Mid-Mass Low-Lying

Spectroscopy via the In-Medium No-Core Shell Model

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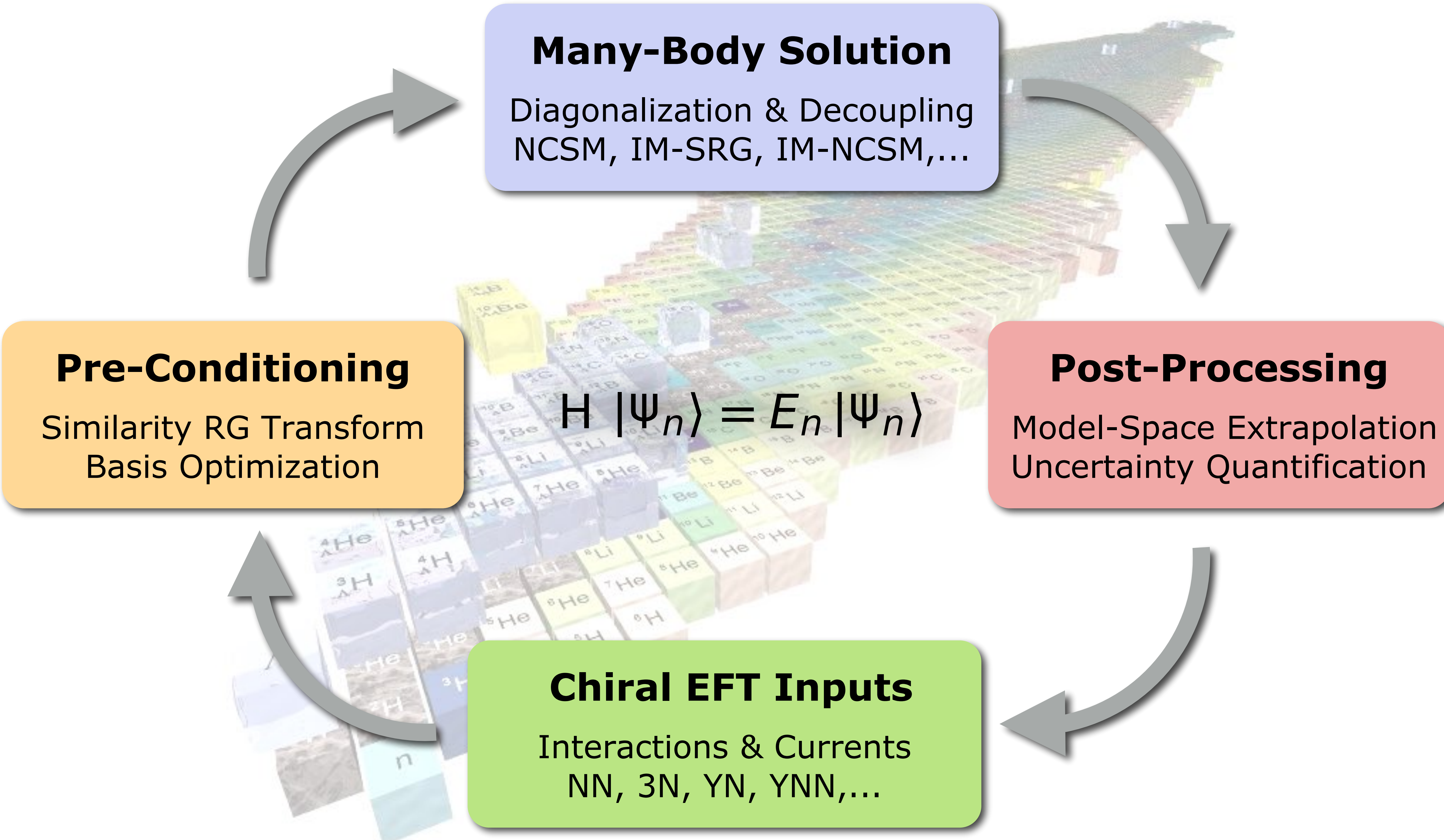
Ab Initio Nuclear Structure Toolbox



Uncertainty Quantification

all theory calculations are affected by systematic uncertainties (some also by statistical uncertainties)

in ab initio methods uncertainties result in a controlled way from truncations

variation of all truncation parameters gives access to systematic UQ

- **chiral EFT uncertainties**
  - assess convergence of observables in dependence of chiral truncation order
  - convergence affected by regulator scheme and scale, degrees of freedom
  - additional uncertainties from fit to experimental data
- **many-body uncertainties**
  - assess convergence of observables with model-space truncation
  - convergence affected by basis choice, truncation scheme, Hamiltonian

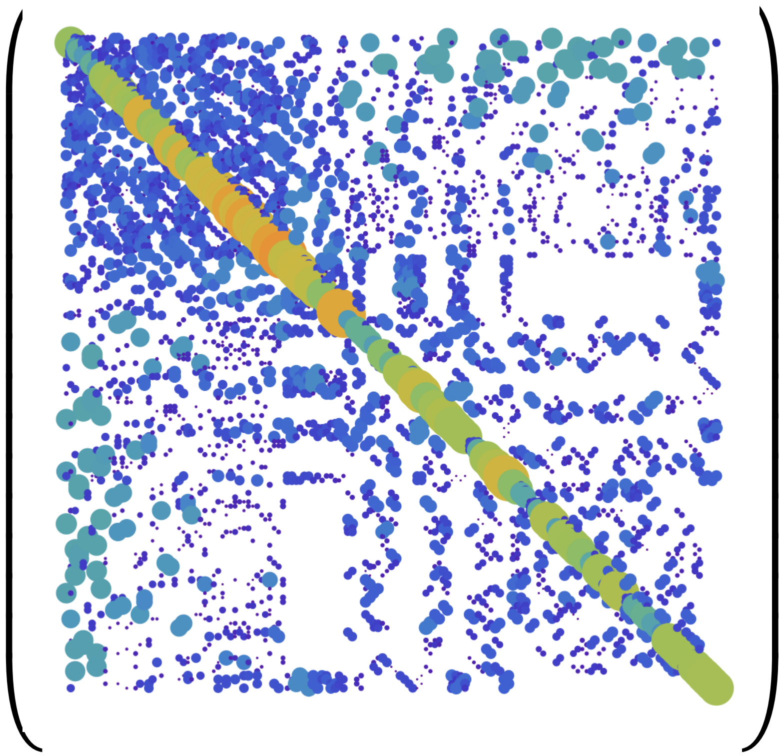
No-Core Shell Model

No-Core Shell Model

Barrett, Vary, Navrátil, Maris, Nogga, Roth,...

no-core shell model is
universal and powerful ab initio approach for
light nuclei (up to A≈25)

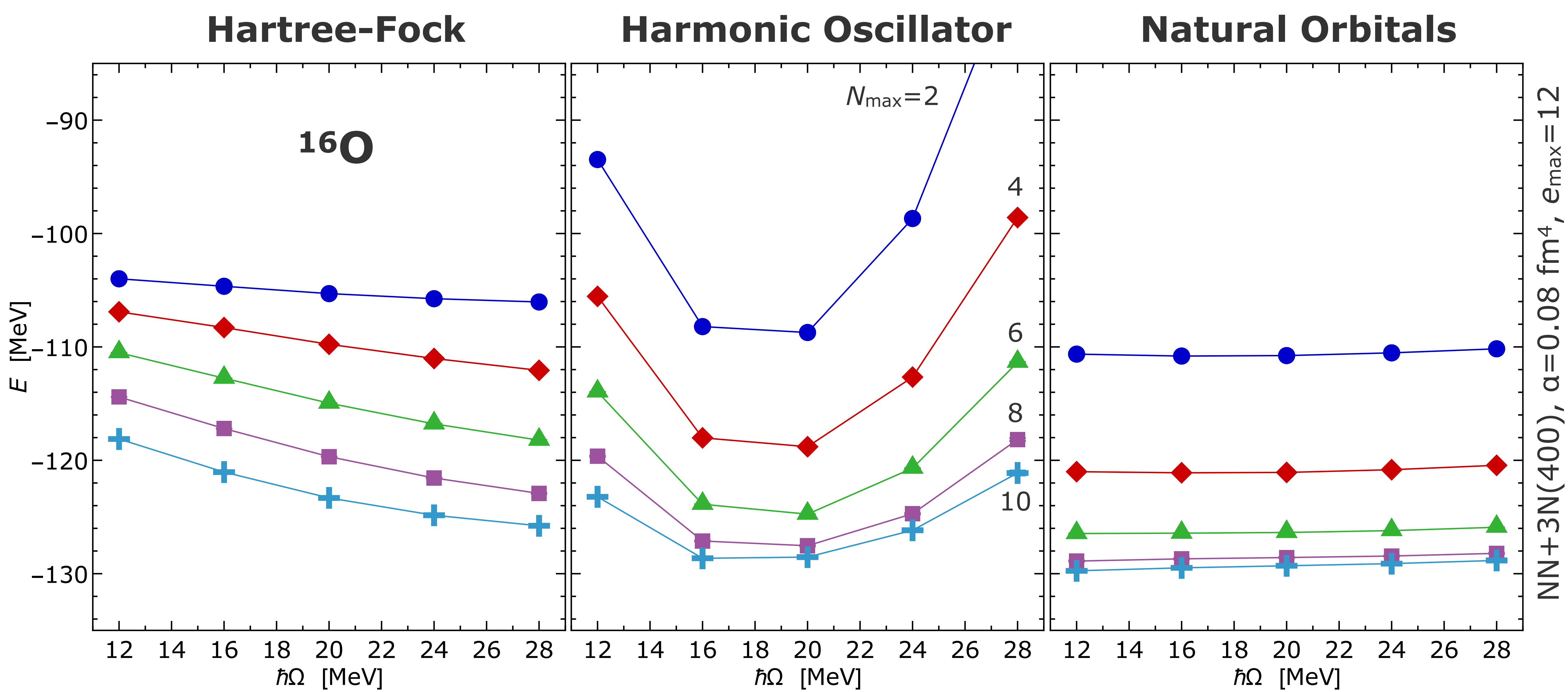
- **idea**: solve eigenvalue problem of Hamiltonian represented in model space of HO Slater determinants truncated w.r.t. HO excitation energy $N_{\max}\hbar\Omega$



$$\begin{pmatrix} \vdots \\ C_{i'}^{(n)} \\ \vdots \end{pmatrix} = E_n \begin{pmatrix} \vdots \\ C_{i}^{(n)} \\ \vdots \end{pmatrix}$$

NCSM Convergence: Energies

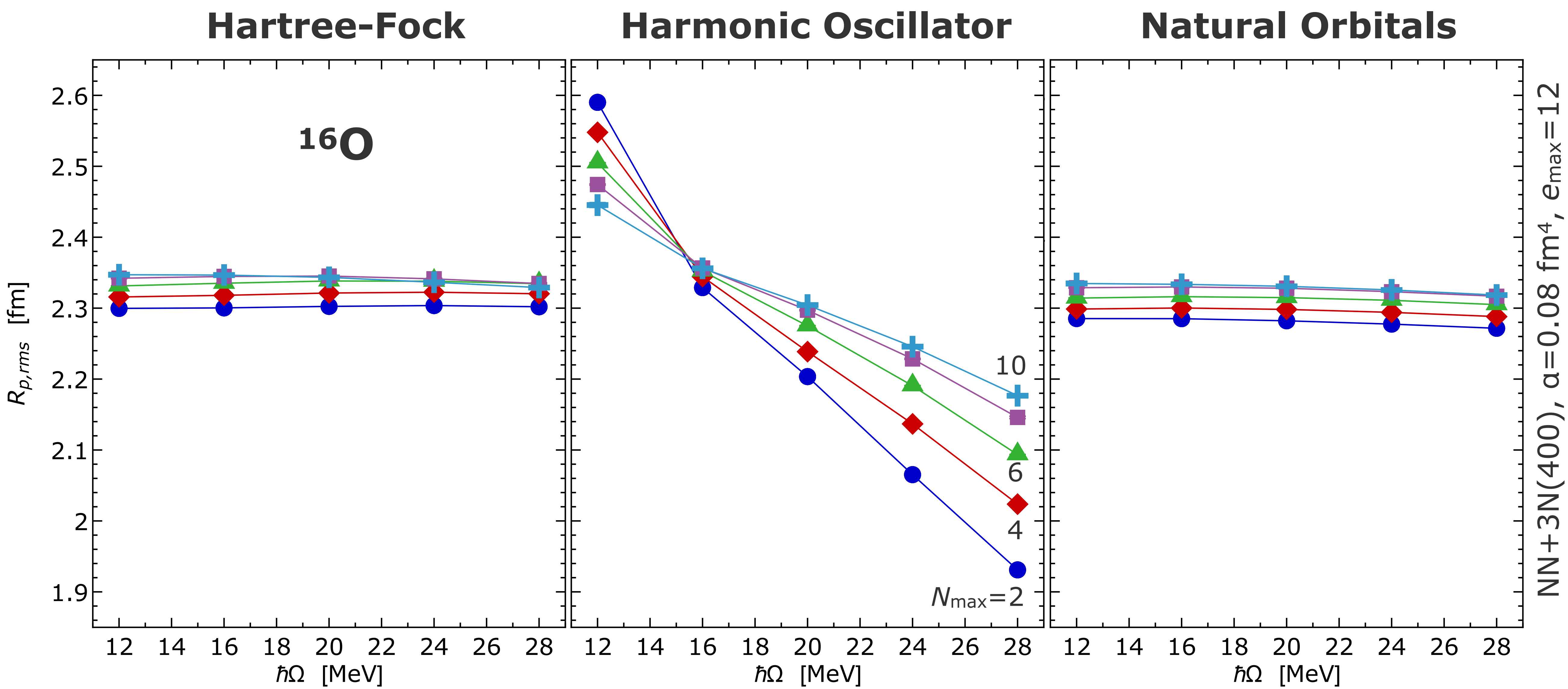
Tichai, Müller, Vobig, Roth; PRC 99, 034321 (2019)



- natural-orbital basis **eliminates frequency dependence** and **accelerates convergence** of NCSM

NCSM Convergence: Radii

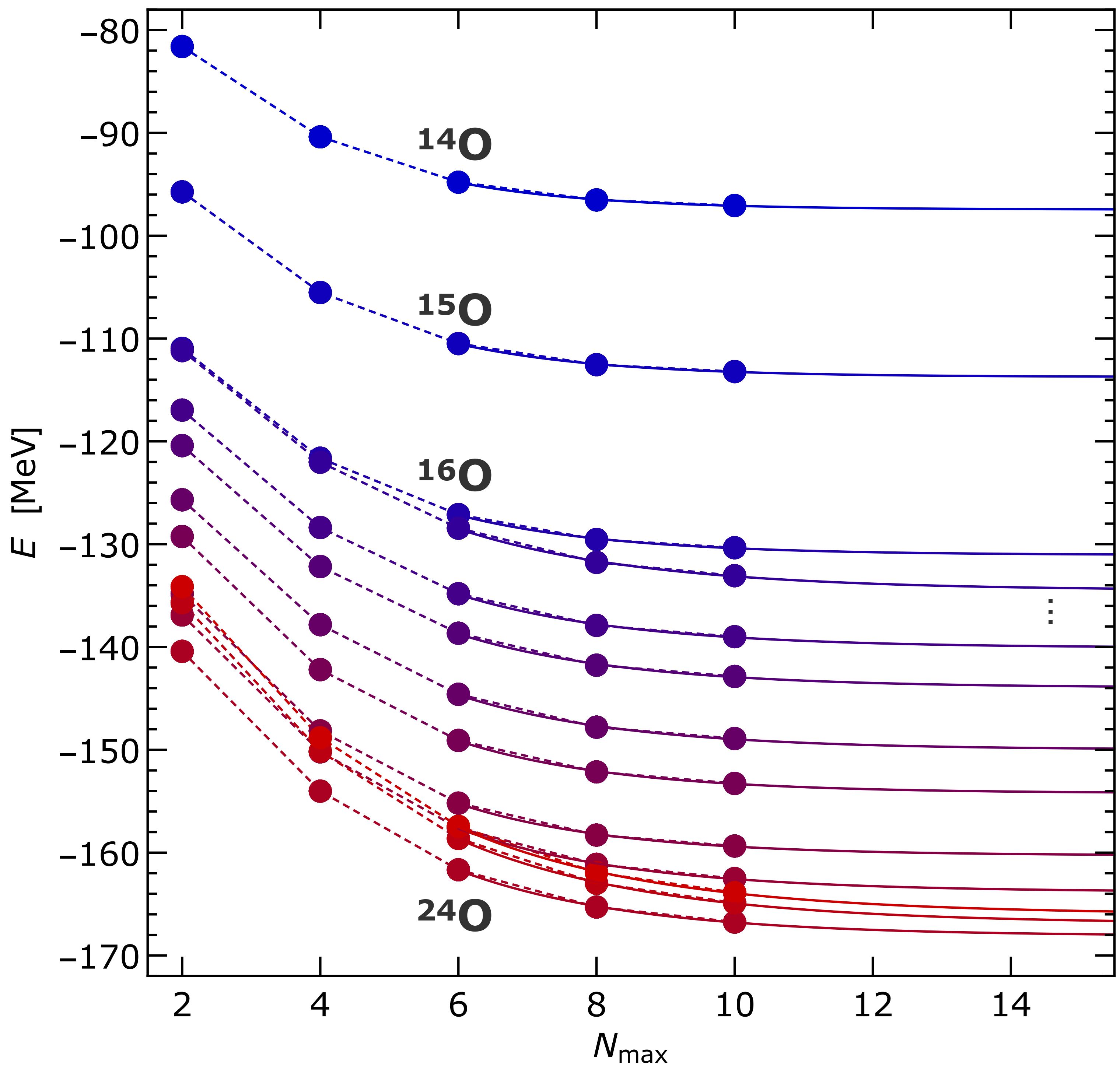
Tichai, Müller, Vobig, Roth; PRC 99, 034321 (2019)



- MBPT natural-orbital basis **eliminates frequency dependence** and **accelerates convergence** of NCSM

Oxygen Isotopes

Tichai, Müller, Vobig, Roth; PRC 99, 034321 (2019)



chiral NN+3N
Λ_{3N}=400 MeV
α=0.08 fm^4
$\hbar\Omega$=20 MeV
e_{max}=12

- excellent convergence with natural-orbital basis for all oxygen isotopes

Oxygen Isotopes

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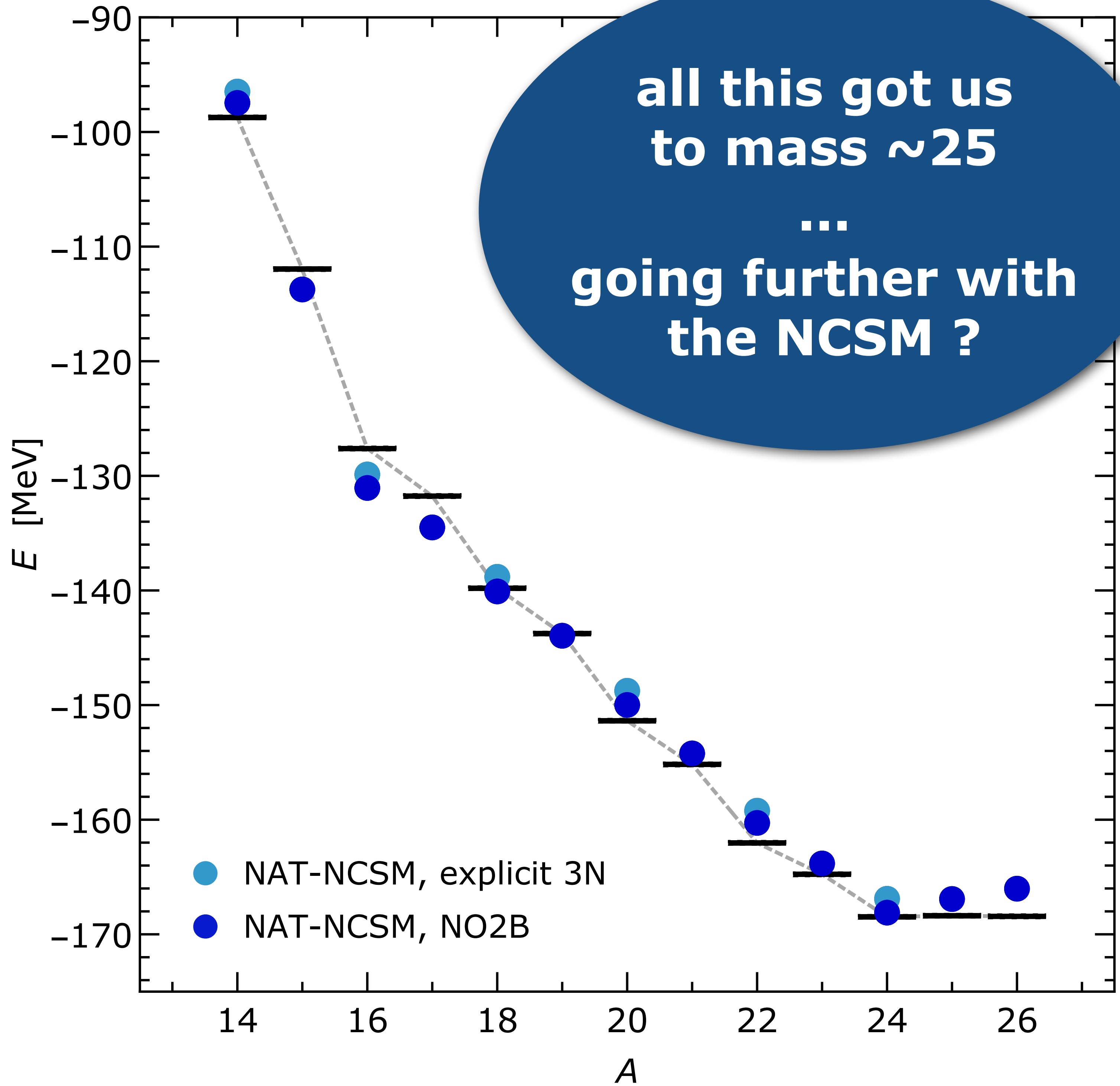

all this got us to mass ~25

...

going further with the NCSM ?

- excellent convergence with natural-orbital basis for all oxygen isotopes
- very good agreement with experimental systematics and dripline
- NO2B instead of explicit 3N causes ~1% overbinding

chiral NN+3N

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$\hbar\Omega$=20 MeV

e_{max}=12

In-Medium NCSM

No-Core Shell Model

Barrett, Vary, Navrátil, Maris, Nogga, Roth,...

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universal and powerful ab initio approach for
light nuclei (up to A≈25)

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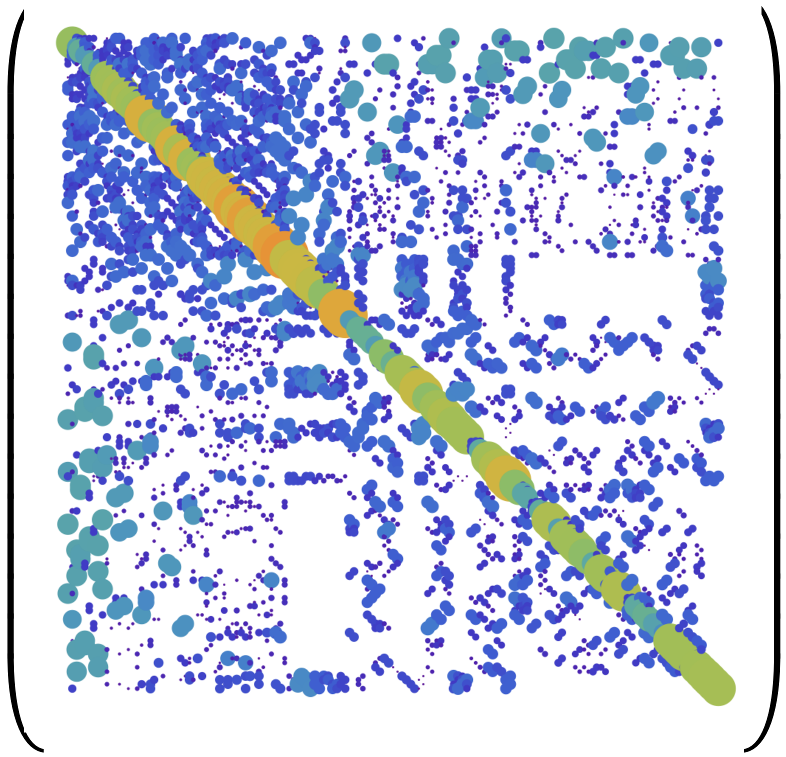

$$\begin{pmatrix}\vdots\\ C_{i'}^{(n)}\\ \vdots\end{pmatrix} = E_n \begin{pmatrix}\vdots\\ C_{i}^{(n)}\\ \vdots\end{pmatrix}$$

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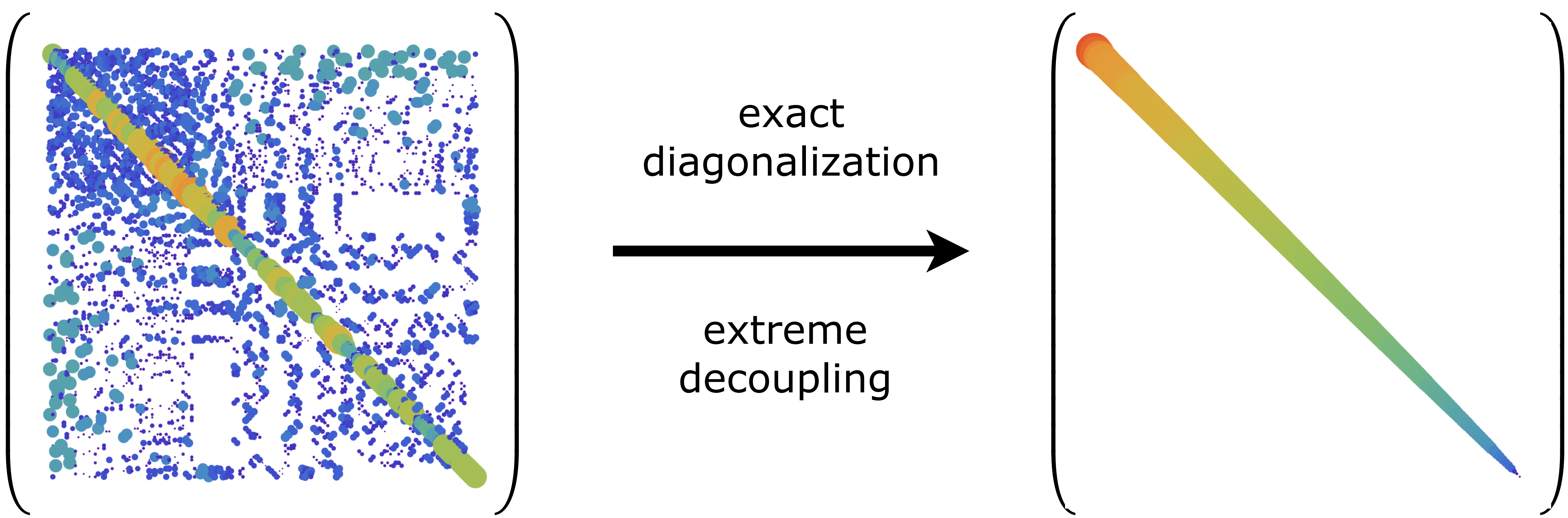
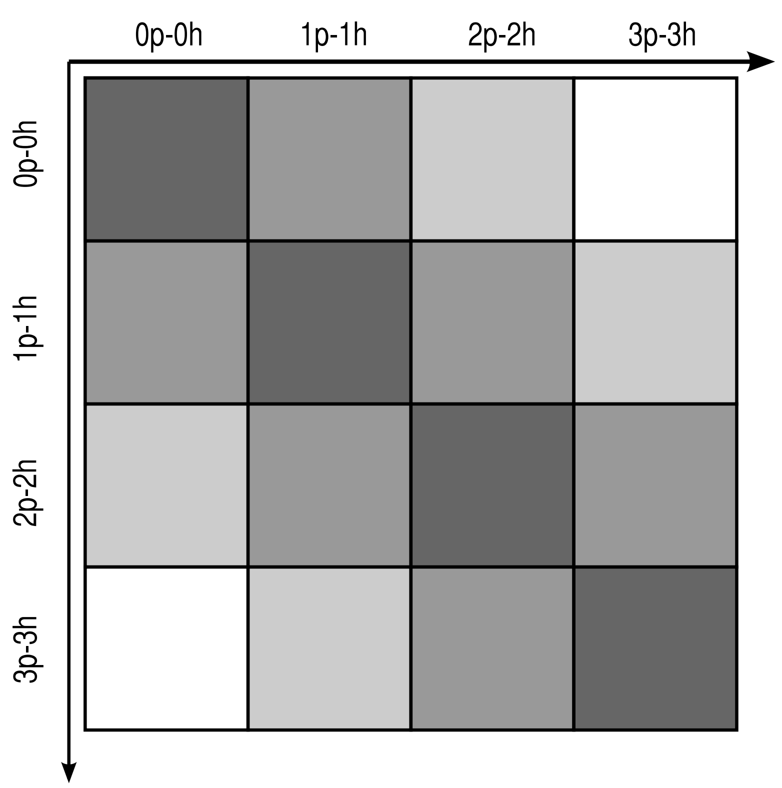


In-Medium SRG

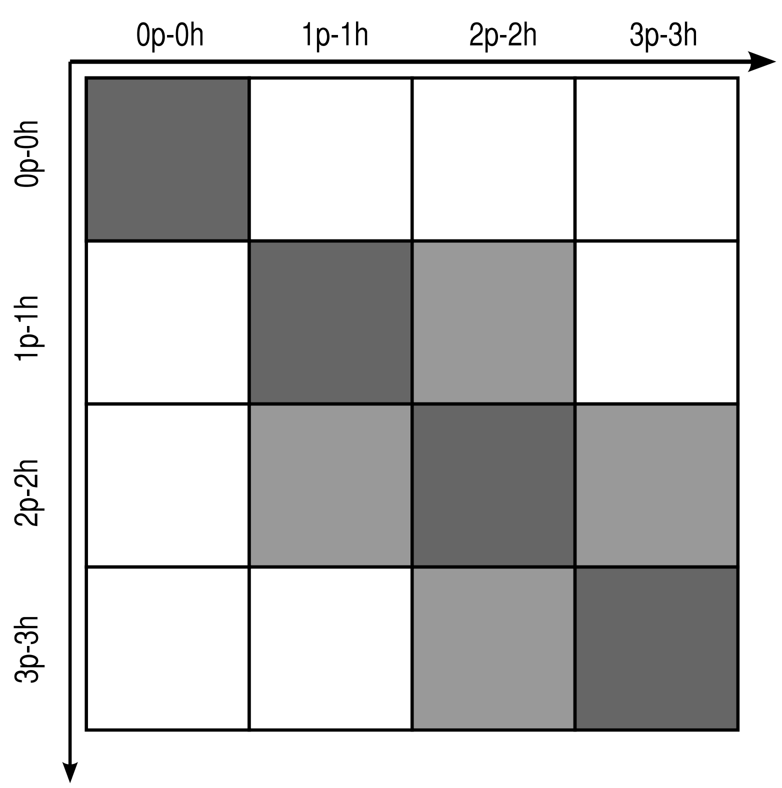
Tsukiyama, Bogner, Schwenk, Hergert,…

decouple reference state from excitations by a unitary transformation of Hamiltonian and other operators

- use IM-SRG to decouple single-determinant reference state for particle-hole excitations, 0p0h matrix-element gives ground-state energy



$$\frac{d}{ds}H(s) = \left[\eta(s), H(s)\right]$$

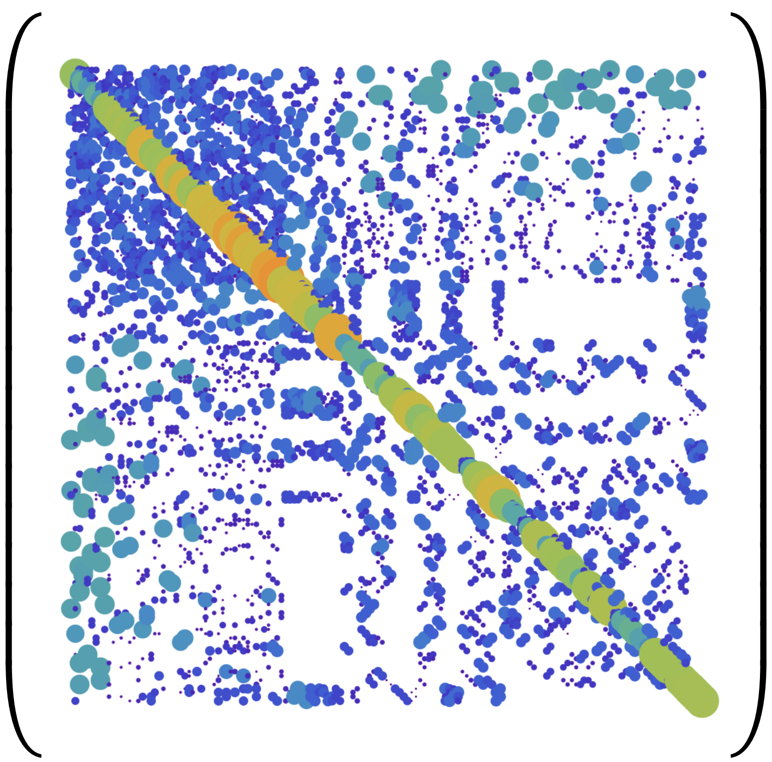


Multi-Reference In-Medium SRG

Hergert, Gebrerufael, Vobig, Mongelli, Roth,…

decouple reference state from excitations by a unitary transformation of Hamiltonian and other operators

- **idea**: use multi-reference formulation of IM-SRG to decouple reference space for rest of model space, i.e., block diagonalize A-body Hamiltonian



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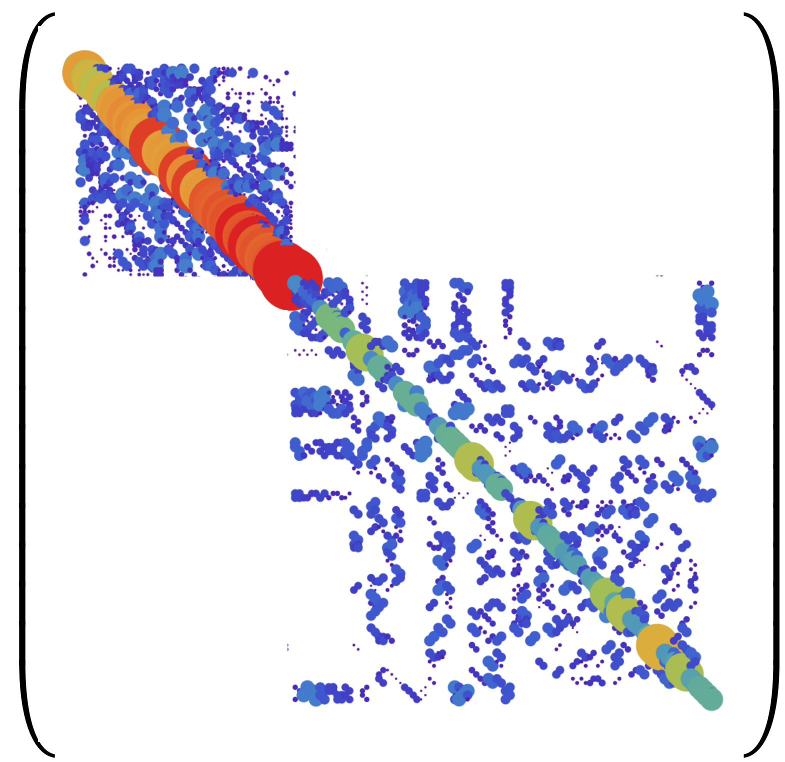
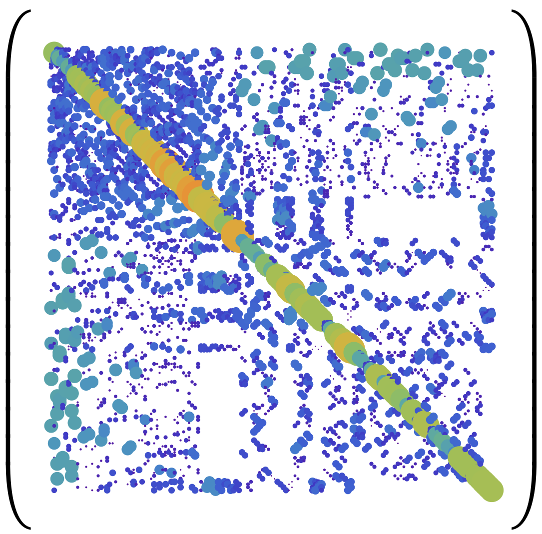
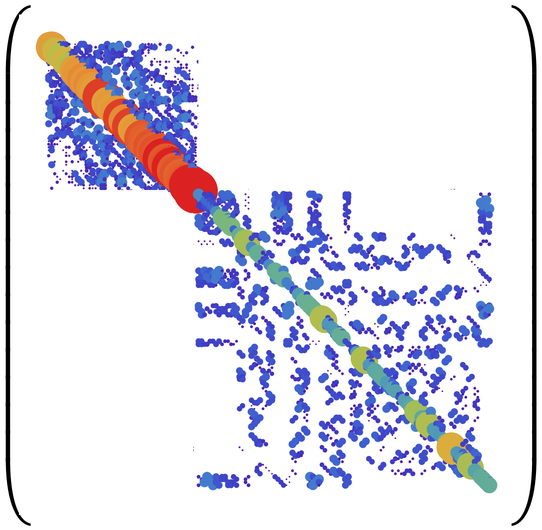


Multi-Reference In-Medium SRG

Hergert, Gebrerufael, Vobig, Mongelli, Roth,...



use SRG flow equations for multi-reference normal-ordered Hamiltonian to decouple reference space



$$\frac{d}{ds}H(s) = \left[\eta(s), H(s)\right]$$

[Kutzelnigg & Mukherjee, 1997]

- Hamiltonian and generator in normal order with respect to multi-determinant reference state, omit residual three-body piece

$$H(s) = E(s) + \sum_{ij} f^i_j(s)\,\tilde{A}^i_j + \frac{1}{4}\sum_{ijkl}\Gamma^{ij}_{kl}(s)\,\tilde{A}^{ij}_{kl} + \cancel{\frac{1}{36}\sum_{ijklmn} W^{ijk}_{lmn}(s)\,\tilde{A}^{ijk}_{lmn}}$$

- define generator to suppress off-diagonal contributions that couple reference state to ph excitations

$$\eta(s) = \left[H(s), H^{\mathrm{d}}(s)\right] = \left[H^{\mathrm{od}}(s), H^{\mathrm{d}}(s)\right]$$

In-Medium NCSM

NCSM
reference state

- ground-state from NCSM at small N_{max} as reference state for multi-reference IM-SRG
- access to all open-shell nuclei and systematically improvable

MR-IM-SRG
decoupling

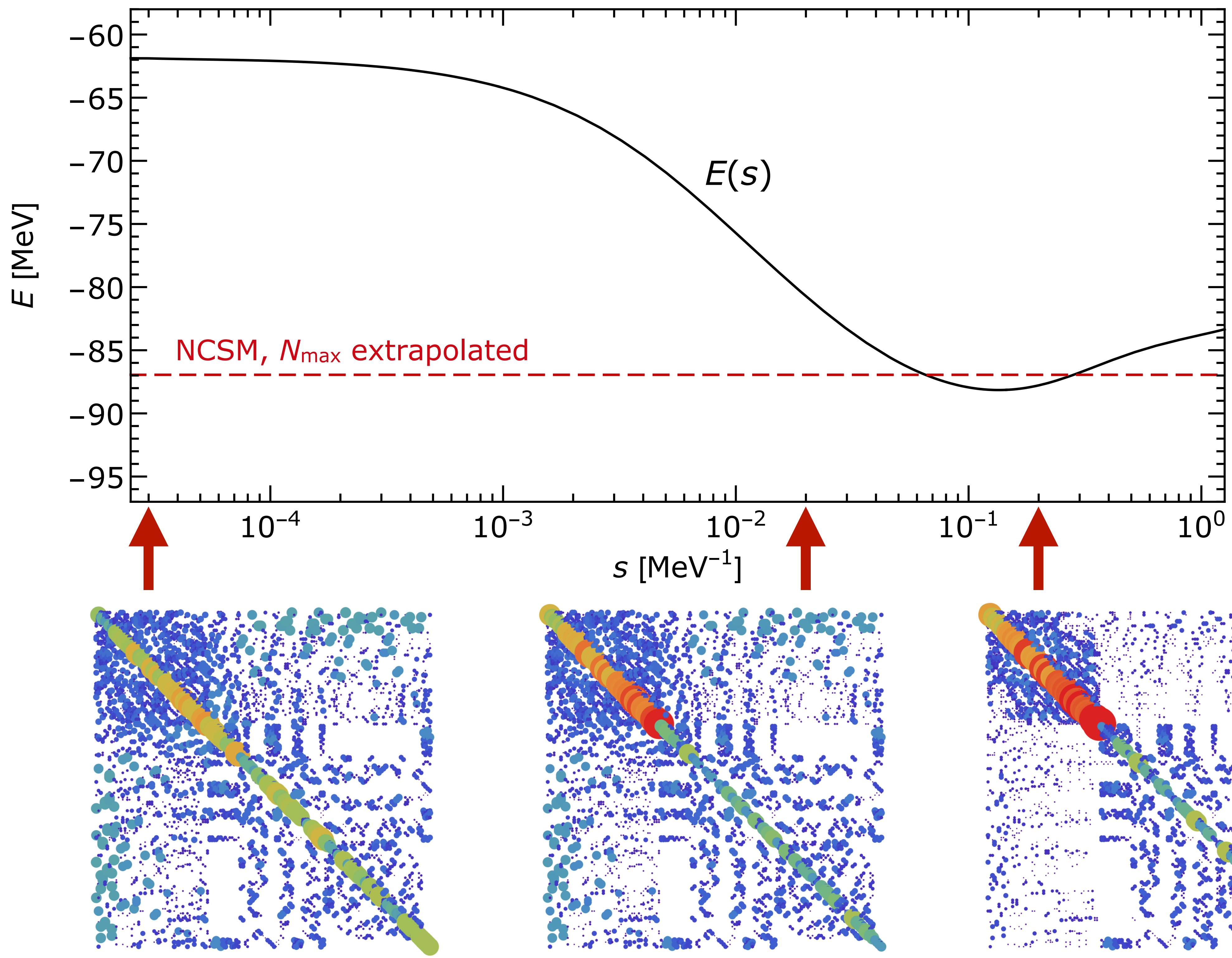
- IM-SRG evolution of multi-reference normal-ordered Hamiltonian and other operators
- decoupling of particle-hole excitations, i.e., pre-diagonalization in many-body space

NCSM
many-body solution

- use in-medium evolved Hamiltonian for a subsequent NCSM calculation
- access to ground and excited states and full suite of observables

In-Medium NCSM: Flow Evolution

Gebrerufael, Vobig, Hergert, Roth; PRL 118, 152503 (2017)



^{12}C

chiral NN+3N

Λ_{3N}=400 MeV

α=0.08 fm^4

$\hbar\Omega$=20 MeV

e_{max}=12

N_{max}=0 reference
HF basis

Hamilton matrix in N_{max}=2 space

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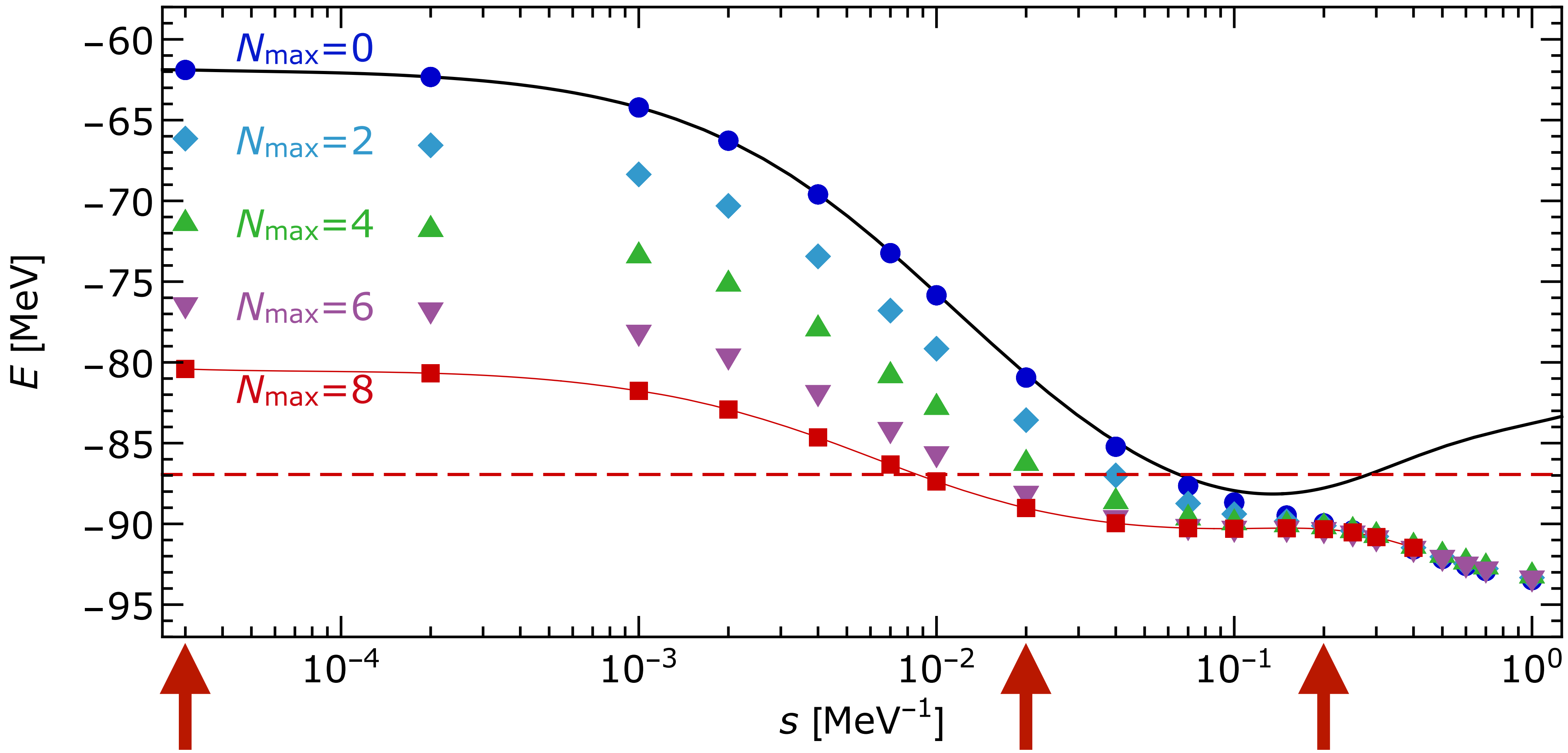

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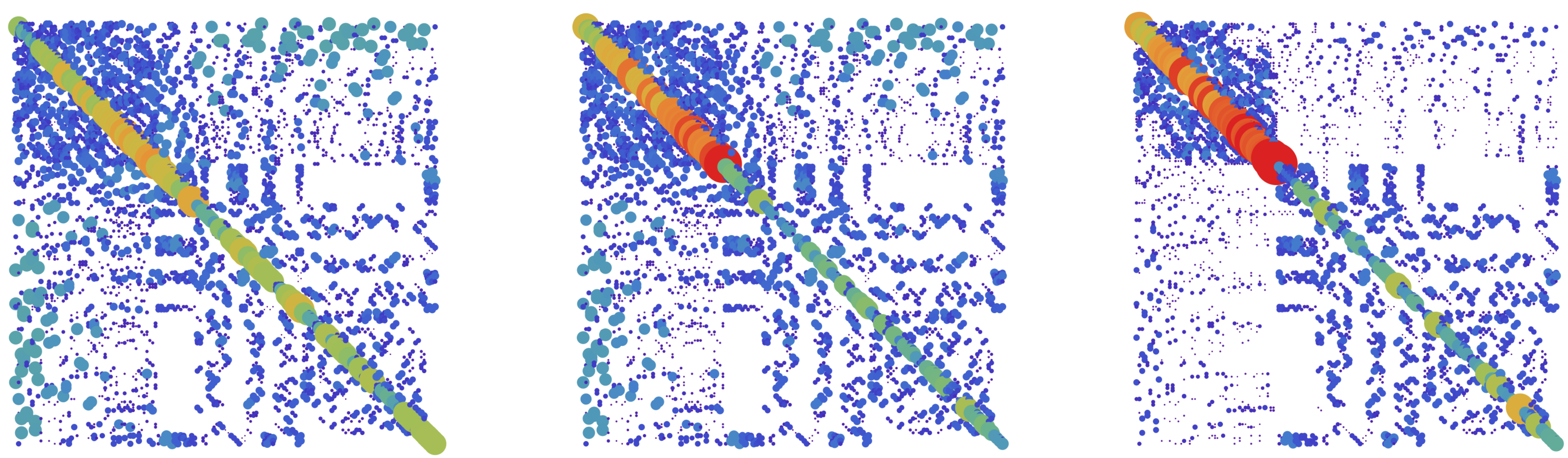

Hamilton matrix in N_{max}=2 space

In-Medium NCSM: Flow Evolution

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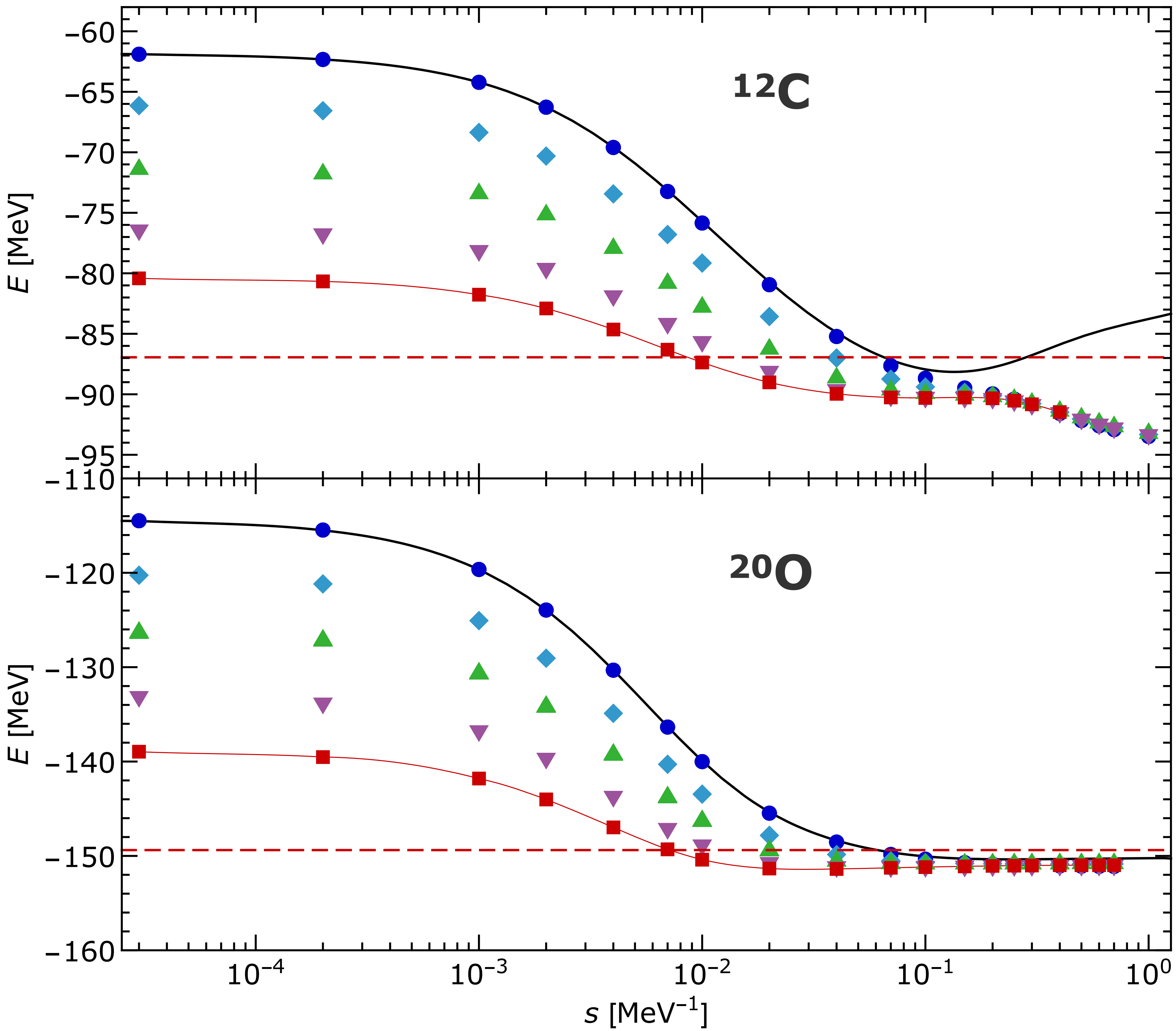

- NCSM convergence is drastically improved
- N_{max}=0 eigenvalues deviated from $E(s)$

chiral NN+3N
Λ_{3N}=400 MeV
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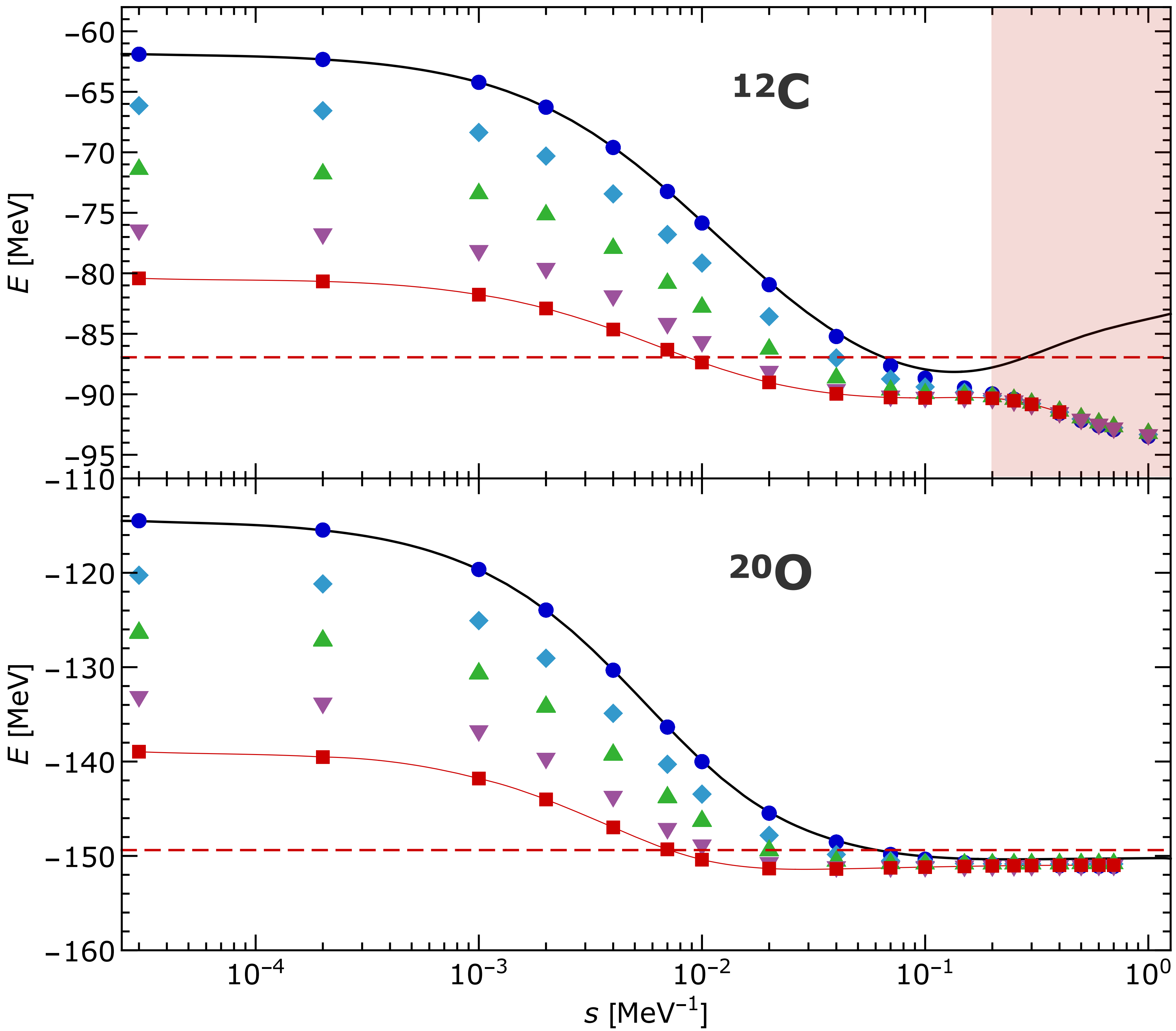
e_{max}=12

HF basis
N_{max}=0 reference state
N_{max}=0,2,4,6,8

In-Medium NCSM: Flow Evolution

Gebrerufael, Vobig, Hergert, Roth; PRL 118, 152503 (2017)



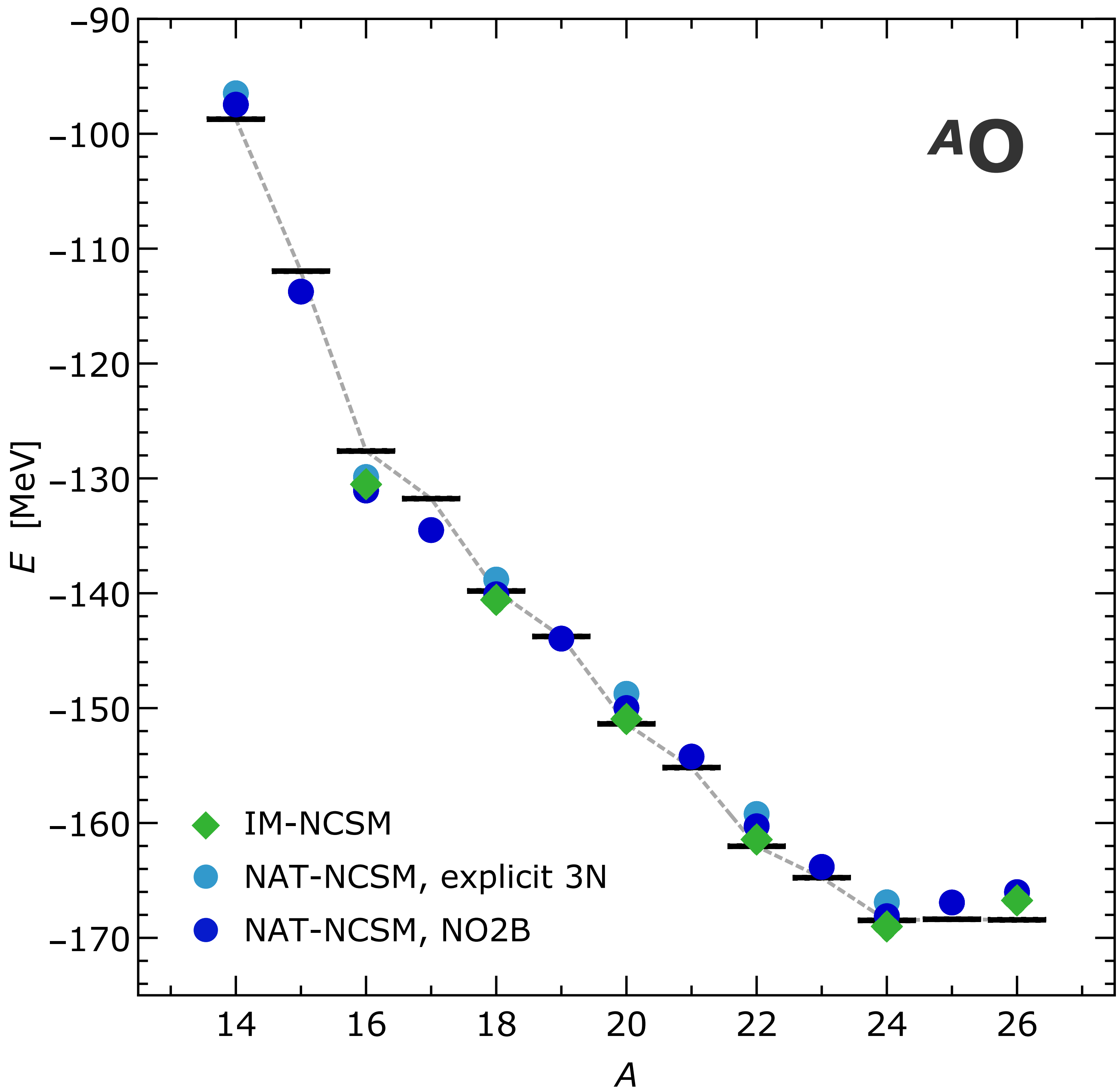
- NCSM convergence is drastically improved
- N_{max}=0 eigenvalues deviated from $E(s)$
- large-s behaviour can be improved by slight modification of generator

chiral NN+3N
Λ_{3N}=400 MeV
α=0.08 fm^4
$\hbar\Omega$=20 MeV
e_{max}=12

HF basis
N_{max}=0 reference state
N_{max}=0,2,4,6,8

IM-NCSM: Oxygen Isotopes

Gebrerufael, Vobig, Hergert, Roth; PRL 118, 152503 (2017)



- excellent agreement with direct NCSM
- IM-SRG evolution limited to *J*=0 reference states and thus even-mass isotopes
- odd-mass nuclei via simple particle attachment or removal in final NCSM run

chiral NN+3N
Λ_{3N}=400 MeV
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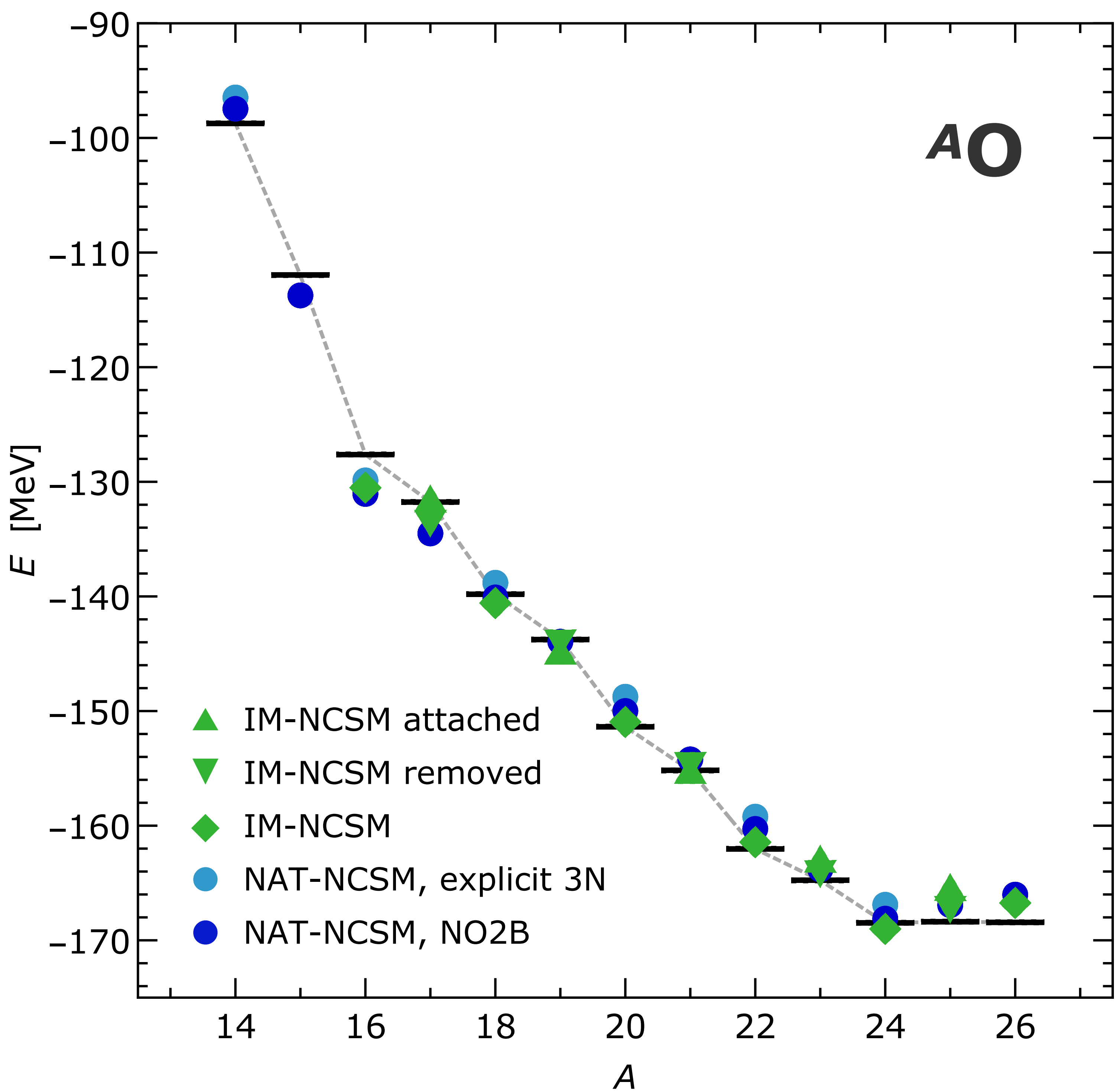
e_{max}=12

HF basis
N_{max}=0 reference

IM-NCSM: Oxygen Isotopes



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chiral NN+3N
$\Lambda_{3N}=400$ MeV
$\alpha=0.08$ fm^4
$\hbar\Omega=20$ MeV
$e_{max}=12$

HF basis
$N_{max}=0$ reference

In-Medium NCSM: Uncertainties

- IM-SRG evolution induces additional uncertainties due to the **truncation** of all normal-ordered operators **at the two-body level**...

  ...NO2B, IM-SRG(2), IM-SRG(M2)

- explicit inclusion of normal-ordered three-body terms is prohibitive in large model spaces (for now)

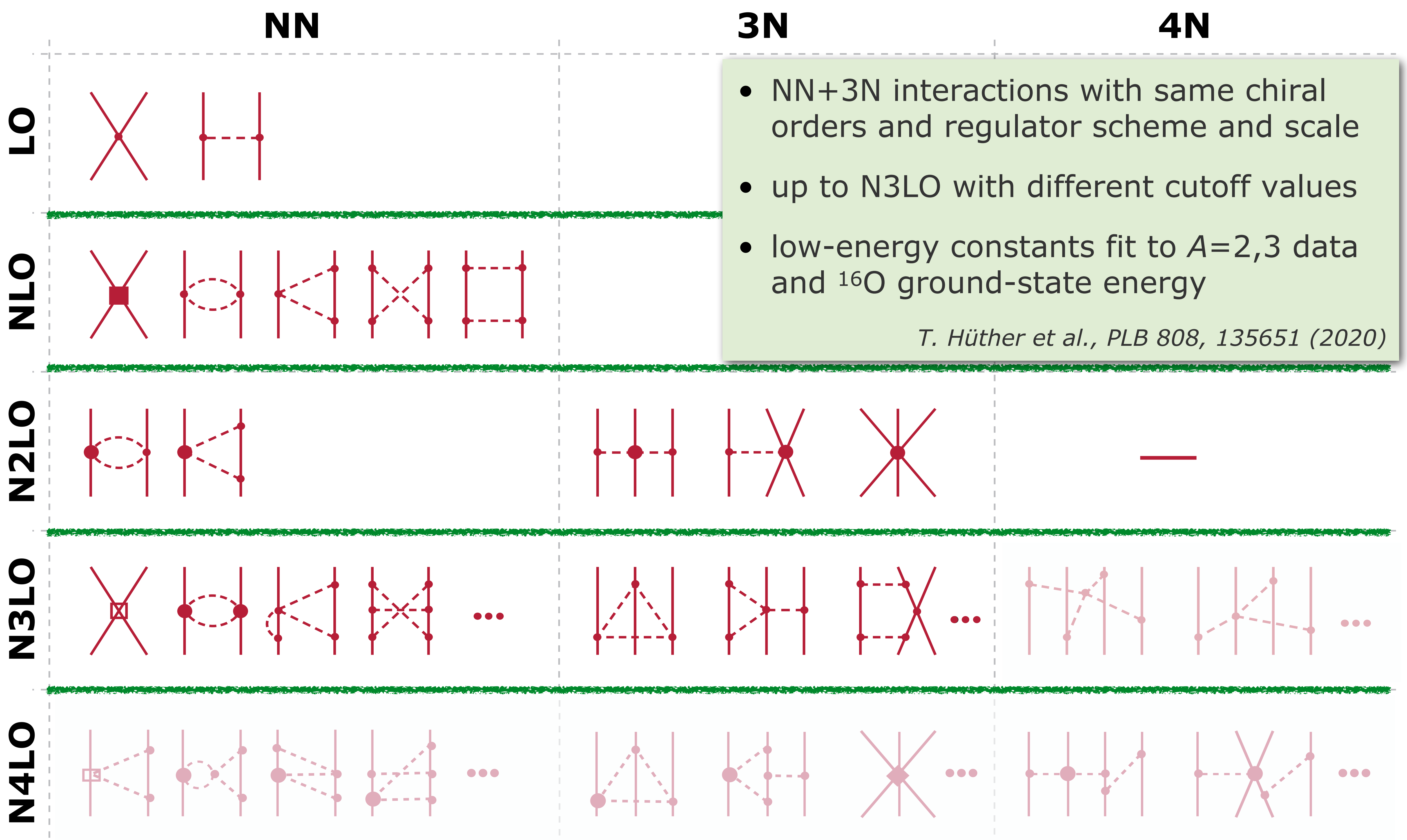
- probe accuracy of NO2B approximation through variation of flow parameter & reference space truncation

- **uncertainty quantification protocol:** perform IM-NCSM calculation for...
  - different reference space truncations: $N_{\mathrm{max}}^{\mathrm{ref}} = 0, 2, 4$
  - different flow parameters: s_{sat} , $s_{\mathrm{sat}}/2$
  - different model-space truncations: $N_{\mathrm{max}} = 0, 2, 4, 6,...$

...maximum difference to next-smaller control parameters gives estimate for many-body uncertainty

Applications with Nonlocal NN+3N Interactions

Family of Non-Local NN+3N Interactions

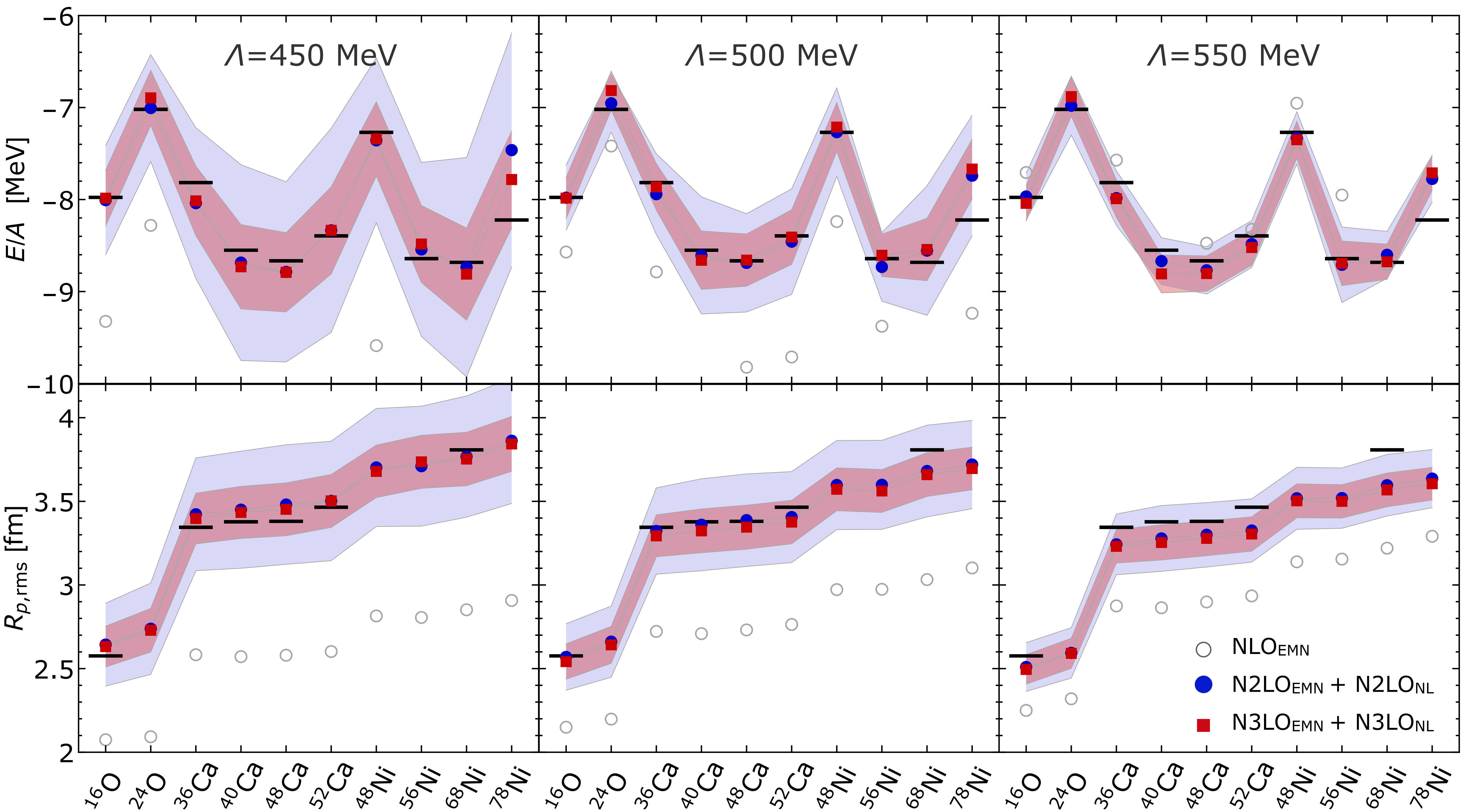


- NN+3N interactions with same chiral orders and regulator scheme and scale
- up to N3LO with different cutoff values
- low-energy constants fit to A=2,3 data and ^{16}O ground-state energy

T. Hüther et al., PLB 808, 135651 (2020)

Medium-Mass Nuclei

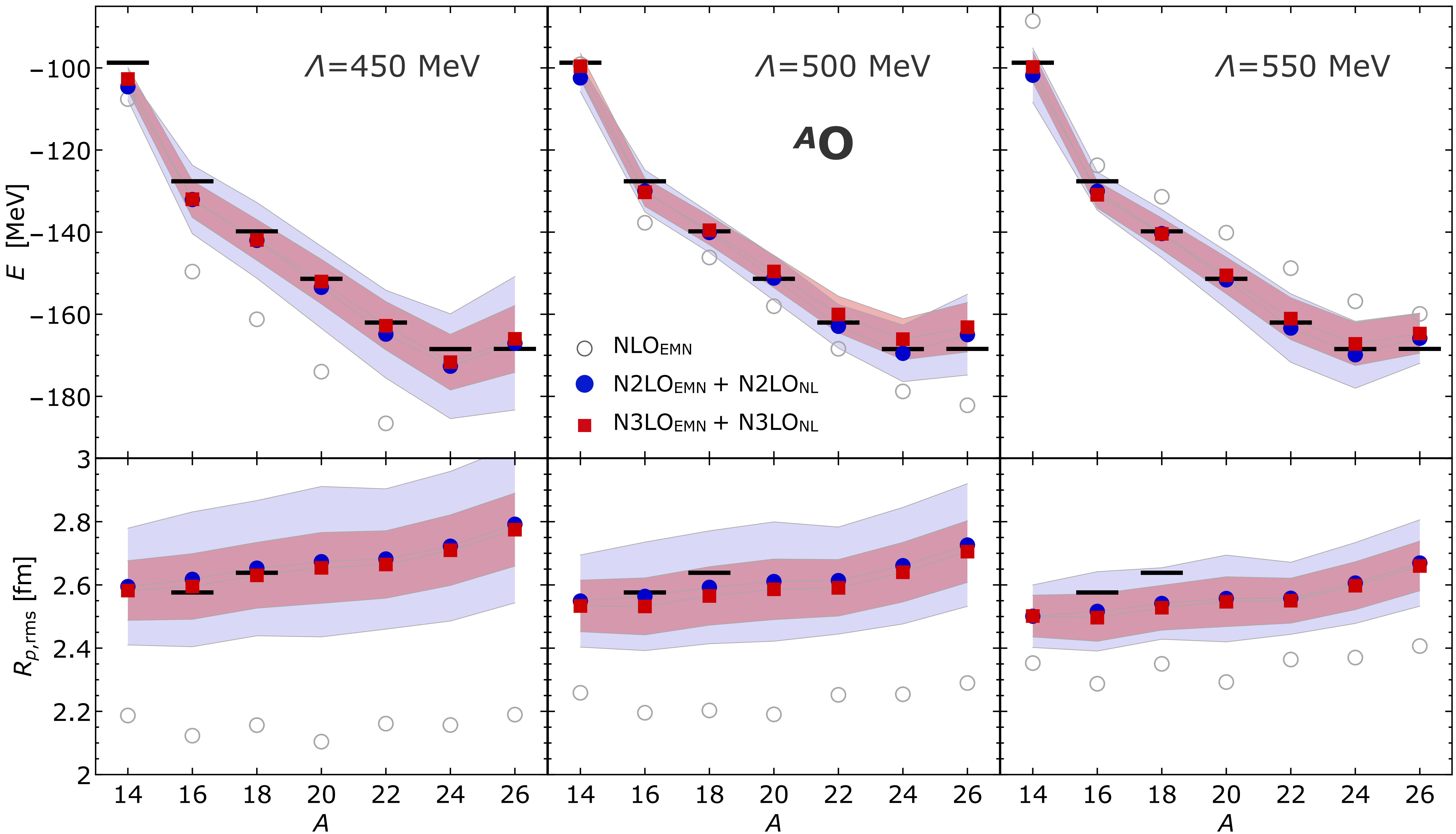
Hüther et al.; PLB 808, 135651 (2020)



IM-SRG(M2), natural orbitals, ħΩ=20 MeV, α=0.04 fm^4, $e_{\max}$=12, $E_{3\max}$=16
error bands show interaction + many-body uncertainties

Oxygen Isotopic Chain

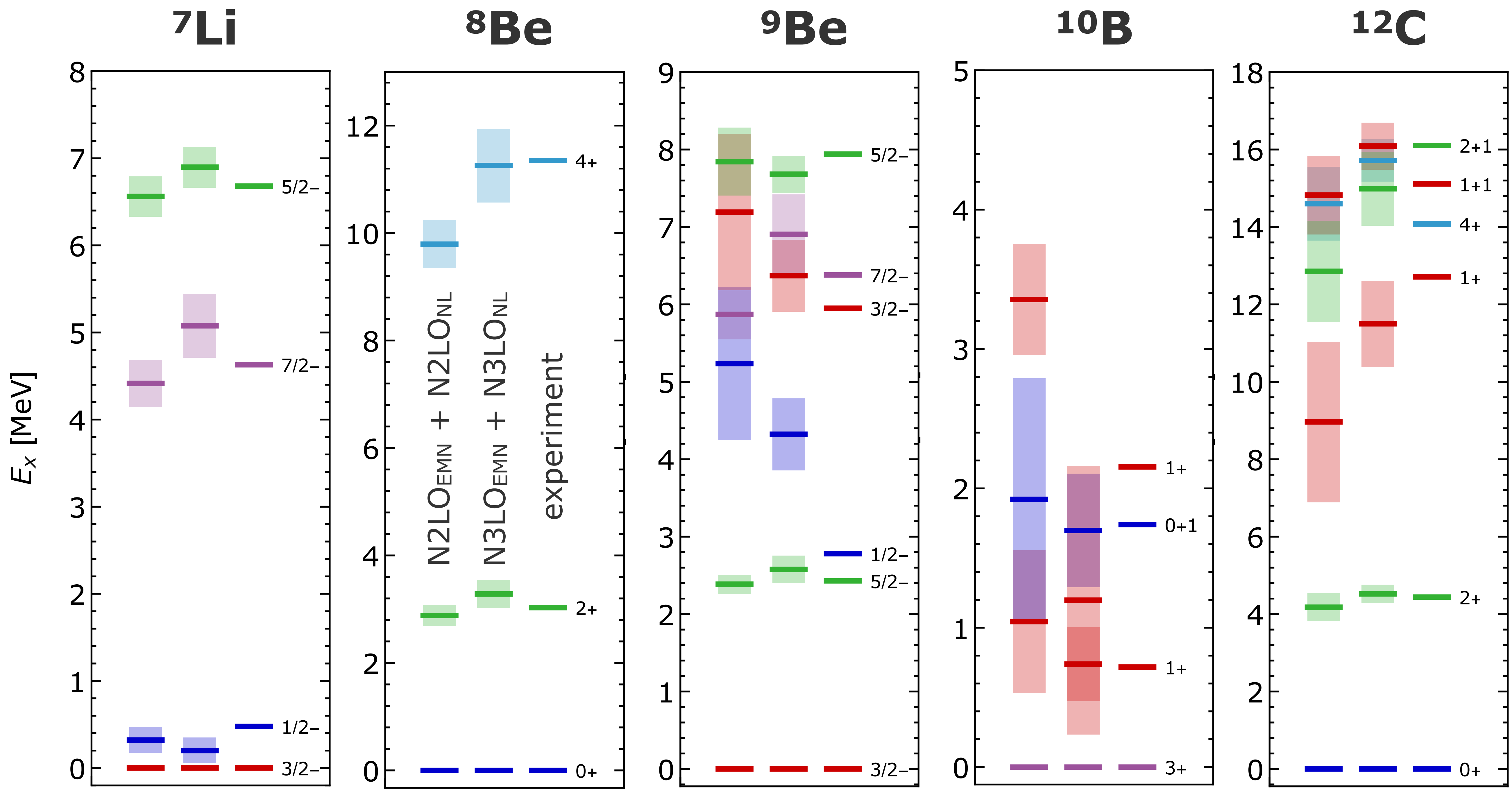
Hüther et al.; PLB 808, 135651 (2020)



IM-NCSM, natural orbitals, ħΩ=20 MeV, α=0.04 fm^4, e_{max}=12, E_{3max}=14, N_{ref}=2
error bands show interaction + many-body uncertainties

p-Shell Spectra

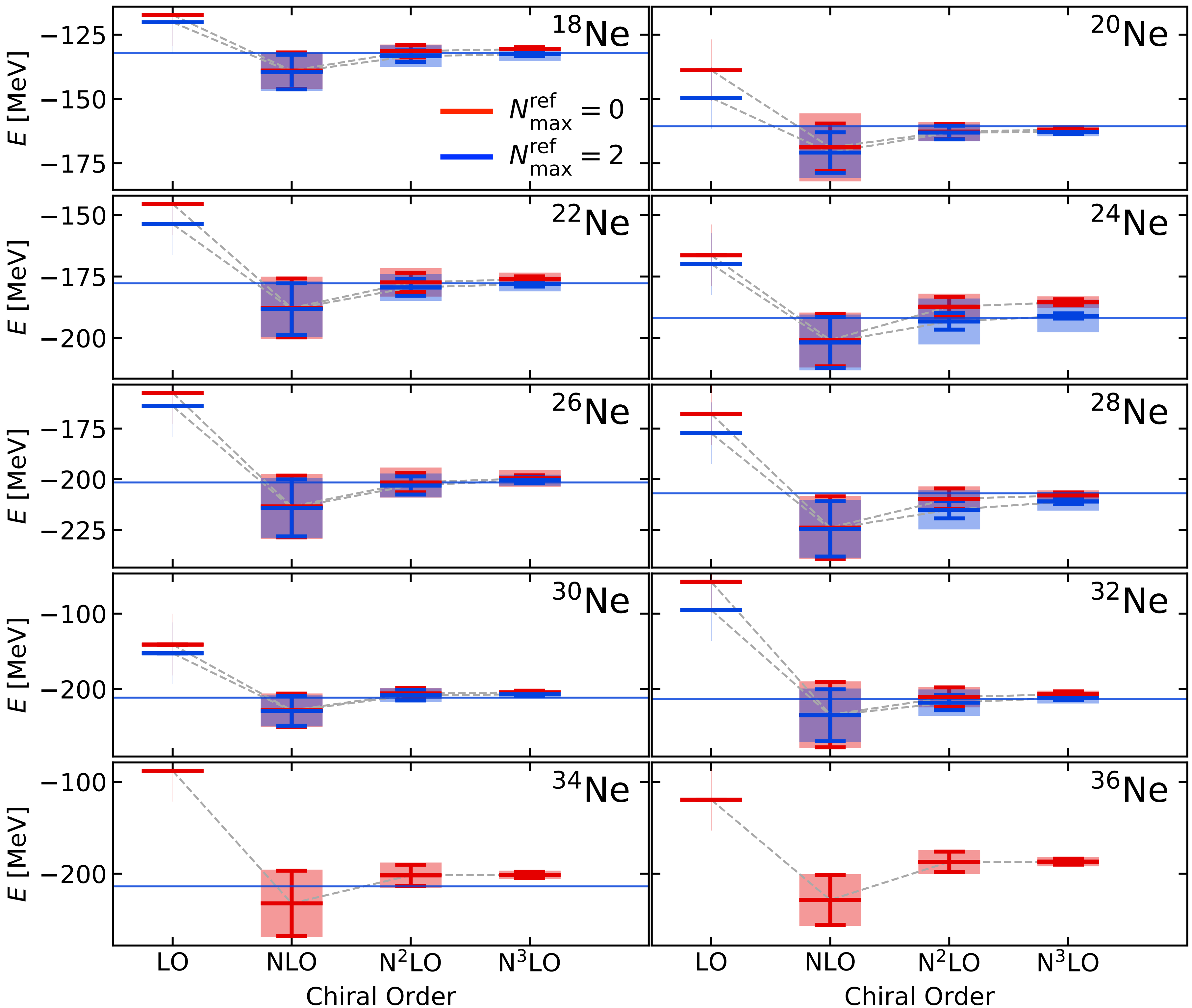
Hüther et al.; PLB 808, 135651 (2020)



NCSM/IM-NCSM, Λ=500 MeV, $\hbar\Omega$=20 MeV
error bands show interaction uncertainties

Applications: Neon Isotopes

Ground-State Energies



- amazing reproduction of experimental energies for all isotopes
- uncertainties under control

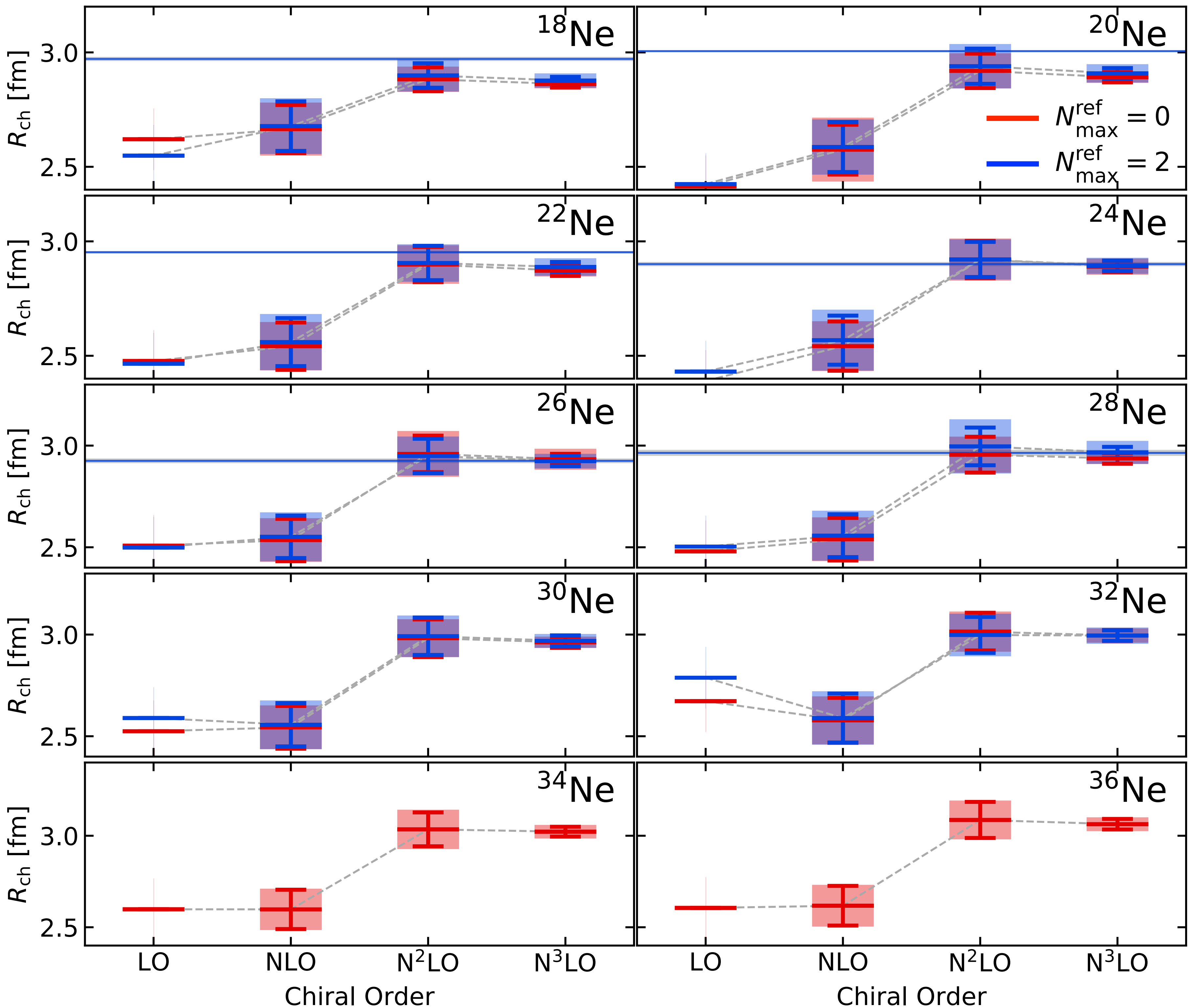
Λ = 500 MeV
α = 0.04 fm^4
$\hbar\Omega$ = 20 MeV
e_{max} = 12
NAT basis

$N^{\text{ref}}_{\text{max}} = 0, 2$
$N_{\text{max}} = 4$

error bars:
68% interaction uncertainties

error bands:
interaction + many-body uncertainties

Charge Radii



- excellent description of radii, slight underestimation for light isotopes
- stable results in N^{2}LO and N^{3}LO

Λ = 500 MeV
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$\hbar\Omega$ = 20 MeV
e_{max} = 12
NAT basis

$N_{max}^{ref} = 0, 2$
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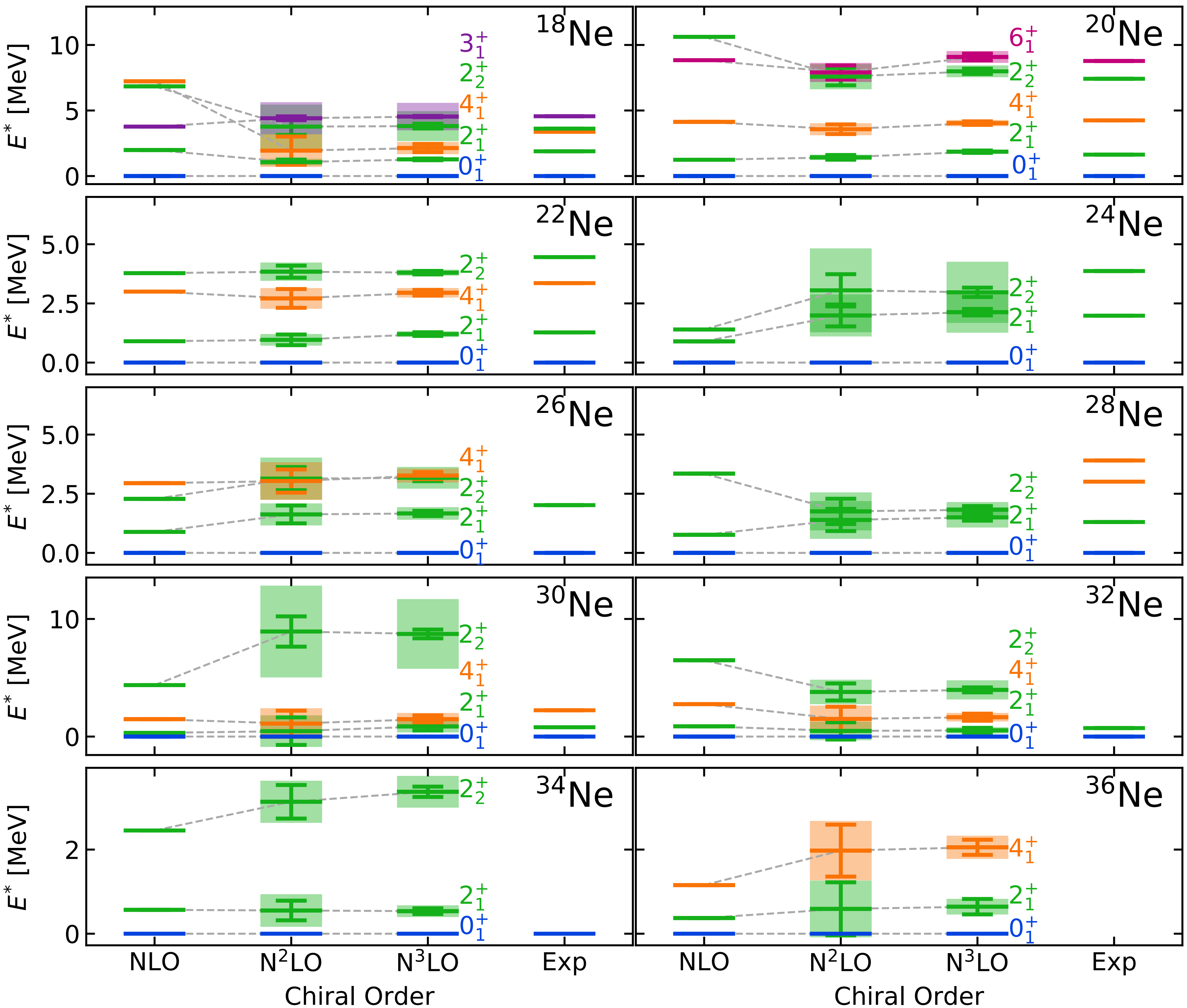
Excitation Energies



- excellent description of excitation spectra

Λ = 500 MeV
α = 0.04 fm^4
$\hbar\Omega$ = 20 MeV
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NAT basis

$N_{max}^{ref} = 2$
$N_{max} = 4$

error bars:
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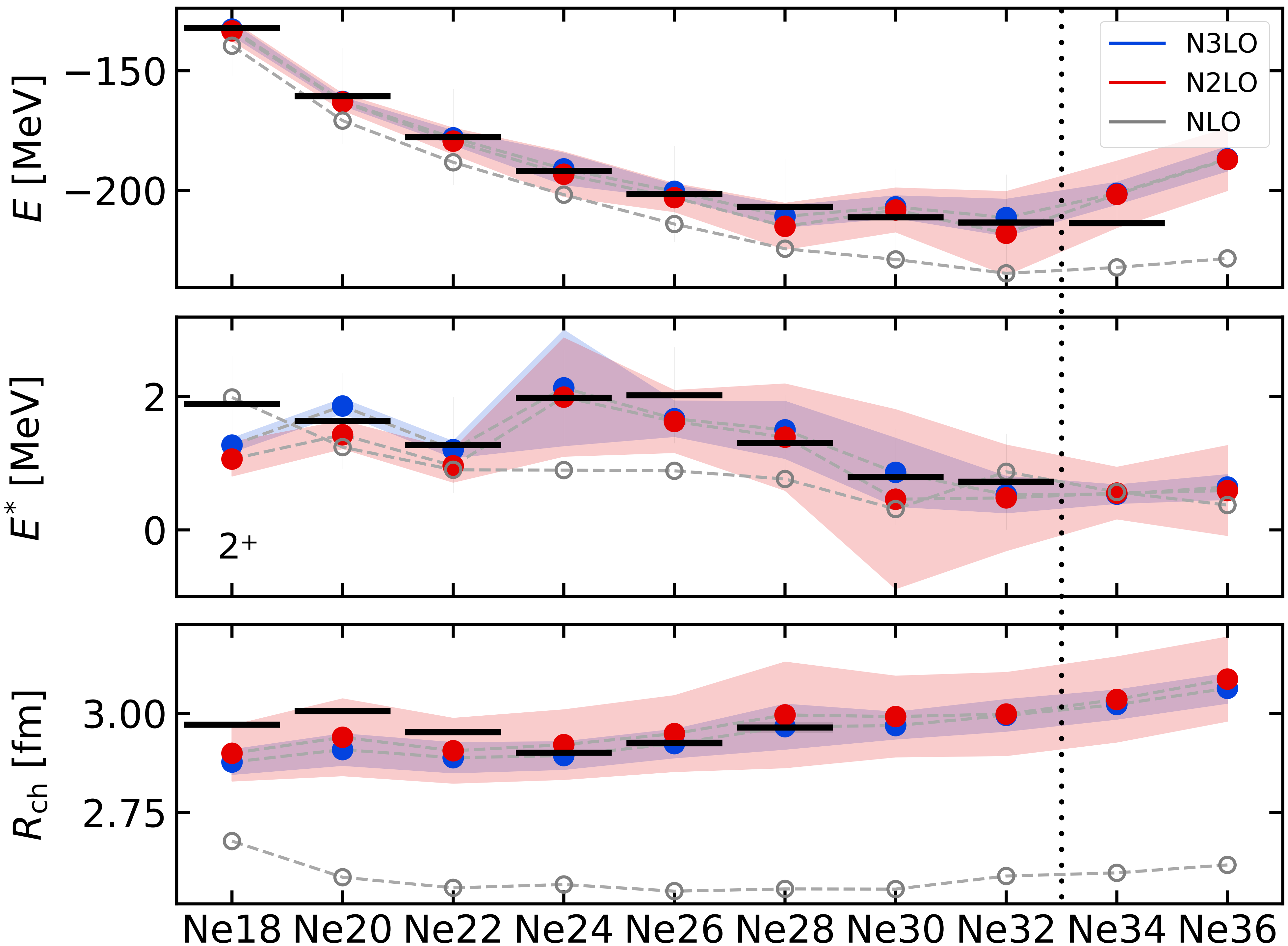
error bands:
interaction + many-body uncertainties

Neon Isotopes: Systematics



error bands:
interaction +
many-body
uncertainties

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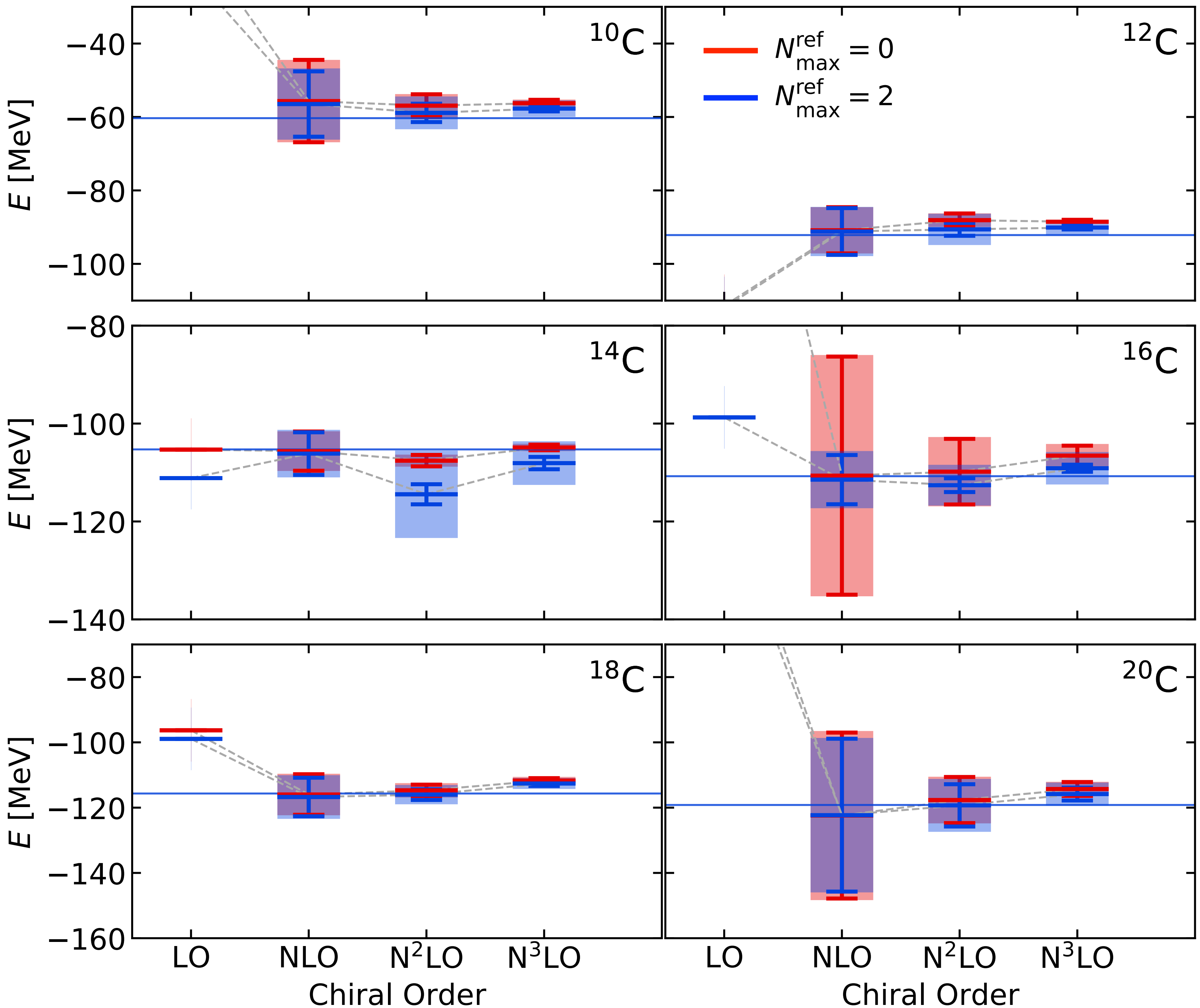
$\hbar\Omega$ = 20 MeV
e_{max} = 12
NAT basis

$N_{max}^{ref} = 2, 0$
$N_{max} = 4, 2$

Applications: Carbon Isotopes

Ground-State Energies



- good reproduction of experimental ground-state energies
- uncertainties under control

Λ = 500 MeV
α = 0.04 fm^4
$\hbar\Omega$ = 20 MeV
e_{max} = 12
NAT basis

$N^{\text{ref}}_{\text{max}} = 0, 2$
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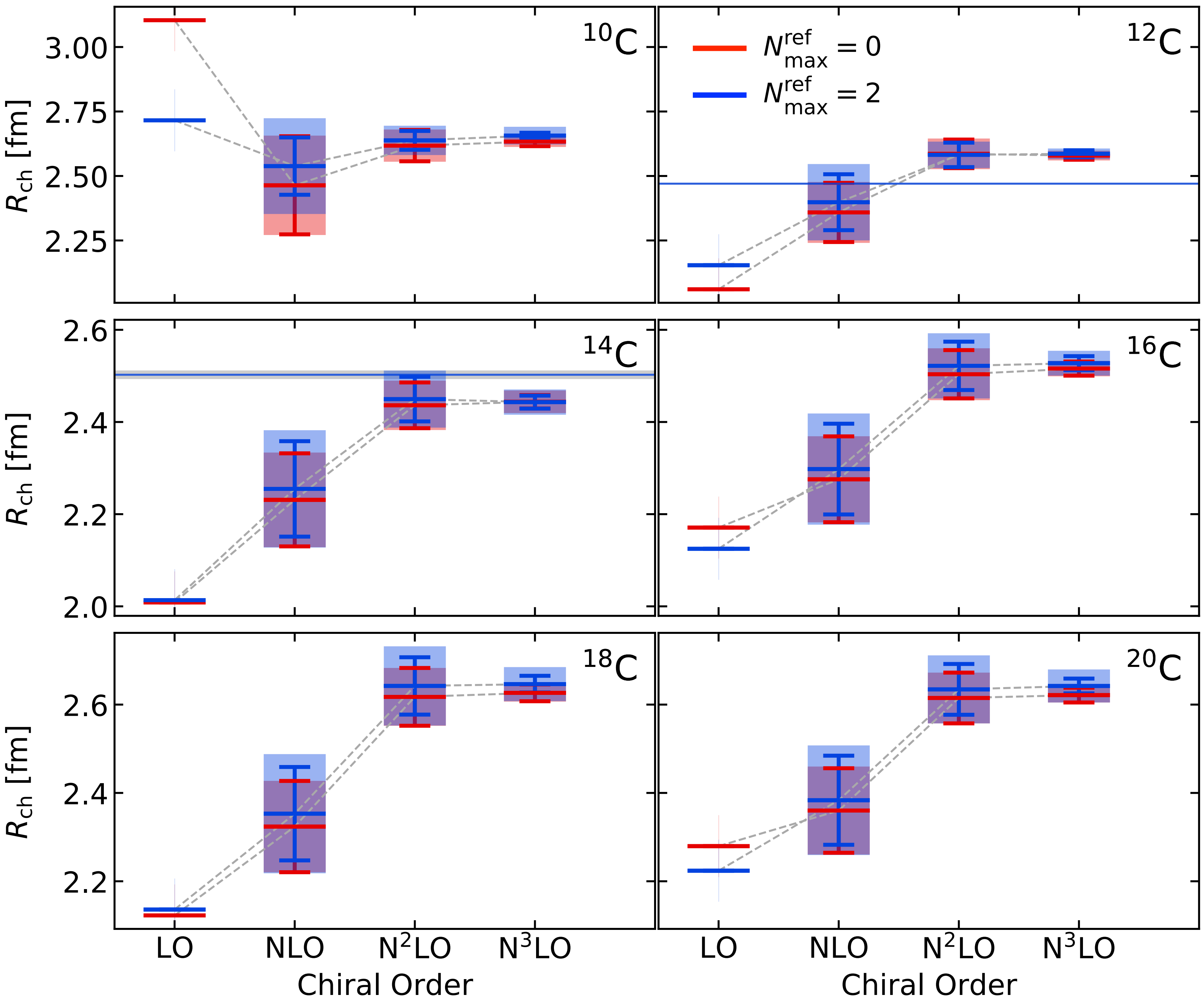
Charge Radii



- slight overprediction of ^{12}C and slight underprediction of ^{14}C charge radius
- stable results in N^{2}LO and N^{3}LO

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NAT basis

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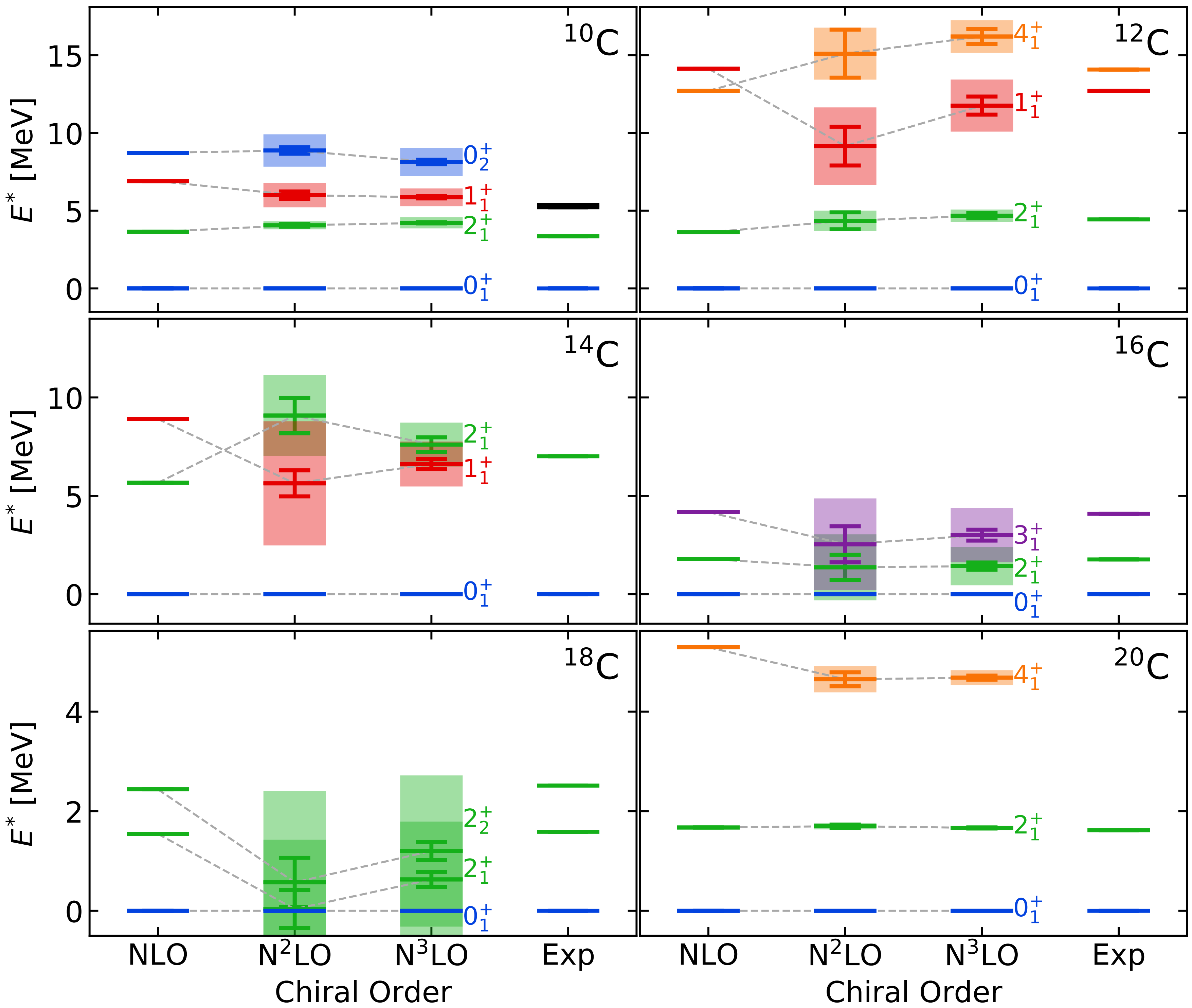
Excitation Spectra



- good overall description of spectra, except cluster states (not shown)
- stable results, uncertainties strongly state dependent

Λ = 500 MeV
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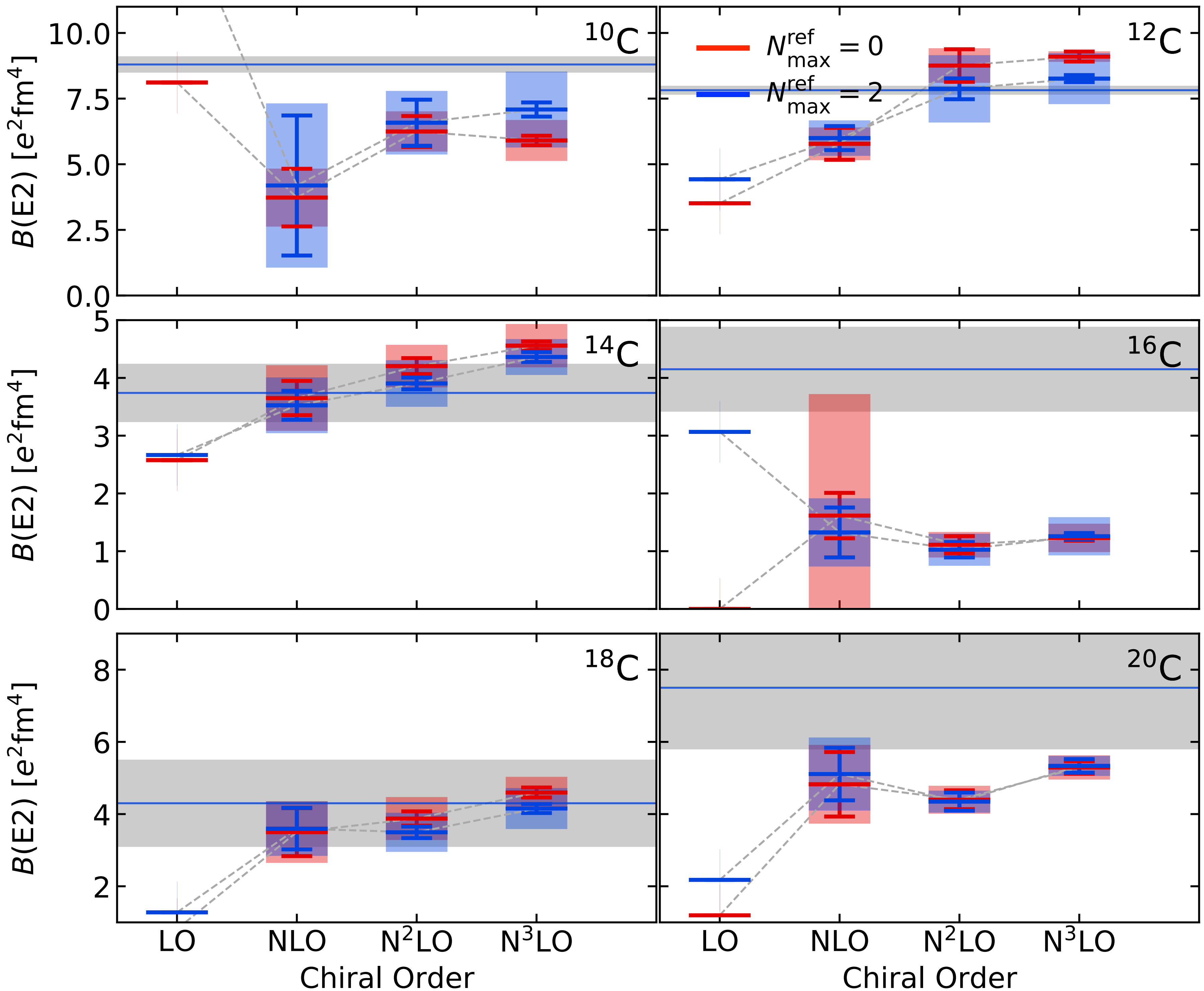
$\hbar\Omega$ = 20 MeV
e_{max} = 12
NAT basis

$N^{ref}_{max} = 2$
$N_{max} = 4$

error bars:
68% interaction uncertainties

error bands:
interaction + many-body uncertainties

B(E2, $2^+ \to 0^+$) Transition Strength



- agreement with experiment within uncertainties
- exception ^{16}C !

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$\hbar\Omega$ = 20 MeV
e_{max} = 12
NAT basis

$N^{ref}_{max} = 0, 2$
$N_{max} = 4$

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error bands:
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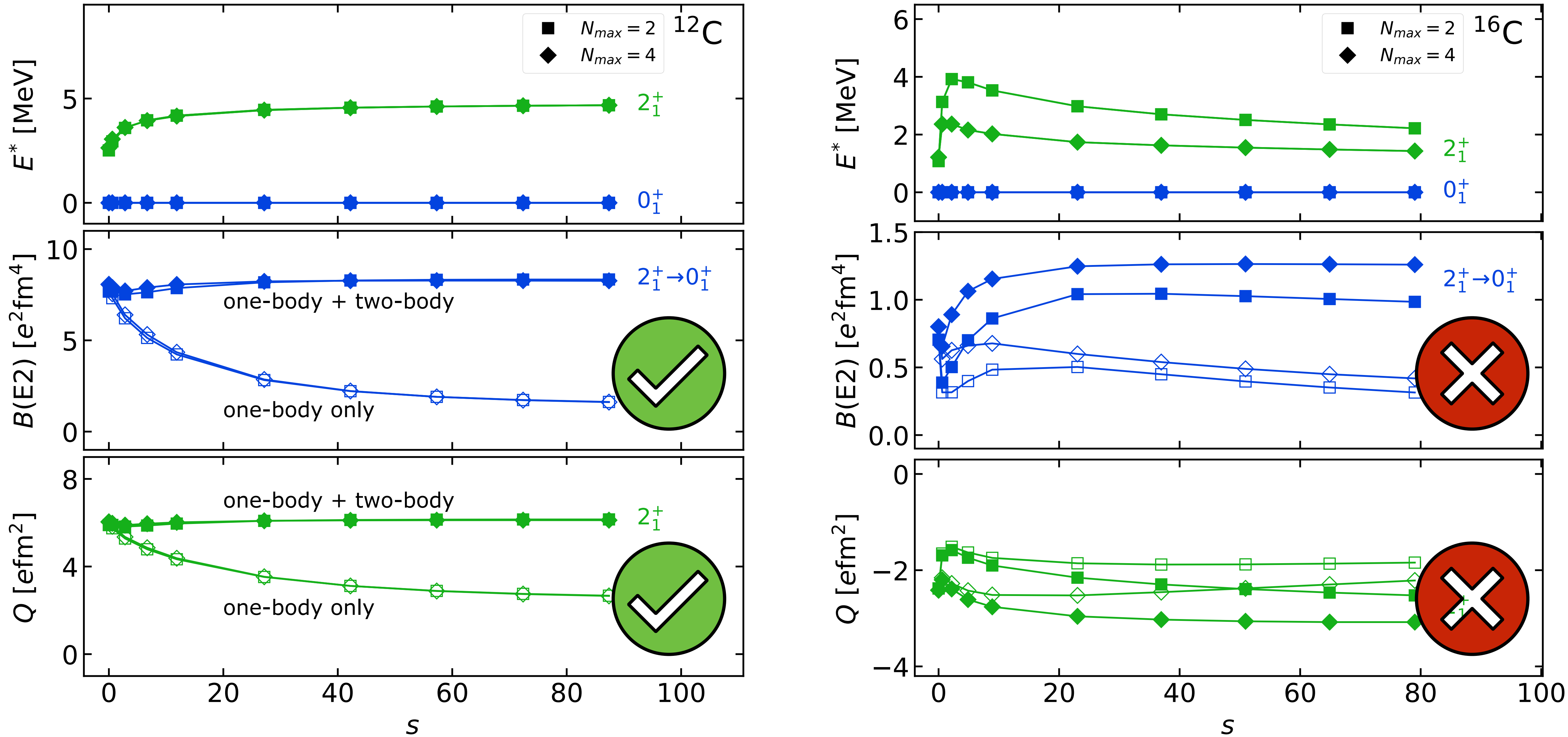
Hierarchy Inversion



- IM-SRG evolution of E2 operator generates dominant (induced) two-body contribution... what about three-body and beyond?
- not a problem, if reference space contains the relevant static correlations

Next Stage: Active-Space IM-CI

- **limitations of IM-NCSM setup**
  - beyond sd-shell, the HO-based $N_{\max}$ truncation does not make sense
  - benefit from optimization of reference space to accommodate specific correlations

- adopt a **more general CI strategy** for the definition of the reference space
  - quantum chemistry: restricted active-space CI methods
  - partitioning of single-particle orbits: hole - active - particle
  - huge flexibility in model-space design

- **perturbative corrections** to account for complete particle space
  - use second-order MCPT with CI eigenstate as 'unperturbed' reference
  - demonstrated successfully with the NCSM-PT *[Tichai et al., PLB 786, 448 (2018)]*

In-Medium CI for Collective Excitations

Collective Excitations

- traditional description via **RPA-type equations of motion methods**

$$|E_\omega\rangle = \mathrm{Q}^\dagger_\omega\,|\mathrm{RPA}\rangle \qquad\qquad \mathrm{Q}_\omega\,|\mathrm{RPA}\rangle = 0$$

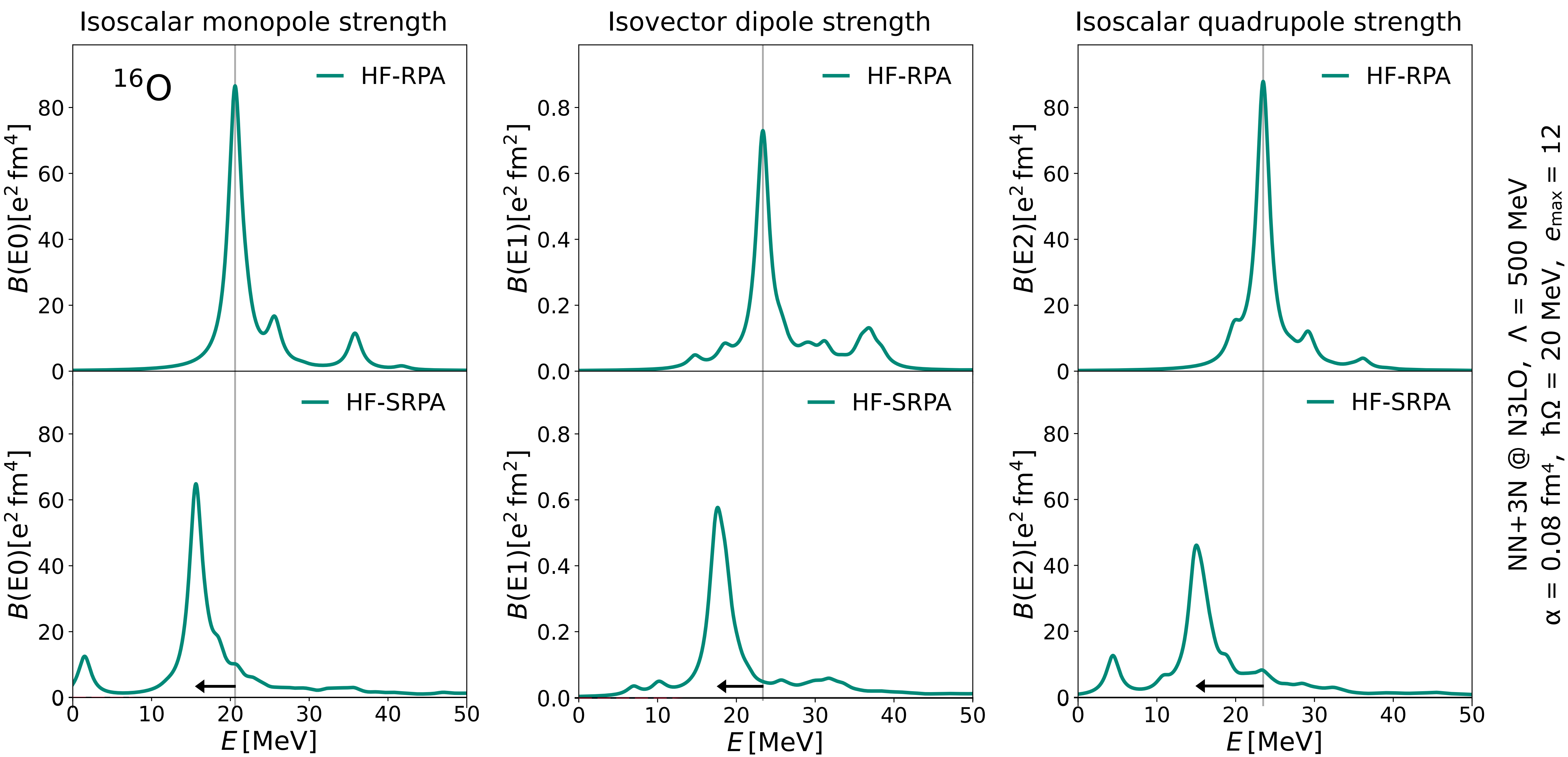
- phonon operator expanded in **particle-hole scheme** including "backwards" terms that imply **ground-state correlations**

$$\begin{aligned}\mathrm{Q}^\dagger_\omega = &\sum_{p,h}\left(X^\omega_{ph}\,\mathrm{a}^\dagger_p\mathrm{a}_h - Y^\omega_{ph}\,\mathrm{a}^\dagger_h\mathrm{a}_p\right) && \textbf{RPA}\\ &+\sum_{pp',hh'}\left(\mathcal{X}^\omega_{php'h'}\,\mathrm{a}^\dagger_p\mathrm{a}_h\mathrm{a}^\dagger_{p'}\mathrm{a}_{h'} - \mathcal{Y}^\omega_{php'h'}\,\mathrm{a}^\dagger_h\mathrm{a}_p\mathrm{a}^\dagger_{h'}\mathrm{a}_{p'}\right) && \textbf{SRPA}\\ &+\ \ldots\end{aligned}$$

- might look old-fashioned, but is a systematic expansion scheme which can be used in an ab initio framework

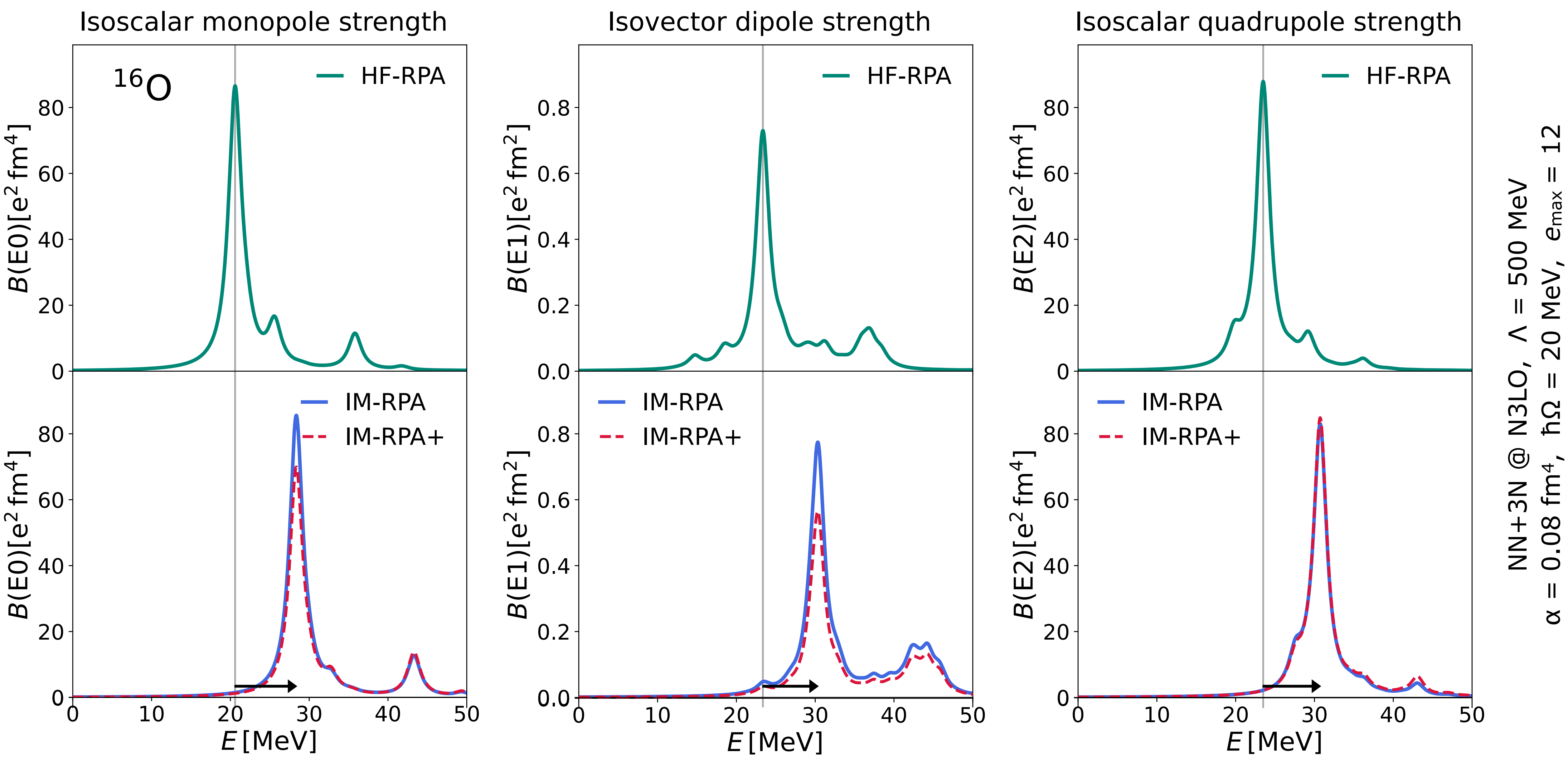
- can we use RPA in connection **with IM-SRG evolved Hamiltonians** and what do we gain... decoupling targets ground state, not high-lying excitations

Standard HF-RPA and HF-SRPA



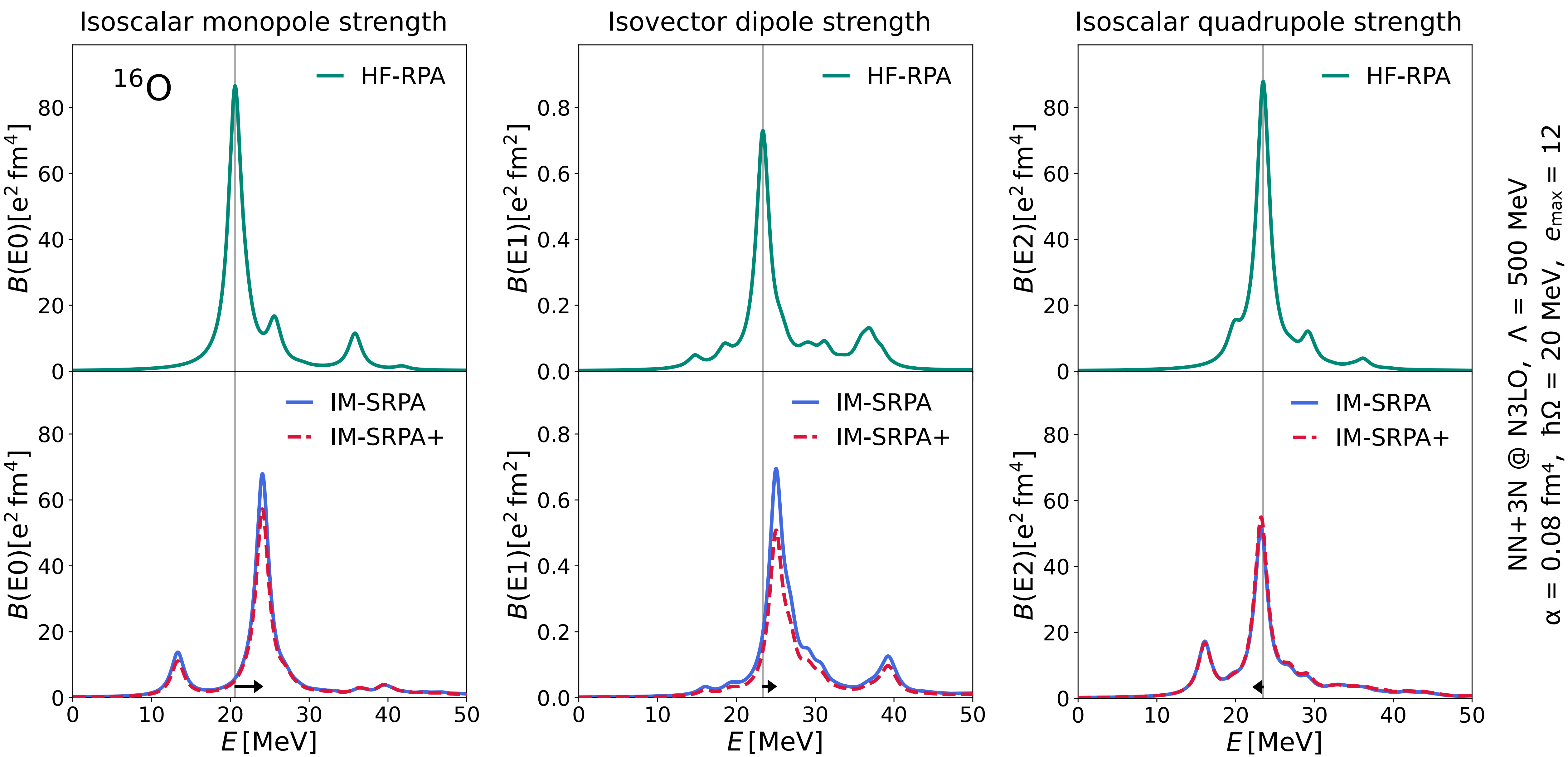
- **SRPA induces unphysical downward shift of resonances**
- 2p2h correlations are included for excited states, but ground state remains at HF level in quasi-boson approximation

SRPA Combined with IM-SRG



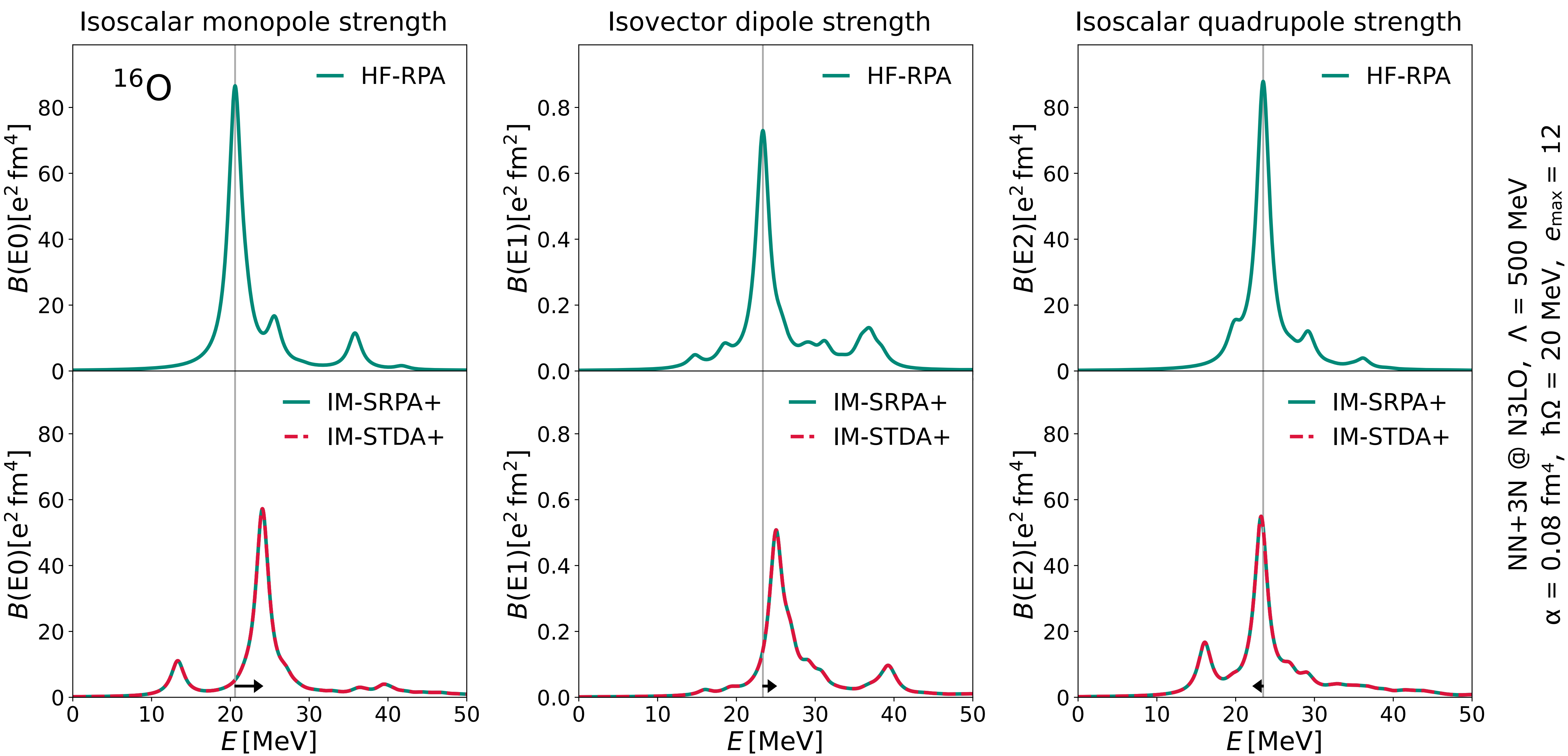
- **IM-SRG evolved Hamiltonian shifts resonances up in energy**
- decoupling designed to account for all ground-state correlations, not so for exited states

SRPA Combined with IM-SRG



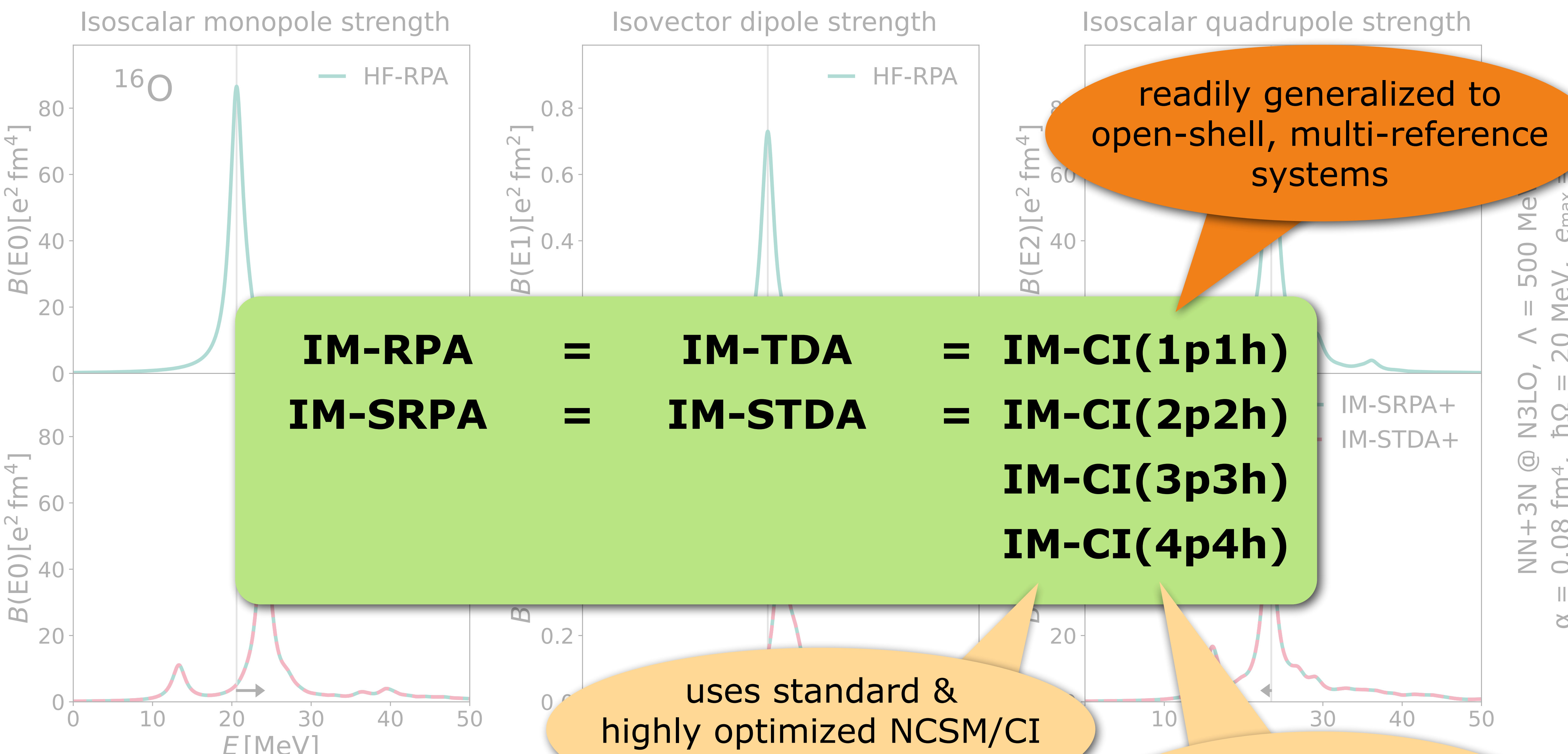
- **SRPA with IM-SRG evolved Hamiltonian moves resonances down**
- building 2p2h correlations explicitly into excited states, ground state is decoupled from the outset

IM-SRPA versus IM-STDA



- **simple (S)TDA calculation becomes equivalent to (S)RPA**
- IM-SRG decoupling suppresses $V_{\text{pp-hh}}$ matrix elements that make up the *B*-matrix, leading to vanishing "backward" amplitudes *Y*

IM for Collective Excitations



IM-RPA = IM-TDA = IM-CI(1p1h)

IM-SRPA = IM-STDA = IM-CI(2p2h)

IM-CI(3p3h)

IM-CI(4p4h)

readily generalized to open-shell, multi-reference systems

uses standard & highly optimized NCSM/CI codebase

combined with Lanczos strength-function method for efficient access to 1000s of excited states

Epilogue

- **thanks to my group and my collaborators**
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