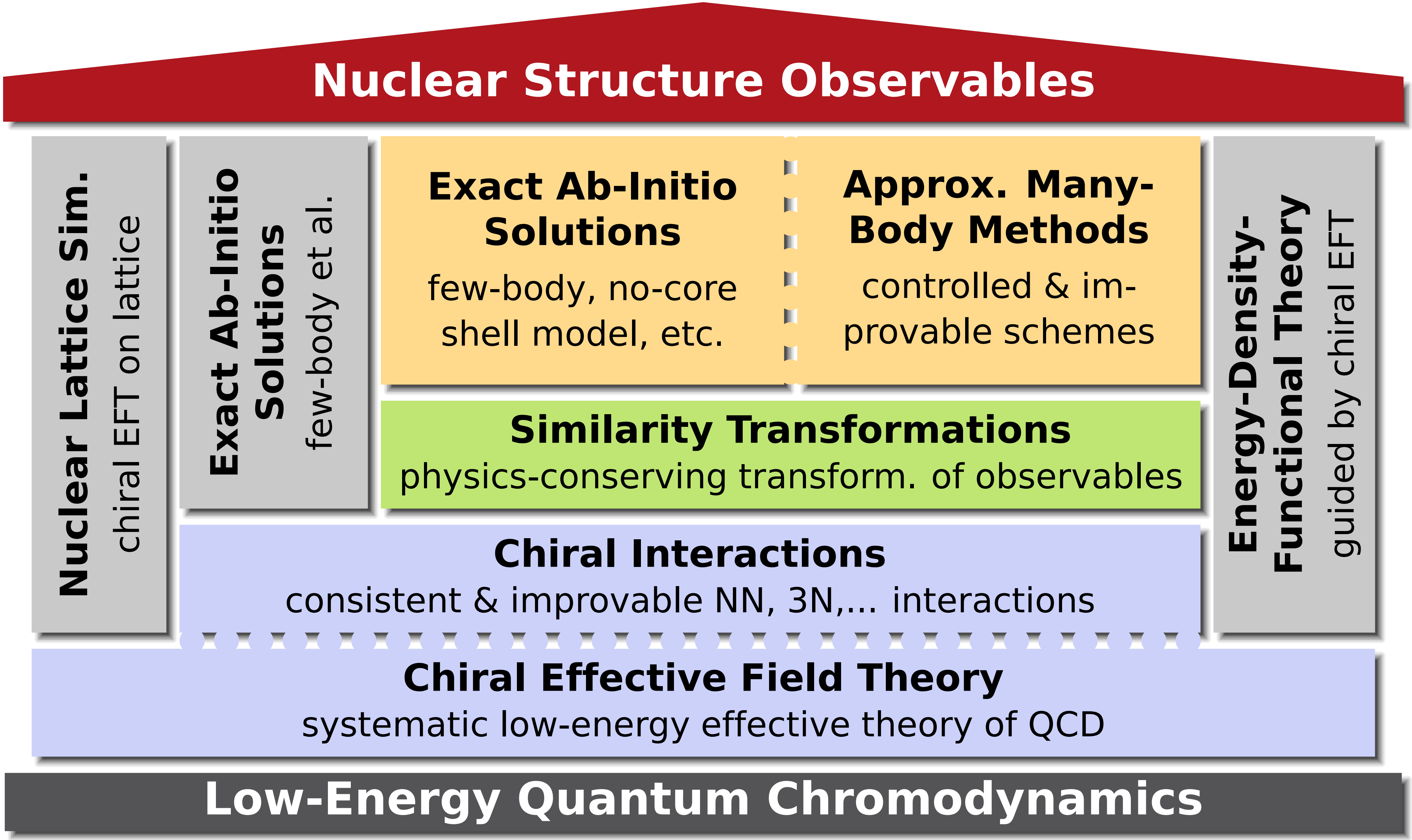
From Chiral EFT Interactions to Nuclear Structure and Reactions

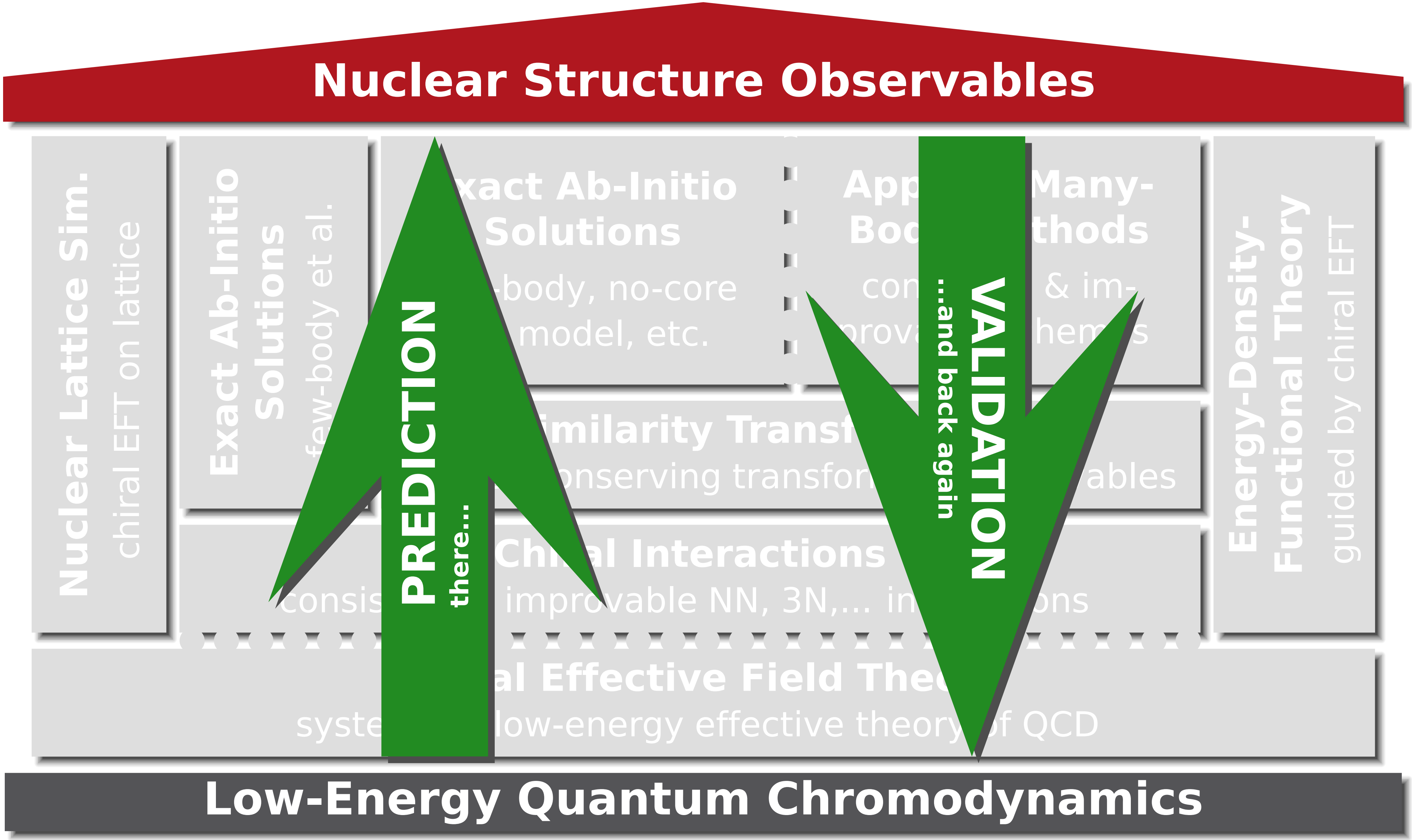
Robert Roth

TECHNISCHE UNIVERSITÄT DARMSTADT

Ab Initio Nuclear Structure



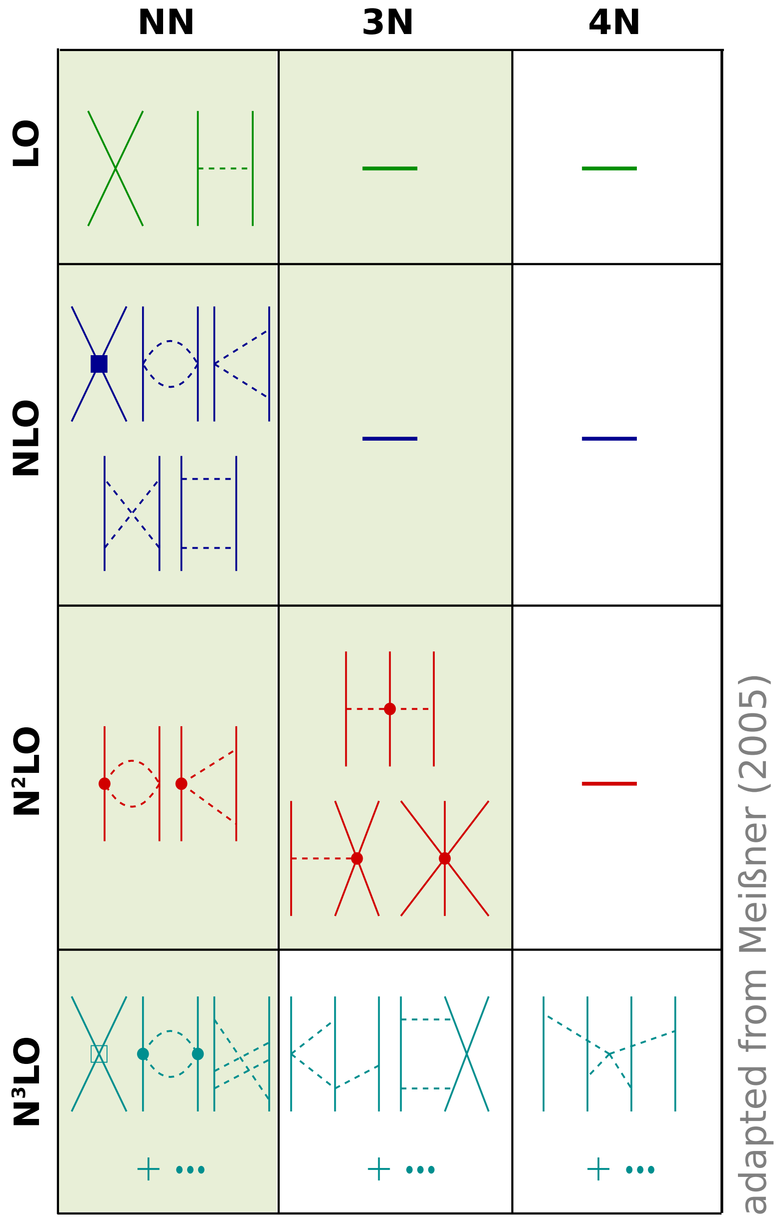
Ab Initio Nuclear Structure



Nuclear Interactions from Chiral EFT

Nuclear Interactions from Chiral EFT

- **chiral EFT perspective**: cf. previous talk by Hermann Krebs
- ab initio nuclear structure theory is the **users community** for chiral EFT Hamiltonians
- present **'standard' Hamiltonian**:
  - NN at N^{3}LO:
    Entem & Machleidt, 500 MeV cutoff
  - 3N at N^{2}LO:
    Navrátil, A=3 fit, 500 MeV cutoff
- ready for **next generation**
  - consistent chiral NN+3N Hamiltonians at N^{3}LO
  - Δ-full chiral EFT, YN interaction,...



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 Hamil

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

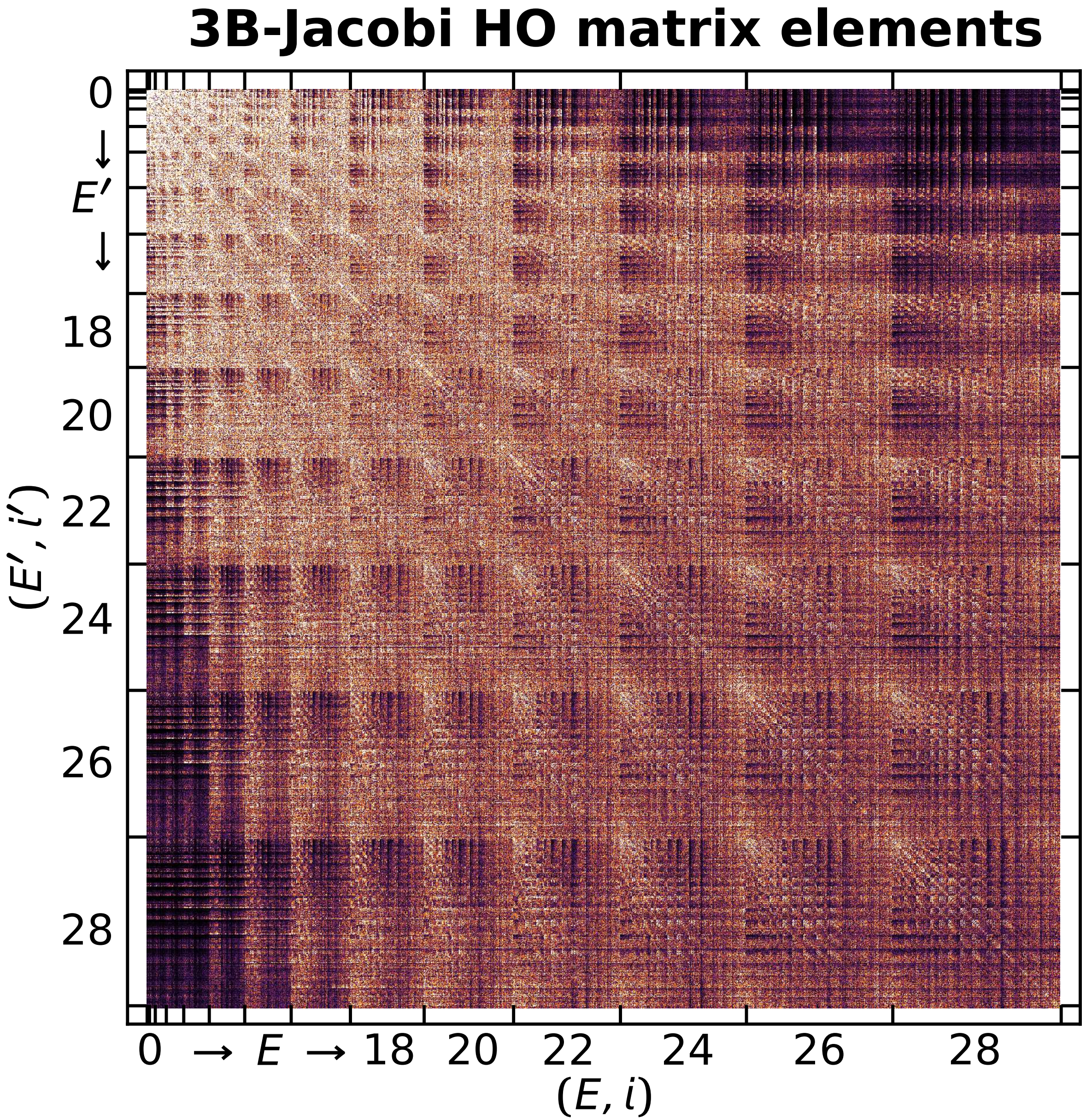
- **evolution equations** for $\widetilde{H}_\alpha$ and U

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

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

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

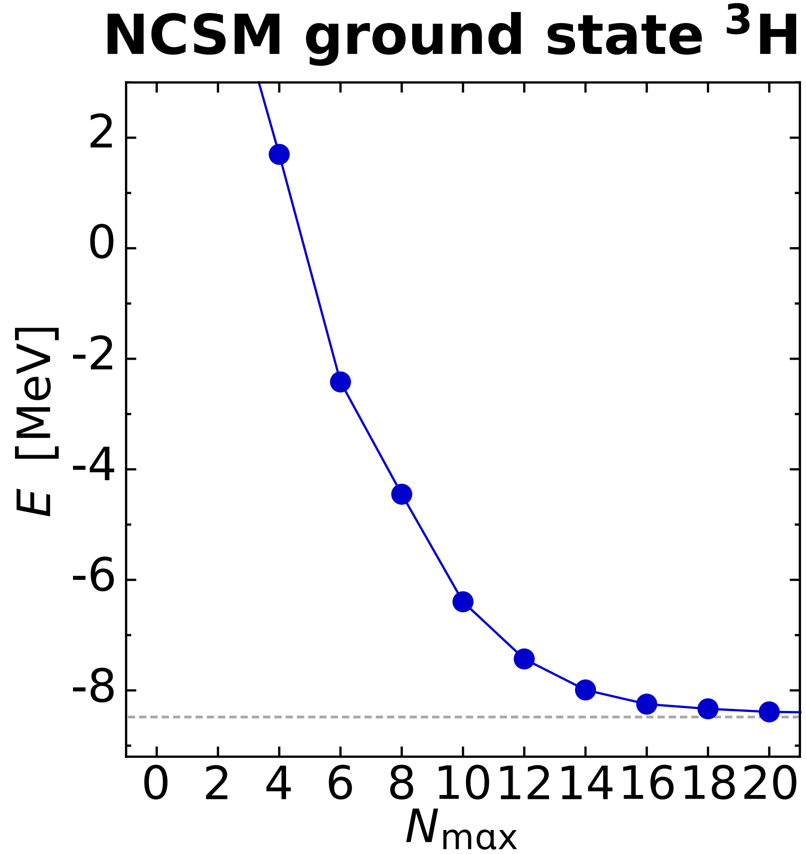
SRG Evolution in Three-Body Space



$$\alpha = 0.000\,\mathrm{fm}^4$$

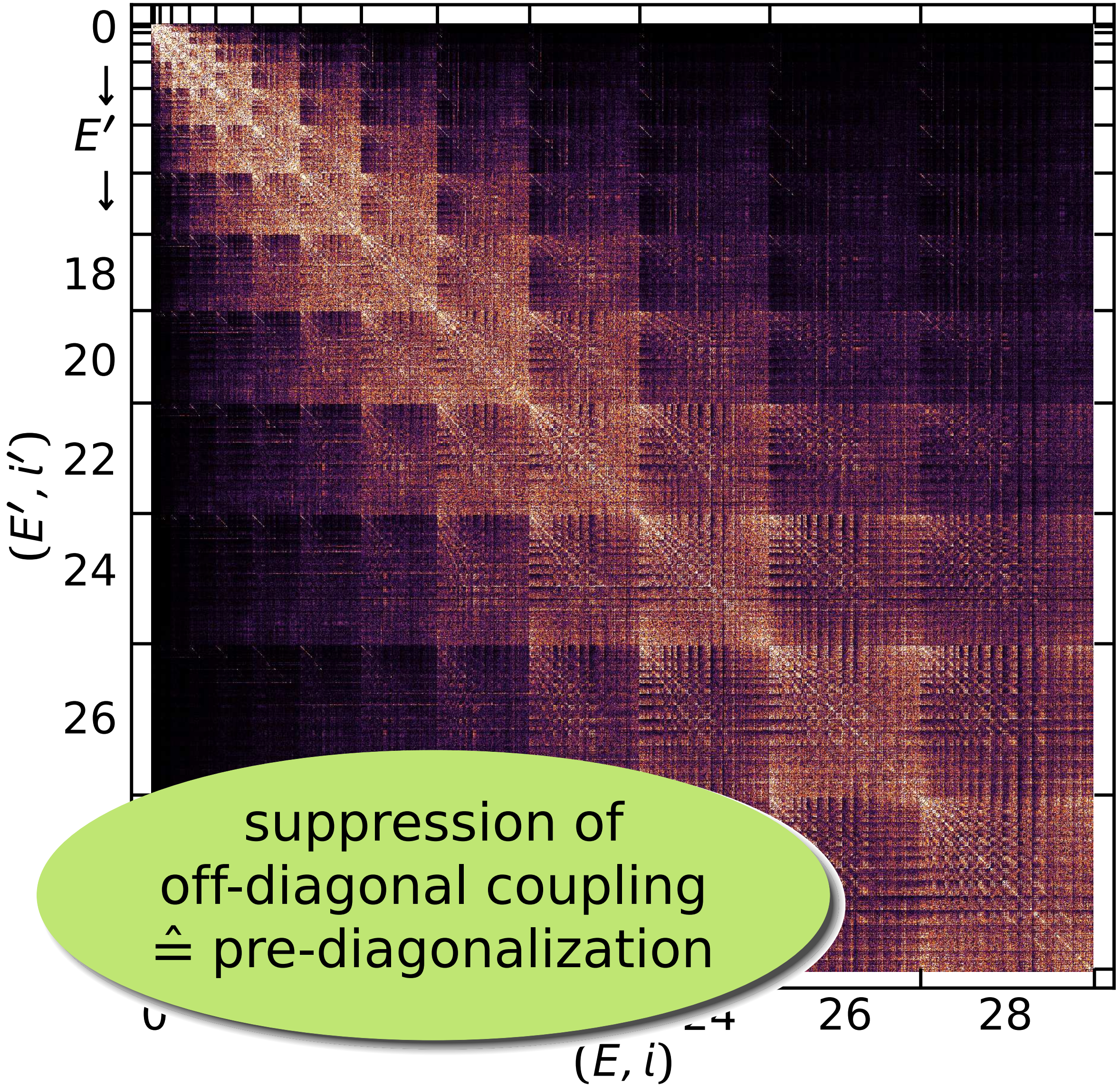
$$\Lambda = \infty\,\mathrm{fm}^{-1}$$

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



SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements



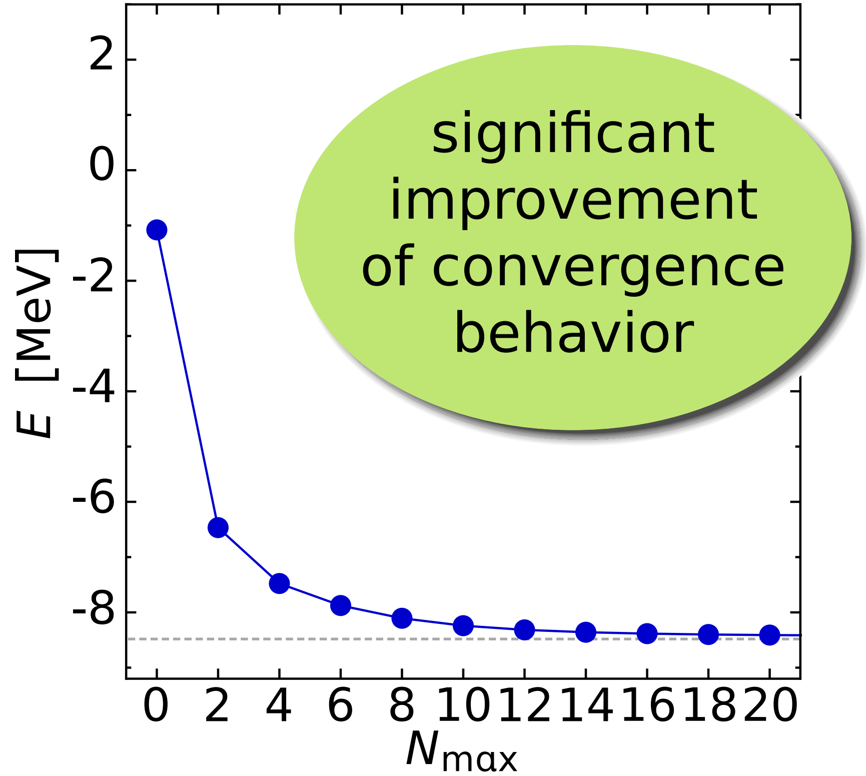
suppression of
off-diagonal coupling
≙ pre-diagonalization

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

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

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

NCSM ground state ^{3}H



significant
improvement
of convergence
behavior

Calculations in *A*-Body Space

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

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

- 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… keep two- and induced three-body terms
- **NN+3N-full**: start with NN+3… and all three-body terms

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

Importance Truncated No-Core Shell Model

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

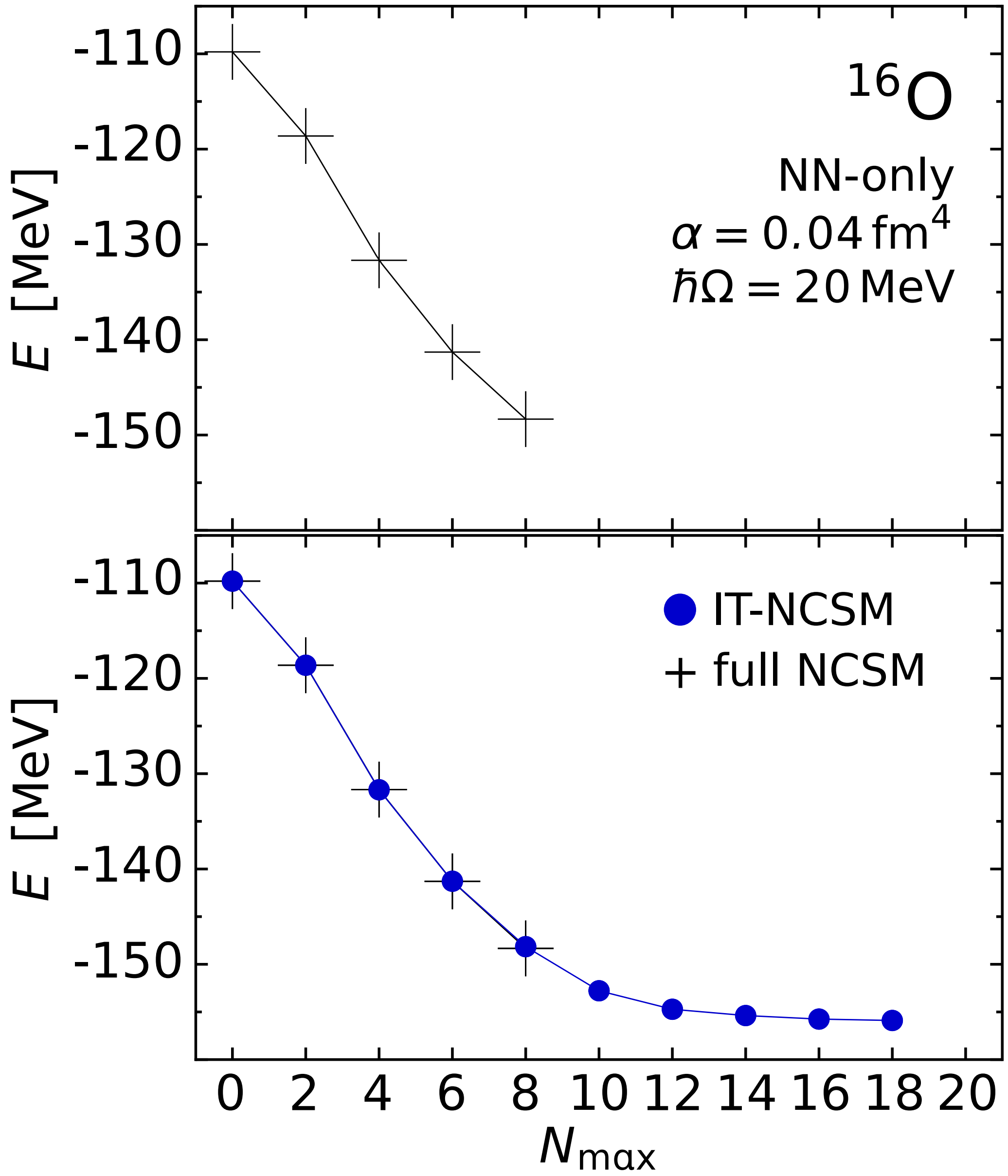
- construct matrix representation of Hamiltonian using a **basis of HO Slater determinants** truncated w.r.t. HO excitation energy $N_{\max}\hbar\Omega$
- solve **large-scale eigenvalue problem** for a few extremal eigenvalues
- **all relevant observables** can be computed from the eigenstates
- range 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 $E_{3\max} = 16$

Importance Truncated NCSM

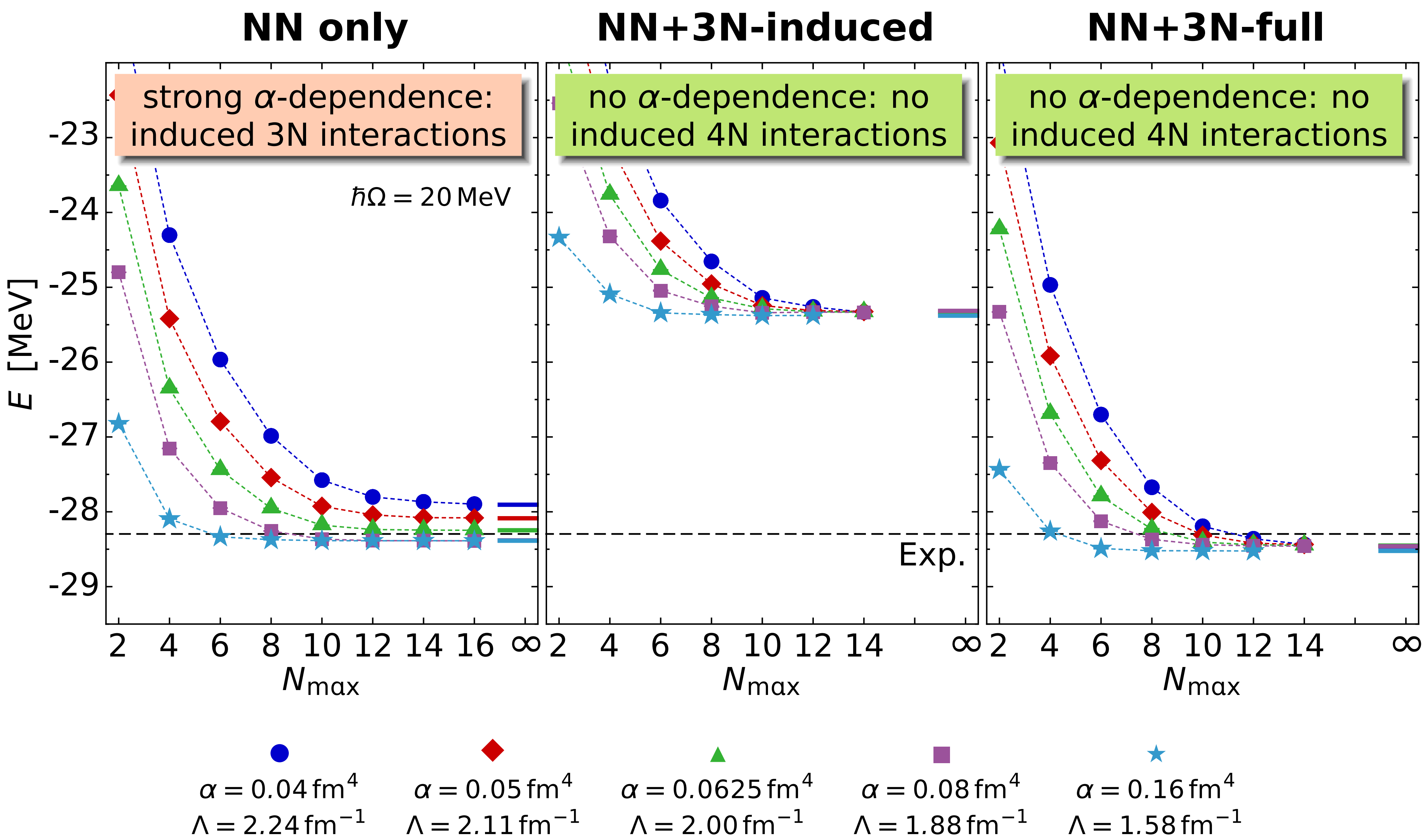
- converged NCSM calculations essentially restricted to lower/mid p-shell
- full $10\hbar\Omega$ calculation for ^{16}O getting very difficult (basis dimension > 10^{10})

Importance Truncation

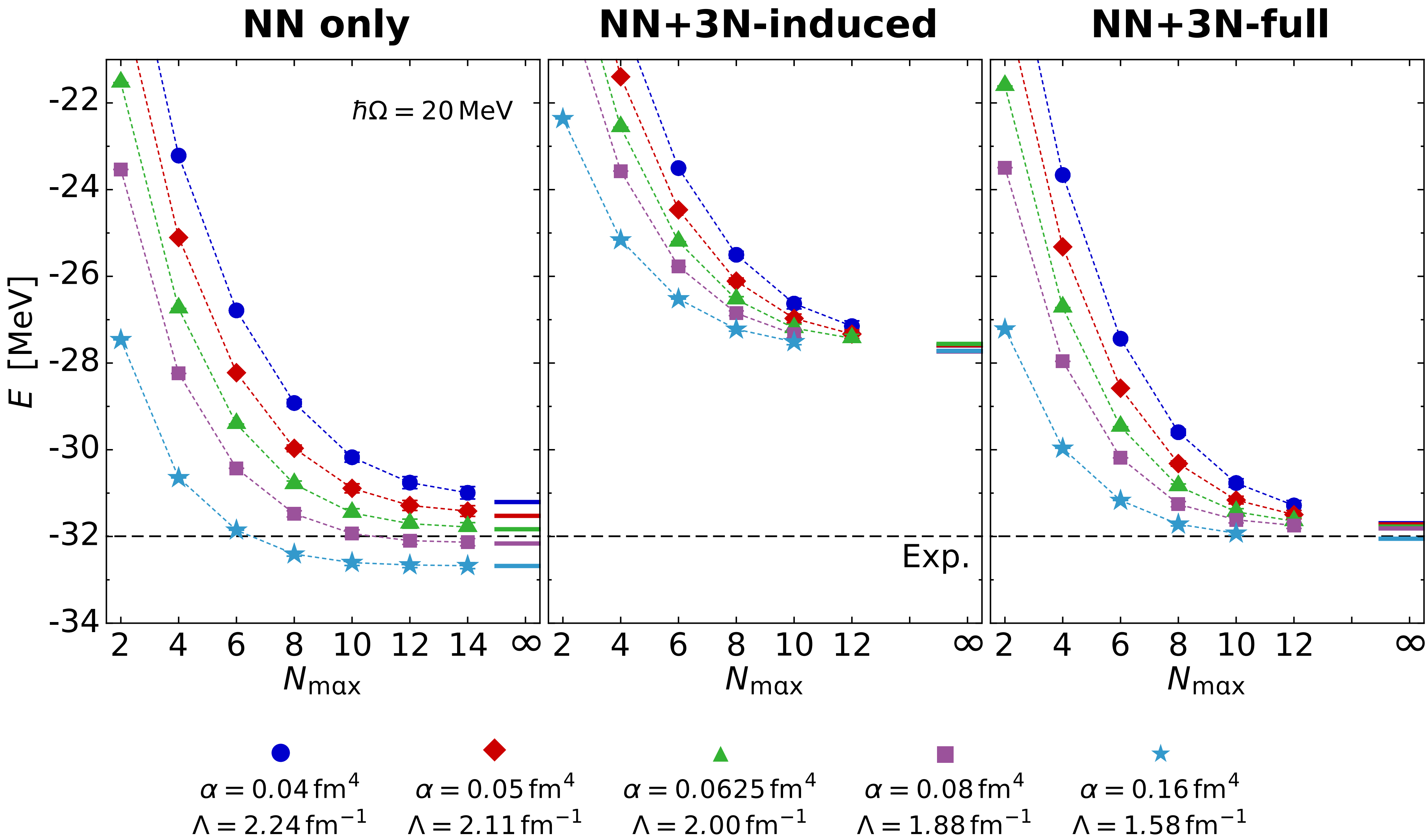
reduce model space to the relevant basis states using an **a priori importance measure** derived from MBPT



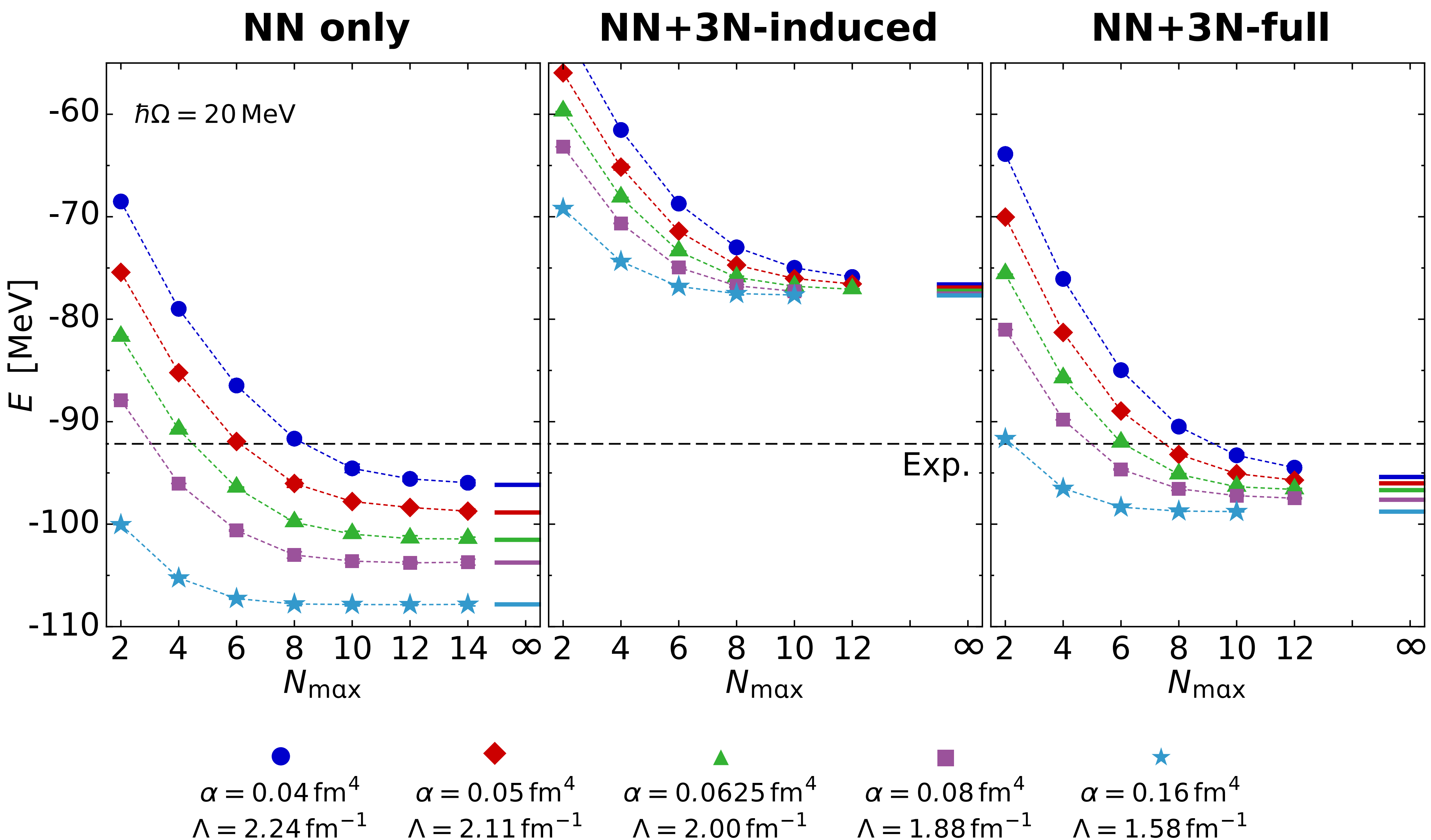
^{4}He: Ground-State Energies



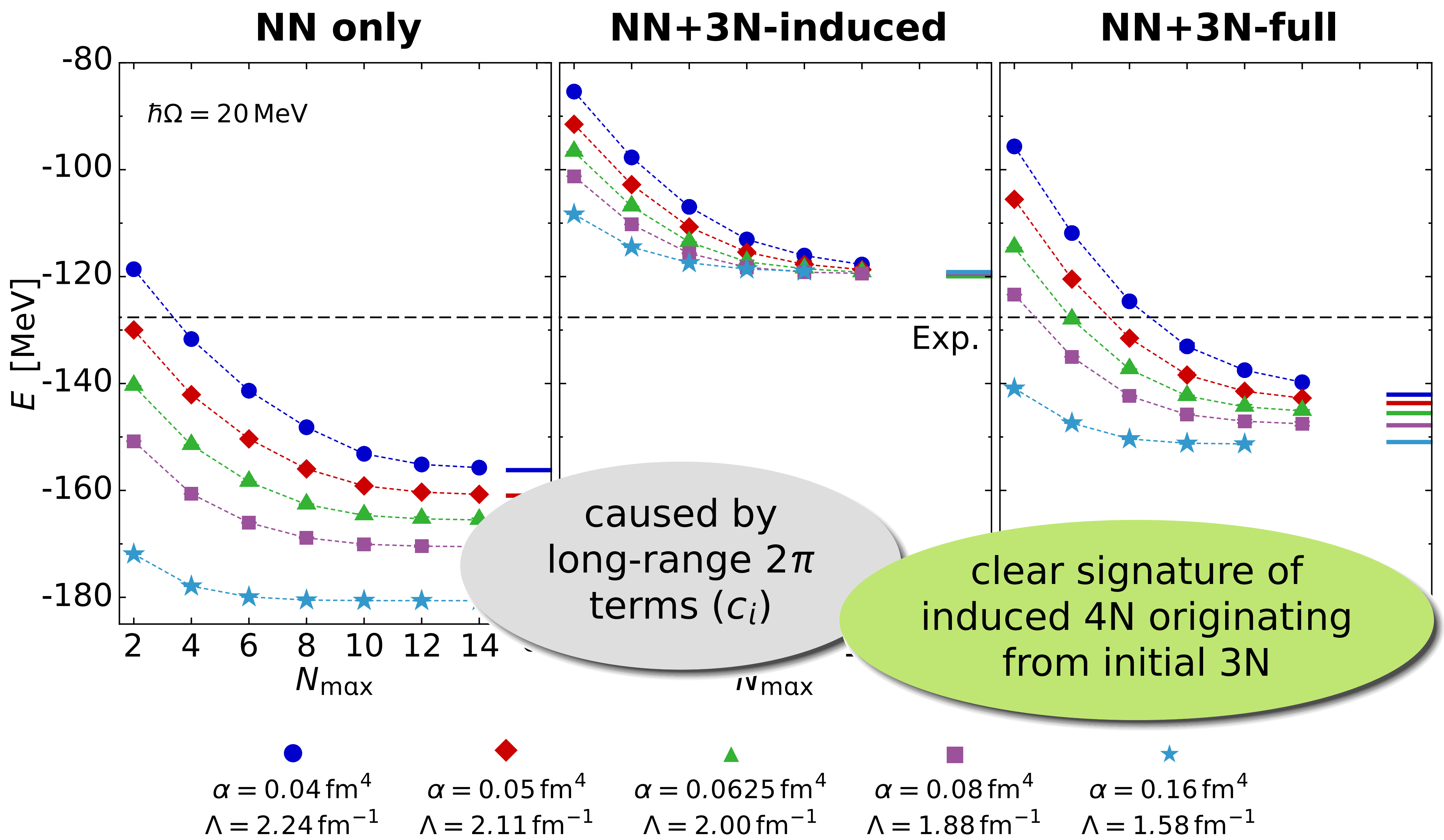
^{6}Li: Ground-State Energies



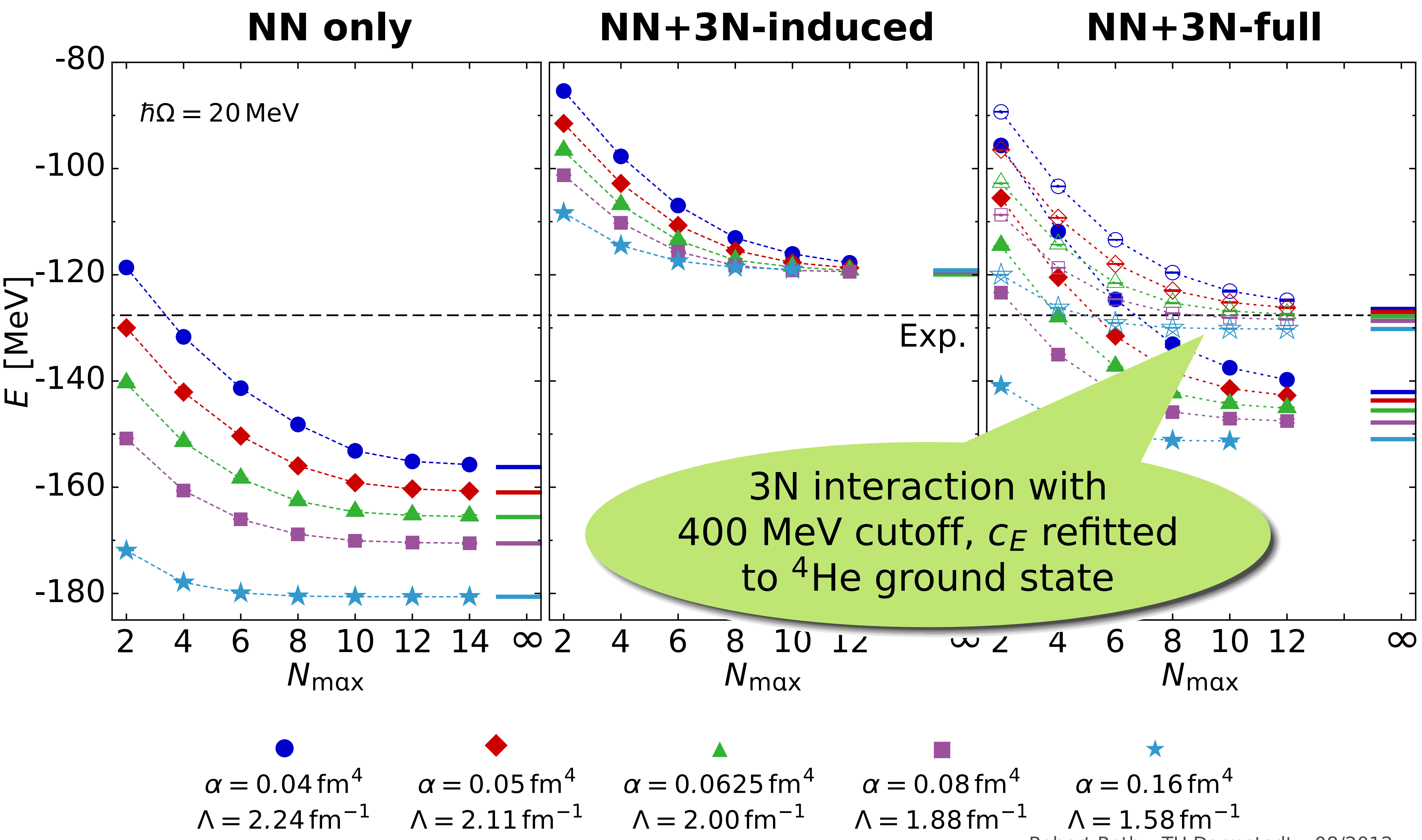
^{12}C: Ground-State Energies



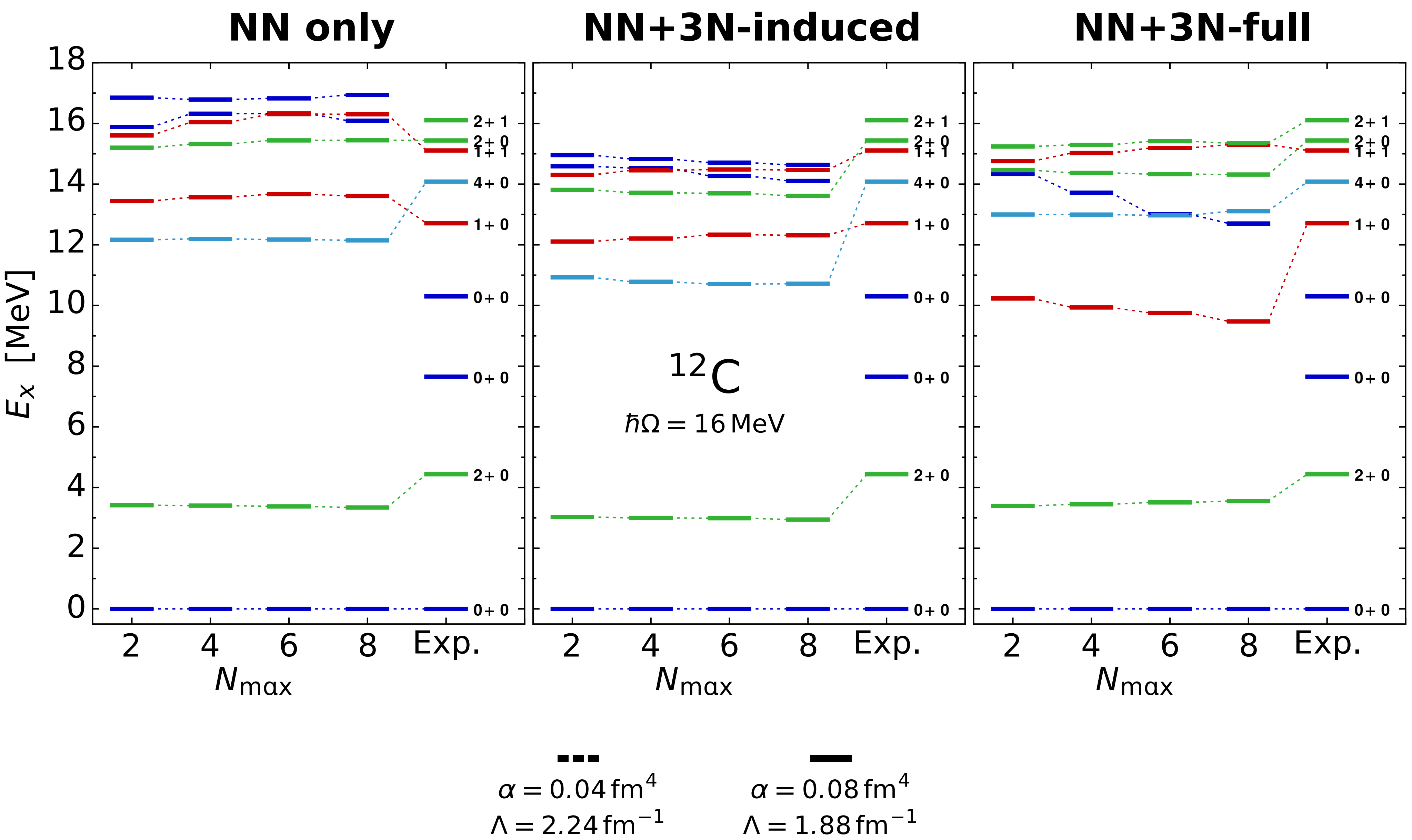
^{16}O: Ground-State Energies



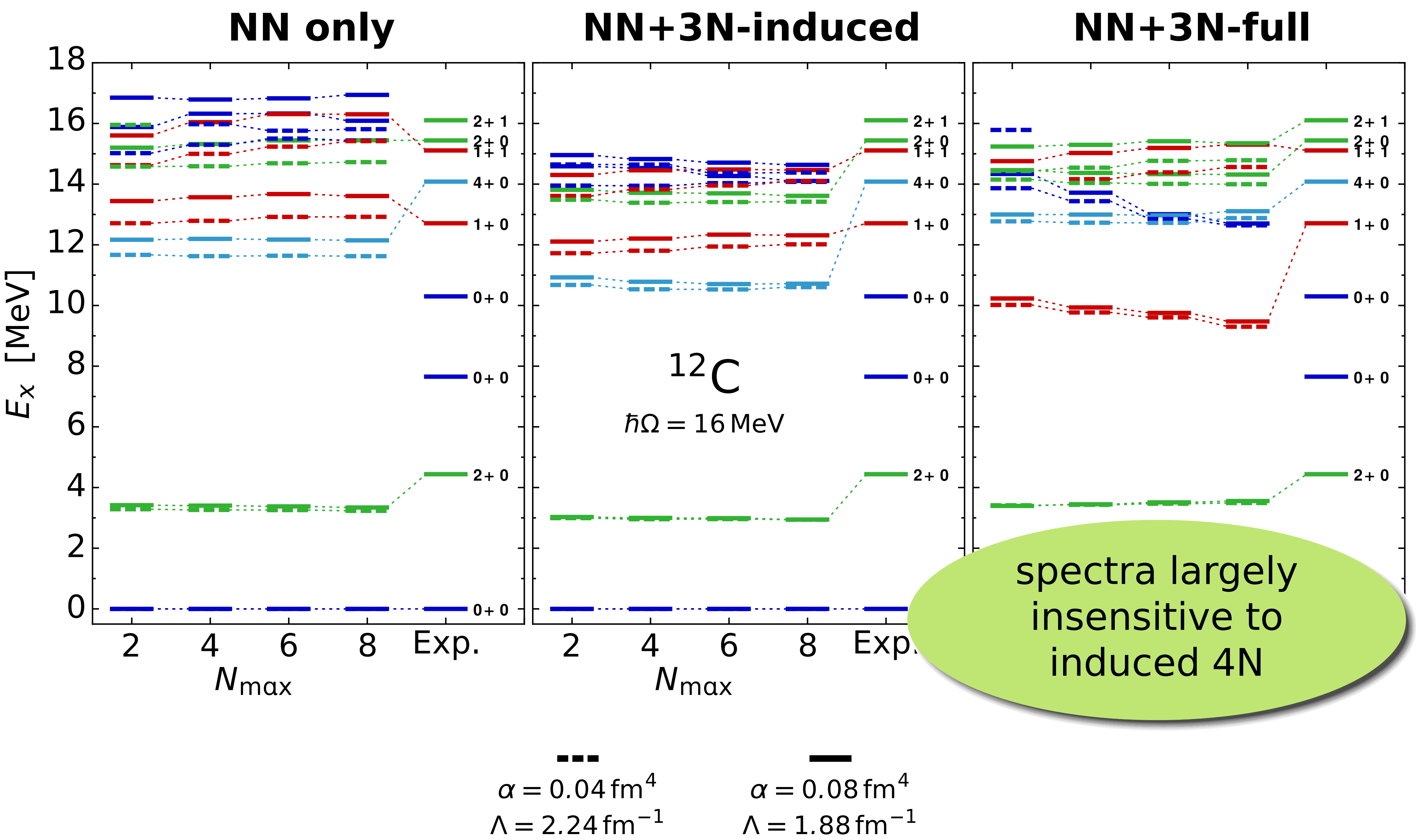
^{16}O: Ground-State Energies



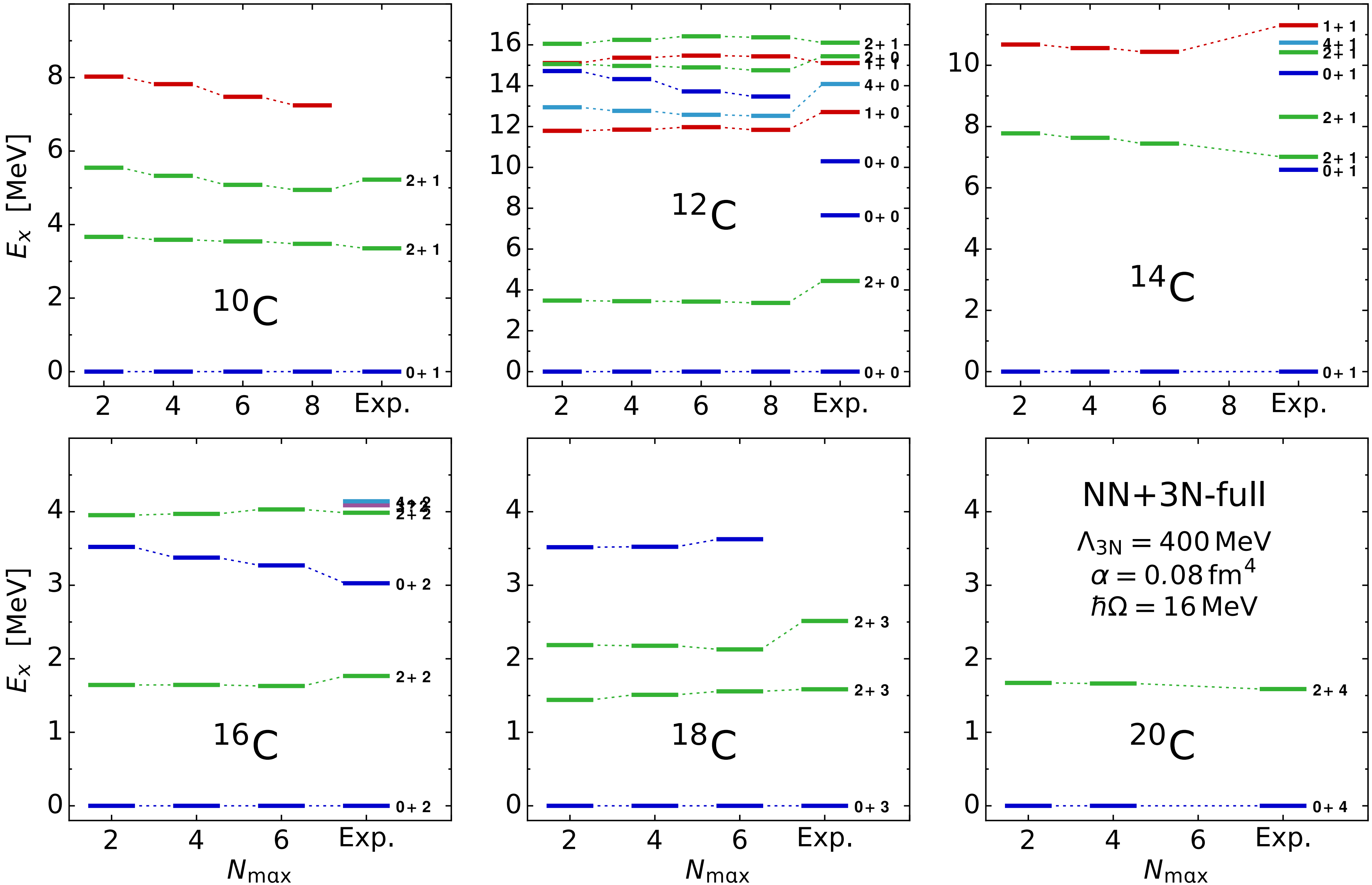
Spectroscopy of ^{12}C



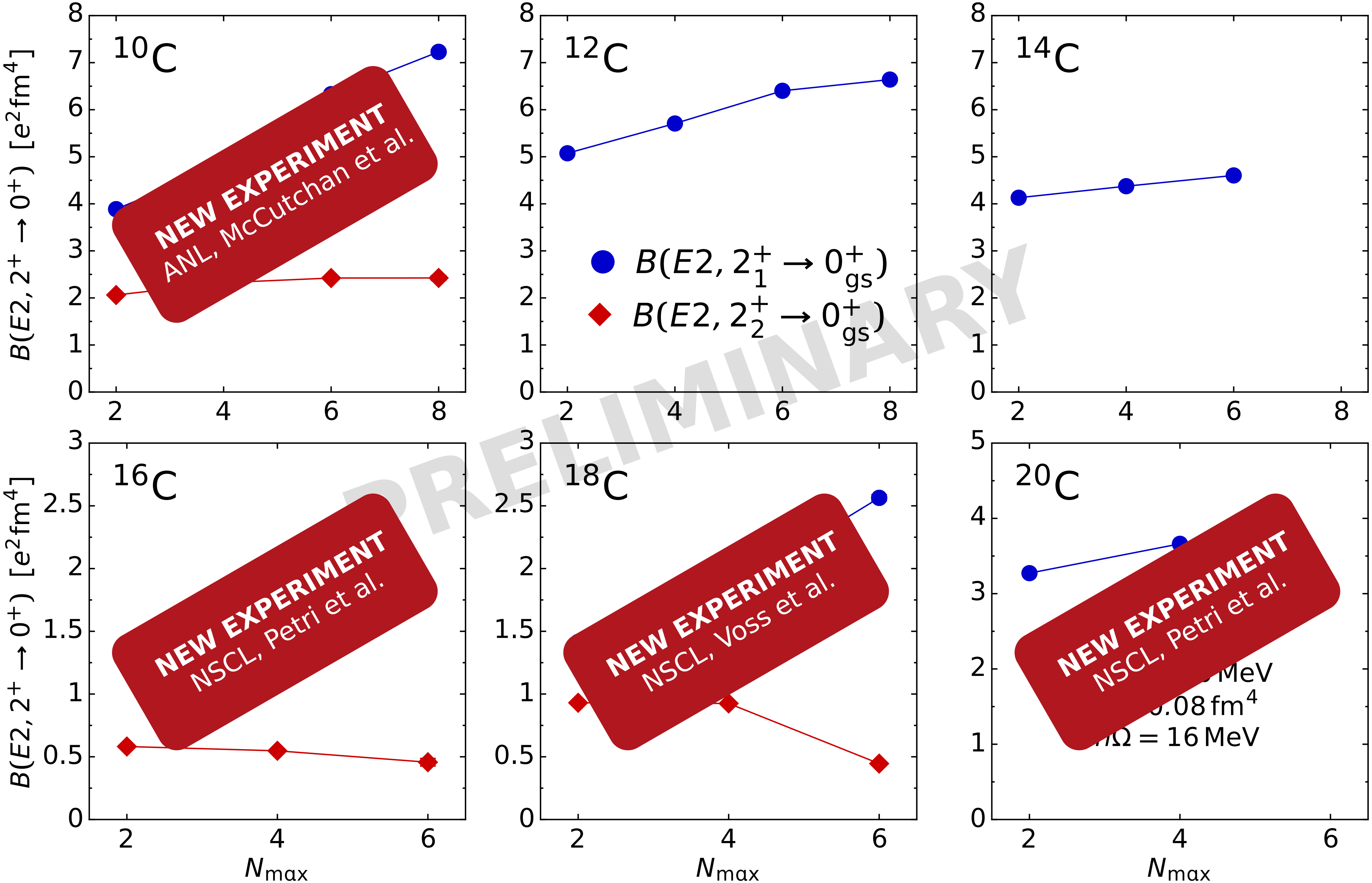
Spectroscopy of ^{12}C



Outlook: Carbon Isotopic Chain



Outlook: Carbon Isotopic Chain



Sensitivity of Nuclear Spectra on Chiral 3N Interactions

Sensitivity on Chiral 3N Interactions

- analyze the sensitivity of spectra on **low-energy constants** (c_i, c_D, c_E) and **cutoff** (Λ) of the chiral 3N interaction at N^{2}LO

- why this is interesting:
  - **impact of N^{3}LO contributions**: some N^{3}LO diagrams can be absorbed into the N^{2}LO structure by shifting the c_i constants

$$\bar{c}_1 = c_1 - \frac{g_A^2 M_\pi}{64\pi F_\pi^2}\,, \quad \bar{c}_3 = c_3 + \frac{g_A^4 M_\pi}{16\pi F_\pi^2}\,, \quad \bar{c}_4 = c_4 - \frac{g_A^4 M_\pi}{16\pi F_\pi^2}$$

  - **uncertainty propagation**: sizable variati... of the c_i from different extractions

$$c_1 = -1.23 \ldots -0.76\,, \quad c_3 = -5.\ldots$$

  - **cutoff dependence**: does t... tion affect nuclear structure obse...

provide **constraints** for the development of chiral Hamiltonians and **quantify theoretical uncertainties**

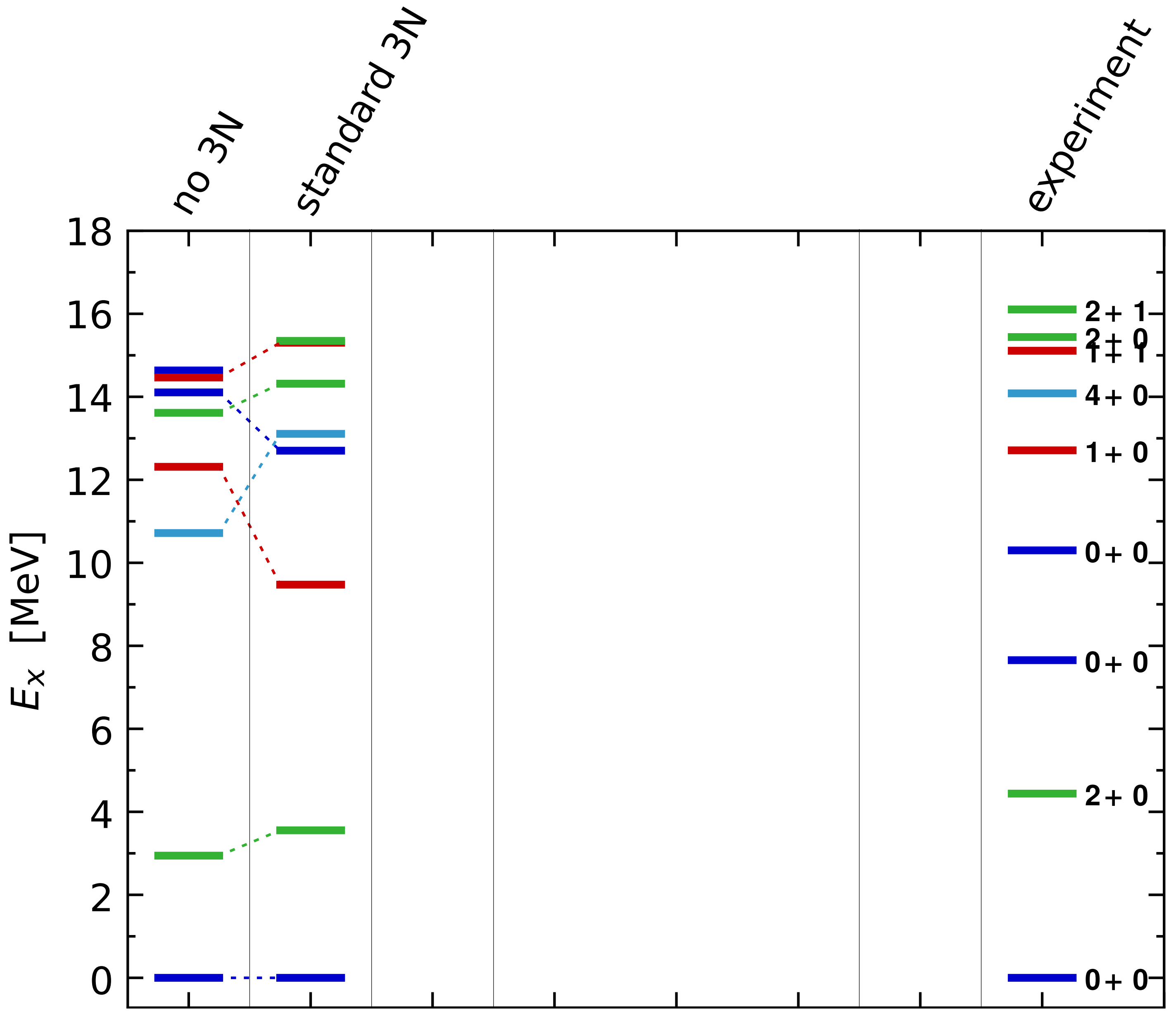
Sensitivity of Spectra on 3N Interactions

- analyze the sensitivity of spectra on **low-energy constants** (c_i, c_D, c_E) and **cutoff** (Λ) of the chiral 3N interaction at N^2LO

	c_1 [GeV^{-1}]	c_3 [GeV^{-1}]	c_4 [GeV^{-1}]	c_D	c_E
standard 3N	−0.81	−3.2	+5.4	−0.2	−0.205
c_i shifted	−0.94	−2.3	+4.5	−0.2	−0.085
c_1 shifted	−0.94	−3.2	+5.4	−0.2	−0.247
c_3 shifted	−0.81	−2.3	+5.4	−0.2	−0.200
c_4 shifted	−0.81	−3.2	+4.5	−0.2	−0.130
$c_D = -1$	−0.81	−3.2	+5.4	−1.0	−0.386
$c_D = +1$	−0.81	−3.2	+5.4	+1.0	−0.038
$\Lambda = 400$ MeV	−0.81	−3.2	+5.4	−0.2	+0.098
$\Lambda = 450$ MeV	−0.81	−3.2	+5.4	−0.2	−0.016

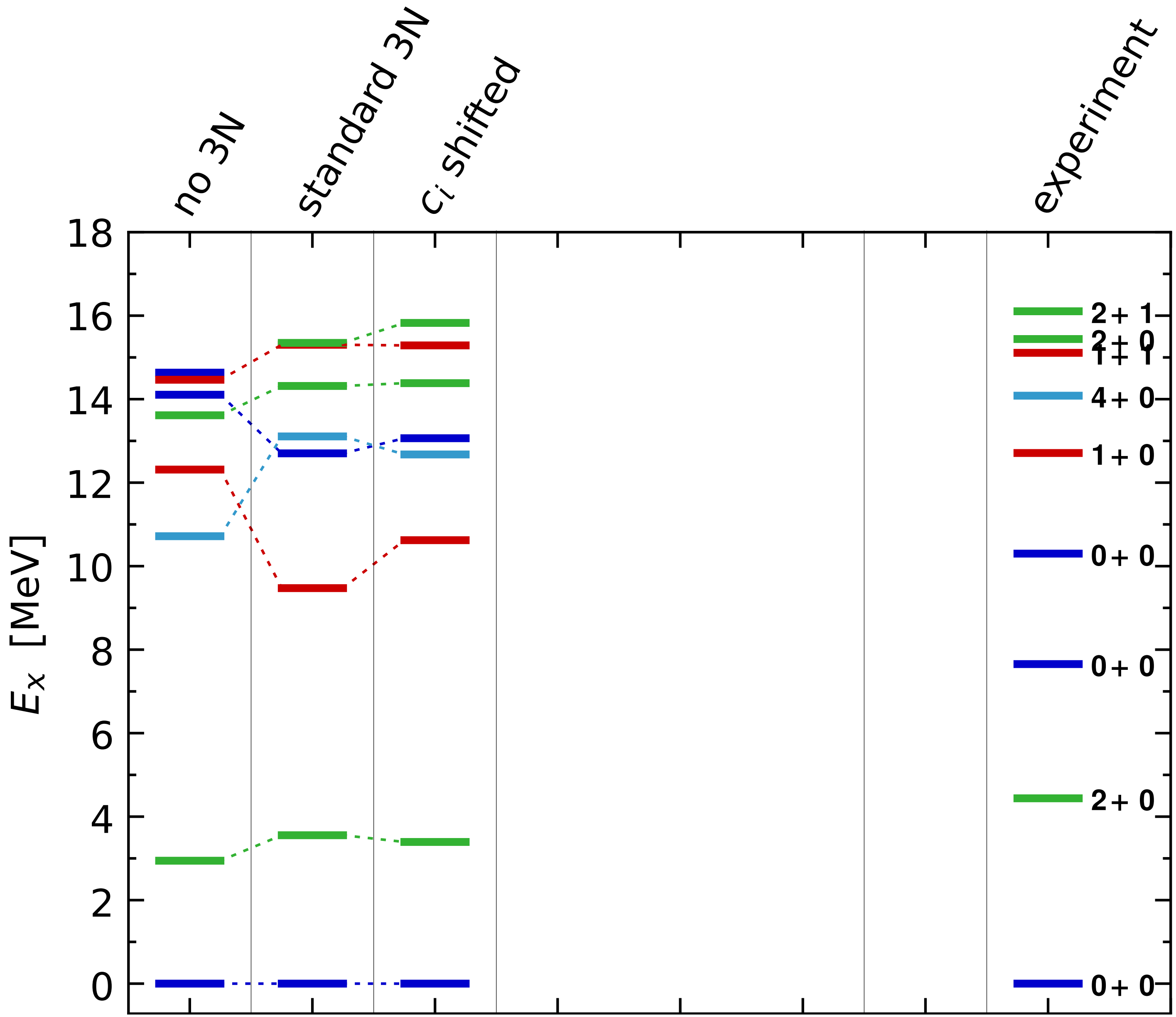
- refit c_E parameter to reproduce ^{4}He ground-state energy

^{12}C : Sensitivity on c_i



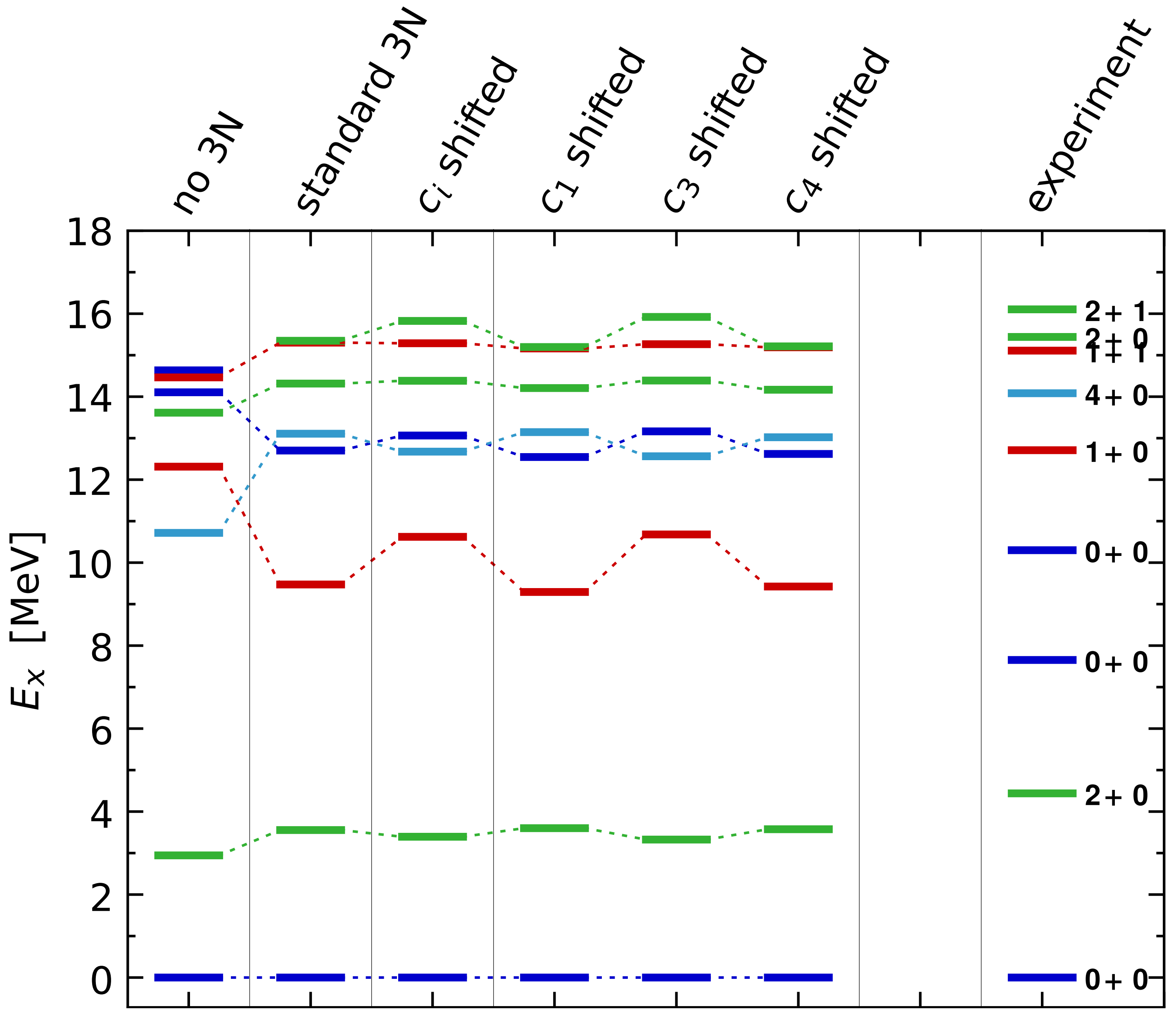
$\hbar\Omega = 16$ MeV
$N_{max} = 8$
$\alpha = 0.08\,fm^4$

^{12}C : Sensitivity on c_i



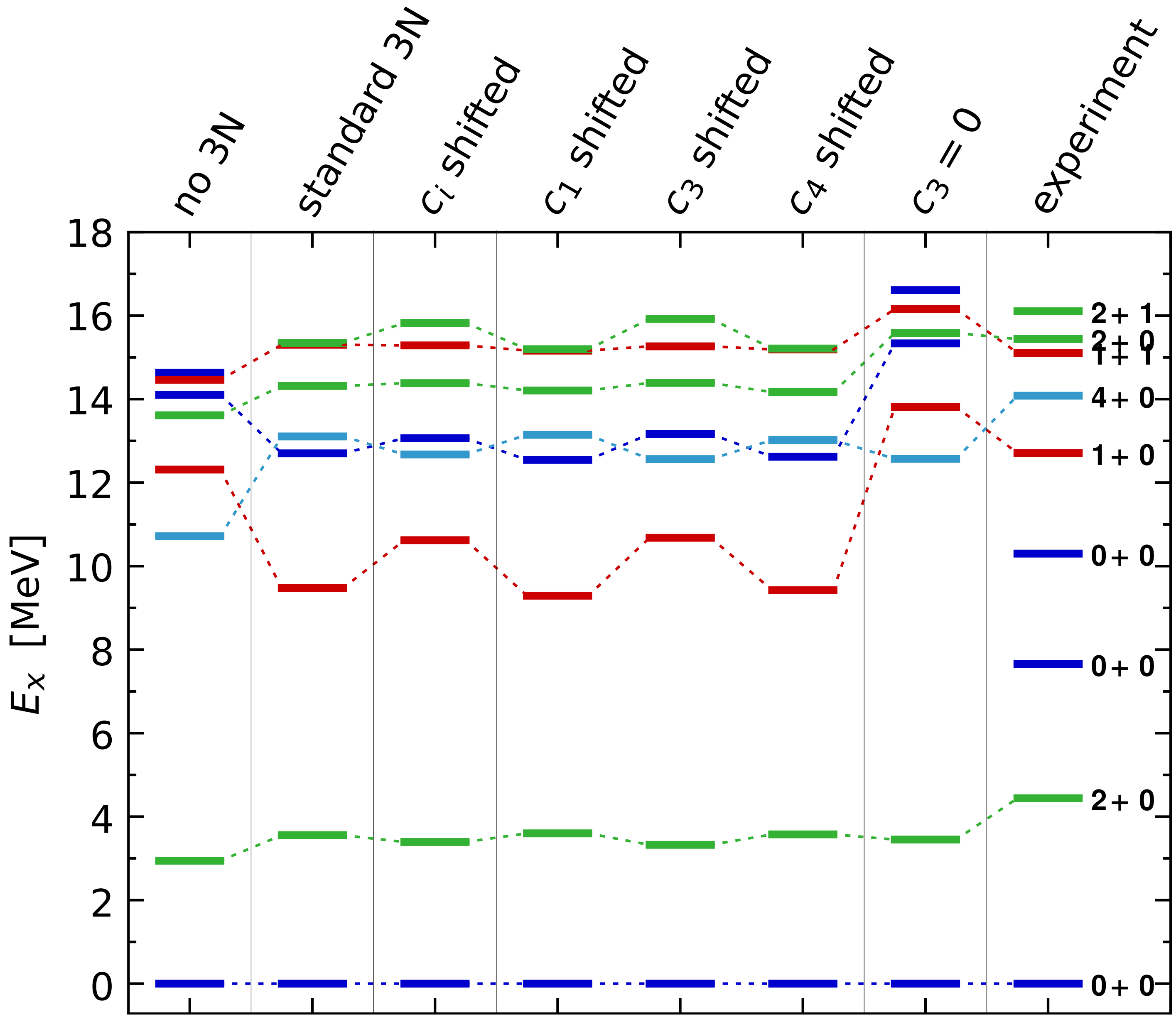
$\hbar\Omega = 16$ MeV
$N_{max} = 8$
$\alpha = 0.08\,fm^4$

^{12}C : Sensitivity on c_i



$\hbar\Omega = 16$ MeV
$N_{max} = 8$
$\alpha = 0.08\,\text{fm}^4$

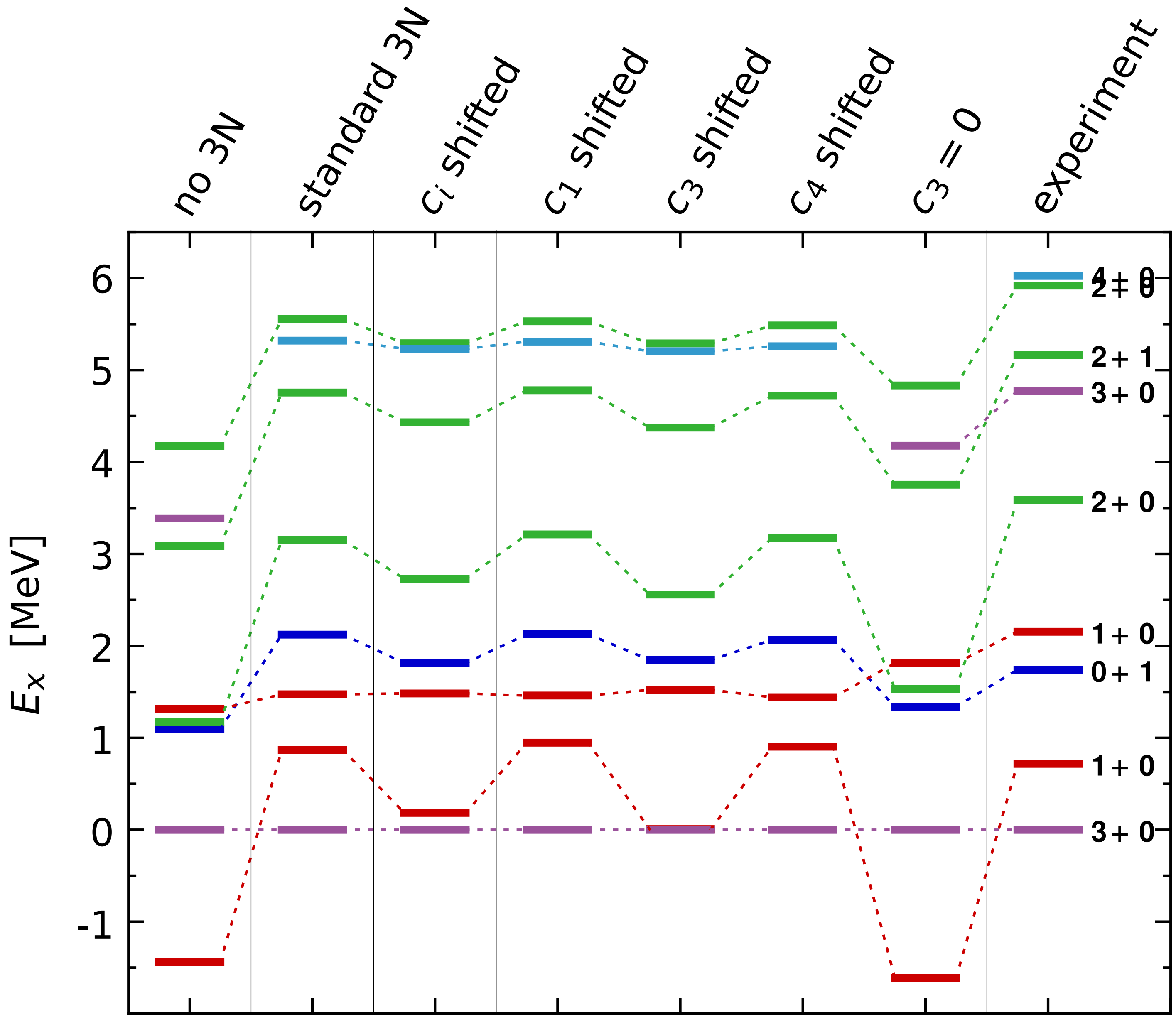
^{12}C : Sensitivity on c_i



- many states are rather c_i-insensitive
- first 1^+ state shows strong c_3-sensitivity

$\hbar\Omega = 16$ MeV
$N_{max} = 8$
$\alpha = 0.08\,\text{fm}^4$

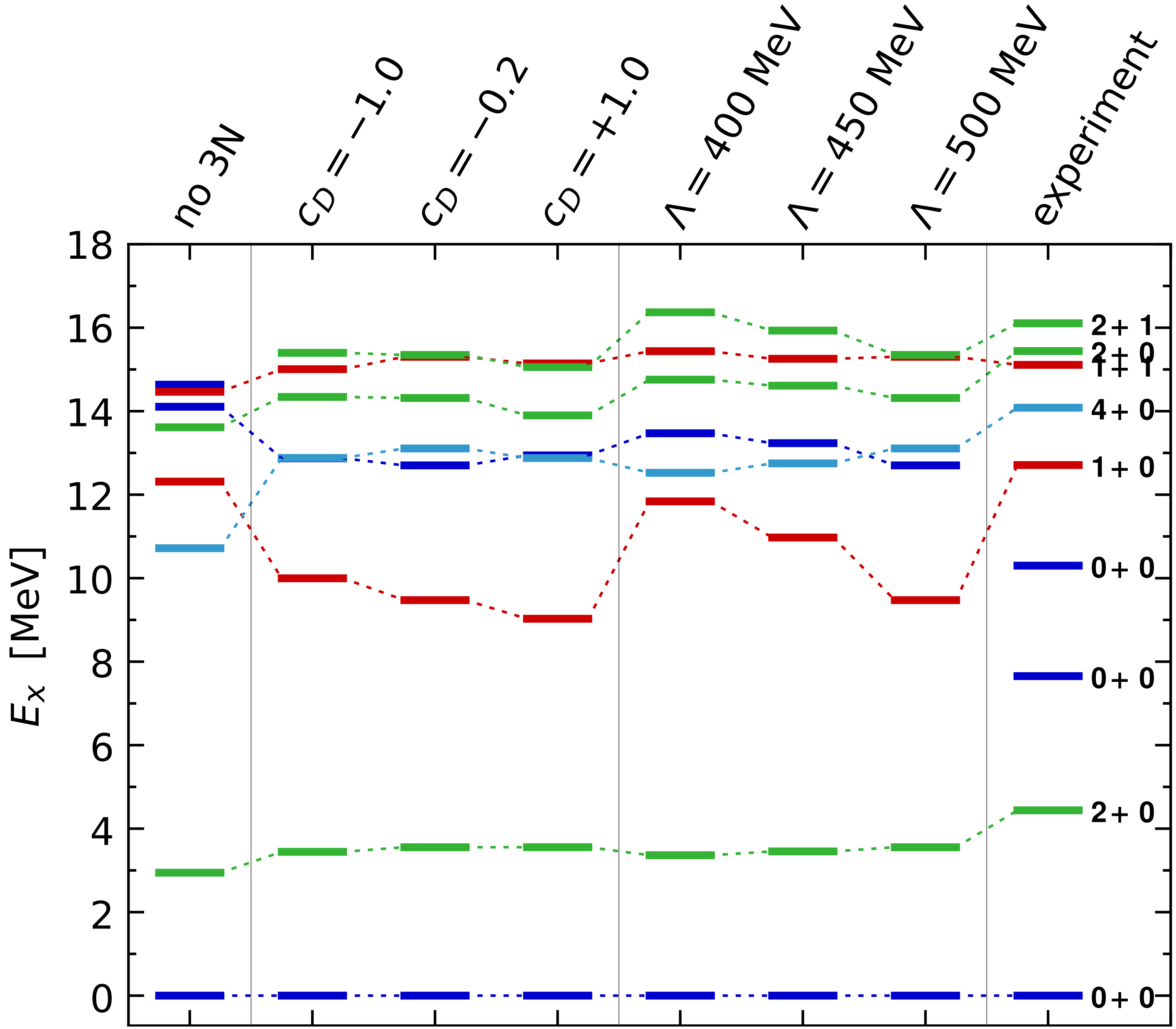
^{10}B : Sensitivity on c_i



- dramatic c_3-sensitivity of first 1^+ state
- opposite energy shift compared to 1^+ in ^{12}C
- second 1^+ very stable

$\hbar\Omega = 16$ MeV
$N_{max} = 8$
$\alpha = 0.08\,\text{fm}^4$

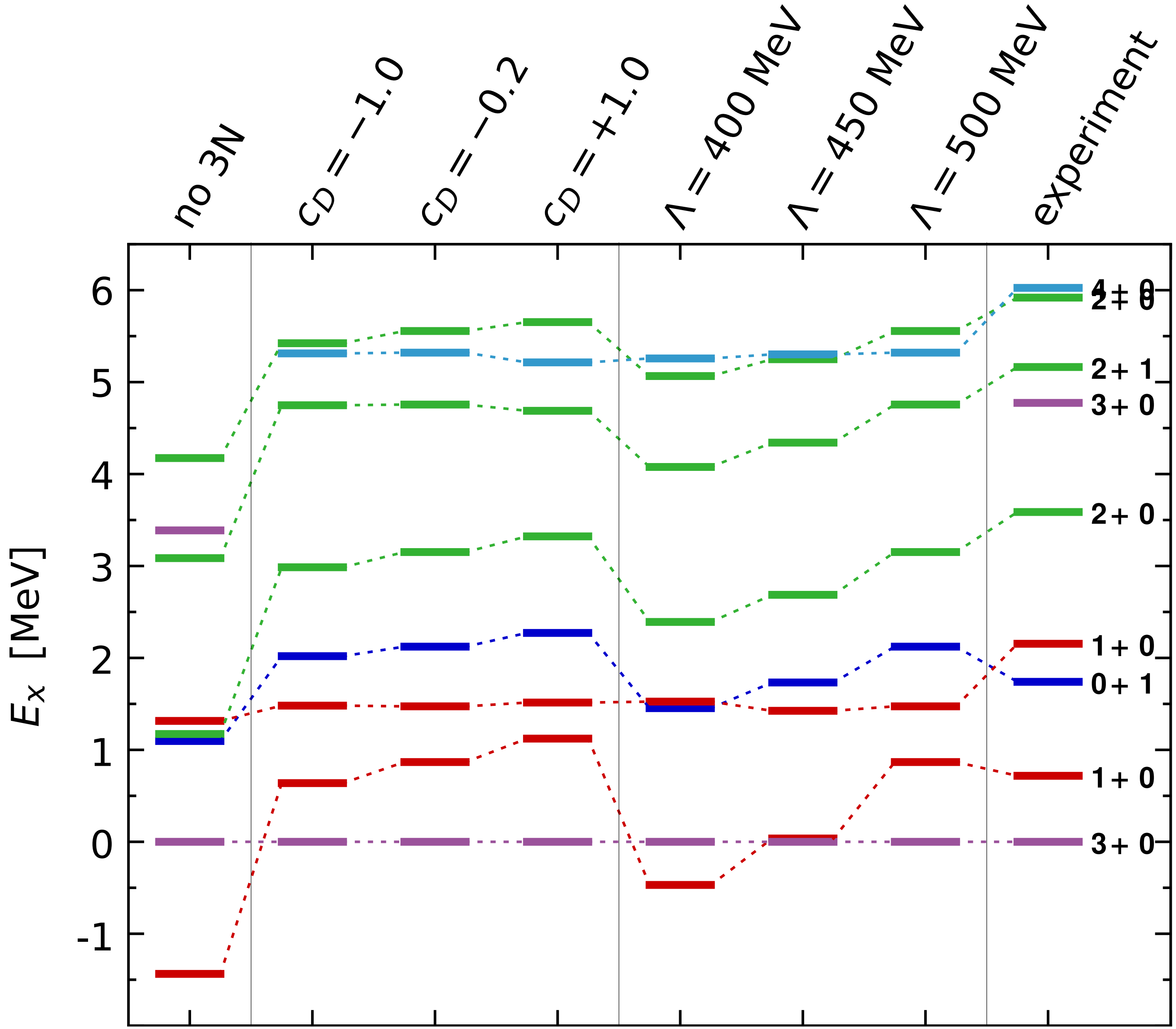
^{12}C : Sensitivity on c_D & Cutoff



- weak dependence on c_D, stronger dependence on Λ
- again first 1^+ state is most sensitive

$\hbar\Omega = 16$ MeV
$N_{max} = 8$
$\alpha = 0.08\,\text{fm}^4$

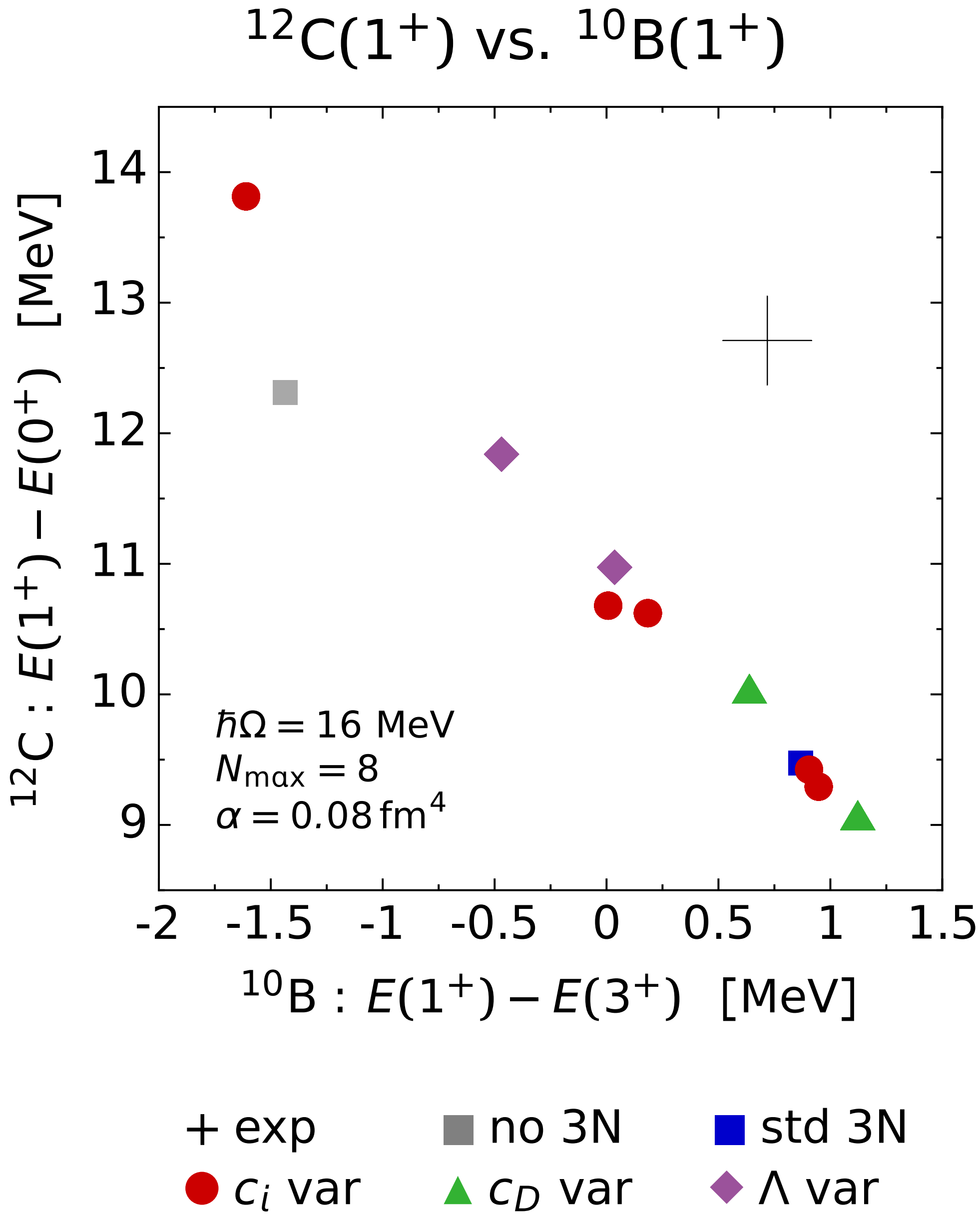
^{10}B : Sensitivity on c_D & Cutoff



- weak dependence on c_D, stronger dependence on Λ
- again first 1^+ state is most sensitive

$\hbar\Omega = 16$ MeV
$N_{max} = 8$
$\alpha = 0.08\,\text{fm}^4$

Sensitivity & Correlation Analysis



- mid-p-shell nuclei provide **powerful test-bed** for chiral 3N interactions
- individual states exhibit a **strong sensitivity** on the details of the 3N interaction
- 3N at N^2LO is **not able** to describe first 1^+ states in $^{10}B/^{12}C$ simultaneously
- **new operator structures** are needed...

Ab Initio Calculations for Heavy Nuclei

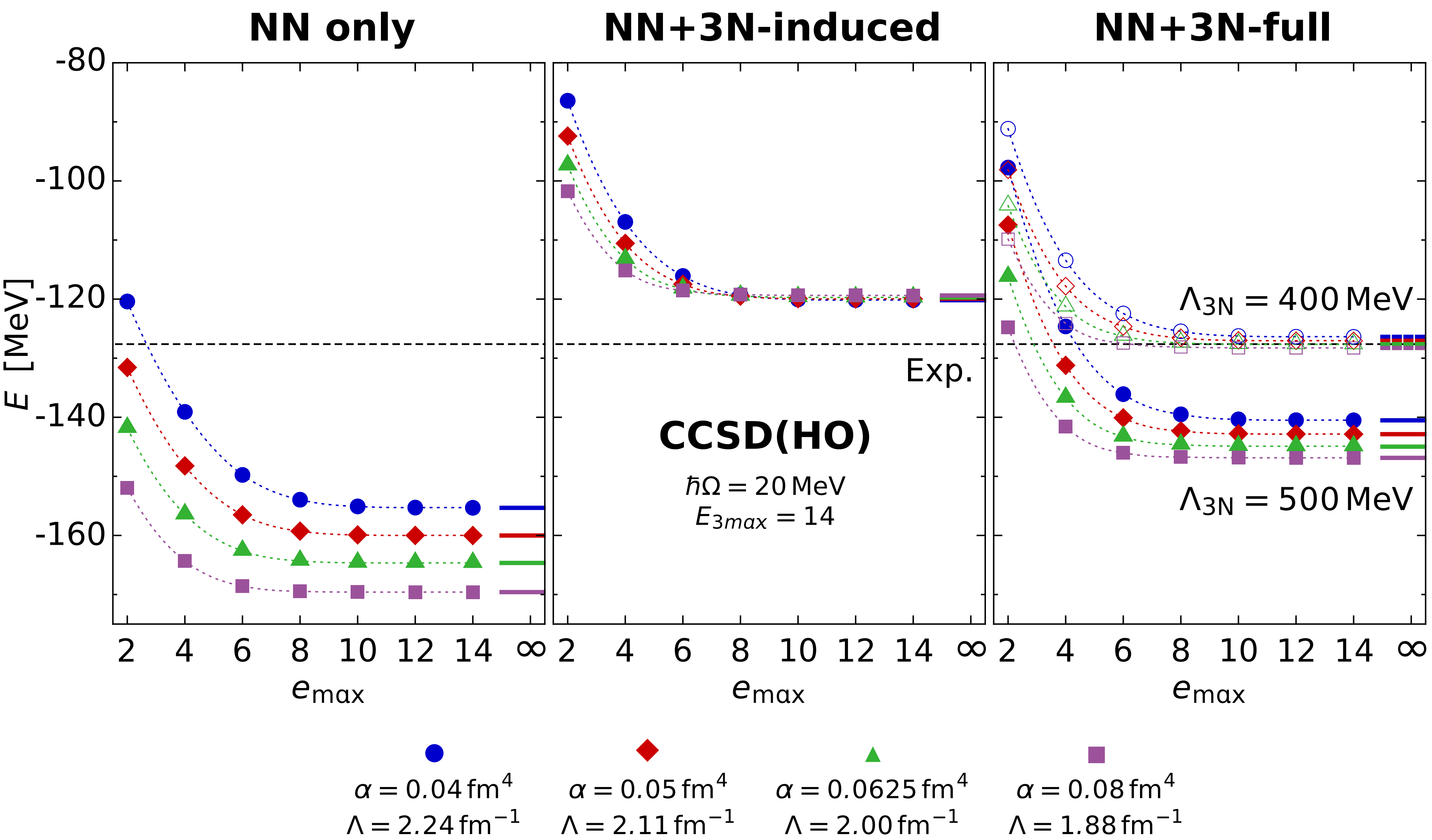
Roth, Binder, Vobig et al. — Phys. Rev. Lett. 109, 052501 (2012)

Heavy Nuclei with 3N Interactions

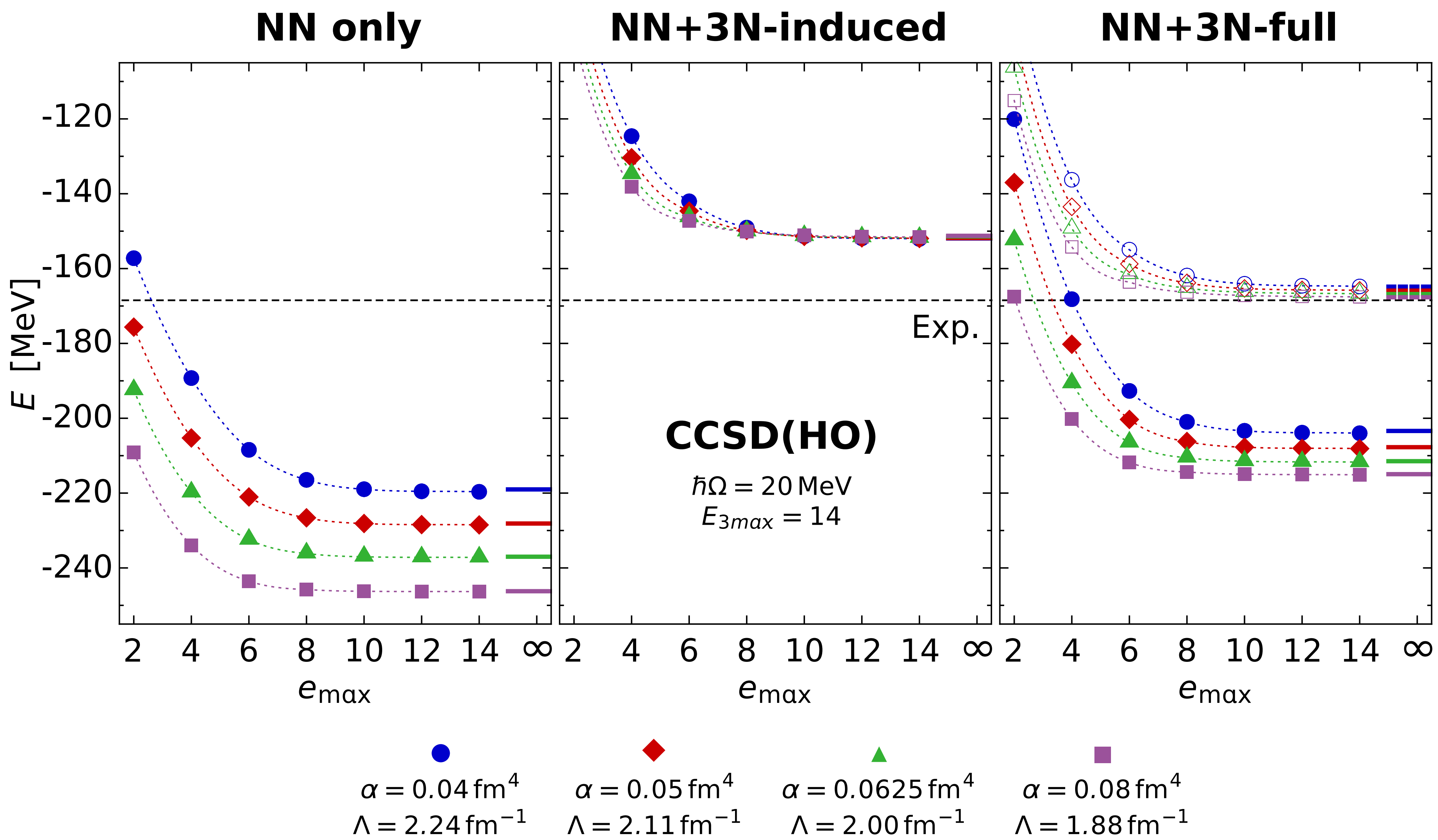
'ab initio' calculations for heavier nuclei require alternative many-body tools and approximate treatment of 3N interactions

- **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

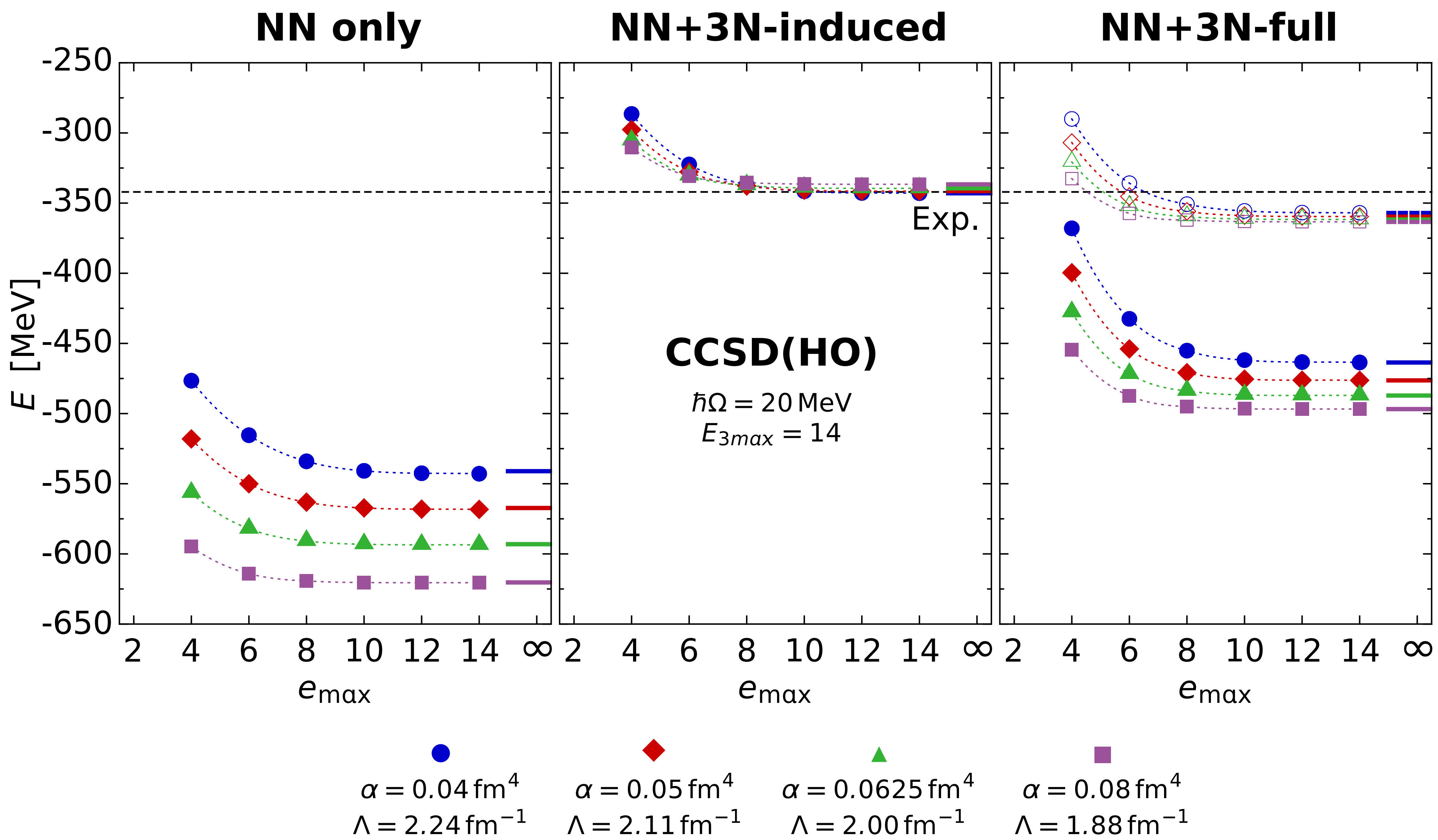
^{16}O: Coupled-Cluster with $3N_{NO2B}$



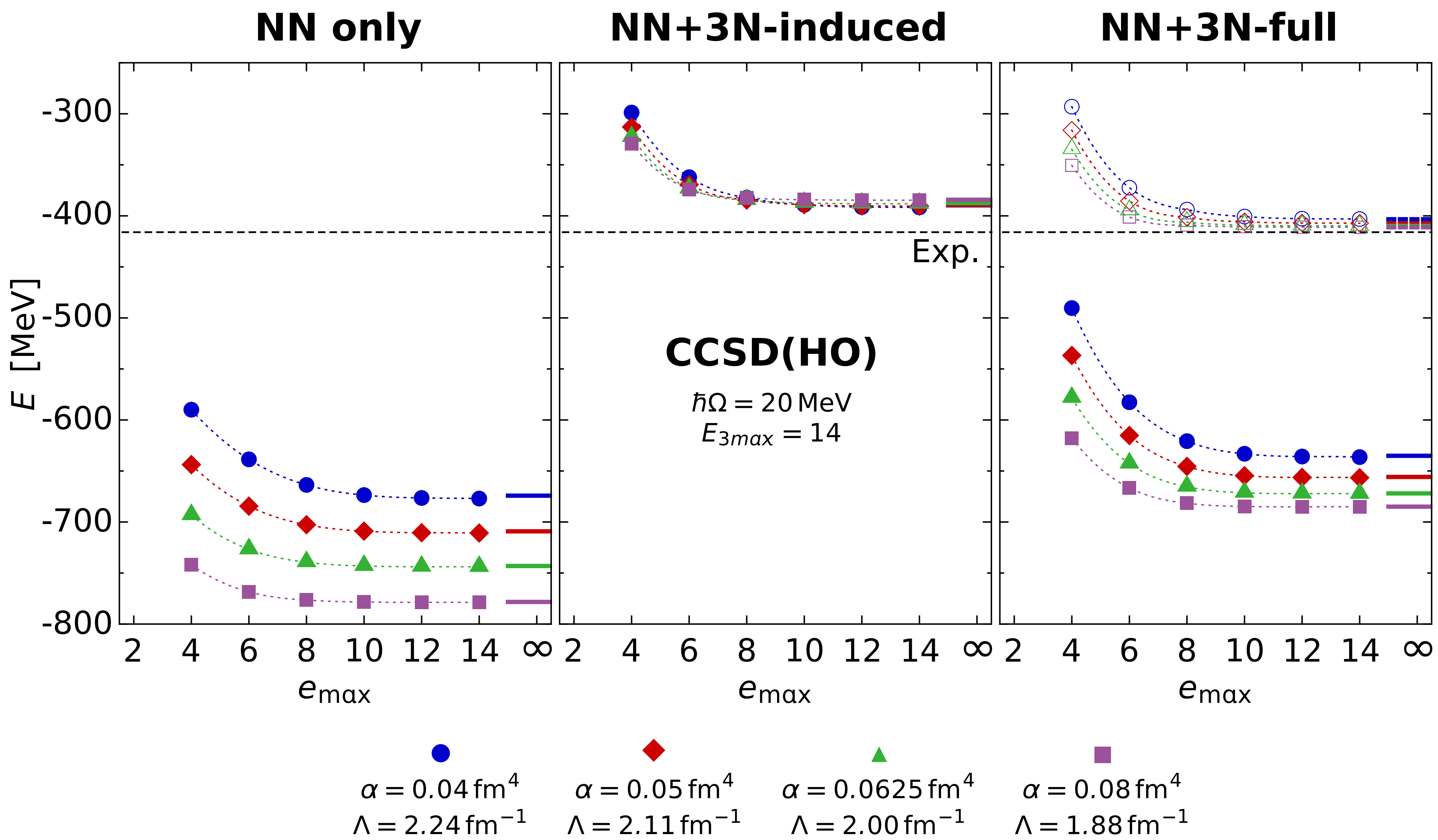
^{24}O: Coupled-Cluster with $3N_{NO2B}$



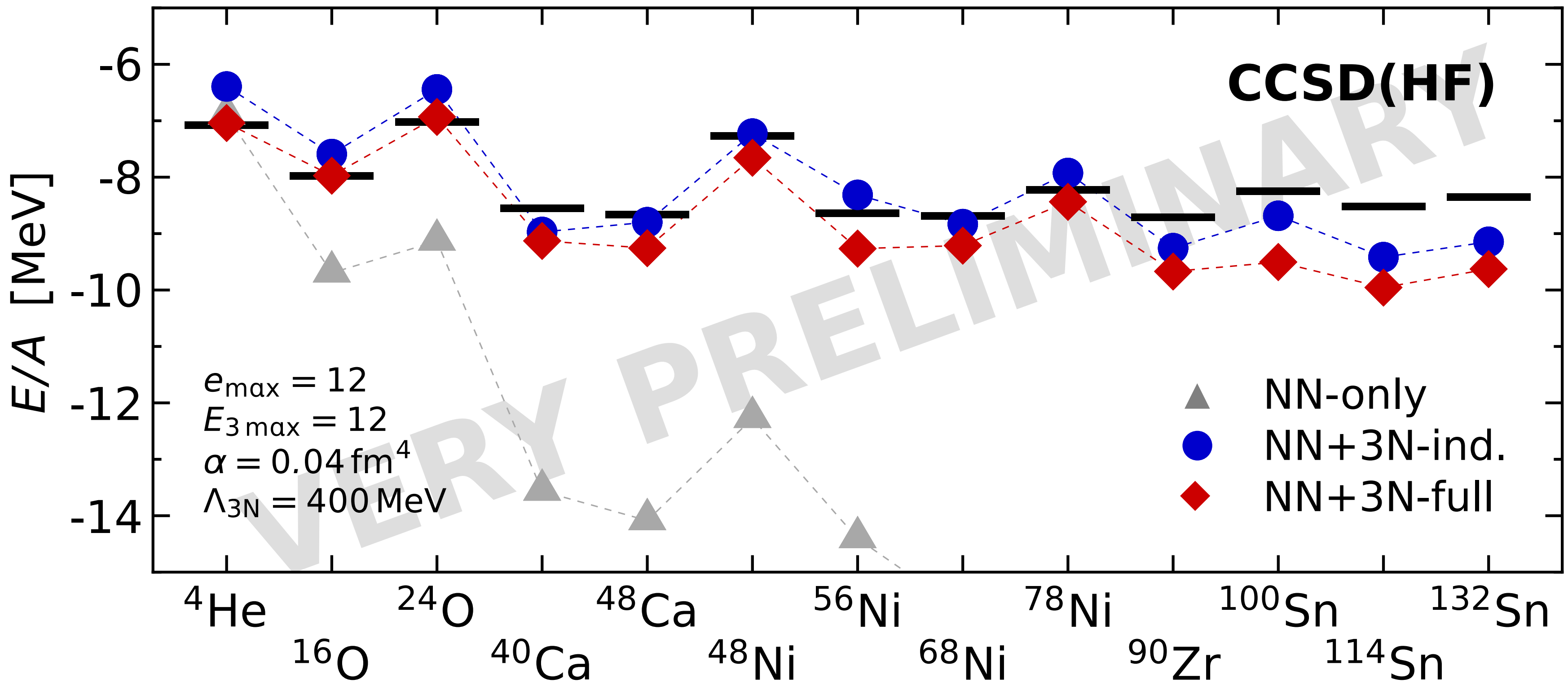
^{40}Ca: Coupled-Cluster with $3N_{NO2B}$



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



Outlook: Chiral 3N for Heavy Nuclei



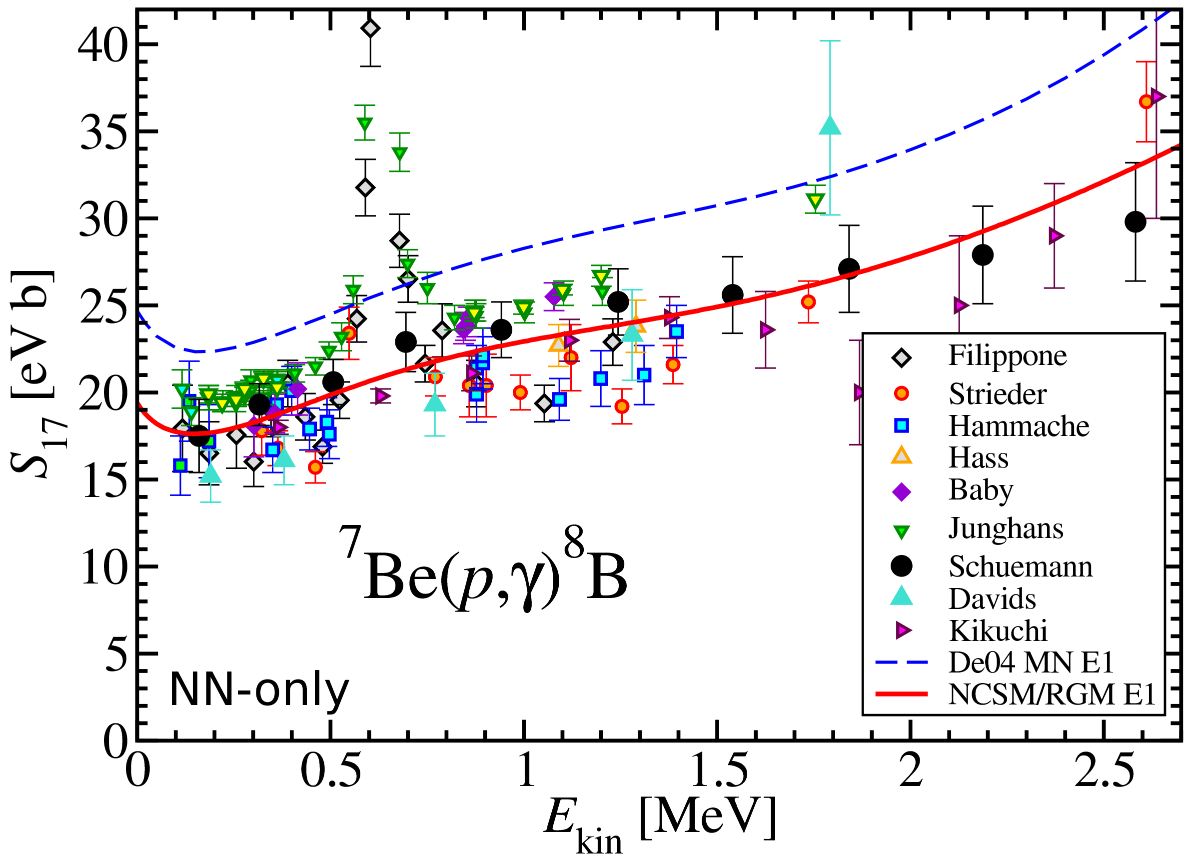
- first ab initio calculations with **chiral NN+3N Hamiltonians for heavy nuclei**
- **realistic mass systematics** without phenomenological adjustments — α-dependence might hold surprises...

Bridge to Ab Initio Reaction Theory

Hupin, Langhammer et al. — in preparation
Navrátil, Roth, Quaglioni — Phys. Lett. B 704, 379 (2011)
Navrátil, Roth, Quaglioni — Phys. Rev. C 82, 034609 (2010)

Bridge to Ab-Initio Reaction Theory

- **NCSM/RGM**: combine Resonating Group Method for description of relative projective-target motion with IT-NCSM for the description of target nucleus



- astrophysical S-factor for proton capture on ^{7}Be
- IT-NCSM wave functions for ^{7}Be for up to 8 eigenstates
- solution of the RGM with kernels involving the full many-body information
- SRG-evolved chiral NN interaction with α adjusted to reproduce ^{8}B energy relative to threshold

Conclusions

Conclusions

- new era of **ab-initio nuclear structure and reaction theory** connected to QCD via chiral EFT
  - chiral EFT as universal starting point... propagate uncertainties & provide feedback
- 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
    Institut für Kernphysik, TU Darmstadt
  - **P. Navrátil**
    TRIUMF Vancouver, Canada
  - J. Vary, P. Maris
    Iowa State University, USA
  - 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

JUROPA — JÜLICH FORSCHUNGSZENTRUM

LOEWE-CSC — CSC Center for Scientific Computing Frankfurt

HOPPER — NERSC

COMPUTING TIME

SFB 634

Deutsche Forschungsgemeinschaft DFG

HIC for FAIR Helmholtz International Center

LOEWE Exzellente Forschung für Hessens Zukunft

HELMHOLTZ GEMEINSCHAFT

Bundesministerium für Bildung und Forschung