Toward *ab initio* determination of charge symmetry breaking strength of Skyrme functionals

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We propose a new approach to determine the strength of the charge symmetry breaking (CSB) term in the framework of Skyrme density functional theory. It is shown that once *ab initio* calculations are available including accurate description of isospin symmetry breaking terms in medium and heavy nuclei, the mass difference of mirror nuclei as well as the neutron-skin thickness of doubly closed shell nuclei can be used to constrain the strength of CSB interaction with an uncertainty less than 6%, separately from other isospin breaking forces. This method opens a new vista of *ab initio* nuclear energy density functionals.

Introduction.—The nuclear mean-field theory or the Energy Density Functionals (EDFs), such as Skyrme [1, 2], Gogny [3, 4], the Michigan-three-range-Yukawa type [5-7], the Fayans ones [8, 9], and the covariant ones [10-12], successfully reproduce many properties of atomic nuclei in the whole region of the nuclear chart, as well as nuclear matter properties related to the equation of state and neutron stars [13-17].

The parameter sets of EDFs introduced in the nuclear density functional theory (DFT) have been determined phenomenologically to reproduce experimental masses and charge radii, as well as nuclear matter properties. To make a link to microscopic approaches of EDFs, *ab initio* determination of such parameters is highly motivated [2, 18-27]. To attain such a goal, novel methods using functional renormalization group [28-36] and inverse Kohn-Sham method [37-39] have also been proposed, although these attempts are still limited.

A sophisticated yet practical approach to pin down the EDF parameters is to combine the *ab initio* calculations with phenomenological EDFs. For instance, the strengths of tensor interaction were determined using a G-matrix calculation [40]. Recently, based on the Skyrme EDF, the strengths of tensor interactions [41] and the charge independence breaking term of the nuclear interaction [42] have also been determined by using the Brueckner Hartree-Fock calculations of proton-neutron drops and symmetric nuclear matter, respectively, with the bare realistic nuclear interaction. Although these terms are not included in the original Skyrme EDF, these attempts and successes are milestones toward constructing *ab initio* EDF. Recently, a systematic construction of nuclear EDFs has been proposed, mimicking the Jacob’s ladder of Coulomb DFT [43] and starting from the local density approximation (LDA) [44].

Even though the isospin symmetry breaking (ISB) terms are small parts of the nuclear interaction, effects of the ISB terms for nuclear properties have gotten attention, for example, for isobaric analog states [42, 45-47], for isobaric multiplet mass equation and the Okamoto-Nolen-Schiffer anomaly in the mirror nuclei mass difference [48-55], and for superallowed $\beta$-decay [56]. The ISB interaction can be divided into two parts, the charge symmetry breaking (CSB) and the charge independence breaking (CIB) interactions [57]. The importance of the ISB interaction in the nuclear structure of $^8\text{Be}$ was also discussed by using the Green’s function Monte Carlo calculation [58]. Hence, the *ab initio* determination of ISB strength of the Skyrme EDF is indispensable and desired toward a comprehensive discussion of ISB effects in the whole nuclear chart.

Our motivation in this Letter is to propose a pragmatic approach to determine the CSB terms of the nuclear interaction adopting the *ab initio* results. We will show that mirror nuclei mass difference $\Delta E_{\text{tot}}$ and the neutron-skin thickness $\Delta R_{np}$ of doubly closed shell nuclei calculated by *ab initio* methods without and with the CSB terms, once they are available, enable us to determine the CSB strength in the Skyrme functional with an uncertainty less than 5% (apart from the uncertainty inherent in the *ab initio* calculations), independently from other isospin breaking forces such as CIB and Coulomb forces. In the previous studies [51, 53], the mass differences of isobars and isotriplets were adopted to pin down the CIB and CSB strengths simultaneously. On the other
hand, in our approach, we will constrain the CSB interaction separately from the other ISB forces. In this way we can set a stricter constrain on the CSB force strength, using the results of \textit{ab initio} calculations.

**CSB and CIB in Skyrme EDF.**—The isospin symmetry breaking of the nuclear interaction can be divided into two parts; the CSB interaction $V_{\text{CSB}} \equiv V_{nn} - V_{pp}$ and the CIB interaction $V_{\text{CIB}} \equiv (V_{nn} + V_{pp})/2 - V_{pn}$, where $V_{pp}$, $V_{nn}$, and $V_{pn}$ denote proton-proton, neutron-neutron, and proton-neutron nuclear interactions, respectively. Origins of the former are mainly proton-neutron mass difference and $\pi^0$-$\eta$ and $\rho^0$-$\omega$ mixings in the meson exchange process, and that of the latter is the mass difference of neutral and charged pions [59–61].

The Skyrme-like zero-range CSB and CIB interactions were introduced in Ref. [62] as

\begin{align}
  v_{\text{CSB}}(\mathbf{r}_1, \mathbf{r}_2) &= \frac{\tau_1 \cdot \tau_2}{4} s_0 (1 + y_0 P_\sigma) \delta (\mathbf{r}_1 - \mathbf{r}_2), \\
  v_{\text{CIB}}(\mathbf{r}_1, \mathbf{r}_2) &= \frac{\tau_1 \cdot \tau_2}{2} u_0 (1 + z_0 P_\sigma) \delta (\mathbf{r}_1 - \mathbf{r}_2),
\end{align}

respectively, where $\tau_i$ is the $i$-direction of isospin operator of nucleon $i$ ($i = 1, 2$) and $P_\sigma = (1 + \sigma \cdot \mathbf{\sigma})/2$ is the spin-exchange operator. This form has been proposed for the sake of simplicity, while momentum-dependent CSB-CIB forces have been discussed in Refs. [53, 55]. One could write a CIB force proportional to the isoscalar form $\hat{T}_{12} = 3\tau_1 \cdot \tau_2 - \mathbf{\tau}_1 \cdot \mathbf{\tau}_2$ [63]. However, the physics would remain the same if the difference between $\hat{T}_{12}$ and the isoscalar part $\tau_1 \tau_2$ can be absorbed in the isospin symmetric part of the (bare or effective) interaction. Thus, in this Letter, we choose $\tau_1 \tau_2$ for the CIB interaction.

Accordingly, the CSB and CIB energy densities are derived as [42, 64]

\begin{align}
  \mathcal{E}_{\text{CSB}}[\rho_p, \rho_n] &= \frac{s_0 (1 - y_0)}{8} (\rho_n^2 - \rho_p^2), \\
  \mathcal{E}_{\text{CIB}}[\rho_p, \rho_n] &= \frac{u_0}{8} \left[ (1 - z_0) (\rho_n^2 + \rho_p^2) - 2 (2 + z_0) \rho_n \rho_p \right],
\end{align}

respectively. In the SAMI-ISB functional [42], $y_0 = z_0 = -1$ are used. The CIB strength $u_0 = 25.8$ MeV fm$^3$ is determined by using the Brueckner Hartree-Fock calculation of the symmetric nuclear matter without and with the CIB part of the AV18 bare interaction [42, 63, 65].

The CSB strength $s_0 = -26.3$ MeV fm$^3$ is determined to reproduce the experimentally measured isobaric analog energy of $^{208}$Pb [42, 66]. In this Letter, since $u_0$ has been already determined microscopically, we propose a way to determine $s_0$ microscopically.

**Mechanism of the behaviors.**—First, the reason why $\Delta E_{0\text{tot}}$ is expected to show a linear dependence on $s_0$ can be described by using the energy densities [Eqs. (2)]. Approximately, the proton density $\rho_p$ of $^{48}$Ca is the same as the neutron density $\rho_n$ of $^{48}$Ni and \textit{vice versa}: $\rho_p^{48}\text{Ca} \simeq \rho_n^{48}\text{Ni}$ and $\rho_p^{48}\text{Ni} \simeq \rho_n^{48}\text{Ca}$. Using these relationships and Eqs. (2), one finds that $\mathcal{E}_{48}\text{Ca} \simeq -\mathcal{E}_{48}\text{Ni}$ and $\mathcal{E}_{\text{CIB}} \simeq \mathcal{E}_{\text{CIB}}$. Consequently, the CSB and CIB contributions to $\Delta E_{0\text{tot}}$ are $\mathcal{E}_{\text{CSB}} - \mathcal{E}_{\text{CSB}} \simeq 2\mathcal{E}_{\text{CSB}}$ and $\mathcal{E}_{\text{CIB}} - \mathcal{E}_{\text{CIB}} \simeq 0$, respectively. Note that deviations from $\mathcal{E}_{\text{CSB}} - \mathcal{E}_{\text{CSB}} = 2\mathcal{E}_{\text{CSB}}$ and $\mathcal{E}_{\text{CIB}} - \mathcal{E}_{\text{CIB}} = 0$ are due to the Coulomb interaction unless the ISB terms are considered.

The neutron-skin thickness $\Delta R_{np}$ is also expected to show a dependence on $s_0$. The CSB interaction between a proton and a neutron is exactly zero. In contrast, the CSB interaction between protons $v_{pp}$ is repulsive, while that between neutrons $v_{nn}$ is attractive, and $v_{pp} \equiv -v_{nn} \sim |s_0|$. As $|s_0|$ becomes larger, the proton-proton repulsive interaction and the neutron-neutron attractive interaction become stronger. Accordingly, the $\rho_p$ expands and $\rho_n$ shrinks, i.e., $R_p$ becomes larger and $R_n$ becomes smaller. Consequently, $\Delta R_{np}$ becomes smaller as $|s_0|$ becomes larger.

**Calculation setup.**—The nuclear energy density consists of four parts: the Coulomb term $\mathcal{E}_{\text{Coul}}$, the isospin symmetric nuclear part $\mathcal{E}_{IS}$, the CSB nuclear part $\mathcal{E}_{\text{CSB}}$, and the CIB nuclear part $\mathcal{E}_{\text{CIB}}$. The Hartree-Fock-Slater approximation (the Coulomb LDA exchange functional) [67, 68] is used for $\mathcal{E}_{\text{Coul}}$ [69]. The SLy4 [70], SLy5 [71], SkM* [71], SAMi [72], and SAMI-ISB [42] functionals are used for $\mathcal{E}_{IS}$ to see whether the choice of functional $\mathcal{E}_{IS}$ affects the $s_0$-dependences of $\Delta R_{np}$ and $\Delta E_{0\text{tot}}$. The CIB part $\mathcal{E}_{\text{CIB}}$ is not considered for SLy4, SLy5, SkM*, and SAMI calculations. In the calculation with the SAMI-ISB functional, two types of calculation are performed; one is with the CIB functional $\mathcal{E}_{\text{CIB}}$ [Eq. (2b)] with the original strength ($u_0 = 25.8$ MeV fm$^3$) and the other is without the CIB functional. Hereafter, the former and latter are referred to as “SAMI-CIB” and “SAMI-noISB” functionals, respectively. On top of these calculations, the CSB functional $\mathcal{E}_{\text{CSB}}$ [Eq. (2a)] is considered. By changing gradually the CSB strength from $s_0 = 0$ to 50 MeV fm$^3$, which will be shown by the figures to be a quite reasonable range, the $s_0$-dependences of $\Delta R_{np}$ and $\Delta E_{0\text{tot}}$ are discussed.

All the calculations are performed by using a code named \textsc{skyrme\_rpa} [73] with $150 \times 0.1$ fm box. Spherical symmetry is assumed and the pairing correlations are not considered since only doubly-magic nuclei are studied.

Before ending this section, the difference among the SAMI, SAMI-noISB, and SAMI-CIB is explained in detail. The SAMI-noISB and SAMI-CIB share the same $\mathcal{E}_{IS}$, while $\mathcal{E}_{\text{CIB}}$ for the former and the latter are $u_0 = 0$ and 25.8 MeV fm$^3$ in Eq. (2b), respectively. When one applies this method, first, one constrains the CIB strength $u_0$ using nuclear matter and, then, constrains the CSB strength $s_0$ using the method proposed in this Letter. Thus, results of the SAMI-CIB shall be referred to. Nevertheless, to see the effect of the order in the fitting, we
One can again remarkably find in Figs. 2 and 3 that $\Delta R_{np}$ for $^{48}$Ca and $^{208}$Pb have also strong linear correlation with $s_0$, as shown by the cross point and the horizontal line, respectively. For comparison, the results calculated with the original SAMi-EDF and experimental data (AME2020) [74] are also shown in Fig. 1. The circle, square, up-triangle, down-triangle, diamond, and pentagon points represent the results calculated with the SLy4, SLy5, SkM*, SAMi, SAMi-noISB, and SAMi-CIB functionals, respectively. For comparison, the results calculated with the original SAMi-EDF and experimental data (AME2020) [74] are also shown in Table I are determined within 0.5% error. Accordingly, among these functionals, the slope $b$ deviates within $\lesssim 6\%$ around the average value of $b$ as shown in Table III. Thus, once $ab\ initio$ results for $\Delta E_{tot}$ calculated without and with the bare CSB interaction, $\Delta E_{tot}^{w/o\ CSB}$ and $\Delta E_{tot}^{w/\ CSB}$, are obtained, using $\delta$, we get $s_0$ as $-s_0 = (\Delta E_{tot}^{w/\ CSB} - \Delta E_{tot}^{w/o\ CSB})/\delta$. Since uncertainty of $\delta$ is less than 6%, the expected uncertainty of $s_0$ is also less than 6%, assuming the uncertainty associated with the $ab\ initio$ calculation is negligible. Note that if the Coulomb interaction is not considered, the parameter $a$ must be zero. Thus, $a$ comes from the Coulomb interaction and its self-consistent effects.

**Neutron-skin thickness.—**Dependence of the neutron-skin thickness, $\Delta R_{np} = R_n - R_p$, of $^{48}$Ca and $^{208}$Pb on the CSB strength $s_0$ are shown in Figs. 2 and 3, respectively, where $R_n$ and $R_p$ are the root-mean-square radii of neutron and proton distributions. The circle, square, up-triangle, down-triangle, diamond, and pentagon points represent the results calculated with the SLy4, SLy5, SkM*, SAMi, SAMi-noISB, and SAMi-CIB functionals, respectively. For comparison, the results calculated with the original SAMi-EDF and experimental data (AME2020) [74] are also shown by the cross points.

The charge radii of $^{48}$Ca and $^{208}$Pb were measured by electron scattering [75] and isotope shift of laser spectroscopy [76]. The neutron radii of $^{48}$Ca and $^{208}$Pb were measured by the proton scattering [77, 78]. The parity-violating assymetry, which is related to the neutron radii, of $^{208}$Pb was also measured by the parity-violating electron scattering (PREX and PREX-II) [79, 80] and that of $^{48}$Ca will be measured as the same manner [81]. Although we do not show the experimental results, the calculated lines span a broad interval which is not incompatible with the experimental findings [82].

One can again remarkably find in Figs. 2 and 3 that $\Delta R_{np}$ for $^{48}$Ca and $^{208}$Pb have also strong linear correlation with $s_0$, as shown by the cross point and the horizontal line, respectively.
relations to the CSB strength $s_0$, and the correlations are universal among the functionals. Hence, these calculated results are fitted to $\Delta R_{np} = a - b s_0$, where fitting parameters for $^{48}$Ca and $^{208}$Pb, shown in fm for $a$ and $\times 10^{-3}$ MeV$^{-1}$ fm$^4$ for $b$. 

Table II. Fitting parameters of $R_{np}$ for $^{48}$Ca and $^{208}$Pb, shown in fm for $a$ and $\times 10^{-3}$ MeV$^{-1}$ fm$^4$ for $b$.

| Functional      | $^{48}$Ca |          | $^{208}$Pb |          |
|-----------------|-----------|----------|-----------|----------|
| SLy4            | +0.1535   | -0.9807  | +0.1595   | -1.0525  |
| SLy5            | +0.1605   | -0.9907  | +0.1622   | -1.0591  |
| SkM*            | +0.1551   | -1.0002  | +0.1686   | -1.1138  |
| SAMi            | +0.1752   | -0.9615  | +0.1466   | -1.0800  |
| SAMi-noISB      | +0.2339   | -0.9131  | +0.1702   | -1.0324  |
| SAMi-CIB        | +0.2372   | -0.9075  | +0.1778   | -1.0255  |

Table III. Averaged values of fitting parameter $b$ for $\Delta E_{tot}$ and $\Delta R_{np}$. Standard deviations of $b$ are also shown as $\Delta b$.

| $\Delta E_{tot}$ | $b$ | $\Delta b$ | $\Delta b/\%$ |
|------------------|----|------------|--------------|
| $(^{48}$Ca)      | -0.3079 | 0.0167    | 5.437 |
| $(^{48}$Pb)      | -0.9589 | 0.0364    | 3.795 |
| $^{208}$Pb       | -1.0605 | 0.0297    | 2.805 |

SAMI-noISB and SAMI-CIB are slightly different from the $b$ of the others. Due to such difference, excluding SAMI-noISB and SAMI-CIB functionals in the derivation of $\bar{b}$ makes slightly smaller deviation $\Delta \bar{b}$, as shown in the Supplemental Material, which indicates that the ISB may not be small enough to be treated perturbatively. Indeed, even if the SAMI-noISB and SAMI-CIB are included, the deviation $\Delta \bar{b}$ is small enough.

One can see the effect of refitting by comparing parameters $b$ derived by SAMI and SAMI-CIB. Since the fitting criteria for $\mathcal{E}_{IS}$ for these two functionals are the same, the difference of $b$ is only due to the ISB terms. The strength $s_0$ can be determined by $\left(\Delta E_{tot}/s_0 - \Delta E_{tot}/w_0/s_0\right)/b$ or $\left(\Delta R_{np}/s_0 - \Delta R_{np}/w_0/s_0\right)/b$. Thus, assuming as known the $ab$ initio values for $\Delta E_{tot}$ and $\Delta R_{np}$ with and without CB effects, the ratio of $s_0$ derived by perturbation ($s_0^{perturb}$) and by refitting ($s_0^{refit}$) reads $s_0^{perturb}/s_0^{refit} = \mathcal{F}_{SAMI-CIB}/\mathcal{F}_{SAMI}$, whose value ranges from 0.90 (derived by $\Delta E_{tot}$) to 0.95 (derived by $\Delta R_{np}$ for $^{208}$Pb). It should be noted that $b^{SAMI-CIB}/b^{SAMI-noISB} \approx 0.99$, and thus fitting for $s_0$ before or after the CIB strength $s_0$ does not matter.

Conclusion.—In this Letter, aiming to construct $ab$ initio Skyrme energy density functional, we discussed the possibility of determination of the strength of Skyrme-like charge-symmetry breaking (CSB) term $s_0$ from the $ab$ initio results. It is found that the mirror nuclei mass difference $\Delta E_{tot}$ and the neutron-skin thickness $\Delta R_{np}$ of $^{48}$Ca and $^{208}$Pb show a linear dependence on $s_0$, while the charge-independence breaking (CIB) term has much smaller effect on these observables. Hence, once $ab$ initio calculations of $\Delta E_{tot}$ and $\Delta R_{np}$ without and with the bare CSB interaction are available, $s_0$ can be determined within 6% accuracy by using $\Delta E_{tot}$ and even within 4% accuracy by using $\Delta R_{np}$. However, $ab$ initio calculations of the isospin symmetry breaking forces have still to be improved [83]. It is important to note that a consistent value for $s_0$ using both methods indicates that our assumption in Eqs. (1) is reasonable, while a difference among the values of $s_0$ derived from $\Delta E_{tot}$ and $\Delta R_{np}$ may hint to the fact that our ansatz for the CSB functional must be improved. The method proposed in this paper is a new feasible way toward $ab$ initio nuclear energy density functionals. Toward such achievement, future collaborations between $ab$ initio and DFT communities are highly desired.
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Supplemental Material for
“Toward ab initio determination of charge symmetry breaking strength of Skyrme functionals”

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In this supplemental material, we show results for 16O, 40Ca, and 48Ni, together with those for 48Ca and 208Pb. We also discuss the effects of the Coulomb interaction.

The mirror nuclei mass difference between 48Ca and 48Ni, \( \Delta E_{\text{tot}} = E_{\text{tot}}^{48\text{Ca}} - E_{\text{tot}}^{48\text{Ni}} \), calculated with the Coulomb interaction are fitted to \( \Delta E_{\text{tot}} = a - b_s \), where the fitting parameters are shown in Table S.1. Meanwhile, the results calculated without the Coulomb interaction are fitted to \( \Delta E_{\text{tot}} = -b_s \), whose parameters \( b \) are also shown there. The CSB strength \( s_0 \) dependences of the neutron-skin thickness \( \Delta R_{np} \) of 16O, 40Ca, and 48Ni are shown in Figs. S.1, S.2, and S.3, respectively. These calculated data are fitted to \( \Delta R_{np} = a - b_s \), where fitting parameters for 16O, 40Ca, 48Ca, 48Ni, and 208Pb are shown in Table S.2. The corresponding results calculated without the Coulomb interaction are fitted to \( \Delta E_{\text{tot}} = -b_s \) (for \( N = Z \) nuclei) or \( \Delta E_{\text{tot}} = a - b_s \) (for \( N \neq Z \) nuclei). The fitting parameters are shown in Table S.3. Note that all the fittings are highly correlated \((r = 1.0000)\).

By using \( b \) shown in Tables S.1 and S.2, the average values \( \bar{b} \) and their standard deviations \( \Delta \bar{b} \) are shown in Table S.4. Results with all the used functionals, i.e., SLy4, SLy5, SkM*, SAMi, SAMi-noISB, and SAMi-CIB, are shown in the column entitled “LDA (All),” while the results without SAMi-noISB and SAMi-CIB are shown in the column entitled “LDA (w/o ISB).” One can find that the CSB strength \( s_0 \) dependence of \( \Delta R_{np} \) is universal in selected nuclei, regardless of \( N < Z \), \( N = Z \), or \( N > Z \). Besides, functional independence of the slope \( b \) also holds among the selected nuclei, and consequently, the standard deviation \( \Delta \bar{b} \) is less than 6% of the averaged value \( \bar{b} \), as discussed in section entitled “Including or excluding SAMi-ISB functional” in the main text.

The Coulomb interaction also breaks isospin symmetry of the atomic nuclei, and therefore, \( \Delta E_{\text{tot}} \) and \( \Delta R_{np} \) becomes finite values even if the ISB terms are not considered. To see the effect of the Coulomb interaction, fitting parameters \( a \) and \( b \) of \( \Delta R_{np} \) calculated without the Coulomb interaction are shown in Table S.3. Note that \( \Delta R_{np} \) for \( N = Z \) nuclei and \( \Delta E_{\text{tot}} \) are exactly zero when neither the CSB nor the Coulomb interaction is switched off. Hence, these data are fitted with constrain \( a = 0 \). The averaged values \( \bar{b} \) and their standard deviation \( \Delta \bar{b} \) are also shown in columns entitled “No Coulomb (All)” and “No Coulomb (w/o ISB)” of Table S.4. It is found that irrespective of the existence of the Coulomb interaction, the parameter \( b \), and accordingly \( \bar{b} \), hardly changes.

Hence, in short, the discussion in the main text hardly changes with respect to the choice of nuclei or the existence of the Coulomb interaction.

| Functional | Coulomb LDA | No Coulomb |
|------------|-------------|------------|
| a (MeV)    | b (fm⁻³)    | b (fm⁻³)   |
| SLy4       | -63.1143    | -0.3234    | -0.3440    |
| SLy5       | -63.1975    | -0.3192    | -0.3397    |
| SkM*       | -63.4399    | -0.3220    | -0.3435    |
| SAMi       | -62.9755    | -0.3133    | -0.3325    |
| SAMi-noISB | -61.6251    | -0.2868    | -0.3039    |
| SAMi-CIB   | -61.3474    | -0.2826    | -0.2998    |
FIG. S.1. Dependence of neutron-skin thickness $\Delta R_{np}$ of $^{16}\text{O}$ on CSB strength $s_0$. For comparison, the result calculated with the original SAMi-ISB is also shown in the cross point.

FIG. S.2. Same as Fig. S.1 but for $^{40}\text{Ca}$.

FIG. S.3. Same as Fig. S.1 but for $^{48}\text{Ni}$.

### TABLE S.2. Fitting parameters of $R_{np} = a - b s_0$ for $^{16}\text{O}$, $^{40}\text{Ca}$, $^{48}\text{Ni}$, and $^{208}\text{Pb}$ shown in fm for $a$ and $b$ calculated with the Coulomb Hartree-Fock-Slater approximation.

| Functional | $^{16}\text{O}$ | $^{40}\text{Ca}$ | $^{48}\text{Ni}$ | $^{208}\text{Pb}$ |
|------------|-----------------|-----------------|-----------------|-----------------|
| SLY4       | $a$ $=-0.0248$ | $b$ $=-0.8884$ | $a$ $=+0.0475$ | $b$ $=-0.9604$ |
| SLY5       | $a$ $=-0.0251$ | $b$ $=-0.9000$ | $a$ $=-0.0480$ | $b$ $=-0.9700$ |
| SkM*       | $a$ $=-0.0251$ | $b$ $=-0.8842$ | $a$ $=-0.0493$ | $b$ $=-0.9893$ |
| SAMi       | $a$ $=-0.0233$ | $b$ $=-0.8542$ | $a$ $=-0.0470$ | $b$ $=-0.9640$ |
| SAMi-noISB | $a$ $=-0.0231$ | $b$ $=-0.8733$ | $a$ $=-0.0459$ | $b$ $=-0.9605$ |
| SAMi-CIB   | $a$ $=-0.0230$ | $b$ $=-0.8585$ | $a$ $=-0.0457$ | $b$ $=-0.9475$ |

### TABLE S.3. Same as Table S.2 but calculated without the Coulomb interaction. In $N = Z$ nuclei, the results are fitted to $\Delta E_{tot} = -b s_0$ instead.

| Functional | $^{16}\text{O}$ | $^{40}\text{Ca}$ | $^{48}\text{Ni}$ | $^{208}\text{Pb}$ |
|------------|-----------------|-----------------|-----------------|-----------------|
| SLY4       | $a$ $=0$       | $b$ $=0$       | $a$ $=0$       | $b$ $=0$       |
| SLY5       | $a$ $=-0.0244$ | $b$ $=0$       | $a$ $=0$       | $b$ $=0$       |
| SkM*       | $a$ $=-0.0244$ | $b$ $=0$       | $a$ $=0$       | $b$ $=0$       |
| SAMi       | $a$ $=-0.0244$ | $b$ $=0$       | $a$ $=0$       | $b$ $=0$       |
| SAMi-noISB | $a$ $=-0.0244$ | $b$ $=0$       | $a$ $=0$       | $b$ $=0$       |
| SAMi-CIB   | $a$ $=-0.0244$ | $b$ $=0$       | $a$ $=0$       | $b$ $=0$       |
TABLE S.4. Averaged values of fitting parameter \( b \) without considering SAMi-noISB nor SAMi-CIB ("w/o ISB" in title) and with all results ("All" in title). Both calculations with Coulomb LDA functional ("LDA" in title) and without Coulomb functional ("No" in title) are shown. Standard deviations of \( b \) are also shown as \( \Delta b \).

| \( \Delta E_{\text{tot}} \) (fm\(^{-1} \)) | LDA (w/o ISB) | LDA (All) | No (w/o ISB) | No (All) |
|----------------------------------------|---------------|------------|---------------|----------|
| \( \Delta b \) | \( b \) | \( \Delta b \) | \( b \) | \( \Delta b \) | \( b \) | \( \Delta b \) |
| \( \Delta R_{np} (^{16}\text{O}) \) (\( \times 10^{-3} \text{ MeV}^{-1} \text{ fm}^4 \)) | -0.3195 | 0.0039 | -0.3079 | 0.0167 | -0.3399 | 0.0046 | -0.3272 | 0.0184 |
| \( \Delta R_{np} (^{40}\text{Ca}) \) (\( \times 10^{-3} \text{ MeV}^{-1} \text{ fm}^4 \)) | -0.8817 | 0.0169 | -0.8761 | 0.0163 | -0.8737 | 0.0187 | -0.8679 | 0.0177 |
| \( \Delta R_{np} (^{44}\text{Ca}) \) (\( \times 10^{-3} \text{ MeV}^{-1} \text{ fm}^4 \)) | -0.9709 | 0.0111 | -0.9653 | 0.0127 | -0.9562 | 0.0102 | -0.9502 | 0.0127 |
| \( \Delta R_{np} (^{48}\text{Ni}) \) (\( \times 10^{-3} \text{ MeV}^{-1} \text{ fm}^4 \)) | -0.9833 | 0.0144 | -0.9544 | 0.0364 | -0.9945 | 0.0141 | -0.9704 | 0.0361 |
| \( \Delta R_{np} (^{208}\text{Pb}) \) (\( \times 10^{-3} \text{ MeV}^{-1} \text{ fm}^4 \)) | -1.1130 | 0.0080 | -1.0775 | 0.0104 | -1.0115 | 0.0118 | -0.9912 | 0.0303 |
| \( \Delta R_{np} (^{208}\text{Pb}) \) (\( \times 10^{-3} \text{ MeV}^{-1} \text{ fm}^4 \)) | -1.0764 | 0.0239 | -1.0605 | 0.0297 | -1.1623 | 0.0297 | -1.1454 | 0.0340 |