News from the Importance Truncated NCSM

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  - Uncertainty Quantification
  - Applications: Carbon & Oxygen Isotopes

- **New Directions**
  - Multi-Reference Normal-Ordering Approximation
  - Importance Truncated Shell Model
  - Ab Initio Description of Hypernuclei

Importance Truncated No-Core Shell Model

Roth, Calci, Langhammer, Binder — in preparation (2013)
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 $N_{\max}\hbar\Omega$
- 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

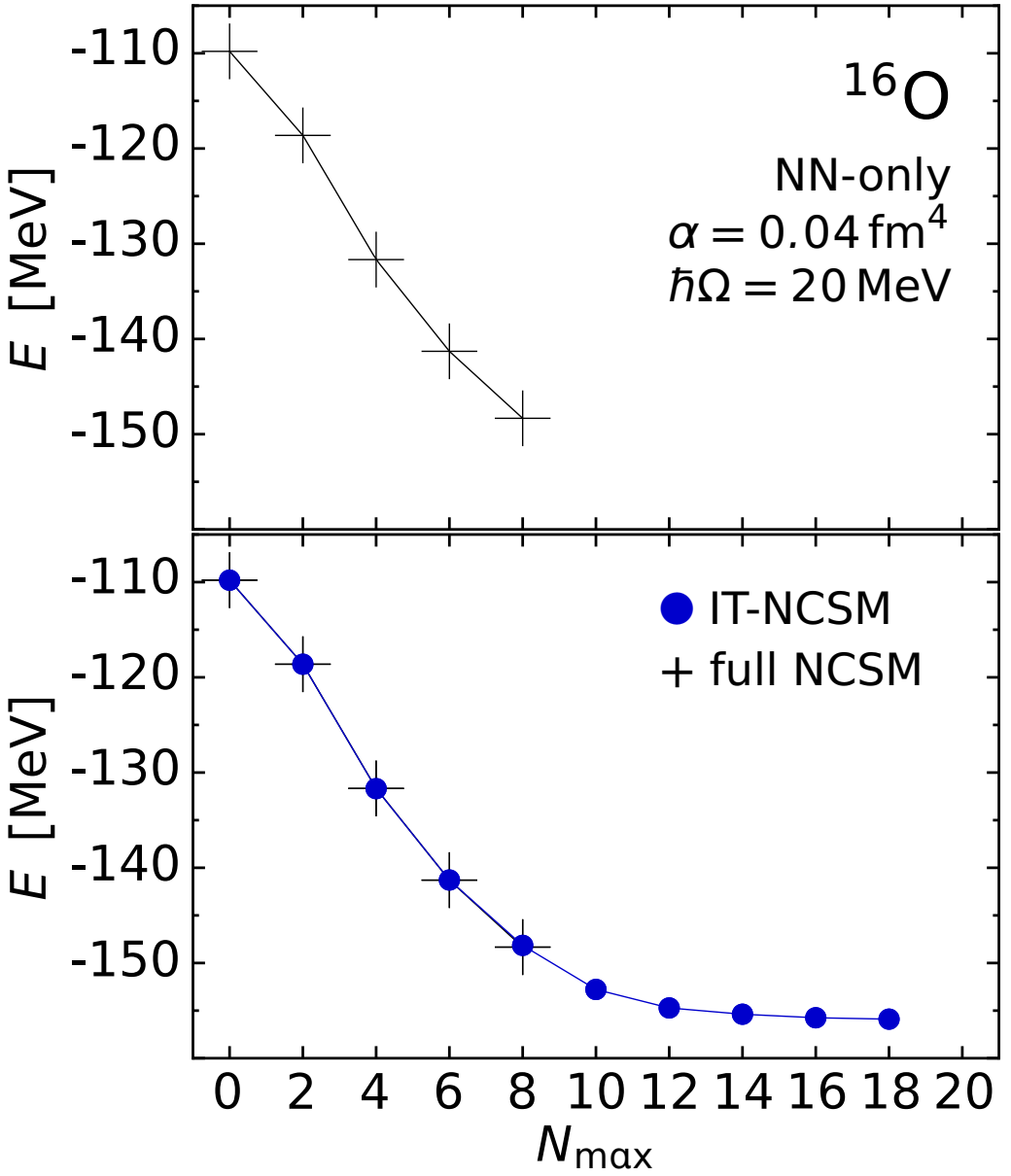
Importance Truncated NCSM

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



Importance Truncation: Basic Idea

- **starting point**: approximation $|\Psi_{\text{ref},m}\rangle$ for the **target states** within a limited reference space $\mathcal{M}_{\text{ref}}$

$$|\Psi_{\text{ref},m}\rangle = \sum_{\nu \in \mathcal{M}_{\text{ref}}} C_{\nu}^{(\text{ref},m)} |\Phi_{\nu}\rangle$$

- **measure the importance** of individual basis state $|\Phi_{\nu}\rangle \notin \mathcal{M}_{\text{ref}}$ via first-order multiconfigurational perturbation theory

$$\frac{\langle \Phi_{\nu}| H |\Psi_{\text{ref},m}\rangle}{\epsilon_{\nu}}$$

- co… …from all basis states

- **solve eigenvalue problem** in … $\mathcal{M}_{\text{IT}}(\kappa_{\text{min}})$ and obtain improved approximation of target state

importance measure only probes 2p2h excitations on top of $\mathcal{M}_{\text{ref}}$ for a two-body Hamiltonian

embed into iterative scheme to access full model space

Importance Truncation: Iterative Scheme

- **property of $N_{\max}$-truncated space**: step from $N_{\max}$ to $N_{\max}+2$ requires 2p2h excitations at most

- **sequential calculation** for a range of $N_{\max}\hbar\Omega$ spaces:

  - ● do full NCSM calculations up to a convenient $N_{\max}$

  - ✪ use components of eigenstates with $|C_\nu^{(m)}| \geq C_{\min}$ as initial $|\Psi_{\text{ref},m}\rangle$

  - ❶ consider all states $|\Phi_\nu\rangle \notin \mathcal{M}_{\text{ref}}$ from an $N_{\max}+2$ space and add those with $|\kappa_\nu^{(m)}| \geq \kappa_{\min}$ to importance-truncated space $\mathcal{M}_{\text{IT}}$

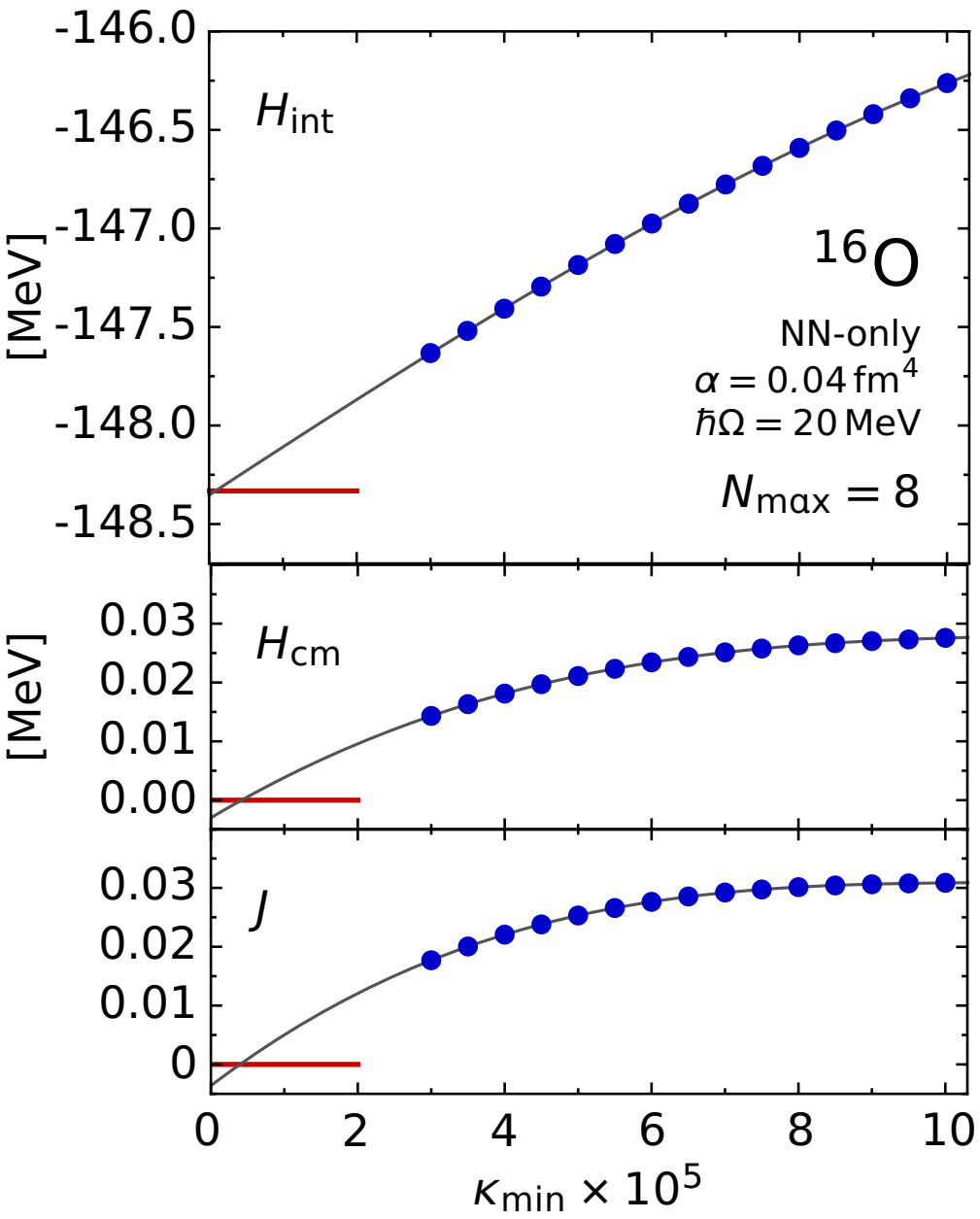
  - ❷ solve eigenvalue problem in $\mathcal{M}_{\text{IT}}$

  - ❸ use components of eigensta

  - ❹ goto ❶

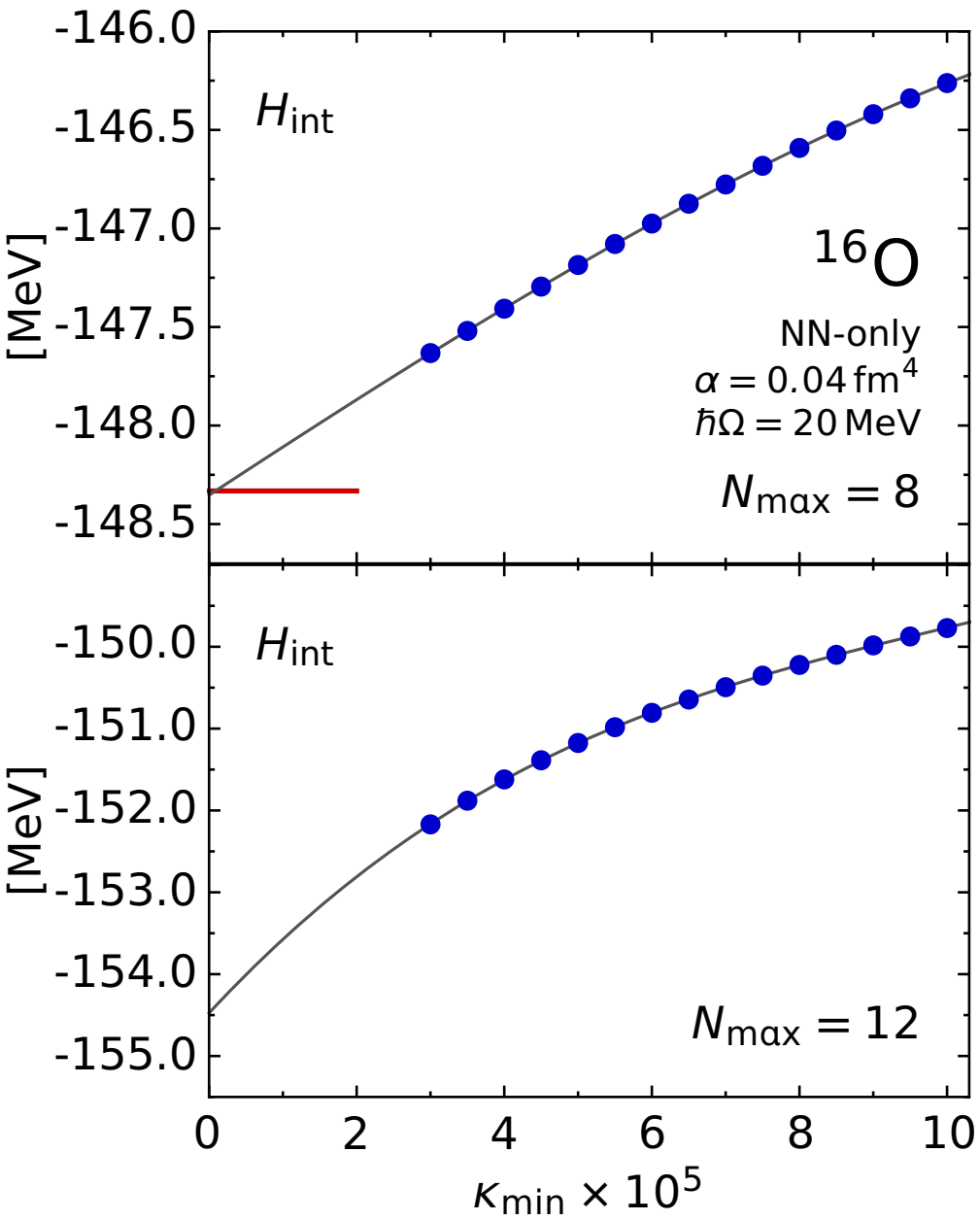
full NCSM space is recovered in the limit $(\kappa_{\min}, C_{\min}) \to 0$

Threshold Extrapolation



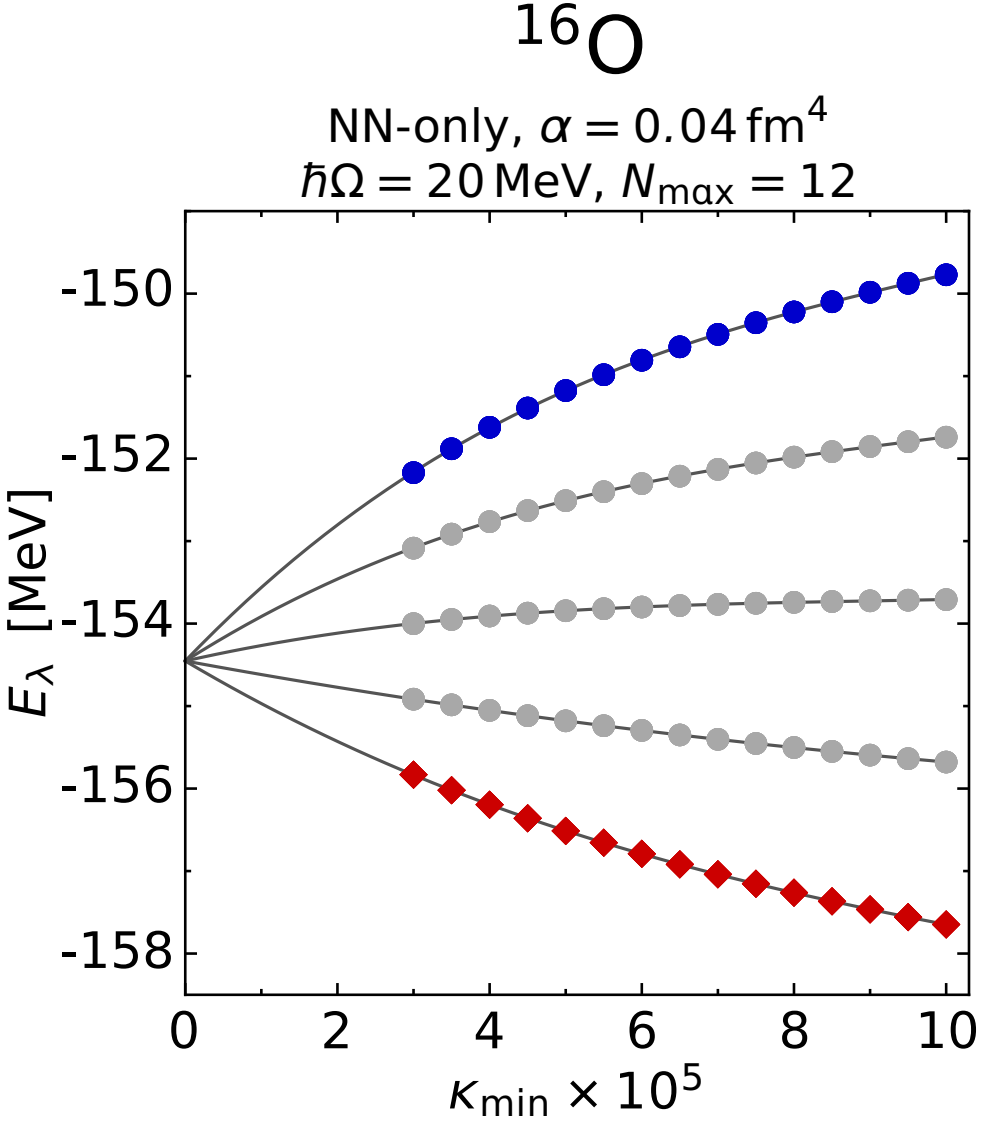
- repeat calculations for a **sequence of importance thresholds** $\kappa_{\rm min}$
- observables show **smooth threshold dependence** and systematically approach the full NCSM limit
- use **a posteriori extrapolation** $\kappa_{\rm min} \to 0$ of observables to account for effect of excluded configurations

Threshold Extrapolation



- repeat calculations for a **sequence of importance thresholds** $\kappa_{\min}$
- observables show **smooth threshold dependence** and systematically approach the full NCSM limit
- use **a posteriori extrapolation** $\kappa_{\min} \rightarrow 0$ of observables to account for effect of excluded configurations

Constrained Threshold Extrapolation



- for free: importance selection gives perturbative energy correction $\Delta_{\mathrm{excl}}(\kappa_{\min})$ accounting for **excluded states**
- formal property

  $\Delta_{\mathrm{excl}}(\kappa_{\min}) \to 0 \quad \text{for} \quad \kappa_{\min} \to 0$

- auxiliary parameter λ defining a family of energy sequences

  $E_\lambda(\kappa_{\min}) = E(\kappa_{\min}) + \lambda \Delta_{\mathrm{excl}}(\kappa_{\min})$

- **simultaneous extrapolation** for family of λ-values with constraint $E_\lambda(0) = E_{\mathrm{extrap}}$

Uncertainty Quantification

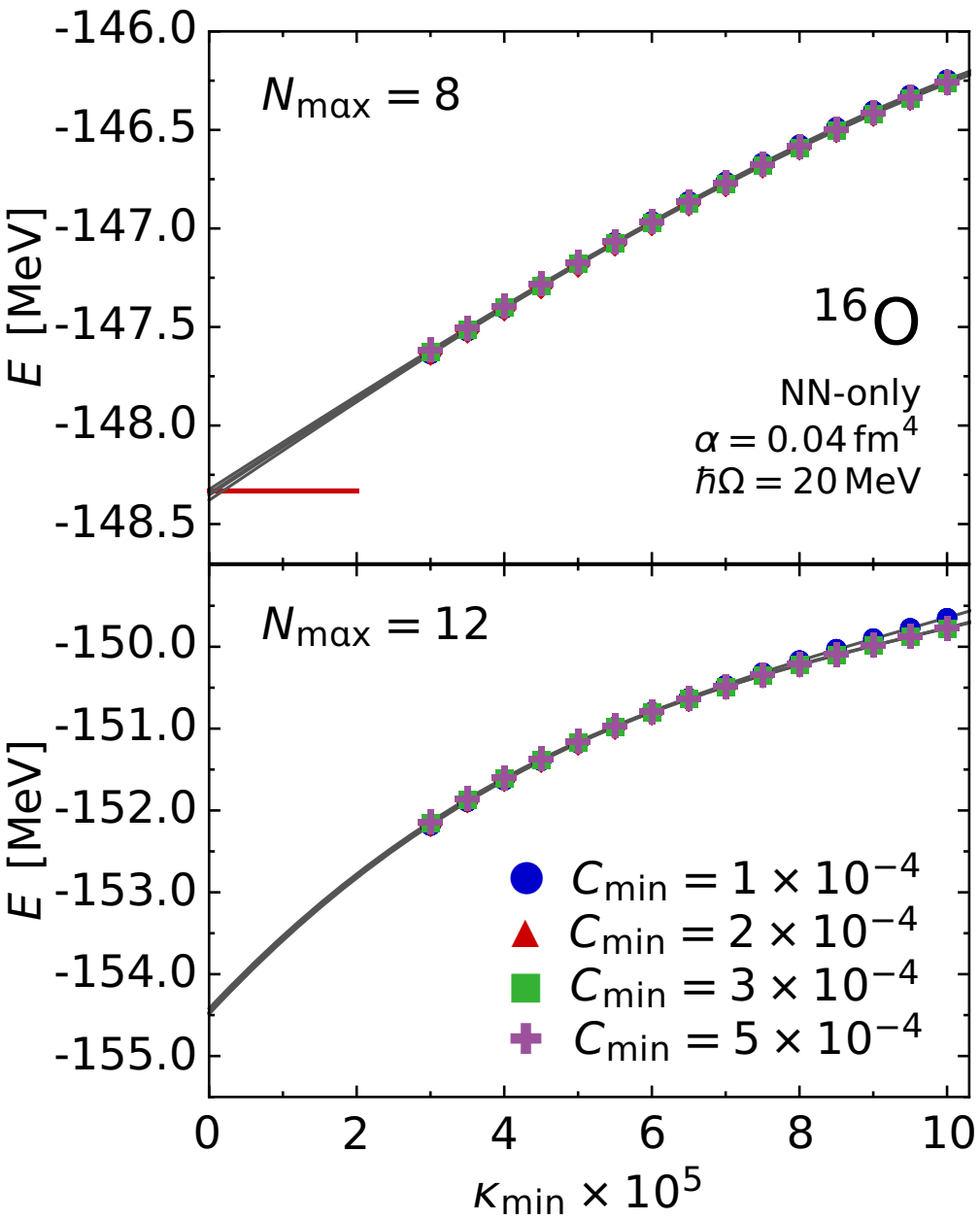
Importance Truncation

- use sequence of $(C_{\min}, \kappa_{\min})$-truncated model spaces
- extrapolate to $\kappa_{\min} \to 0$ using poynomial ansatz or more refined constrained extrapolation scheme
- uncertainty estimate derived from extrapolation protocol
- **systematic uncertainty** absent in full NCSM

Model-Space Truncation

- use sequence of $N_{\max}$-truncated model spaces
- extrapolate to $N_{\max} \to \infty$ using exponential ansatz or more elaborate extrapolation schemes
- uncertainty estimate derived from extrapolation protocol
- same **extrapolation uncertainties** as in full NCSM

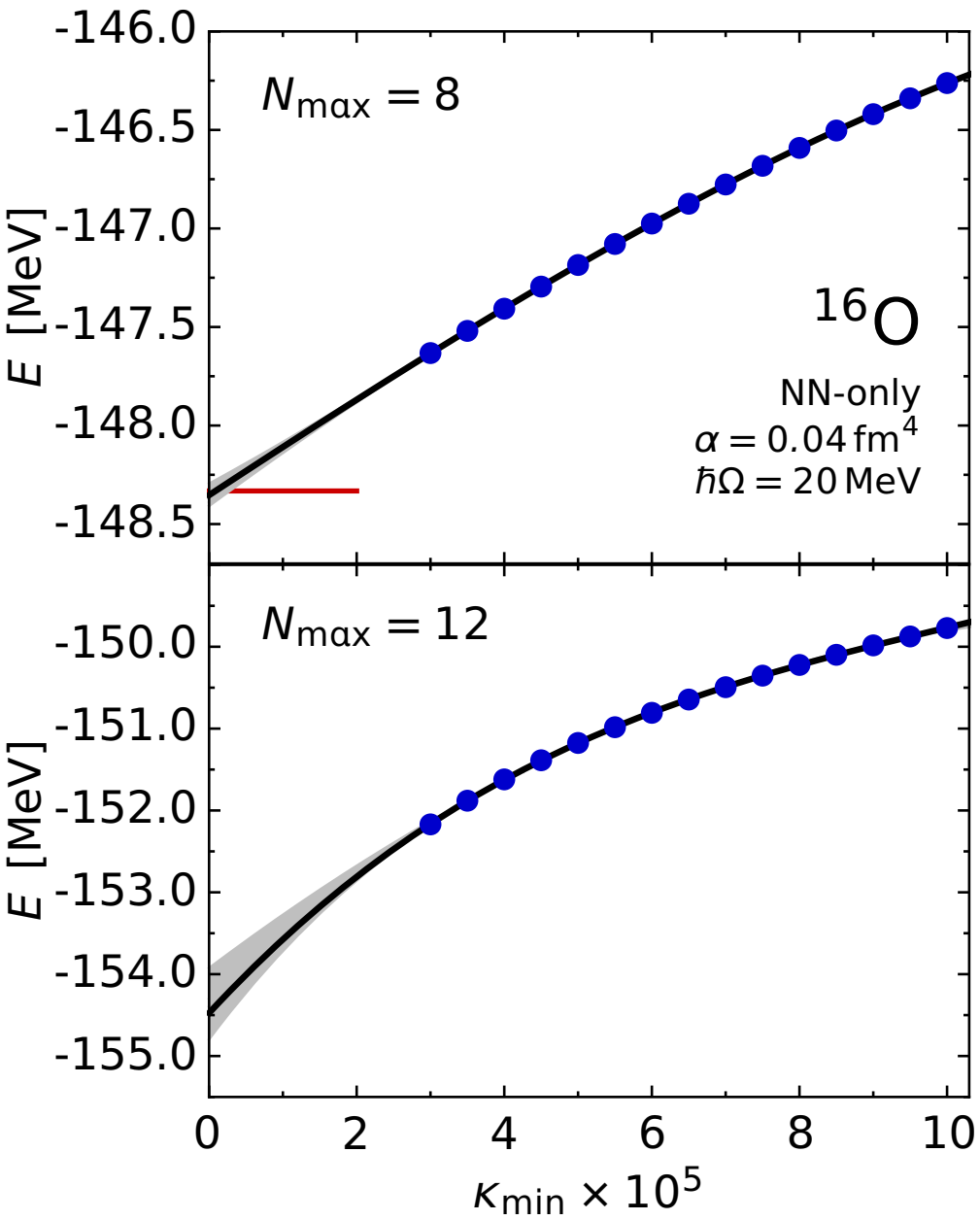
Comment on C_{min} Truncation



- truncation of reference state to components with $|C_\nu| \geq C_{min}$
- technical reason: importance selection phase scales with $(\dim \mathcal{M}_{ref})^2$
- typically $C_{min} = 2 \times 10^{-4}$

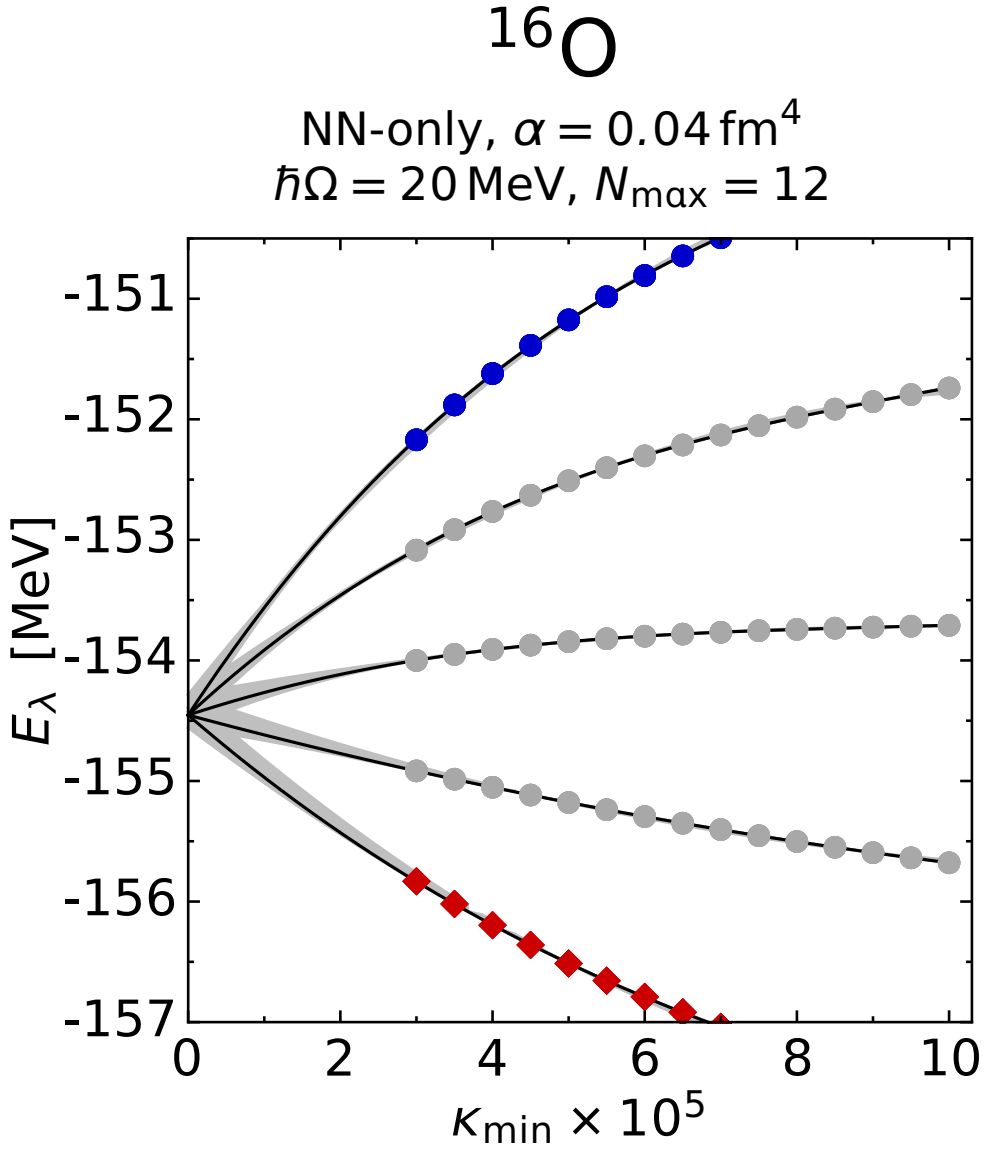
practically no influence on threshold extrapolated energies

Protocol: Simple $\kappa_{\min}$ Extrapolation



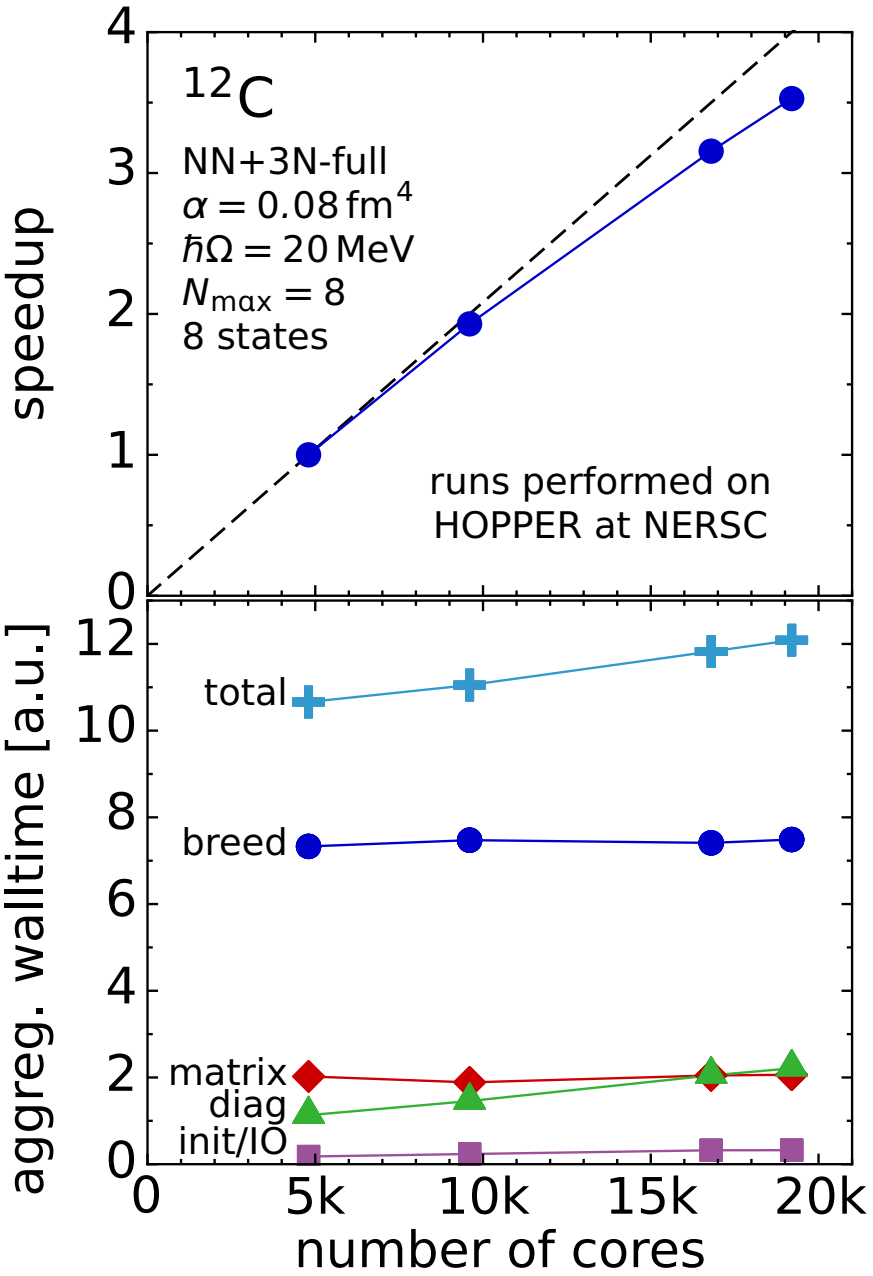
- perform IT-NCSM calculations for range of $\kappa_{\min}$-values, typically $\kappa_{\min} = 3, 3.5, \ldots, 10 \times 10^{-5}$
- extrapolation $\kappa_{\min} \to 0$ using polynomial $P_p(\kappa_{\min})$ fit to full $\kappa_{\min}$-set, typically of order $p = 3$
- generate uncertainty band from set of alternative extrapolations
  - P_{p-1} and P_{p+1} extrapolations using full $\kappa_{\min}$-range
  - P_p extrapolations with lowest and lowest two $\kappa_{\min}$-points dropped
- quote standard deviation as nominal uncertainty

Protocol: Constrained $\kappa_{\min}$ Extrapolation



- select a few λ-values to get symmetrical approach towards common $E_{\mathrm{extrap}} = E_\lambda(\kappa_{\min} = 0)$
- constrained simultaneous extrapolation $\kappa_{\min} \to 0$ using polynomial $P_p(\kappa_{\min})$, typically of order $p = 3$
- generate uncertainty band from set of constrained extrapolations
  - P_{p-1} and P_{p+1} extrapolations using full $\kappa_{\min}$-range
  - P_p extrapolations with lowest and lowest two $\kappa_{\min}$-points dropped
  - P_p extrapolations with smallest and largest λ-set dropped
- std. deviation gives uncertainty

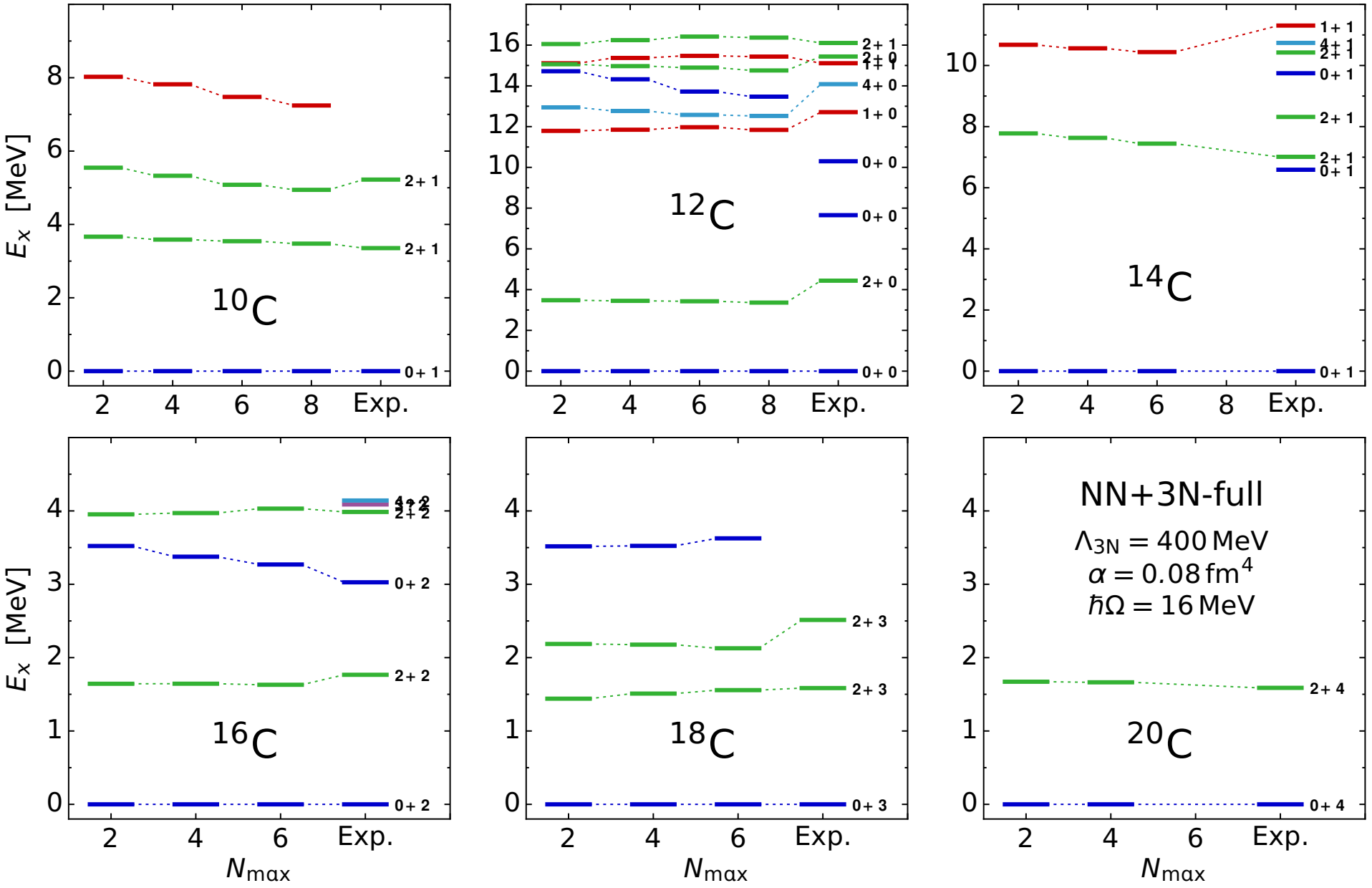
Computational Aspects



- hybrid OpenMP/MPI implementation of IT-NCSM developed from scratch (no ‘vintage’ code pieces)
- capable of using large sets of JT-coupled 3N matrix elements
- efficient on-the-fly decoupling of NN,3N,4N matrix elements
  - first GPU version looks extremely promising (with Vary et al.)
- dynamic load balancing and automatic checkpointing/restart capabilities
- very good scaling behavior

Ab Initio Calculations for p- and sd-Shell Nuclei

Spectroscopy of Carbon Isotopes



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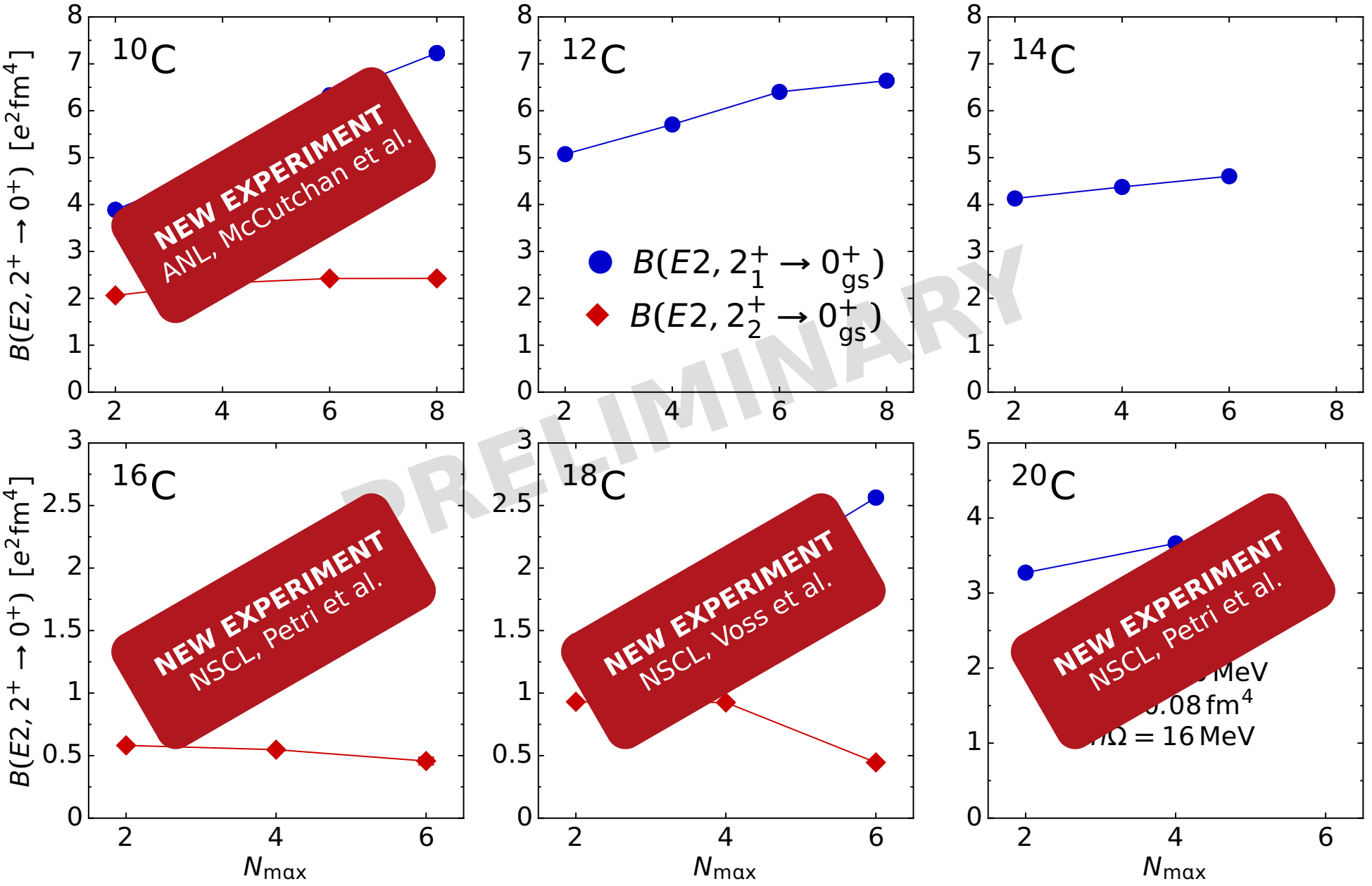
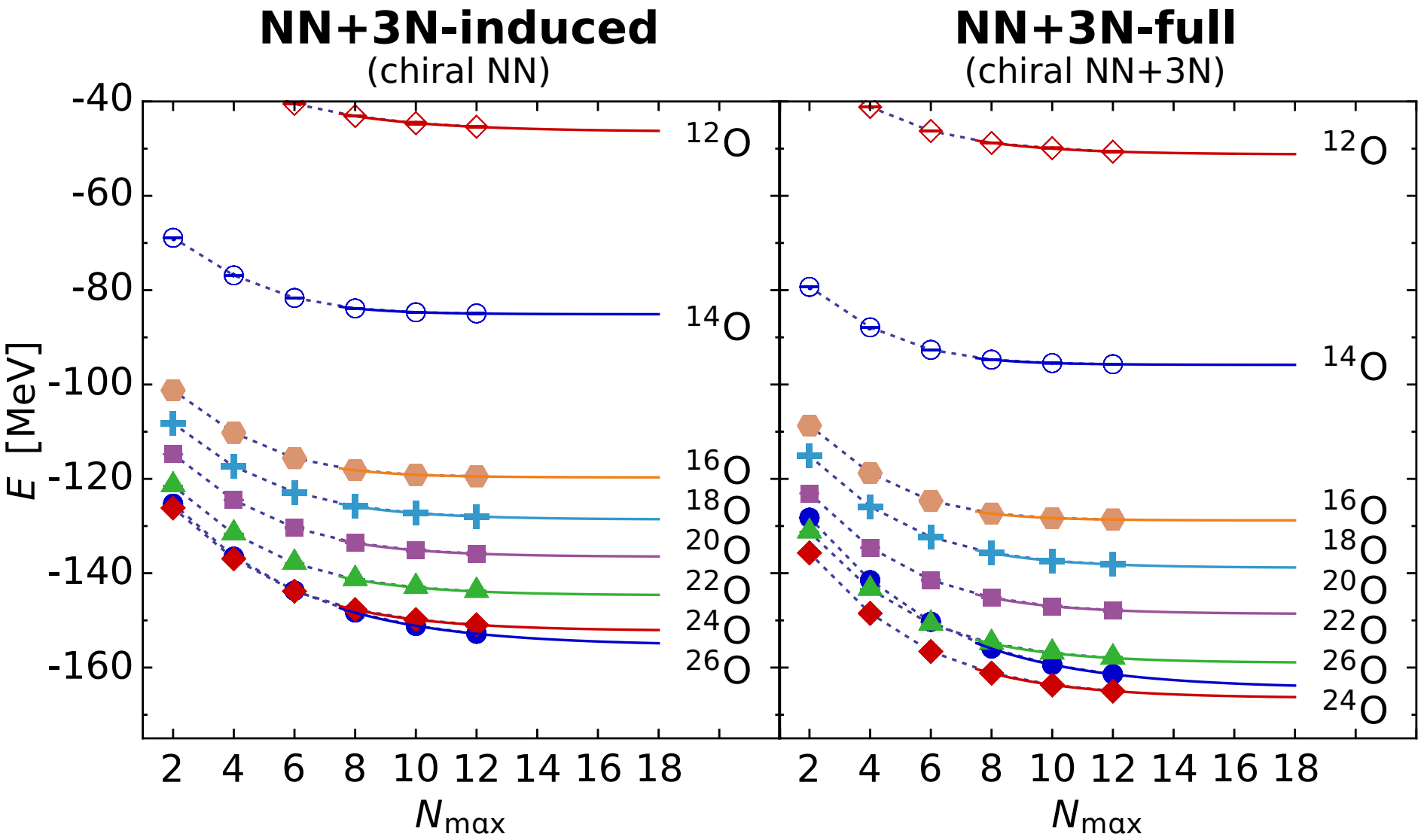


Ground States of Oxygen Isotopes

Hergert, Binder, Calci, Langhammer, Roth; in prep.



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

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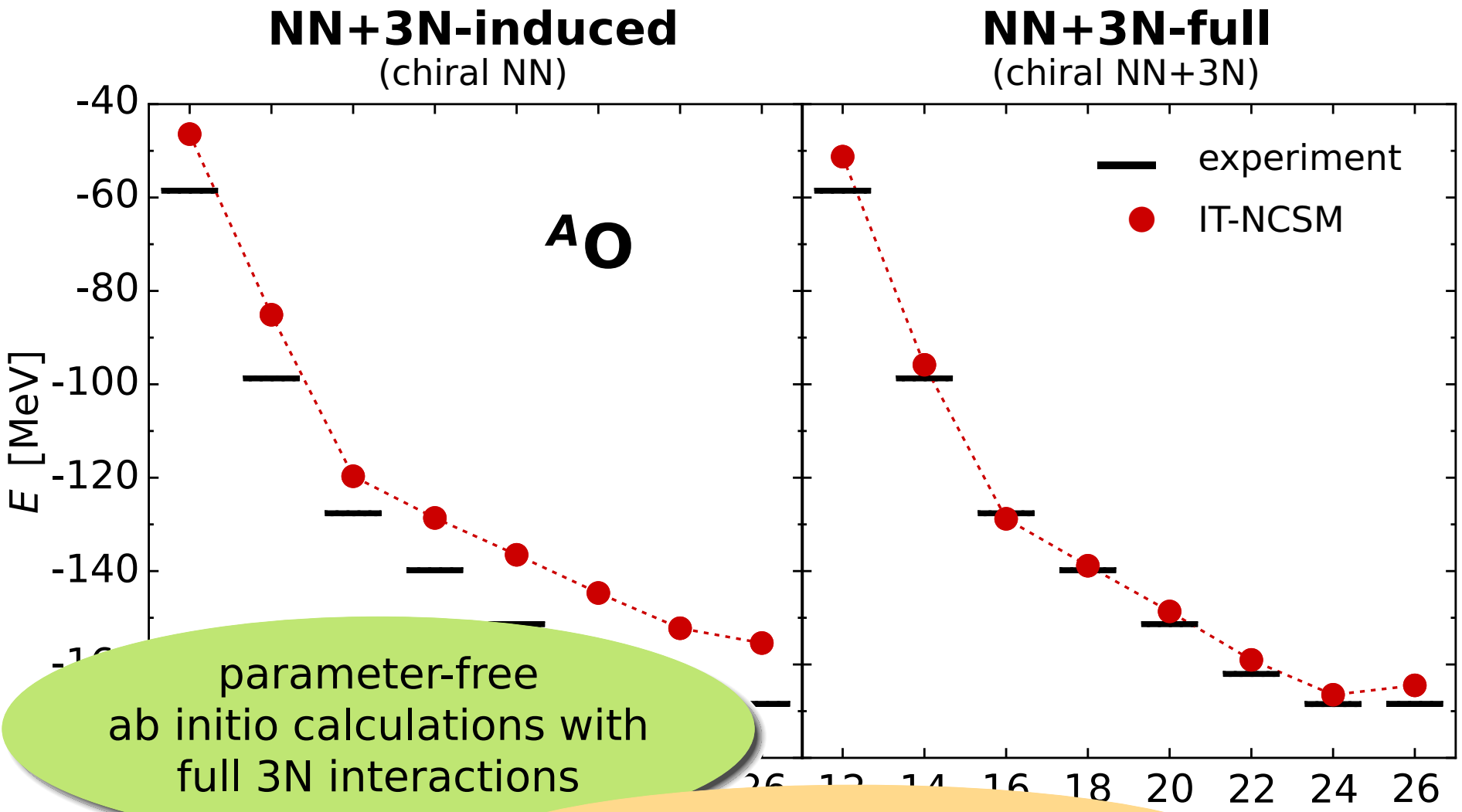

parameter-free
ab initio calculations with
full 3N interactions

highlights predictive power
of chiral NN+3N Hamiltonians

$\Lambda_{3N} = 400$ MeV, [illegible] optimal $\hbar\Omega$

Ground States of Oxygen Isotopes

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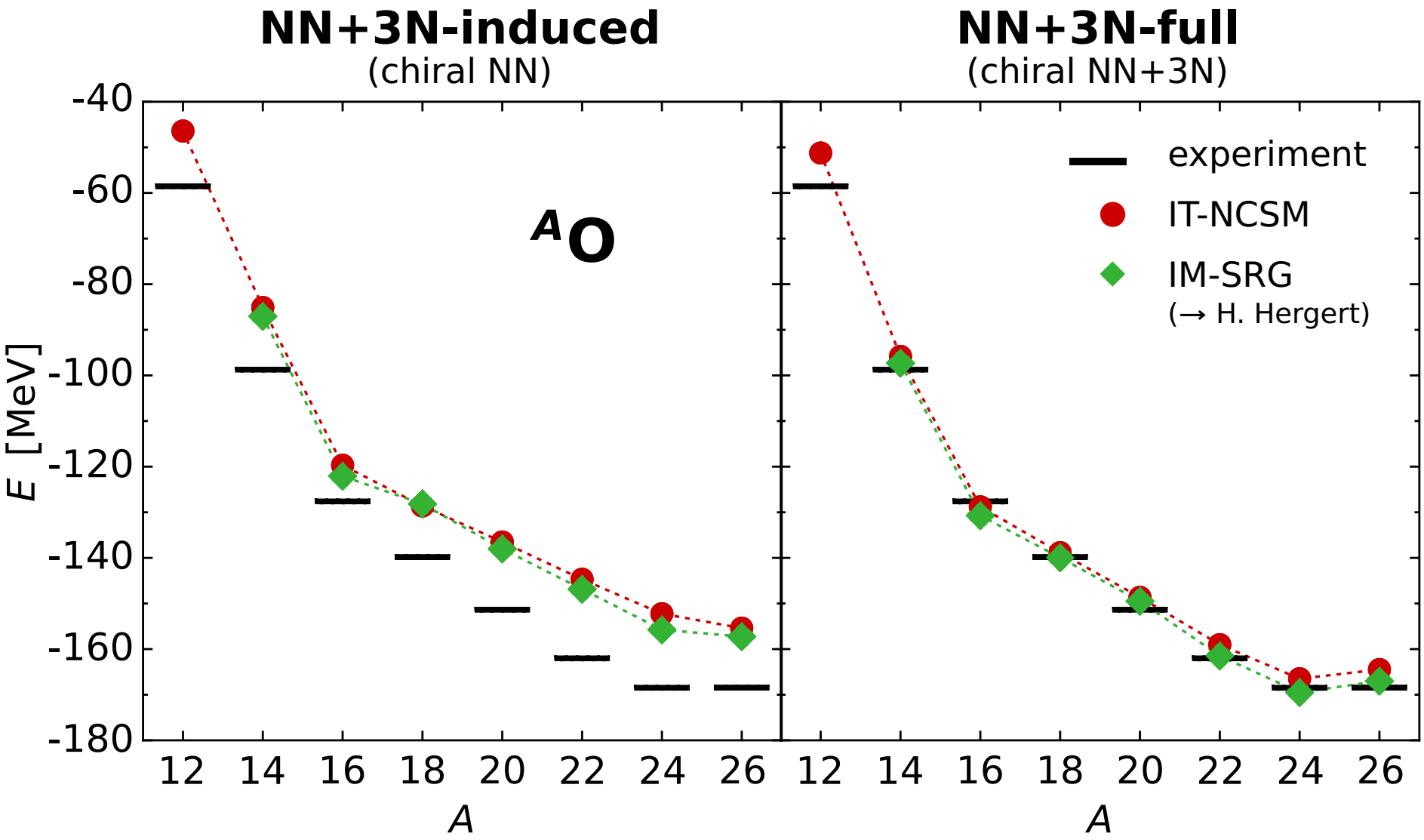

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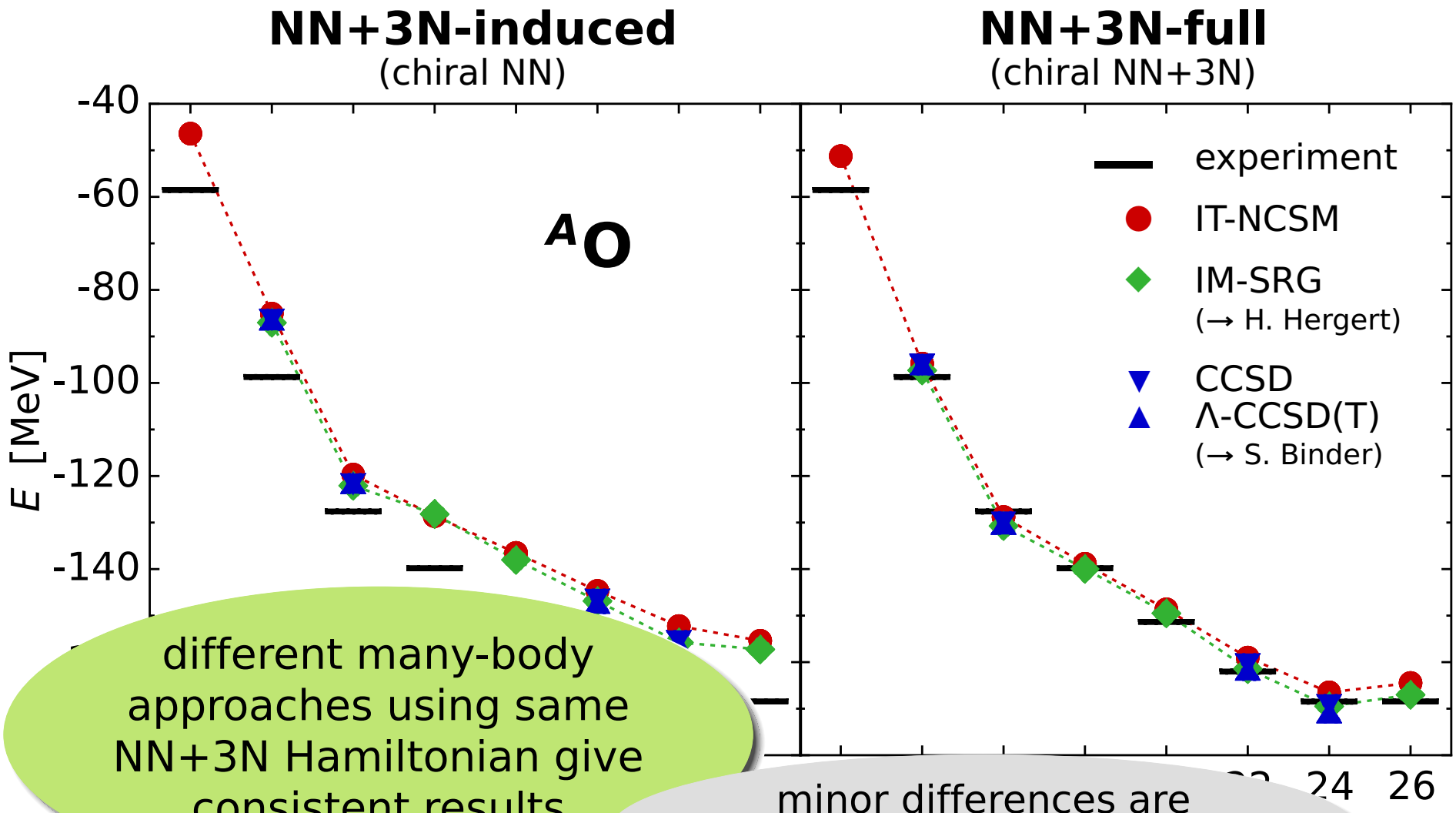


different many-body approaches using same NN+3N Hamiltonian give consistent results

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

$\Lambda_{3N} = 400$ MeV, $\alpha = 0.08\,\mathrm{fm}^{-1}$, $E_{3\,max} = 14$, optimal $\hbar\Omega$

Multi-Reference Normal Ordering

with

Eskendr Gebrerufael

Motivation: Normal Ordering

avoid formal and computational challenges of including explicit 3N terms in many-body calculations

- circumvent **formal extension of many-body method** to include explicit 3N interactions
- avoid the **increase of computational cost** caused by inclusion of explicit 3N interactions
- **normal-ordered two-body approximation** works very well for closed-shell systems (→ S. Binder)
- can we do the same for **open-shell nuclei**?

Normal Ordering of 3N Interaction

- **starting point**: three-body operator in second-quantized form with respect to the zero-body vacuum $|0\rangle$

$$V_{3N} = \frac{1}{36} \sum_{abc,\bar{a}\bar{b}\bar{c}} V^{abc}_{\bar{a}\bar{b}\bar{c}} \, A^{abc}_{\bar{a}\bar{b}\bar{c}}$$

$$V^{abc}_{\bar{a}\bar{b}\bar{c}} = \langle abc | V_{3N} | \bar{a}\bar{b}\bar{c} \rangle \qquad A^{abc}_{\bar{a}\bar{b}\bar{c}} = a^\dagger_a a^\dagger_b a^\dagger_c \, a_{\bar{c}} a_{\bar{b}} a_{\bar{a}}$$

- **single-reference normal ordering**: assume reference state $|\Phi_{SR}\rangle$ given by a single Slater determinant
  - standard toolbox: Wick theorem, contractions, etc.

- **multi-reference normal ordering**: assume reference state $|\Phi_{MR}\rangle$ given by a superposition of Slater determinants
  - generalized Wick theorem and n-tupel contractions proposed by Mukherjee & Kutzelnigg (1997)

Multi-Reference Normal Ordering

- **three-body operator in normal-ordered form** with respect to multi-reference state $|\Phi_{\mathrm{MR}}\rangle$

$$V_{3N} = W + \sum_{c,\bar{c}} W^{c}_{\bar{c}} \, \widetilde{A}^{c}_{\bar{c}} + \frac{1}{4} \sum_{bc,\bar{b}\bar{c}} W^{bc}_{\bar{b}\bar{c}} \, \widetilde{A}^{bc}_{\bar{b}\bar{c}} + \frac{1}{36} \sum_{abc,\bar{a}\bar{b}\bar{c}} W^{abc}_{\bar{a}\bar{b}\bar{c}} \, \widetilde{A}^{abc}_{\bar{a}\bar{b}\bar{c}}$$

  where $\widetilde{A}^{\circ\circ\circ}_{\circ\circ\circ}$ indicates multi-reference normal ordered string of creation and annihilation operators (abstract concept)

- matrix elements of **normal-ordered *n*-body contributions** involve one-, two- and three-body density matrices for $|\Phi_{\mathrm{MR}}\rangle$

$$W = \frac{1}{36} \sum_{abc,\bar{a}\bar{b}\bar{c}} V^{abc}_{\bar{a}\bar{b}\bar{c}} \, \rho^{abc}_{\bar{a}\bar{b}\bar{c}} \qquad W^{c}_{\bar{c}} = \frac{1}{4} \sum_{ab,\bar{a}\bar{b}} V^{abc}_{\bar{a}\bar{b}\bar{c}} \, \rho^{ab}_{\bar{a}\bar{b}}$$

$$W^{bc}_{\bar{b}\bar{c}} = \sum_{a,\bar{a}} V^{abc}_{\bar{a}\bar{b}\bar{c}} \, \rho^{a}_{\bar{a}} \qquad W^{abc}_{\bar{a}\bar{b}\bar{c}} = V^{abc}_{\bar{a}\bar{b}\bar{c}}$$

Multi-Reference Normal Ordering

- discard normal-ordered three-body contribution to define the **normal-ordered two-body (NO2B) approximation**

$$V_{\mathrm{NO2B}} = W + \sum_{c,\bar{c}} W^{c}_{\bar{c}}\, \tilde{A}^{c}_{\bar{c}} + \frac{1}{4} \sum_{bc,\bar{b}\bar{c}} W^{bc}_{\bar{b}\bar{c}}\, \tilde{A}^{bc}_{\bar{b}\bar{c}}$$

- converted back into **vacuum normal order** with respect to $|0\rangle$

$$V_{\mathrm{NO2B}} = \bar{V} + \sum_{c,\bar{c}} \bar{V}^{c}_{\bar{c}}\, A^{c}_{\bar{c}} + \frac{1}{4} \sum_{bc,\bar{b}\bar{c}} \bar{V}^{bc}_{\bar{b}\bar{c}}\, A^{bc}_{\bar{b}\bar{c}}$$

with new matrix elements

$$\bar{V} = \frac{1}{36} \sum_{abc,\bar{a}\bar{b}\bar{c}} V^{abc}_{\bar{a}\bar{b}\bar{c}} \left(\rho^{abc}_{\bar{a}\bar{b}\bar{c}} - 18\, \rho^{a}_{\bar{a}}\, \rho^{bc}_{\bar{b}\bar{c}} + 36\, \rho^{a}_{\bar{a}}\, \rho^{b}_{\bar{b}}\, \rho^{c}_{\bar{c}} \right)$$

$$\bar{V}^{c}_{\bar{c}} = \frac{1}{4} \sum_{ab,\bar{a}\bar{b}} V^{abc}_{\bar{a}\bar{b}\bar{c}} \left(\rho^{ab}_{\bar{a}\bar{b}} - 4\, \rho^{a}_{\bar{a}}\, \rho^{b}_{\bar{b}} \right) \qquad \bar{V}^{bc}_{\bar{b}\bar{c}} = \sum_{a,\bar{a}} V^{abc}_{\bar{a}\bar{b}\bar{c}}\, \rho^{a}_{\bar{a}}$$

Single-Reference Normal Ordering

- **single-reference normal ordering** is recovered by pugging in density matrices for a single Slater-determinant

$$\rho^{a}_{\bar{a}} = n_a \delta^{a}_{\bar{a}}$$
$$\rho^{ab}_{\bar{a}\bar{b}} = \rho^{a}_{\bar{a}}\,\rho^{b}_{\bar{b}} - \rho^{b}_{\bar{a}}\,\rho^{a}_{\bar{b}}$$
$$\rho^{abc}_{\bar{a}\bar{b}\bar{c}} = \ldots$$

- three-body operator in **single-reference NO2B approximation** converted back into vacuum representation

$$\mathrm{V_{NO2B}} = \bar{V} + \sum_{c,\bar{c}} \bar{V}^{c}_{\bar{c}}\,\mathrm{A}^{c}_{\bar{c}} + \frac{1}{4}\sum_{bc,\bar{b}\bar{c}} \bar{V}^{bc}_{\bar{b}\bar{c}}\,\mathrm{A}^{bc}_{\bar{b}\bar{c}}$$

with simplified matrix elements

$$\bar{V} = \frac{1}{6}\sum_{abc} V^{abc}_{abc}\, n_a n_b n_c \qquad \bar{V}^{c}_{\bar{c}} = -\frac{1}{2}\sum_{ab} V^{abc}_{ab\bar{c}}\, n_a n_b \qquad \bar{V}^{bc}_{\bar{b}\bar{c}} = \sum_{a} V^{abc}_{a\bar{b}\bar{c}}\, n_a$$

IT-NCSM with MR-NO2B Approximation

❶ perform NCSM with explicit 3N interaction for small $N_{\max}$

- ground state defines the reference state $|\Phi_{\mathrm{MR}}\rangle$
- no explicit information on excited states enters

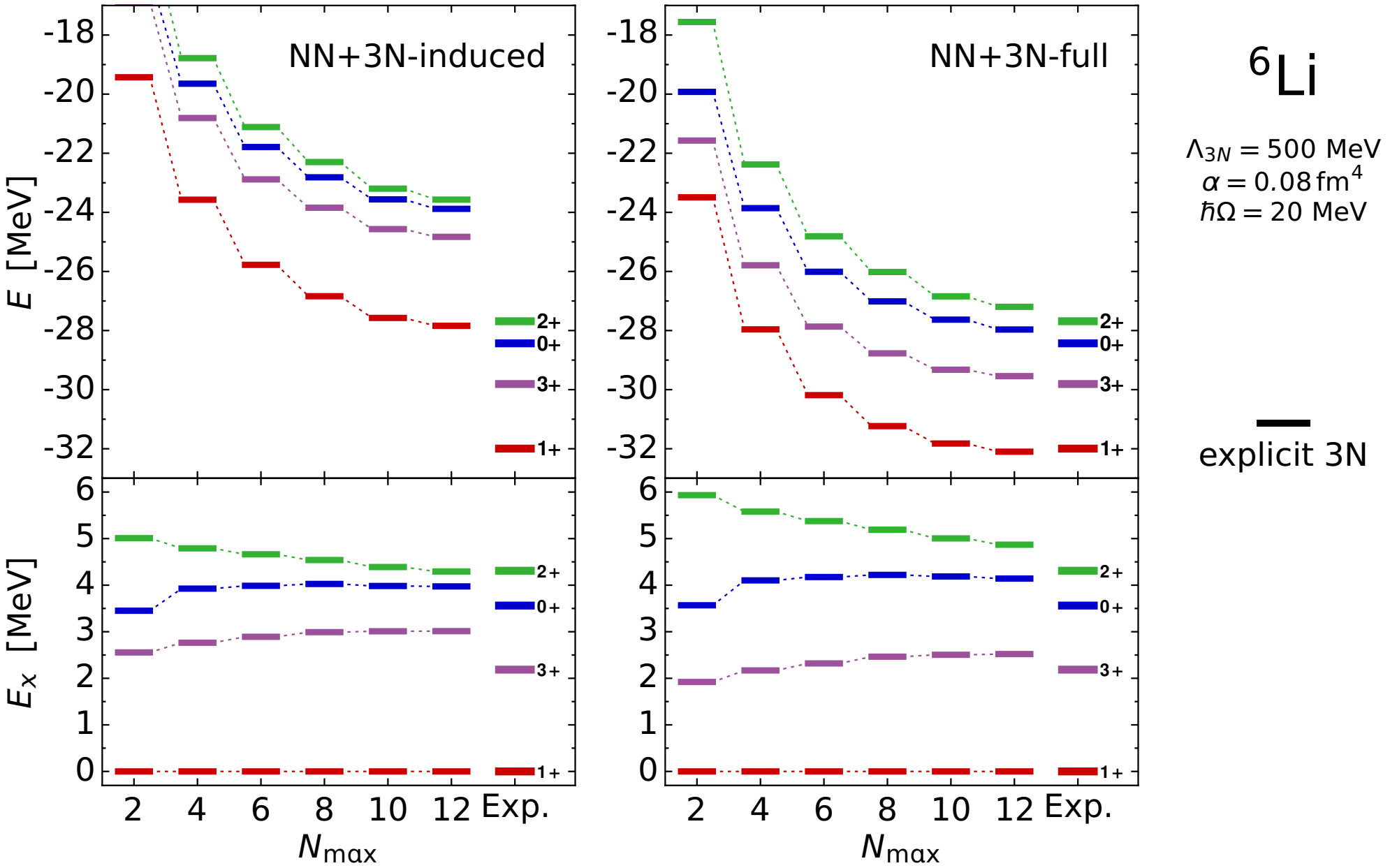
❷ compute zero-, one- and two-body matrix elements of MR-NO2B approximation

- density matrices for $|\Phi_{\mathrm{MR}}\rangle$ can be precomputed and stored
- three-body density matrix is not need explicitly

❸ perform NCSM or IT-NCSM calculation up to large $N_{\max}$ using MR-NO2B approximation

- same computational cost as a simple NN-only calculation
- larger model spaces become accessible

Benchmark: ^{6}Li

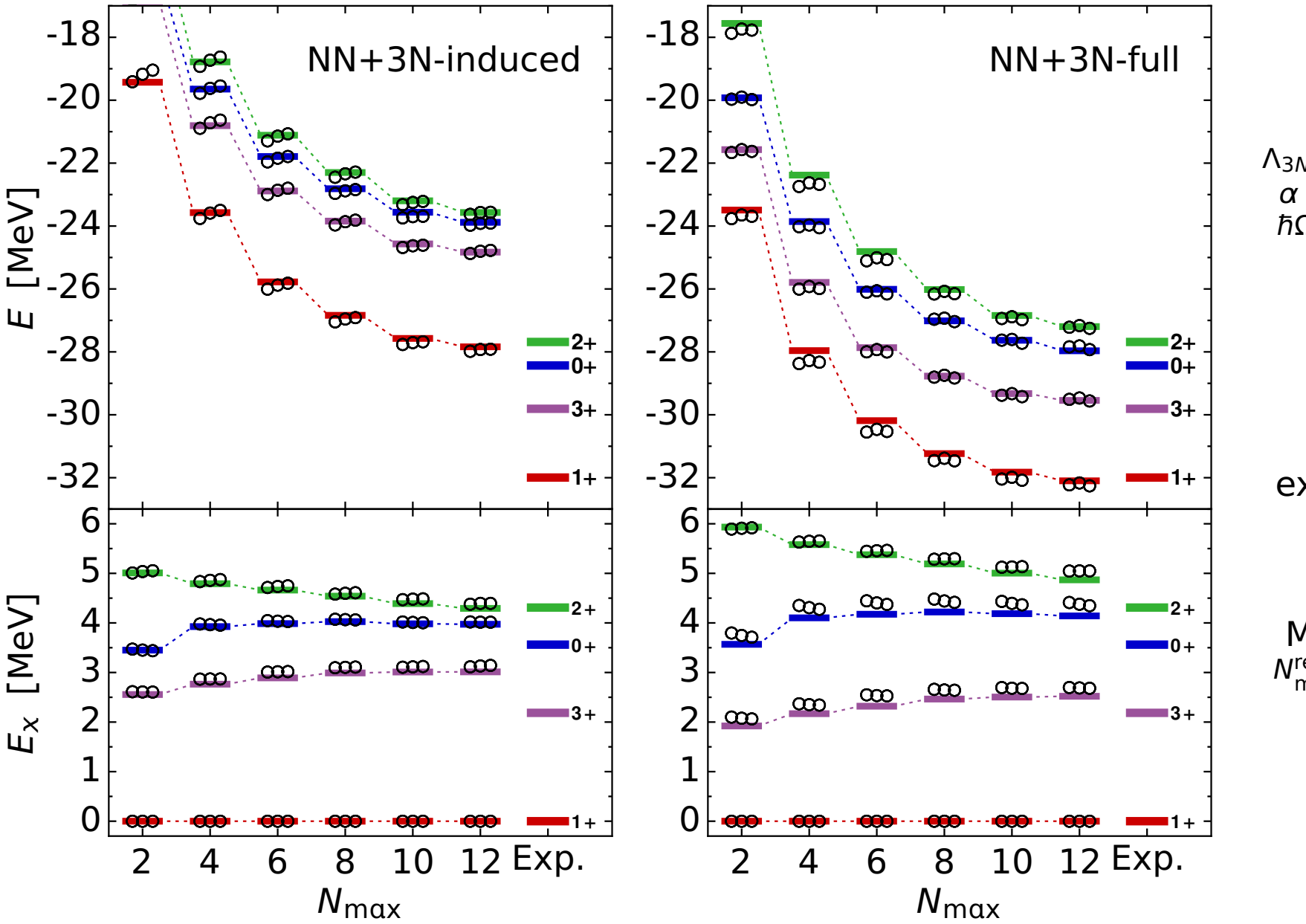


^{6}Li

$\Lambda_{3N} = 500$ MeV
$\alpha = 0.08\,\mathrm{fm}^4$
$\hbar\Omega = 20$ MeV

explicit 3N

Benchmark: ^{6}Li



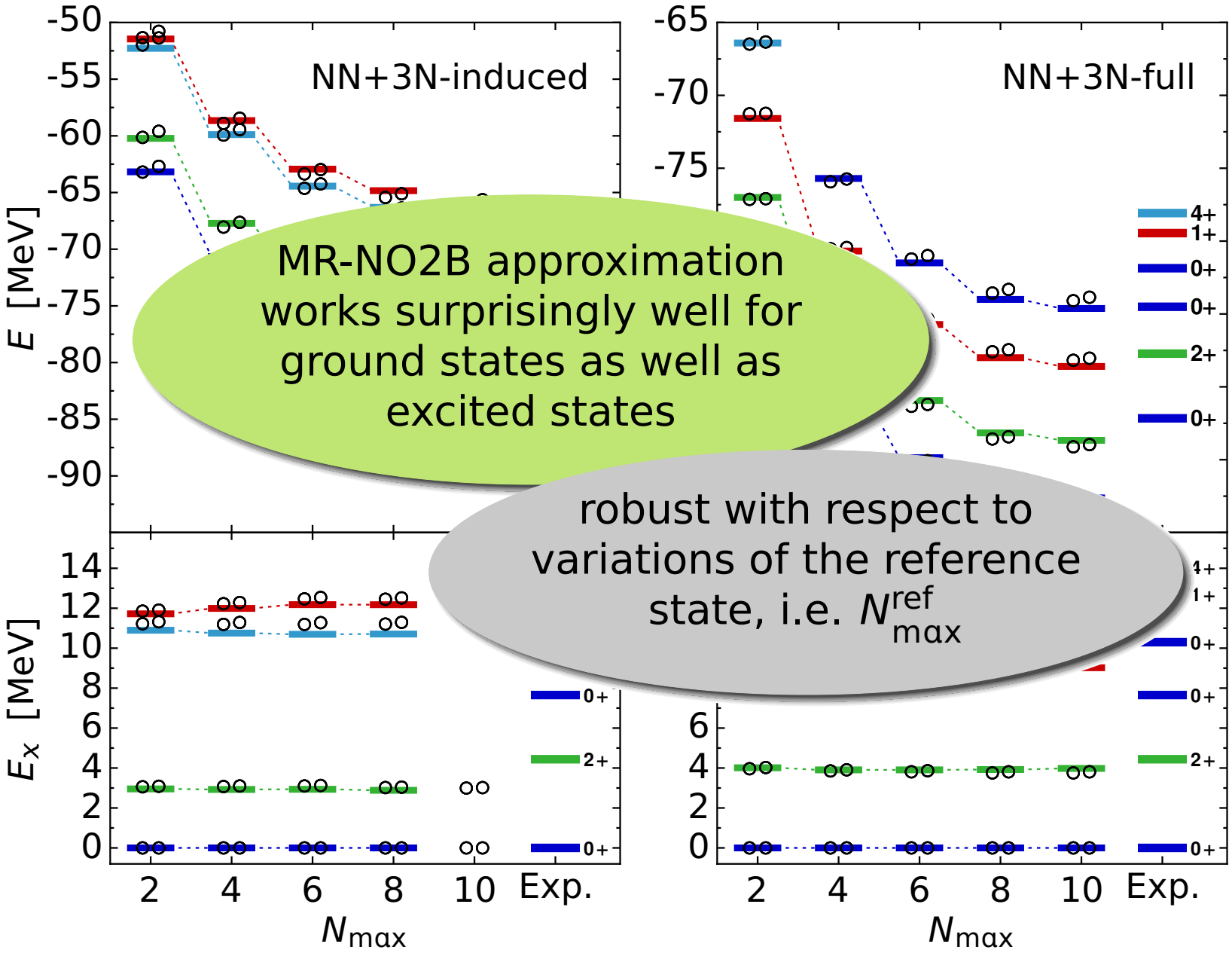
^{6}Li

$\Lambda_{3N} = 500$ MeV
$\alpha = 0.08\,\mathrm{fm}^4$
$\hbar\Omega = 20$ MeV

explicit 3N

MR-NO2B
$N_{max}^{ref} = 2, 4, 6$

Benchmark: ^{12}C



MR-NO2B approximation works surprisingly well for ground states as well as excited states

robust with respect to variations of the reference state, i.e. $N_{\max}^{\mathrm{ref}}$

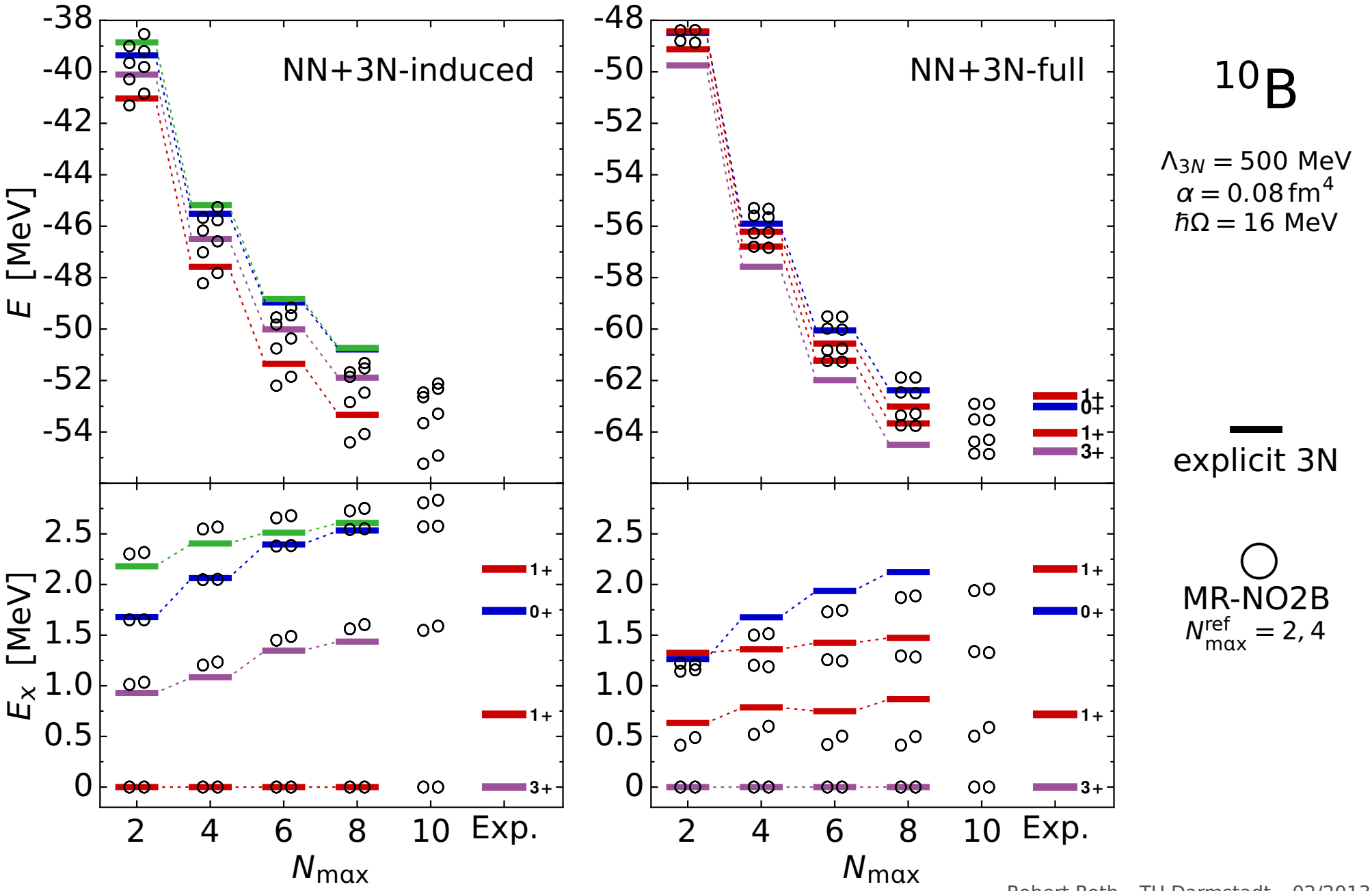
^{12}C

$\Lambda_{3N} = 500$ MeV
$\alpha = 0.08\,\mathrm{fm}^4$
$\hbar\Omega = 20$ MeV

explicit 3N

MR-NO2B
$N_{\max}^{\mathrm{ref}} = 2, 4$

Challenge: ^{10}B



Importance-Truncated Shell Model

with

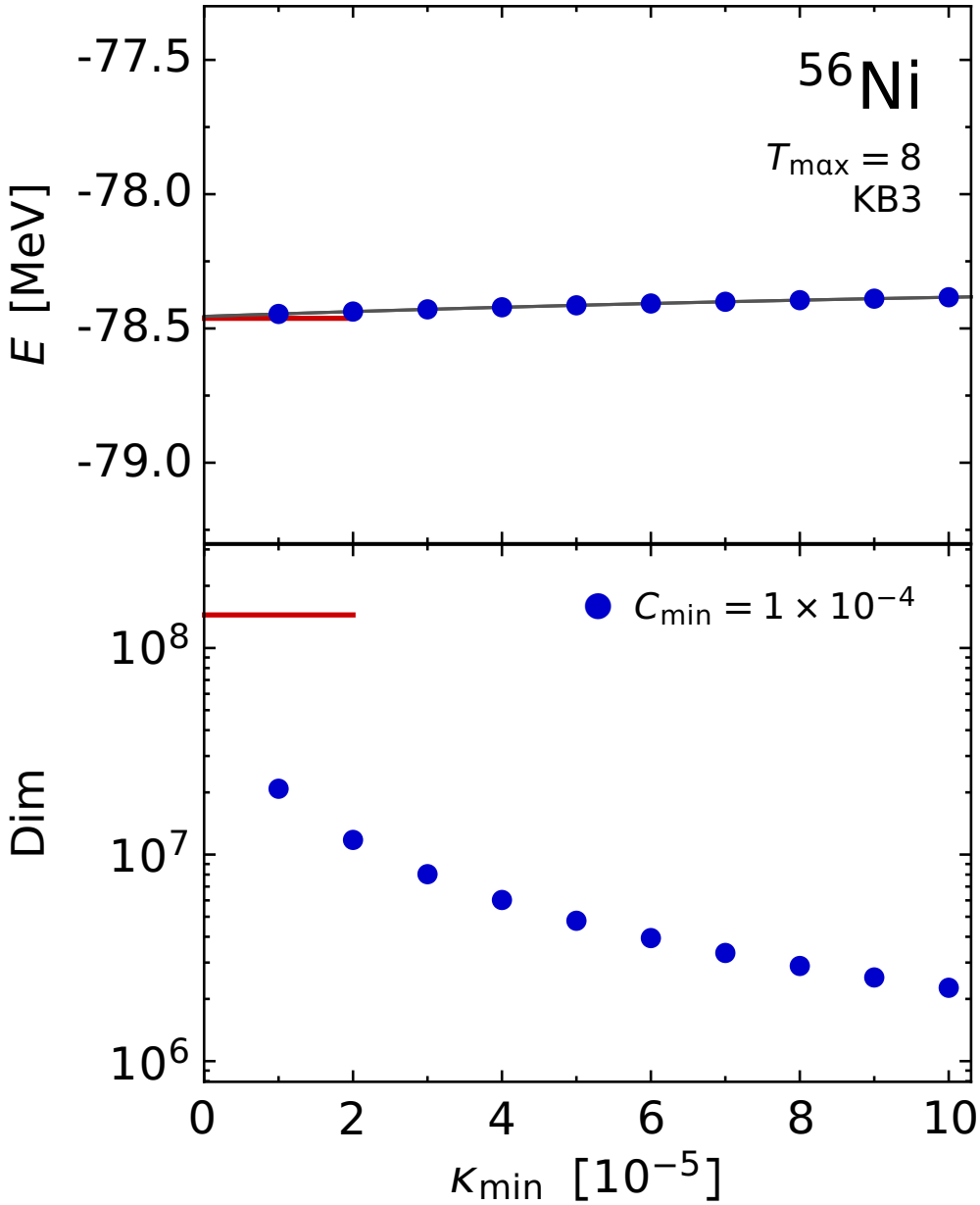
Christina Stumpf

Motivation: Importance Truncated SM

valence-space shell model suffers
from the same limitation as the NCSM:
model-space dimension

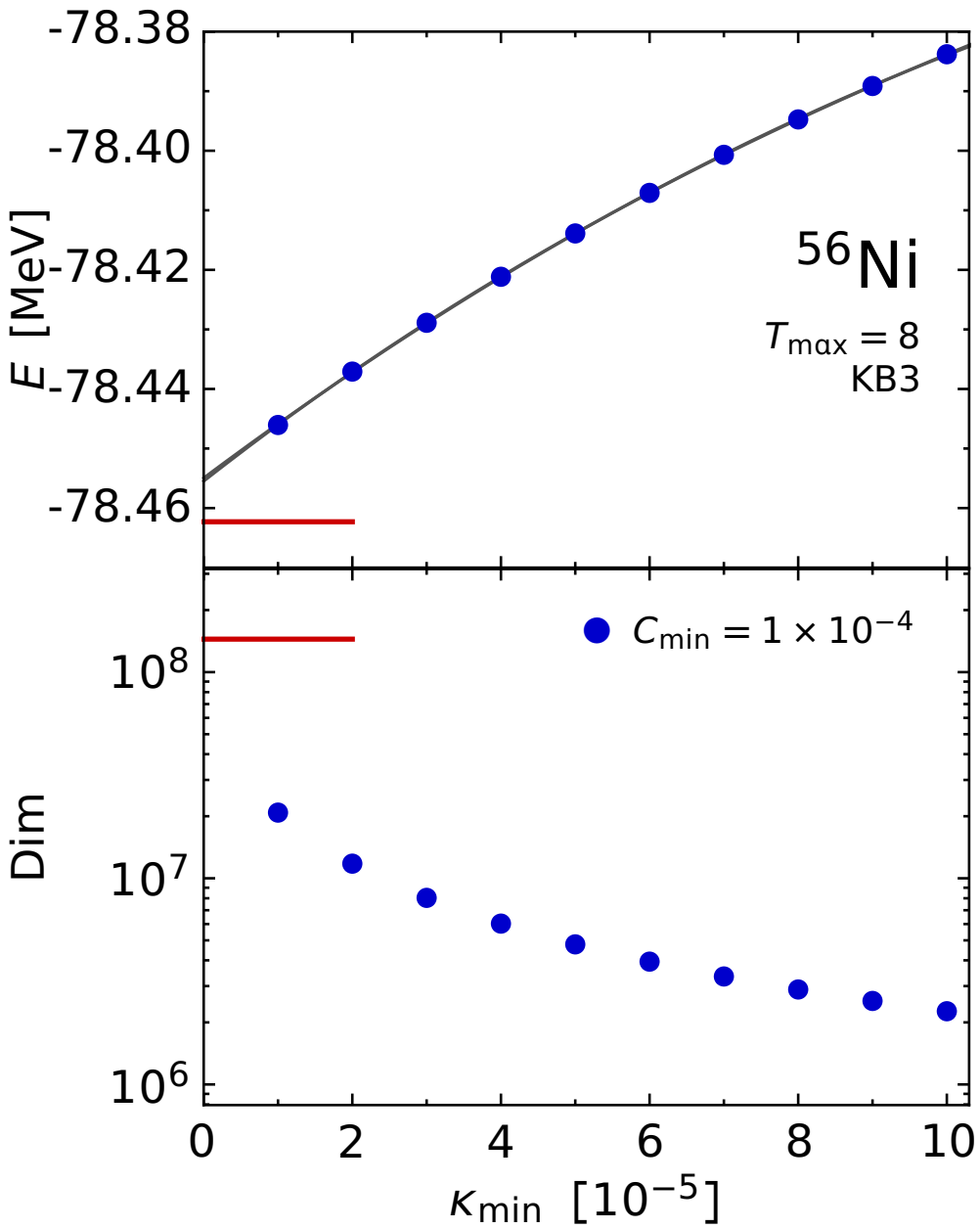
- concept of importance truncation can be **transferred directly to valence-space shell model**
- **new IT-SM code** based on our existing optimized IT-NCSM code
- use T_{max} **truncation** instead of N_{max} to set up iterative scheme
- start with full calculation at small T_{max} to define initial reference state and iteratively increase T_{max} in steps of 2

Test Case: ^{56}Ni in *pf* Valence-Space



- very weak κ_{min}-dependence of energies
- dimension reduced by one order of magnitude

Test Case: ^{56}Ni in *pf* Valence-Space



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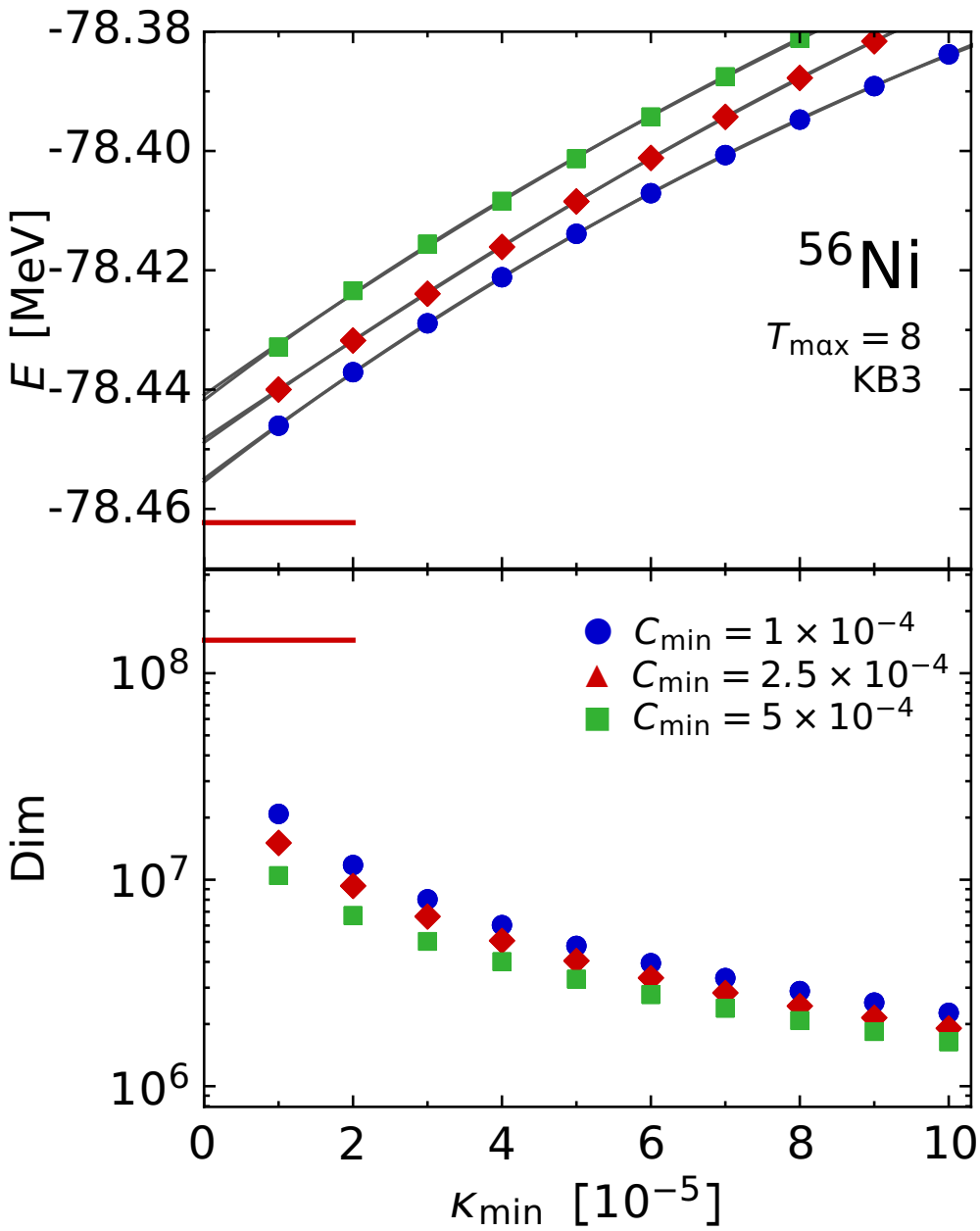
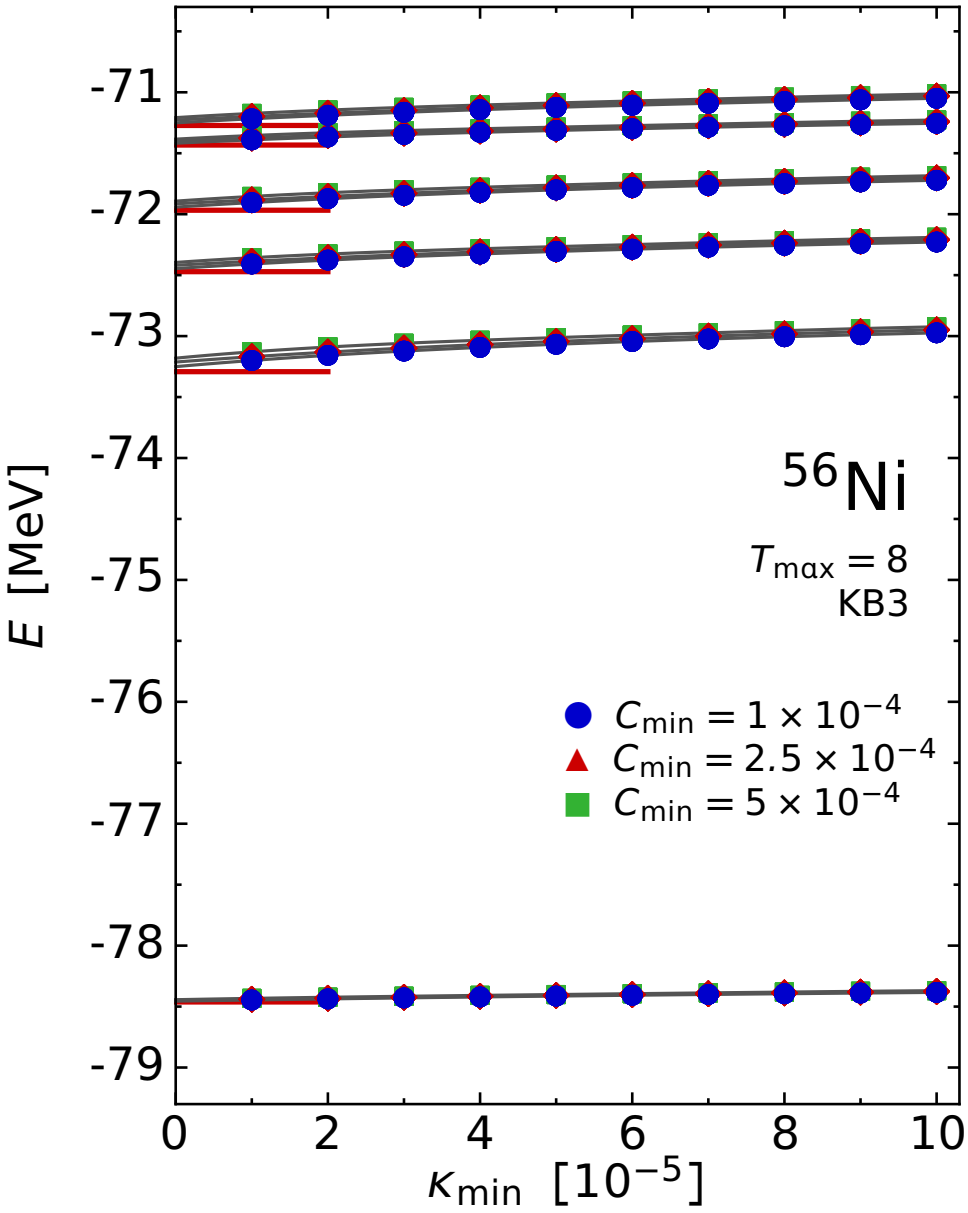


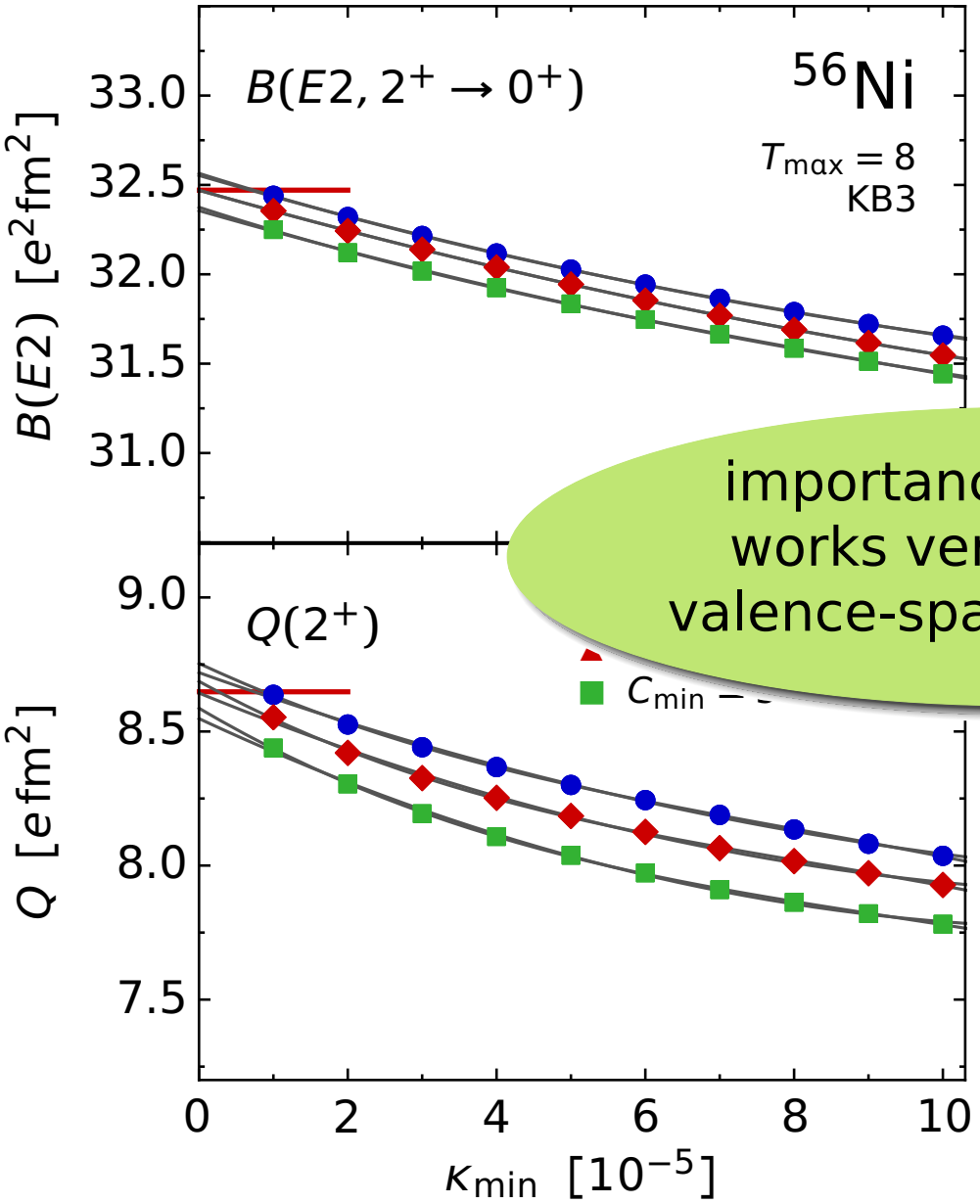
- very weak $\kappa_{\min}$-dependence of energies
- dimension reduced by one order of magnitude
- reference-space truncation induces ~ 5 keV deviation

Test Case: ^{56}Ni in *pf* Valence-Space



- very weak $\kappa_{\min}$-dependence of energies
- dimension reduced by one order of magnitude
- reference-space truncation induces ~ 5 keV deviation
- excitation spectrum is accessible with the same accuracy

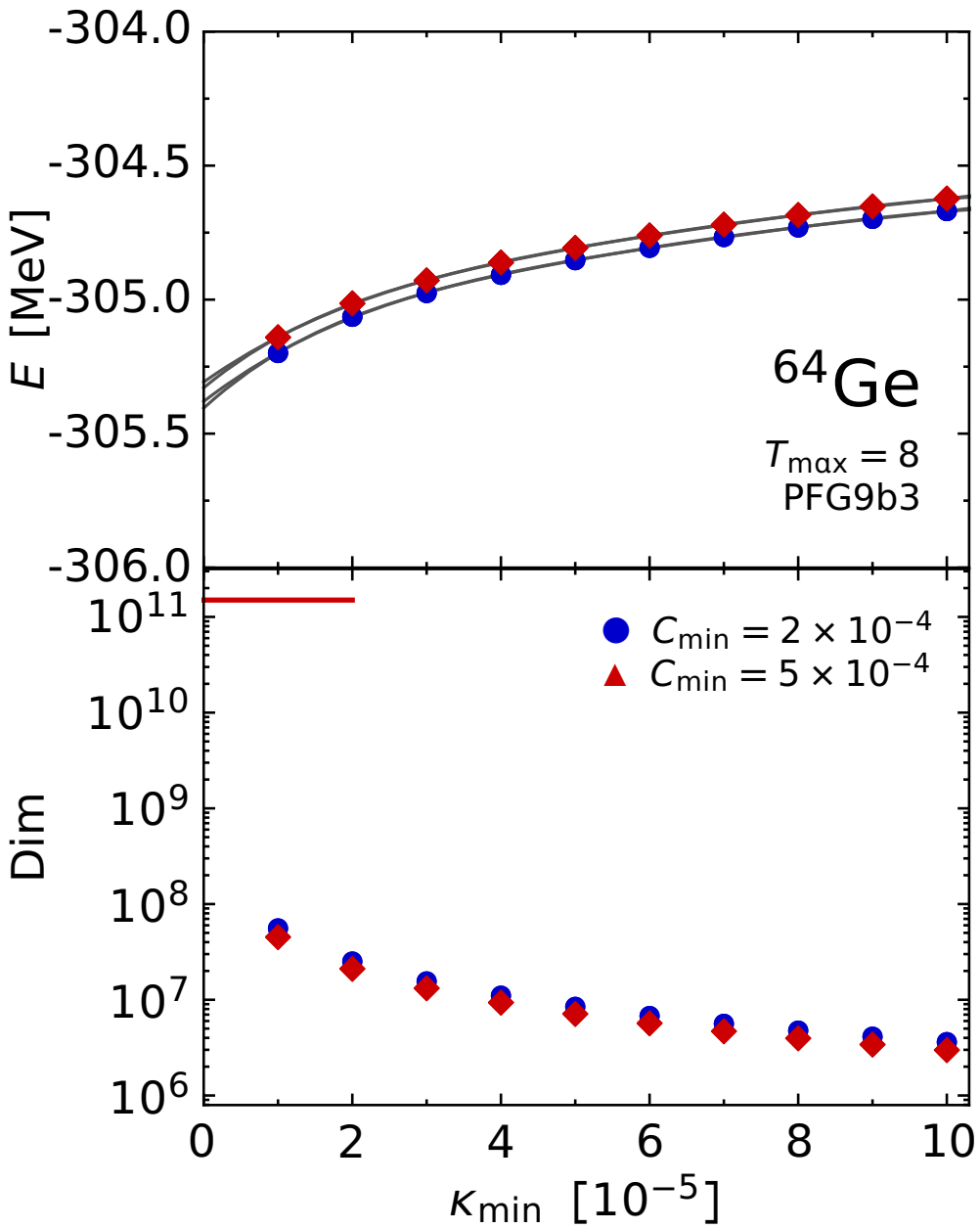
Test Case: ^{56}Ni in *pf* Valence-Space



importance truncation works very well in the valence-space shell model

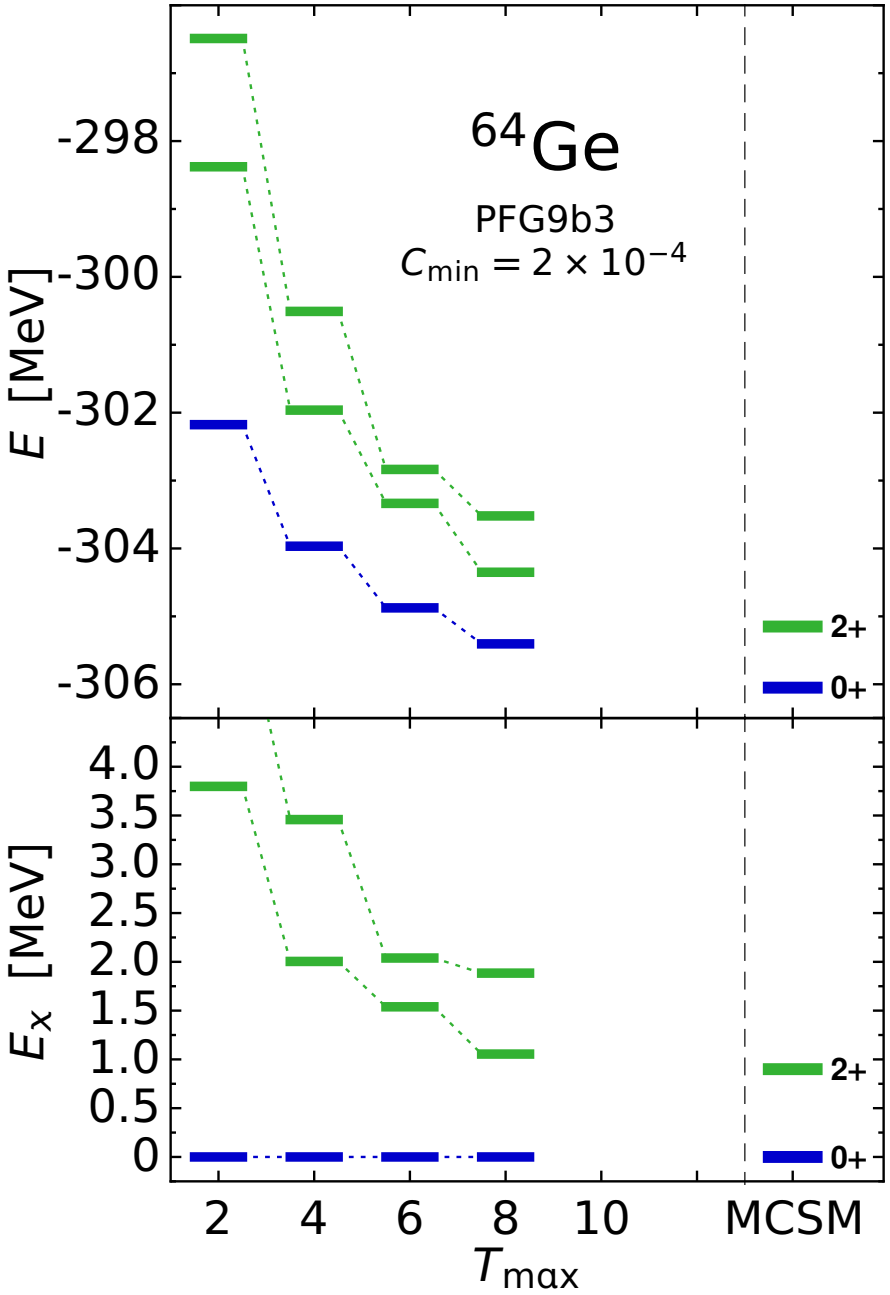
- very weak κ_{min}-dependence of energies
- dimension reduced by one order of magnitude
- truncation in- eviation
- ation spectrum is accessible with the same accuracy
- spectroscopic observables are equally well described

Challenge: ^{64}Ge in $pfg_{9/2}$ Valence-Space



- beyond the reach of the full shell model for $T_{max} > 4$
- moderate κ_{min}-dependence of energies
- dimension reduced by several orders of magnitude

Challenge: ^{64}Ge in $pfg_{9/2}$ Valence-Space



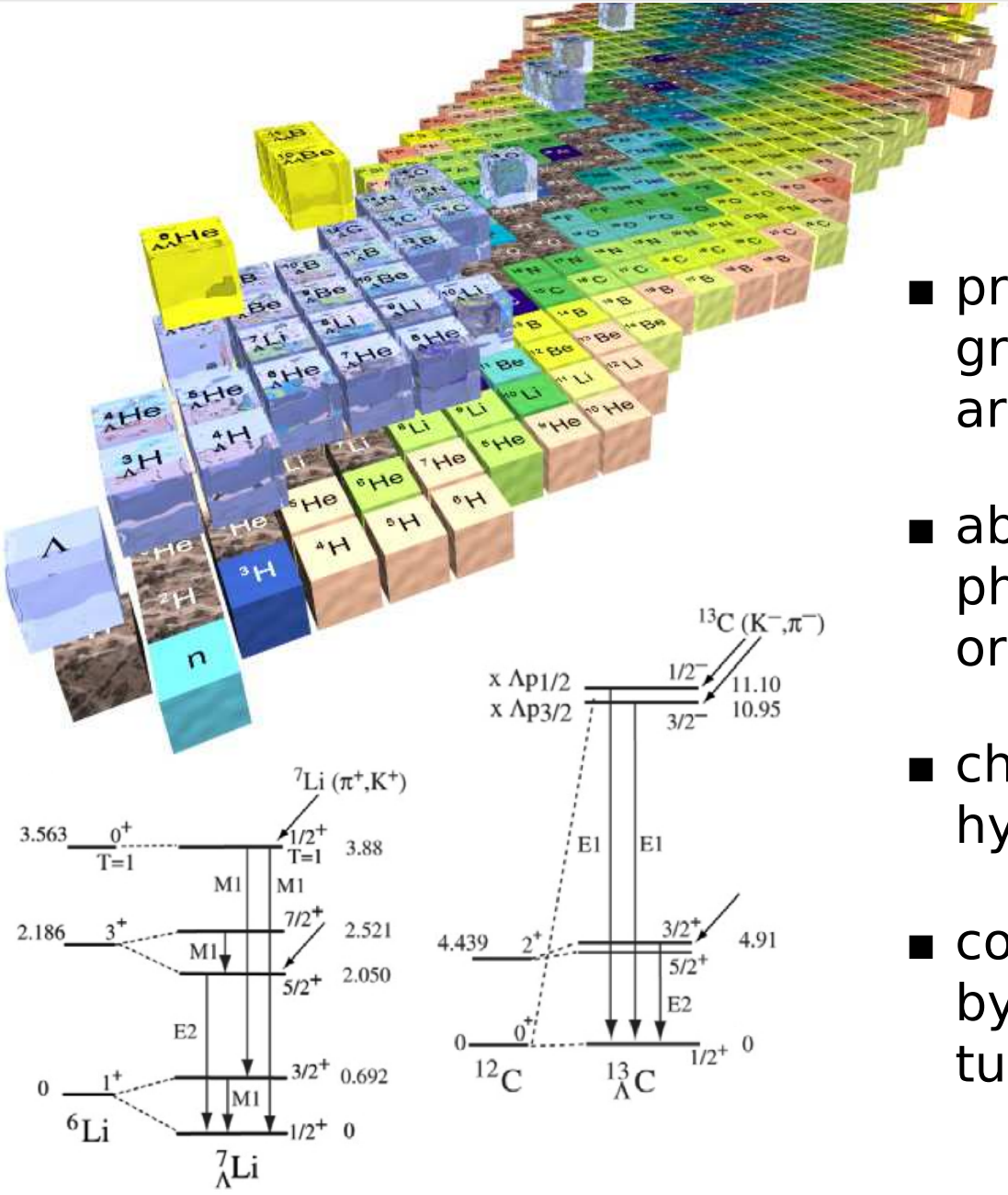
- beyond the reach of the full shell model for $T_{max} > 4$
- moderate κ_{min}-dependence of energies
- dimension reduced by several orders of magnitude
- results consistent with Monte Carlo Shell Model (MCSM) by Otsuka et al.
- IT-SM calculations for larger T_{max} are on their way...

Ab Initio Hypernuclear Structure

with

Roland Wirth

Motivation: Hypernuclear Structure



- precision data on hypernuclear ground states and spectroscopy are available
- ab initio few-body ($A \lesssim 4$) and phenomenological shell model or cluster calculations so far
- chiral EFT interactions including hyperons are being constructed
- constrain YN & YY interaction by ab initio hypernuclear structure calculations

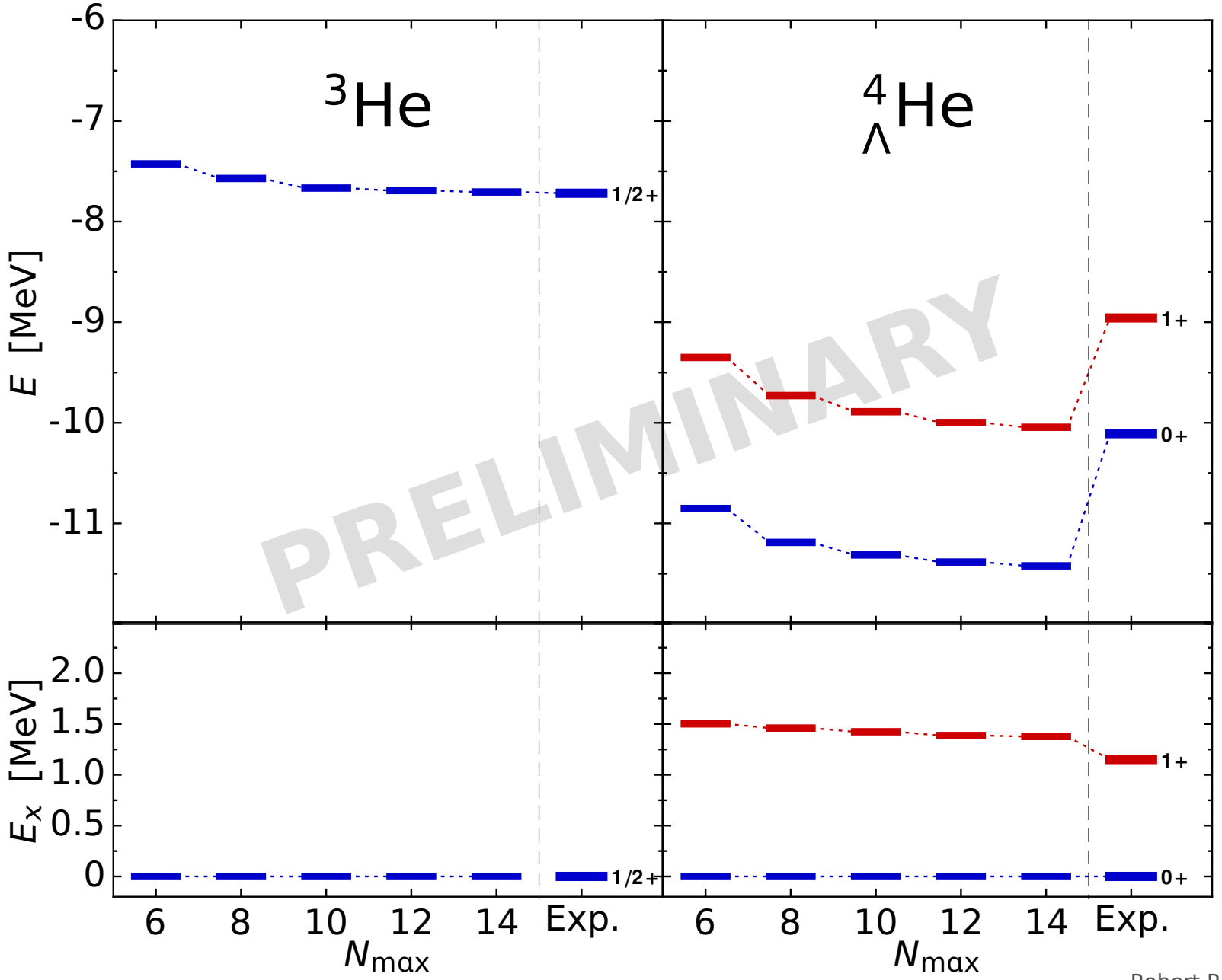
Ab Initio Toolbox

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

- **Similarity Renormalization Group**
  - consistent SRG-evolution of NN, 3N, YN interactions
  - using particle basis and including ΛΣ-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: ${}^{4}_{\Lambda}$He



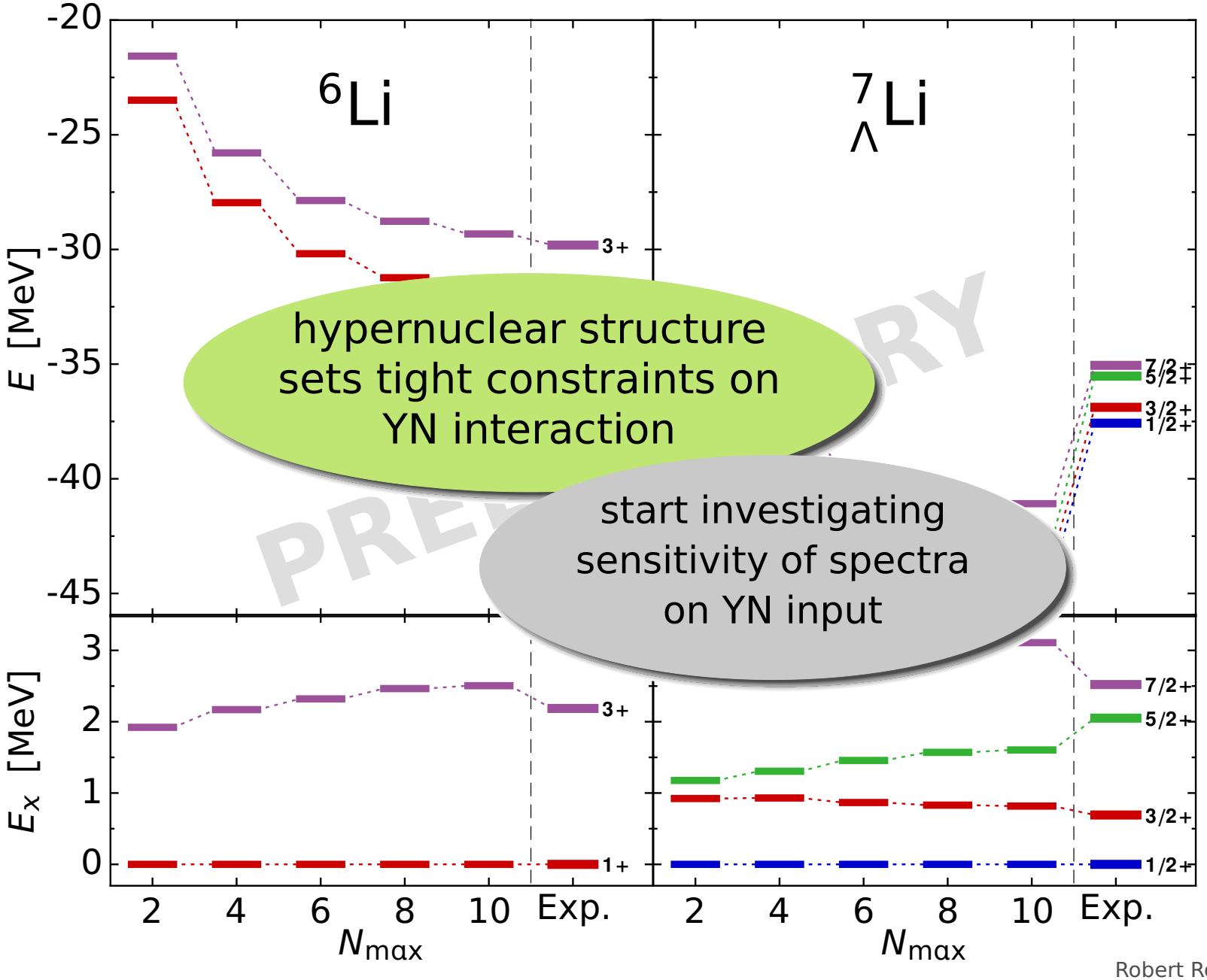
NN @ N3LO
Entem&Machleidt
$\Lambda_{NN} = 500$ MeV

3N @ N2LO
Navratil
$\Lambda_{3N} = 500$ MeV
triton fit

YN @ LO
Haidenbauer et al.
$\Lambda_{YN} = 600$ MeV
scatt. & hypertriton

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

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



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Conclusions

Conclusions

- importance truncation pushes the limit for **ab initio NCSM calculations** into the sd-shell
  - controlled and quantified uncertainties
  - preserves all the goodies of the full NCSM
  - carbon and oxygen isotopic chains up to the drip lines

- several **new directions**
  - multi-reference normal-ordering for approximate inclusion of 3N
  - importance truncation for the valence-space shell model
  - first ab initio calculations for p-shell hypernuclei

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

Epilogue

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LOEWE-CSC — CSC Center for Scientific Computing Frankfurt
HOPPER — NERSC
COMPUTING TIME

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DFG

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Helmholtz International Center

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Exzellente Forschung für Hessens Zukunft

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