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## N3LO $NN$ interaction adjusted to light nuclei in *ab initio* approach



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### ABSTRACT

We use phase-equivalent transformations to adjust off-shell properties of similarity renormalization group evolved chiral effective field theory  $NN$  interaction (Idaho N3LO) to fit selected binding energies and spectra of light nuclei in an *ab initio* approach. We then test the transformed interaction on a set of additional observables in light nuclei to verify that it provides reasonable descriptions of these observables with an apparent reduced need for three- and many-nucleon interactions.

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An *ab initio* description of nuclear structure and reactions is one of the mainstays of modern nuclear theory [1]. It is based on a rapid development of supercomputer facilities and recent advances in the utilization of high-performance computing systems [2]. Modern *ab initio* nuclear theory has opened a wide range of nuclear phenomena that can be evaluated to high precision using realistic nucleon–nucleon ( $NN$ ) and three-nucleon ( $NNN$ ) interactions. In particular, *ab initio* approaches, such as the No-Core Shell Model (NCSM) [3], the Green's Function Monte Carlo (GFMC) [4] and the Coupled-Cluster Theory [5], are able to reproduce properties of a large number of atomic nuclei with mass up to  $A = 16$  and selected heavier nuclear systems around closed shells. Very important progress has been achieved in the *ab initio* description of reactions with light nuclei, in particular, by combining the NCSM with the Resonating Group Method [6].

The *ab initio* theory requires a high-quality realistic inter-nucleon interaction providing an accurate description of  $NN$  scattering data and predictions for binding energies, spectra and other observables in light nuclei. A number of meson-exchange potentials sometimes supplemented with phenomenological terms to achieve high accuracy in fitting  $NN$  data, e.g., CD-Bonn [7], Nijmegen [8], Argonne [9], have been developed that should be

used together with modern  $NNN$  forces such as Urbana [10,11], Illinois [12], Tucson–Melbourne [13–15] to reproduce properties of many-body nuclear systems. A very important step in the theory of inter-nucleon interactions in nuclei is the emergence of realistic  $NN$  and  $NNN$  interactions tied to QCD via chiral effective field theory ( $\chi$ EFT) [16–20].

Three-nucleon forces require a significant increase of computational resources in order to diagonalize a many-body Hamiltonian matrix since the  $NNN$  interaction increases the number of non-zero matrix elements approximately by a factor of 30 in the case of  $p$ -shell nuclei [21,22]. As a result, one needs to restrict the basis space in many-body calculations when  $NNN$  forces are involved which makes the predictions less precise. *Ab initio* many-body studies benefit from the use of recently developed purely two-nucleon interactions such as INOY (Inside Nonlocal Outside Yukawa) [23,24] and JISP ( $J$ -matrix Inverse Scattering Potential) [25–28] types which are fitted not only to the  $NN$  data but also to binding energies of  $A = 3$  and heavier nuclei. At the fundamental level, these  $NN$  interactions are supported by the work of Polyzou and Glöckle [29] who demonstrated that a given  $NN$  interaction is equivalent at the  $A = 3$  level to some other  $NN$  interaction augmented by  $NNN$  interactions, where the two  $NN$  interactions are related through a phase-equivalent transformation (PET). It seems reasonable then to exploit this freedom and strive to minimize the need for the explicit introduction of three- and

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higher-body forces. Endeavors along these lines have resulted in the design of INOY and JISP inter-nucleon interaction models.

Conventional realistic meson-exchange  $NN$  interactions [7–9] and  $NN$  interactions obtained via  $\chi$ EFT [18] present convergence challenges in many-body calculations. A modern tool to soften the  $NN$  interaction and hence to improve the convergence, is the Similarity Renormalization Group (SRG) technique [30,31]. The SRG softening guarantees a monotonic convergence of many-body calculations as a function of increasing basis space size and makes it possible to extrapolate the results to the infinite basis space thus improving essentially an accuracy of theoretical predictions. We note that the SRG softening of  $NN$  interaction induces  $NNN$  and, generally, four-nucleon ( $4N$ ), five-nucleon, etc., forces.

We develop here an  $NN$  interaction based on  $\chi$ EFT able to describe light nuclei without explicit use of  $NNN$  forces and with good convergence of many-body *ab initio* calculations. This interaction which we hereafter refer to as Daejeon16  $NN$  interaction should be useful for a wide range of applications in nuclear structure and nuclear reactions. We start from the Idaho N3LO  $\chi$ EFT  $NN$  force [18] SRG-evolved with the flow parameter  $\lambda = 1.5 \text{ fm}^{-1}$  and apply to it various PETs with continuous parameters searching for an optimal set of PET parameters providing a good description of light nuclei. In our approach, we assume that our selected PETs are generating  $NNN$  forces which cancel the combined effect of the ‘intrinsic’  $NNN$  interaction and the  $NNN$  force induced by the SRG transformation. Insofar as the PETs also provide a good fit to nuclei with  $A = 4$ , and beyond, we interpret that success as an indication that effects of neglected  $4N$  forces, and beyond, are also minimized.

The technique used to construct the Daejeon16 interaction has much in common with the one utilized in constructing the JISP6 [26,27] and JISP16 [28]  $NN$  interactions. In particular, we use the PETs of the same type – mixing lowest components of the interaction matrix in the oscillator basis which were suggested in [32,33]. A minor difference is that these PETs are utilized in the oscillator basis with the frequency  $\hbar\Omega = 25 \text{ MeV}$  while  $\hbar\Omega = 40 \text{ MeV}$  was used in the JISP6 and JISP16 case. More important differences are the use of the SRG-evolved Idaho N3LO interaction instead of the ISTP interaction of Ref. [25] for PETs and a more accurate fitting to nuclear energies due to the use of the extrapolation technique of Ref. [34] instead of a combination of results obtained with OLS-transformed and ‘bare’ interaction in Refs. [26–28].

We note here that the JISP16  $NN$  interaction appeared to be very successful in describing light nuclei (see a summary of the JISP16 results for  $p$ -shell nuclei in Refs. [35,36]). In particular, the accuracies of  $^{14}\text{F}$  binding energy and spectrum predictions [37] based on this interaction were later confirmed by the first experimental study of this nucleus in Ref. [38]. However, the fit of the JISP16 interaction to light nuclei was performed in 2006 with supercomputers of that era and hence within bases that are small by today’s standards. In addition, those calculations were performed without the use of the extrapolation technique to the infinite model space which was introduced later. As a result, the JISP16 interaction was found to be less accurate in the description of nuclei with mass  $A > 12$  and of some exotic light nuclei far away from  $N = Z$  (see, e.g., Refs. [35,36]). We note also that JISP16 is a completely phenomenological  $NN$  interaction whose design starts from the inverse scattering fit to the  $NN$  data [25] without any underlying physics model. The Daejeon16  $NN$  interaction is free from these drawbacks. Its fit to the many-body nuclear data is more accurate and it is obtained from the N3LO interaction of Ref. [18] by means of a well-defined SRG transformation and PETs. As a result, one can obtain the effective operators, e.g., electroweak operators, that should be used in *ab initio* studies of many-body nuclear sys-

**Table 1**

PET angles (in degrees) defining the Daejeon16  $NN$  interaction in various  $NN$  partial waves.

| Wave  | $^1s_0$ | $^3sd_1$ | $^1p_1$ | $^3p_0$ | $^3p_1$ | $^3pf_2$ | $^3d_2$ |
|-------|---------|----------|---------|---------|---------|----------|---------|
| Angle | −2.997  | 4.461    | 5.507   | 1.785   | 4.299   | −2.031   | 7.833   |

tems with Daejeon16 by applying the same SRG transformation and PETs to the ‘bare’ operators consistent with the  $\chi$ EFT theory. We note that such SRG and PET transformations of the two-body chiral EFT electroweak operators can be included straightforwardly in future applications. It is also worth noting here that the SRG transformation and PETs do not affect the description of  $NN$  data and deuteron binding energy provided by the Idaho N3LO  $NN$  interaction.

We admit that, although it may be possible to weaken three-, four- and many-body interactions by performing PETs with fits to selected observables, one cannot in general eliminate them completely. These interactions have a natural size in the context of chiral EFT suggesting that reduction below that size amounts to fine tuning which could succeed on a limited scale as we demonstrate here. However, one anticipates that other observables, such as properties of heavier nuclei, may or may not be improved relative to experiment but further effort is needed to test such behaviors.

As noted above, we start from the Idaho N3LO  $\chi$ EFT  $NN$  interaction [18], SRG-evolve it with the flow parameter  $\lambda = 1.5 \text{ fm}^{-1}$  and apply to it PETs of the type utilized in Ref. [25–28] using the oscillator basis with  $\hbar\Omega = 25 \text{ MeV}$ . The PETs are mixing the lowest oscillator components of the wave function in each  $NN$  partial wave; in case of coupled  $^3sd_1$  and  $^3pf_2$  waves we mix by PETs the lowest  $s$  and  $p$  components, respectively. The Daejeon16  $NN$  interaction is designed to be charge- and isospin-independent, hence the  $pn$  component after the PET is used to obtain the Daejeon16 interaction in all  $NN$  partial waves in  $nn$ ,  $pn$  and  $pp$  channels; in the latter case it should be supplemented by the Coulomb interaction.

The set of PET parameters in each partial wave is obtained by the fit to binding energies of  $^3\text{H}$ ,  $^4\text{He}$ ,  $^6\text{Li}$ ,  $^8\text{He}$ ,  $^{10}\text{B}$ ,  $^{12}\text{C}$  and  $^{16}\text{O}$  nuclei and to excitation energies of a few narrow excited states: the two lowest excited states with  $(J^\pi, T) = (3^+, 0)$  and  $(0^+, 1)$  in  $^6\text{Li}$  and the first excited states  $(1^+, 0)$  in  $^{10}\text{B}$  and  $(2^+, 0)$  in  $^{12}\text{C}$ . We minimize the root-mean-square (rms) deviation of weighted differences of the calculated energies from target values using the POUNDerS derivative-free algorithm [39] as implemented in [40, 41]. The many-body calculations are performed within the NCSM using the code MFDn [42–44]. To save computational resources, the minimization is performed using NCSM calculations with relatively small basis spaces; the target values in the fit are the energies in respective nuclei in these small basis spaces which are expected to result in correct experimental values after performing the extrapolations of Ref. [34] to the infinite model space. The modification of the  $NN$  interaction by PETs changes the convergence rate of NCSM calculations in each nucleus individually. Therefore after the initial fit we recalculate all targeted nuclei with the obtained interaction in a set of larger basis spaces, adjust the target energy values and perform a new fit; recalculations in larger basis spaces with the new version of the  $NN$  interaction result in a further adjustment of the target values and in a new fit, etc.

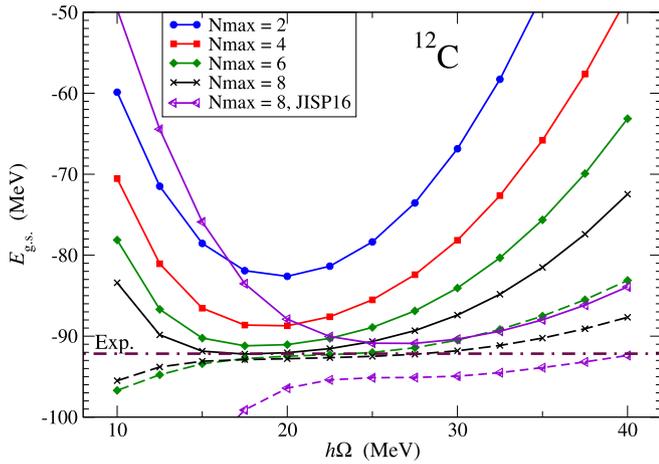
The set of PET angles resulting from this multi-step fit and defining the Daejeon16  $NN$  interaction is presented in Table 1, the definition of these PET angles is given in Refs. [25–28].<sup>1</sup> The

<sup>1</sup> We note that we mix here by PETs the two lowest  $s$  components in the coupled  $^3sd_1$  waves while PETs utilized in Refs. [25–28] mix the lowest  $s$  with the lowest  $d$  components.

**Table 2**

Binding energies (in MeV) of nuclei obtained with Daejeon16  $NN$  interaction using Extrapolation B of Ref. [34] with estimated uncertainty of the extrapolation (in parentheses), the optimal  $\hbar\Omega$  (in MeV) for the extrapolation and the largest  $N_{\max}$  value used in NCSM calculations. The JISP16 results are given for comparison. The experimental data are taken from Ref. [46].

| Nucleus         | Nature  | Daejeon16             |               |            | JISP16    |               |            |
|-----------------|---------|-----------------------|---------------|------------|-----------|---------------|------------|
|                 |         | Theory                | $\hbar\Omega$ | $N_{\max}$ | Theory    | $\hbar\Omega$ | $N_{\max}$ |
| $^3\text{H}$    | 8.482   | 8.442(+0.003, -0.000) | 12.5          | 16         | 8.370(3)  | 15            | 20         |
| $^3\text{He}$   | 7.718   | 7.744(+0.005, -0.000) | 12.5          | 16         | 7.667(5)  | 17.5          | 20         |
| $^4\text{He}$   | 28.296  | 28.372(0)             | 17.5          | 16         | 28.299(0) | 22.5          | 18         |
| $^6\text{He}$   | 29.269  | 29.39(3)              | 12.5          | 14         | 28.80(5)  | 17.5          | 16         |
| $^8\text{He}$   | 31.409  | 31.28(1)              | 12.5          | 14         | 29.9(2)   | 20            | 14         |
| $^6\text{Li}$   | 31.995  | 31.98(2)              | 12.5          | 14         | 31.48(3)  | 20            | 16         |
| $^{10}\text{B}$ | 64.751  | 64.79(3)              | 17.5          | 10         | 63.9(1)   | 22.5          | 10         |
| $^{12}\text{C}$ | 92.162  | 92.9(1)               | 17.5          | 8          | 94.8(3)   | 27.5          | 10         |
| $^{16}\text{O}$ | 127.619 | 131.4(7)              | 17.5          | 8          | 145(8)    | 35            | 8          |



**Fig. 1.**  $^{12}\text{C}$  ground state energy in NCSM calculations obtained with Daejeon16  $NN$  interaction with  $N_{\max}$  values ranging from 2 to 8 as a function of  $\hbar\Omega$  (solid lines) and Extrapolation B results from basis spaces up to respective  $N_{\max}$  value (dashed lines). The  $N_{\max} = 8$  results obtained with JISP16  $NN$  interaction are given for comparison. The horizontal dash-dotted line shows the experimental  $^{12}\text{C}$  ground state energy [46].

Daejeon16 interaction is defined in all  $NN$  partial waves with total angular momentum  $J \leq 6$ ; the interaction in all partial waves not listed in Table 1 is the SRG-evolved Idaho N3LO interaction without a PET. For practical use, we refer to a FORTRAN code generating the Daejeon16  $NN$  interaction matrix elements in the oscillator basis with  $\hbar\Omega = 25$  MeV [45].

*Ab initio* NCSM calculations with the Daejeon16  $NN$  interaction demonstrate a fast convergence as is illustrated by Fig. 1 where we present the results obtained in NCSM basis spaces with excitation quanta  $N_{\max}$  ranging from 2 to 8 as functions of  $\hbar\Omega$ . We show in Fig. 1 also the results of extrapolation to infinite NCSM model space for each  $\hbar\Omega$  (Extrapolations B of Ref. [34]) derived from the NCSM results from 3 successive basis spaces up to  $N_{\max} = 6$  and 8. The NCSM results are seen to converge as  $N_{\max}$  increases around the minimum of the  $\hbar\Omega$  dependence. This minimum for  $N_{\max} = 6$  and 8 is very close to the extrapolated values and the  $\hbar\Omega$  dependence is weak around the minimum. These convergence patterns are due to the small value of the SRG flow parameter  $\lambda = 1.5 \text{ fm}^{-1}$  and are consistent with the study of convergence for various  $\lambda$  values of Ref. [47]. For comparison, we show in Fig. 1 the  $N_{\max} = 8$  results and respective extrapolations obtained with JISP16 interaction. JISP16 was designed to be a very soft interaction providing a fast convergence of *ab initio* studies. Nevertheless, it is seen that the extrapolated values are much farther from the NCSM JISP16

**Table 3**

Excitation energies (in MeV) of some nuclei obtained with Daejeon16  $NN$  interaction using Extrapolation B of Ref. [34] with estimation of uncertainty (in parentheses) for the absolute energy of the respective state, the optimal  $\hbar\Omega$  (in MeV) for the extrapolation of the excited state and the largest  $N_{\max}$  value used in NCSM calculations. The JISP16 results are given for comparison. The experimental data are taken from Ref. [46].

| Nucleus, level                | Nature         | Daejeon16 |               |            | JISP16 |               |            |    |
|-------------------------------|----------------|-----------|---------------|------------|--------|---------------|------------|----|
|                               |                | Theory    | $\hbar\Omega$ | $N_{\max}$ | Theory | $\hbar\Omega$ | $N_{\max}$ |    |
| $^6\text{He}$<br>( $0^+, 1$ ) | 0              | 0         |               |            | 0      |               |            |    |
|                               | ( $2^+, 1$ )   | 1.797     | 1.91(5)       | 12.5       | 14     | 2.3(1)        | 17.5       | 16 |
| $^6\text{Li}$                 | ( $1^+_1, 0$ ) | 0         |               |            | 0      |               |            |    |
|                               | ( $3^+_1, 0$ ) | 2.186     | 1.91(1)       | 12.5       | 14     | 2.55(7)       | 20         | 16 |
|                               | ( $0^+, 1$ )   | 3.563     | 3.50(4)       | 12.5       | 14     | 3.65(6)       | 17.5       | 16 |
|                               | ( $2^+, 0$ )   | 4.312     | 4.4(3)        | 12.5       | 14     | 4.5(2)        | 20         | 16 |
|                               | ( $2^+, 1$ )   | 5.366     | 5.36(7)       | 12.5       | 14     | 5.9(1)        | 17.5       | 16 |
|                               | ( $1^+_2, 0$ ) | 5.65      | 5.0(4)        | 12.5       | 14     | 5.4(2)        | 17.5       | 16 |
| $^{10}\text{B}$               | ( $3^+_1, 0$ ) | 0         |               |            | 0      |               |            |    |
|                               | ( $1^+_1, 0$ ) | 0.718     | 0.5(1)        | 15         | 10     | 0.9(2.4)      | 22.5       | 10 |
|                               | ( $0^+, 1$ )   | 1.740     | 1.74(7)       | 17.5       | 10     | 1.8(1.4)      | 25         | 8  |
|                               | ( $1^+_2, 0$ ) | 2.154     | 2.8(2)        | 17.5       | 10     | 4.1(1.7)      | 30         | 10 |
|                               | ( $2^+_1, 0$ ) | 3.587     | 4.3(2)        | 15         | 10     | 3.8(2)        | 27.5       | 10 |
|                               | ( $3^+_2, 0$ ) | 4.774     | 5.1(7)        | 17.5       | 10     | 5.6(3)        | 22.5       | 10 |
| $^{12}\text{C}$               | ( $0^+, 0$ )   | 0         |               |            | 0      |               |            |    |
|                               | ( $2^+, 0$ )   | 4.439     | 4.57(15)      | 17.5       | 8      | 3.9(4)        | 27.5       | 10 |

results than in the case of Daejeon16, hence the Daejeon16  $NN$  interaction provides a much better convergence than JISP16.

We present in Table 2 the extrapolated results of NCSM calculations of binding energies of several  $s$ - and  $p$ -shell nuclei. Daejeon16 is seen from Table 2 to provide an accurate description of these binding energies. In particular, Daejeon16 describes the bindings generally better than the JISP16  $NN$  interaction whose results are also shown in Table 2 for comparison. The main drawbacks of the JISP16 interaction – overbinding of nuclei at the end of  $p$  shell such as  $^{16}\text{O}$  and too strong decrease of binding energies as  $|N - Z|$  increases, e.g., underbinding of  $^6\text{He}$  and  $^8\text{He}$  – are much less pronounced in the case of Daejeon16. As a manifestation of the fast convergence of Daejeon16 calculations, the same precision of binding energy extrapolations is achieved in smaller basis spaces as compared with JISP16.

Spectra of  $^6\text{Li}$  and  $^{10}\text{B}$  together with excitation energies of the first excited states in  $^6\text{He}$  and  $^{12}\text{C}$  are shown in Table 3. Note, only two lowest narrow excited states in  $^6\text{Li}$  and the first excited states in  $^{10}\text{B}$  and  $^{12}\text{C}$  were involved in the fit. We calculate the un-

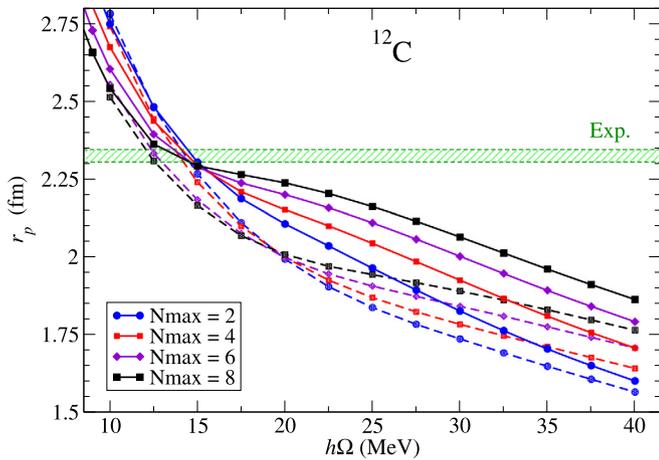


Fig. 2.  $^{12}\text{C}$  point-proton radius as a function of  $\hbar\Omega$  obtained with Daejeon16 (solid lines) and JISP16 (dashed lines)  $NN$  interactions in NCSM calculations with various  $N_{\text{max}}$  values. The shaded area shows the experimental value with its uncertainties [48].

certainties of excitation energies as uncertainties of extrapolations of absolute energies of respective levels. The uncertainties of the absolute energies include the uncertainty of the overall binding energy and that uncertainty (listed in Table 3) is conservative when quoted as the uncertainty for excitation energies due to cancellations of the systematic error contributions. Note that the precision of excitation energies obtained with Daejeon16 is generally better than the precision of the excitation energies obtained with JISP16 reflecting the faster convergence of *ab initio* calculations with Daejeon16.

The spectra of light nuclei shown in Table 3 are well reproduced by Daejeon16. The ordering of levels is correct with an exception of a wide ( $\Gamma = 1.5$  MeV) ( $1_2^+, 0$ ) state in  $^6\text{Li}$  for which ordering in the spectrum is uncertain due to large error bars of its extrapolated energy overlapping the neighboring narrow ( $2^+, 1$ ) state. We note that it is widely accepted that the spin of the  $^{10}\text{B}$  ground state cannot be reproduced without an explicit use of  $NNN$  interactions. Our calculations with Daejeon16 demonstrate that the  $^{10}\text{B}$  ground state spin can be obtained using only two-nucleon interaction which, however, mimics the effects of  $NNN$  forces by modification of its off-shell properties by means of PETs. The correct spin of the  $^{10}\text{B}$  ground state may also be reproduced by the JISP16  $NN$  interaction, however the uncertainties of extrapolations of JISP16 results (see Table 3) prevent a definitive conclusion about the ordering of the lowest ( $3_1^+, 0$ ) and ( $1_1^+, 0$ ) states in  $^{10}\text{B}$ .

The JISP16 interaction typically underestimates rms radii of nuclei. As is seen in Fig. 1, the  $\hbar\Omega$ -dependence of NCSM eigenenergies obtained with Daejeon16 interaction has a minimum at a much smaller  $\hbar\Omega$  value than in the case of the JISP16  $NN$  interaction. This is true not only for  $^{12}\text{C}$  but also for other nuclei as is illustrated by Tables 2 and 3 where we present optimal  $\hbar\Omega$  values for Extrapolation B which are close to the minima of respective  $\hbar\Omega$ -dependences. This feature suggests that the rms nuclear radii obtained with Daejeon16 will be closer to experiment since smaller  $\hbar\Omega$  values correspond to larger rms radii of basis oscillator functions. The rms radii obtained in NCSM calculations are  $N_{\text{max}}$  and  $\hbar\Omega$ -dependent (see Fig. 2 where we present the  $^{12}\text{C}$  point-proton rms radii  $r_p$  obtained with Daejeon16 interaction in comparison with those from JISP16). The  $\hbar\Omega$  dependencies of rms radii obtained with a given interaction with different  $N_{\text{max}}$  values tend to cross each other approximately at the same point. We use these crossing points as rough estimates of the converged radius as has been suggested in Ref. [49]. We note here that the extrapolation technique for nuclear rms radii was recently suggested [50]. How-

ever, this technique was not tested for nuclei with masses  $A > 2$  and requires results from very large  $\hbar\Omega$  values ( $\hbar\Omega > 49$  MeV were utilized in Ref. [50]) which were not used in our study. We note also that a detailed study of Ref. [51] of the  $^{12}\text{C}$  point-proton rms radius with JISP16 interaction using a version of NCSM with Woods–Saxon basis resulted in a value of 2.08(7) fm, which agrees with  $r_p \approx 2.04$  fm that is the crossing point of JISP16 curves in Fig. 2. The crossing of the Daejeon16 curves suggests  $r_p \approx 2.29$  fm that is much closer to the experimental result of 2.32(2) fm [48].

In conclusion, we propose a realistic  $NN$  interaction Daejeon16 based on a SRG-transformed chiral N<sup>3</sup>LO interaction that provides a good description of various observables in light nuclei without  $NNN$  forces and also generates rapid convergence in *ab initio* calculations. We anticipate that this interaction will be useful for a wide range of applications to nuclear structure and reactions.

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