Ab Initio Studies with Chiral NN+3N Hamiltonians

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From QCD to Nuclear Structure

Nuclear Structure

Low-Energy QCD

From QCD to Nuclear Structure

Nuclear Structure

NN+3N Interaction from Chiral EFT

Low-Energy QCD

- chiral EFT based on the relevant degrees of freedom & symmetries of QCD
- provides consistent NN, 3N,... interaction plus currents
- initial Hamiltonian:
  - NN at N^3LO
    Entem & Machleidt, 500 MeV cutoff
  - 3N at N^2LO
    Navrátil, A=3 fit, 500 MeV cutoff

From QCD to Nuclear Structure

Nuclear Structure

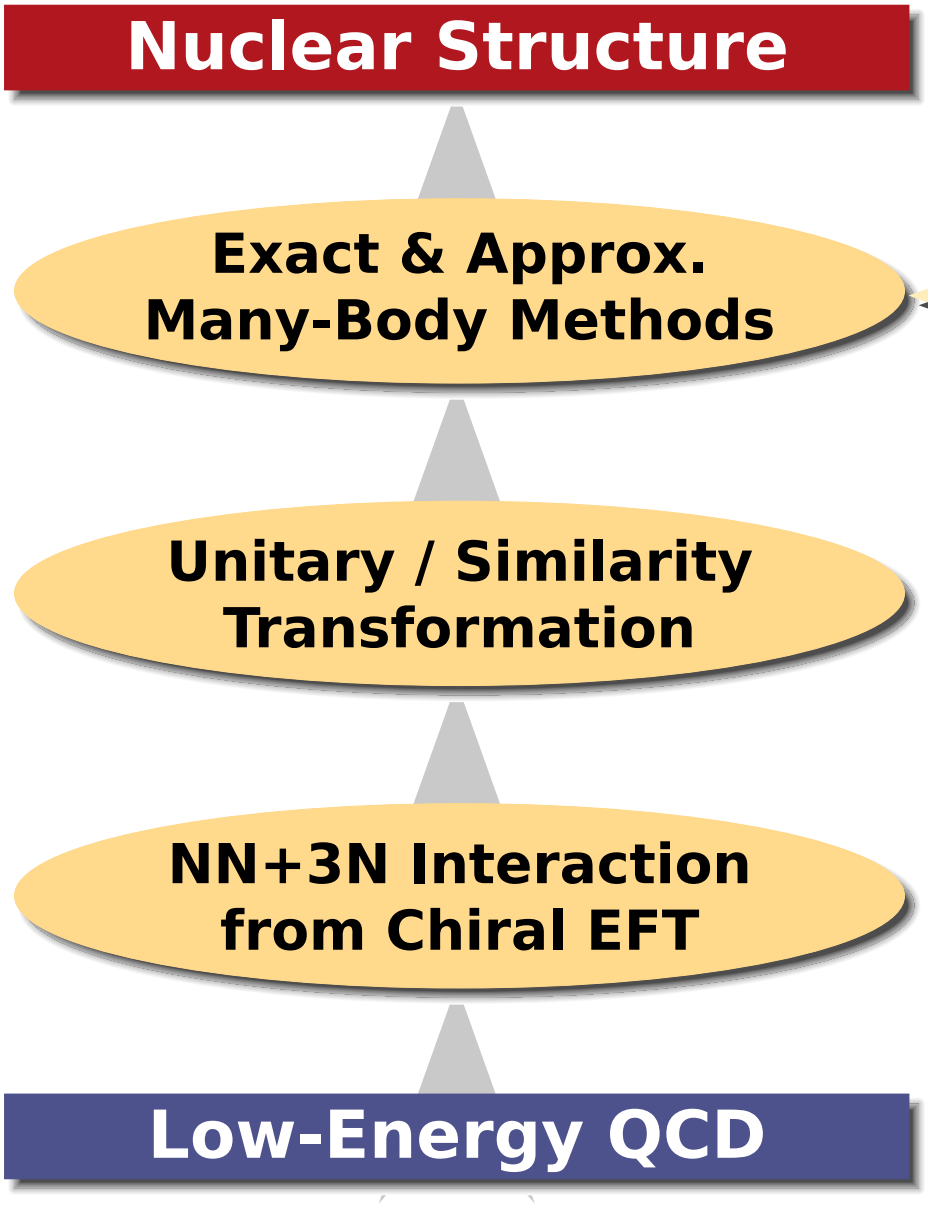
Unitary / Similarity Transformation

NN+3N Interaction from Chiral EFT

Low-Energy QCD

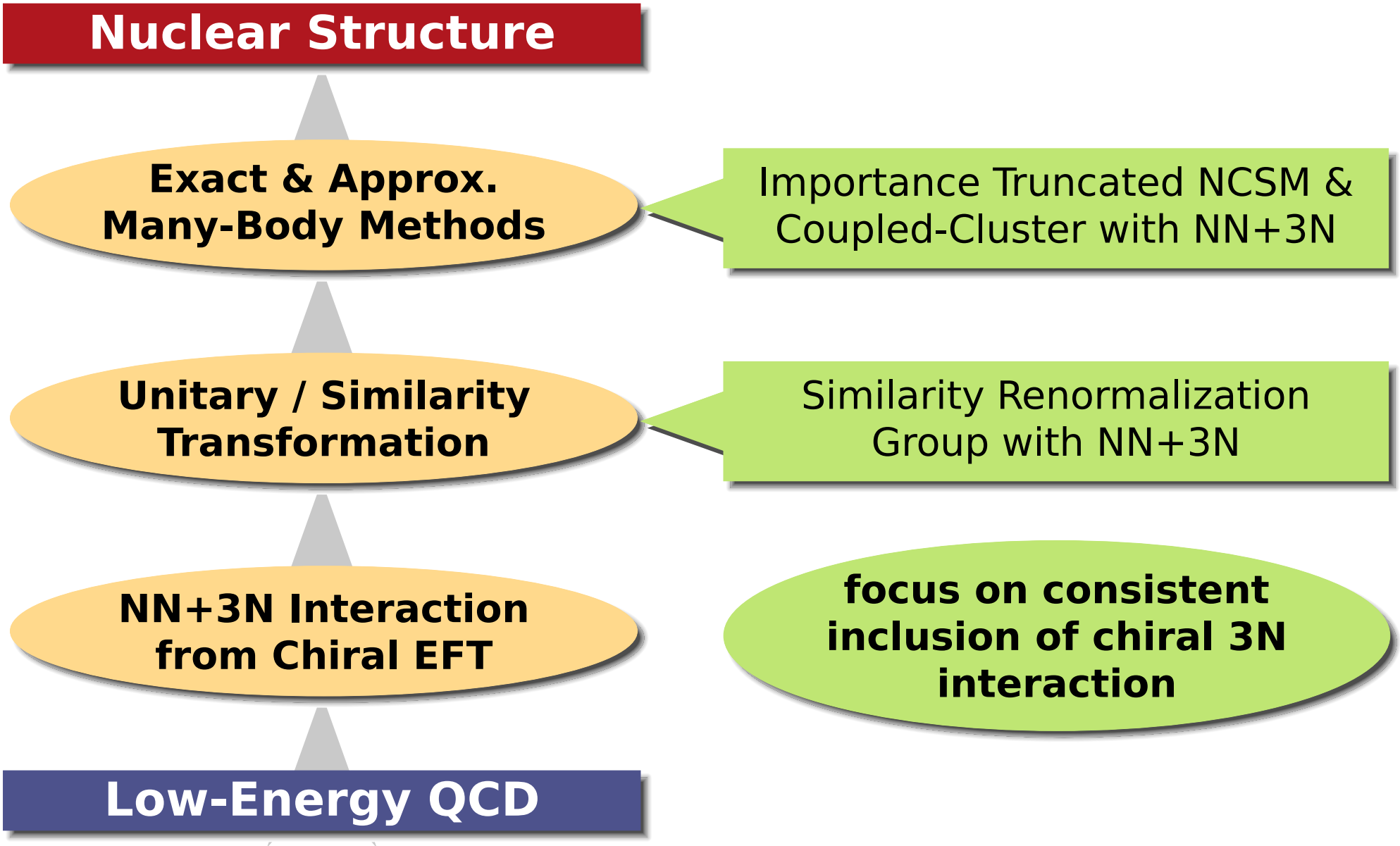
- adapt Hamiltonian to truncated low-energy model space
  - tame short-range correlations
  - improve convergence behavior
- transform Hamiltonian & observables consistently

From QCD to Nuclear Structure



- accurate solution of the many-body problem for light & intermediate masses (NCSM, CC,...)
- controlled approximations for heavier nuclei (MBPT,...)
- all rely on truncated model spaces & benefit from unitary transformation

From QCD to Nuclear Structure



Similarity Renormalization Group

Roth, Langhammer, Calci et al. — Phys. Rev. Lett. 107, 072501 (2011)
Roth, Neff, Feldmeier — Prog. Part. Nucl. Phys. 65, 50 (2010)
Roth, Reinhardt, Hergert — Phys. Rev. C 77, 064033 (2008)
Hergert, Roth — Phys. Rev. C 75, 051001(R) (2007)

Similarity Renormalization Group

continuous transformation driving
Hamiltonian to band-diagonal form
with respect to a chosen basis

simplicity and flexibility are great advantages of the SRG approach

solve SRG evolution equations using two- & three-body matrix representation

- **unitary transformation** of Hami

$$\widetilde{H}_\alpha = U_\alpha^\dagger H U_\alpha$$

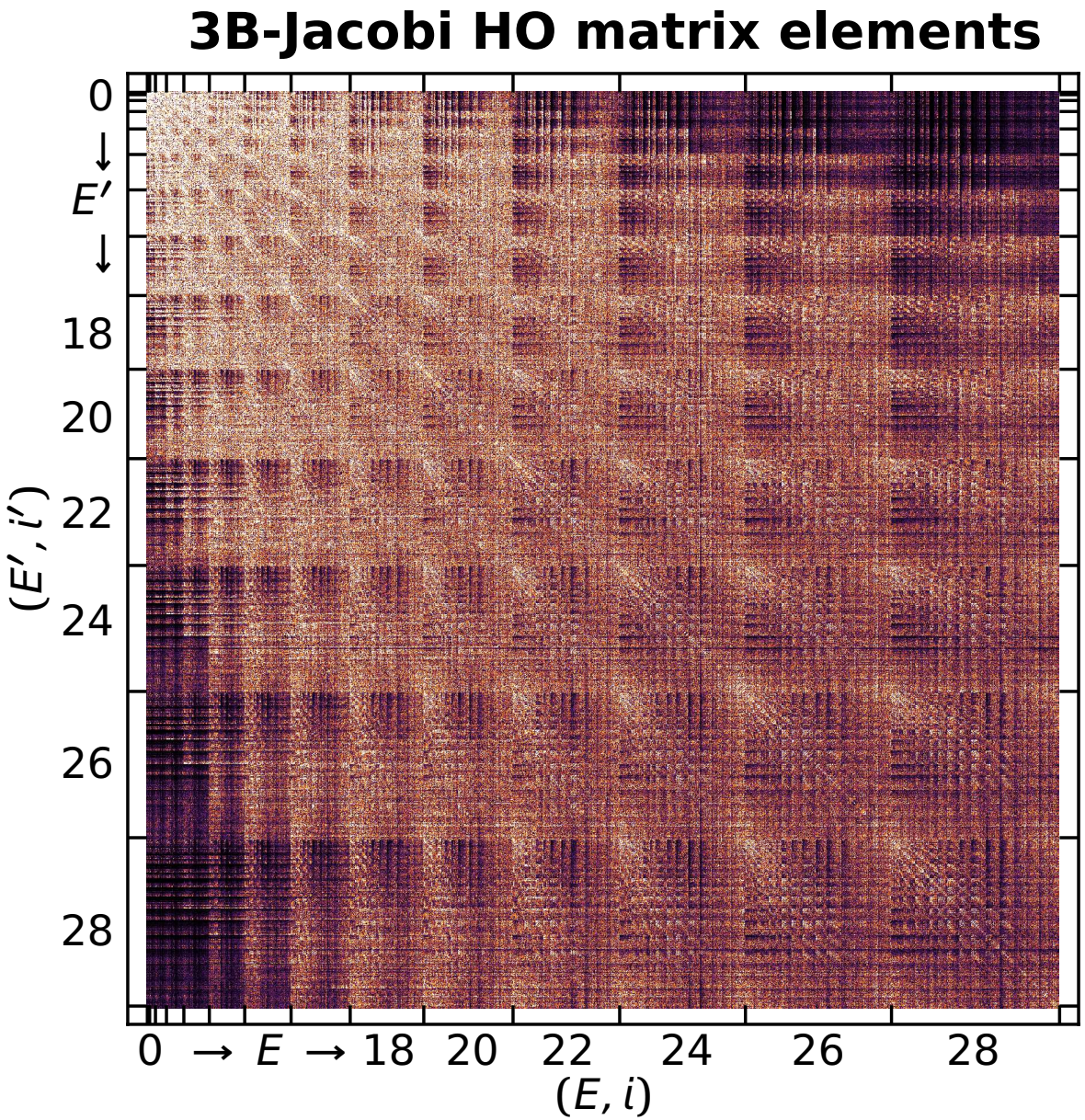
- **evolution equations** for $\widetilde{H}_\alpha$ and U

$$\frac{d}{d\alpha}\widetilde{H}_\alpha = [\eta_\alpha, \widetilde{H}_\alpha]$$

- **dynamic generator**: commutator with the operator in whose eigenbasis H shall be diagonalized

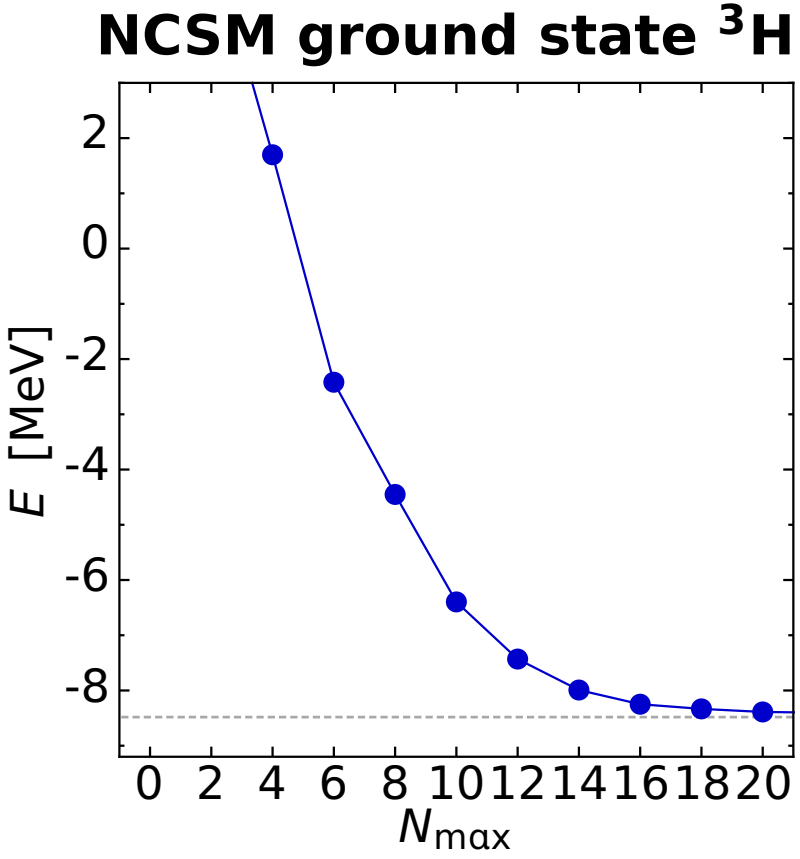
$$\eta_\alpha = (2\mu)^2 [T_{\text{int}}, \widetilde{H}_\alpha]$$

SRG Evolution in Three-Body Space



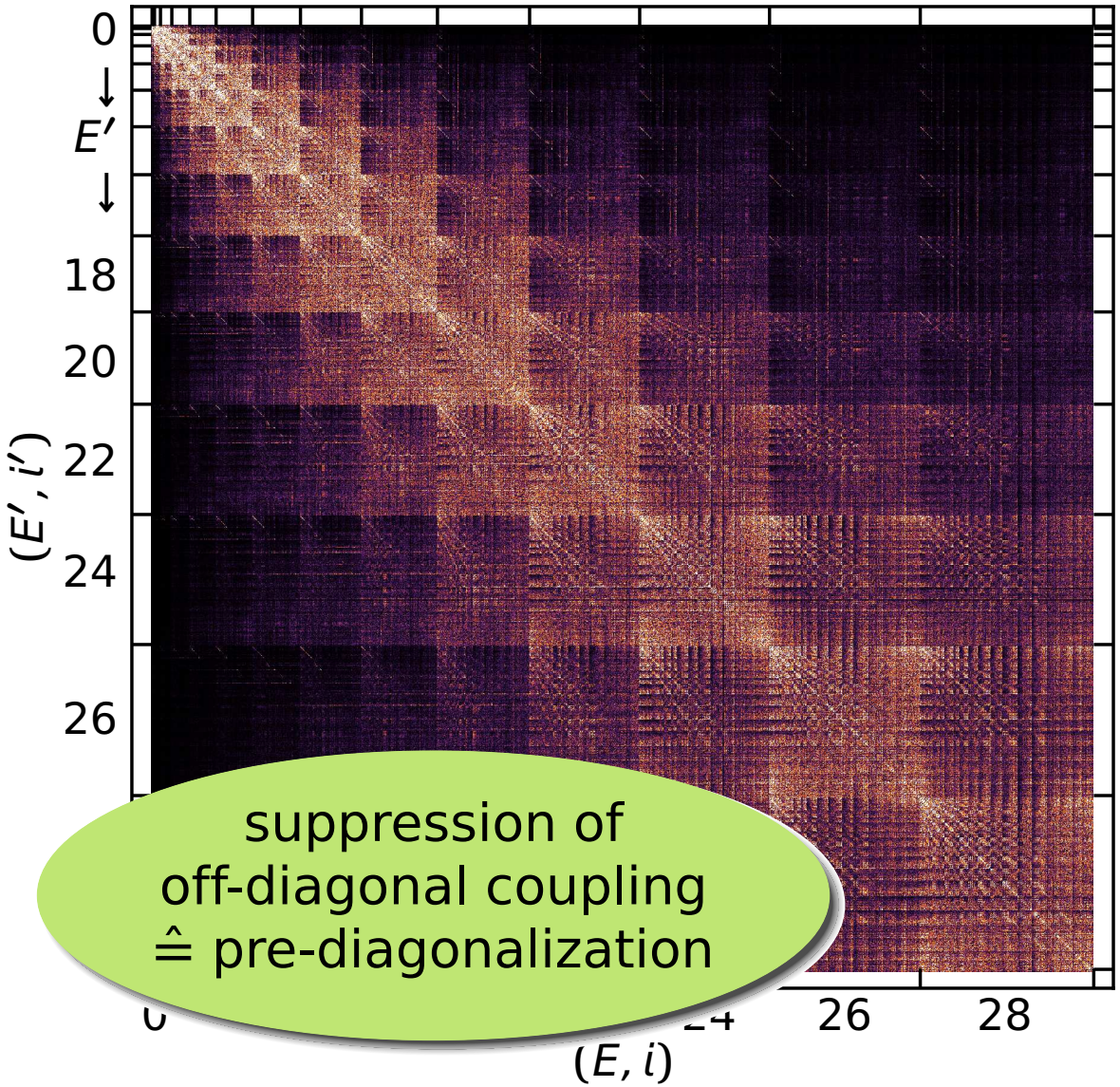
$$\alpha = 0.000\,\mathrm{fm}^4$$
$$\Lambda = \infty\,\mathrm{fm}^{-1}$$

$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 28\,\mathrm{MeV}$



SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements



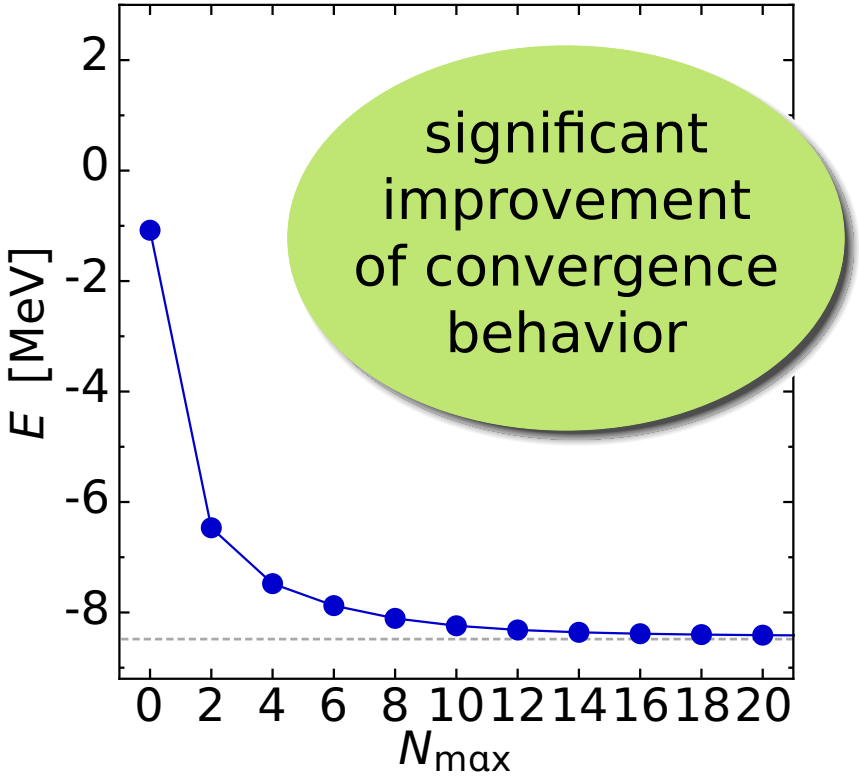
suppression of
off-diagonal coupling
≙ pre-diagonalization

$\alpha = 0.320\,\mathrm{fm}^4$

$\Lambda = 1.33\,\mathrm{fm}^{-1}$

$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 28\,\mathrm{MeV}$

NCSM ground state ^{3}H



significant
improvement
of convergence
behavior

Calculations in *A*-Body Space

- evolution **induces *n*-body contributions** $\widetilde{\mathrm{H}}_\alpha^{[n]}$ to Hamiltonian

$$\widetilde{\mathrm{H}}_\alpha = \widetilde{\mathrm{H}}_\alpha^{[1]} + \widetilde{\mathrm{H}}_\alpha^{[2]} + \widetilde{\mathrm{H}}_\alpha^{[3]} + \widetilde{\mathrm{H}}_\alpha^{[4]} + \ldots$$

- truncation of cluster series inevitable — formally destroys unitarity and invariance of energy eigenvalues (independence of α)

Three SRG-Evolved Hamiltonians

- **NN only**: start with NN initial Hamiltonian and keep two-body terms only
- **NN+3N-induced**: start with NN initial Ham[illegible] keep two- and induced three-body terms
- **NN+3N-full**: start with NN+3[illegible] and all three-body terms

α-variation provides a **diagnostic tool** to assess the contributions of omitted many-body interactions

Importance Truncated NCSM

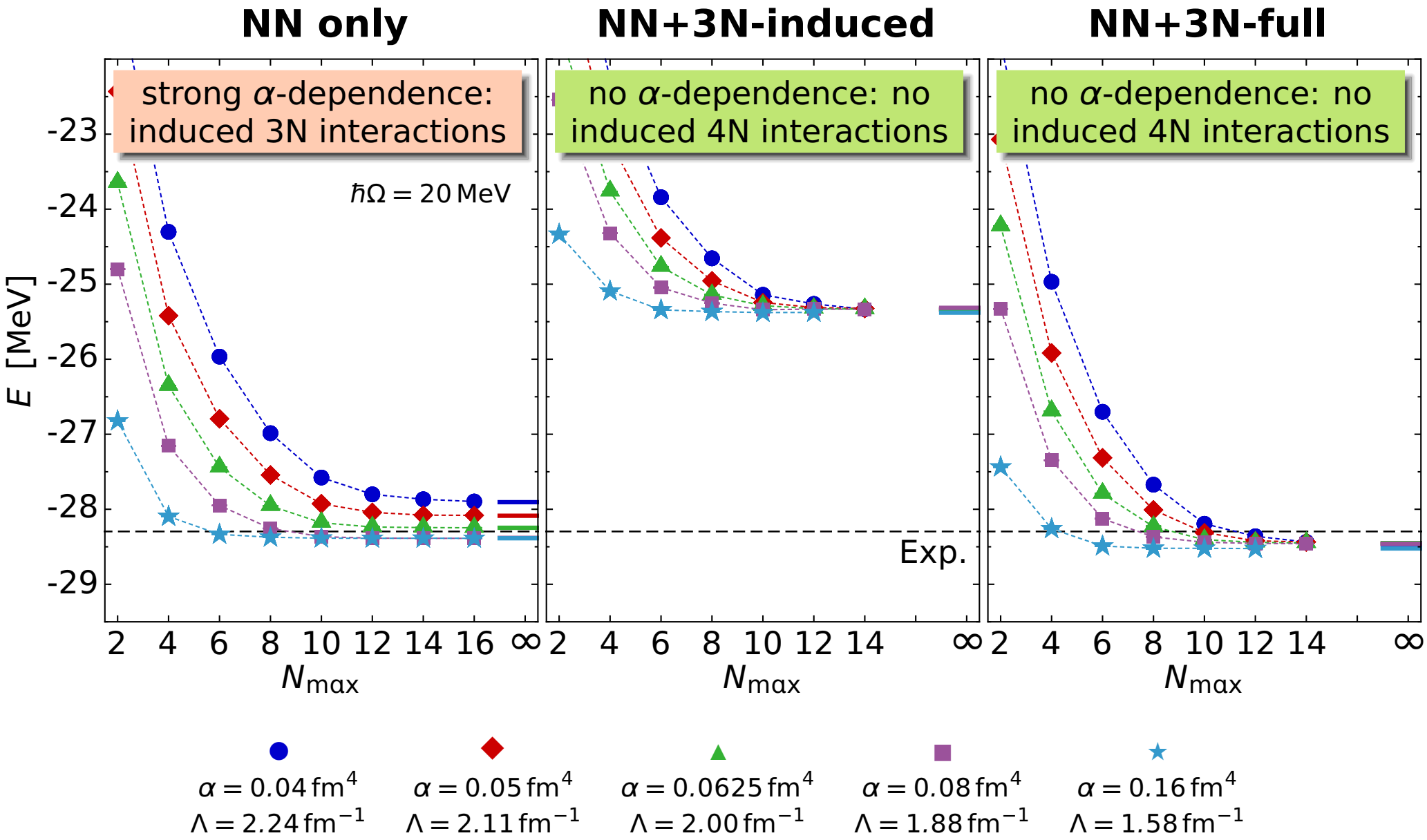
Roth, Langhammer, Calci et al. — Phys. Rev. Lett. 107, 072501 (2011)
Navrátil, Roth, Quaglioni — Phys. Rev. C 82, 034609 (2010)
Roth — Phys. Rev. C 79, 064324 (2009)
Roth, Gour & Piecuch — Phys. Lett. B 679, 334 (2009)
Roth, Gour & Piecuch — Phys. Rev. C 79, 054325 (2009)
Roth, Navrátil — Phys. Rev. Lett. 99, 092501 (2007)

Importance Truncated NCSM

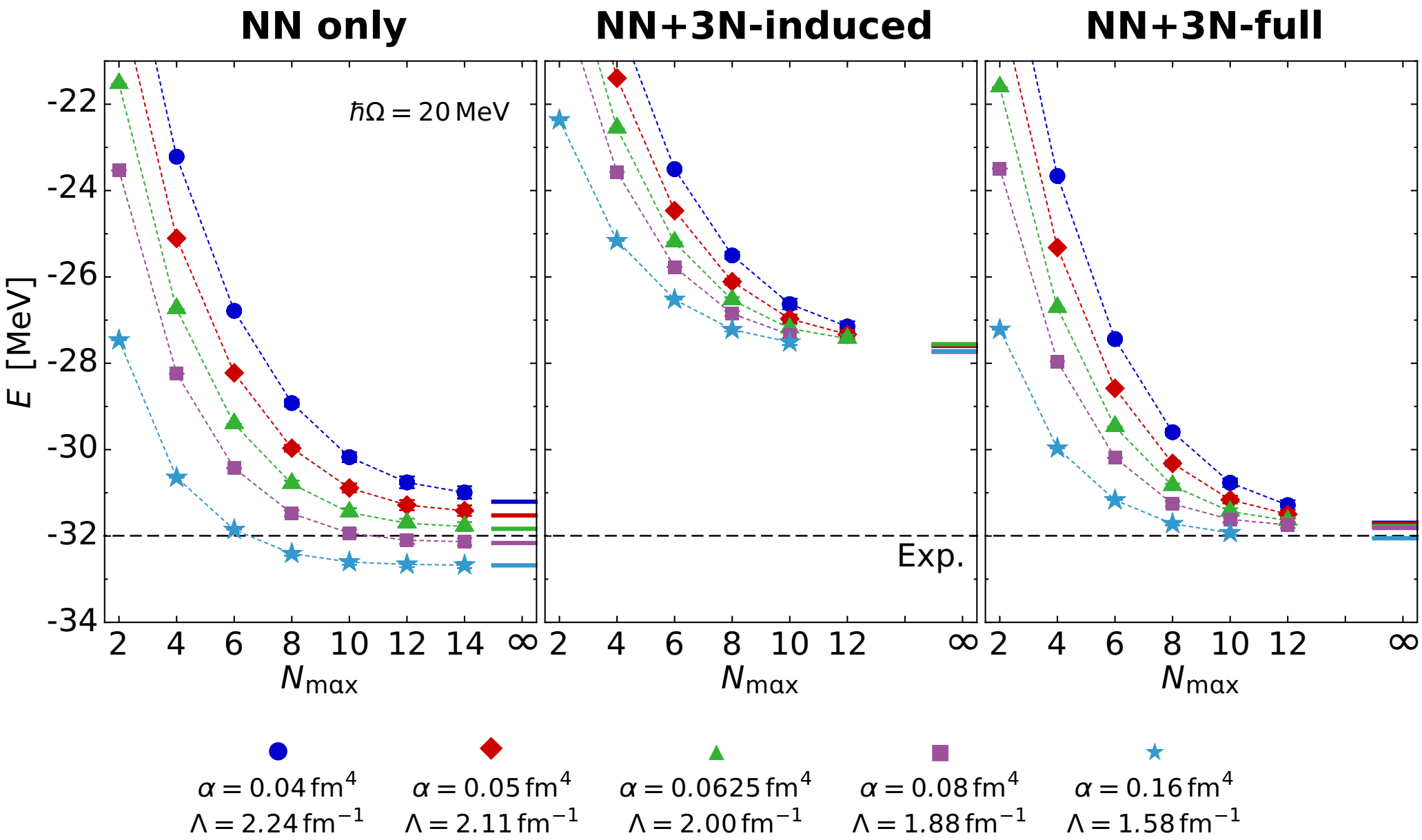
NCSM is one of the most powerful and universal exact ab-initio methods

- construct matrix representation of Hamiltonian using a **basis of HO Slater determinants** truncated w.r.t. HO excitation energy $N_{\max}\hbar\Omega$
- solve **large-scale eigenvalue problem** for a few extremal eigenvalues
- **all relevant observables** can be computed from the eigenstates
- range of applicability limited by **factorial growth** of basis with $N_{\max}$ & A
- adaptive **importance truncation** extends the range of NCSM by reducing the model space to physically relevant states
- we have developed a **parallelized IT-NCSM/NCSM code** capable of handling 3N matrix elements up to $E_{3\,\max} = 16$

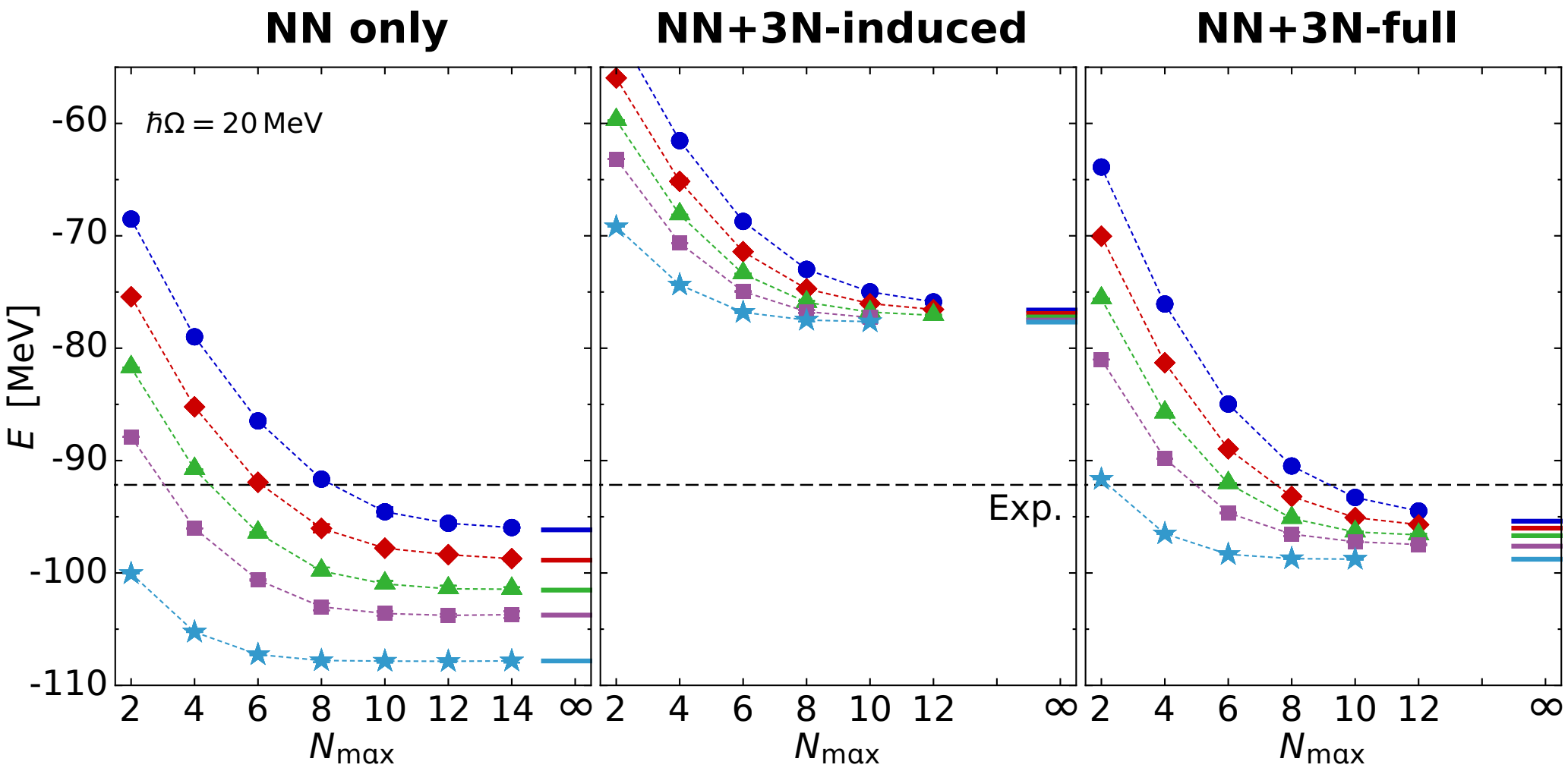
^{4}He: Ground-State Energies



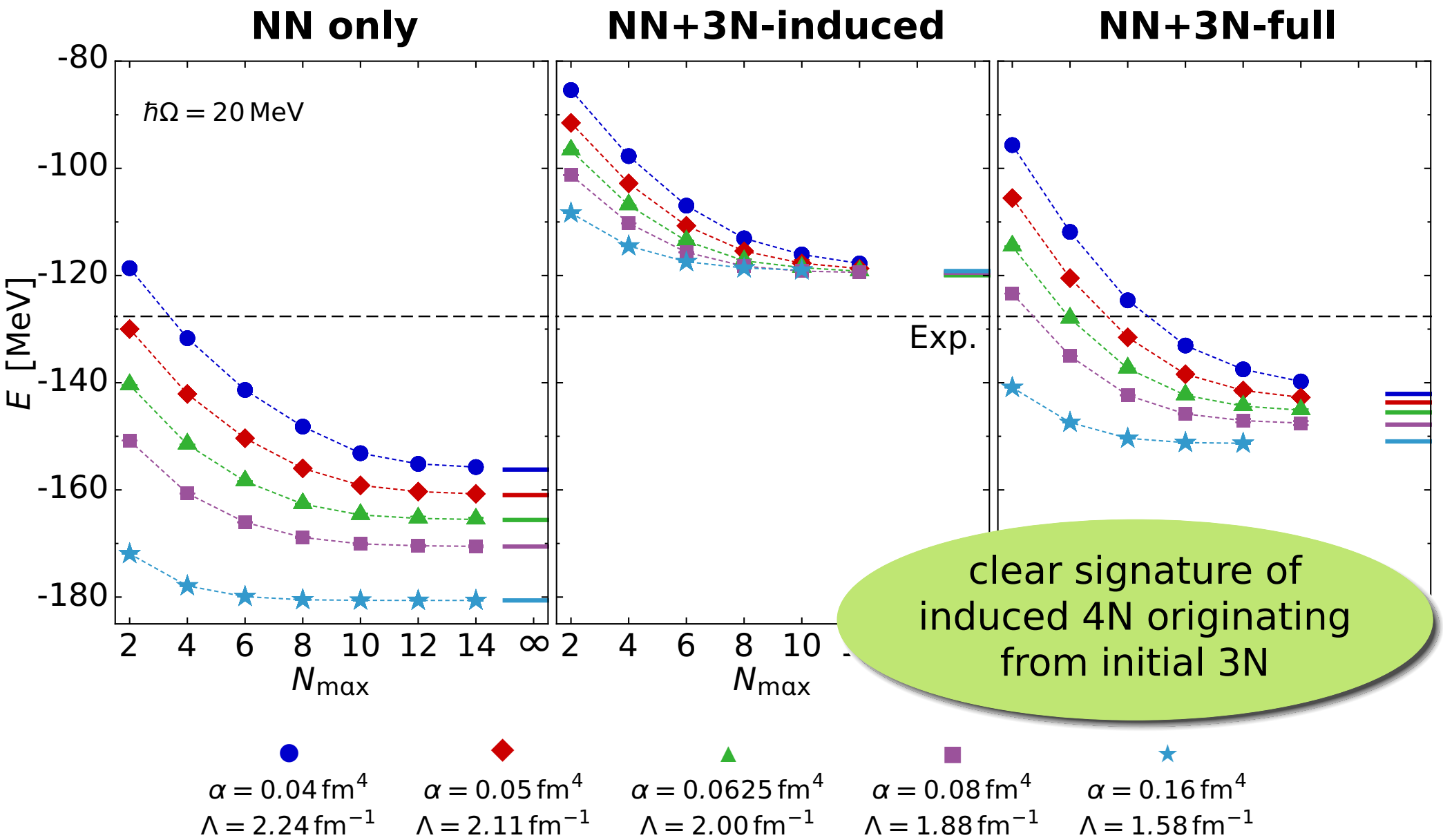
^{6}Li: Ground-State Energies



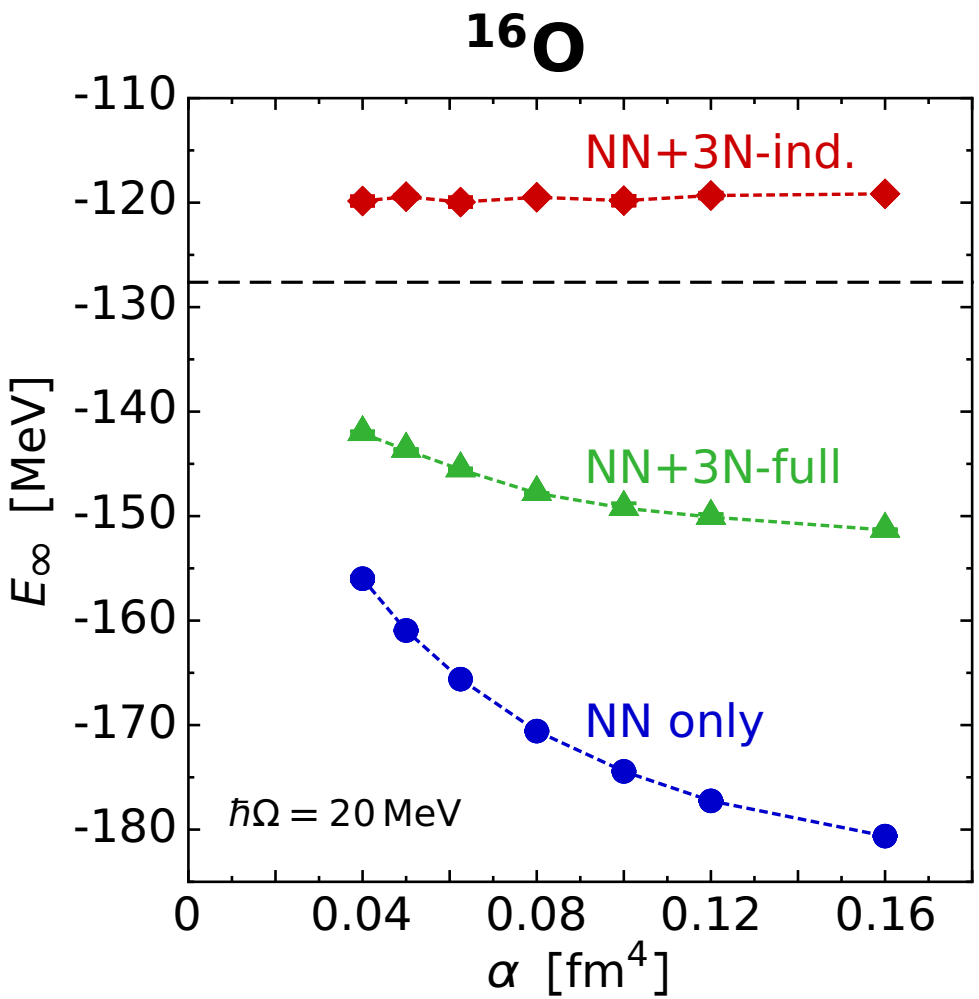
^{12}C: Ground-State Energies



^{16}O: Ground-State Energies

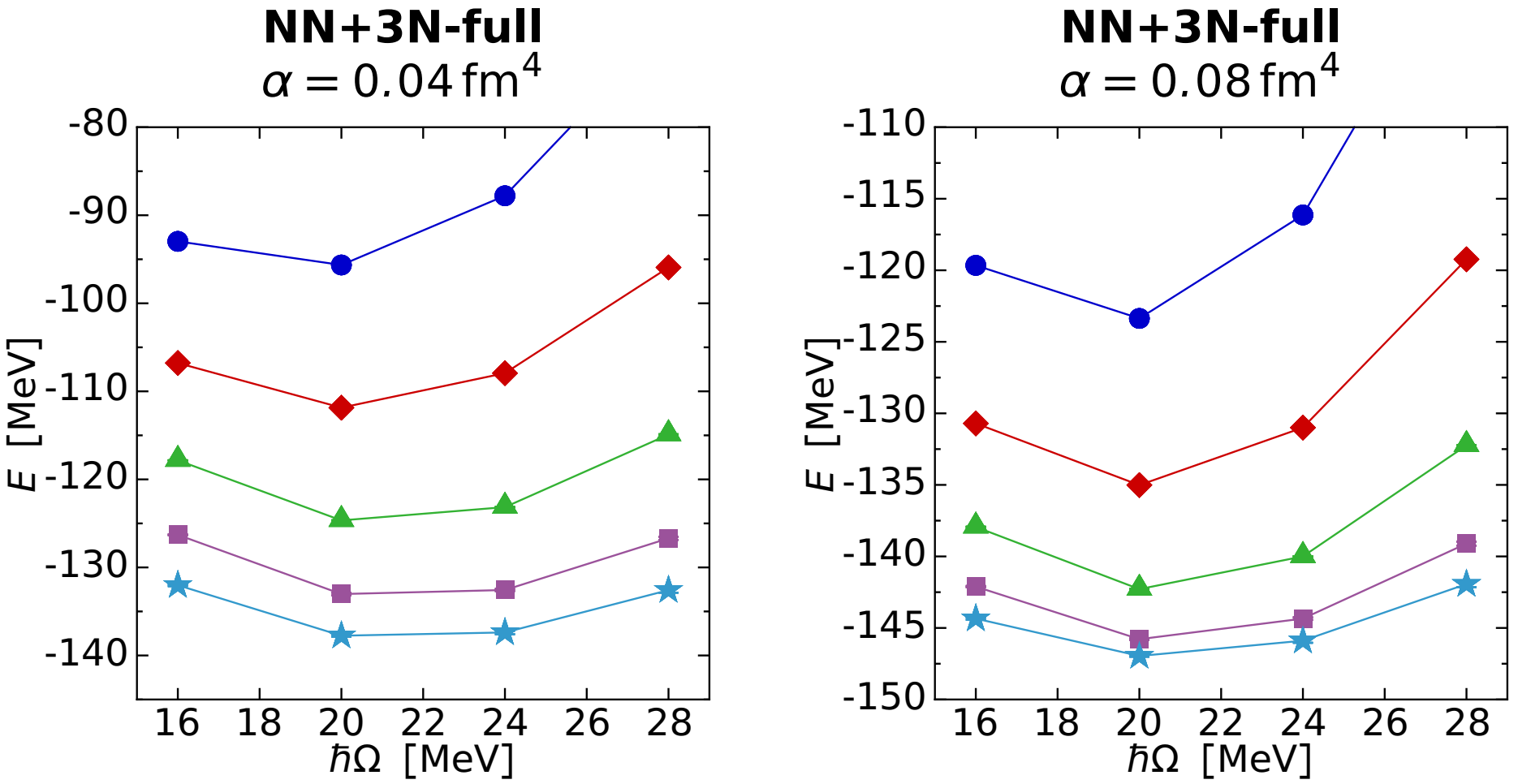


^{16}O: Energy vs. Flow Parameter

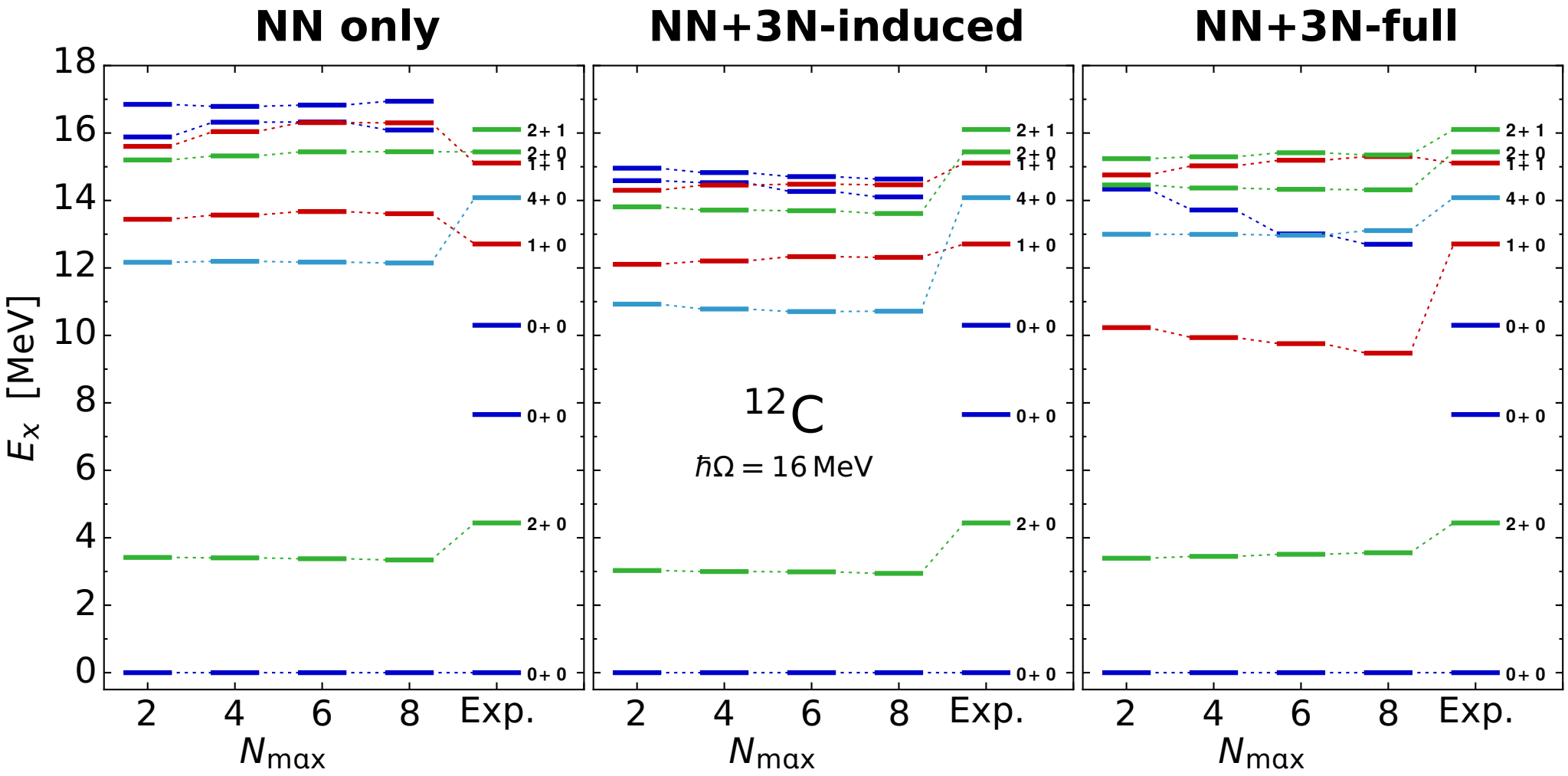


- **initial NN Hamiltonian**
  - induced 3N interactions are significant
  - no indication of induced 4N
  - NN+3N-induced unitarily equivalent to initial NN
- **initial NN+3N Hamiltonian**
  - induced 4N interactions are sizable in upper p-shell
  - generated by long-range 2π terms of initial 3N interaction

^{16}O: Frequency Dependence



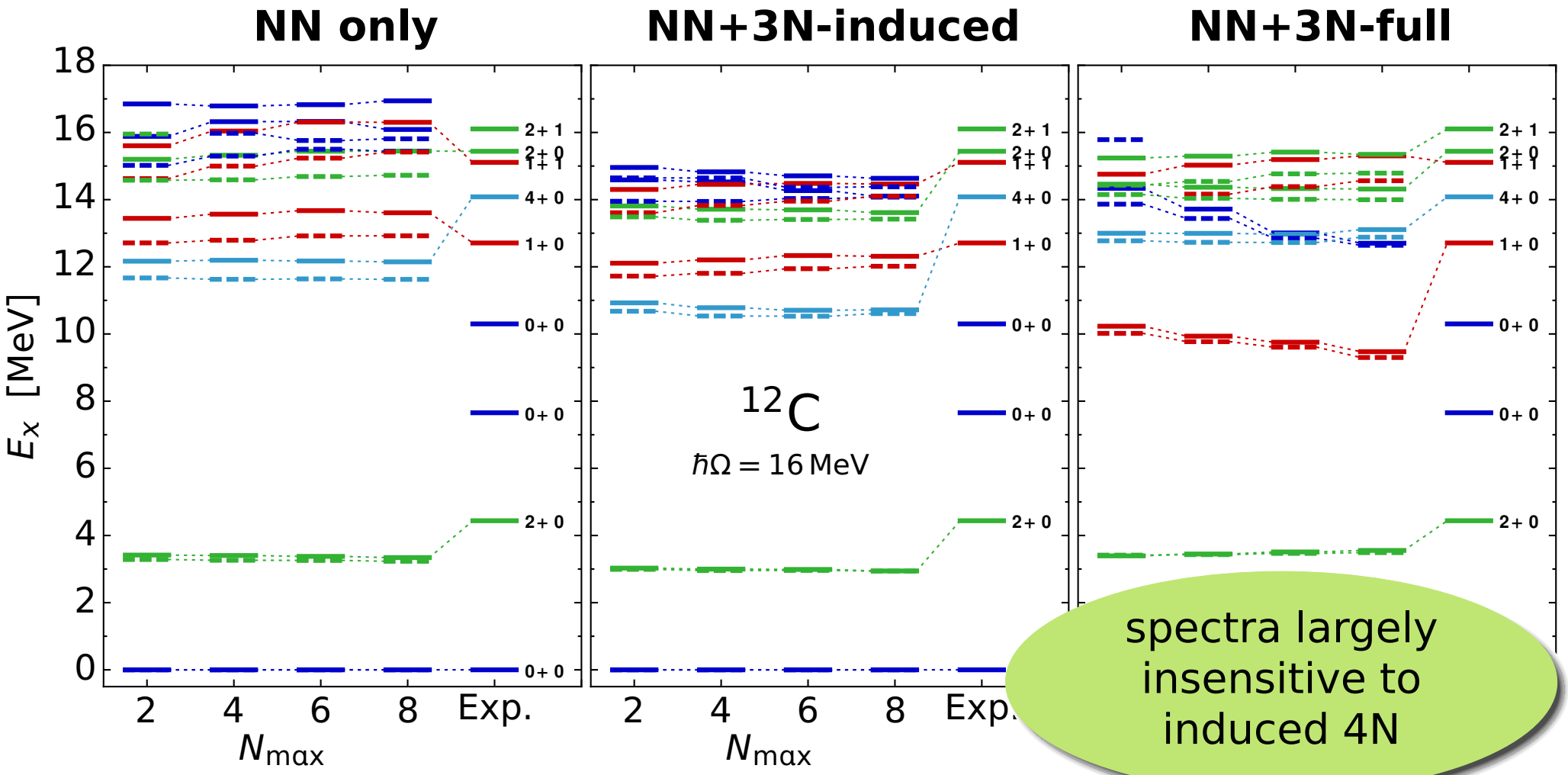
Spectroscopy of ^{12}C



$\alpha = 0.04\,\mathrm{fm}^4$
$\Lambda = 2.24\,\mathrm{fm}^{-1}$

$\alpha = 0.08\,\mathrm{fm}^4$
$\Lambda = 1.88\,\mathrm{fm}^{-1}$

Spectroscopy of ^{12}C



Where do we go from here?

- beyond the lightest nuclei, **SRG-induced 4N contributions** affect the absolute energies (but not the excitation energies)
- with the inclusion of the leading 3N interaction we already obtain a **very reasonable description** of spectra (and ground states)

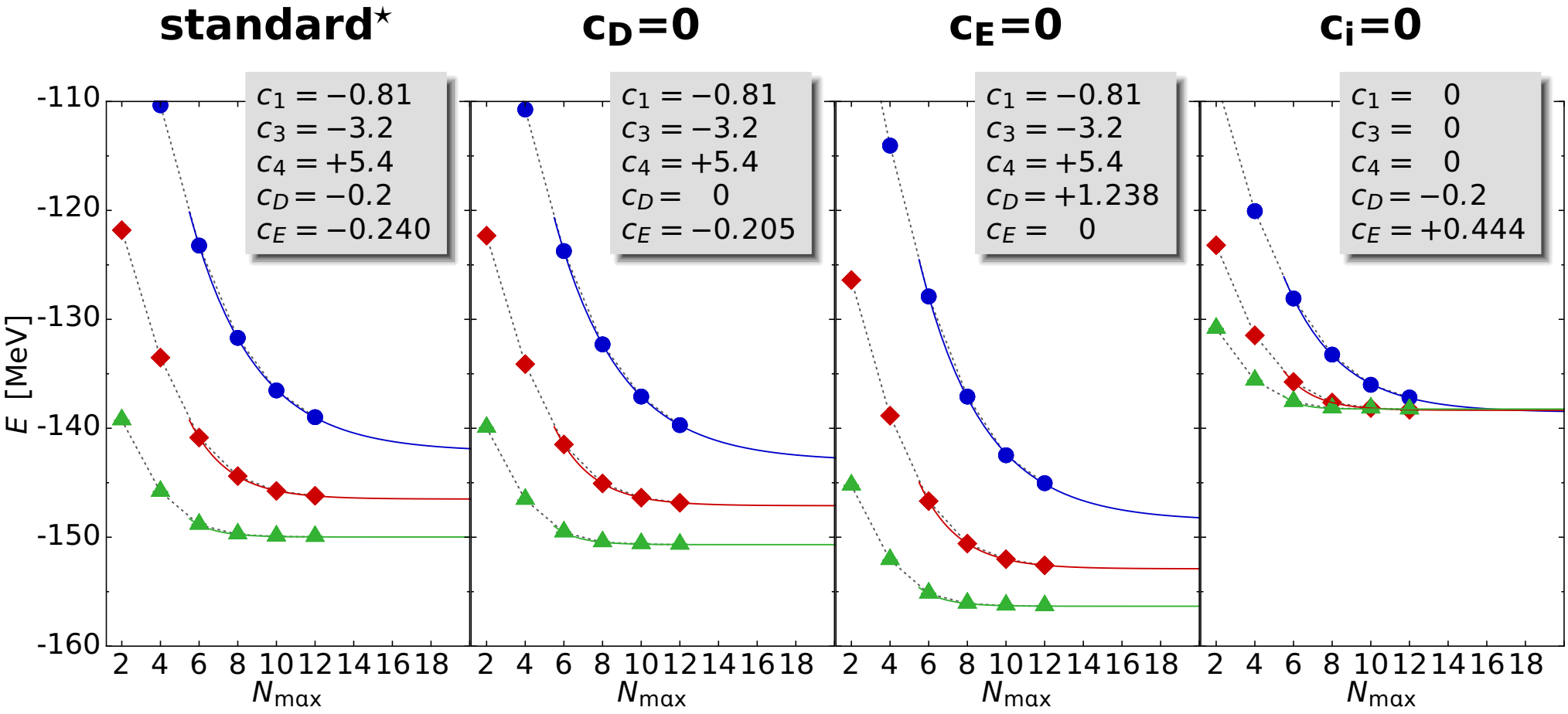
SRG Transformation

- Which parts of the initial 3N cause the induced 4N contributions ?
- Can we find alternative SRG generators with suppressed induced 4N ?

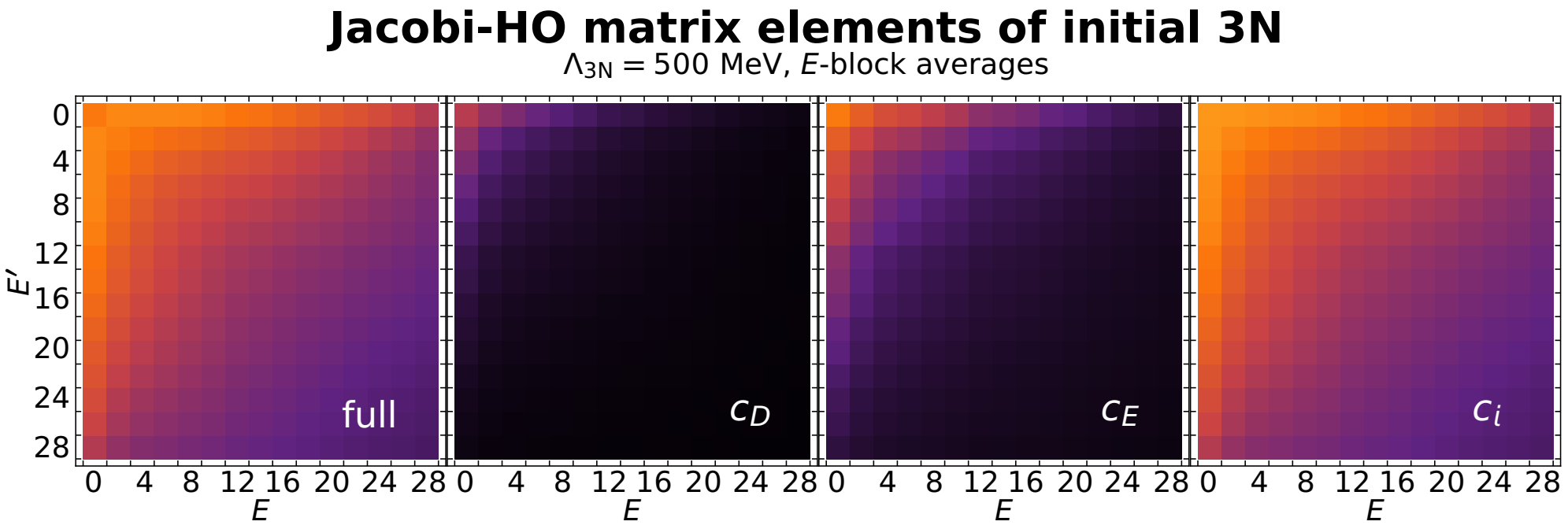
Chiral NN+3N Interactions

- How sensitive is the spectroscopy on specifics of the 3N interaction (cutoff, c_i's) ?
- How does the inclusion of the subleading 3N terms affect the picture ?

^{16}O: Origin of Induced 4N



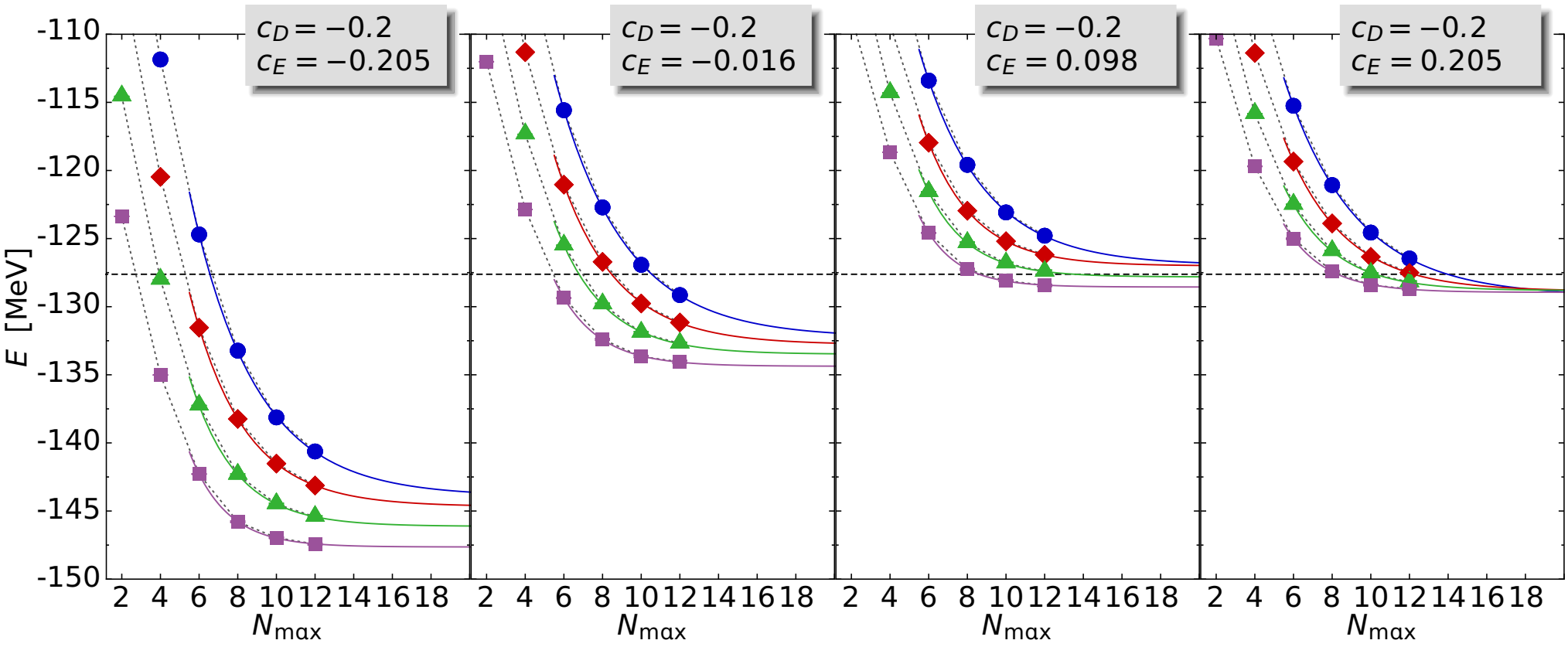
Origin of Induced 4N



- off-diagonal matrix elements dominated by c_i (c_3 and c_4) terms
- suppress initial off-diagonal matrix elements by:
  - lowering initial 3N cutoff Λ_{3N}
  - changing regulator function or scheme

^{16}O: Lowering the Initial 3N Cutoff

refitted 3N interaction with modified 3N cutoff



$\alpha = 0.04\,\mathrm{fm}^4$ $\Lambda = 2.24\,\mathrm{fm}^{-1}$

$\alpha = 0.05\,\mathrm{fm}^4$ $\Lambda = 2.11\,\mathrm{fm}^{-1}$

$\alpha = 0.0625\,\mathrm{fm}^4$ $\Lambda = 2.00\,\mathrm{fm}^{-1}$

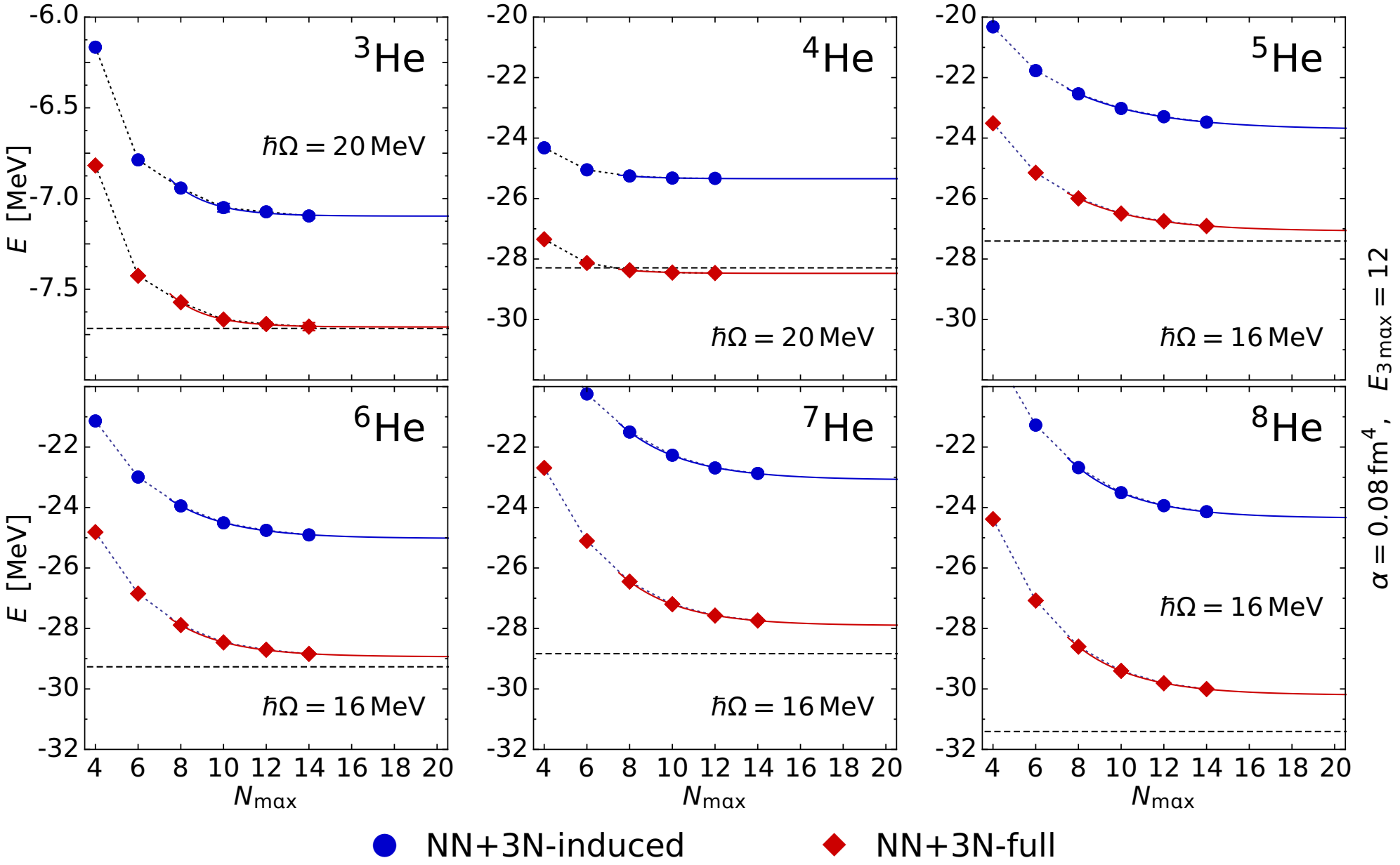
$\alpha = 0.08\,\mathrm{fm}^4$ $\Lambda = 1.88\,\mathrm{fm}^{-1}$

NN+3N-full
$\hbar\Omega = 20\,\mathrm{MeV}$

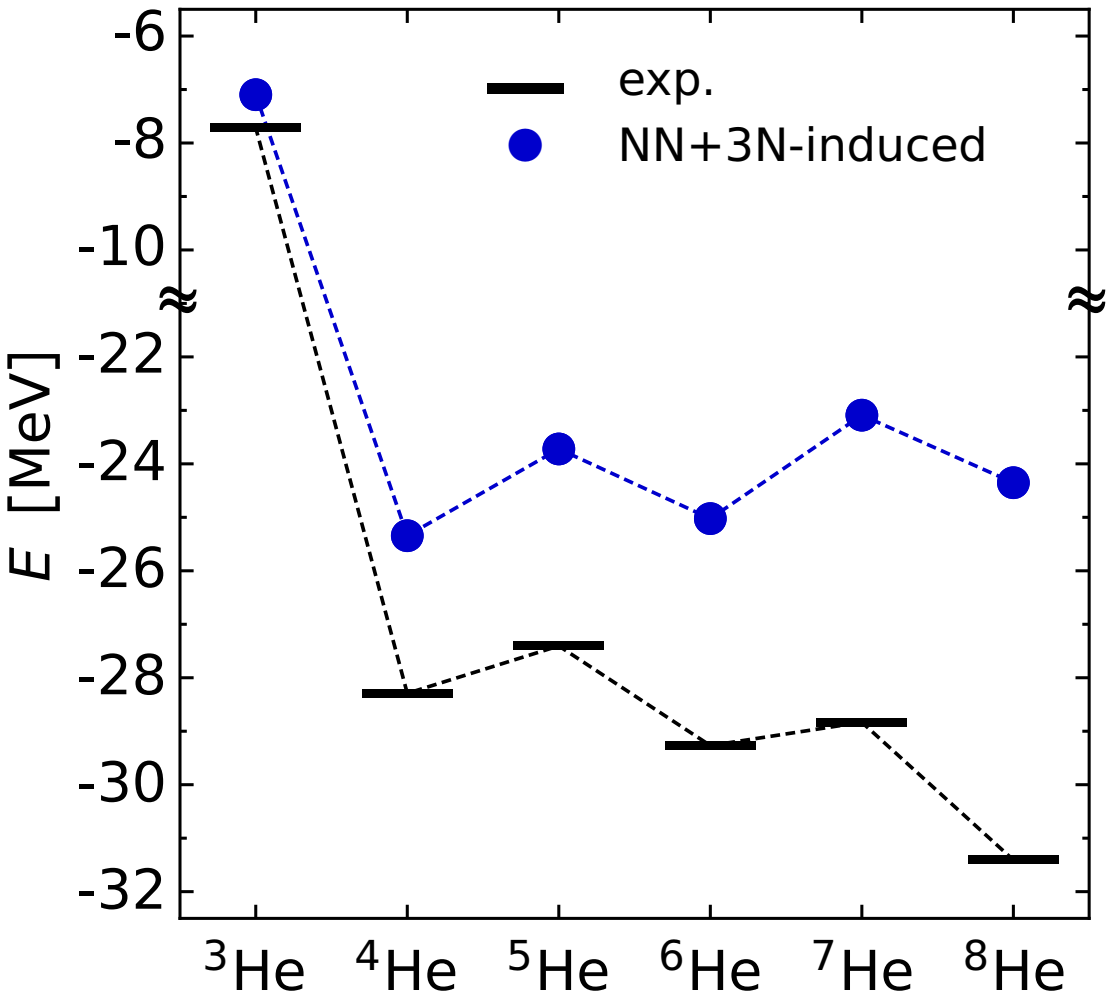
Outlook: Physics Applications

(work in progress... all preliminary)

Outlook: Ground-States of Helium Isotopes



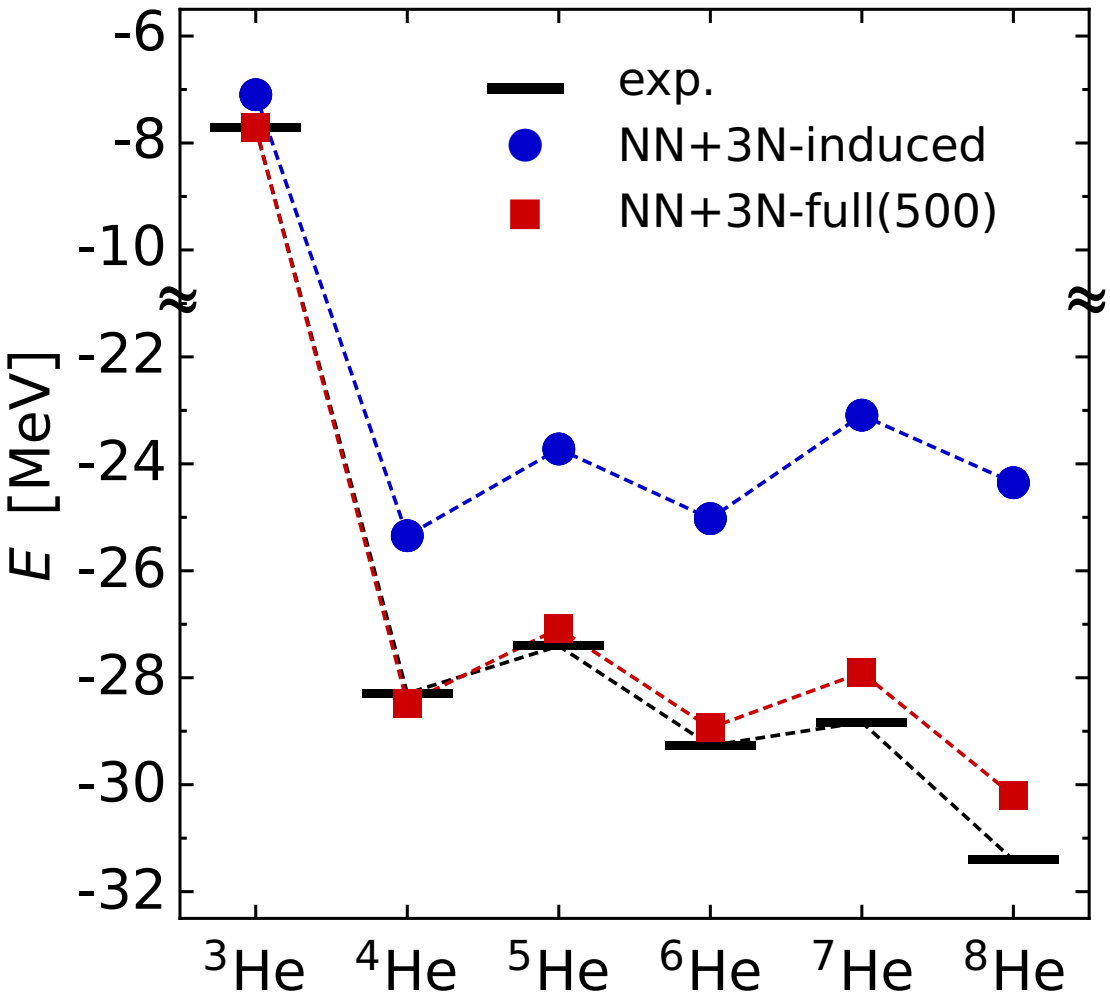
Outlook: Ground-States of Helium Isotopes



$\alpha = 0.08\,\mathrm{fm}^4,\ E_{3\,\mathrm{max}} = 12$

- chiral NN interaction cannot reproduce mass systematics

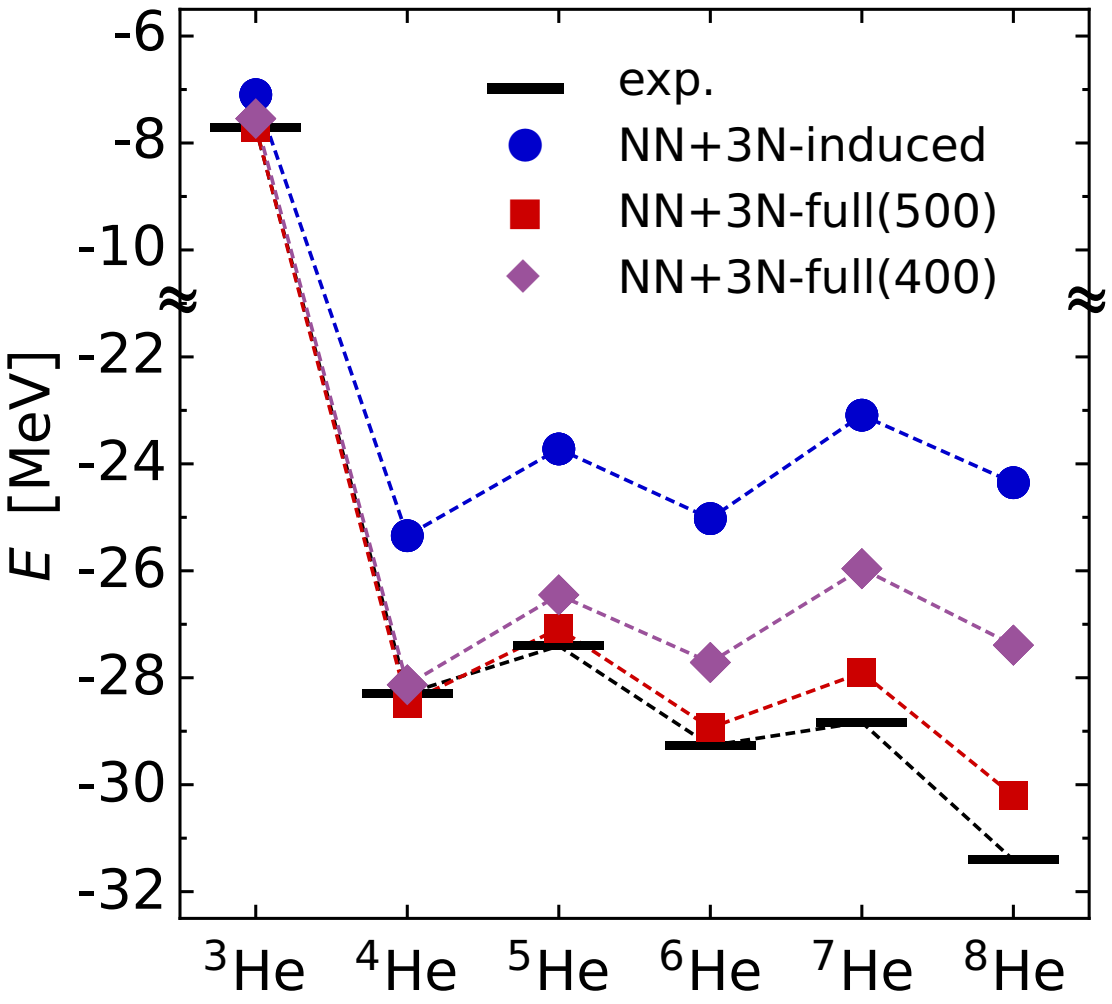
Outlook: Ground-States of Helium Isotopes



$\alpha = 0.08\,\mathrm{fm}^4,\ E_{3\,\mathrm{max}} = 12$

- chiral NN interaction cannot reproduce mass systematics
- inclusion of chiral 3N gives a **very good systematic agreement**

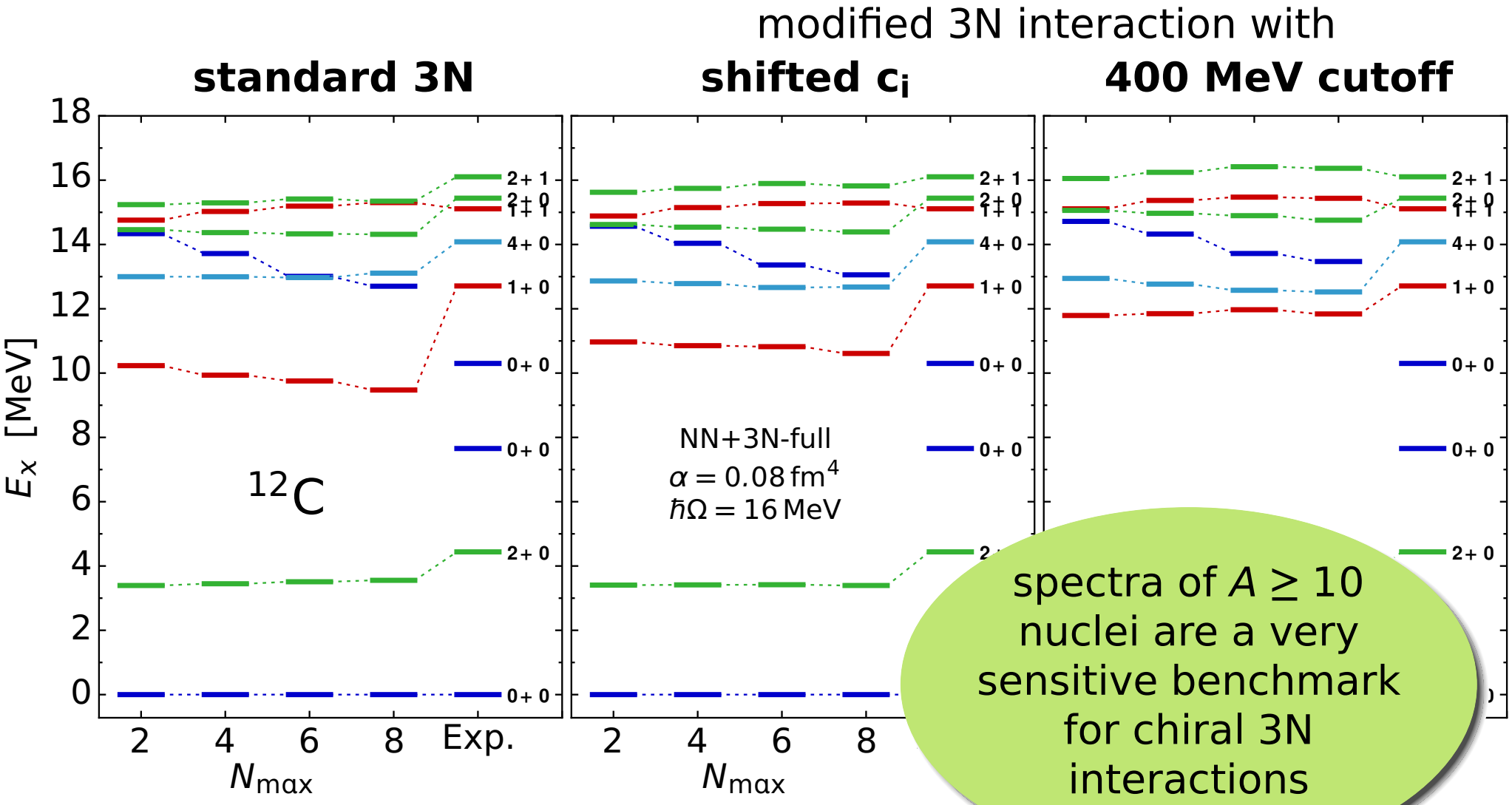
Outlook: Ground-States of Helium Isotopes



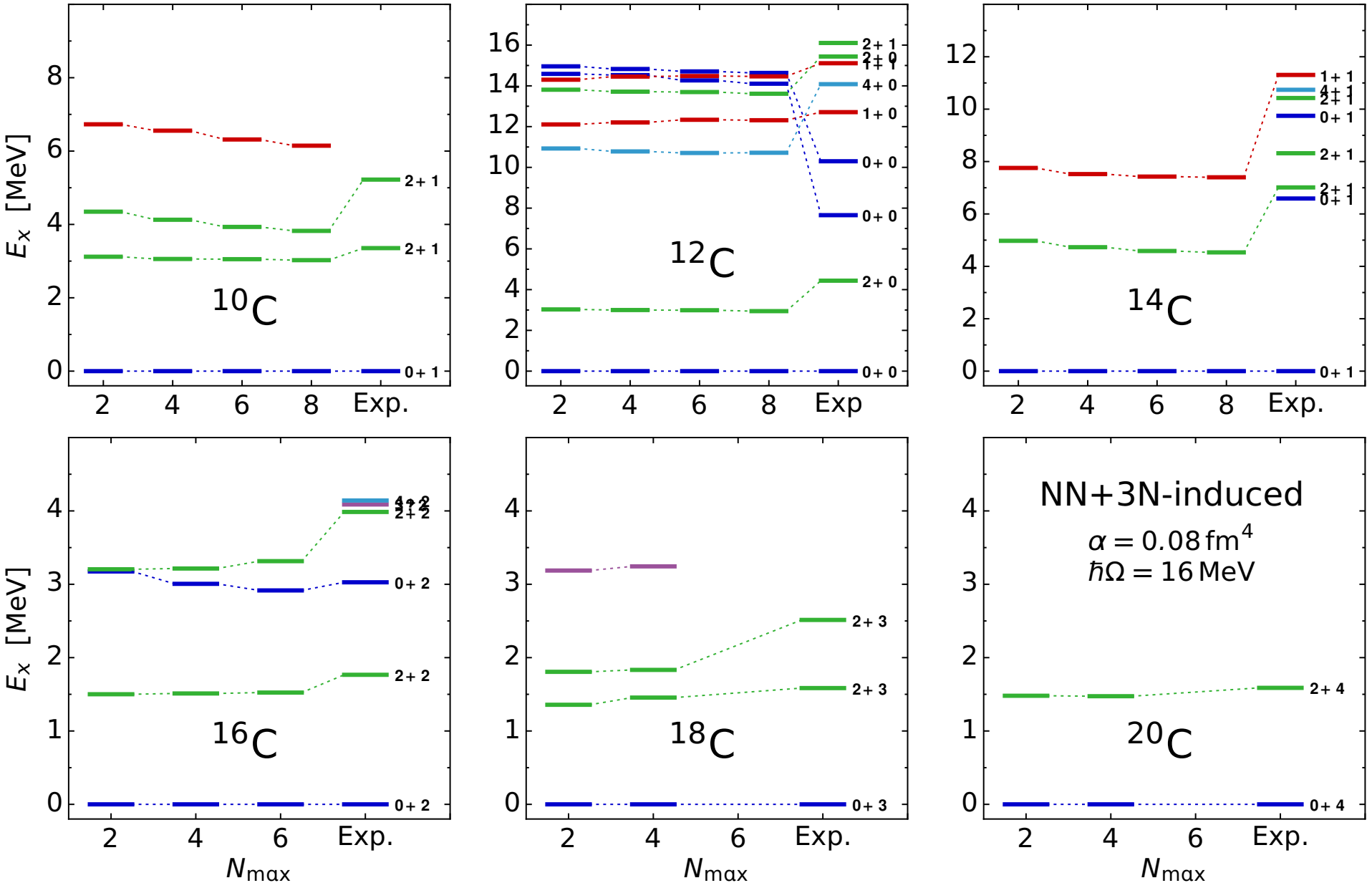
$\alpha = 0.08\,\mathrm{fm}^4,\ E_{3\mathrm{max}} = 12$

- chiral NN interaction cannot reproduce mass systematics
- inclusion of chiral 3N gives a **very good systematic agreement**
- sensitive to details of the initial 3N interaction, e.g. the cutoff
- next: **consistent coupling to continuum** within NCSMC

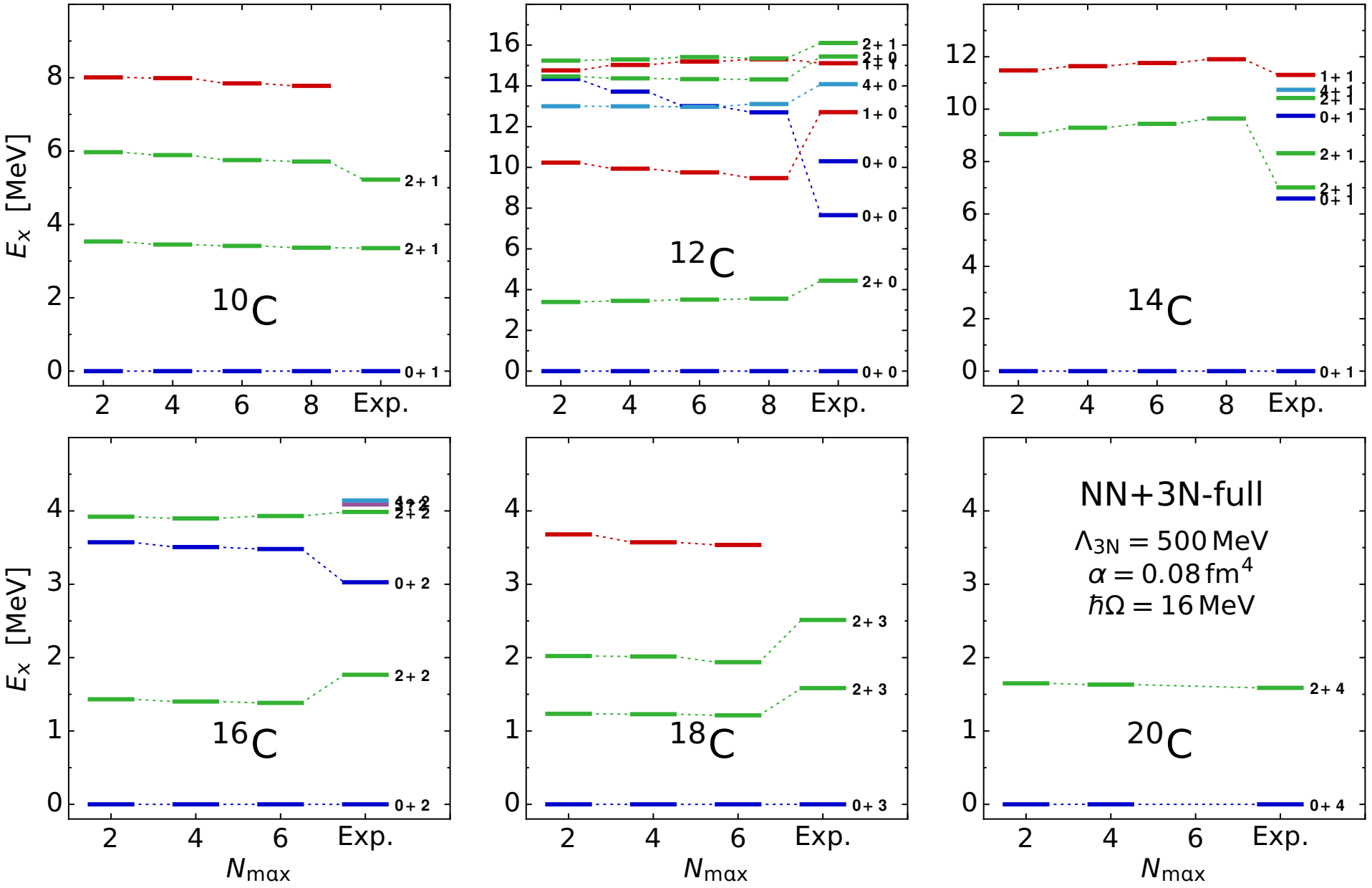
Outlook: Sensitivity on Initial 3N



Outlook: Carbon Isotopic Chain



Outlook: Carbon Isotopic Chain



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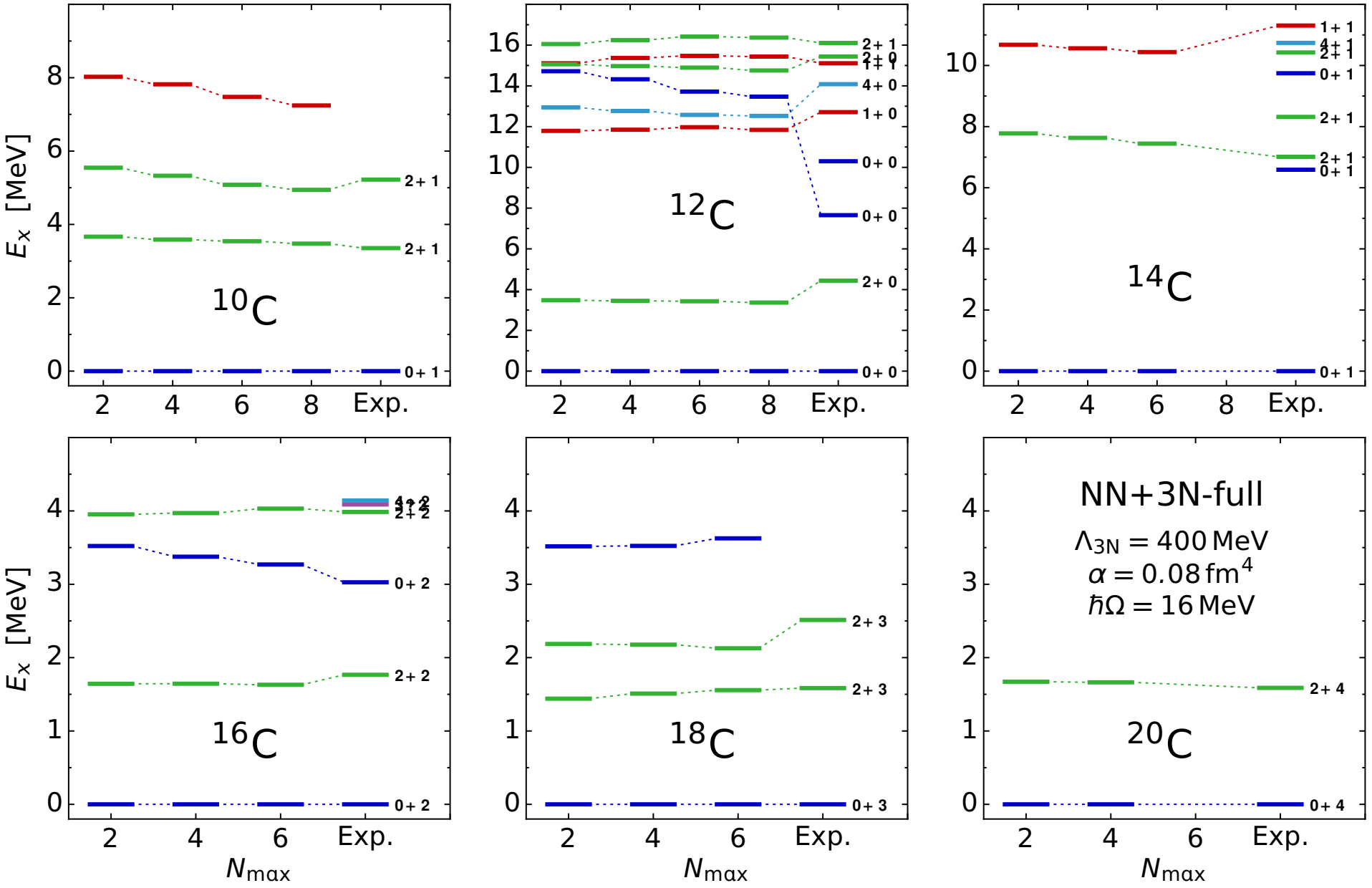
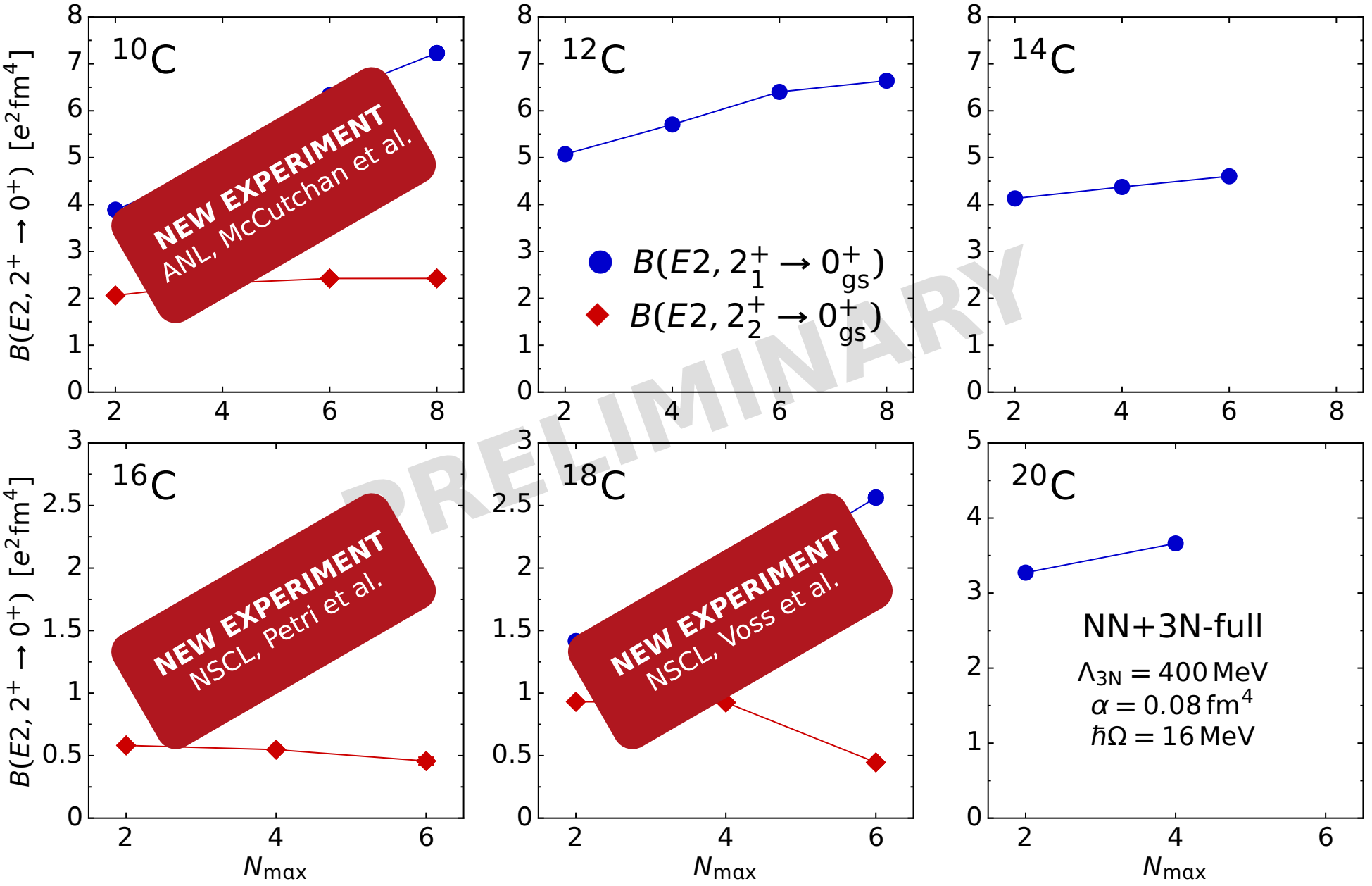
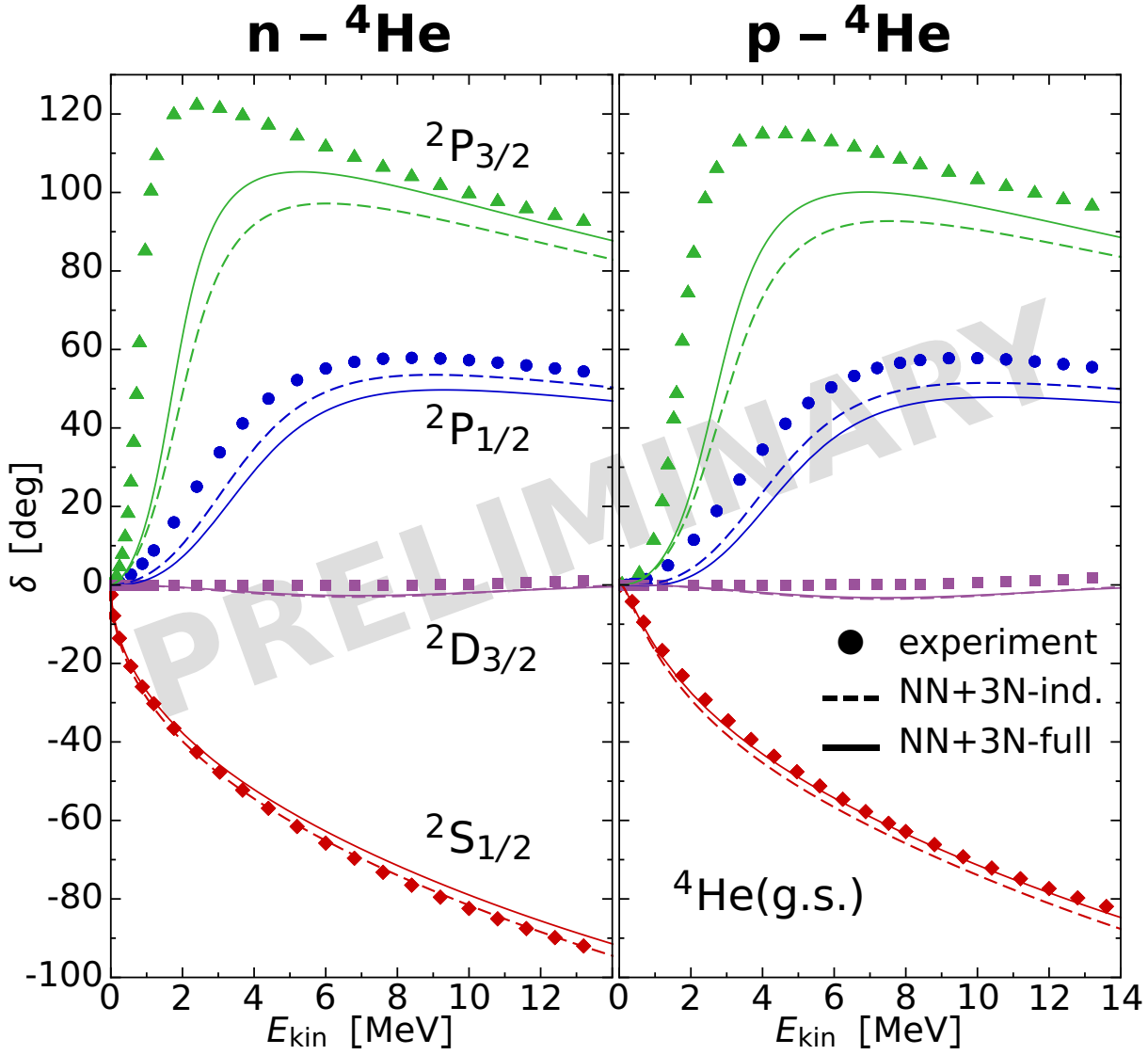


Outlook: Carbon Isotopic Chain



Outlook: Ab Initio Reactions with Chiral 3N



$N_{max} = 8,\ E_{3\,max} = 10,\quad \hbar\Omega = 20$ MeV

- inclusion of **full 3N interactions** into NCSM/RGM & NCSMC (see Petr Navrátil's talk)
- development of a new computational scheme for kernels... completed
- first proof-of-principle calculations... done
- initial 3N **increases spin-orbit splittings**

Normal-Ordered 3N Interaction & Coupled-Cluster Method

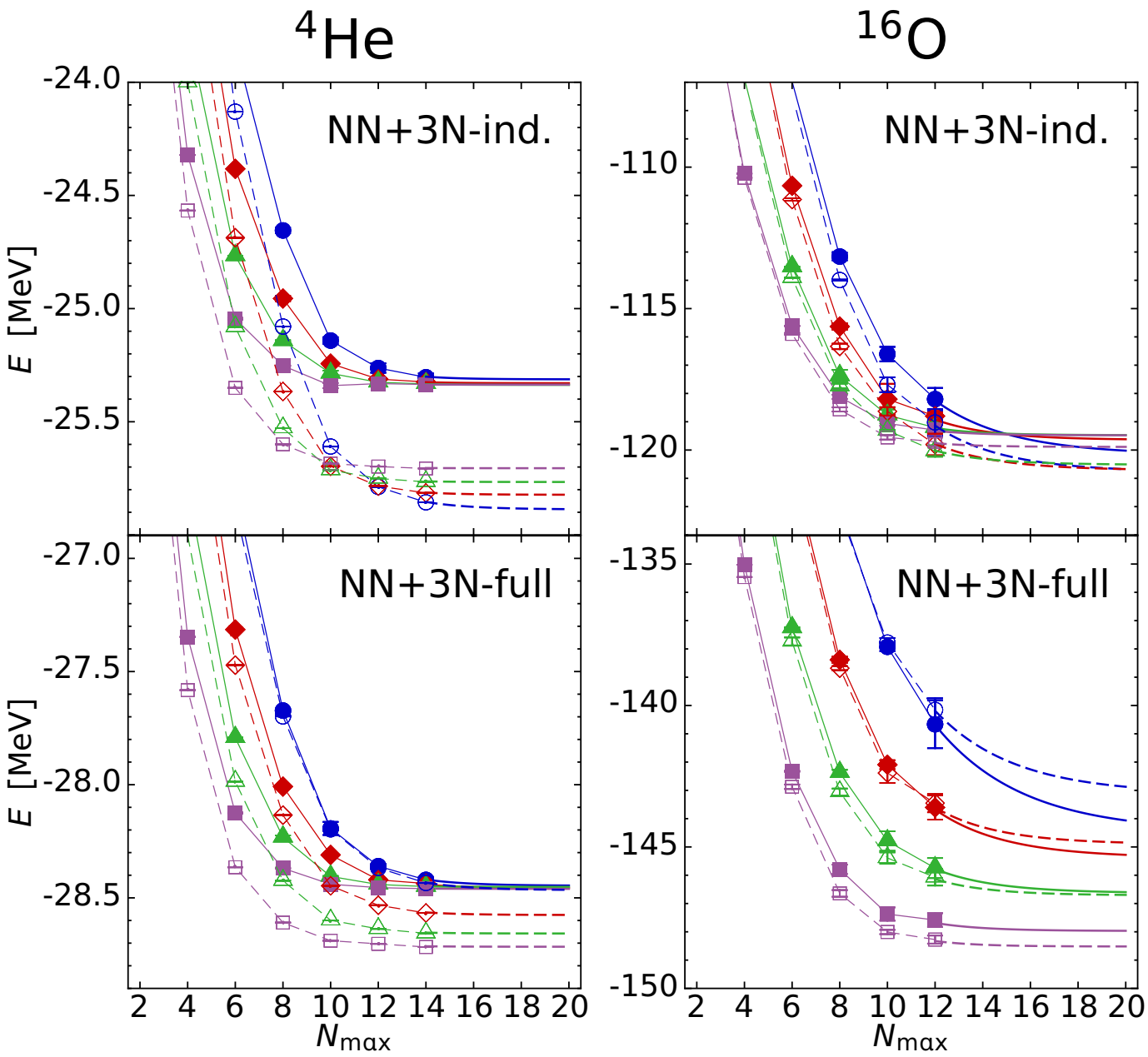
Roth, Binder, Vobig et al. — arXiv: 1112.0287 (2011)

Heavy Nuclei with 3N Interactions

‘ab initio’ calculations for heavier nuclei require alternative many-body tools and approximate treatment of 3N interactions

- **coupled-cluster method** for ground states of closed-shell nuclei
  - exponential ansatz for many-body states using singles and doubles excitations (CCSD)
- **normal-ordering approximation** of the 3N interaction truncated at the two-body level
  - summation over reference state converts part of 3N interaction to zero-, one- and two-body terms
- both approximations are controlled and systematically improvable

Benchmark of Normal-Ordered 3N



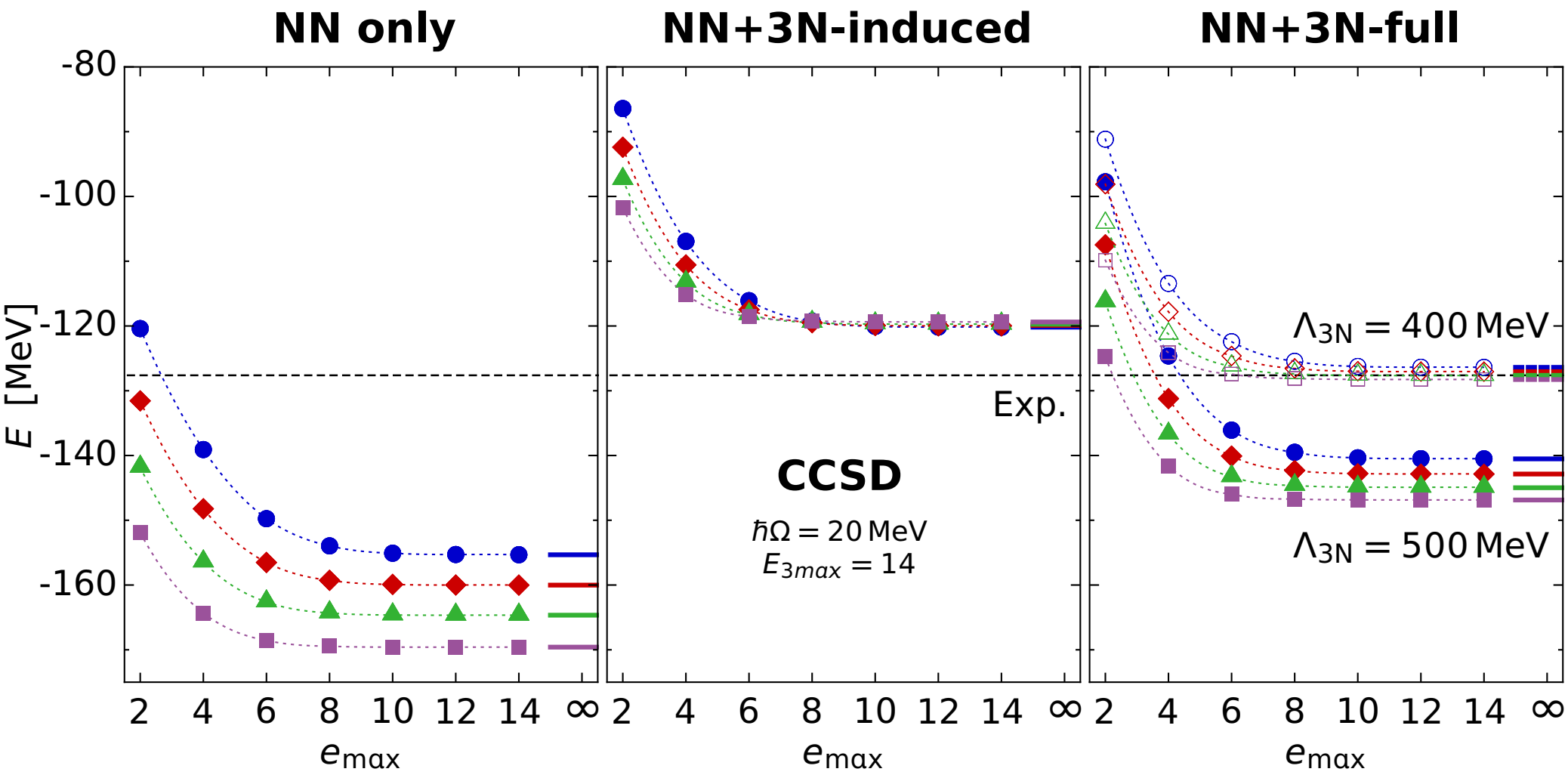
- compare IT-NCSM results with full 3N to normal-ord. 3N truncated at the 2B level
- typical deviations up to 2% for ^{4}He and 1% for ^{16}O

full / NO2B

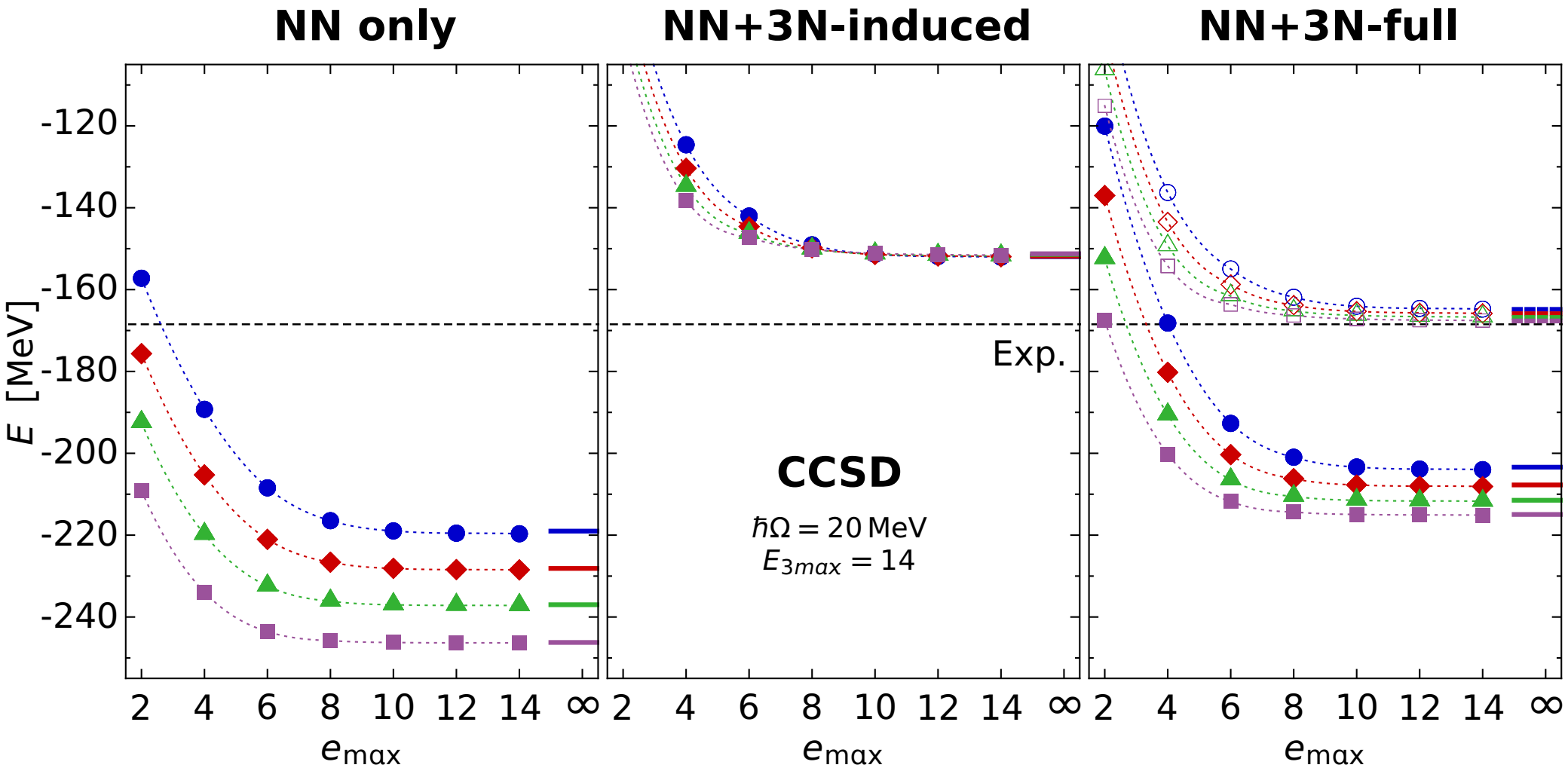
● / ○	$\alpha = 0.04\,\mathrm{fm}^4$
◆ / ◇	$\alpha = 0.05\,\mathrm{fm}^4$
▲ / △	$\alpha = 0.0625\,\mathrm{fm}^4$
■ / □	$\alpha = 0.08\,\mathrm{fm}^4$

$\hbar\Omega = 20\,\mathrm{MeV}$

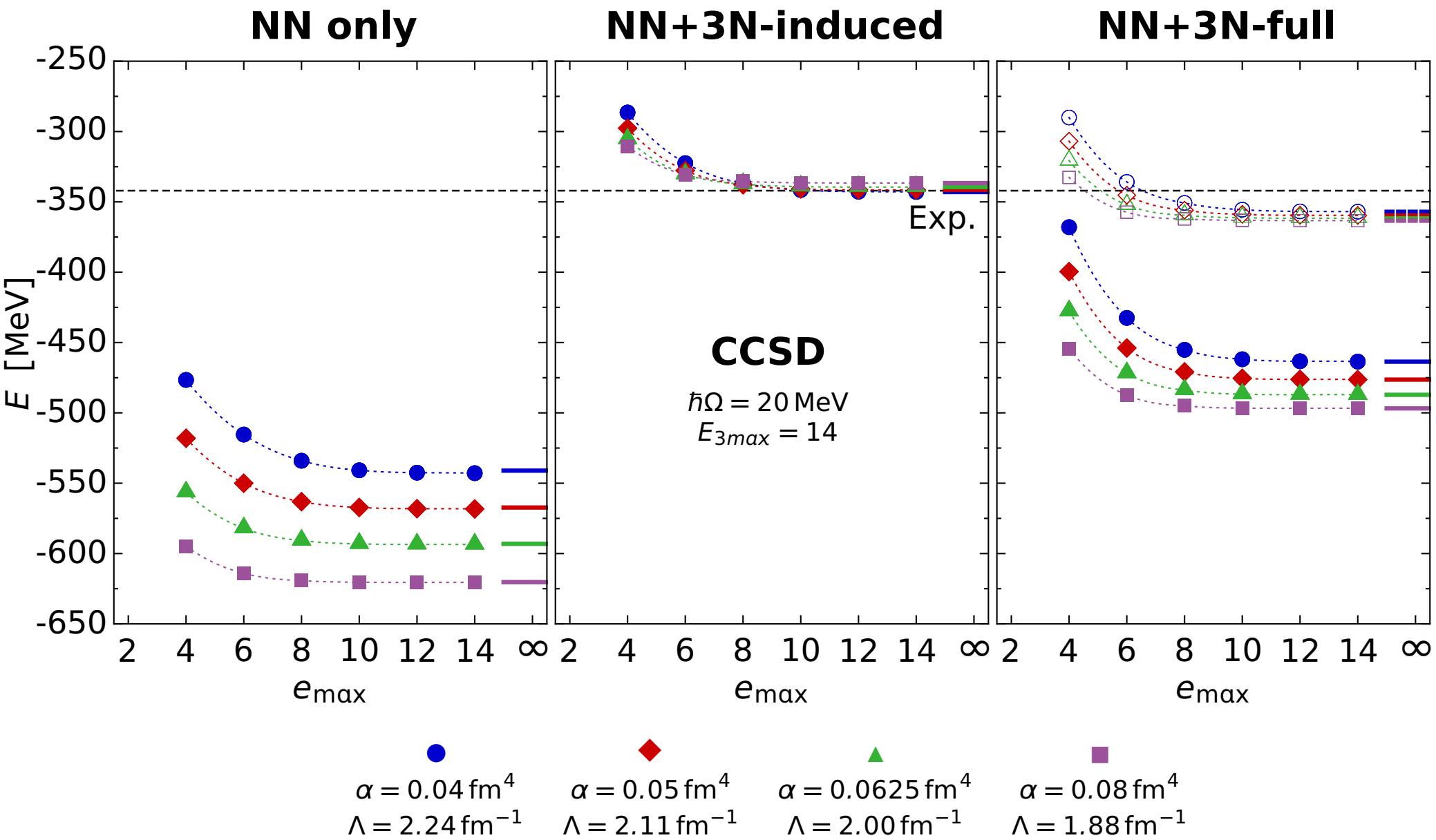
^{16}O: Coupled-Cluster with 3N$_{NO2B}$



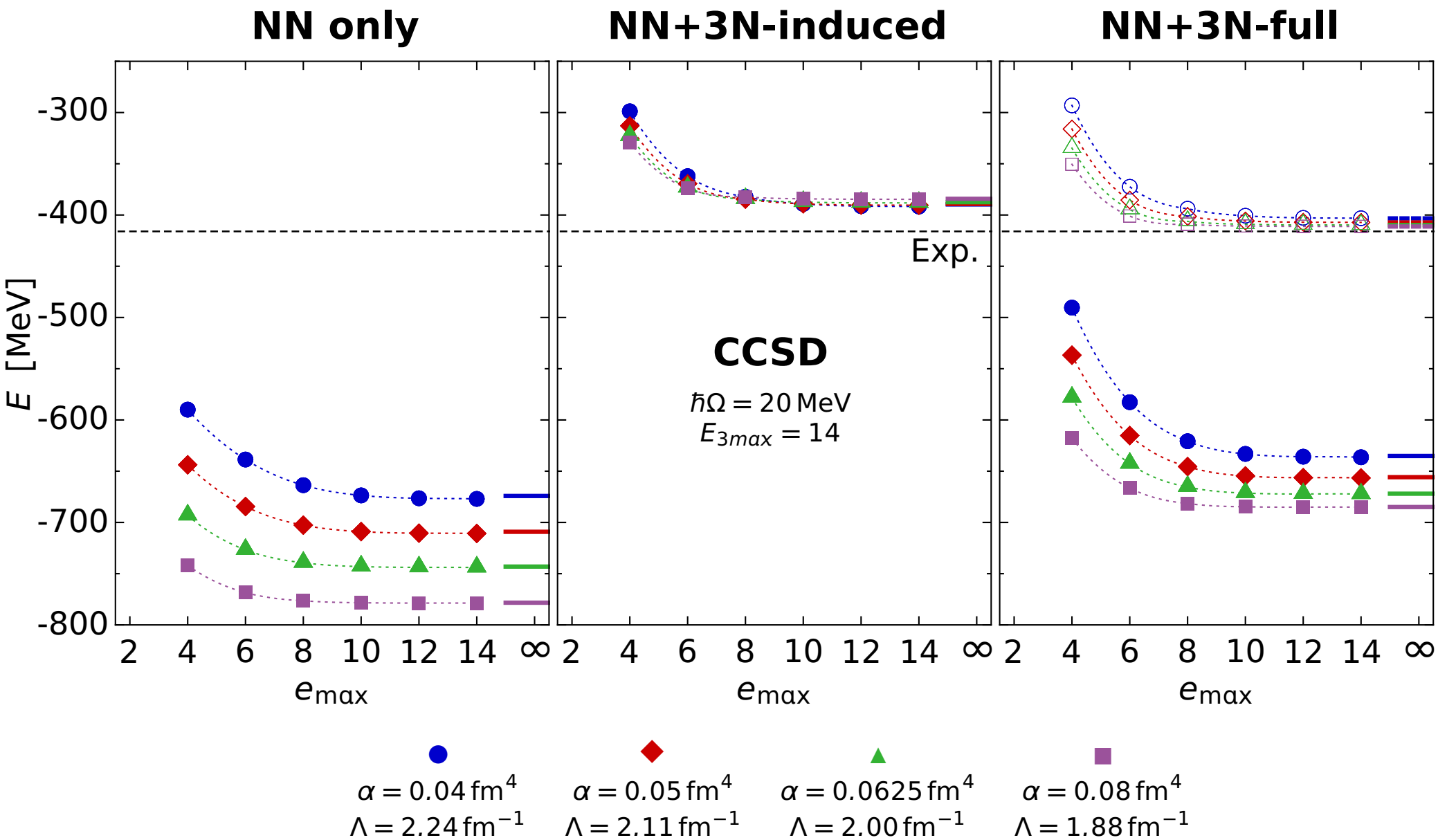
^{24}O: Coupled-Cluster with 3N$_{NO2B}$



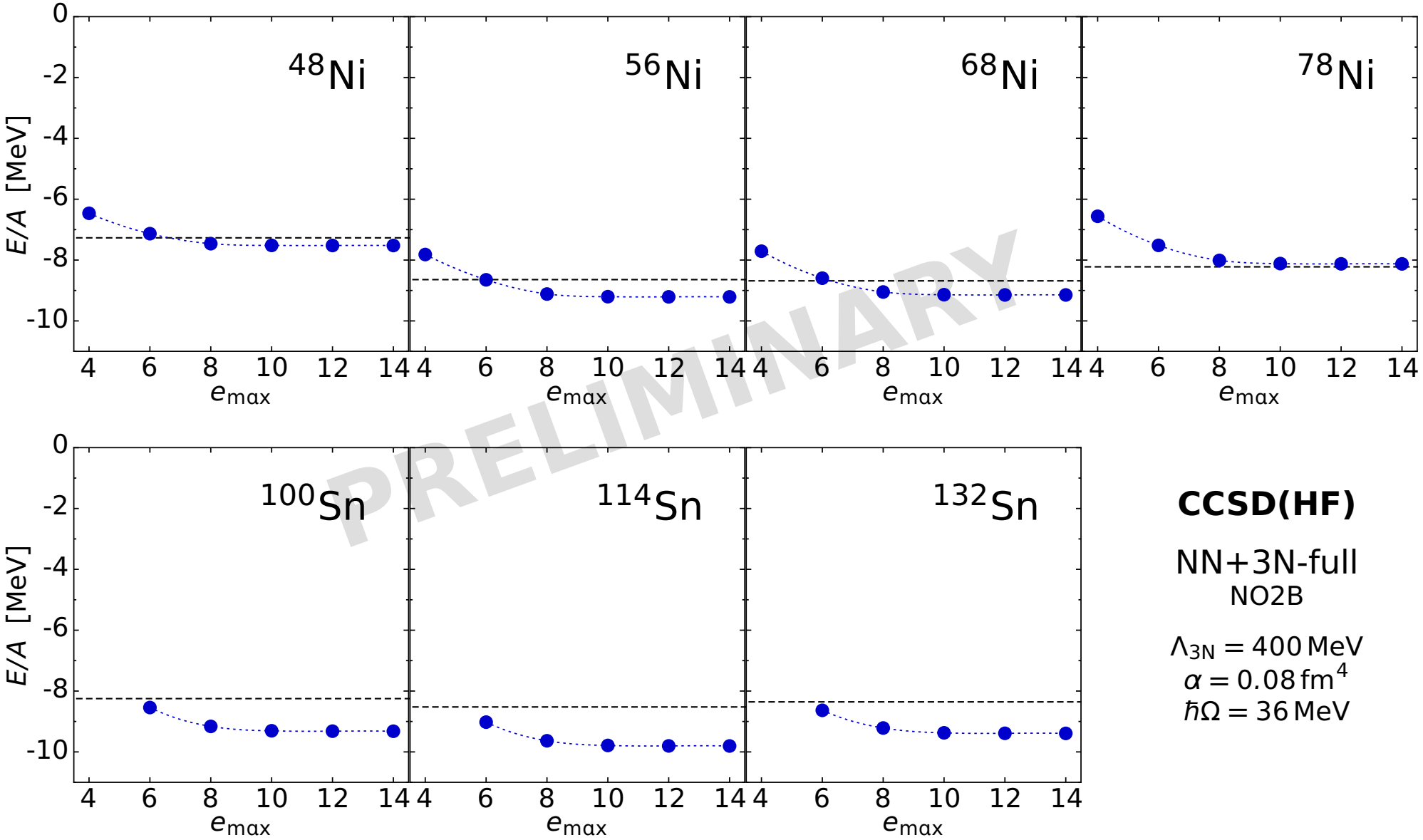
^{40}Ca: Coupled-Cluster with $3N_{NO2B}$



^{48}Ca: Coupled-Cluster with 3N$_{NO2B}$



Outlook: Chiral 3N for Heavy Nuclei



CCSD(HF)

NN+3N-full
NO2B

$\Lambda_{3N} = 400\,\mathrm{MeV}$
$\alpha = 0.08\,\mathrm{fm}^4$
$\hbar\Omega = 36\,\mathrm{MeV}$

Conclusions

Conclusions

- new era of **ab-initio nuclear structure and reaction theory** connected to QCD via chiral EFT
  - chiral EFT as universal starting point... some issues remain
- consistent **inclusion of 3N interactions** in similarity transformations & many-body calculations
  - breakthrough in computation & handling of 3N matrix elements
- **innovations in many-body theory**: extended reach of exact methods & improved control over approximations
  - versatile toolbox for different observables & mass ranges
- many **exciting applications** ahead...

Epilogue

- **thanks to my group & my collaborators**

  - **S. Binder**, **A. Calci**, B. Erler, E. Gebrerufael, A. Günther, H. Krutsch, **J. Langhammer**, S. Reinhardt, C. Stumpf, R. Trippel, K. Vobig, R. Wirth
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  - S. Quaglioni
    LLNL Livermore, USA
  - P. Piecuch
    Michigan State University, USA
  - H. Hergert, K. Hebeler
    Ohio State University, USA
  - P. Papakonstantinou
    IPN Orsay, F
  - C. Forssén
    Chalmers University, Sweden
  - H. Feldmeier, T. Neff
    GSI Helmholtzzentrum

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LOEWE – Landes-Offensive zur Entwicklung Wissenschaftlich-ökonomischer Exzellenz

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HOPPER — NERSC

COMPUTING TIME