From Chiral EFT Interactions to Nuclear Structure... and Back

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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

- chiral EFT based on the relevant degrees of freedom & symmetries of QCD
- provides consistent NN, 3N,... interaction plus currents

Low-Energy QCD

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

Nuclear Structure

Exact & Approx. Many-Body Methods

Unitary / Similarity Transformation

NN+3N Interaction from Chiral EFT

Low-Energy QCD

- 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

Nuclear Structure

Exact & Approx. Many-Body Methods

Unitary / Similarity Transformation

NN+3N Interaction from Chiral EFT

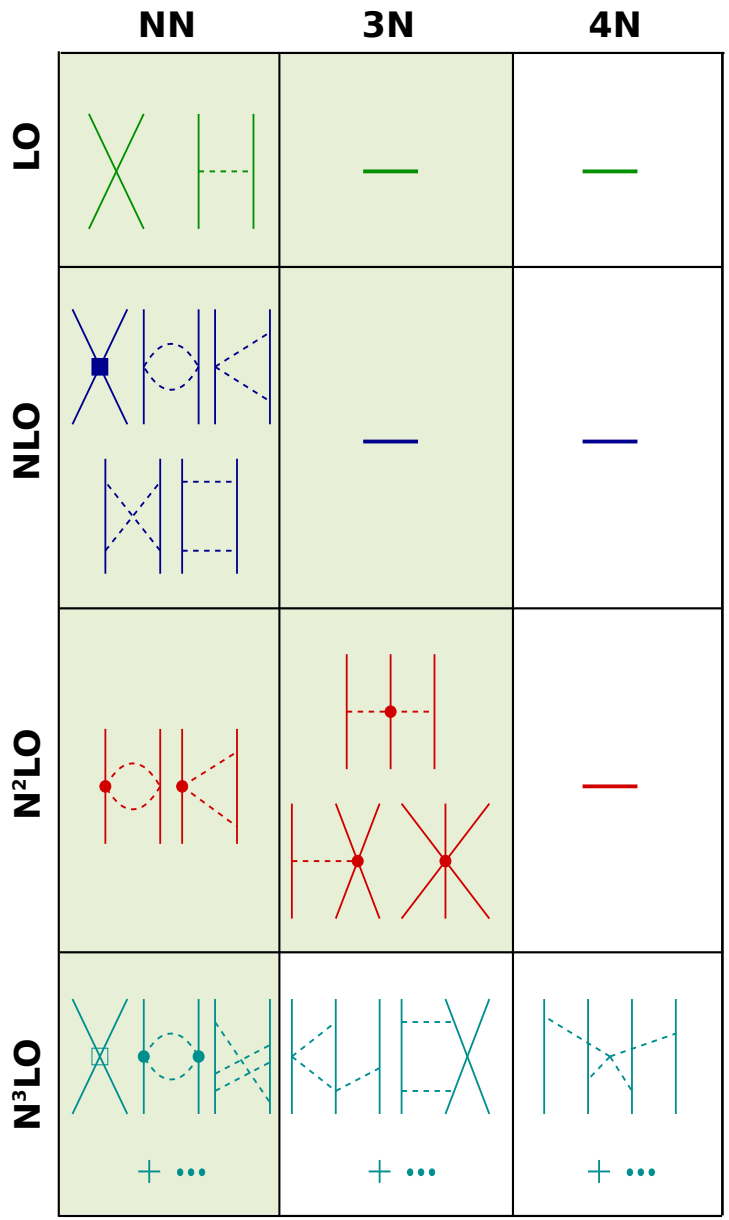
Low-Energy QCD

Nuclear Interactions from Chiral EFT

Nuclear Interactions from Chiral EFT

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

- **standard Hamiltonian**:
  - NN at N3LO:
    Entem & Machleidt, 500 MeV cutoff
  - 3N at N2LO:
    Navrátil, A=3 fit, 500 MeV cutoff
- **variations**:
  - 3N at N2LO:
    modified cutoff or LECs, A=3,4 refit
- **alternatives**:
  - consistent NN+3N at N2LO:
    Epelbaum, POUNDerS
  - consistent NN+3N at N3LO:
    LENPIC collaboration
  - Δ-full chiral EFT, YN interaction,...



Similarity Renormalization Group

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 uncorrelated basis

simplicity and flexibility are great advantages of the SRG approach

- **unitary transformation** of Hami

$$H_\alpha = U_\alpha^\dagger H U_\alpha \qquad U_\alpha$$

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

- **evolution equations** for H_α and U

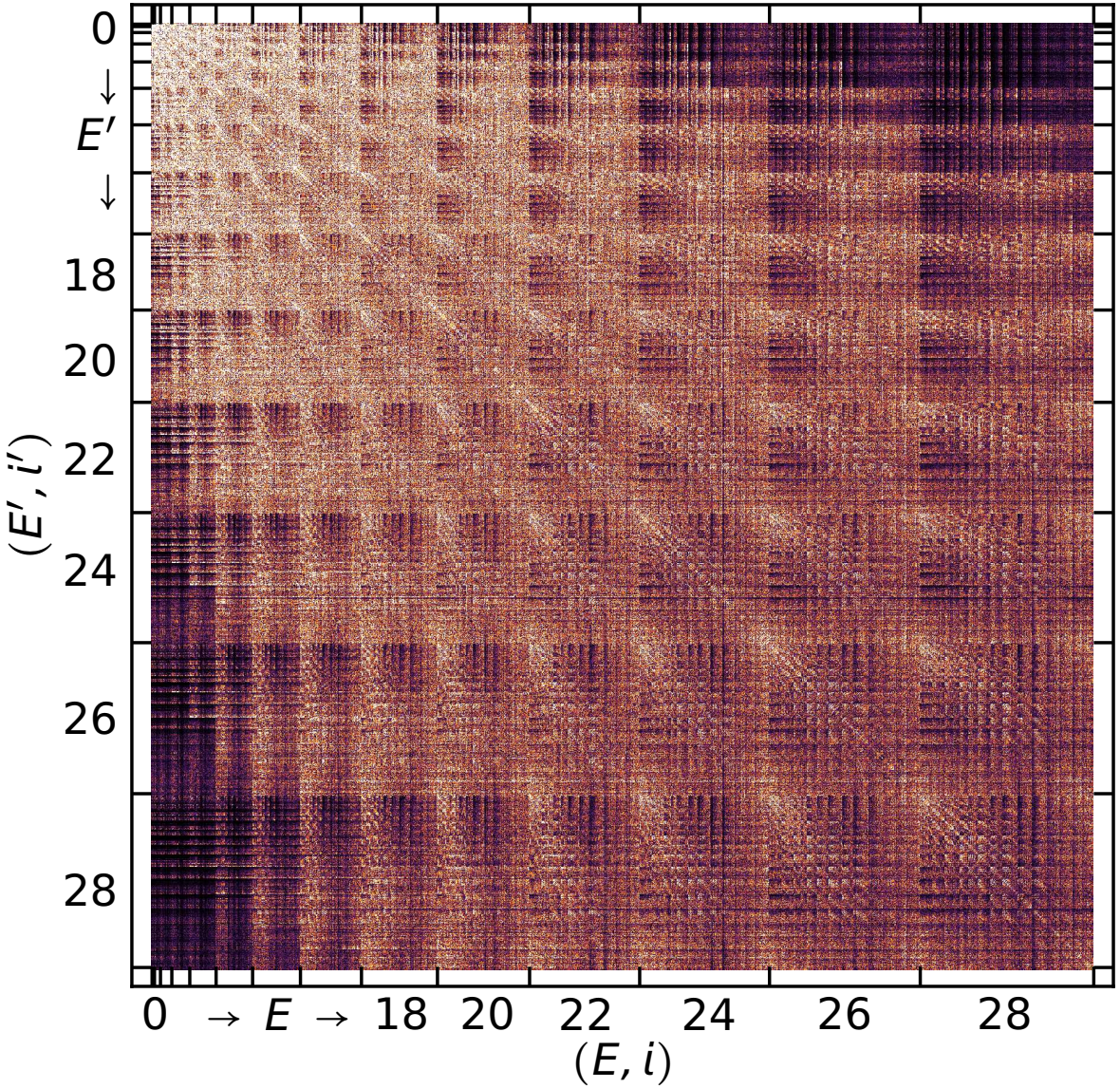
$$\frac{d}{d\alpha} H_\alpha = \left[\eta_\alpha, H_\alpha\right]$$

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

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

SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements

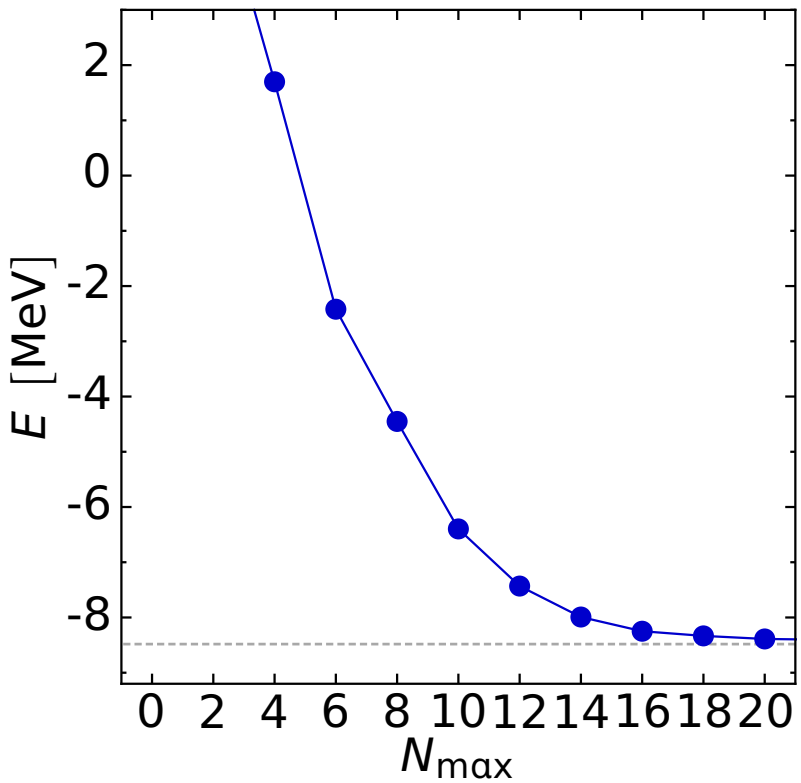


$\alpha = 0.000\,\mathrm{fm}^4$

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

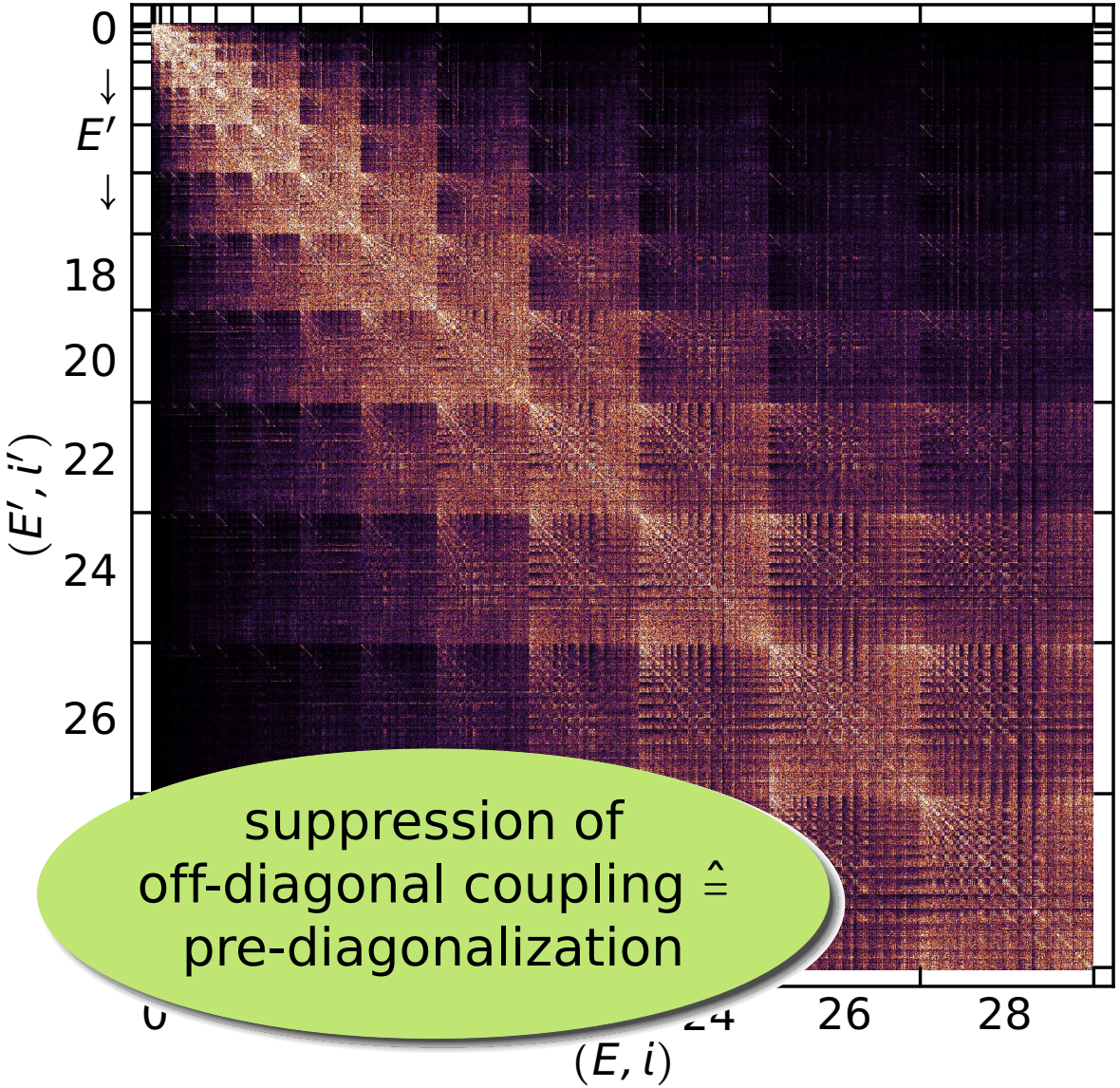
$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 28\,\mathrm{MeV}$

NCSM ground state ^{3}H



SRG Evolution in Three-Body Space

3B-Jacobi HO matrix elements



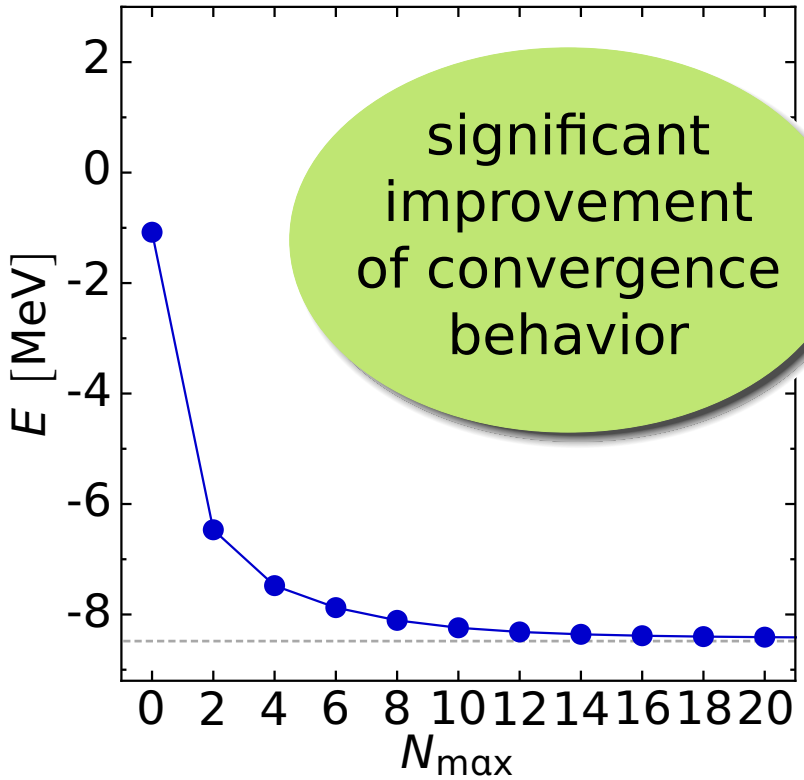
suppression of off-diagonal coupling ≙ pre-diagonalization

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

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

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

NCSM ground state ^{3}H



significant improvement of convergence behavior

Hamiltonian in A-Body Space

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

$$\mathrm{H}_\alpha = \mathrm{H}_\alpha^{[1]} + \mathrm{H}_\alpha^{[2]} + \mathrm{H}_\alpha^{[3]} + \mathrm{H}_\alpha^{[4]} + \mathrm{H}_\alpha^{[5]} + \ldots$$

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

- flow-parameter α provides **diagnostic tool** to assess neglected higher-order contributions

SRG-Evolved Hamiltonians

$\mathbf{NN_{only}}$	use initial NN, keep evolved NN
$\mathbf{NN + 3N_{ind}}$	use initial NN, keep evolved NN+3N
$\mathbf{NN + 3N_{full}}$	use initial NN+3N, keep evolved NN+3N
$\mathbf{NN + 3N_{full} + 4N_{ind}}$	use initial NN+3N, keep evolved NN+3N+4N

Importance Truncated No-Core Shell Model

No-Core Shell Model

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

NCSM is one of the most powerful and universal ab initio many-body 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 $E_{3\,\max} = 16$

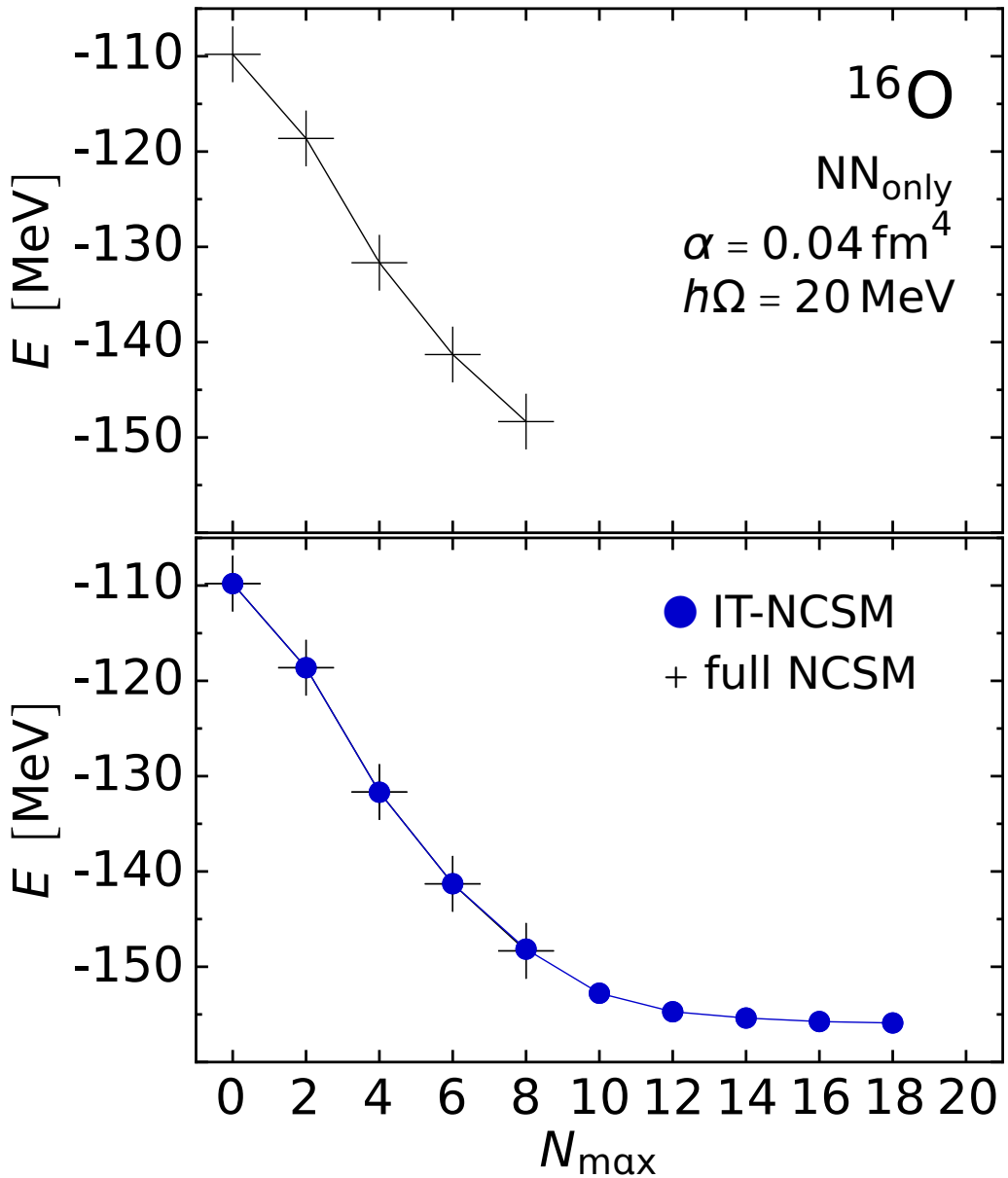
Importance Truncated NCSM

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

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

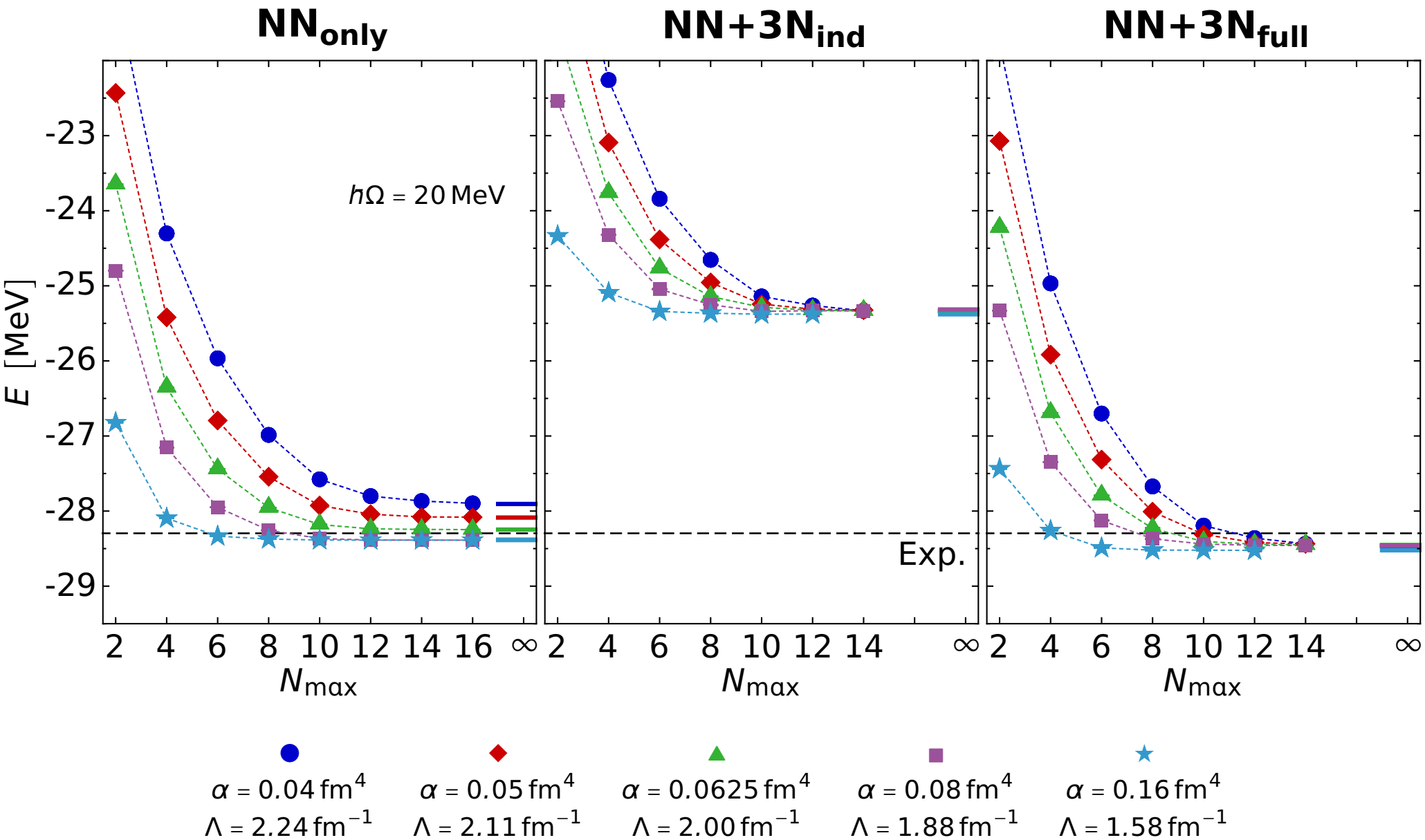
Importance Truncation

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



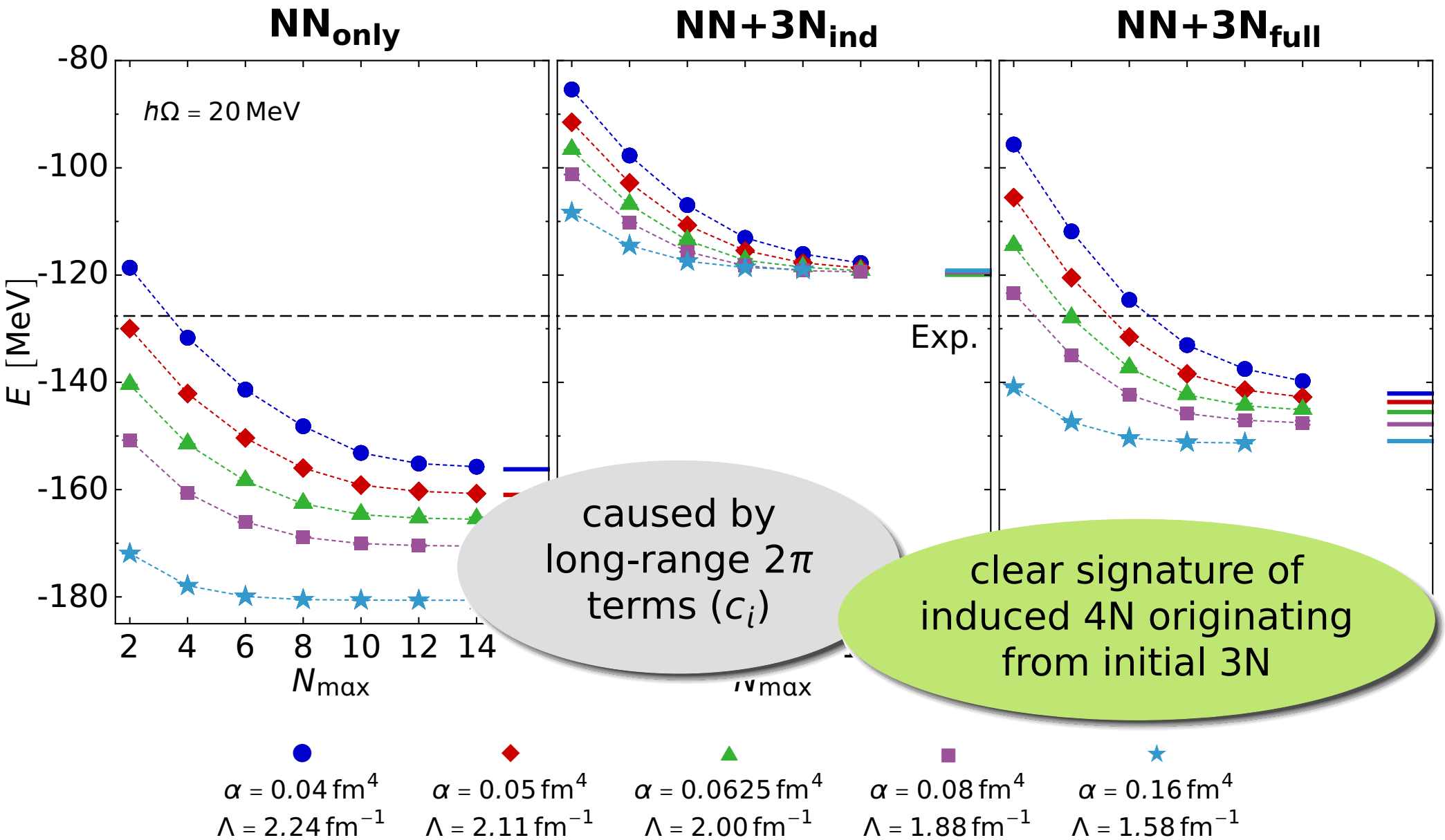
^{4}He: Ground-State Energies

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



^{16}O: Ground-State Energies

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

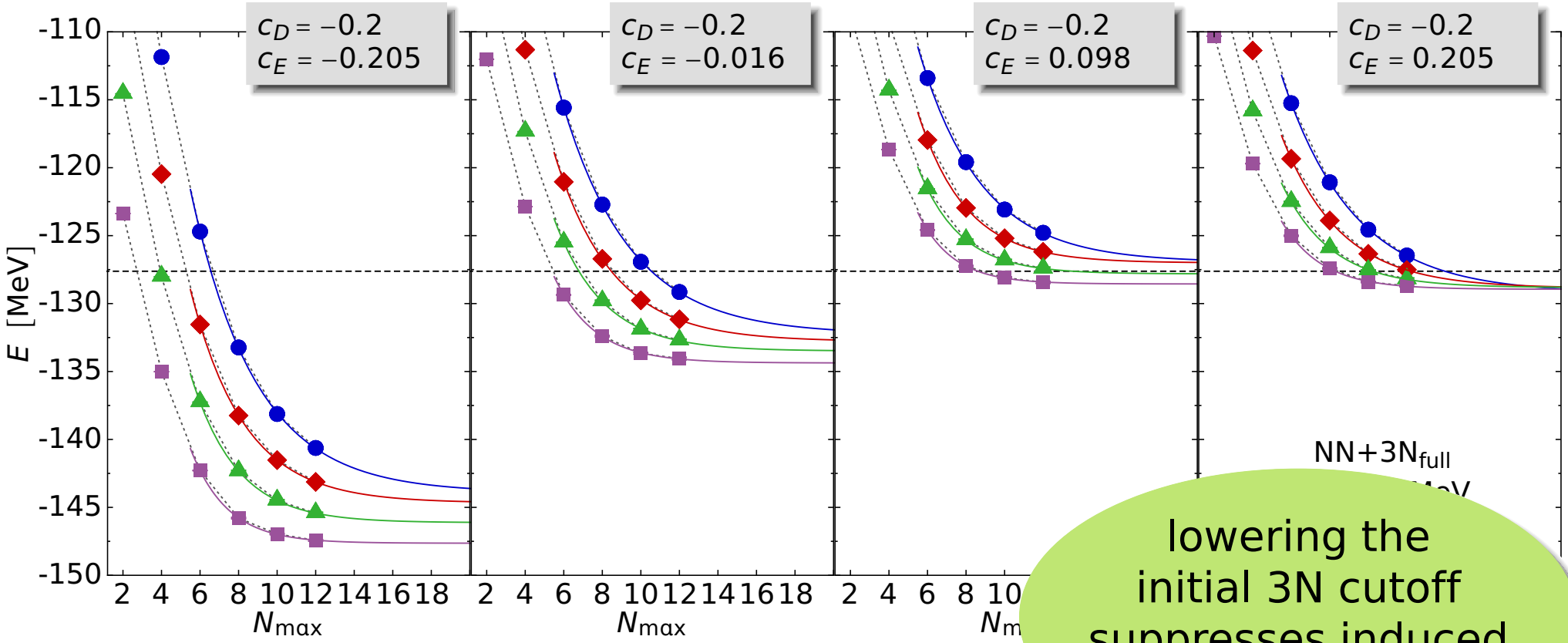


^{16}O: Lowering the Initial 3N Cutoff

standard

reduced 3N cutoff
(c_E refit to ^{4}He binding energy)

500 MeV **450 MeV** **400 MeV** **350 MeV**



lowering the initial 3N cutoff suppresses induced 4N terms

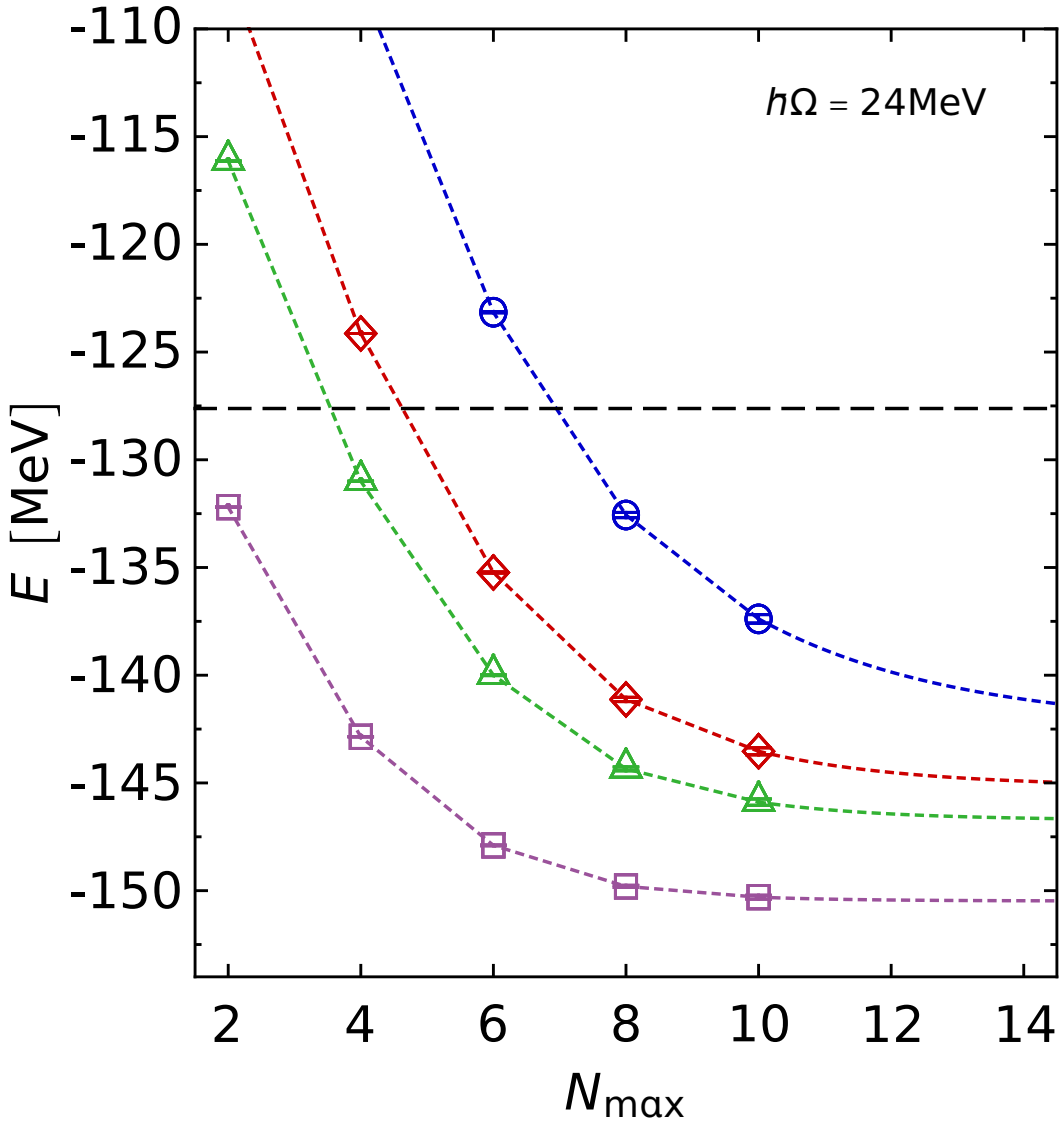
● $\alpha = 0.04\,\mathrm{fm}^4$ $\Lambda = 2.24\,\mathrm{fm}^{-1}$

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

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

α [illegible] $\Lambda = 1.88\,\mathrm{fm}$ [illegible]

^{16}O: Explicit Inclusion of Induced 4N

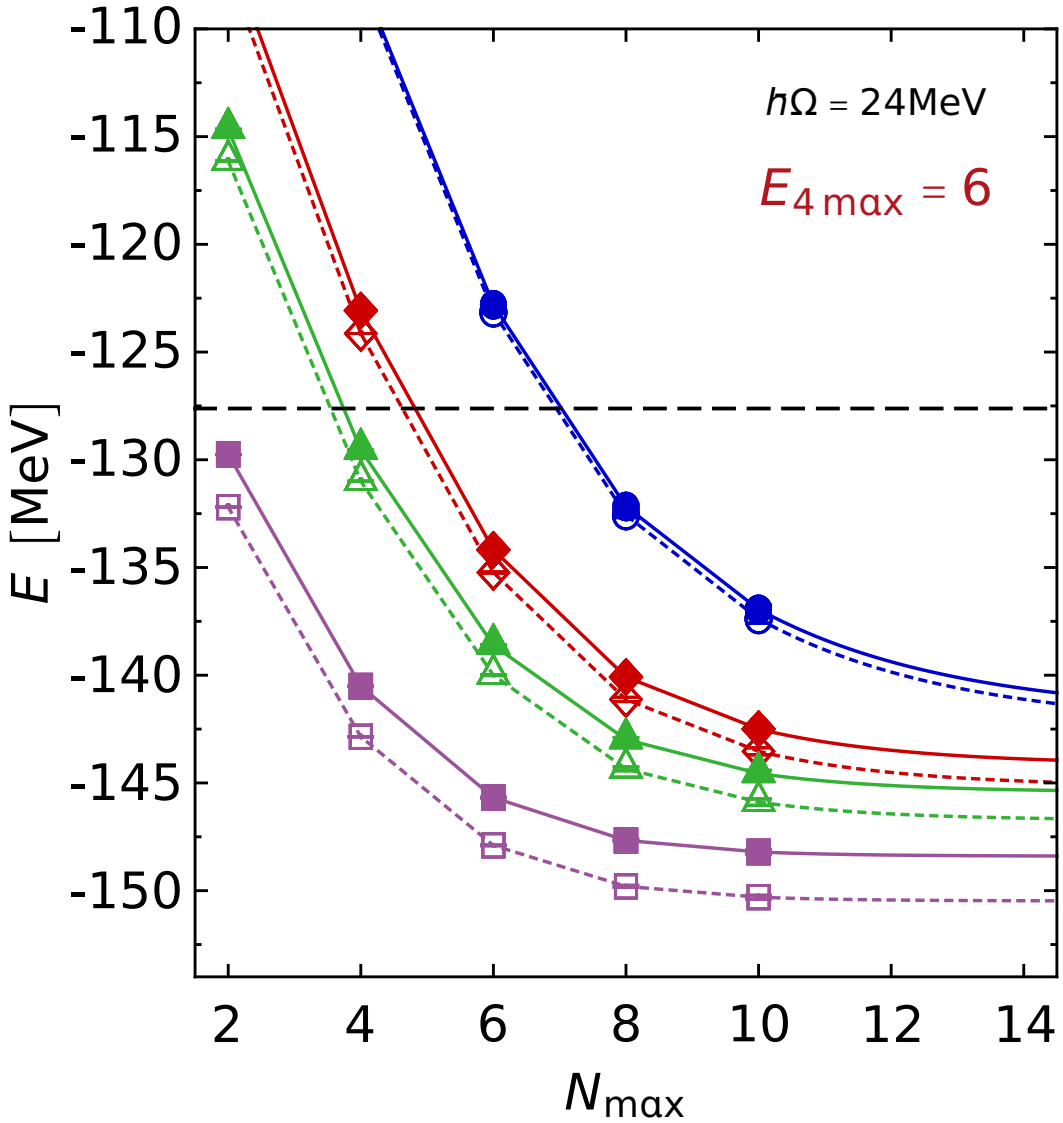


- induced 4N from SRG evolution in four-body Jacobi-HO
- transformation to *m*- or *JT*-scheme 4N matrix elements
- explicit 4N terms in IT-NCSM

NN+3N$_{\mathbf{full}}$

- $\alpha = 0.04\,\mathrm{fm}^4$
- $\alpha = 0.0625\,\mathrm{fm}^4$
- $\alpha = 0.08\,\mathrm{fm}^4$
- $\alpha = 0.16\,\mathrm{fm}^4$

^{16}O: Explicit Inclusion of Induced 4N



- induced 4N from SRG evolution in four-body Jacobi-HO
- transformation to *m*- or *JT*-scheme 4N matrix elements
- explicit 4N terms in IT-NCSM

NN+3N$_{\mathbf{full}}$

NN+3N$_{\mathbf{full}}$+4N$_{\mathbf{ind}}$ (0^+0)

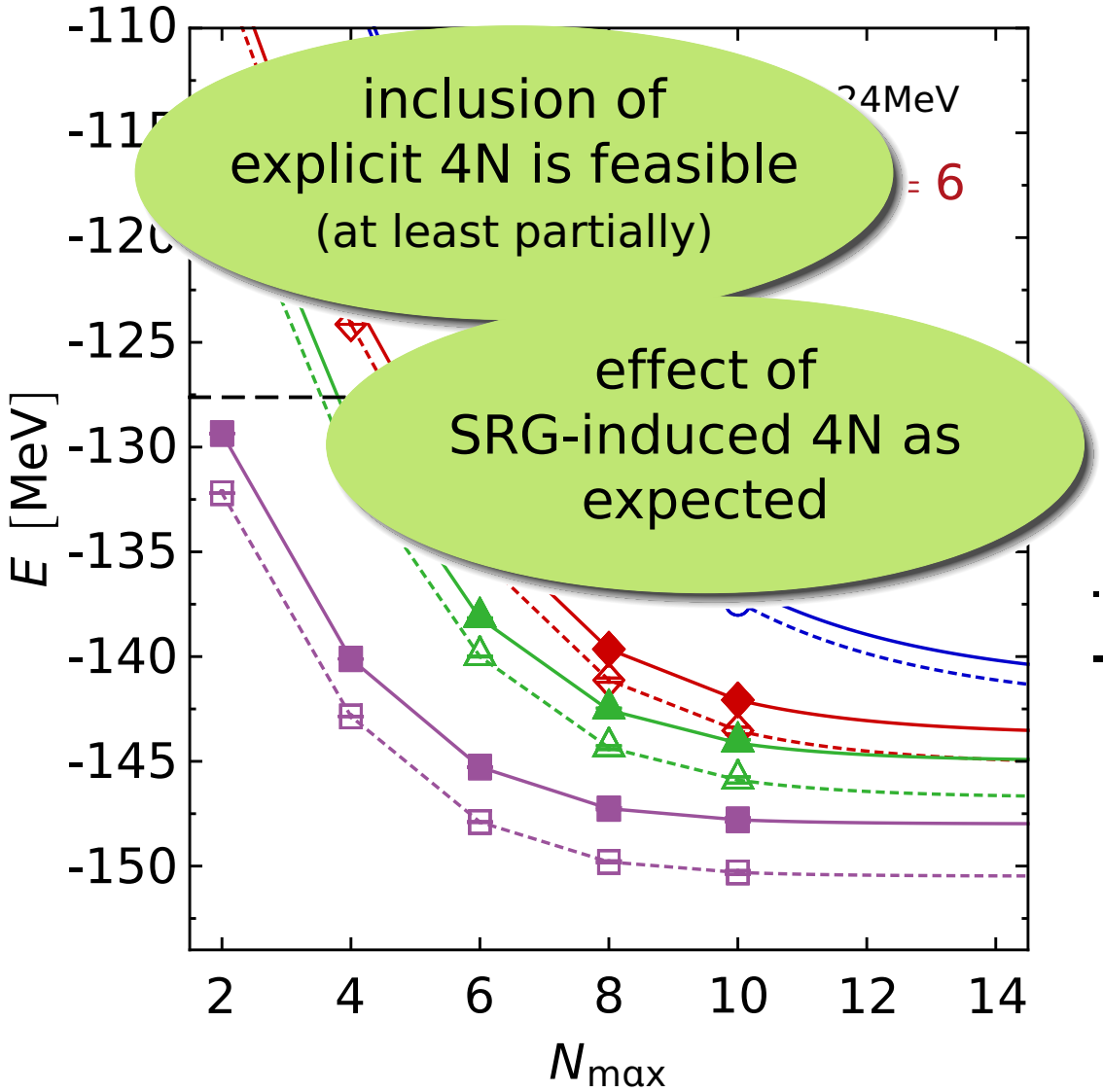
$\alpha = 0.04\,\mathrm{fm}^4$

$\alpha = 0.0625\,\mathrm{fm}^4$

$\alpha = 0.08\,\mathrm{fm}^4$

$\alpha = 0.16\,\mathrm{fm}^4$

^{16}O: Explicit Inclusion of Induced 4N



- induced 4N from SRG evolution in four-body Jacobi-HO
- transformation to *m*- or *JT*-scheme 4N matrix elements
- explicit 4N terms in IT-NCSM

NN+3N$_{\mathbf{full}}$

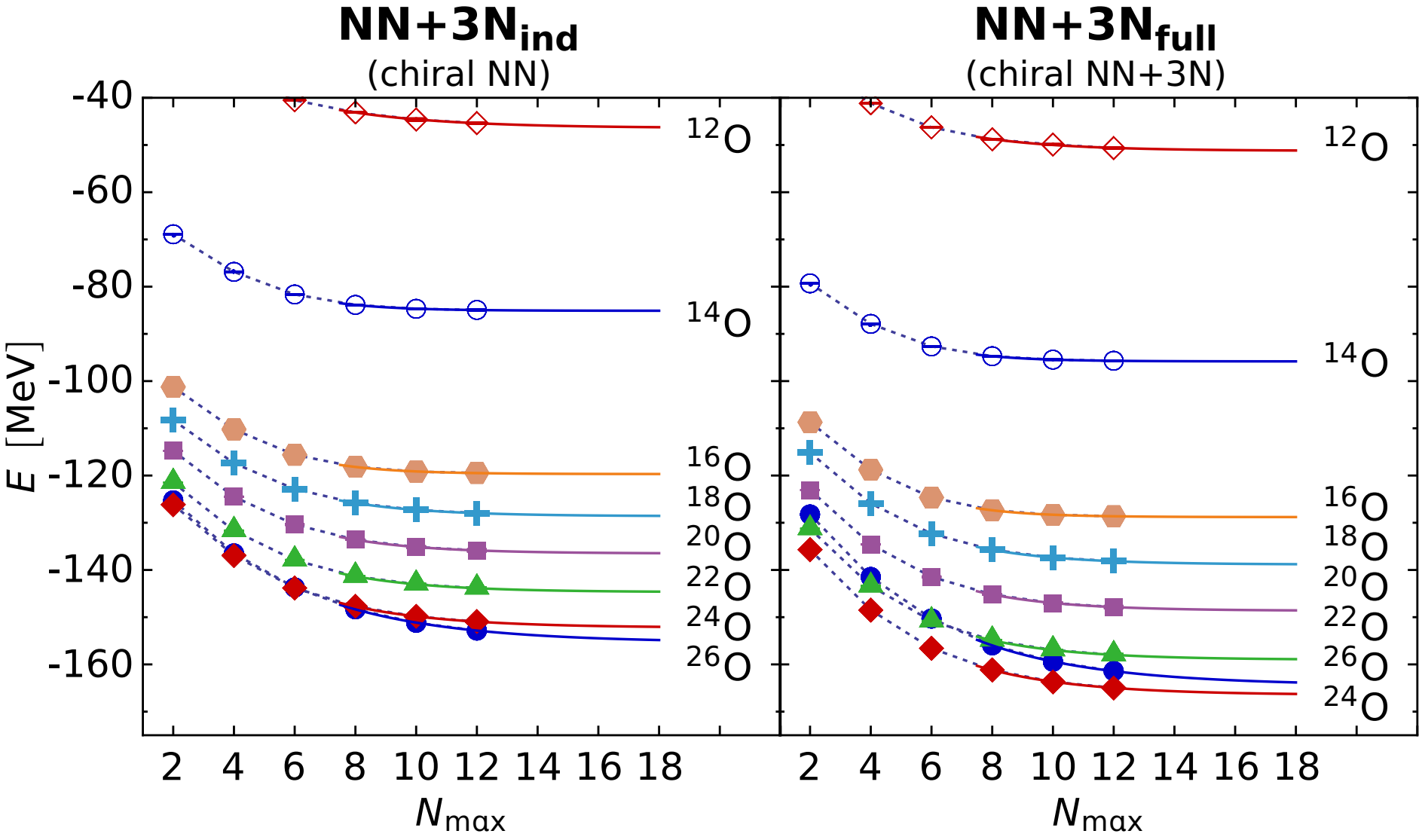
NN+3N$_{\mathbf{full}}$+4N$_{\mathbf{ind}}$ $(0^+0, 0^-0, 0^+1)$

- $\alpha = 0.04\,\mathrm{fm}^4$
- $\alpha = 0.0625\,\mathrm{fm}^4$
- $\alpha = 0.08\,\mathrm{fm}^4$
- $\alpha = 0.16\,\mathrm{fm}^4$

Ab Initio IT-NCSM Calculations for p- and sd-Shell Nuclei

Ground States of Oxygen Isotopes

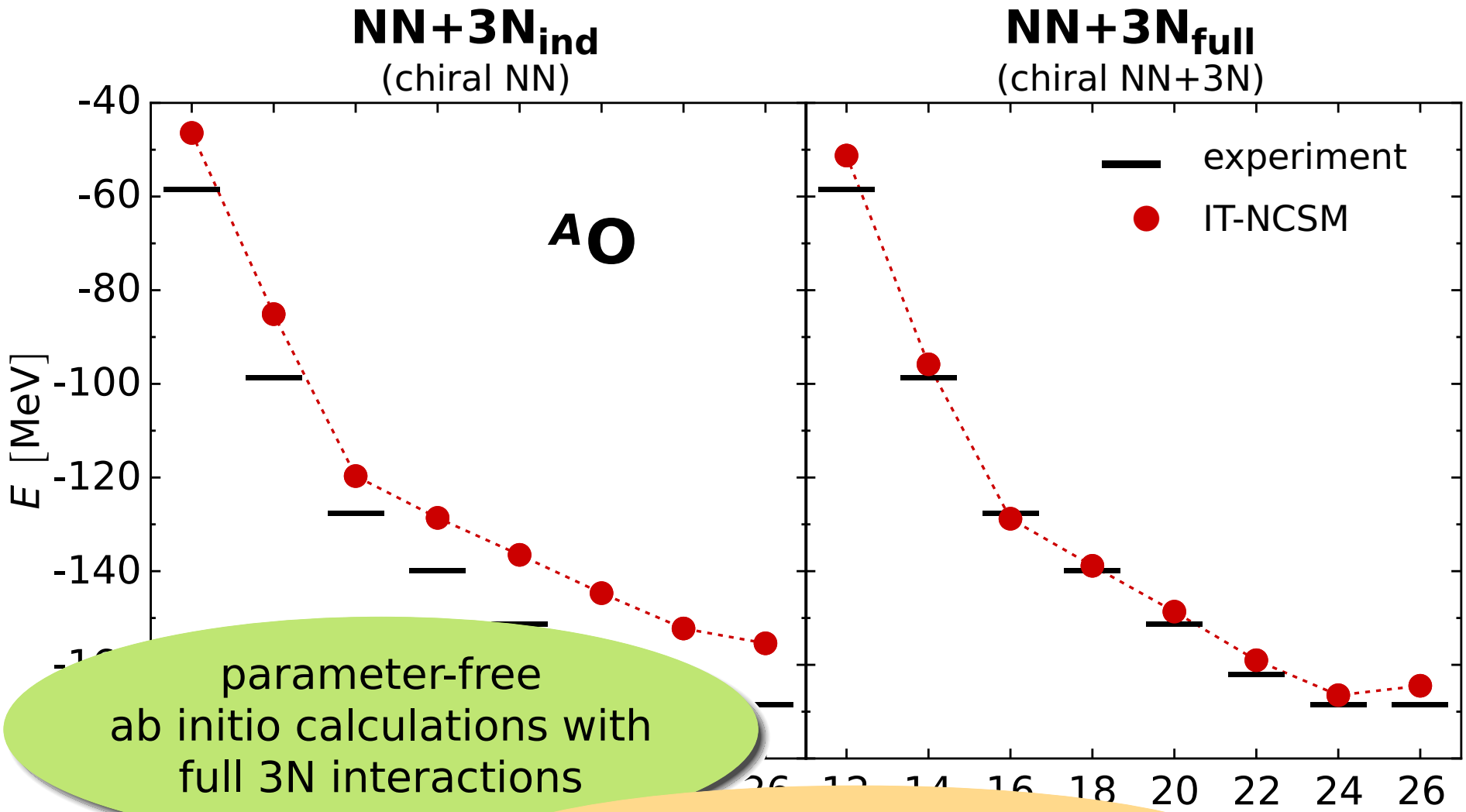
Hergert et al., PRL 110, 242501 (2013)



$\Lambda_{3N} = 400$ MeV, $\alpha = 0.08\,\mathrm{fm}^4$, $E_{3\,max} = 14$, optimal $\hbar\Omega$

Ground States of Oxygen Isotopes

Hergert et al., PRL 110, 242501 (2013)



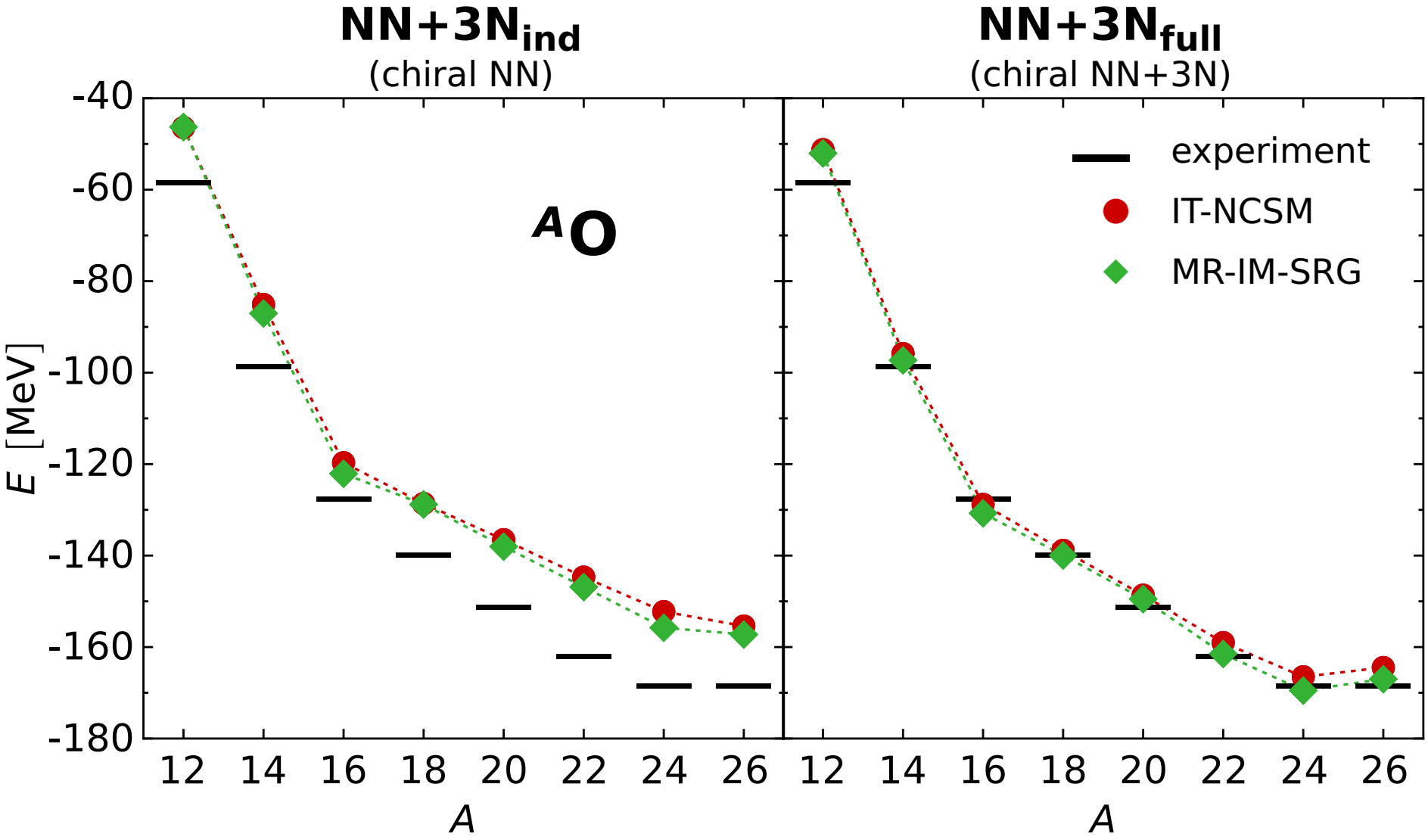
parameter-free
ab initio calculations with
full 3N interactions

highlights predictive power
of chiral NN+3N Hamiltonians

Λ_{3N} = 400 MeV, α = optimal $\hbar\Omega$

Ground States of Oxygen Isotopes

Hergert et al., PRL 110, 242501 (2013)



$\Lambda_{3N} = 400$ MeV, $\alpha = 0.08\,\text{fm}^4$, $E_{3\,max} = 14$, optimal $\hbar\Omega$

Ground States of Oxygen Isotopes

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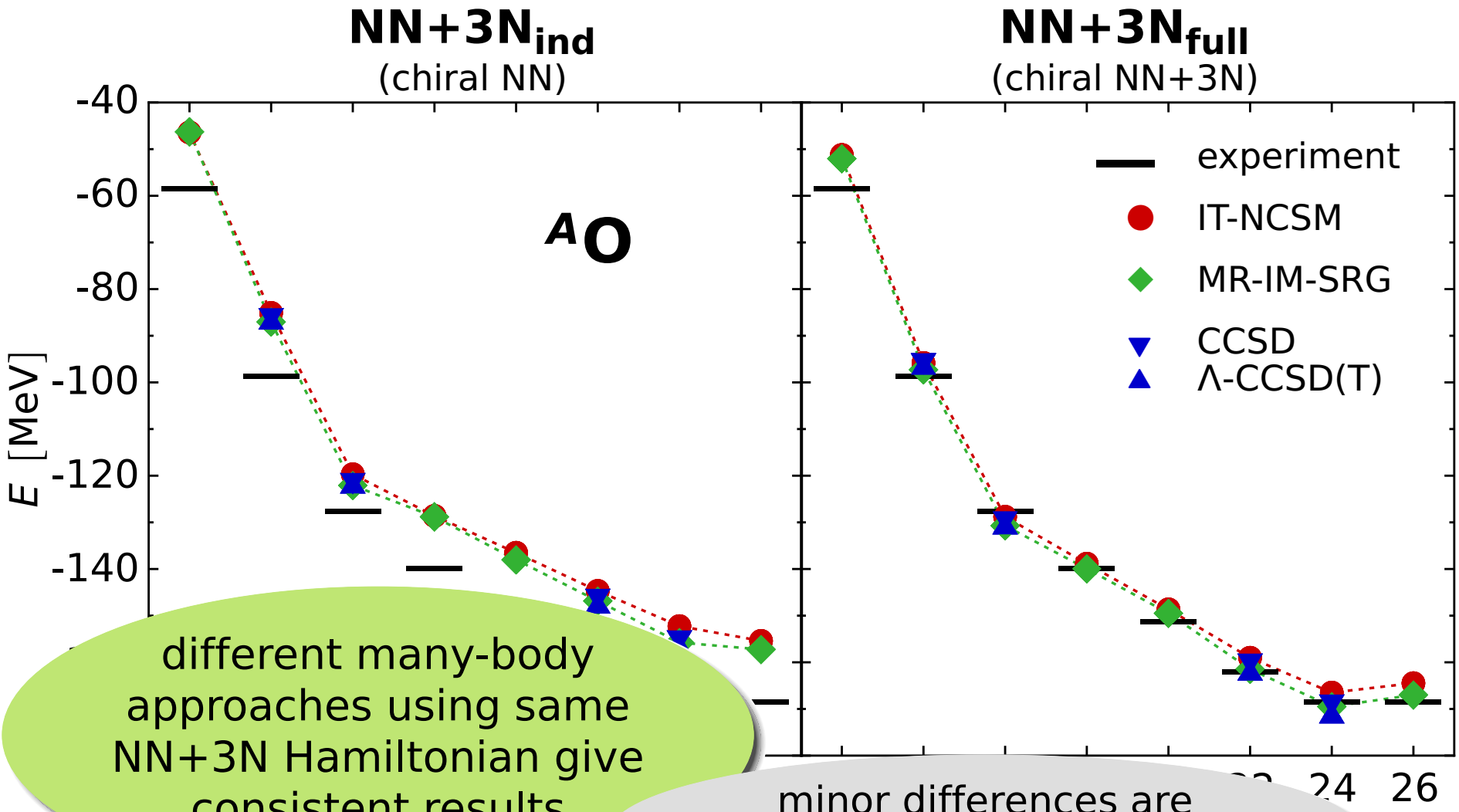


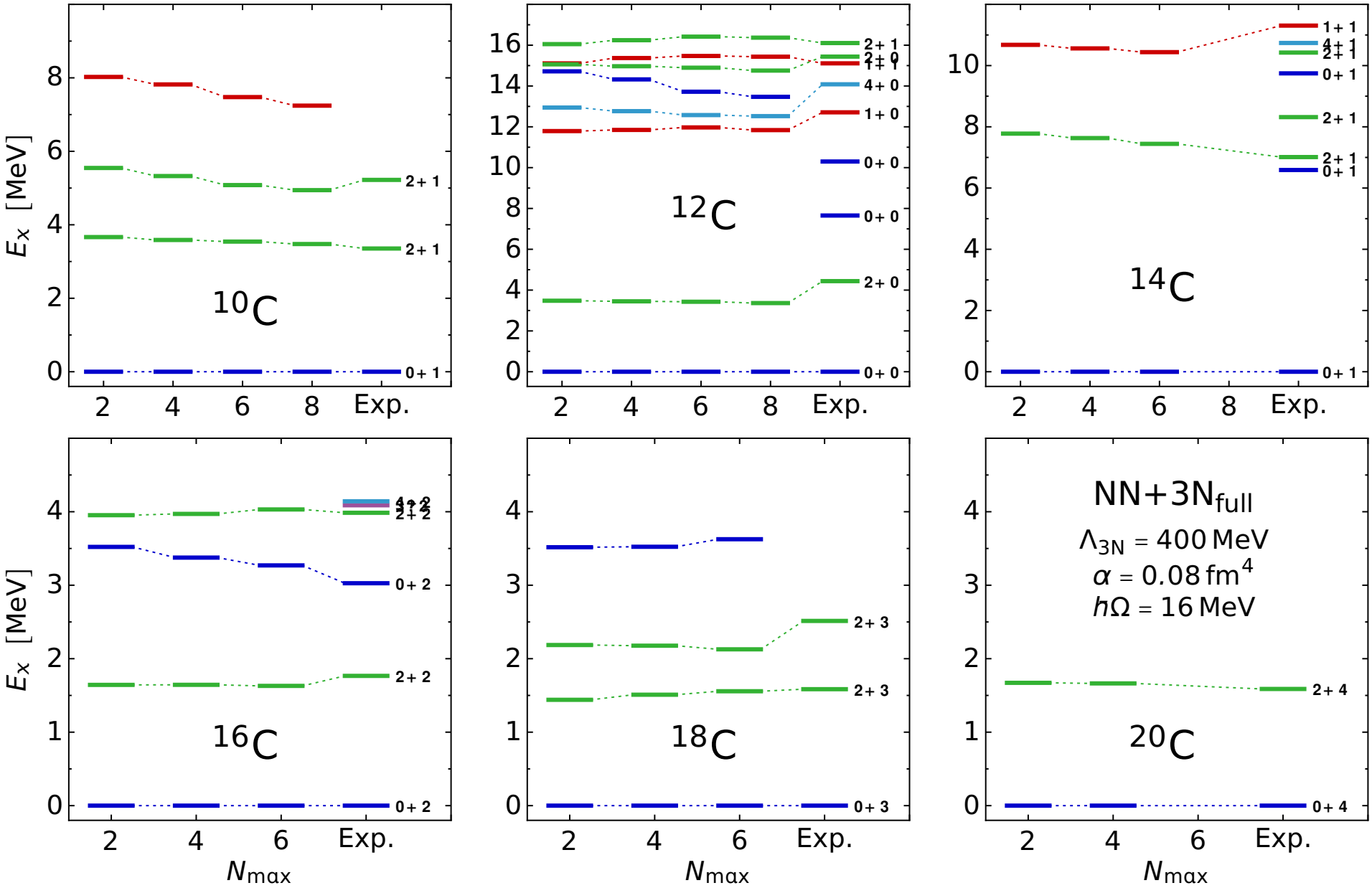
different many-body approaches using same NN+3N Hamiltonian give consistent results

minor differences are understood (NO2B, $E_{3\,max}$,...)

Λ_{3N} = 400 MeV, α = 0.08 fm^{-}, $E_{3\,max}$ = 14, optimal $\hbar\Omega$

Spectroscopy of Carbon Isotopes

Forssen et al., JPG 40, 055105 (2013); Roth et al., in prep.

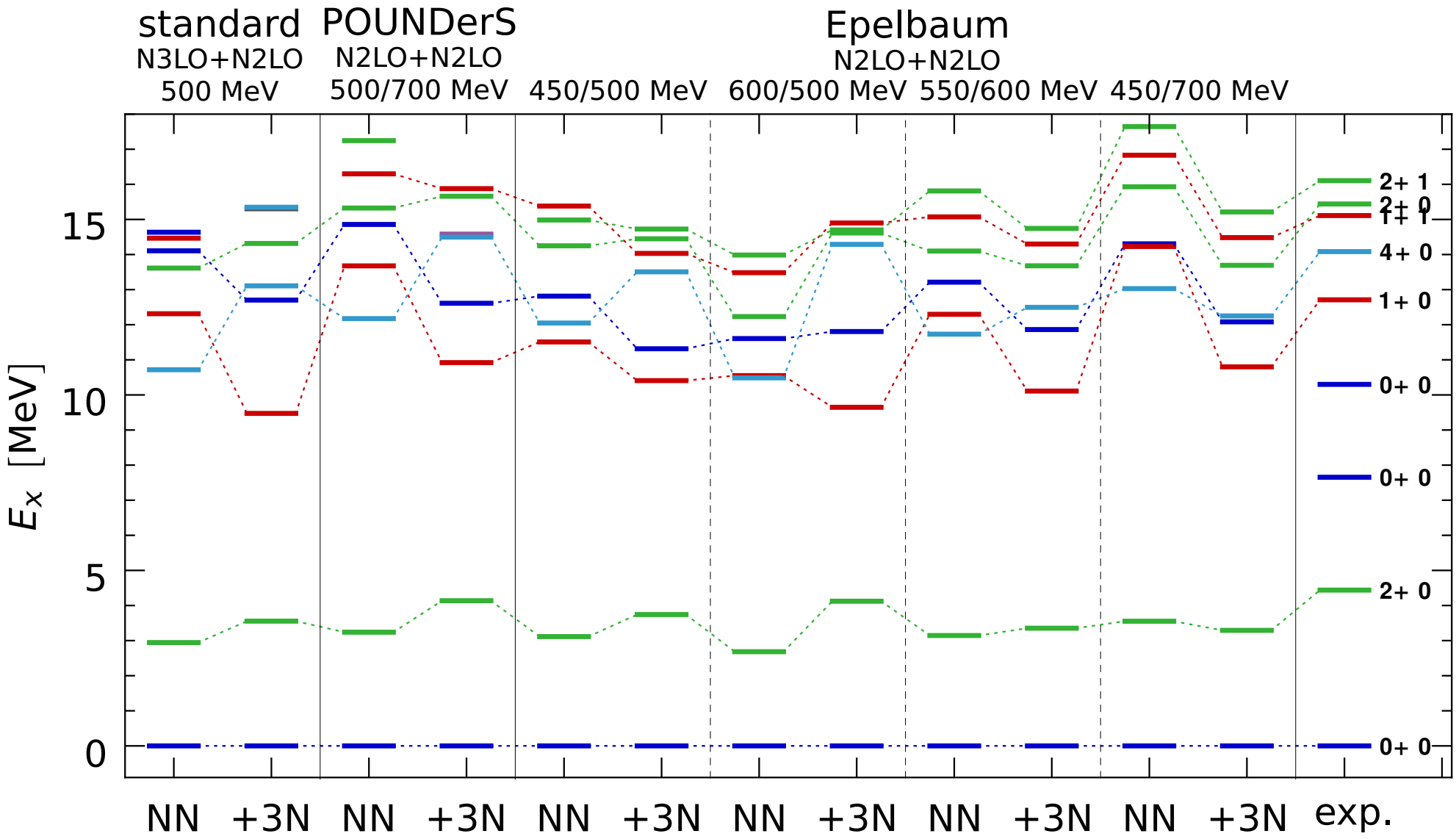


Towards Consistent Chiral N3LO Hamiltonians

Technical Aspects

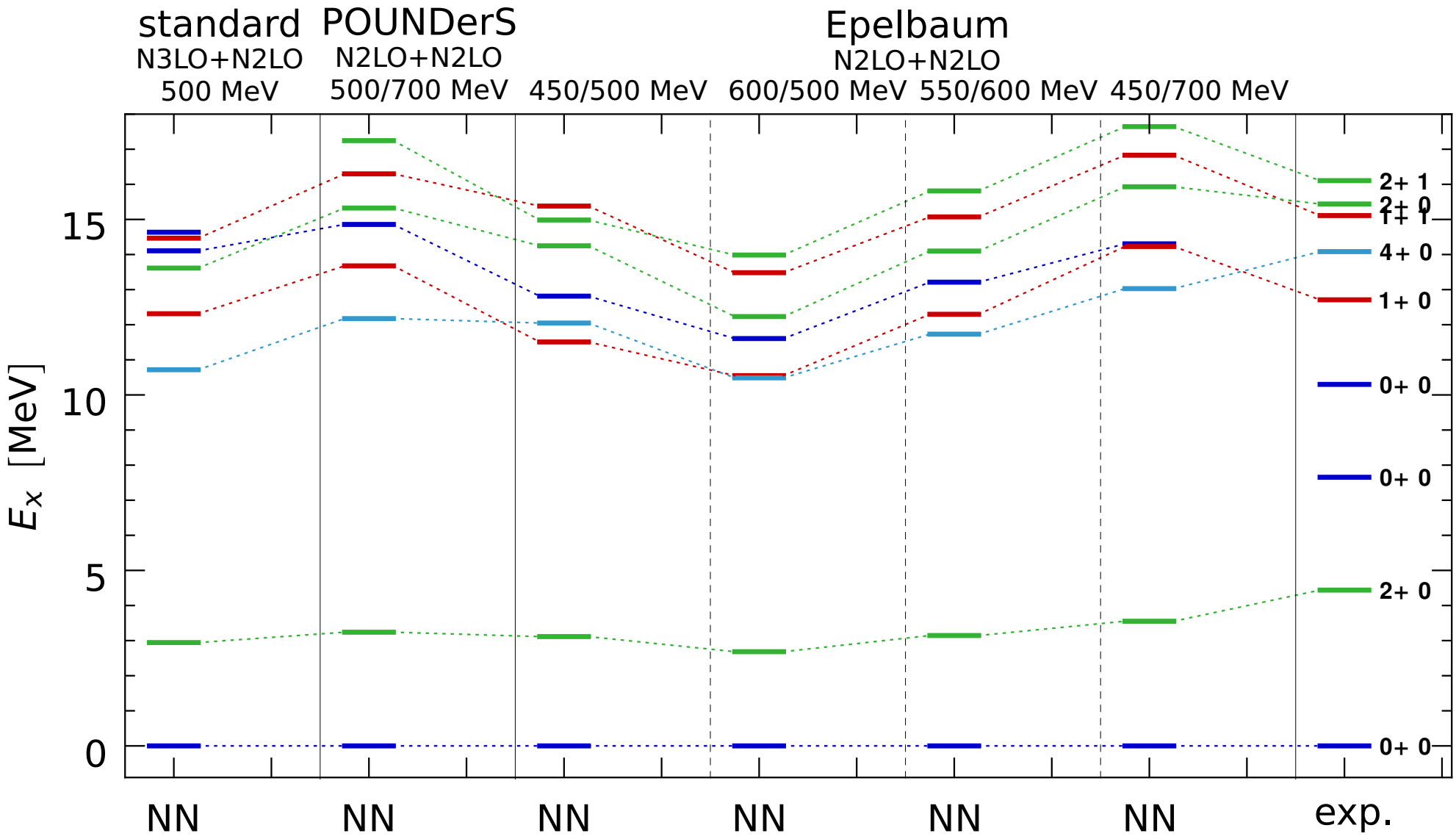
- **starting point**: numerical 3N matrix elements in partial-wave Jacobi-momentum basis
  - numerical partial-wave decomposition of Skibinski et al.
  - ongoing collaborative effort to produce N2LO/N3LO matrix elements (LENPIC: Cracow, Bochum, Bonn, Jülich, Ohio SU, Iowa SU, Darmstadt)
- **interface**: 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 ~ 10 (~ 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



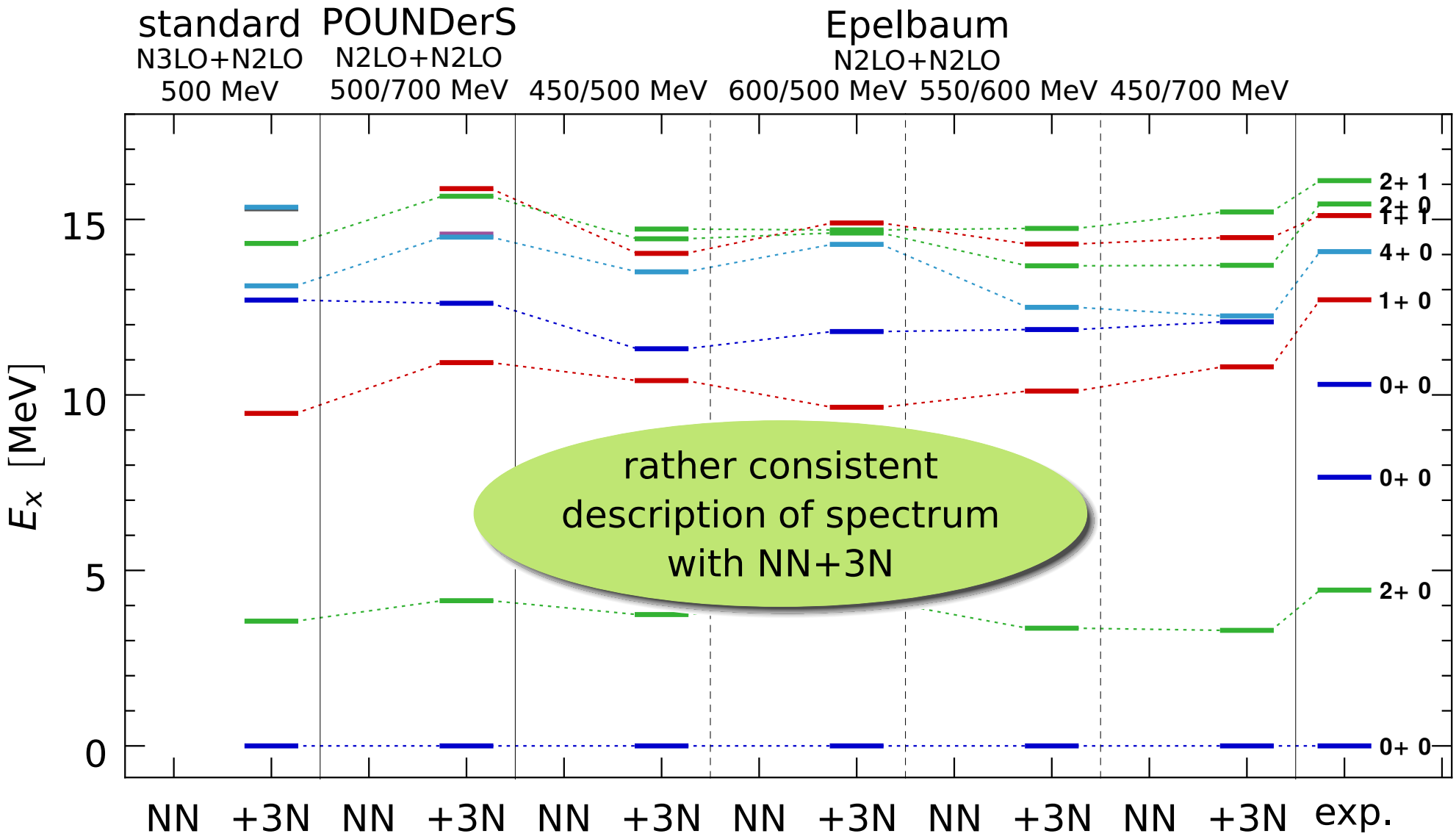
$N_{max} = 8,\ \alpha = 0.08\,\mathrm{fm}^4,\ \hbar\Omega = 16$ MeV

^{12}C: Consistent N2LO Hamiltonians



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

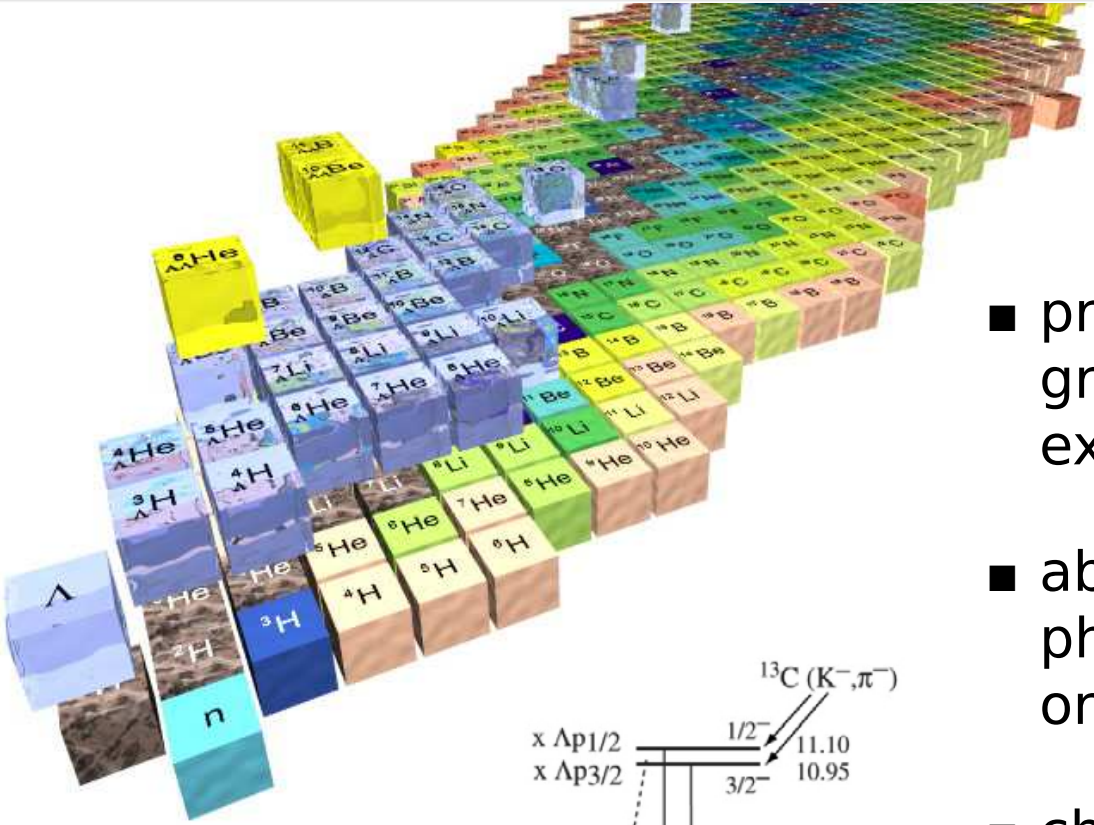
^{12}C: Consistent N2LO Hamiltonians

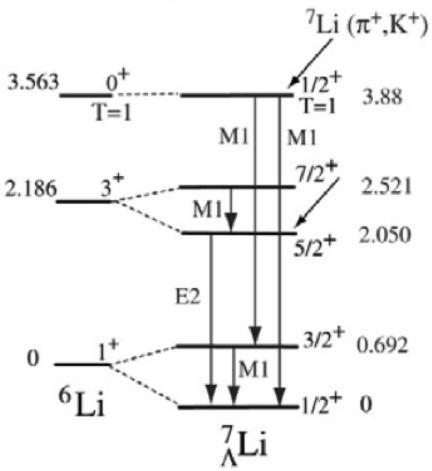


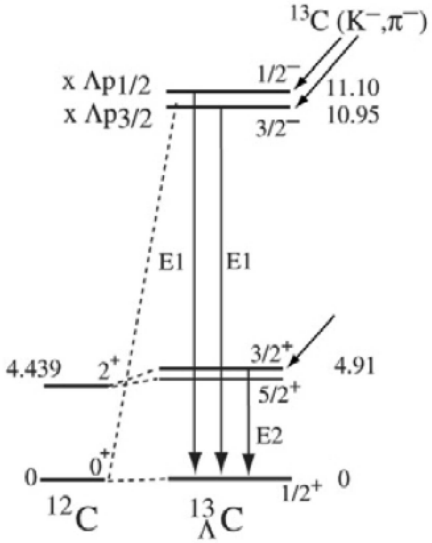
$N_{max} = 8,\ \alpha = 0.08\,\mathrm{fm}^4,\ \hbar\Omega = 16$ MeV

Ab Initio
Hyper-Nuclear Structure

Motivation: Hyper-Nuclear Structure







- precision data on hypernuclear ground states and spectroscopy exists
- ab initio few-body ($A \lesssim 4$) and phenomenological shell model or cluster calculations so far
- chiral EFT interactions including hyperons at LO,NLO are available (Haidenbauer, et al.)
- constrain YN & YY interaction by ab initio hypernuclear structure calculations

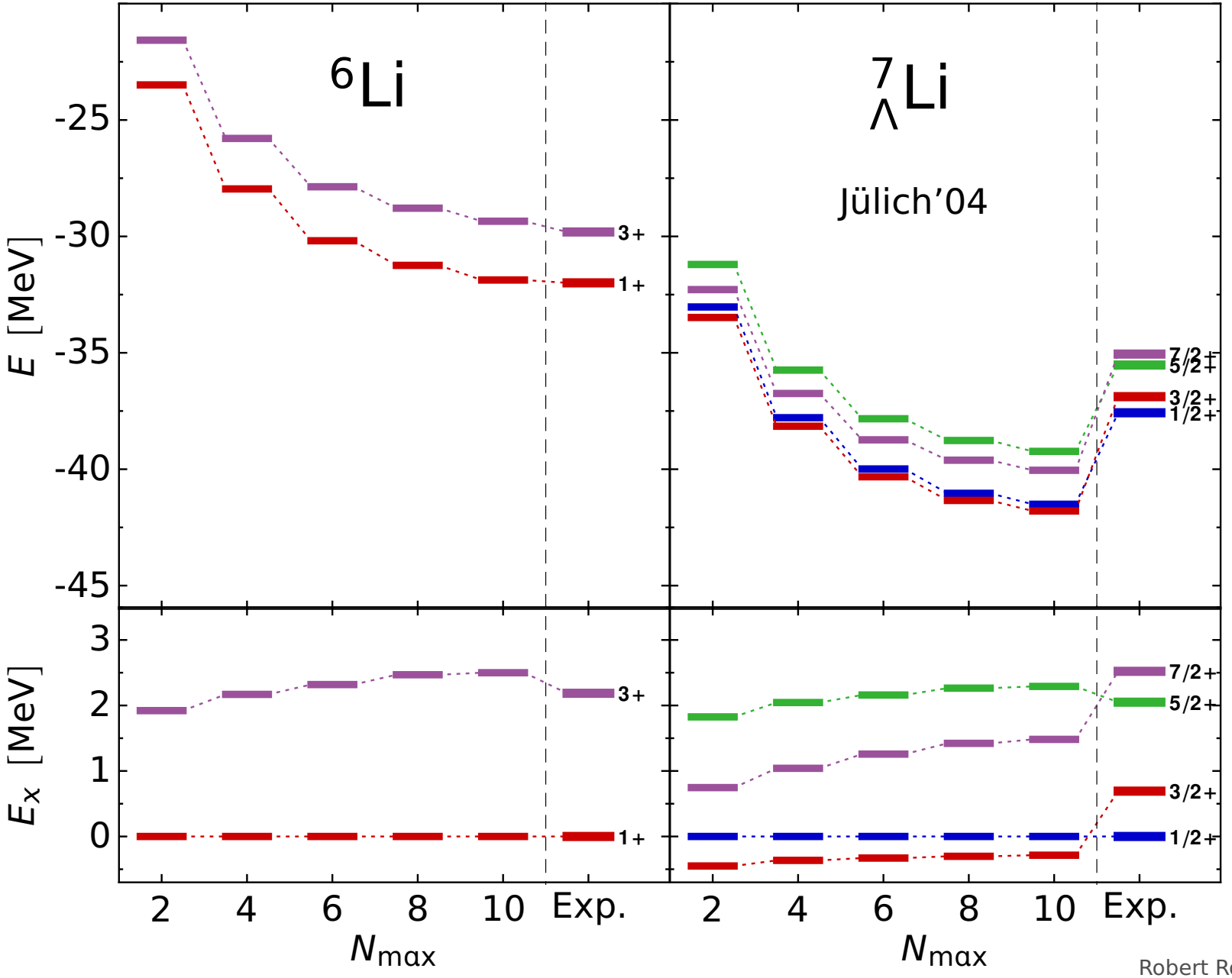
Ab Initio Toolbox

- **Hamiltonian from chiral EFT**
  - NN+3N: standard chiral Hamiltonian (Entem&Machleidt, Navrátil)
  - YN: LO chiral interaction (Haidenbauer et al.), NLO is available

- **Similarity Renormalization Group**
  - consistent SRG-evolution of NN, 3N, YN interactions
  - using particle basis and including $\Lambda\Sigma$-coupling (larger matrices)
  - Λ-Σ mass difference and $p\Sigma^{\pm}$ Coulomb included consistently

- **Importance Truncated No-Core Shell Model**
  - include explicit $(p, n, \Lambda, \Sigma^{+}, \Sigma^{0}, \Sigma^{-})$ with physical masses
  - larger model spaces easily tractable with importance truncation
  - all p-shell single-Λ hypernuclei are accessible

Application: ${}^{7}_{\Lambda}$Li



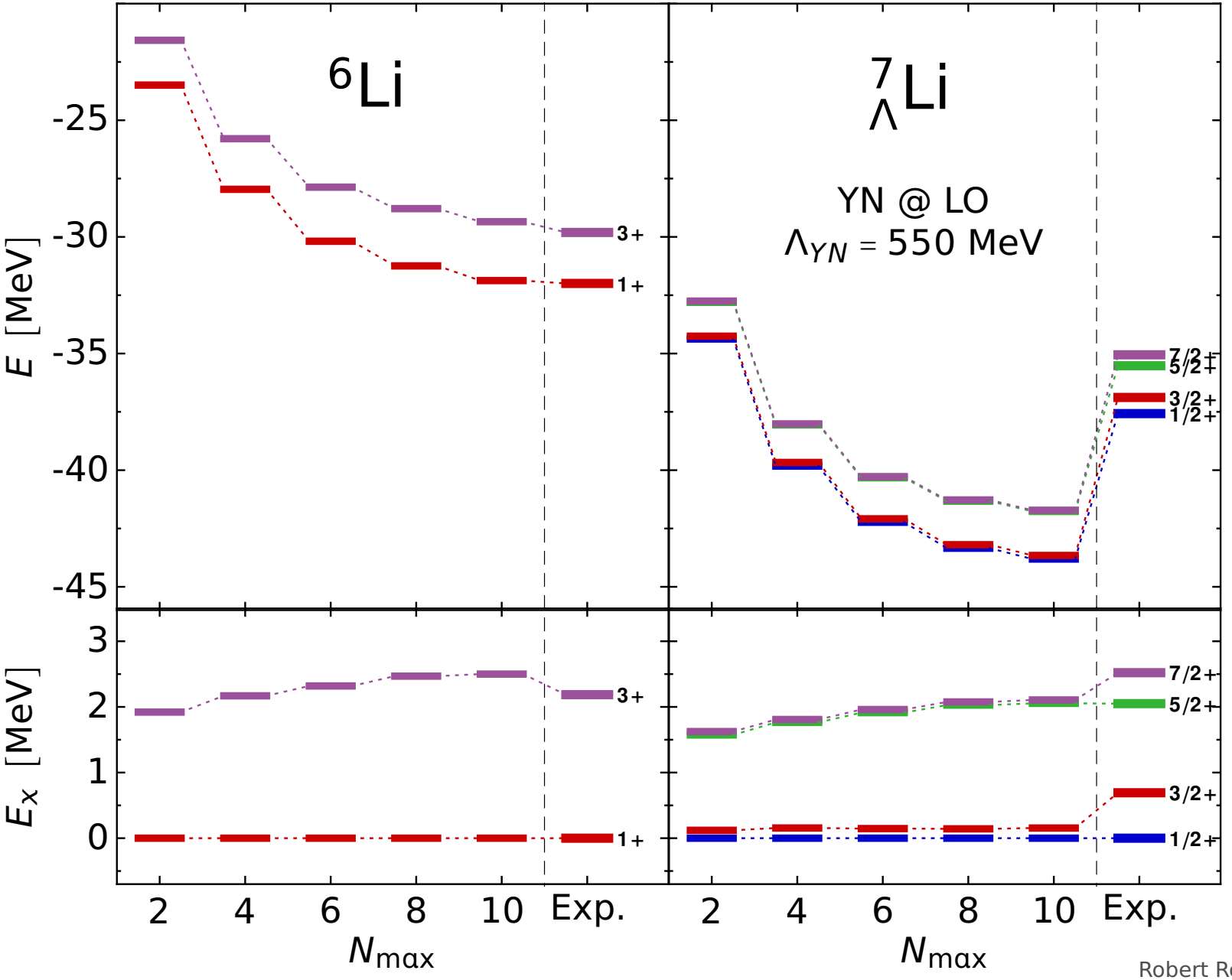
NN @ N3LO
Entem&Machleidt
Λ_{NN} = 500 MeV

3N @ N2LO
Navratil
Λ_{3N} = 500 MeV
triton fit

Jülich'04
Haidenbauer et al.
scatt. & hypertriton

$\alpha = 0.08\,\mathrm{fm}^4$
$\hbar\Omega = 20$ MeV

Application: ${}^{7}_{\Lambda}$Li



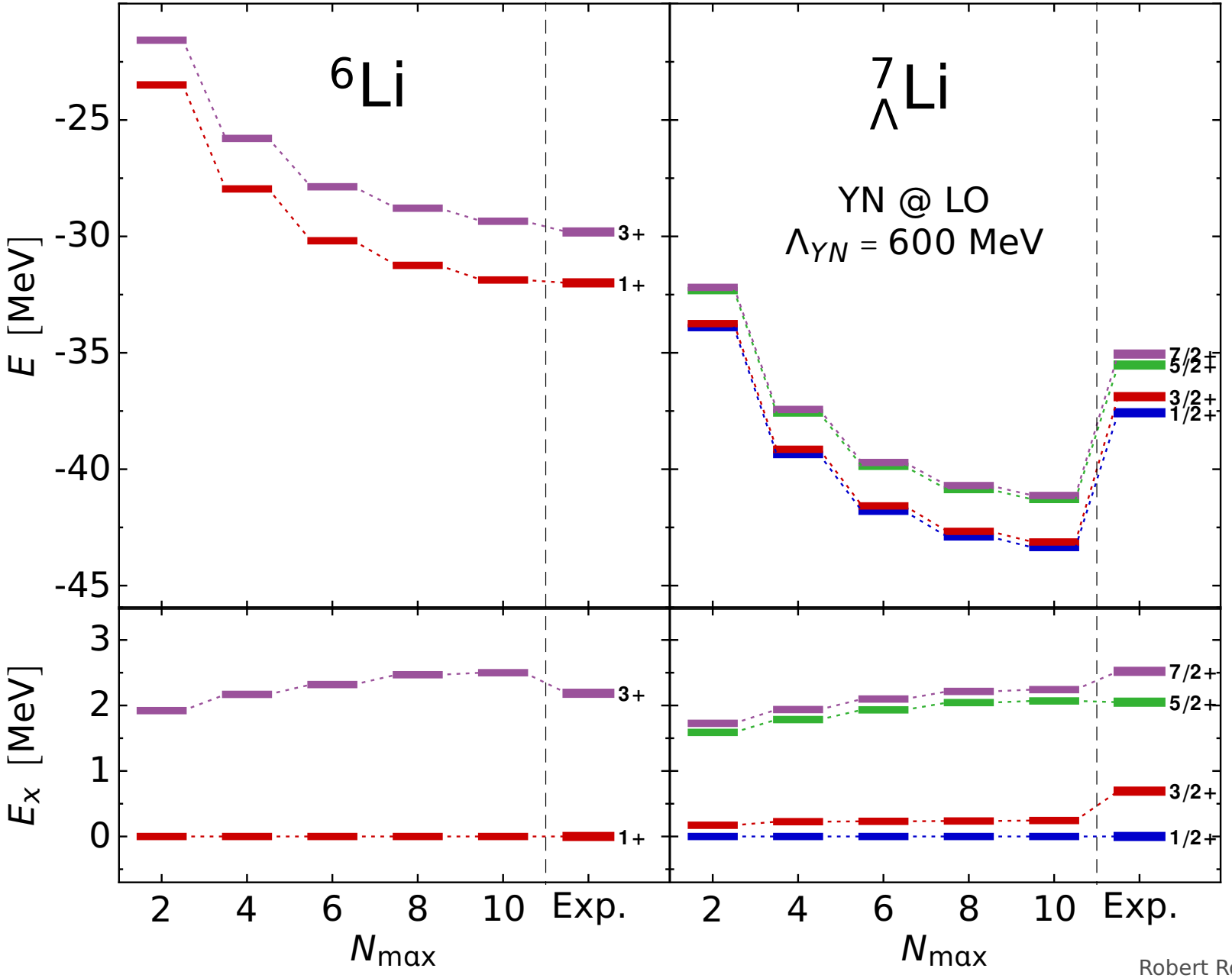
NN @ N3LO
Entem&Machleidt
Λ_{NN} = 500 MeV

3N @ N2LO
Navratil
Λ_{3N} = 500 MeV
triton fit

YN @ LO
Haidenbauer et al.
Λ_{YN} = 550 MeV
scatt. & hypertriton

$\alpha = 0.08\,\mathrm{fm}^4$
$\hbar\Omega$ = 20 MeV

Application: ${}^{7}_{\Lambda}$Li



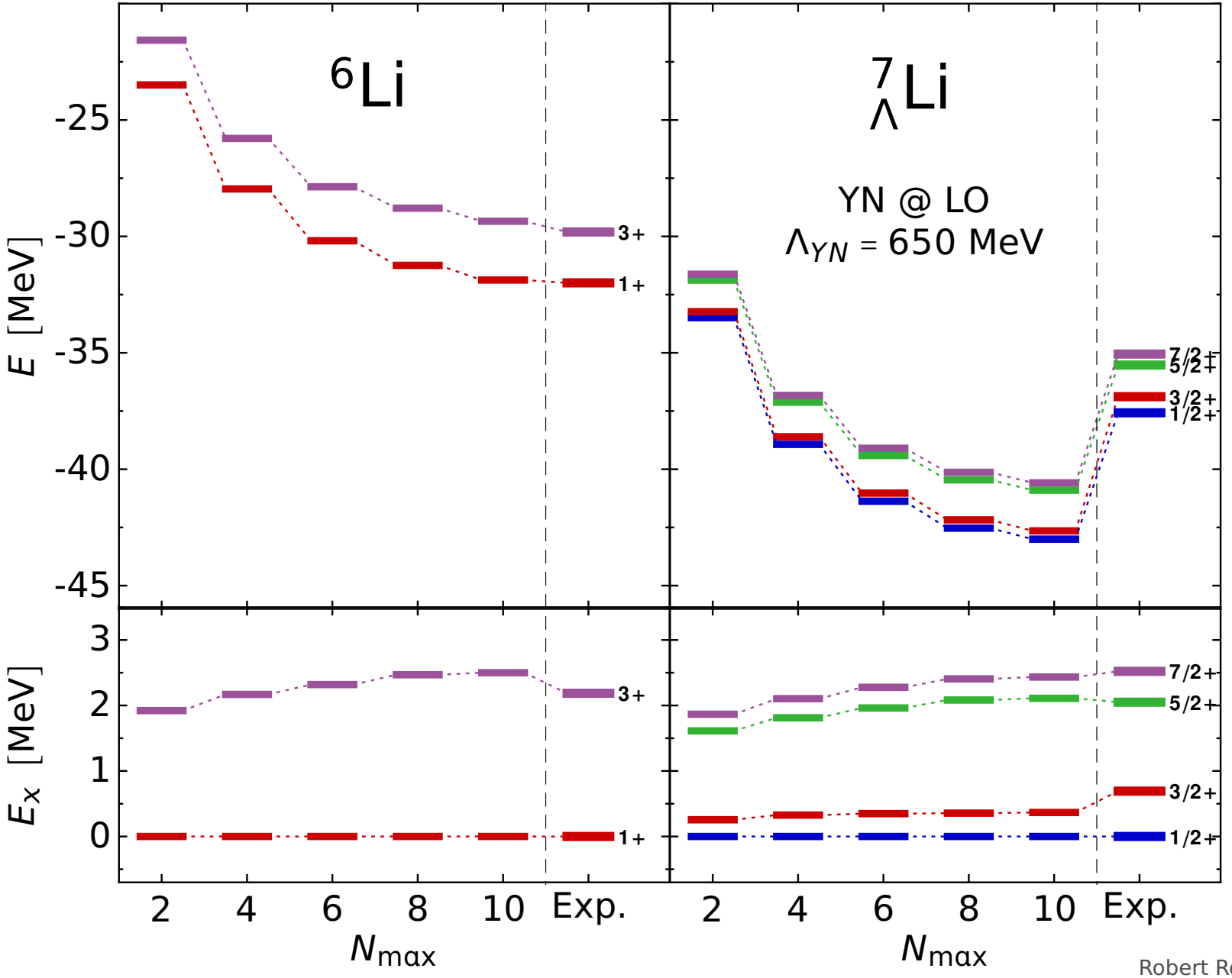
NN @ N3LO
Entem&Machleidt
Λ_{NN} = 500 MeV

3N @ N2LO
Navratil
Λ_{3N} = 500 MeV
triton fit

YN @ LO
Haidenbauer et al.
Λ_{YN} = 600 MeV
scatt. & hypertriton

$\alpha = 0.08\,\mathrm{fm}^4$
$\hbar\Omega$ = 20 MeV

Application: ${}^{7}_{\Lambda}$Li



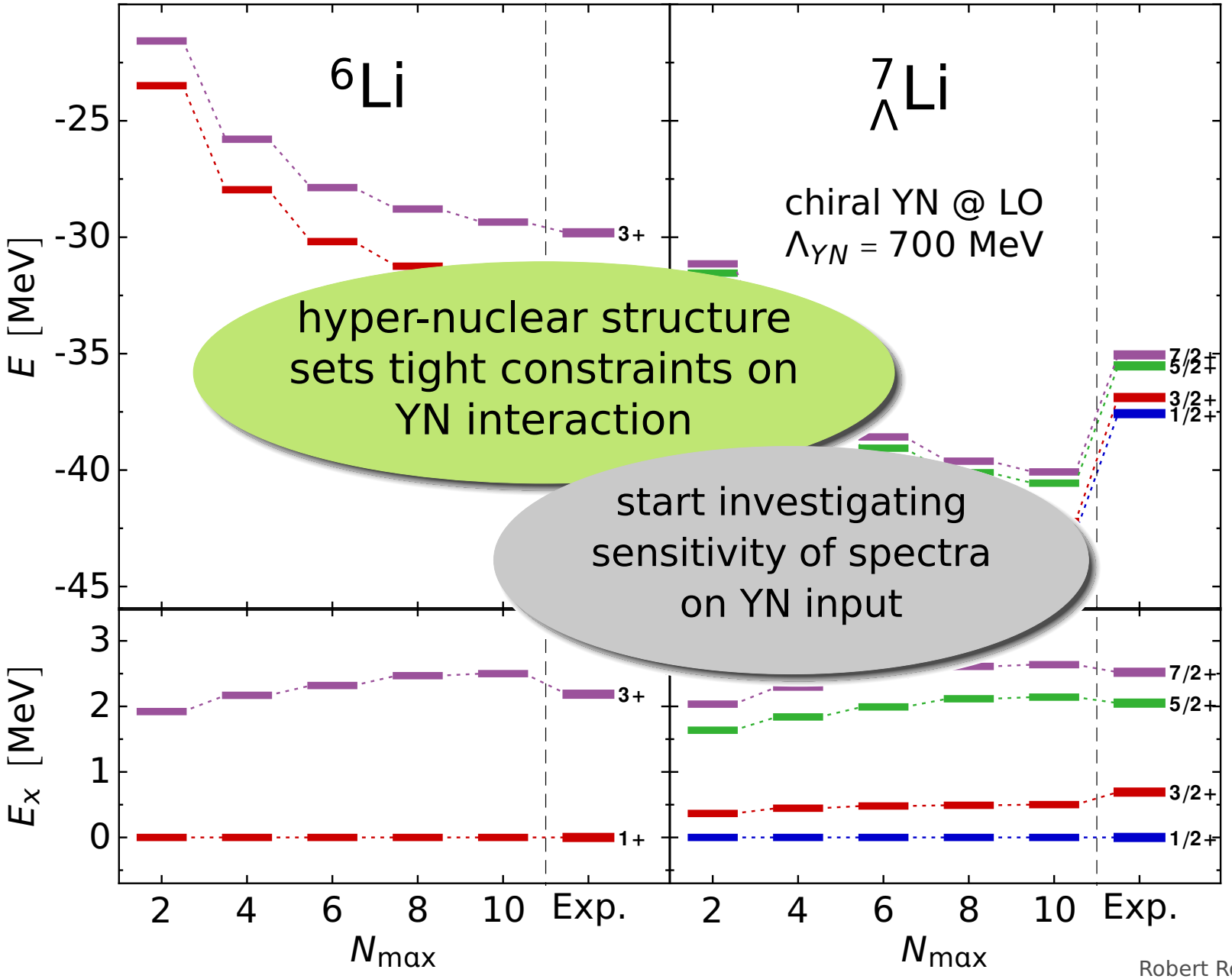
NN @ N3LO
Entem&Machleidt
Λ_{NN} = 500 MeV

3N @ N2LO
Navratil
Λ_{3N} = 500 MeV
triton fit

YN @ LO
Haidenbauer et al.
Λ_{YN} = 650 MeV
scatt. & hypertriton

$\alpha = 0.08\,\mathrm{fm}^4$
$\hbar\Omega$ = 20 MeV

Application: ${}^{7}_{\Lambda}$Li



NN @ N3LO
Entem&Machleidt
Λ_{NN} = 500 MeV

3N @ N2LO
Navratil
Λ_{3N} = 500 MeV
triton fit

YN @ LO
Haidenbauer et al.
Λ_{YN} = 700 MeV
scatt. & hypertriton

$\alpha = 0.08\,\mathrm{fm}^4$
$\hbar\Omega$ = 20 MeV

New Horizons...

- **nuclear structure theory connected to QCD via chiral EFT**
  - chiral EFT as universal, controlled and improvable starting point
  - consistent and optimized interactions at N2LO, N3LO,...
  - consistent similarity transformation of Hamiltonian and observables

- **innovations in ab initio many-body theory**
  - consistent inclusion of 3N (and 4N) interactions
  - precision structure and spectroscopy in p- and sd-shell (IT-NCSM,...)
  - access to the medium-mass regime (CC, IM-SRG,...)
  - ab initio hyper-nuclear structure
  - bridge to reaction theory (NCSM/RGM, NCSMC)
  - uncertainty quantification, error propagation, feedback cycle

- **many exciting applications ahead...**

Epilogue

- **thanks to my group & my collaborators**
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    Chalmers University, Sweden
  - H. Feldmeier, T. Neff
    GSI Helmholtzzentrum

LENPIC
Low-Energy Nuclear Physics International Collaboration

SFB 634

Deutsche Forschungsgemeinschaft
DFG

HIC for FAIR
Helmholtz International Center

LOEWE
Exzellente Forschung für Hessens Zukunft

HELMHOLTZ GEMEINSCHAFT

Bundesministerium für Bildung und Forschung

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