In-Medium No-Core Shell Model

- Developments & Applications -

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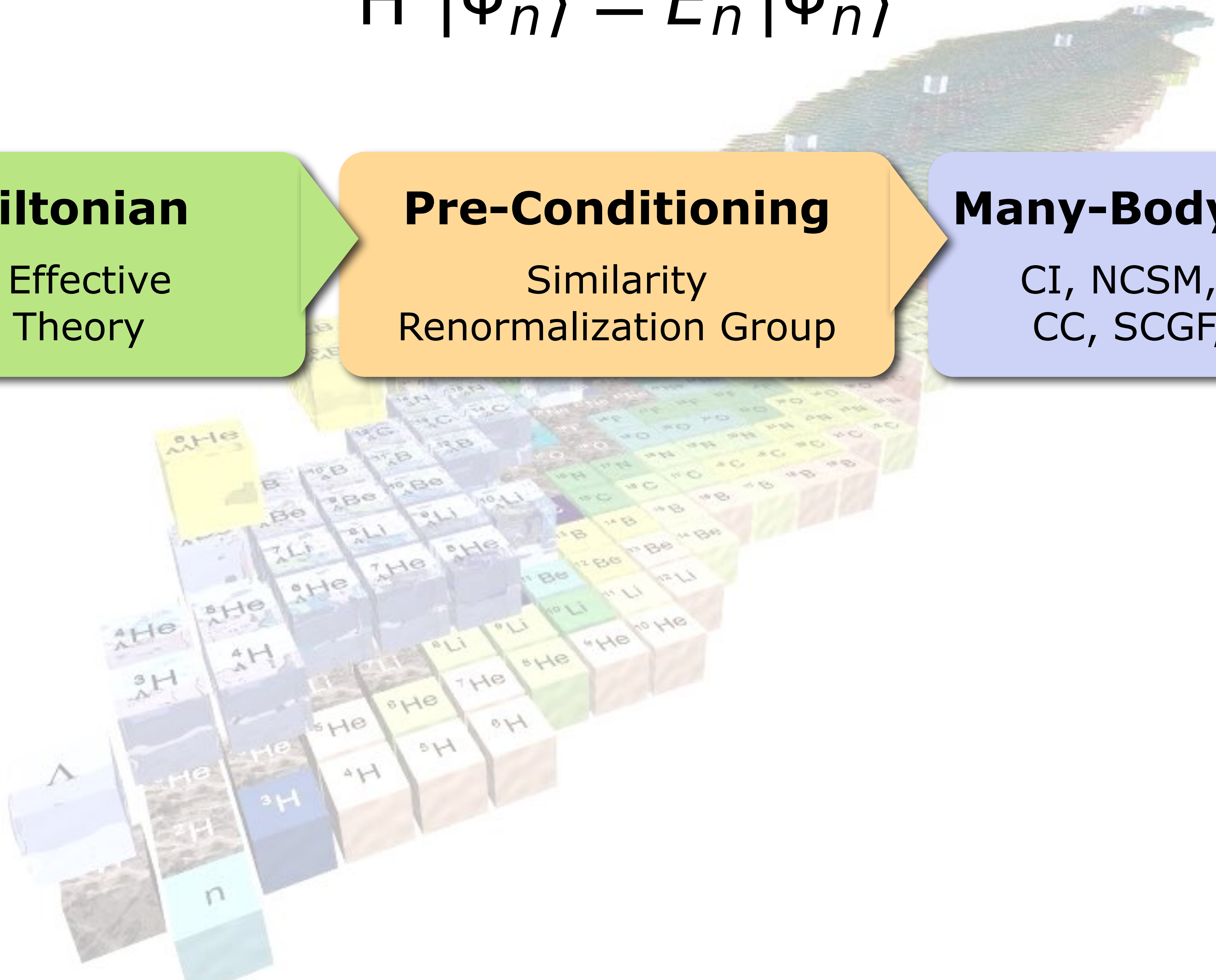
Ab Initio Nuclear Structure Theory

$$H \; |\Psi_n\rangle = E_n \, |\Psi_n\rangle$$



Hamiltonian

Chiral Effective Field Theory

Pre-Conditioning

Similarity Renormalization Group

Many-Body Solution

CI, NCSM, IM-SRG, CC, SCGF, MBPT...

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Many-Body Solution

CI, NCSM, IM-SRG, CC, SCGF, MBPT...

- unitary transformation of all operators as preparatory step
- drastically improves convergence of many-body calculation
- induces many-body terms that have to be monitored

Ab Initio Nuclear Structure Theory

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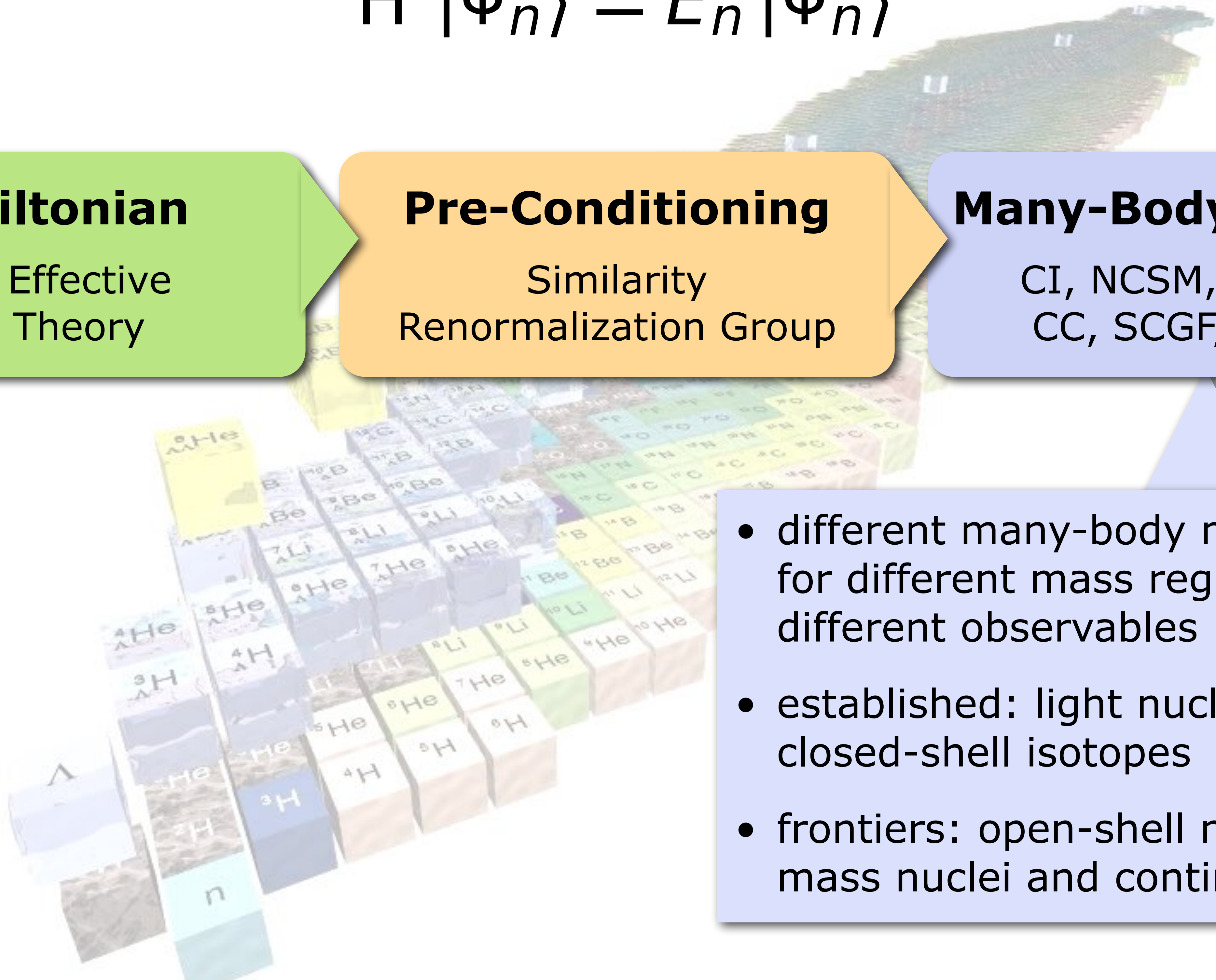

Hamiltonian

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Many-Body Solution

CI, NCSM, IM-SRG, CC, SCGF, MBPT...

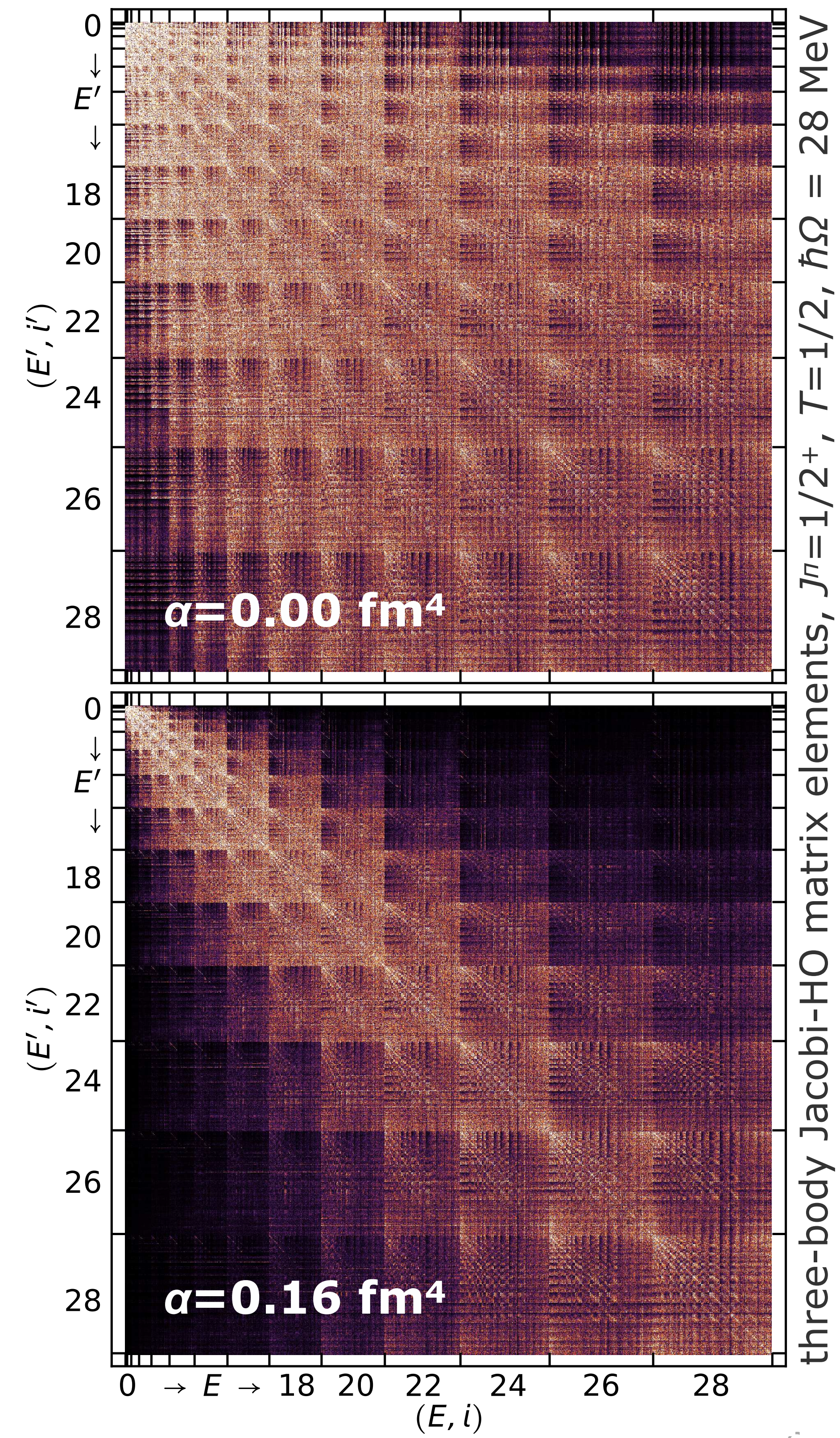
- different many-body methods for different mass regions and different observables
- established: light nuclei and closed-shell isotopes
- frontiers: open-shell medium-mass nuclei and continuum

Similarity Renormalization Group

Similarity Renormalization Group

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

continuous unitary transformation driving Hamiltonian towards diagonal form



- unitary transformation via flow equation

$$H_\alpha = U_\alpha^\dagger H\, U_\alpha \quad \rightarrow \quad \frac{d}{d\alpha} H_\alpha = [\eta_\alpha, H_\alpha]$$

$$O_\alpha = U_\alpha^\dagger O\, U_\alpha \quad \rightarrow \quad \frac{d}{d\alpha} O_\alpha = [\eta_\alpha, O_\alpha]$$

- dynamic generator determines physics of transformation

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

- solve flow equation using matrix representation in two- and three-body space

Similarity Renormalization Group

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

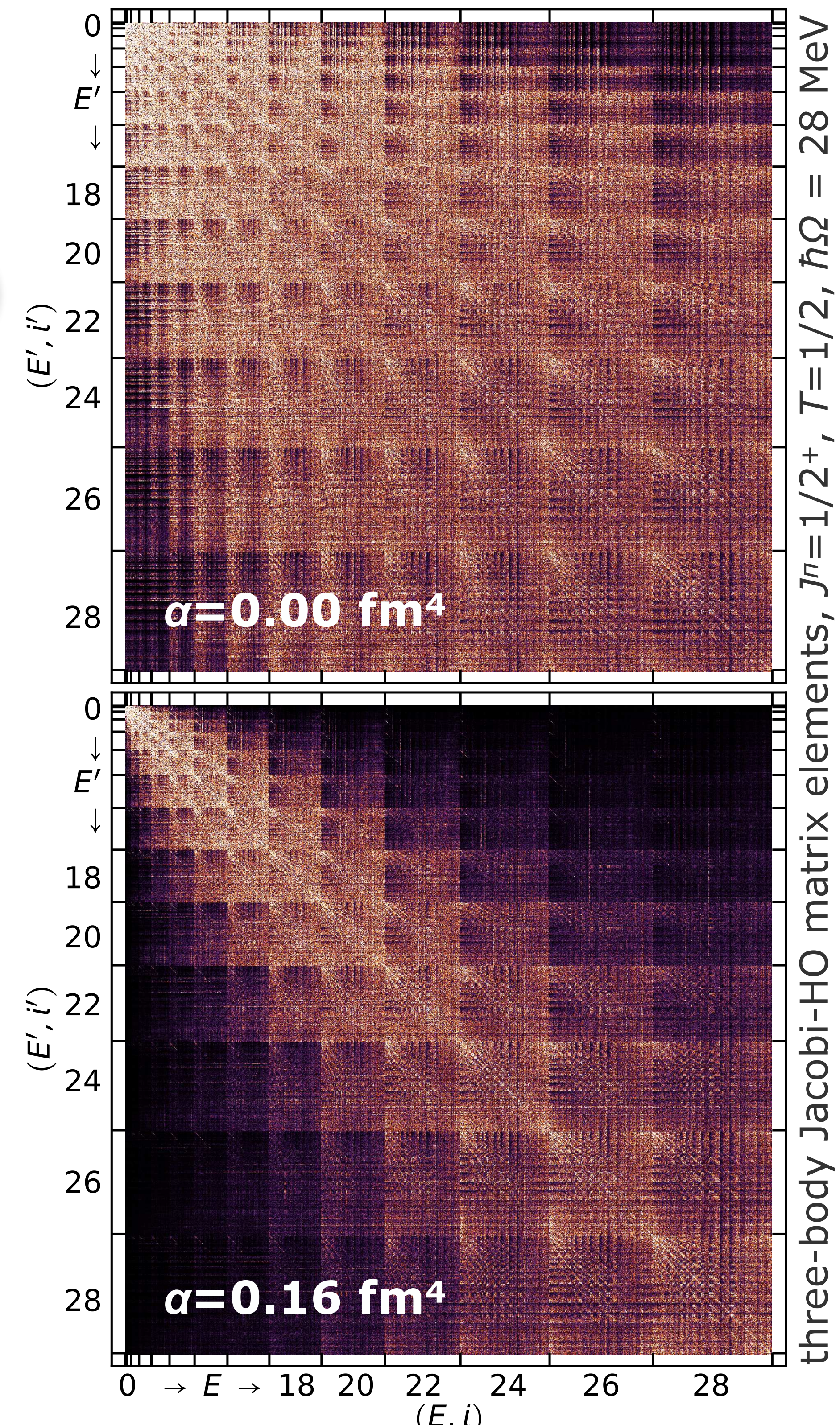
pro:
improves convergence of many-body calculations

con:
induces many-body interactions

- need to truncate evolved Hamiltonian

$$H_\alpha = H_\alpha^{[1]} + H_\alpha^{[2]} + H_\alpha^{[3]} + H_\alpha^{[4]} + \cdots$$

- variation of flow parameter provides diagnostic for omitted many-body terms
- state of the art:
  - keep all terms **up to the three-body level** consistently
  - consistently **evolve all relevant operators**, e.g. electromagnetic operators



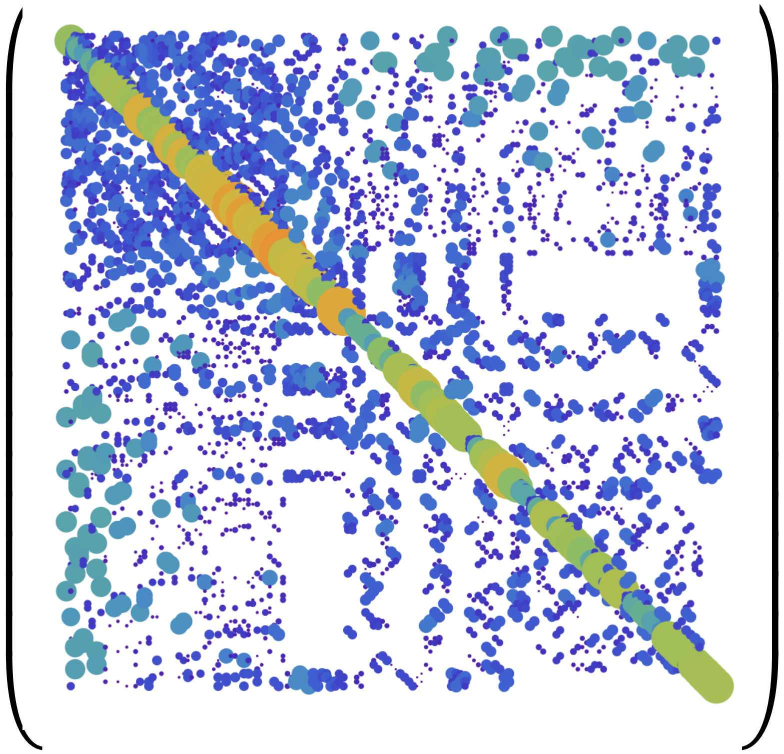
No-Core Shell Model

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 $N_{\max}\hbar\Omega$



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

No-Core Shell Model

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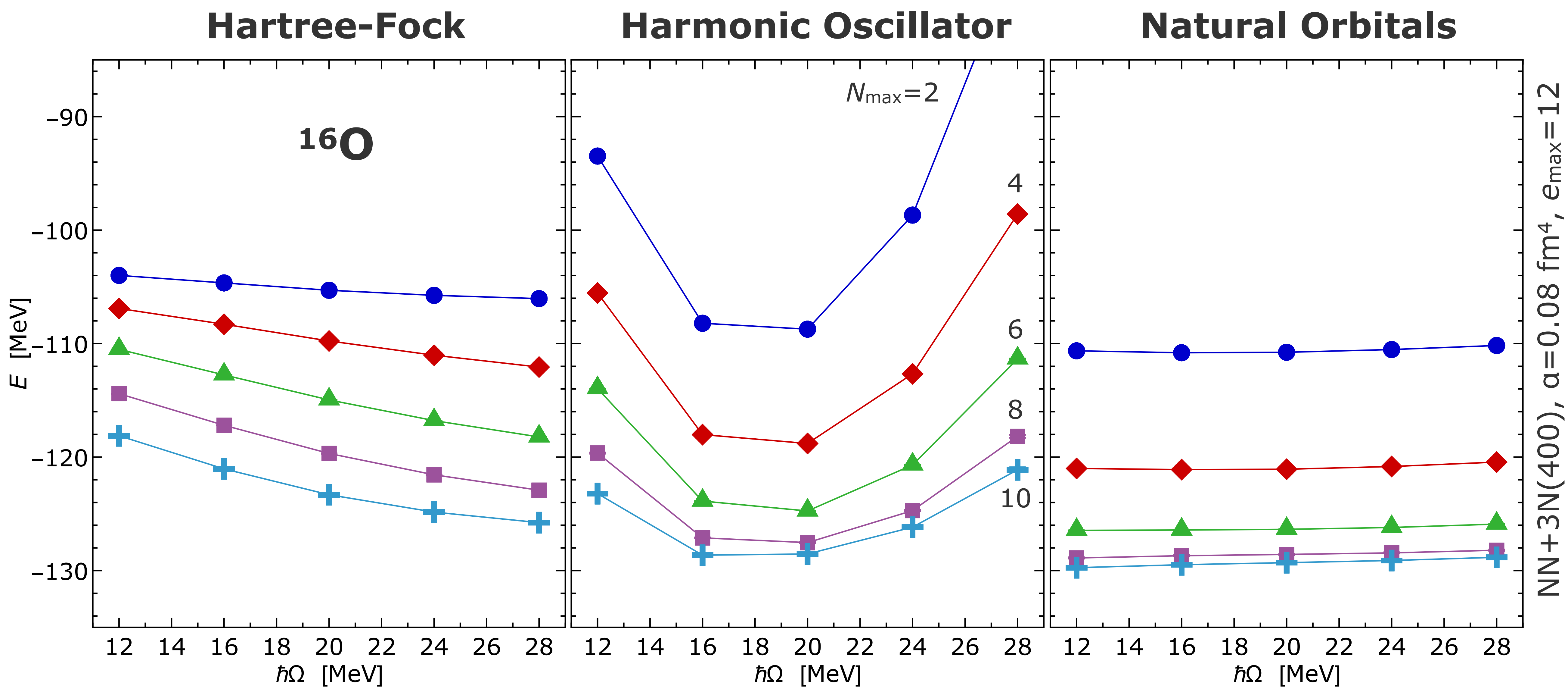
- **idea**: solve eigenvalue problem of Hamiltonian represented in model space of HO Slater determinants truncated w.r.t. HO excitation energy $N_{max}\hbar\Omega$
  - convergence of observables w.r.t. N_{max} is the only limitation and source of uncertainty
- **importance truncation**: reduce NCSM model space to physically relevant basis states and extrapolate to full space a posteriori
  - increases the range of applicability of NCSM significantly
- **alternative basis sets**: optimize to enhance model-space convergence or to include continuum physics
  - single-particle basis: natural orbitals, Gamow states
  - many-body basis: resonating group method with binary clusters

NCSM Convergence: Energies

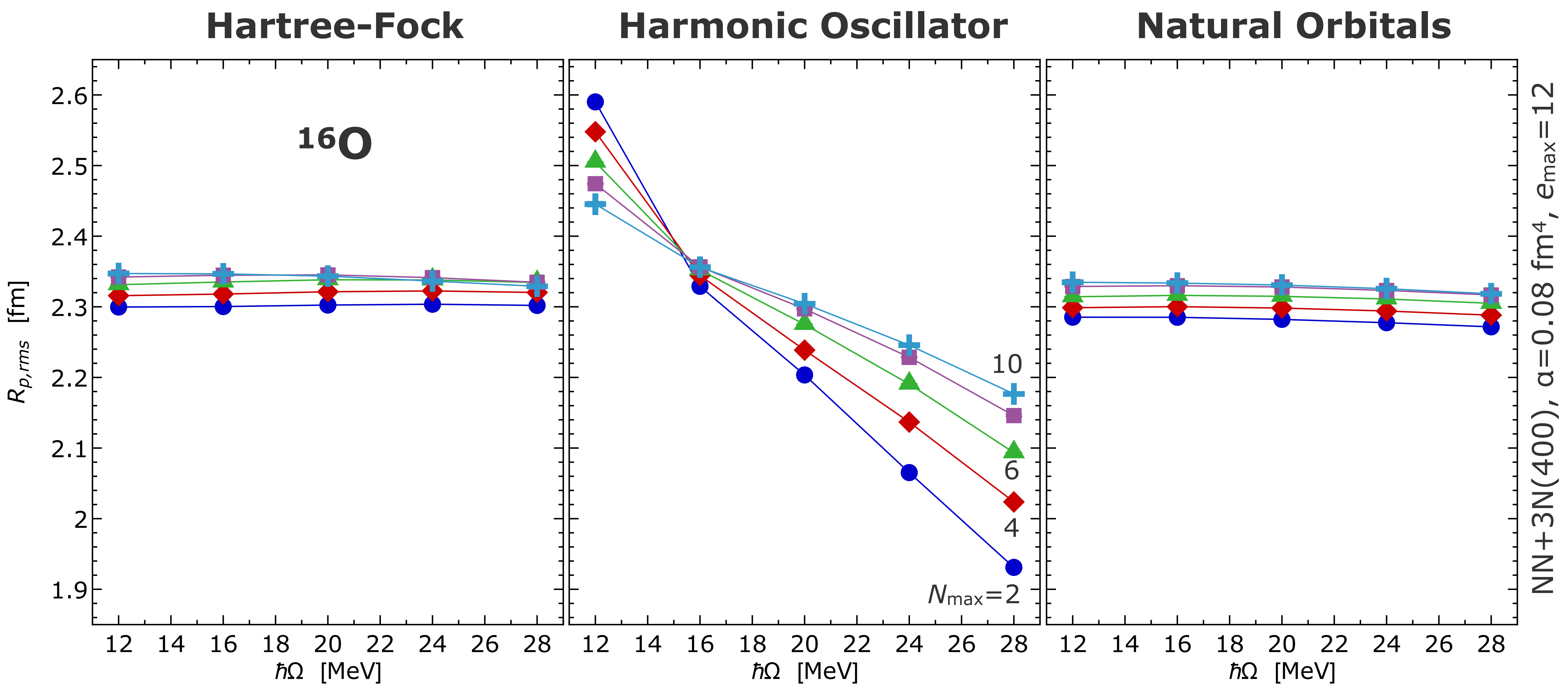
Tichai, Müller, Vobig, Roth; PRC 99, 034321 (2019)



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

NCSM Convergence: Radii

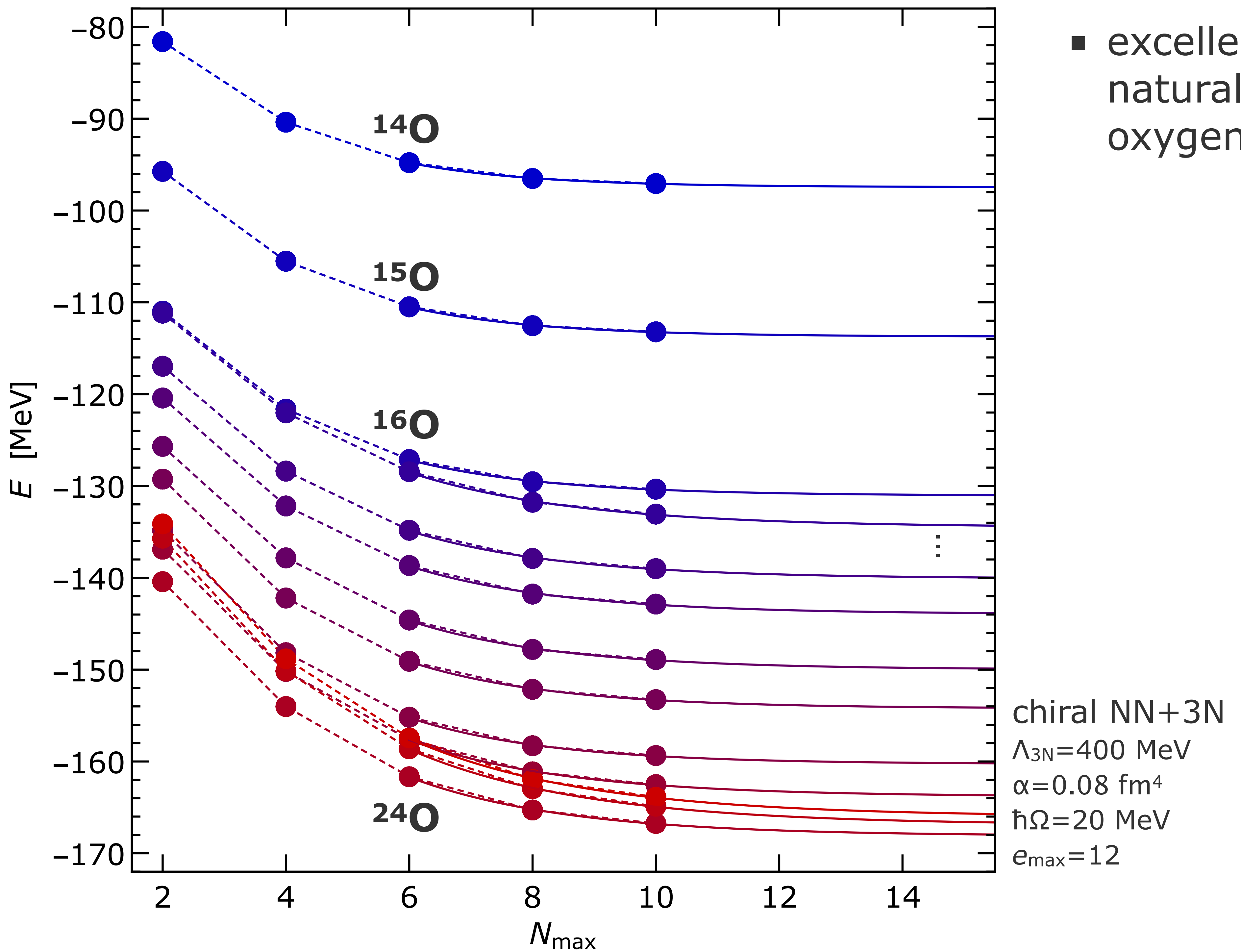
Tichai, Müller, Vobig, Roth; PRC 99, 034321 (2019)



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

Oxygen Isotopes

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



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

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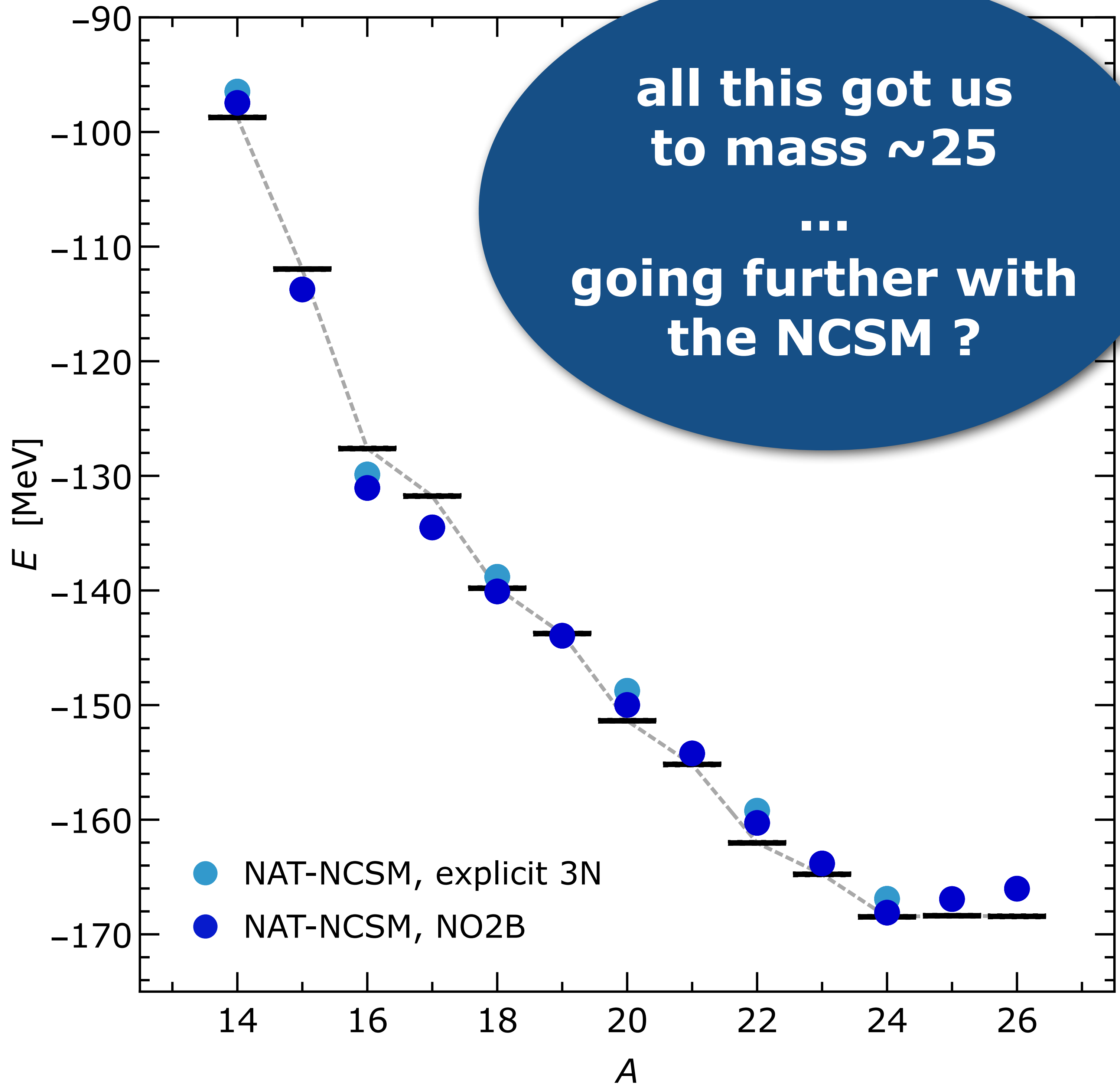

all this got us to mass ~25

...

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

In-Medium NCSM

No-Core Shell Model

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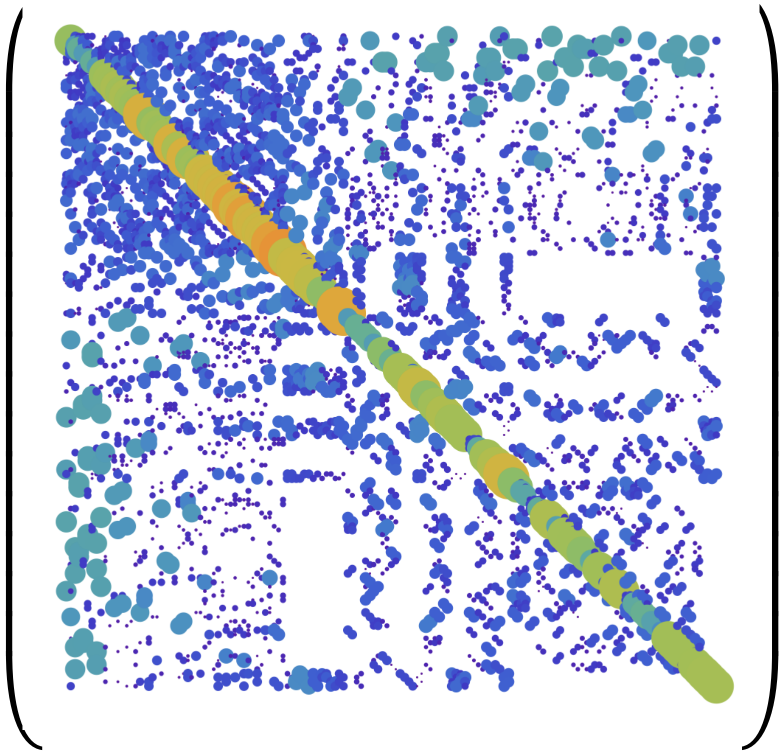

$$\begin{pmatrix} \vdots \\ C^{(n)}_{i'} \\ \vdots \end{pmatrix} = E_n \begin{pmatrix} \vdots \\ C^{(n)}_{i} \\ \vdots \end{pmatrix}$$

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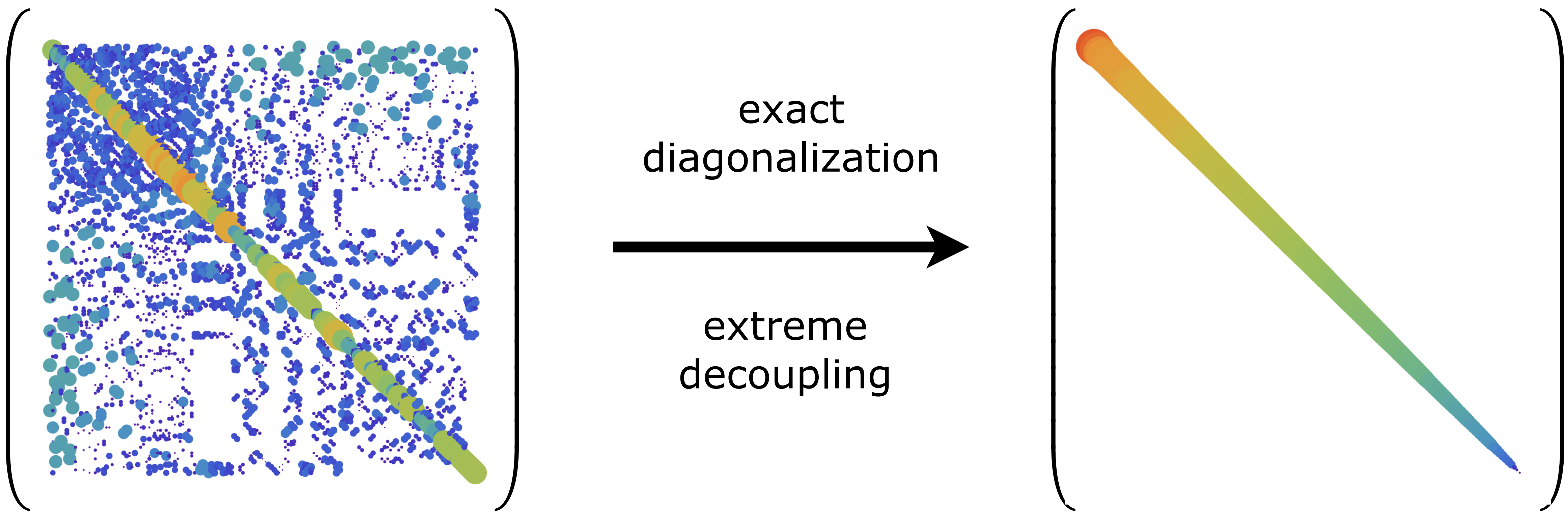
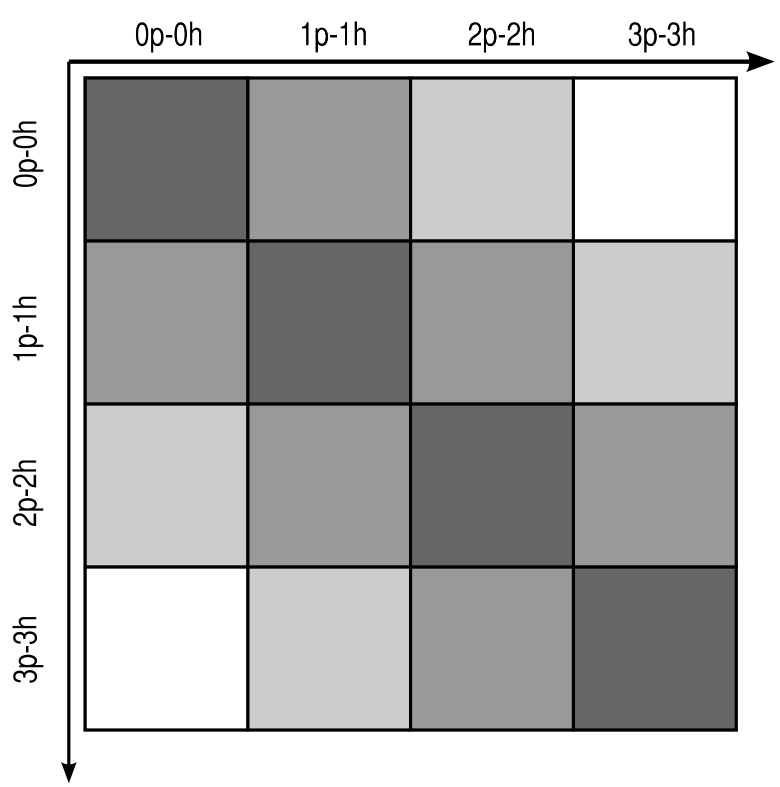


In-Medium SRG

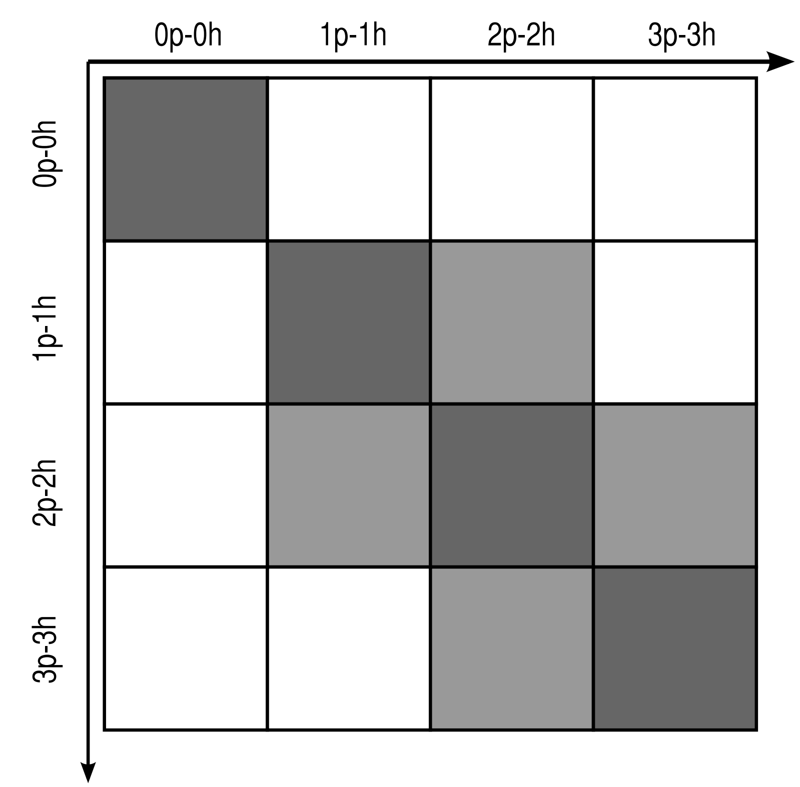
Tsukiyama, Bogner, Schwenk, Hergert,…

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



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

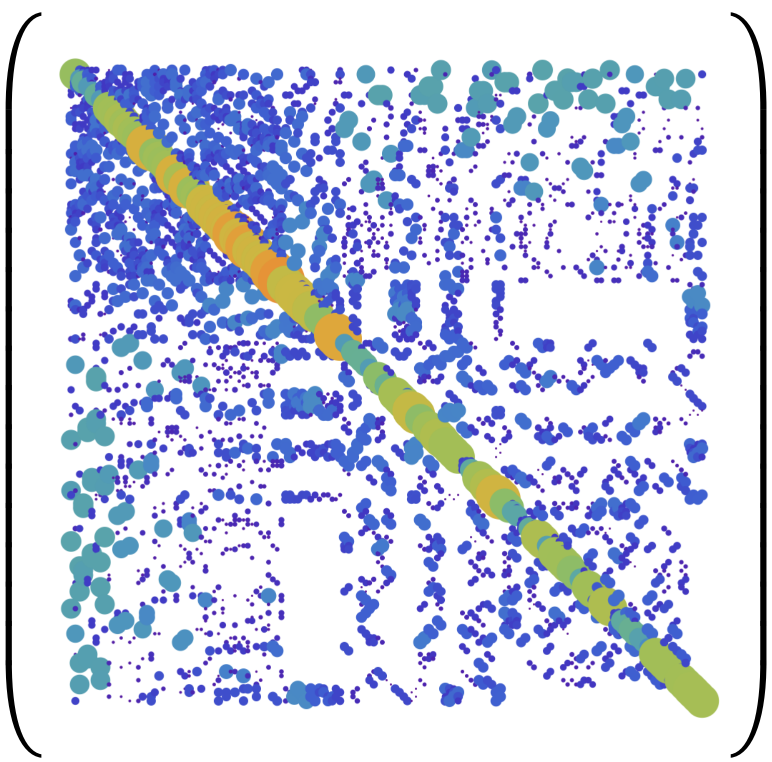


Multi-Reference In-Medium SRG

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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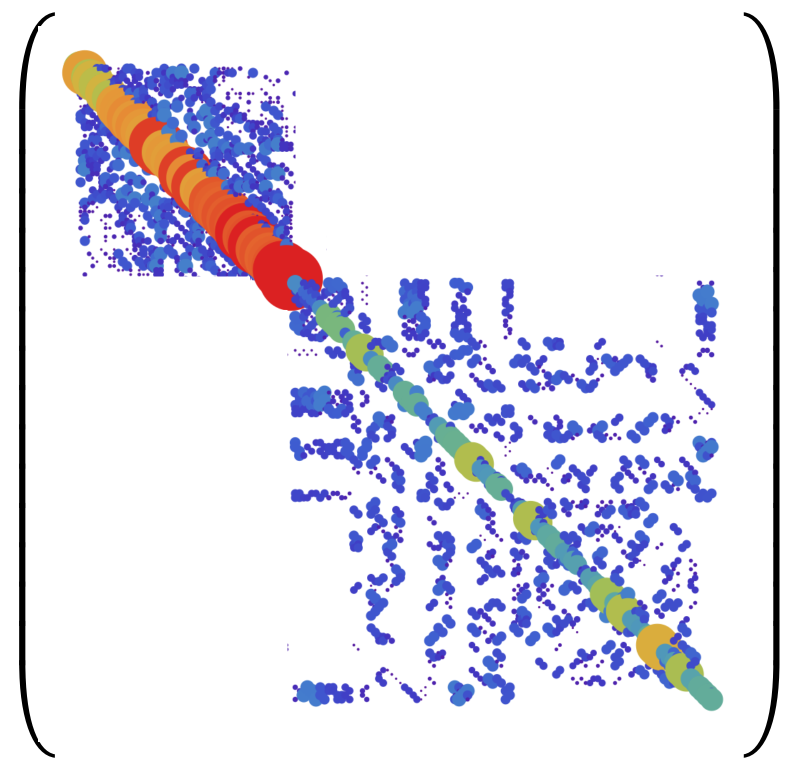

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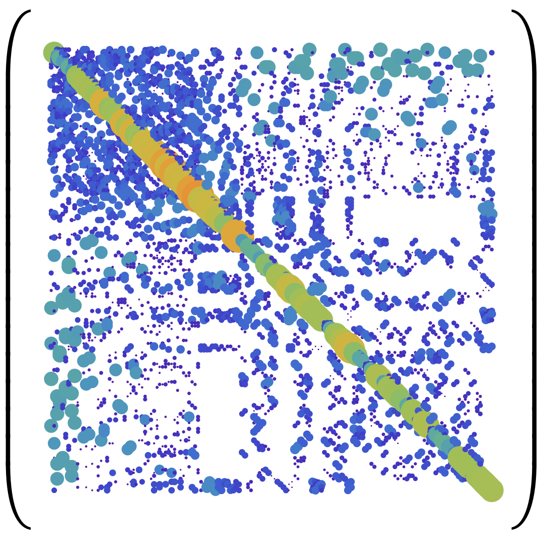
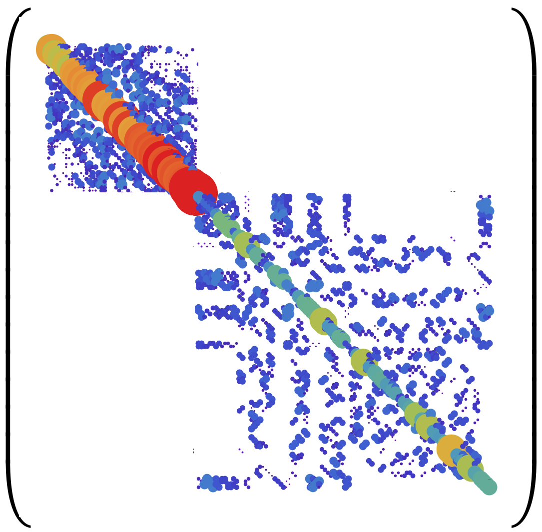
Hergert, Gebrerufael, Vobig, Mongelli, Roth,...



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

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

- 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

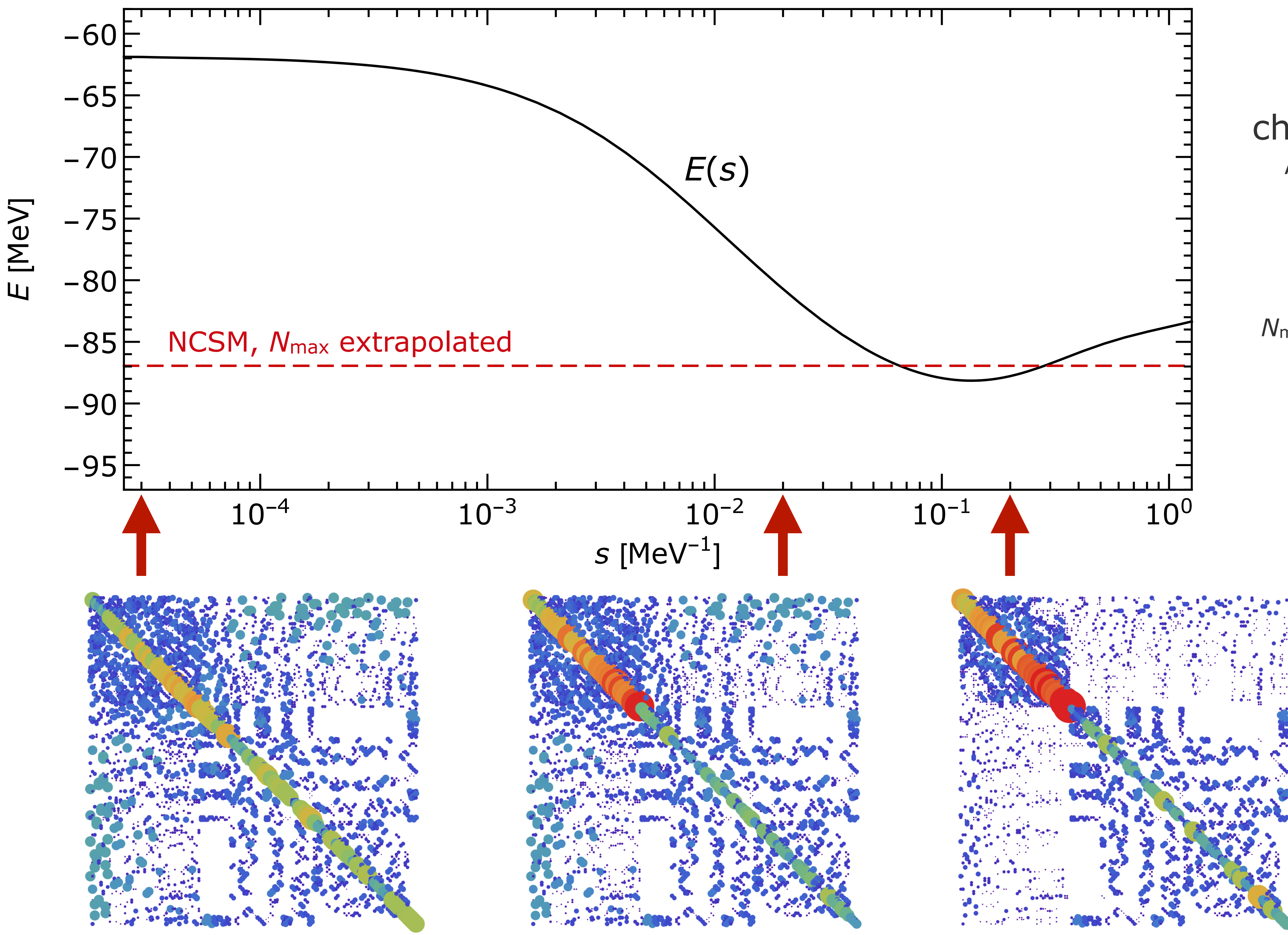
- IM-SRG evolution of multi-reference normal-ordered Hamiltonian and other operators
- decoupling of particle-hole excitations, i.e., pre-diagonalization in many-body space

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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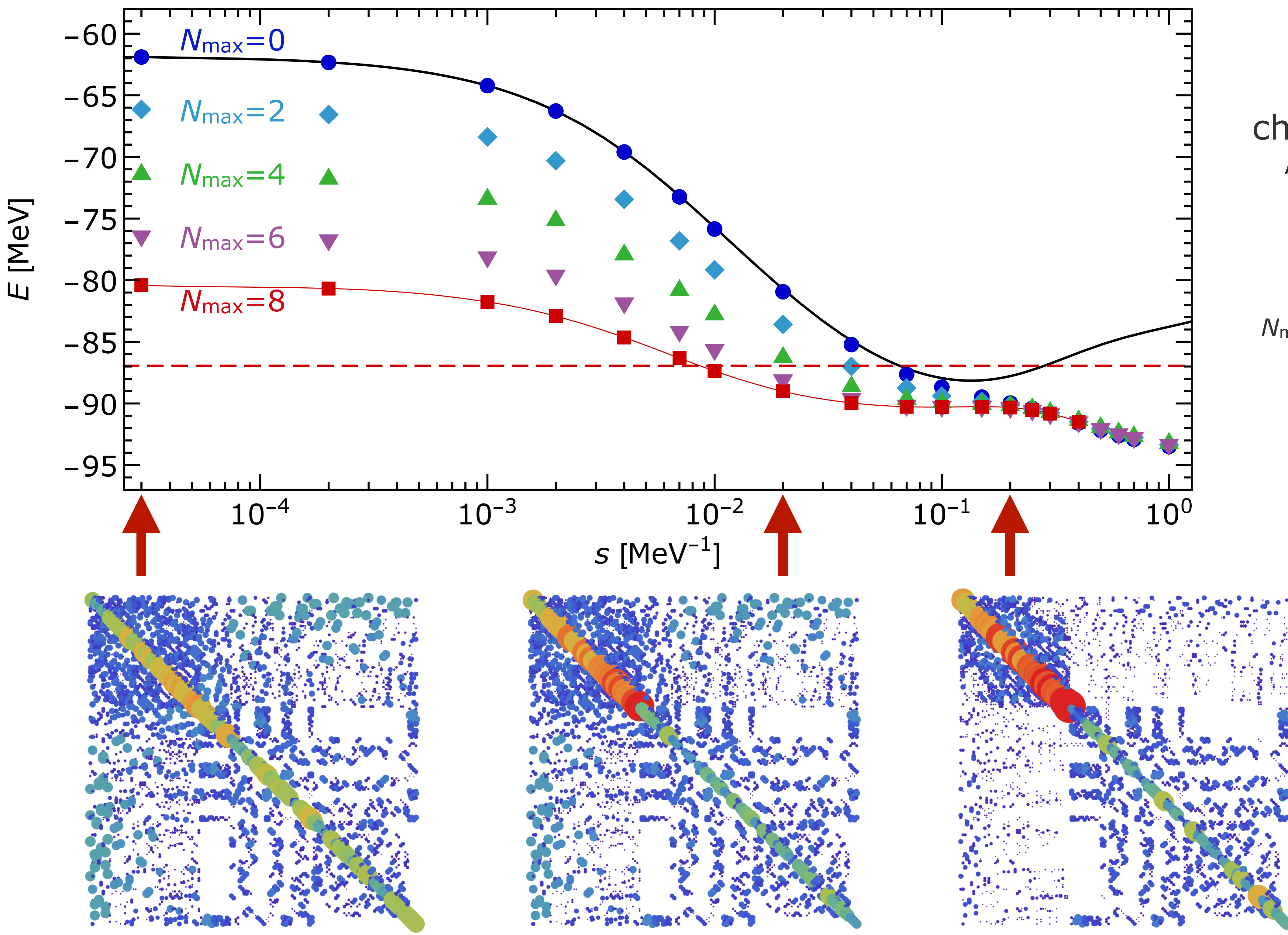

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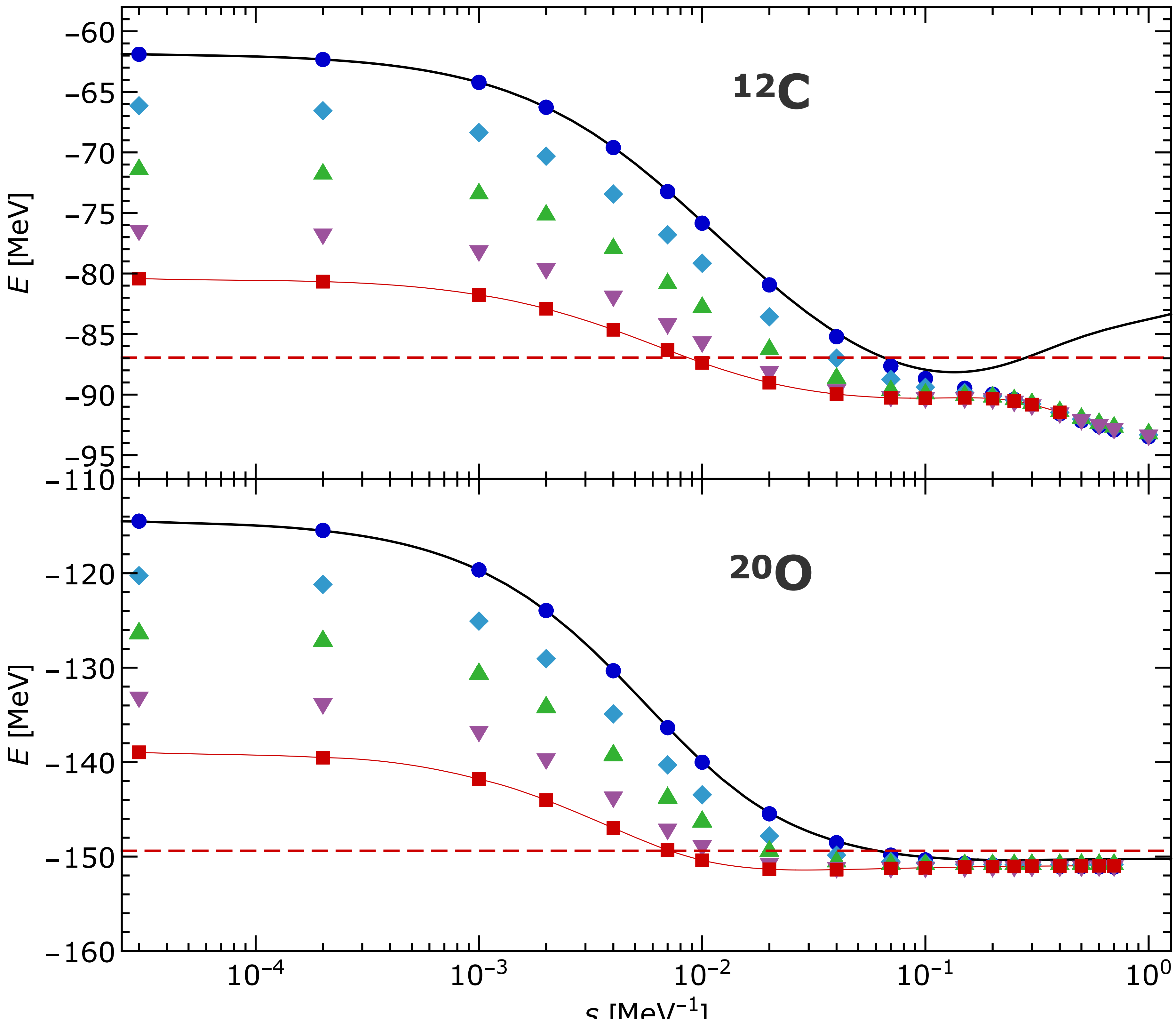

- NCSM convergence is drastically improved
- N_{max}=0 eigenvalues deviated from $E(s)$

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

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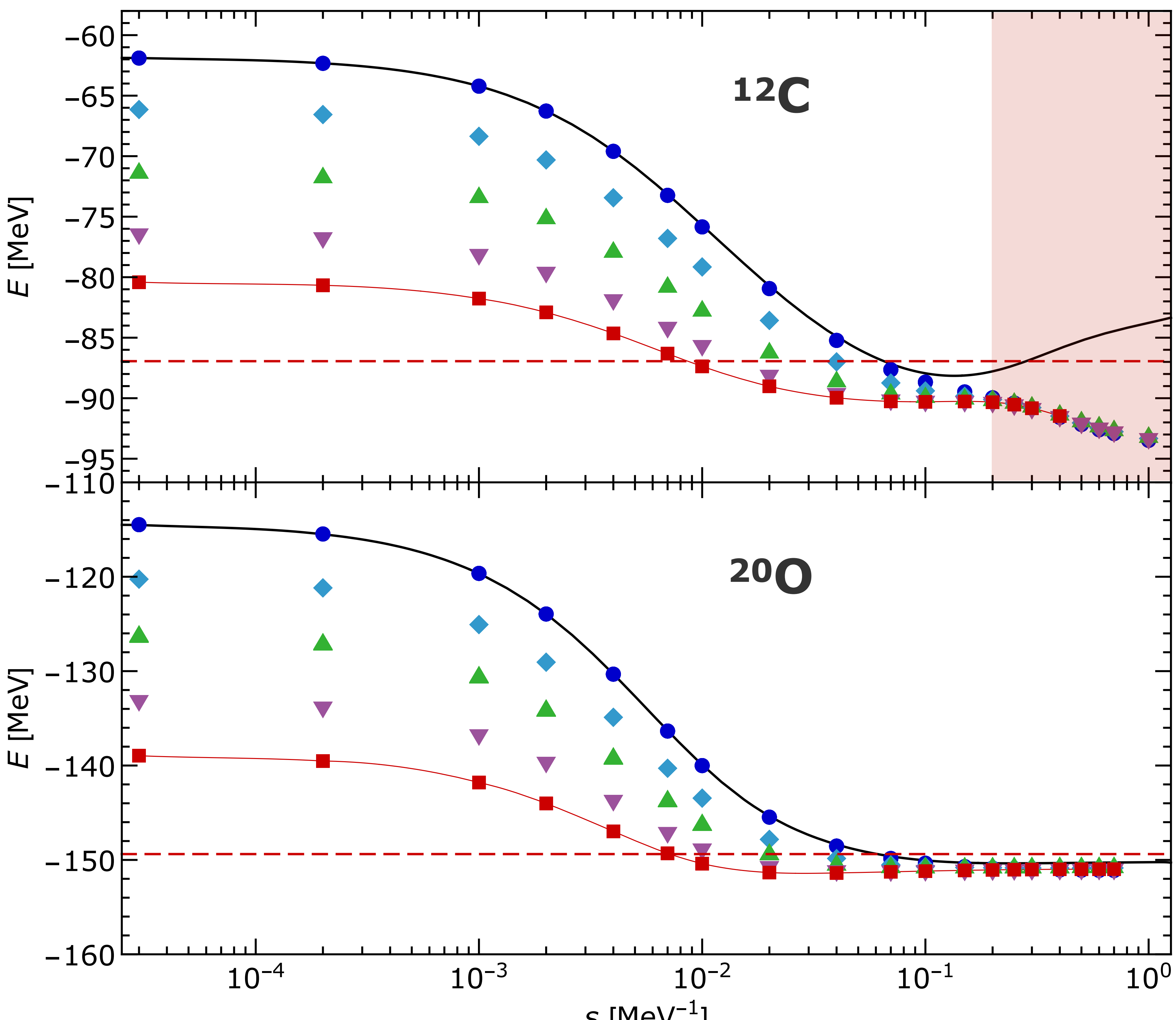

- NCSM convergence is drastically improved
- N_{max}=0 eigenvalues deviated from $E(s)$
- induced many-body contributions might affect large-s results

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e_{max}=12

HF basis
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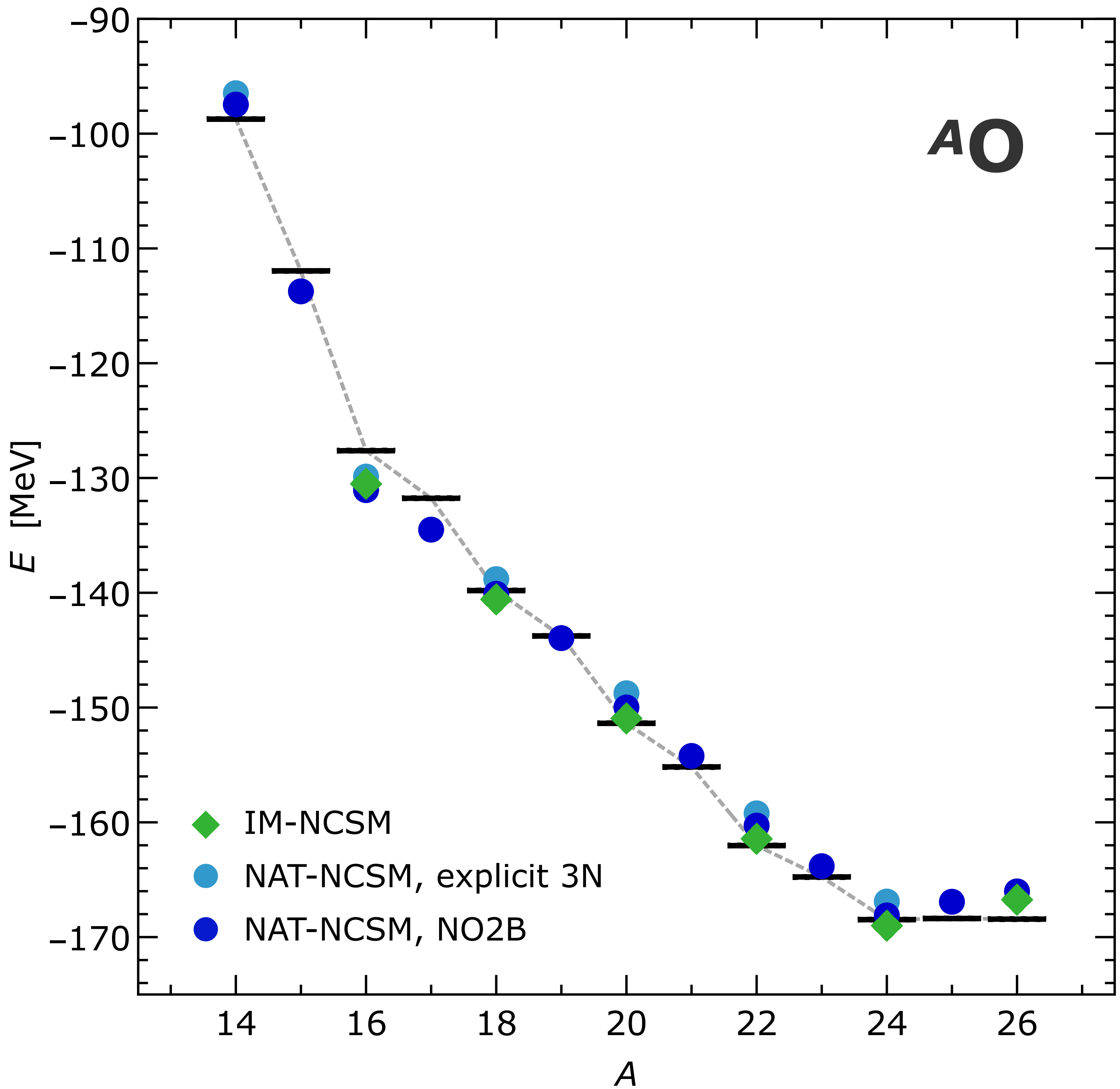
IM-NCSM: Oxygen Isotopes

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
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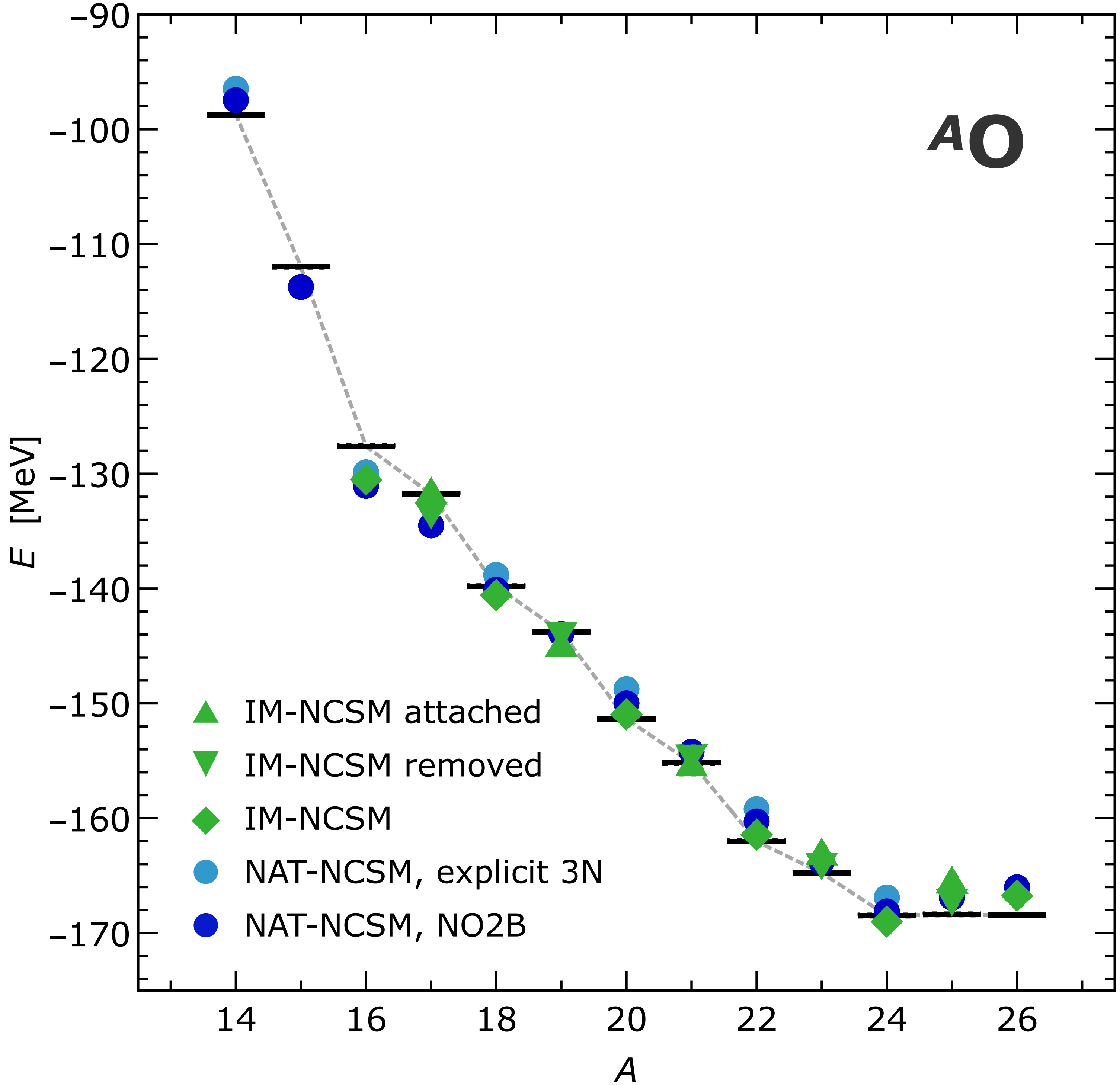
Vobig, Mongelli, Roth; in prep.



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HF basis
N_{max}=0 reference

In-Medium NCSM: Magnus Formulation

Magnus, Comm. Pure Appl. Math. 7, 649 (1954); Morris et al., PRC 92, 034331 (2015)

- classical formulation of flow equation **impractical** for treatment of several different observables (energies, radii, E2, M1,...)

- formulation of flow-equation for **Magnus operator** Ω(s)

$$U(s) = e^{-\Omega(s)} \qquad \frac{d}{ds}\Omega(s) = \sum_{k=0}^{\infty} \frac{B_k}{k!} \left[\Omega(s), \eta(s)\right]_k$$

- **transformation of observables** via Baker-Campbell-Hausdorff series

$$O(s) = e^{+\Omega(s)}\, O\, e^{-\Omega(s)} = \sum_{n=0}^{\infty} \frac{1}{n!}\left[\Omega(s), O\right]_n$$

- **computational benefits**
  - system of ODEs only for Magnus operator, reduces computational cost significantly
  - extraction of evolved observables is simple post-processing step
  - nested commutator series converge quickly
  - necessity for treatment of non-scalar operators (elmag. multipole operators)

In-Medium NCSM: Refinements

Vobig et al., in preparation

- **optimized decoupling pattern**
  - standard generators also induce a decoupling within the reference space
  - include full reference space into diagonal part, no decoupling of excitations within reference space
  - eliminates anomalies in large-s regime

- **particle-attached particle-removed scheme**
  - angular-momentum-coupled formulation of flow equations needs scalar density matrix (J=0 reference state) to be efficient
  - odd-A nuclei cannot be targeted directly, therefore...
    - use adjacent even-A parent nucleus for definition of reference state and solution of flow equations (with odd-A prefactors in Hamiltonian)
    - perform final NCSM calculation for odd-A target nucleus
  - monitor N_{max} convergence for different possible parent nuclei

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 for realistic applications

- 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: $N_{\text{max}}^{\text{ref}} = 0, 2, 4$
  - different flow parameters: s_{sat} , $s_{\text{sat}}/2$
  - different model-space truncations: $N_{\text{max}} = 0, 2, 4, 6,...$

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

Applications with
Nonlocal NN+3N Interactions

Nonlocal Interactions

Hüther et al.; PLB 808, 135651 (2020)

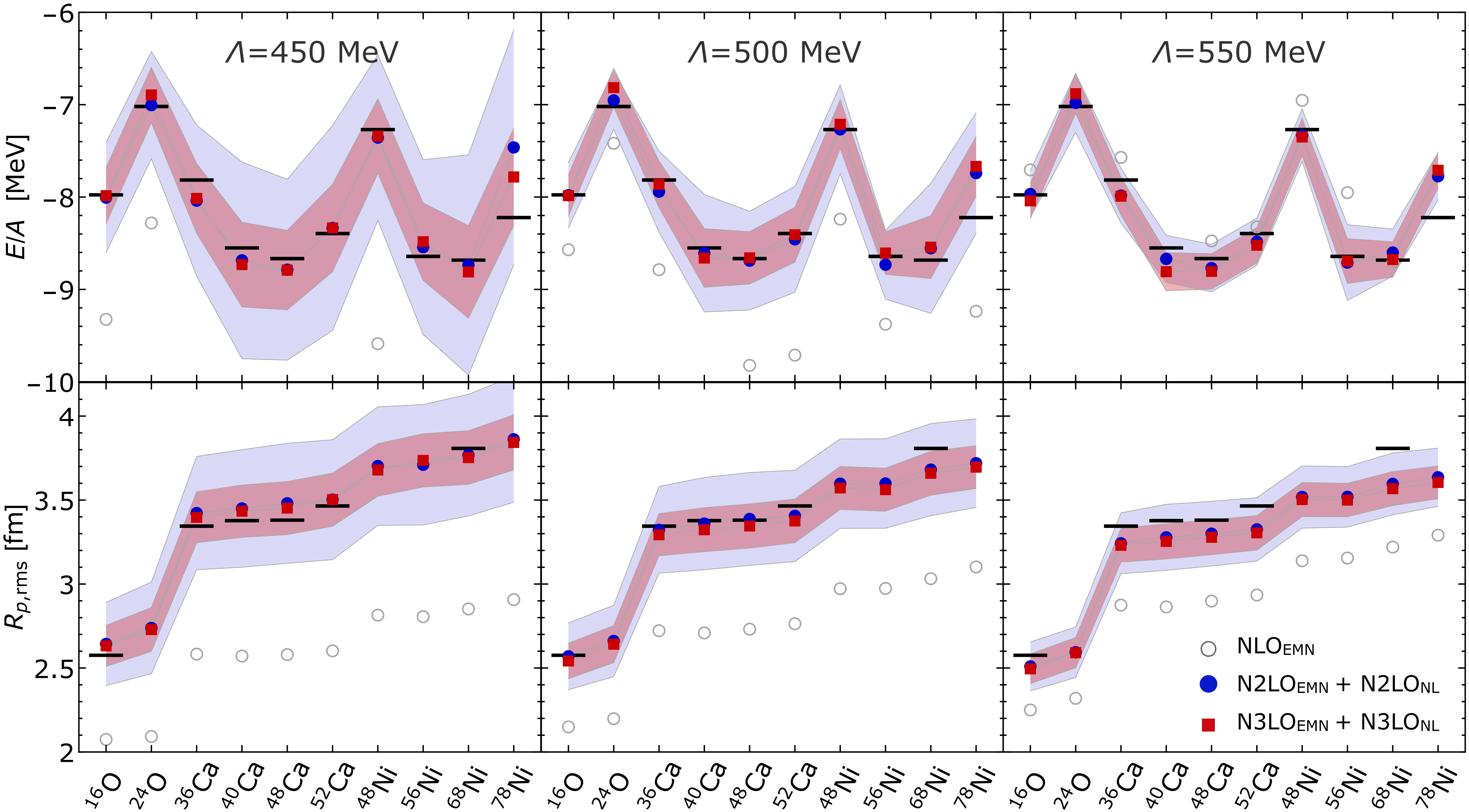
- **start from chiral NN interaction by Entem, Machleidt & Nosyk** *PRC 96, 024004 (2017)*
  - LO to N3LO
  - non-local regulator
  - cutoff 450, 500, 550 MeV
  - accurate reproduction of NN scattering data up to ~300 MeV

- **supplement non-local 3N interaction at N2LO and N3LO**
  - N2LO or N3LO
  - non-local regulator, compatible with NN interaction
  - cutoff 450, 500, 550 MeV, same as NN interaction

- **determine 3N low-energy constants**
  - c_E fit to triton binding energy
  - determine c_D from ^{16}O ground-state energy in IM-SRG

Medium-Mass Nuclei

Hüther et al.; PLB 808, 135651 (2020)

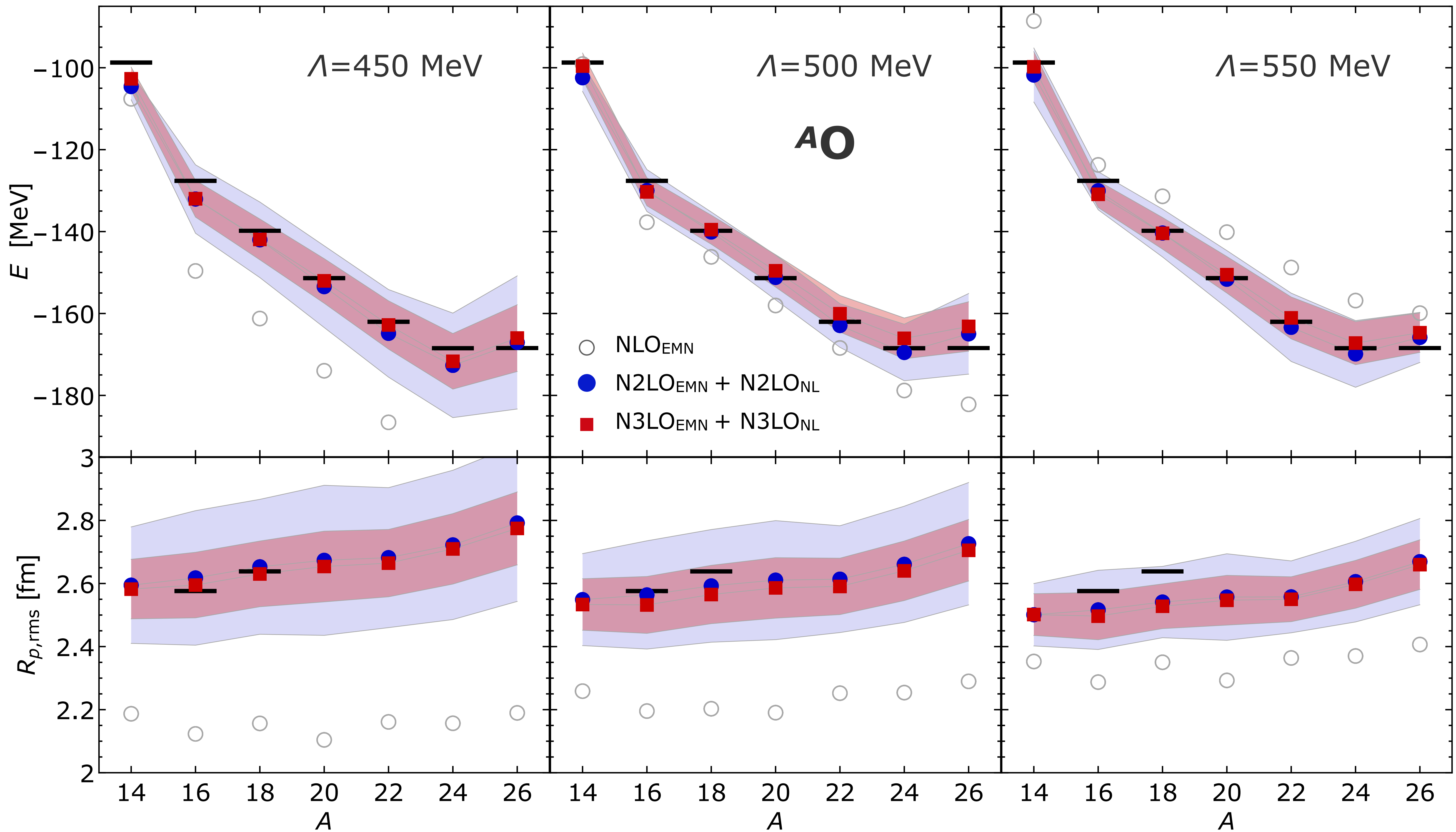


IM-SRG(M2), natural orbitals, ħΩ=20 MeV, α=0.04 fm^4, e_{max}=12, E_{3max}=16

error bands show interaction + many-body uncertainties

Oxygen Isotopic Chain

Hüther et al.; PLB 808, 135651 (2020)

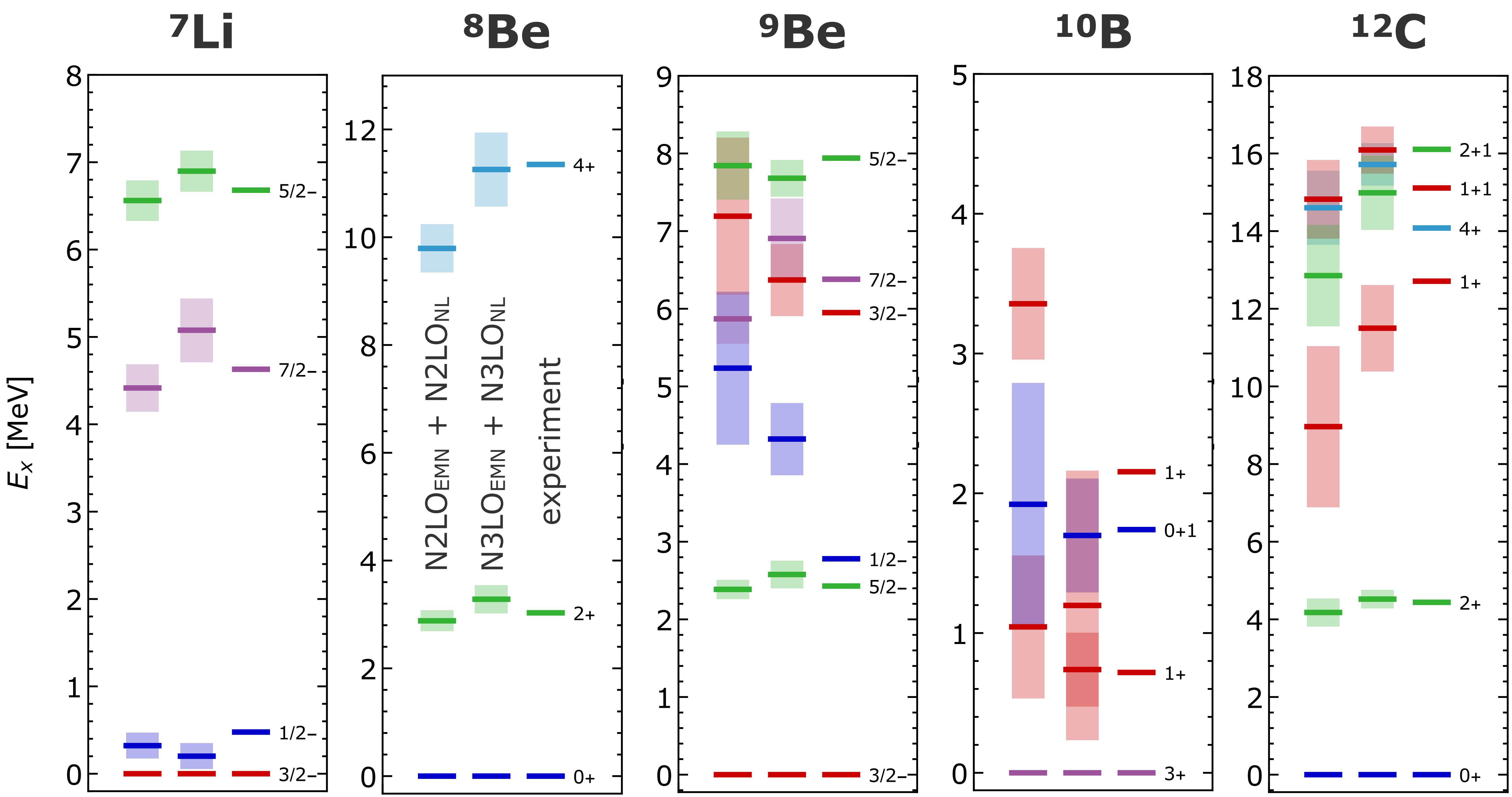


IM-NCSM, natural orbitals, $\hbar\Omega$=20 MeV, α=0.04 fm⁴, e_{max}=12, E_{3max}=14, N_{ref}=2

error bands show interaction + many-body uncertainties

p-Shell Spectra

Hüther et al.; PLB 808, 135651 (2020)

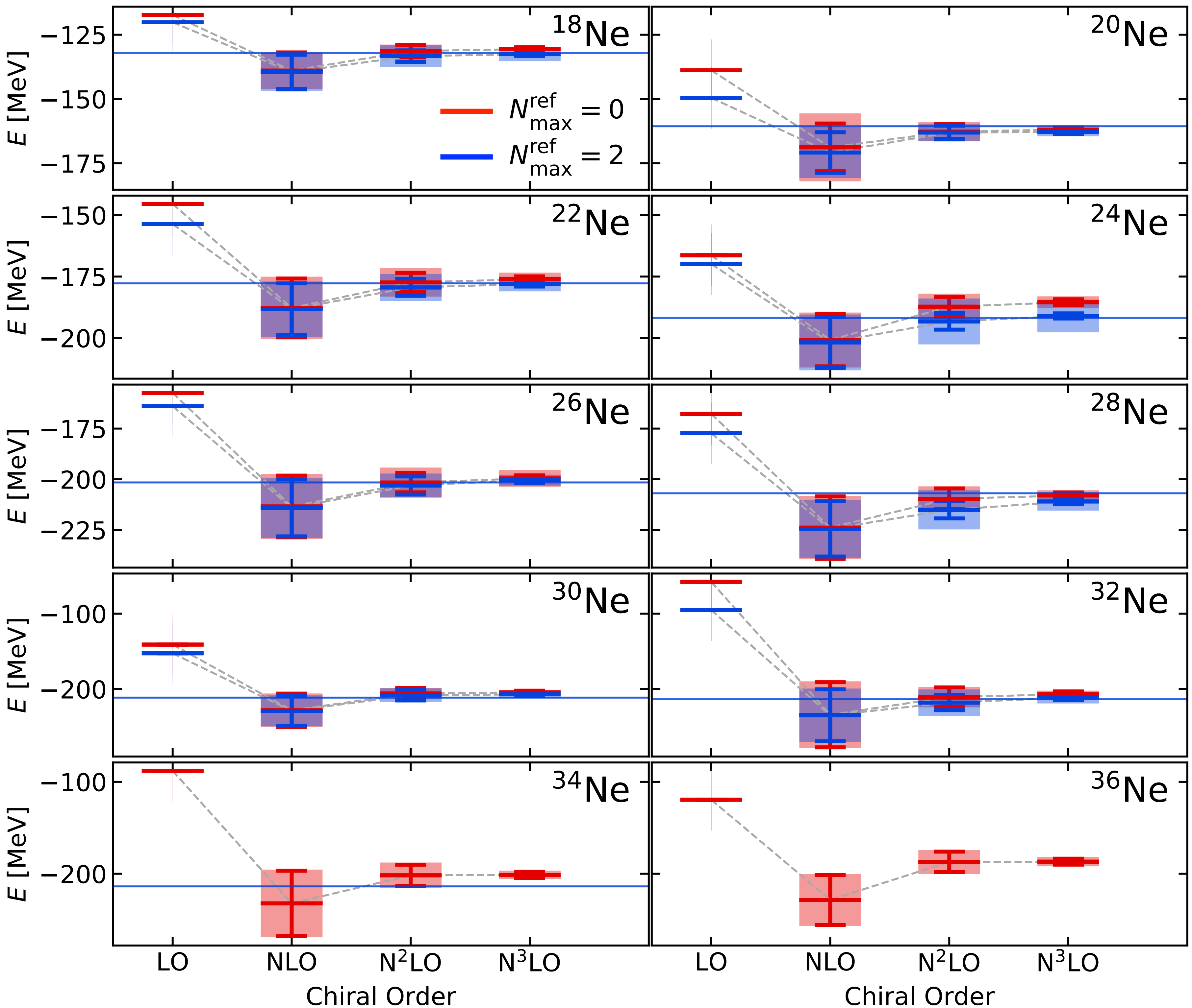


NCSM/IM-NCSM, Λ=500 MeV, ħΩ=20 MeV
error bands show interaction uncertainties

Applications: Neon Isotopes

Ground-State Energies

Mongelli et al., in preparation



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

Λ = 500 MeV
α = 0.04 fm^4
ħΩ = 20 MeV
e_{max} = 12
NAT basis

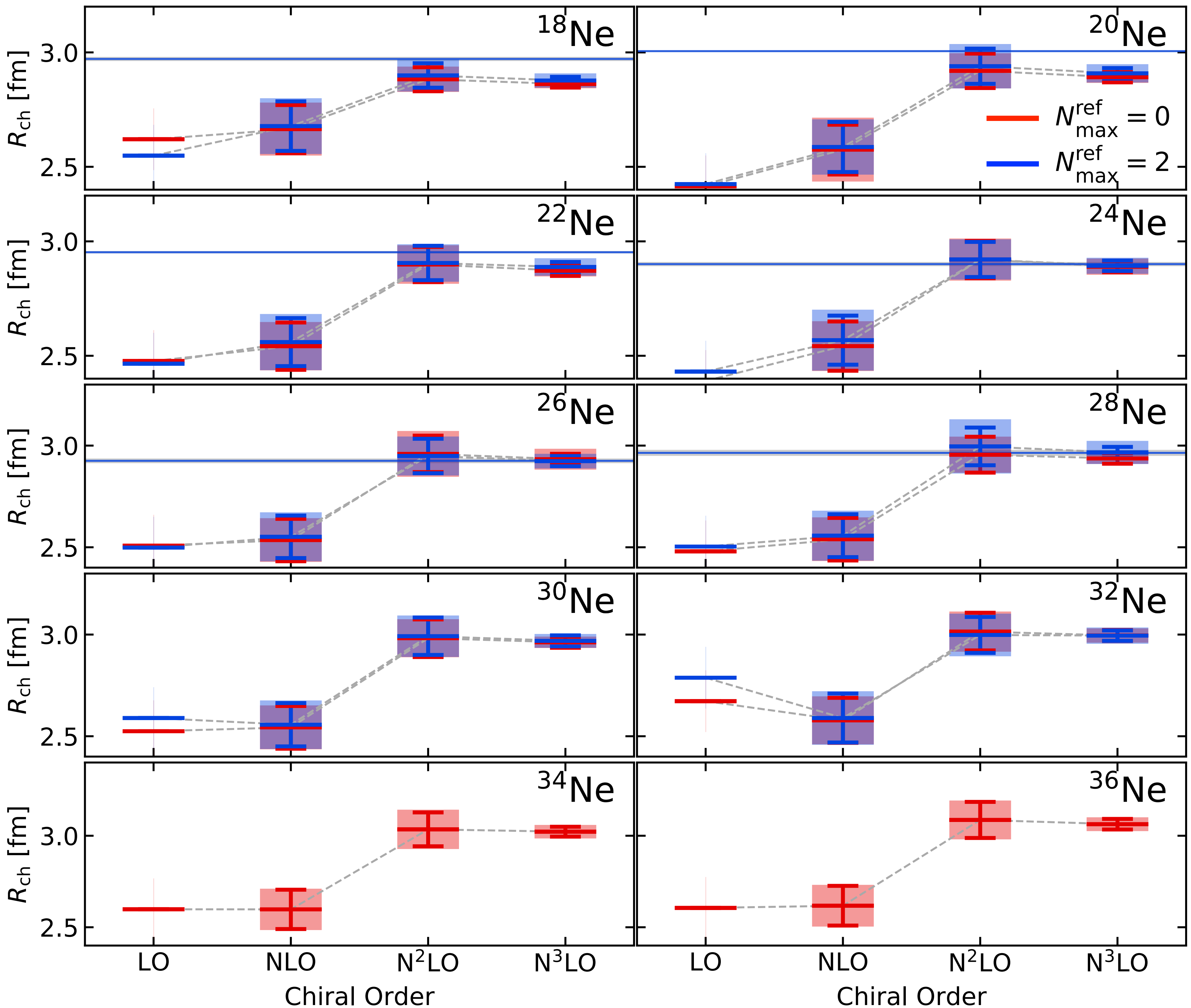
$N^{ref}_{max} = 0, 2$
$N_{max} = 4$

error bars:
68% interaction uncertainties

error bands:
interaction + many-body uncertainties

Charge Radii

Mongelli et al., in preparation



- excellent description of radii, slight underestimation for light isotopes
- stable results in N²LO and N³LO

Λ = 500 MeV
α = 0.04 fm⁴
$\hbar\Omega$ = 20 MeV
e_{max} = 12
NAT basis

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

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68% interaction uncertainties

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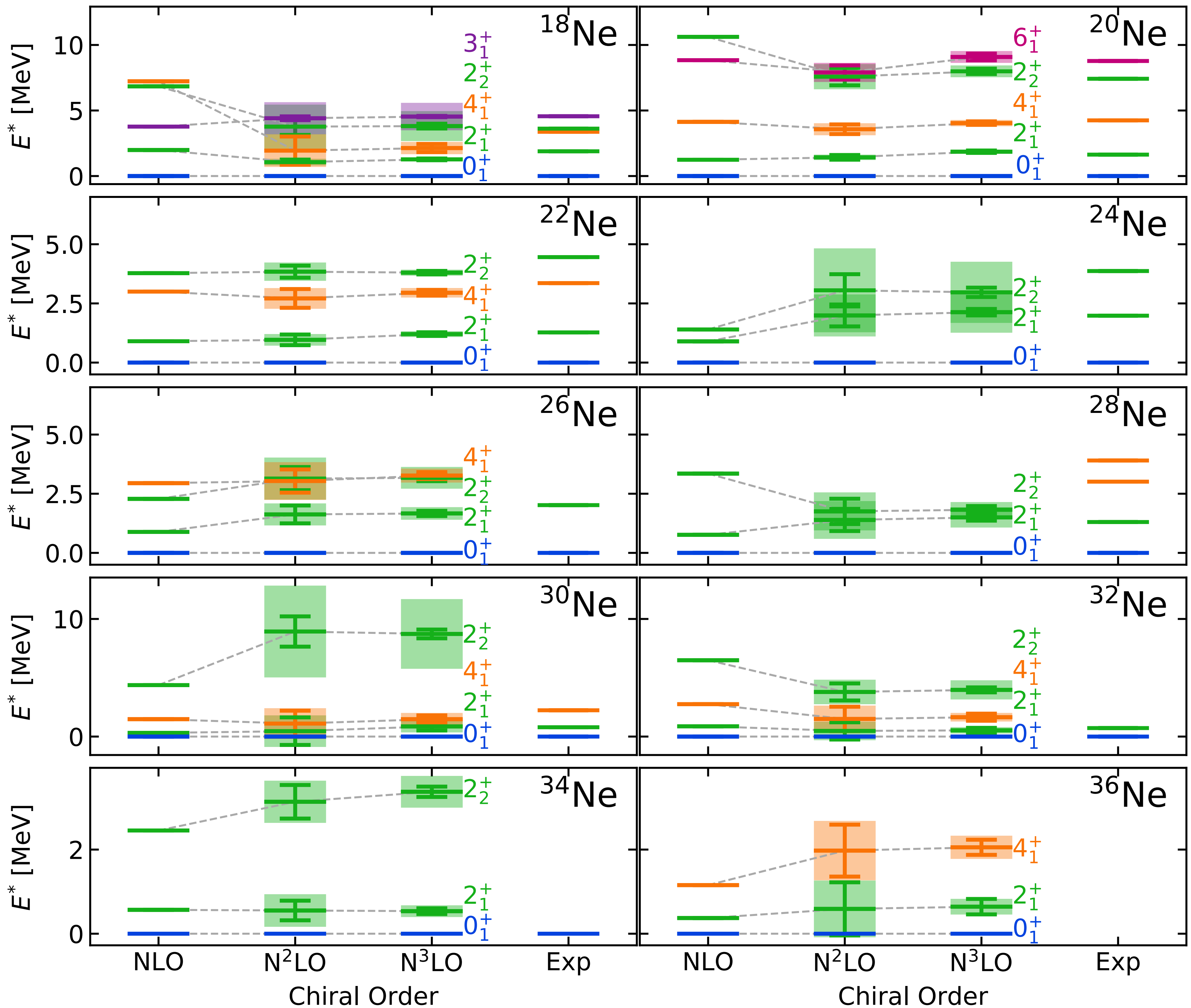
interaction + many-body uncertainties

Excitation Energies

Mongelli et al., in preparation



- excellent description of excitation spectra

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

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

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68% interaction uncertainties

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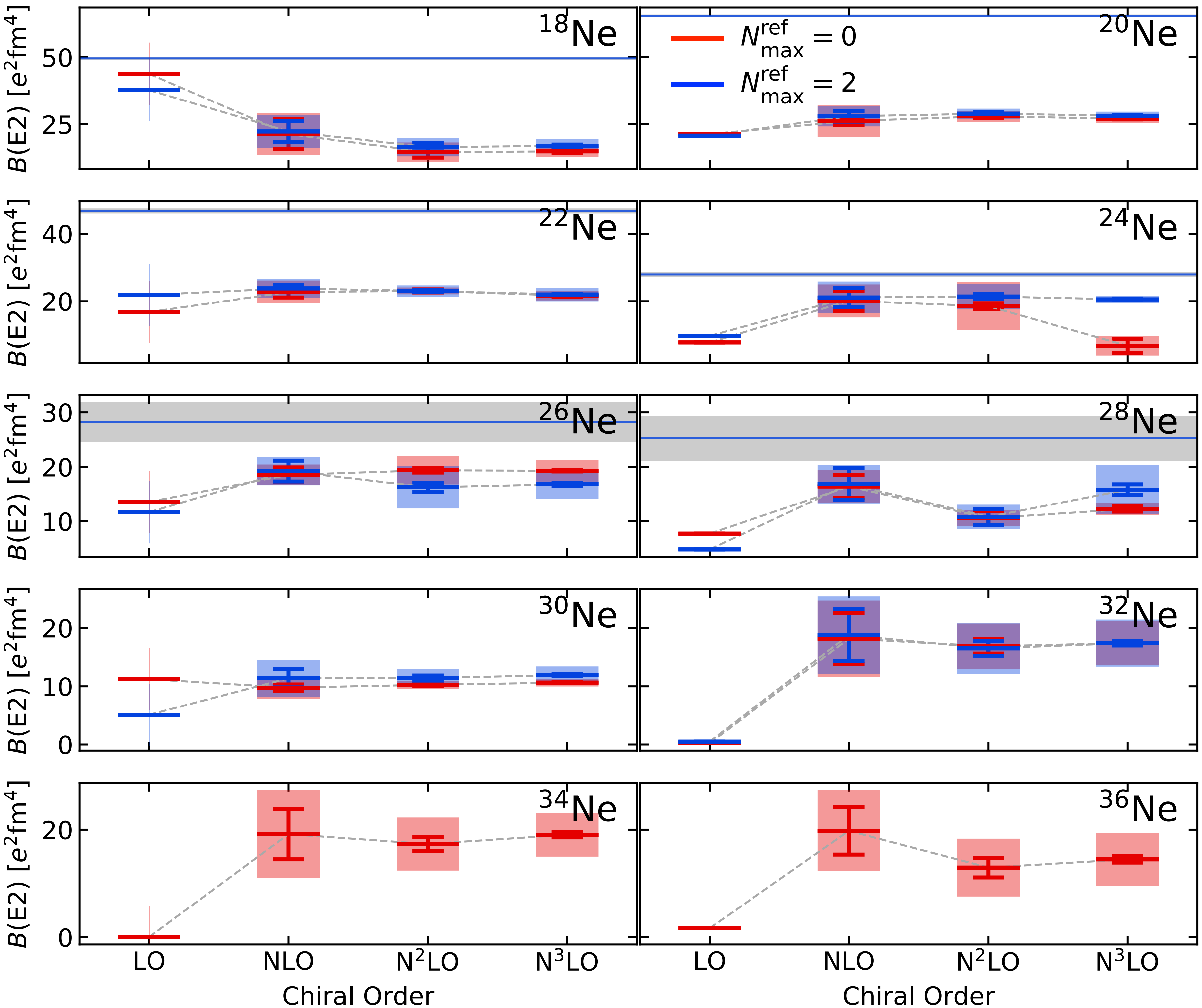
B(E2, 2⁺ → 0⁺) Transition Strength

Mongelli et al., in preparation



- significant under-estimation of B(E2) all over the place
- hierarchy inversion
- missing 'collectivity'

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

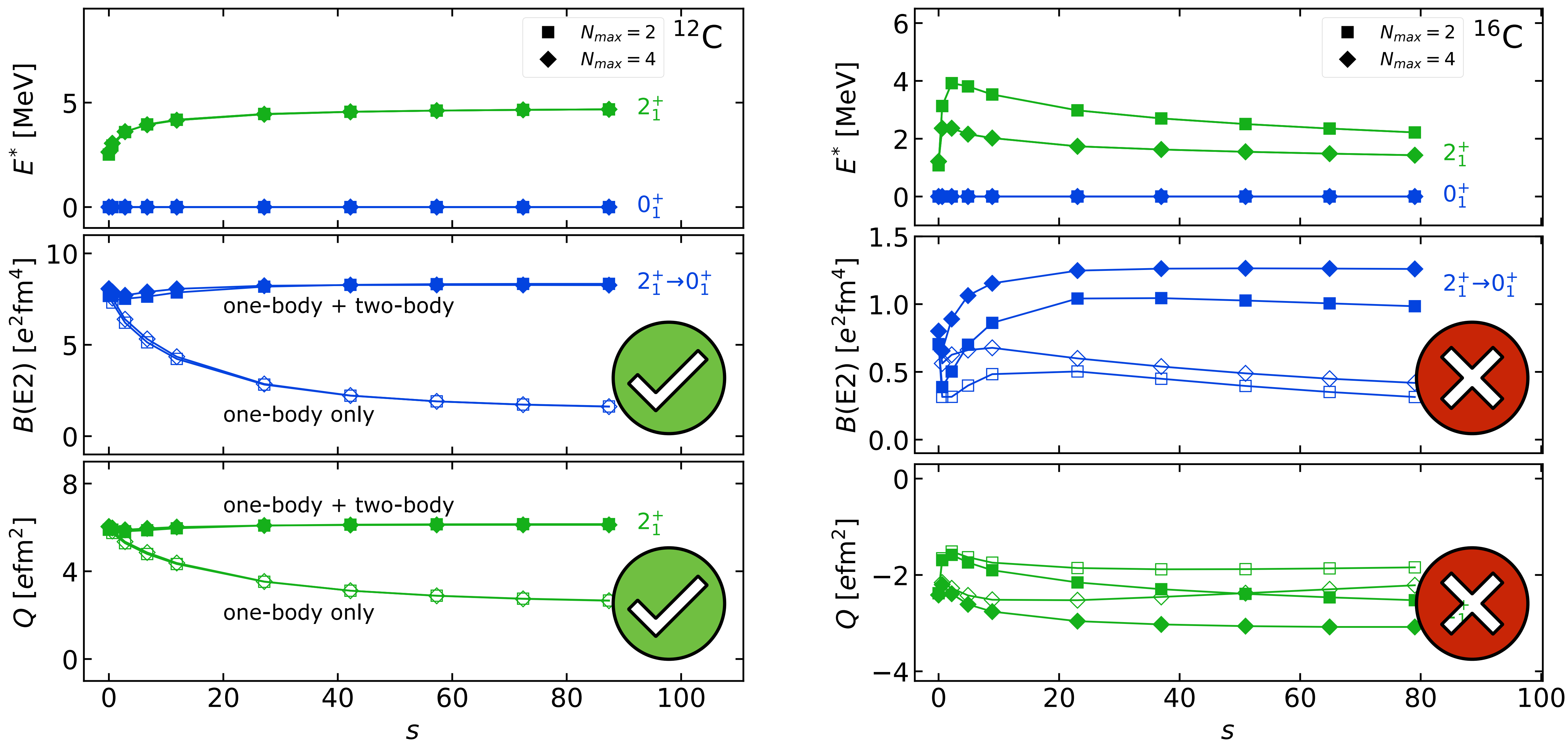
$N^{ref}_{max} = 0, 2$
$N_{max} = 4$

error bars:
68% interaction uncertainties

error bands:
interaction + many-body uncertainties

Hierarchy Inversion

Mongelli et al., in preparation



- 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 ^{40}Ca, 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
  - truncate many-body basis w.r.t. number of particle and hole states

- **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)]*

Epilogue

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