge radii.