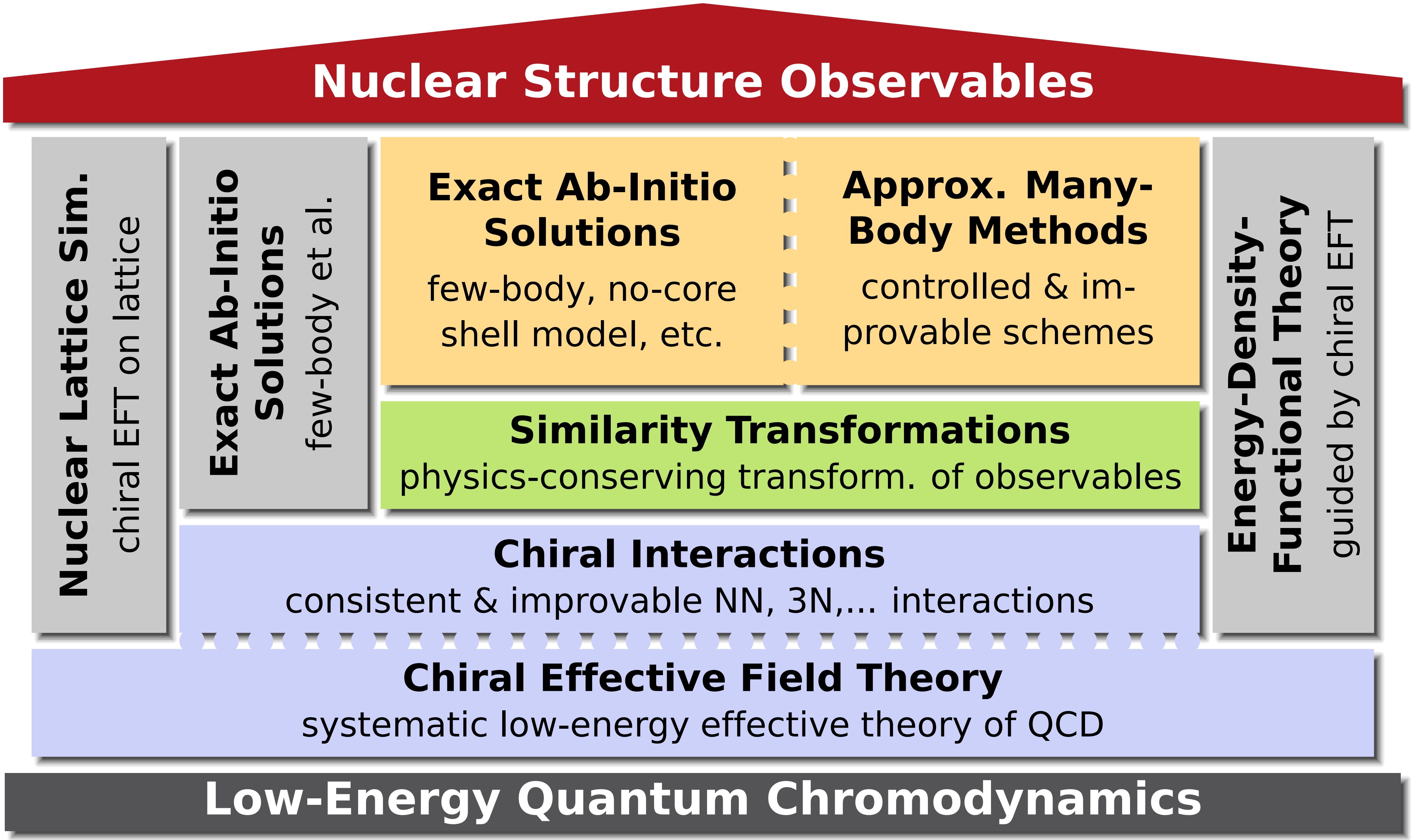
Chiral Three-Nucleon Interactions and the Structure of 'Light' Nuclei

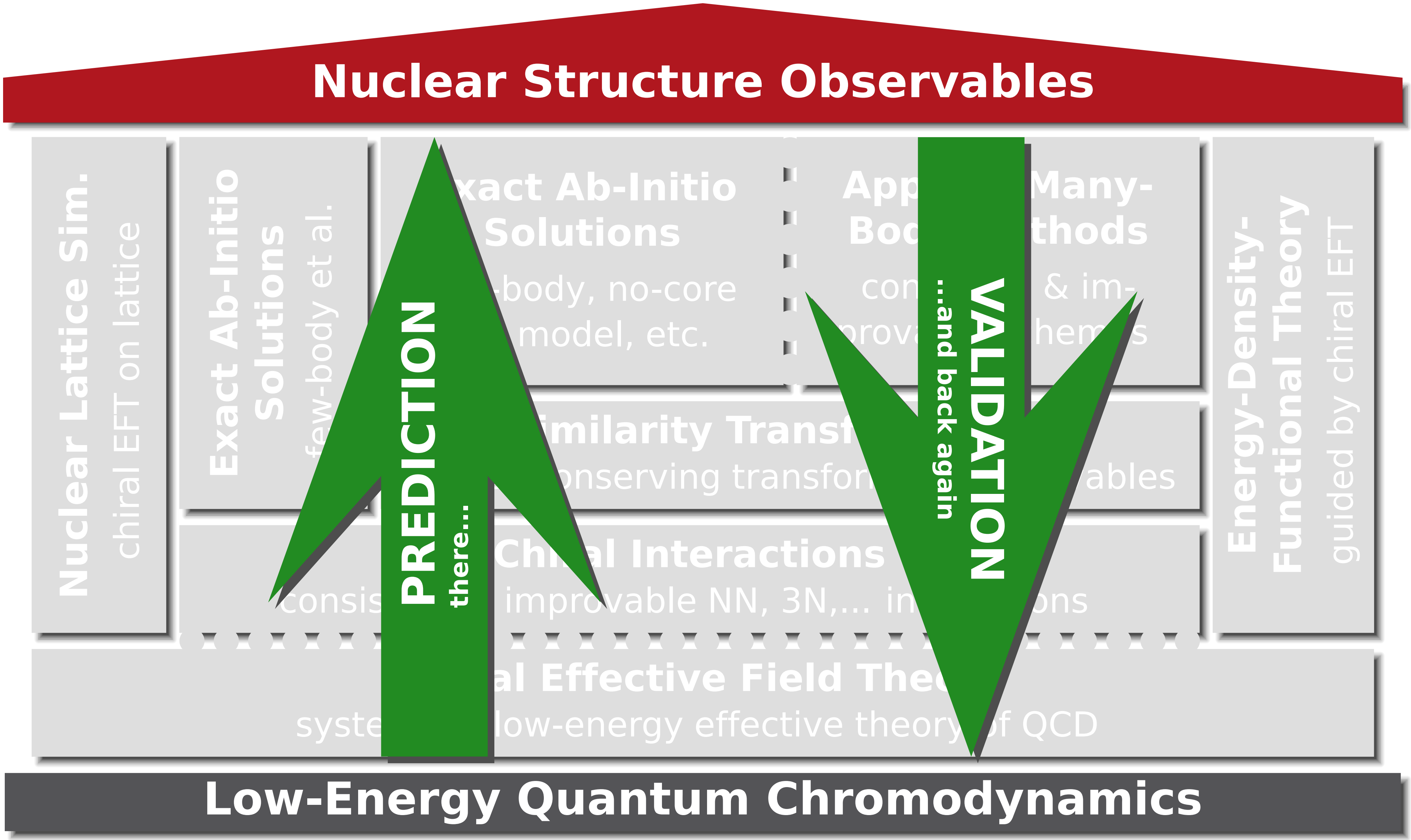
Robert Roth

TECHNISCHE UNIVERSITÄT DARMSTADT

Ab Initio Nuclear Structure



Ab Initio Nuclear Structure

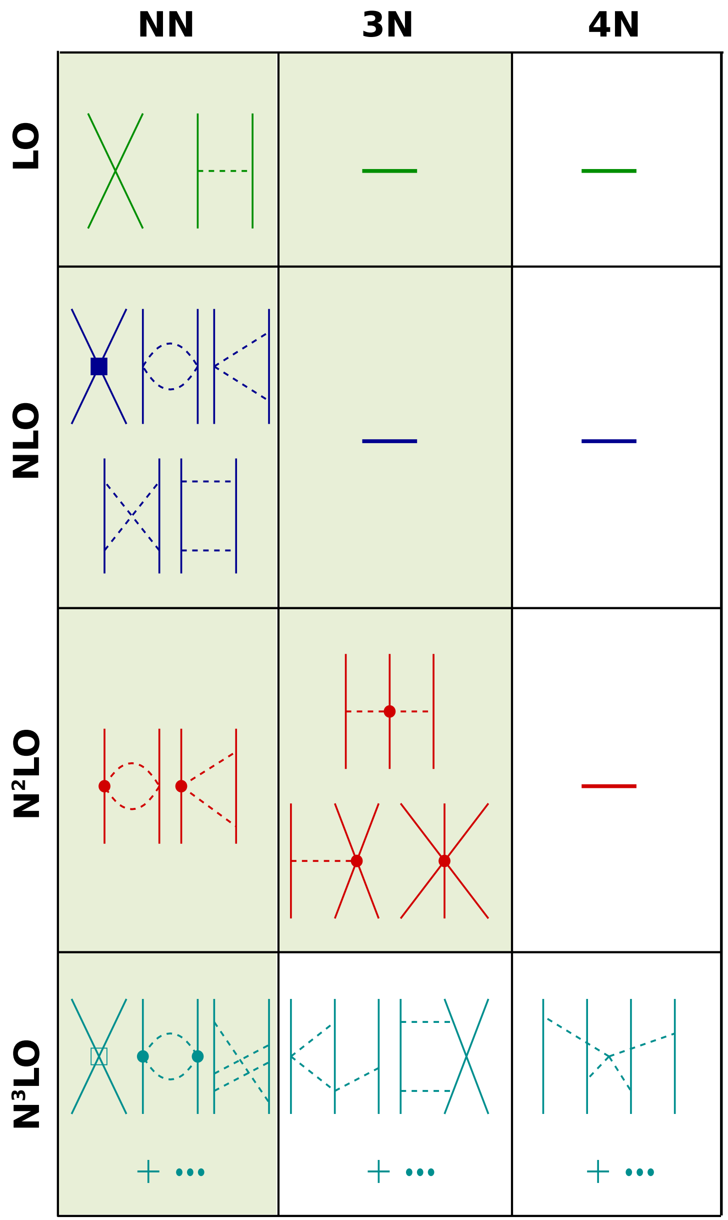


Nuclear Interactions from Chiral EFT

Nuclear Interactions from Chiral EFT

Weinberg, van Kolck, Machleidt, Entem, Meißner, Epelbaum, Krebs, Bernard,...

- low-energy **effective field theory** for relevant degrees of freedom (π,N) based on symmetries of QCD
- long-range **pion dynamics** explicitly
- short-range physics absorbed in **contact terms**, low-energy constants fitted to experiment (NN, πN,...)
- hierarchy of **consistent NN, 3N,... interactions** (plus currents)
- many **ongoing developments**
  - 3N interaction at N3LO, N4LO,...
  - explicit inclusion of Δ-resonance
  - YN- & YY-interactions
  - formal issues: power counting, renormalization, cutoff choice,...



Chiral NN+3N Hamiltonians

- **standard Hamiltonian:**
  - NN at N3LO: Entem / Machleidt, 500 MeV cutoff
  - 3N at N2LO: Navrátil, local, 500 MeV cutoff, fit to $T_{1/2}(^3\text{H})$ and $E(^3\text{H}, {}^3\text{He})$

- **standard Hamiltonian with modified 3N:**
  - NN at N3LO: Entem / Machleidt, 500 MeV cutoff
  - 3N at N2LO: Navrátil, local, with modified LECs and cutoffs, refit to $E(^4\text{He})$

- **consistent N2LO Hamiltonian:**
  - NN at N2LO: Epelbaum et al., 450,...,600 MeV cutoff
  - 3N at N2LO: Epelbaum et al., nonlocal, 450,...,600 MeV cutoff

- **consistent N3LO Hamiltonian:**
  - coming soon...

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

Wegner, Glazek, Wilson, Perry, Bogner, Furnstahl, Hergert, Roth, Jurgenson, Navratil,...

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

simplicity and flexibility
are great advantages of
the SRG approach

- **unitary transformation** of Hamil

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

- **evolution equations** for $\widetilde{H}_\alpha$ and U_α depending on generator η_α

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

- **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

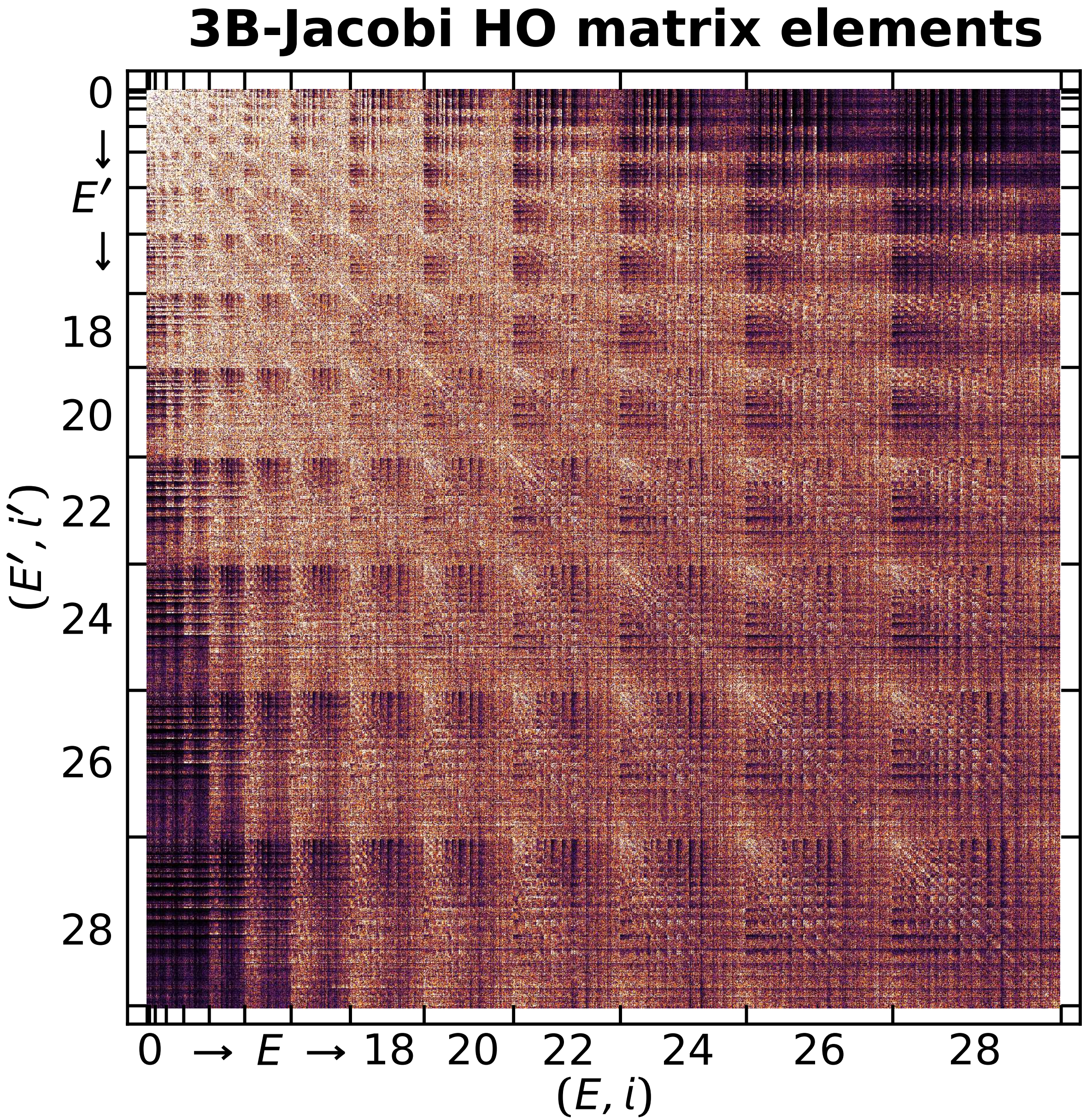
- represent operator equation in **three-body Jacobi basis**
  - harmonic oscillator: antisymm. Jacobi HO states $|EiJ^\pi T\rangle$
  - momentum space: Jacobi momentum states $|pq\alpha\rangle$ → K. Hebeler

- system of **coupled evolution equations** for each $(J^\pi T)$-block

$$\frac{d}{d\alpha}\langle EiJ^\pi T|\,\widetilde{H}_\alpha\,|E'i'J^\pi T\rangle = (2\mu)^2 \sum_{E'',i''}^{E_{SRG}} \sum_{E''',i'''}^{E_{SRG}} \Big[\langle Ei...|\,T_{int}\,|E''i''...\rangle \langle E''i''...|\,\widetilde{H}_\alpha\,|E'''i'''...\rangle \langle E'''i'''...|\,\widetilde{H}_\alpha\,|E'i'...\rangle - 2\langle Ei...|\,\widetilde{H}_\alpha\,|E''i''...\rangle \langle E''i''...|\,T_{int}\,|E'''i'''...\rangle \langle E'''i'''...|\,\widetilde{H}_\alpha\,|E'i'...\rangle + \langle Ei...|\,\widetilde{H}_\alpha\,|E''i''...\rangle \langle E''i''...|\,\widetilde{H}_\alpha\,|E'''i'''...\rangle \langle E'''i'''...|\,T_{int}\,|E'i'...\rangle \Big]$$

- we use HO with $E_{SRG} = 40$ for $J \leq 5/2$ and ramp down for larger J, sufficient for p-shell nuclei with $\hbar\Omega \gtrsim 16$ MeV

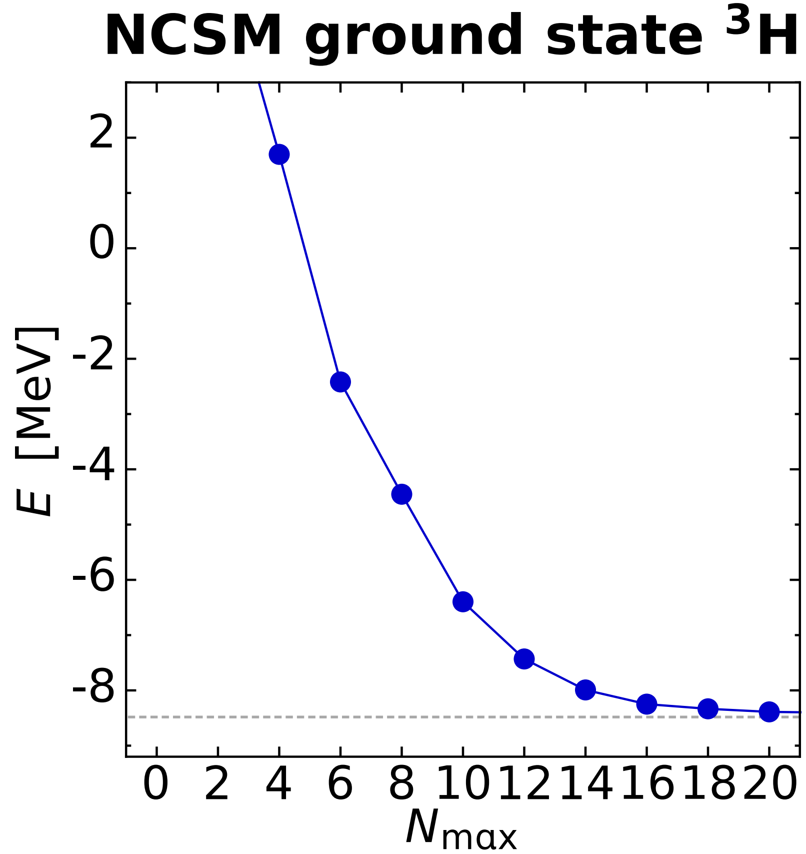
SRG Evolution in Three-Body Space



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

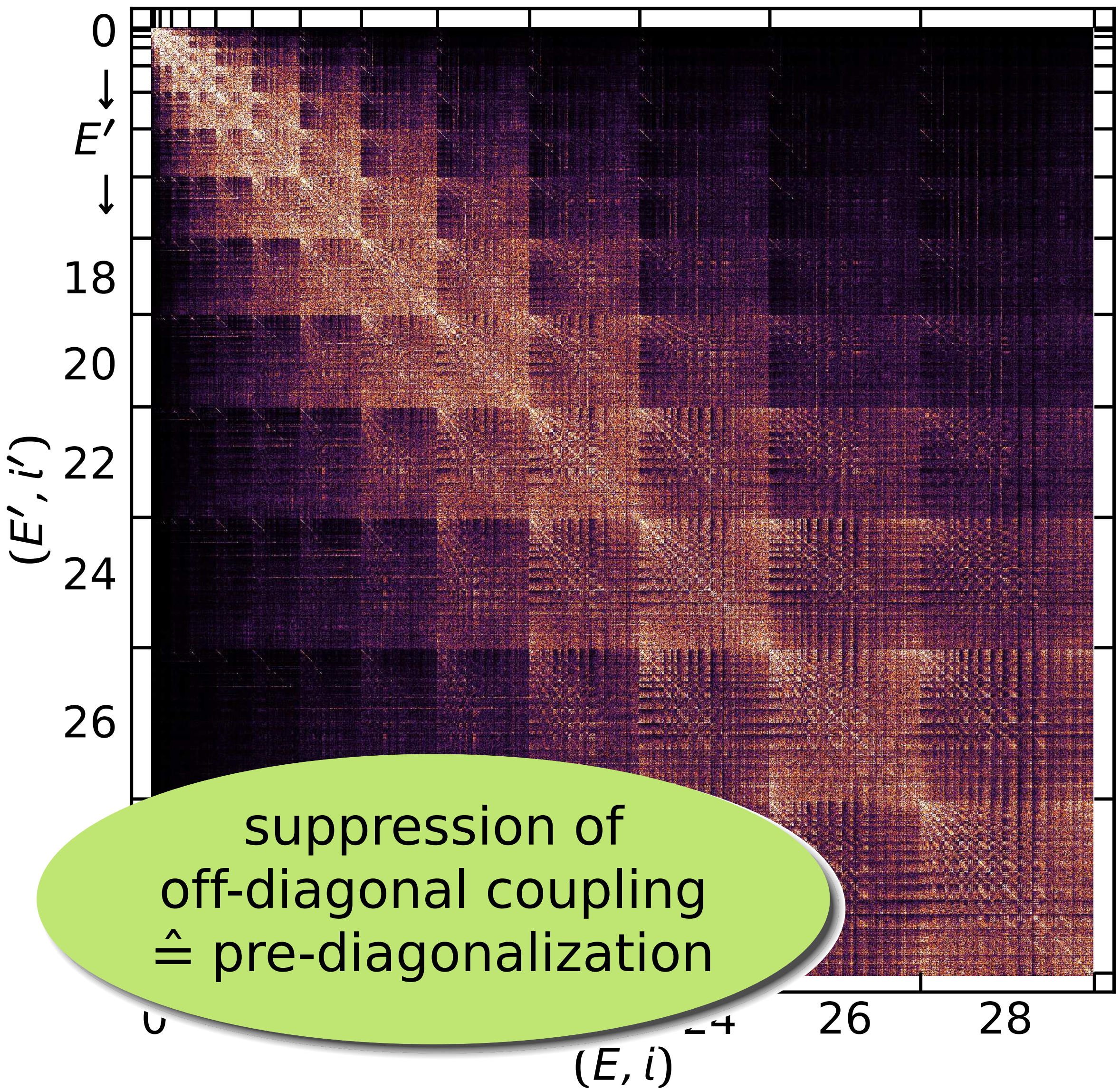
$\Lambda = \infty\,\text{fm}^{-1}$

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



SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements



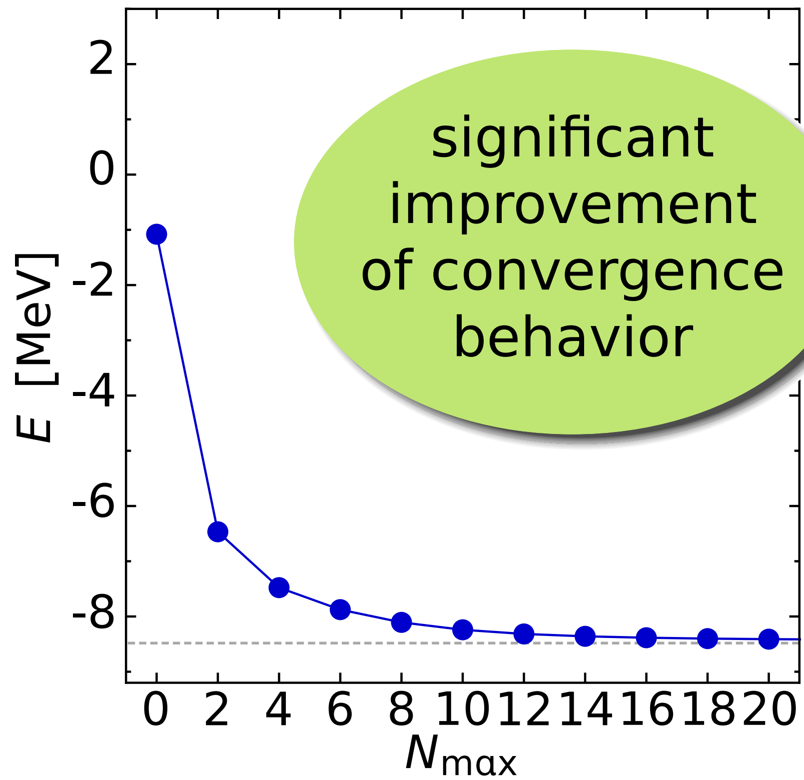
suppression of
off-diagonal coupling
≙ pre-diagonalization

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

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

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

NCSM ground state ^{3}H



significant
improvement
of convergence
behavior

Calculations in *A*-Body Space

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

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

- 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[...] [...]d 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

Sounds easy, but...

❶ initial 3B-Jacobi HO matrix elements of chiral 3N interactions

- direct computation using Petr Navratil's ManyEff code (N2LO)
- conversion of partial-wave decomposed moment-space matrix elements of Epelbaum et al. (N2LO, N3LO,...)

❷ SRG evolution in 2B/3B space and cluster decomposition

- efficient implementation using adaptive ODE solver & BLAS; largest JT-block takes a few hours on single node

❸ transformation of 2B/3B Jacobi HO matrix elements into JT-coupled representation

- transform directly into JT-coupled scheme; highly efficient implementation; can handle $E_{3\,\text{max}} = 16$ in JT-coupled scheme

❹ data management and on-the-fly decoupling in many-body codes

- optimized storage scheme for fast on-the-fly decoupling; can keep all matrix elements up to $E_{3\,\text{max}} = 16$ in memory; suitable for GPUs

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)

No-Core Shell Model

Barrett, Vary, Navratil, Maris, Nogga, Roth,...

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 $N_{\text{max}}\hbar\Omega$
- 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 $E_{3\,\text{max}} = 16$

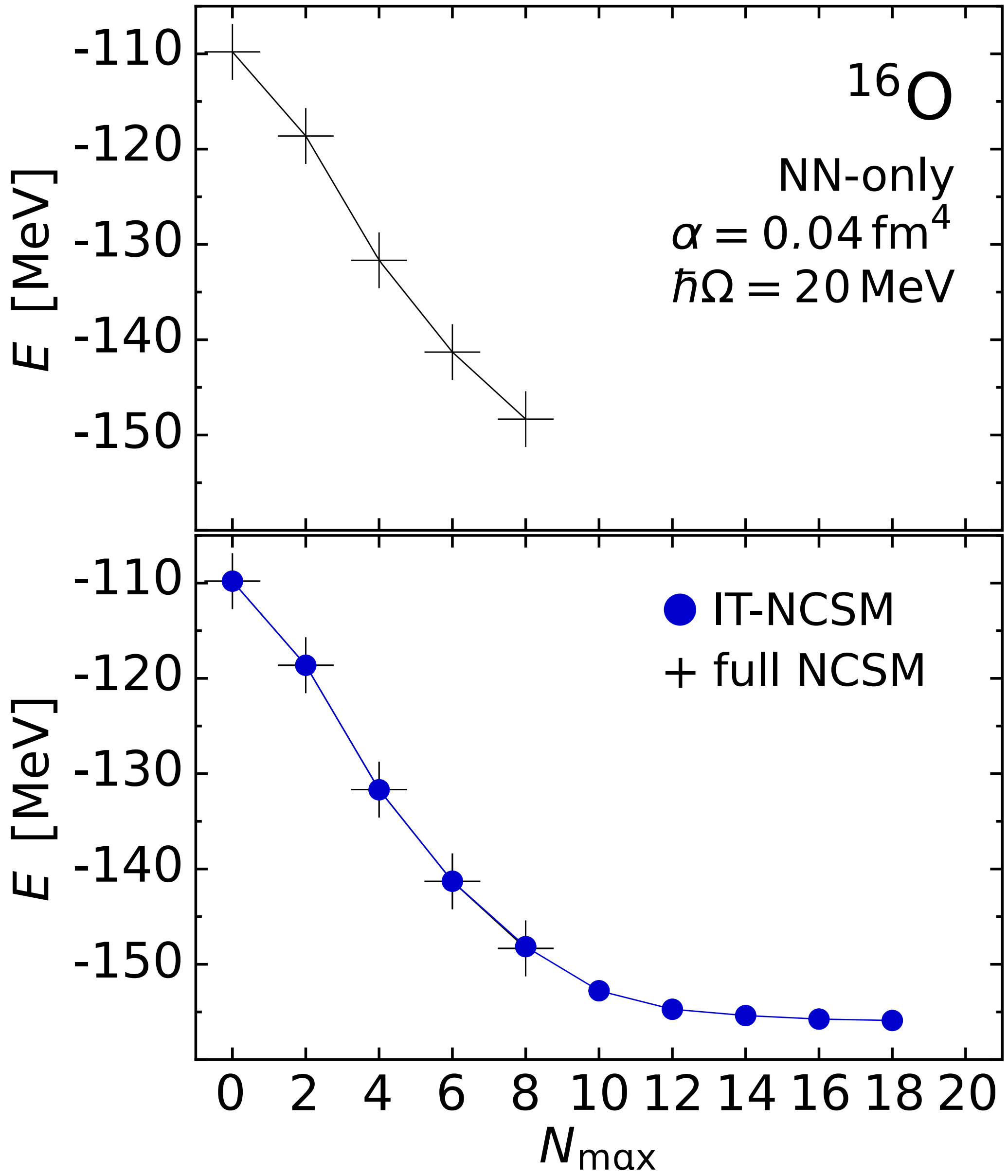
Importance Truncated NCSM

Roth, PRC 79, 064324 (2009); PRL 99, 092501 (2007)

- 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})

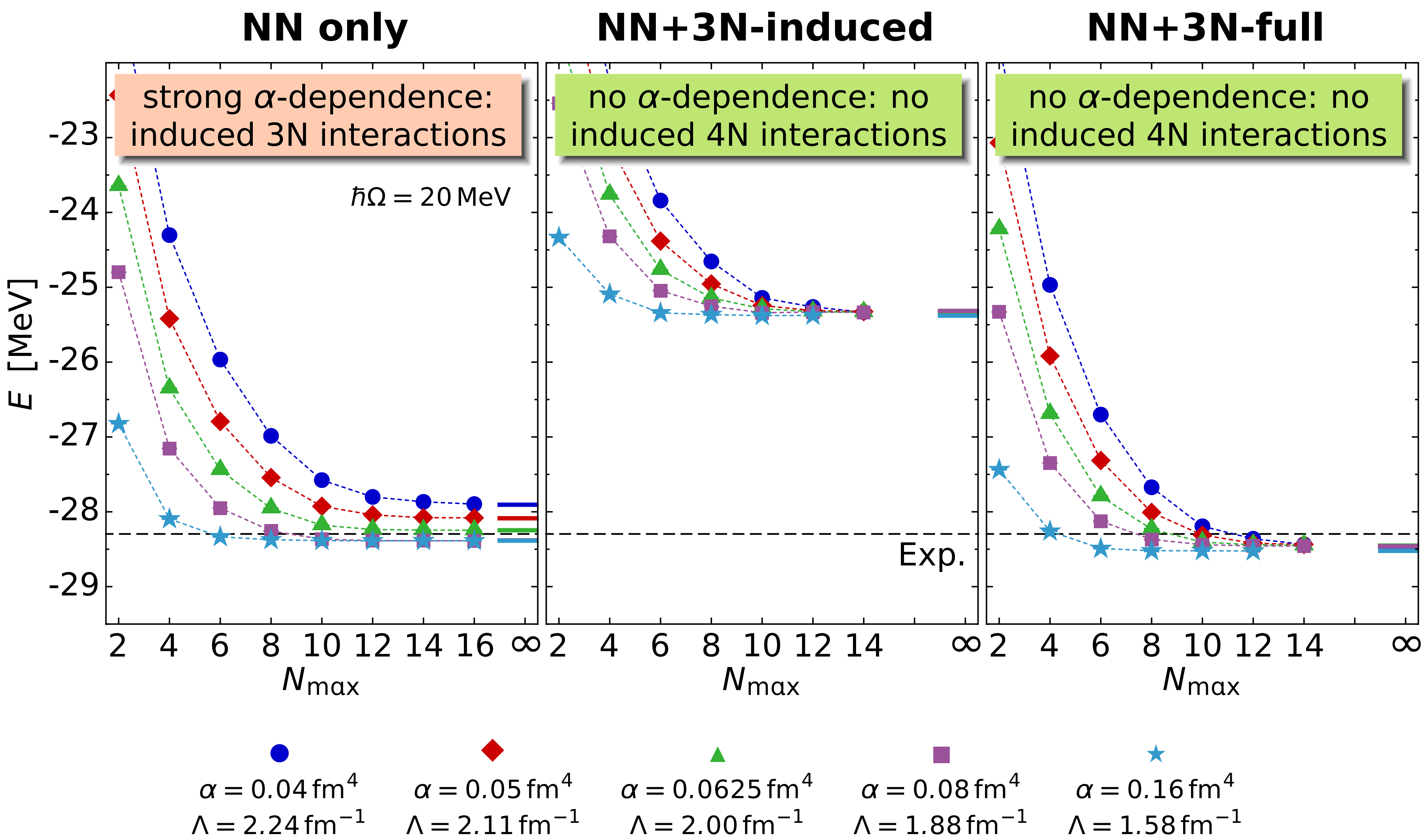
Importance Truncation

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



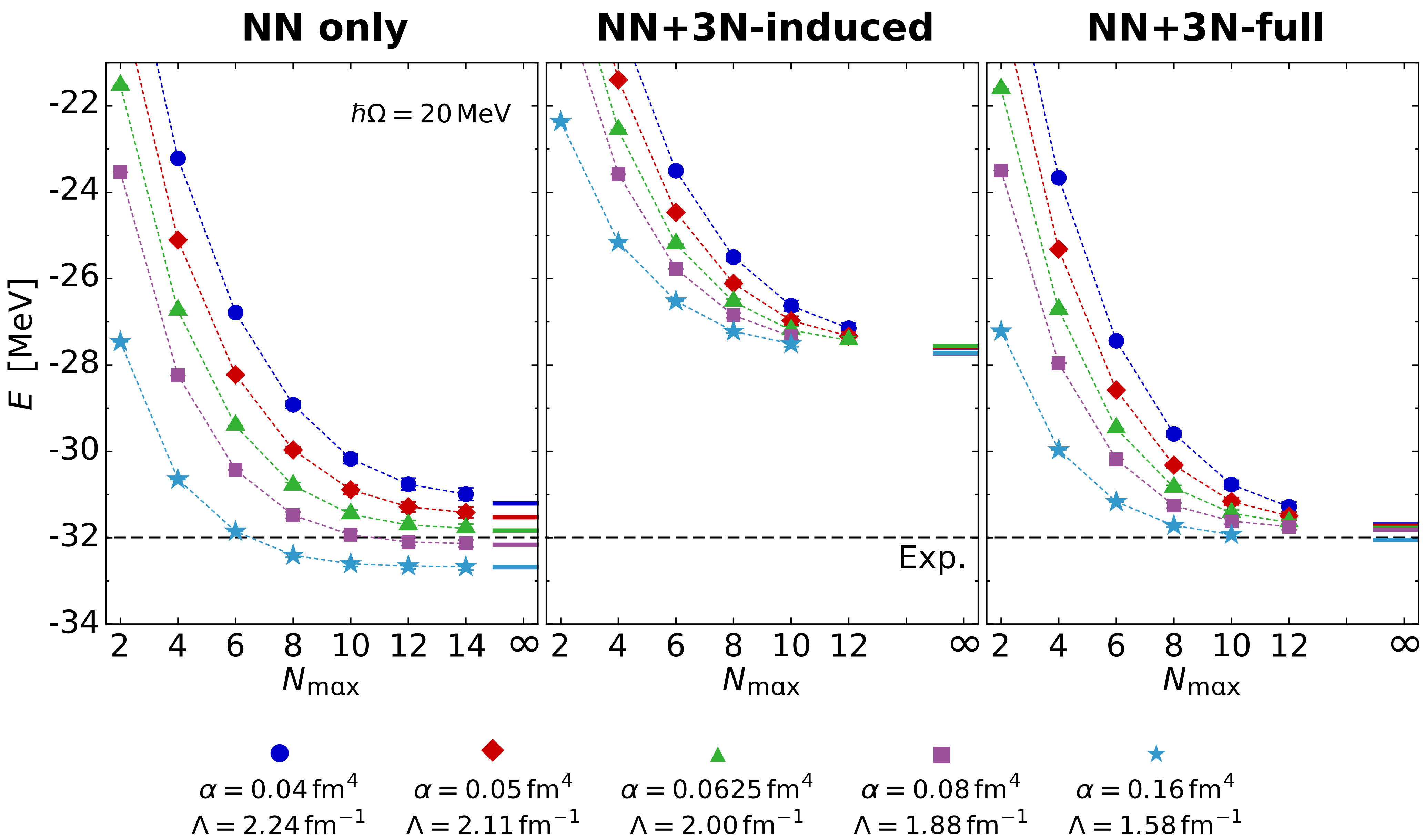
^{4}He: Ground-State Energies

Roth, et al; PRL 107, 072501 (2011)



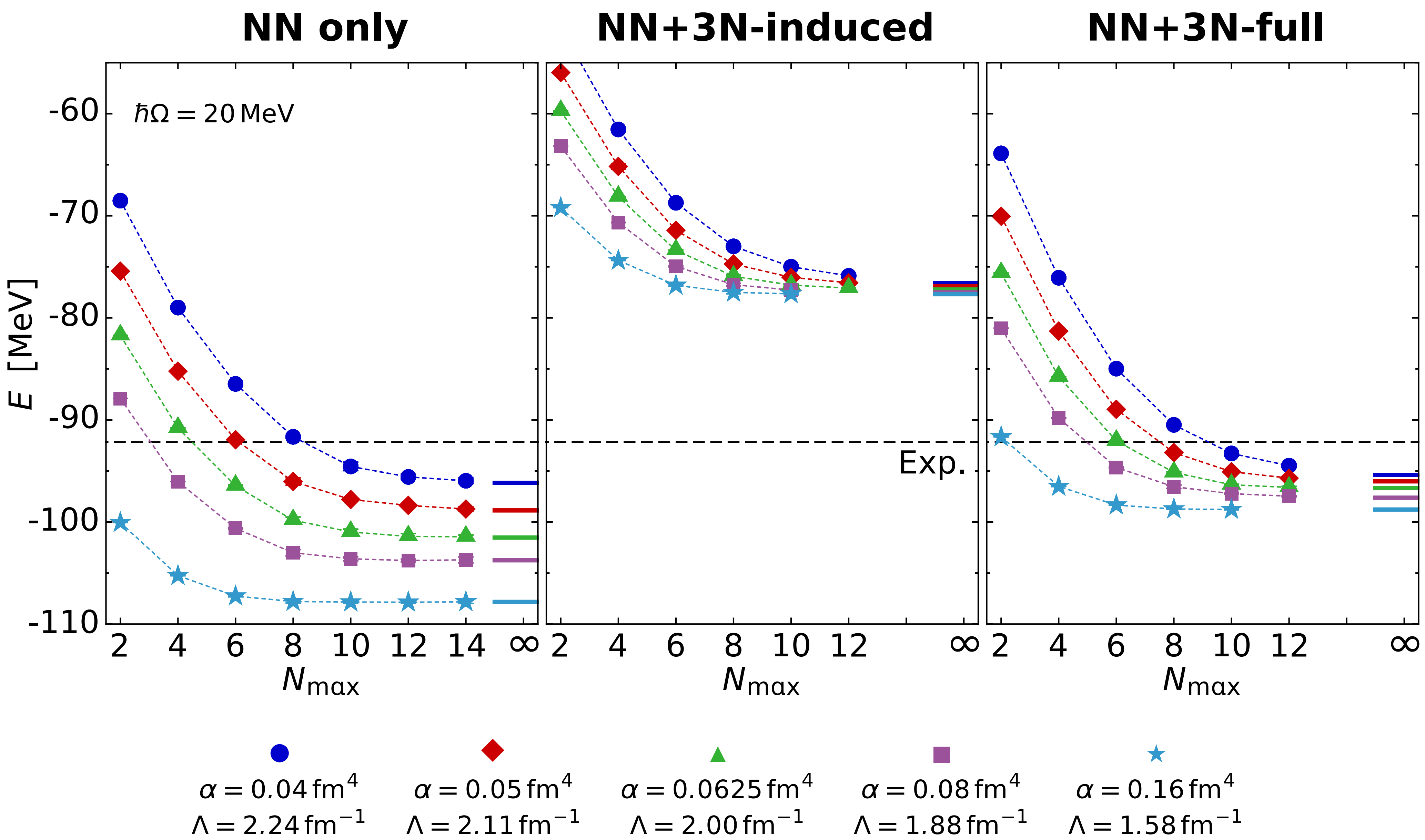
^{6}Li: Ground-State Energies

Roth, et al; PRL 107, 072501 (2011)



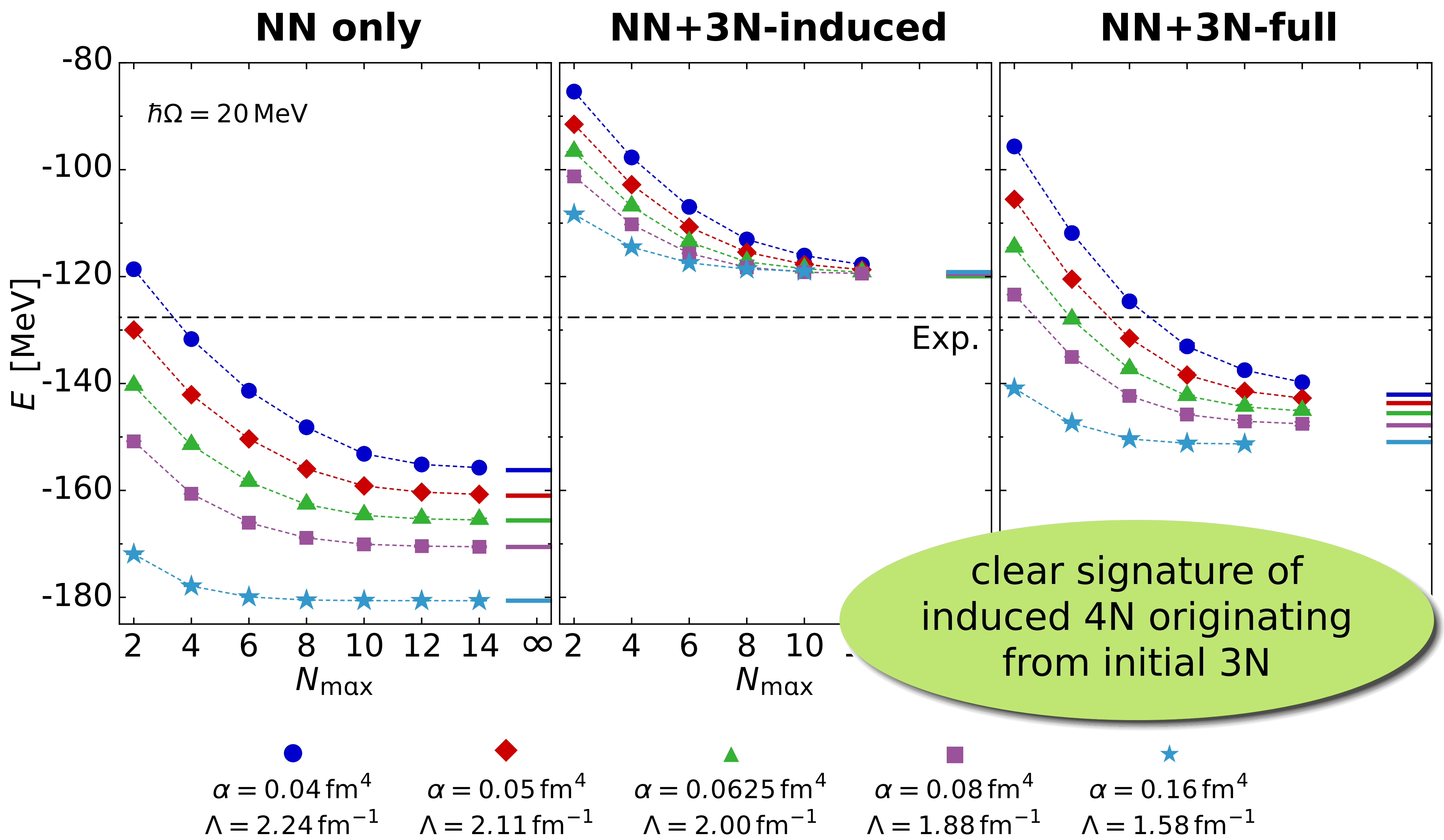
^{12}C: Ground-State Energies

Roth, et al; PRL 107, 072501 (2011)



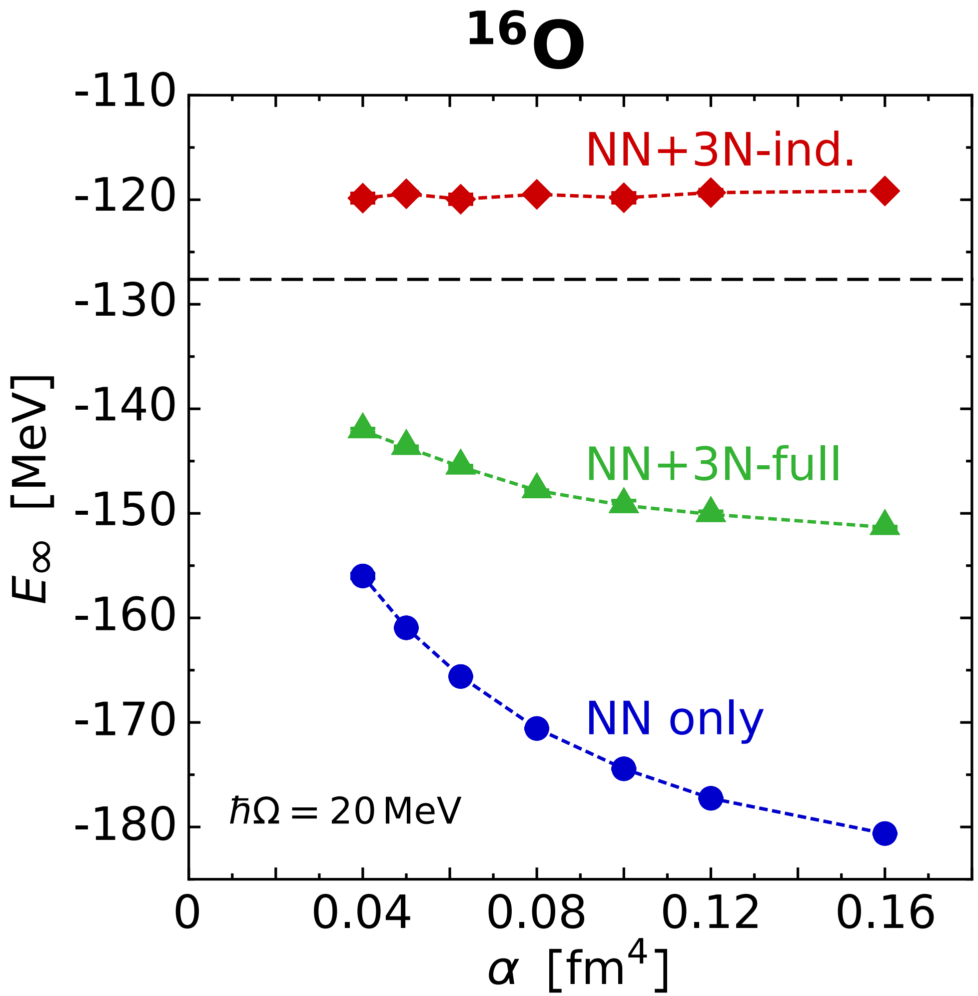
^{16}O: Ground-State Energies

Roth, et al; PRL 107, 072501 (2011)



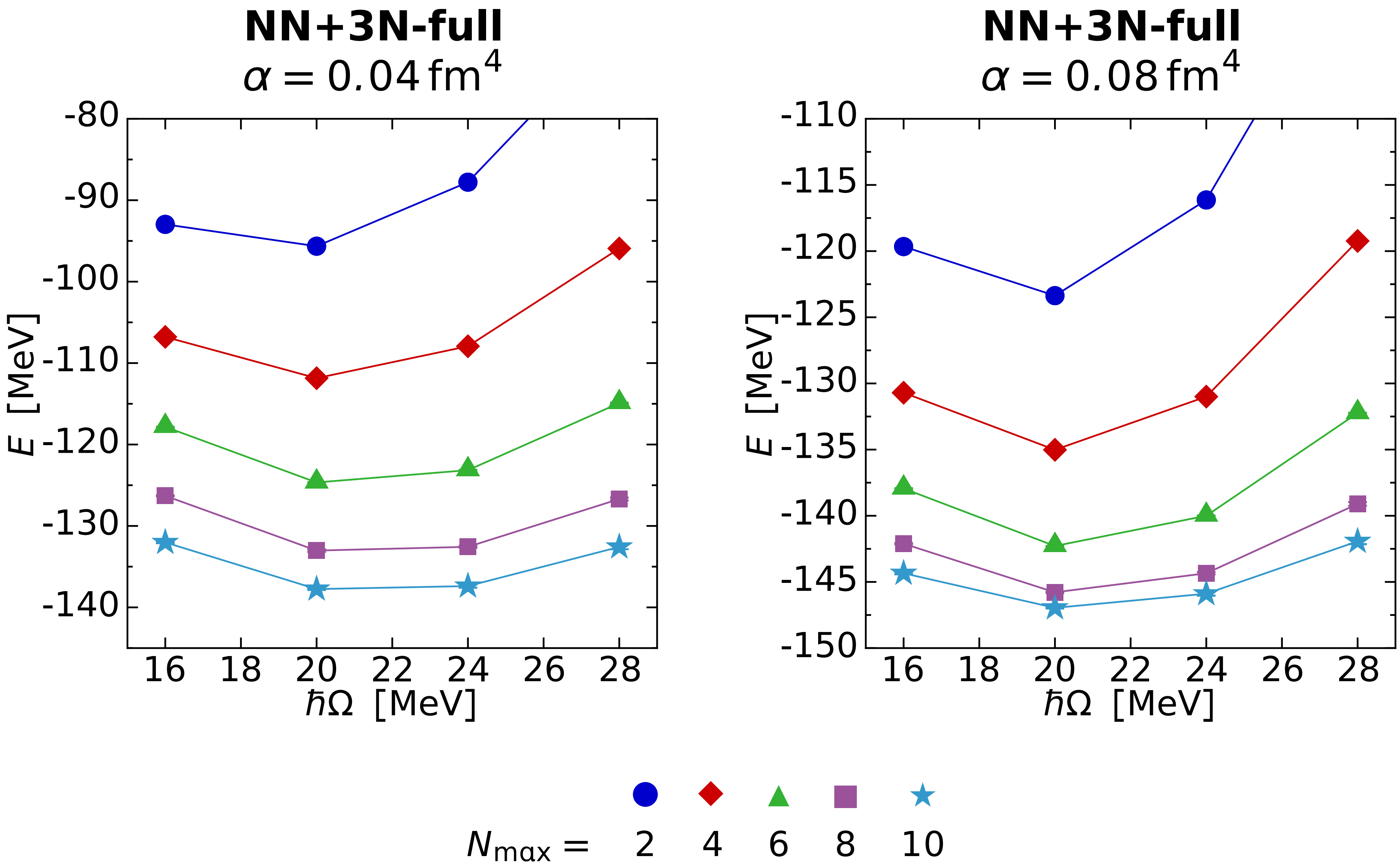
^{16}O: Energy vs. Flow Parameter

Roth, et al; PRL 107, 072501 (2011)



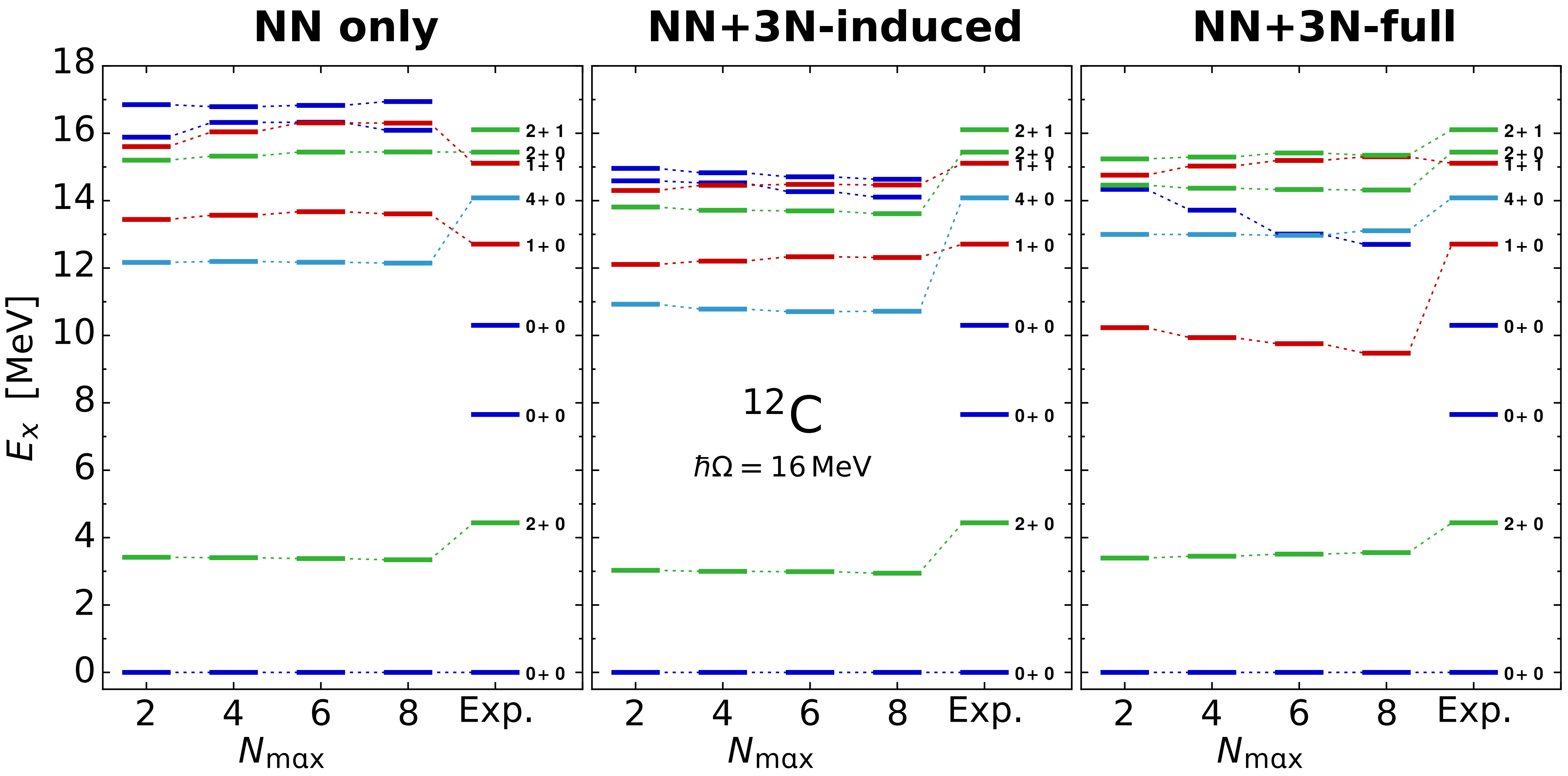
- **initial NN Hamiltonian**
  - induced 3N interactions are significant
  - no indication of induced 4N
  - NN+3N-induced unitarily equivalent to initial NN
- **initial NN+3N Hamiltonian**
  - induced 4N interactions are sizable in upper p-shell

^{16}O: Frequency Dependence



Spectroscopy of ^{12}C

Roth, et al; PRL 107, 072501 (2011)

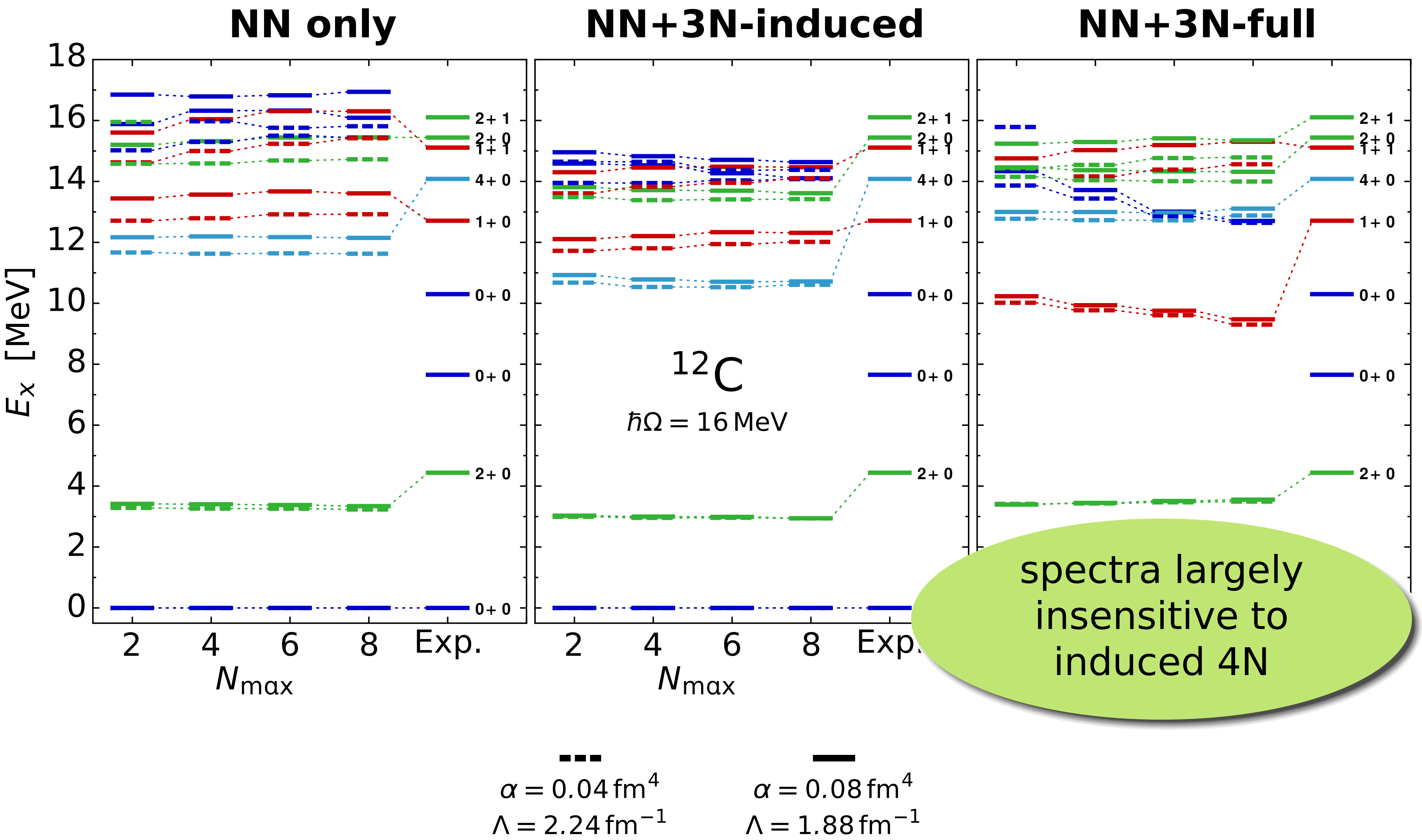


$\alpha = 0.04\,\text{fm}^4$
$\Lambda = 2.24\,\text{fm}^{-1}$

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

Spectroscopy of ^{12}C

Roth, et al; PRL 107, 072501 (2011)



Where do we go from here?

- beyond light 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 **good 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 ?

Origin of
Induced 4N Interaction

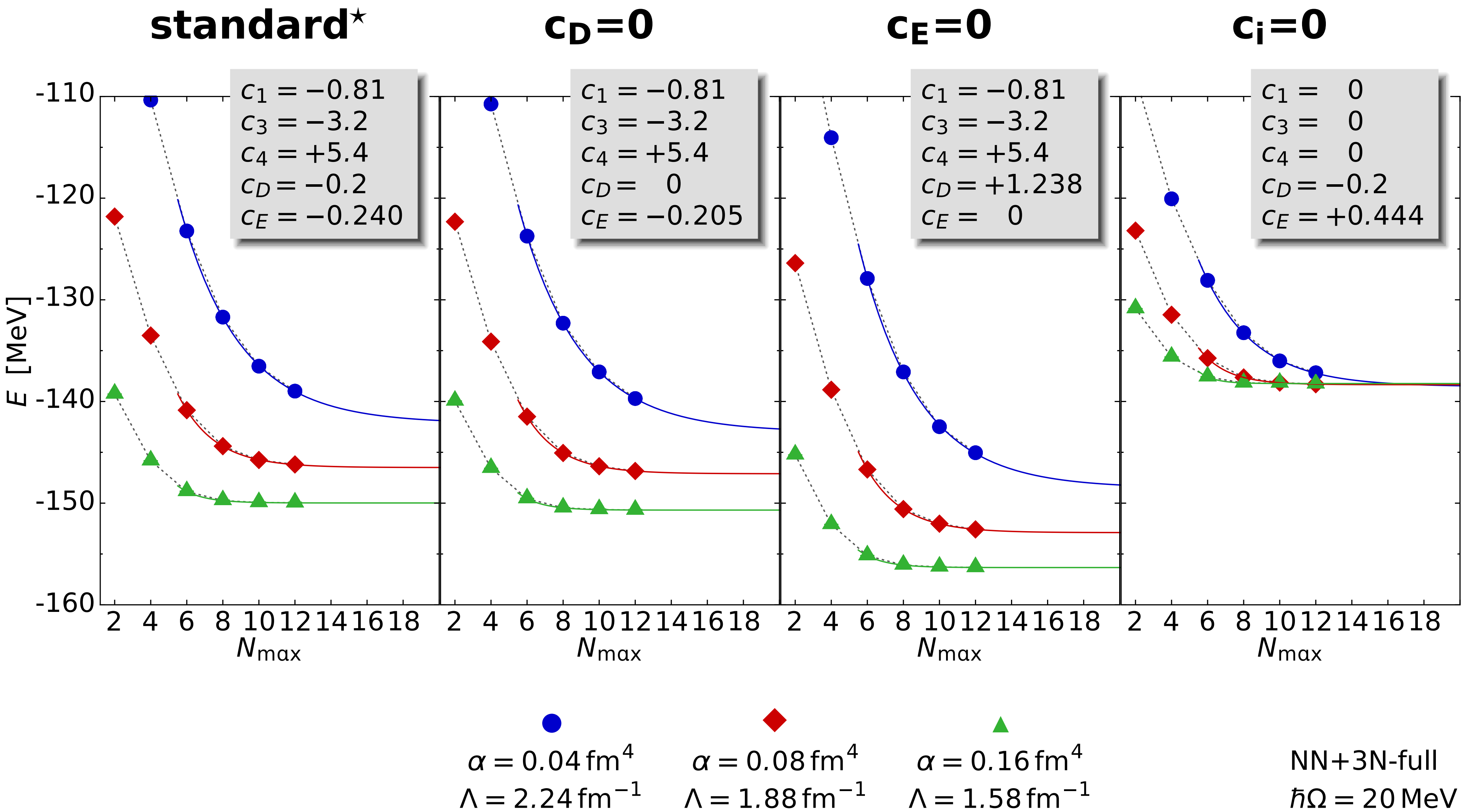
Origin of Induced 4N

- analyze the origin of the induced 4N terms by **switching off individual contributions** of the 3N interaction

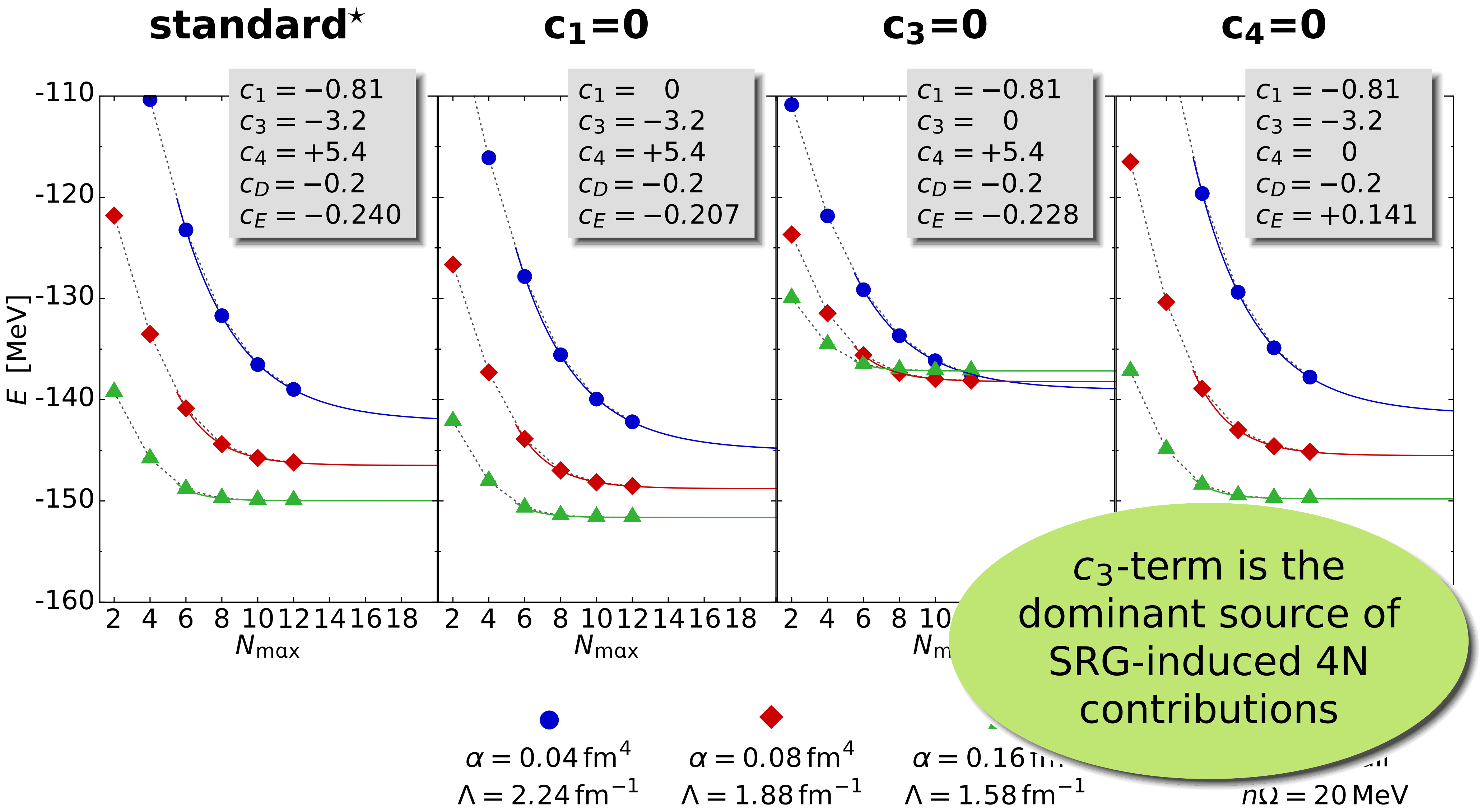
	c_1 [GeV^{-1}]	c_3 [GeV^{-1}]	c_4 [GeV^{-1}]	c_D	c_E
std*	-0.81	-3.2	$+5.4$	-0.2	-0.240
$c_D = 0$	-0.81	-3.2	$+5.4$	0	-0.205
$c_E = 0$	-0.81	-3.2	$+5.4$	$+1.238$	0
$c_i = 0$	0	0	0	-0.2	$+0.444$
$c_1 = 0$	0	-3.2	$+5.4$	-0.2	-0.207
$c_3 = 0$	-0.81	0	$+5.4$	-0.2	-0.228
$c_4 = 0$	-0.81	-3.2	0	-0.2	$+0.141$

- refit c_E (or c_D) parameter to reproduce ^{4}He ground-state energy

^{16}O: Origin of Induced 4N

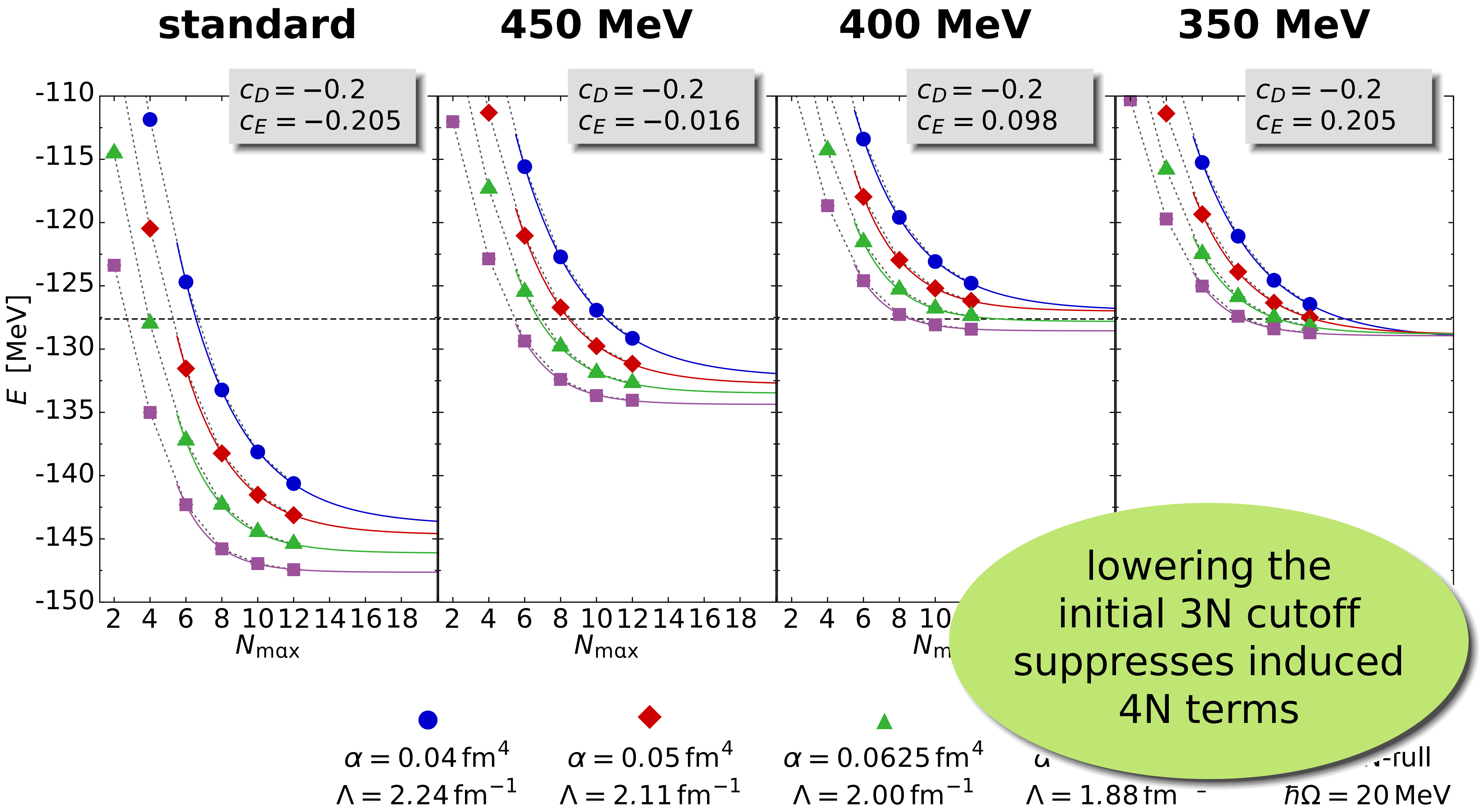


^{16}O: Origin of Induced 4N



c_3-term is the dominant source of SRG-induced 4N contributions

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



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 N2LO

- why this is interesting:
  - **impact of N3LO contributions**: some N3LO diagrams can be absorbed into the N2LO 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 variations of the c_i from different extractions (also affects NN

$$c_1 = -1.23 \dots -0.76\,, \quad c_3 = -5.9$$

  - **cutoff dependence**: does
tion affect nuclear structure obs

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

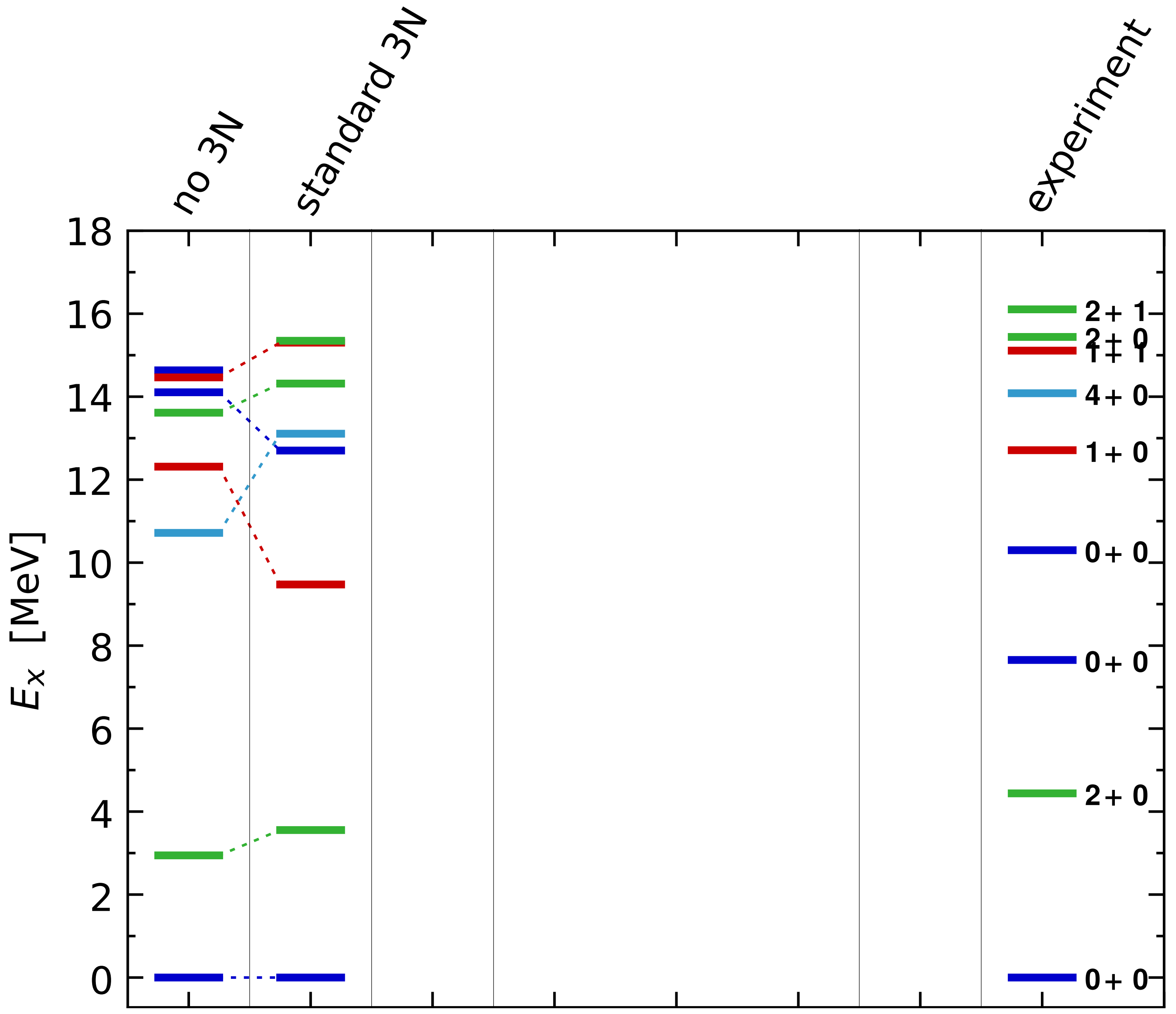
Sensitivity of Spectra on 3N Interactions

- 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

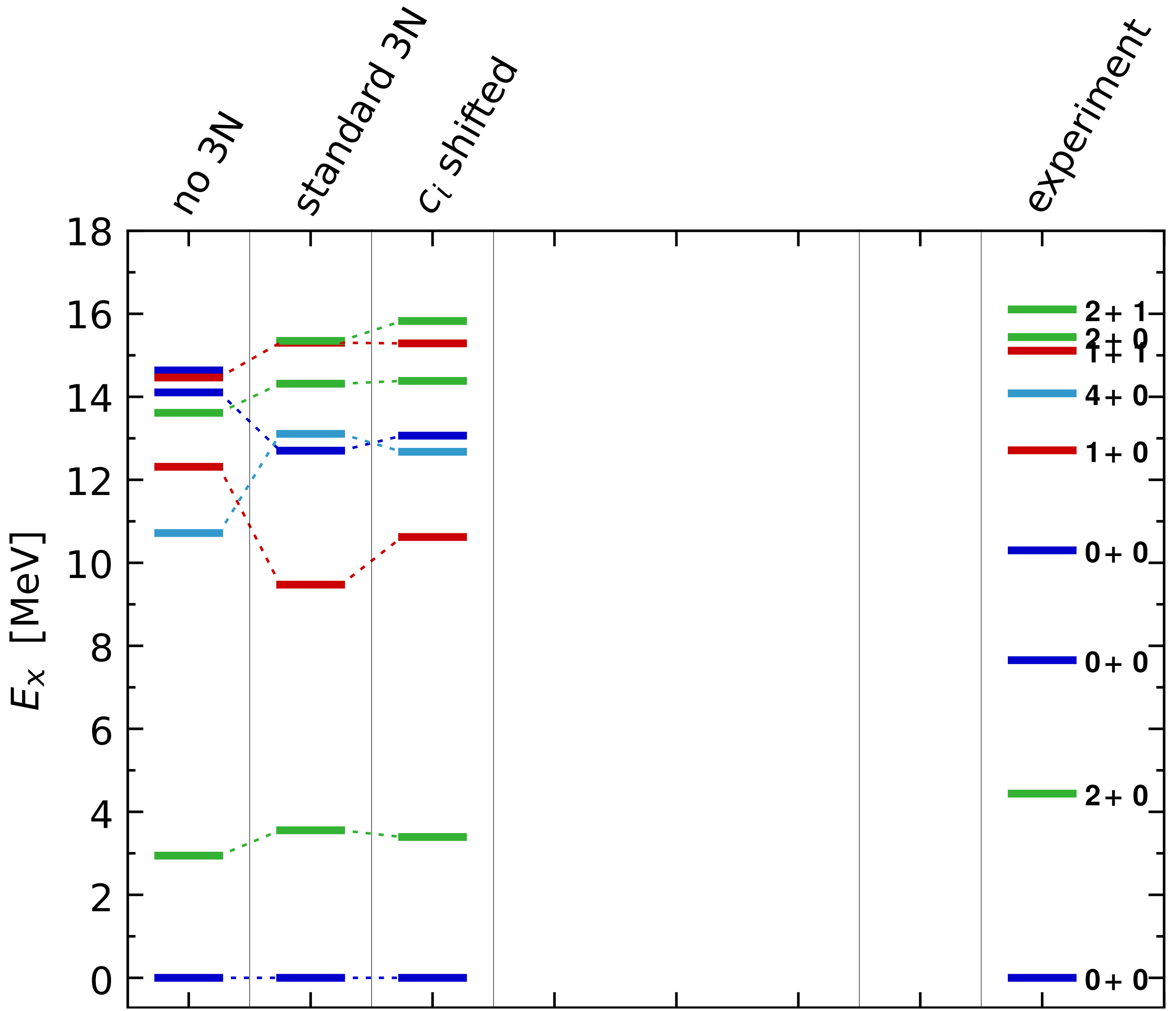
- refit c_E parameter to reproduce ^{4}He ground-state energy

^{12}C : Sensitivity on c_i



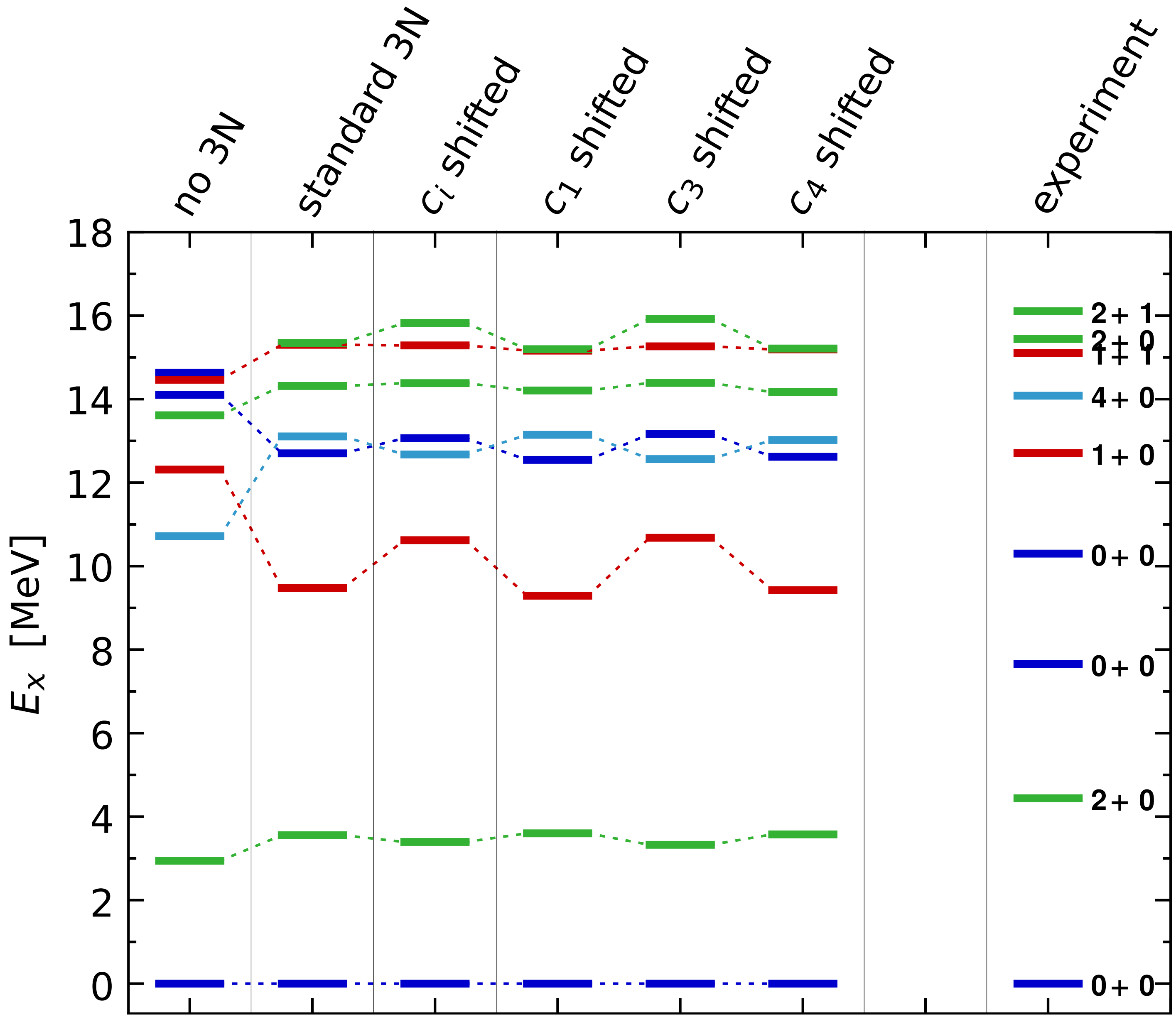
$\hbar\Omega = 16$ MeV
$N_{max} = 8$
$\alpha = 0.08\,\text{fm}^4$

^{12}C : Sensitivity on c_i



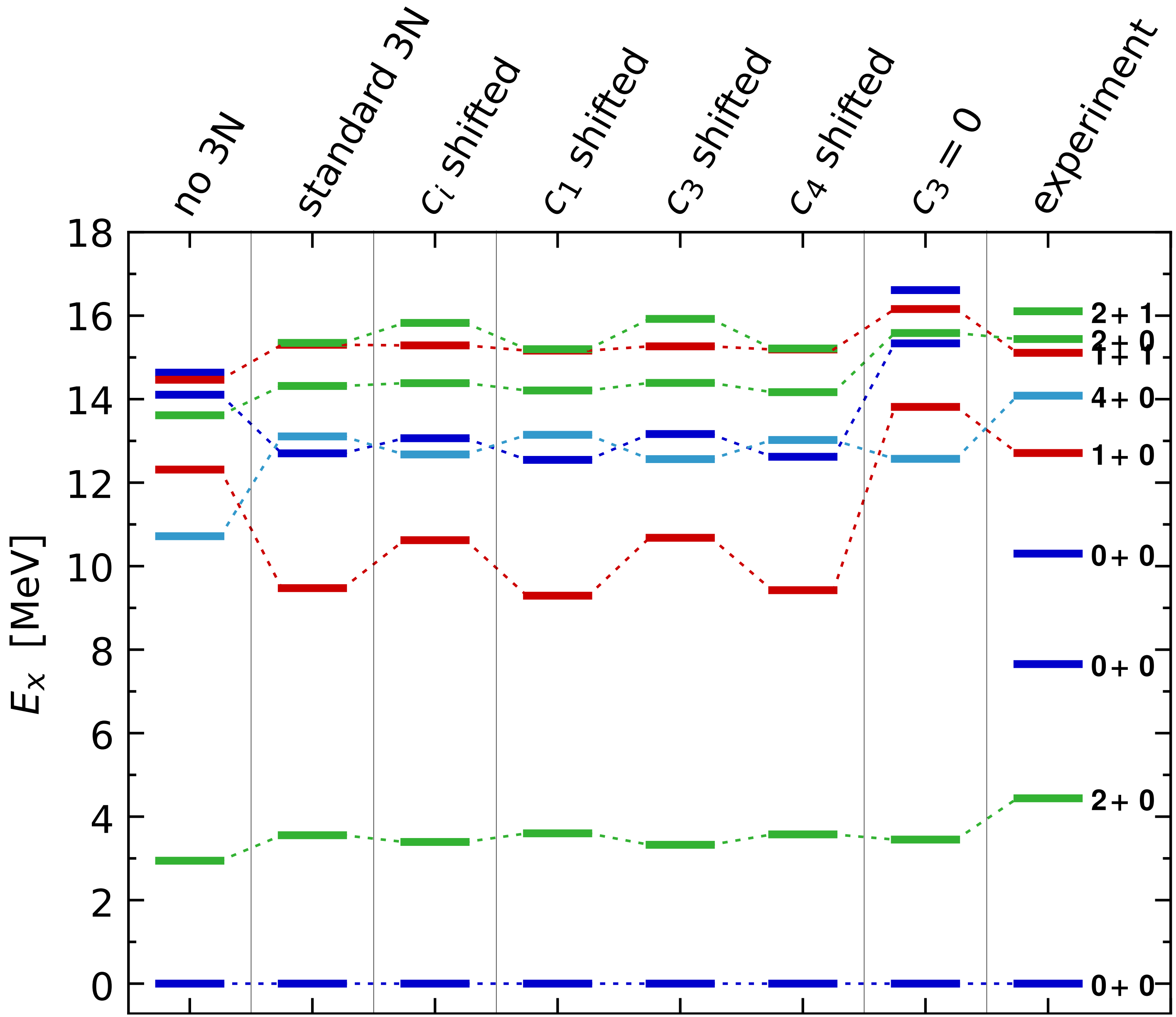
$\hbar\Omega = 16$ MeV
$N_{max} = 8$
$\alpha = 0.08\,\mathrm{fm}^4$

^{12}C : Sensitivity on c_i



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

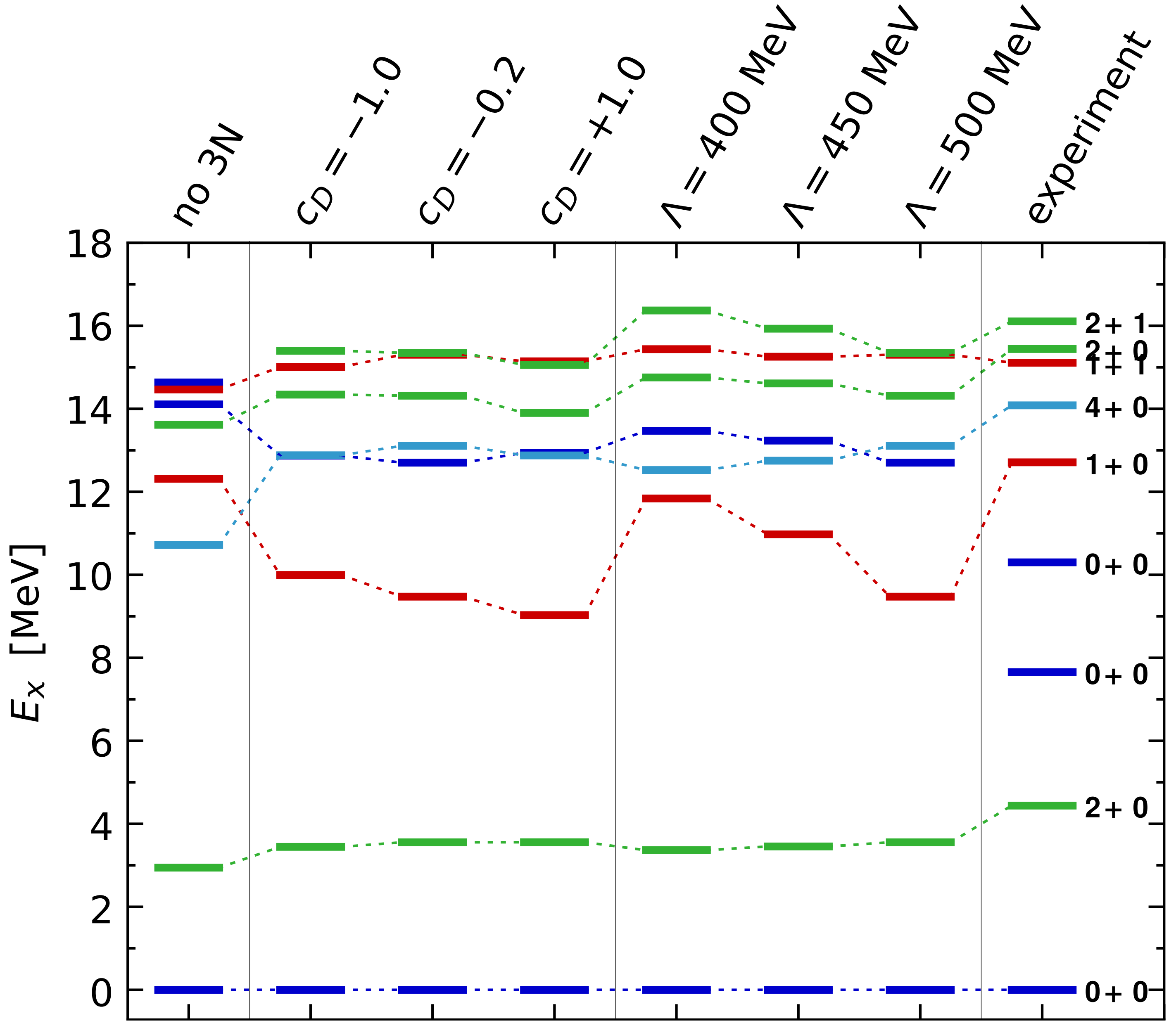
^{12}C : Sensitivity on c_i



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

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

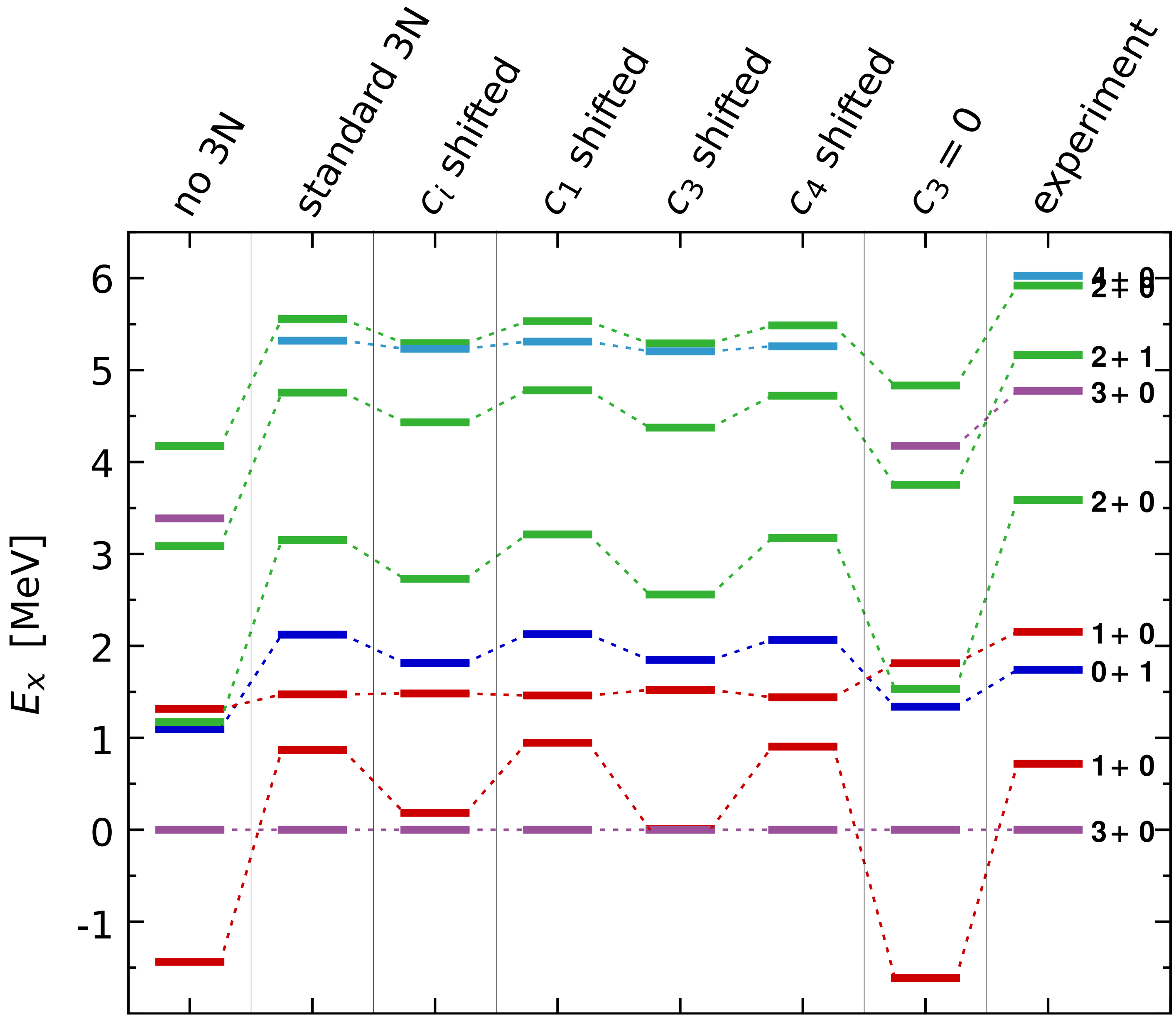
^{12}C : Sensitivity on c_D & Cutoff



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

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

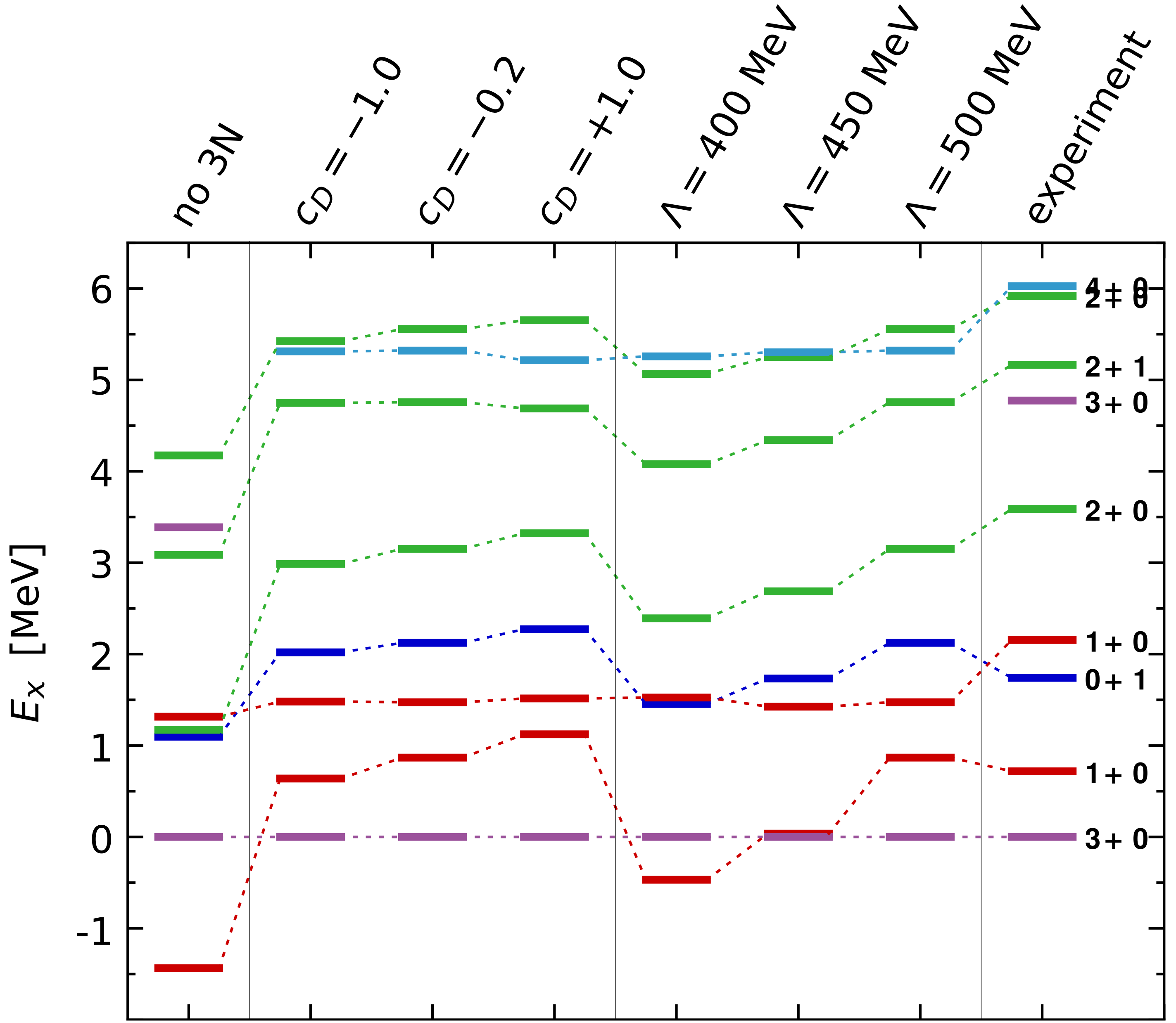
^{10}B : Sensitivity on c_i



- 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
$N_{\max} = 8$
$\alpha = 0.08\,\text{fm}^4$

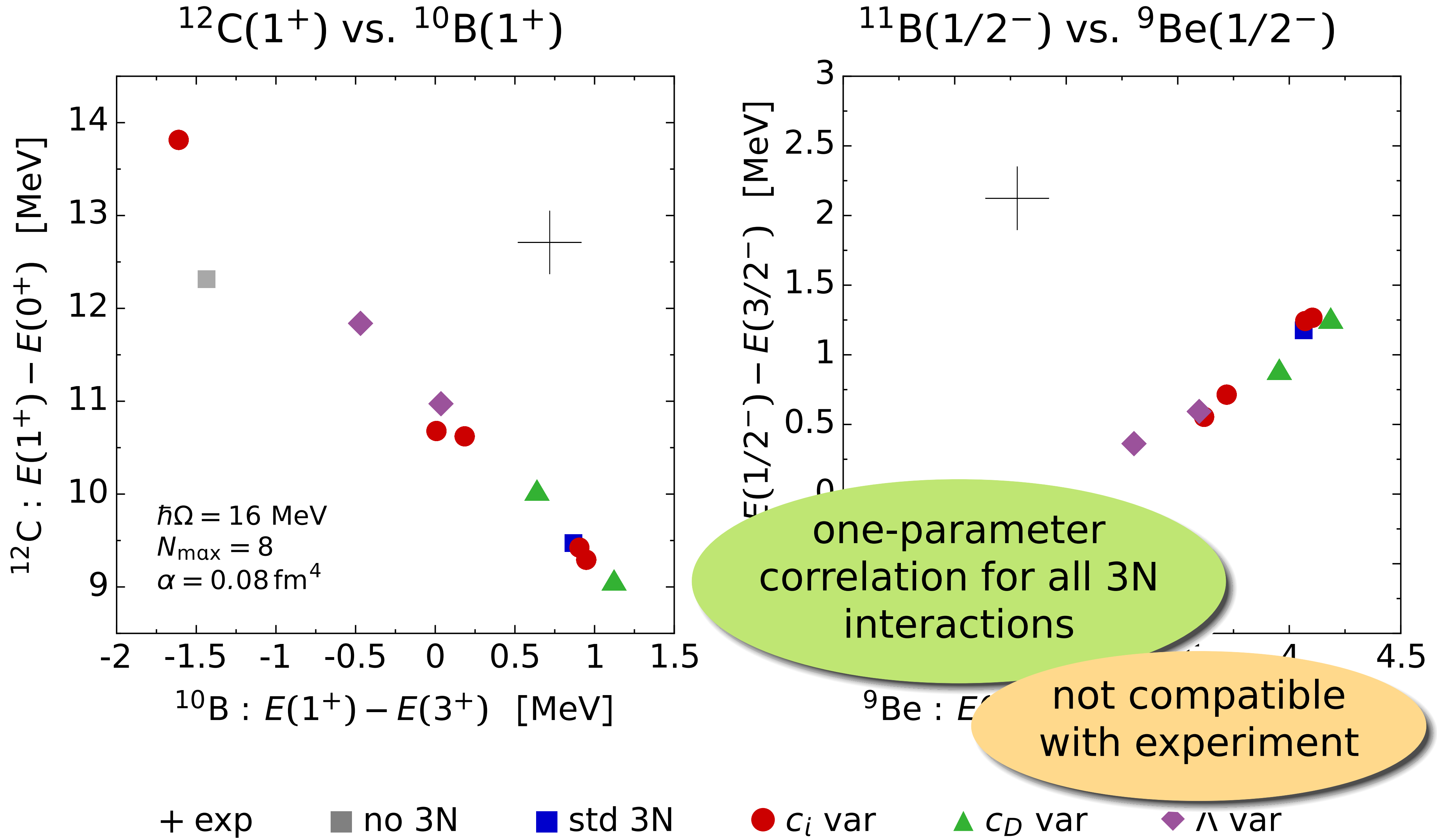
^{10}B : Sensitivity on c_D & Cutoff



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

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

Correlation Analysis



one-parameter correlation for all 3N interactions

not compatible with experiment

The Message...

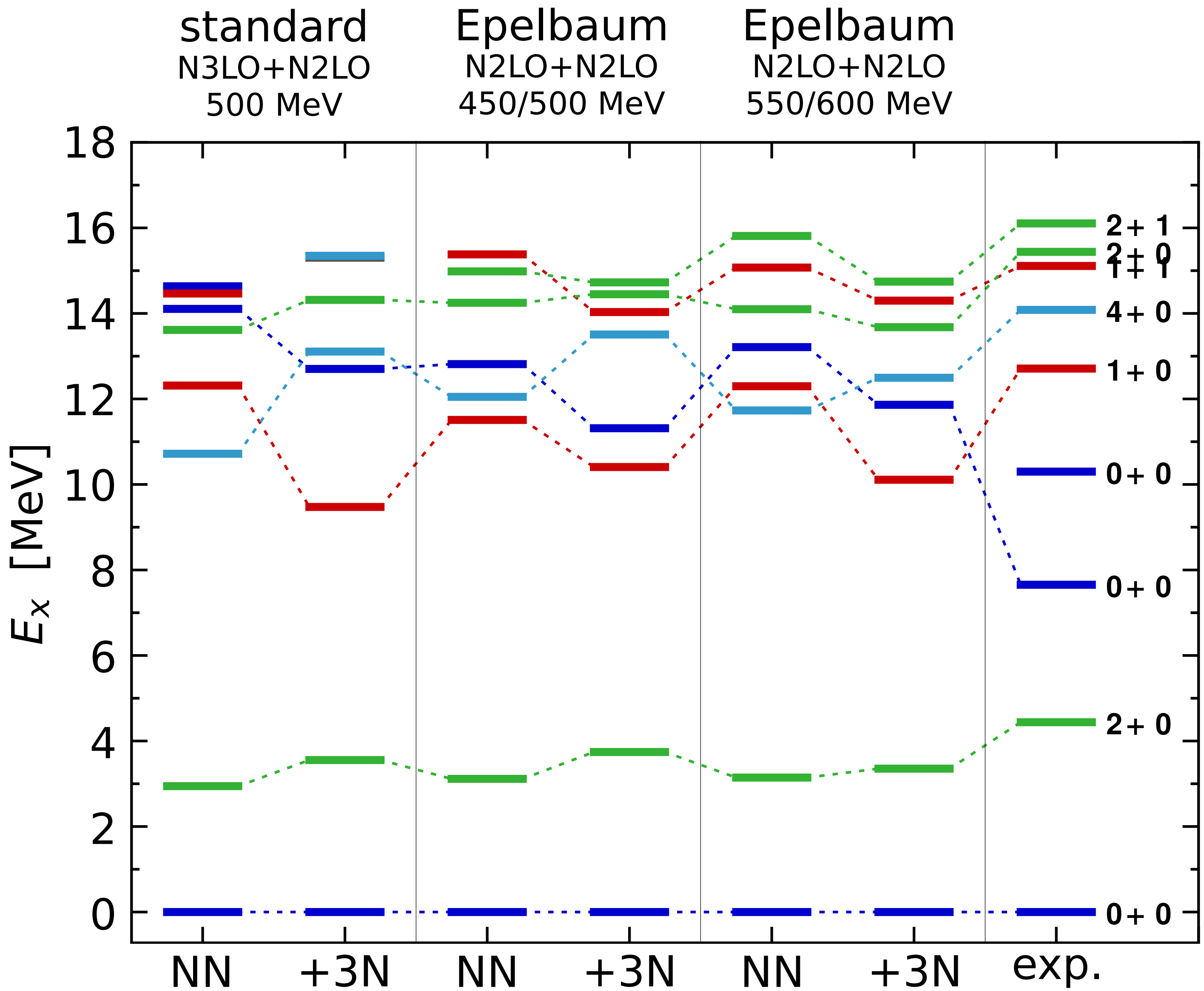
- mid-p-shell nuclei provide **powerful test-bed** for chiral 3N interactions
- individual excited states exhibit a **strong sensitivity** on the details of the 3N interaction
- **c_3 term** drives structural changes of the spectrum (probably through spin-orbit and tensor effects)
- **not able** to describe first 1^+ states in $^{10}B/^{12}C$ and first $1/2^-$ states in $^{9}Be/^{11}B$ simultaneously with 3N at N2LO
- **new operator structures** are needed... N3LO, N4LO, Δ-full !

Towards Next-Generation Chiral Hamiltonians

Technical Aspects

- **starting point**: numerical 3N matrix elements in partial-wave Jacobi-momentum basis
  - numerical partial-wave decomposition of Skibinski et al.
  - ongoing collaborative effort to produce N2LO/N3LO matrix elements (Cracow, Bochum, Bonn, Ohio SU, Iowa SU, Darmstadt)
- **interface**: transformation into Jacobi-HO representation implemented and validated
  - SRG evolution can be done in Jacobi-momentum or HO basis
- **first application**: consistent NN+3N Hamiltonian at N2LO
  - NN at N2LO: Epelbaum et al., cutoffs 450,...,600 MeV, phase-shift fit χ^2/dat $\sim$ 10 ($\sim$ 1) up to 300 MeV (100 MeV)
  - 3N at N2LO: Epelbaum et al., cutoffs 450,...,600 MeV, nonlocal, fit to $a(nd)$ and $E(^3\mathrm{H})$, included up to J=7/2

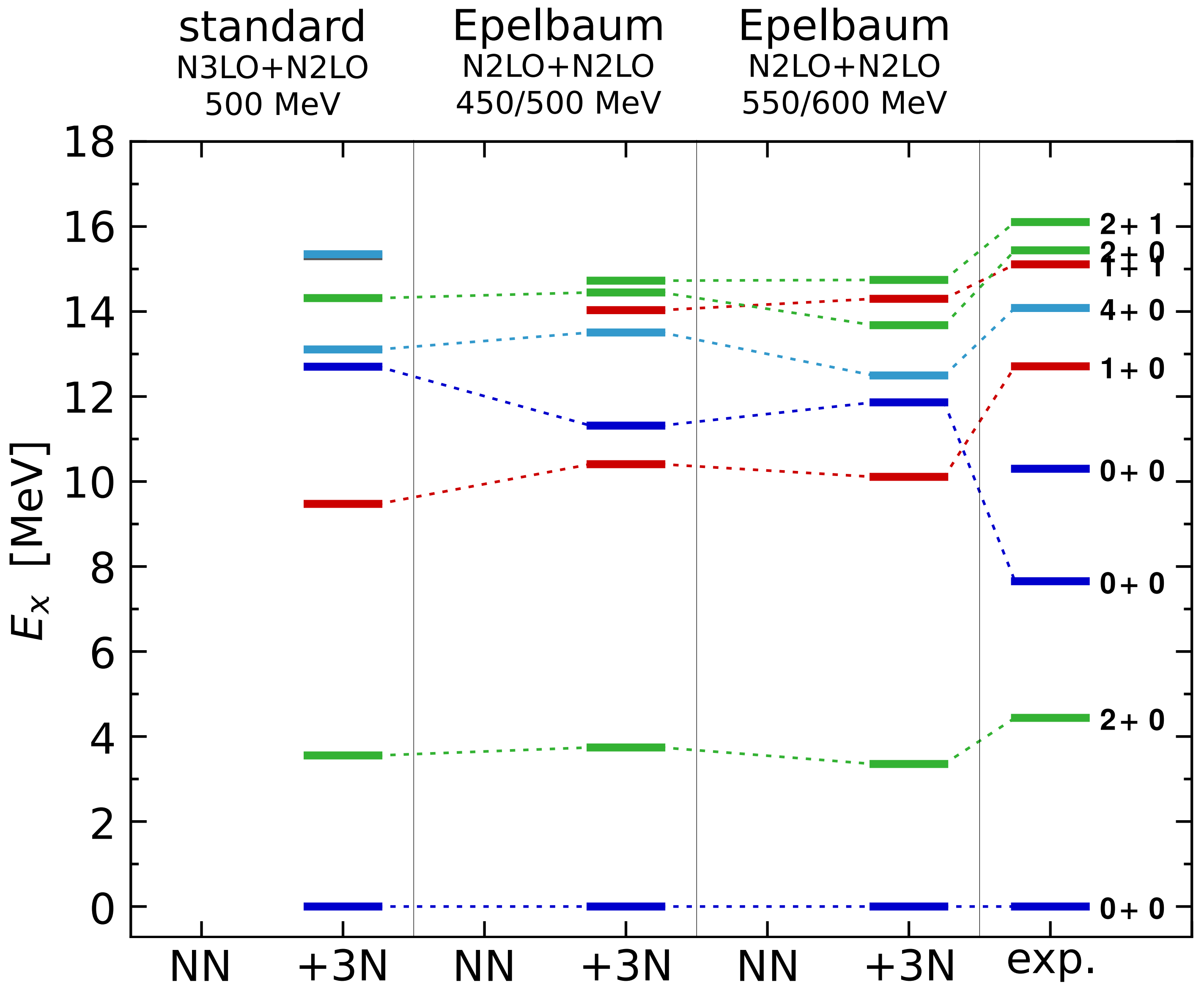
^{12}C : Consistent N2LO Hamiltonians



- rather consistent description with different NN+3N Hamiltonians

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

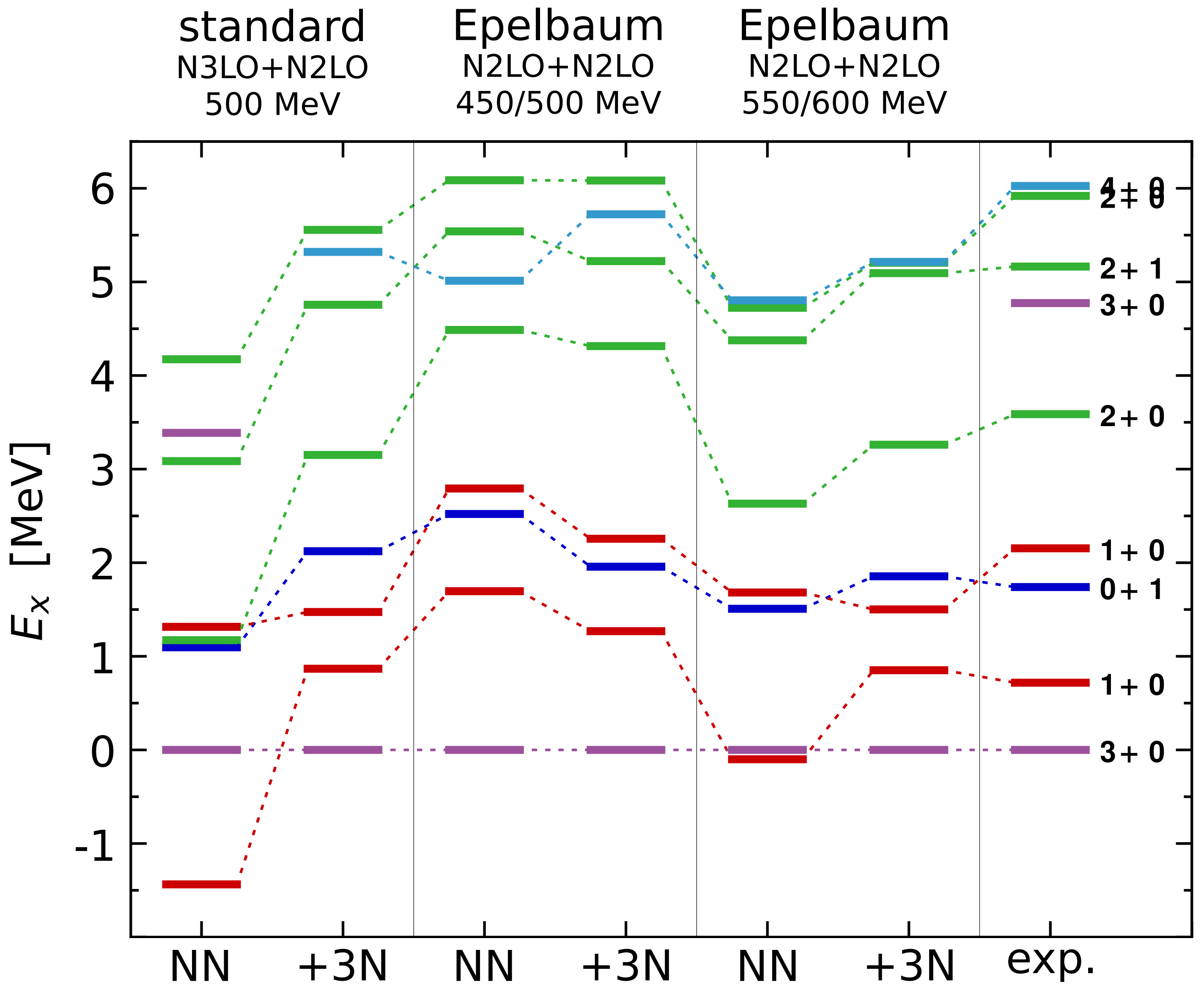
^{12}C : Consistent N2LO Hamiltonians



- rather consistent description with different NN+3N Hamiltonians

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

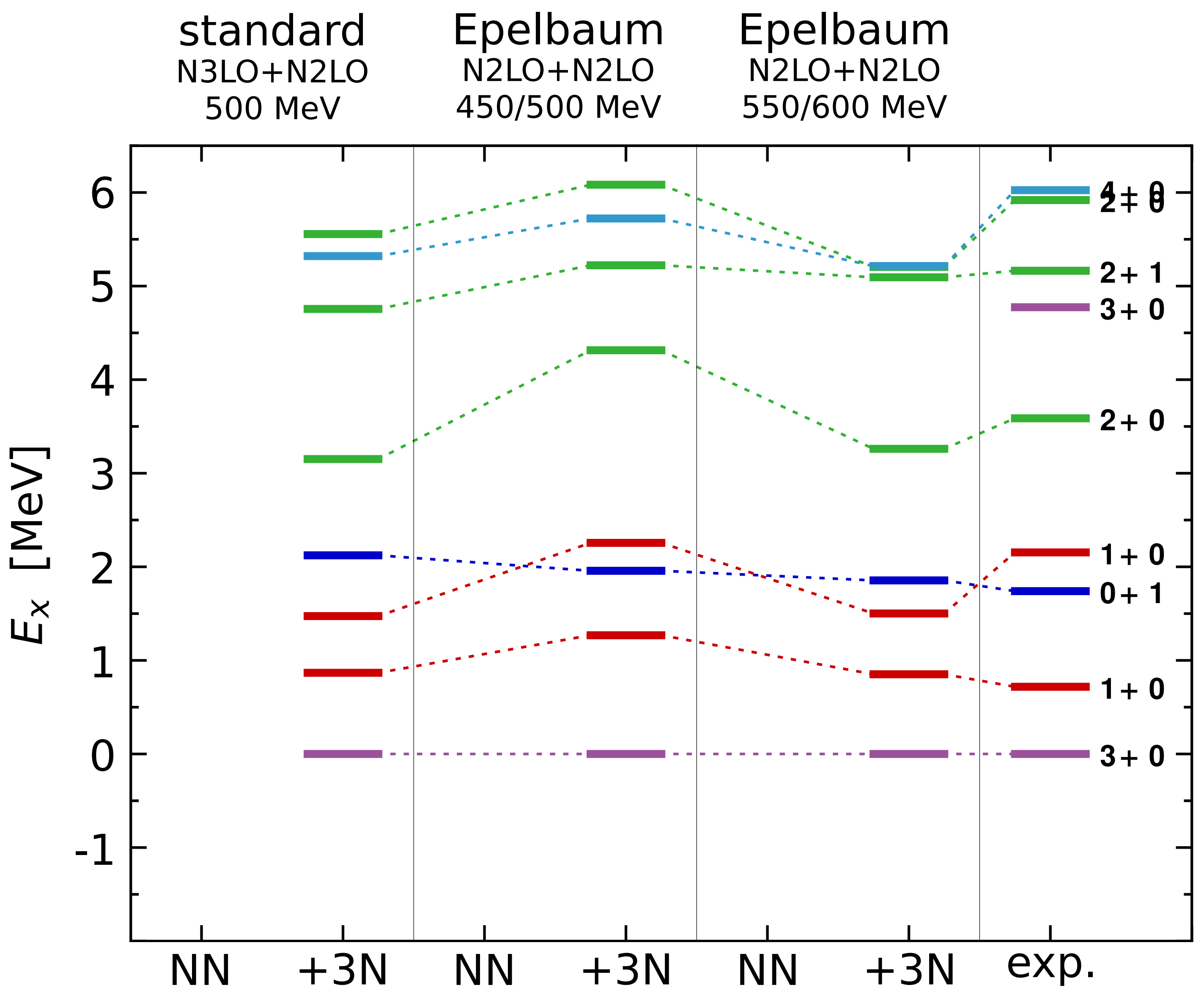
^{10}B : Consistent N2LO Hamiltonians



- large variations at NN level
- more consistent description with NN+3N

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

^{10}B : Consistent N2LO Hamiltonians



- large variations at NN level
- more consistent description with NN+3N

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

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 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