In-Medium No-Core Shell Model:
Updates & Applications

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Ab Initio Nuclear Structure Theory

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

Hamiltonian

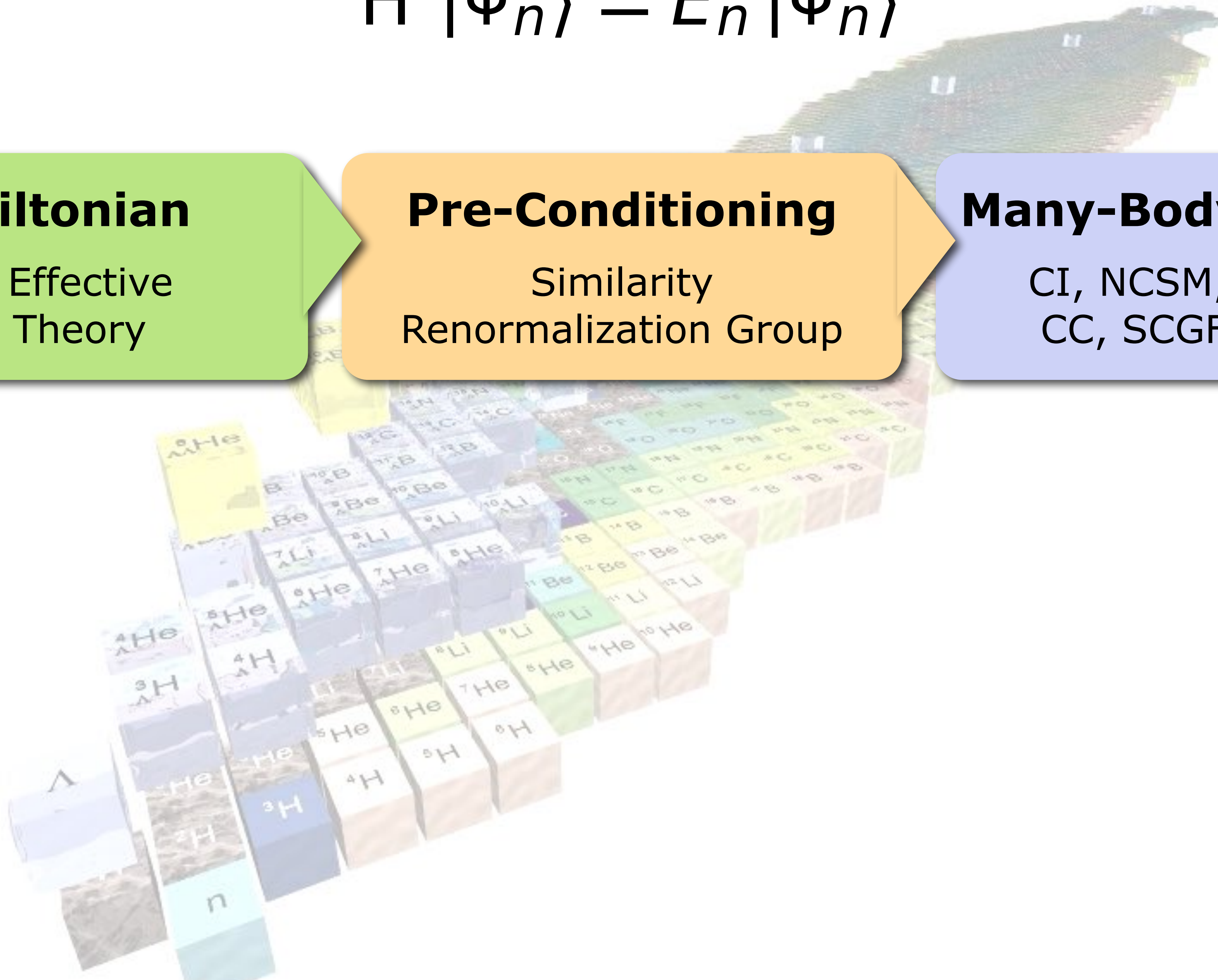
Chiral Effective Field Theory

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...

- focus on families of chiral NN+3N interactions up to N3LO
- systematic variation of chiral order and cutoff
- quantification of truncation uncertainties via Bayesian methods

Ab Initio Nuclear Structure Theory

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Many-Body Solution

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

- use standard free-space SRG for all operators
- interactions we use require pre-diagonalization for controlled many-body convergence

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...

- focus on NCSM-based approaches because of versatility
- use multi-reference IM-SRG as additional convergence booster
- hybrid approaches entail more difficult uncertainty quantification

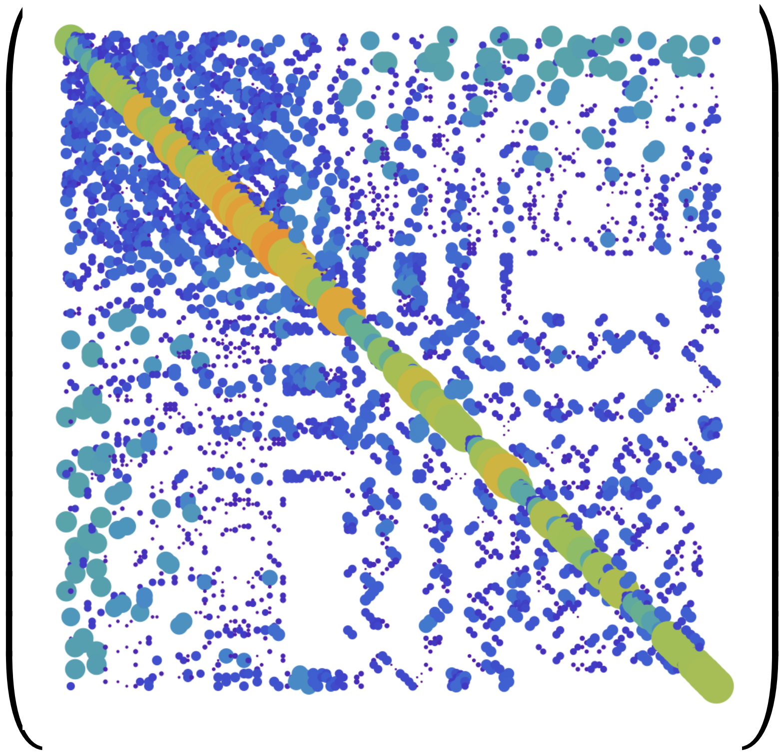
No-Core Shell Model

No-Core Shell Model

Barrett, Vary, Navrátil, Maris, Forseen, Johnson, 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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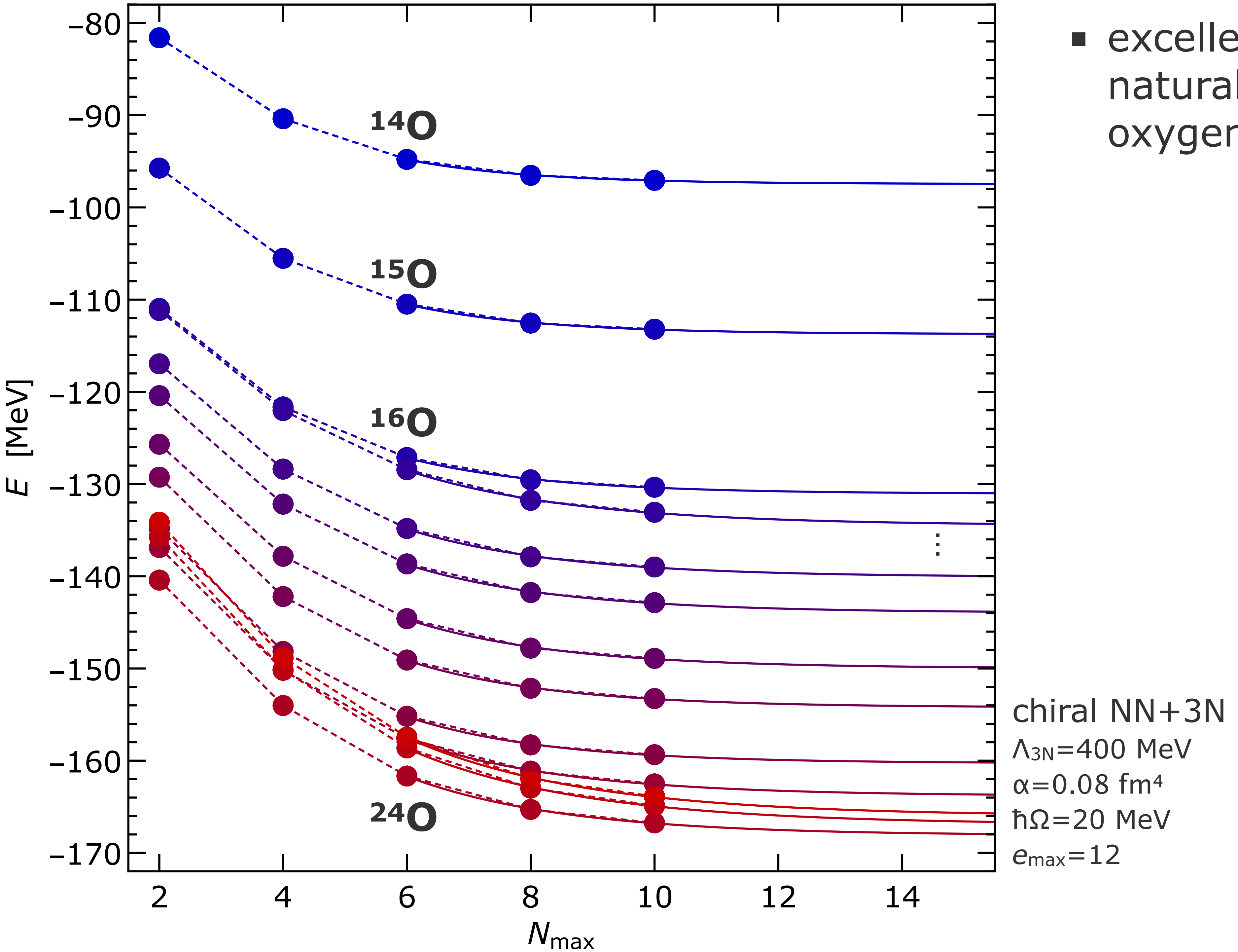
- **idea**: solve eigenvalue problem of Hamiltonian represented in model space of HO Slater determinants truncated w.r.t. HO excitation energy $N_{\text{max}}\hbar\Omega$
  - convergence of observables w.r.t. N_{max} is the only limitation and source of uncertainty
- **importance truncation**: reduce 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
  - single-particle basis: natural orbitals, Coulomb-Sturmian, et al.

Oxygen Isotopes

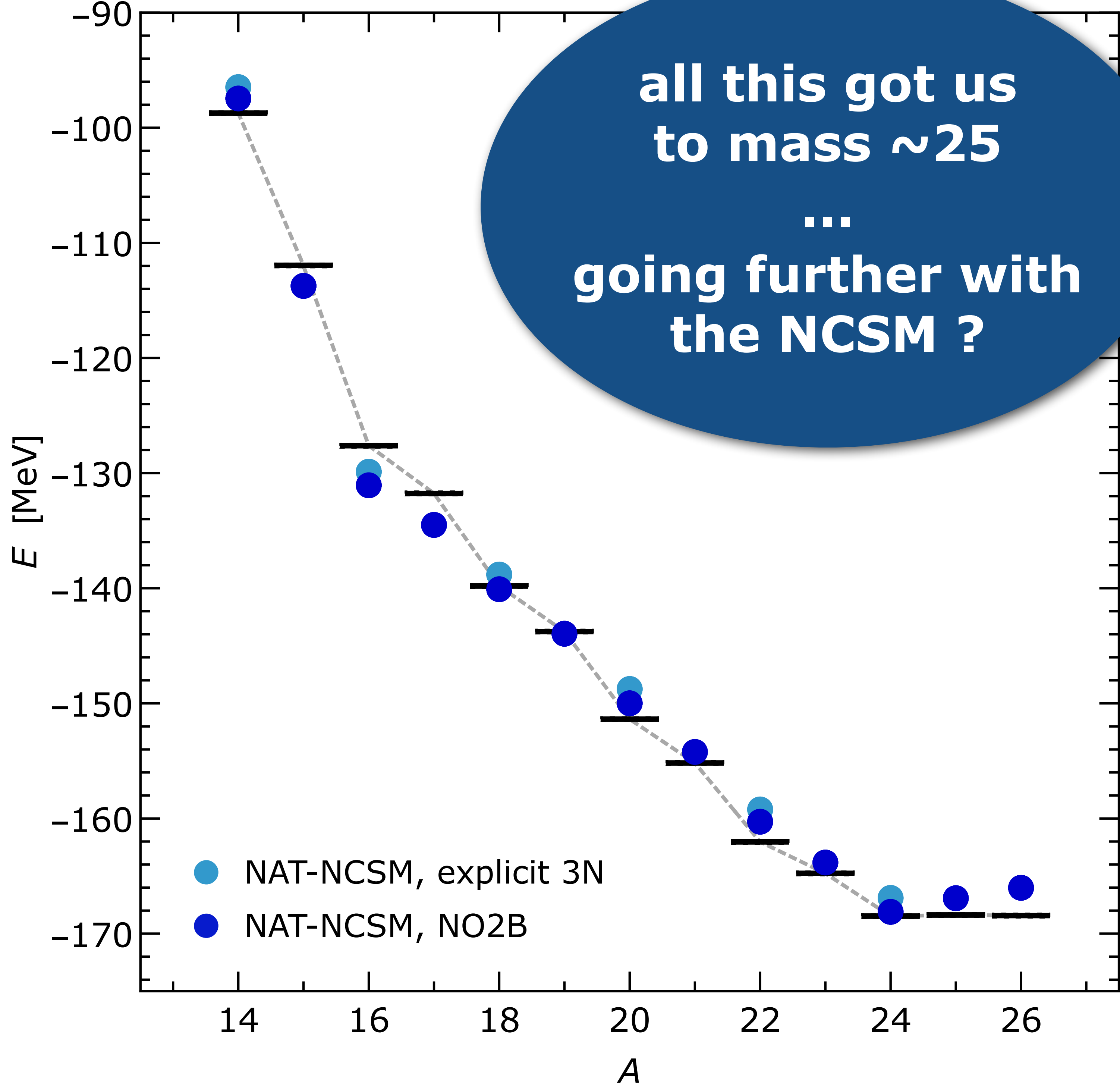
Tichai, Müller, Vobig, Roth; PRC 99, 034321 (2019)



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

Oxygen Isotopes

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



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

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

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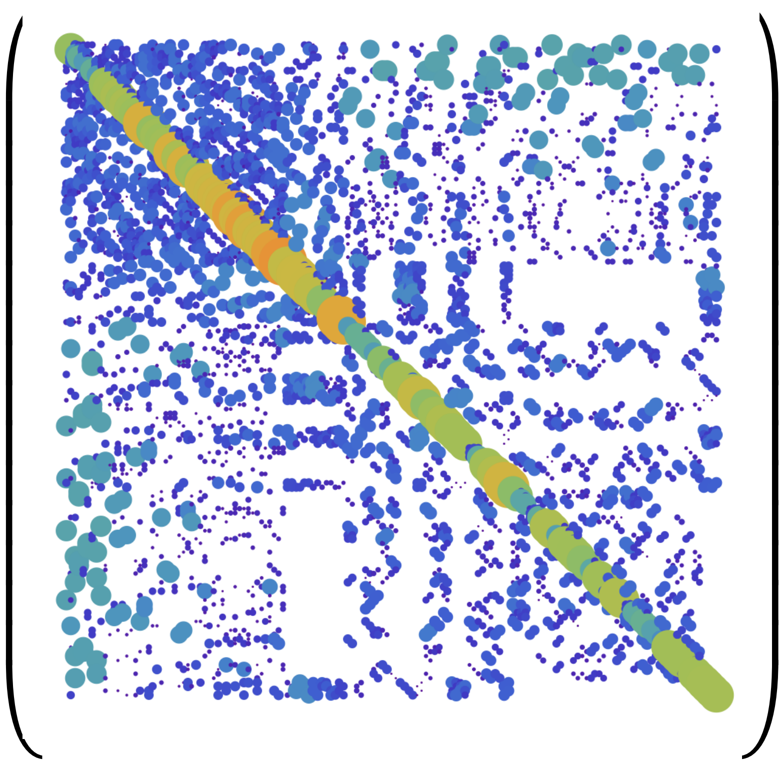

$$\begin{pmatrix} \vdots \\ C_{i'}^{(n)} \\ \vdots \end{pmatrix} = E_n \begin{pmatrix} \vdots \\ C_{i}^{(n)} \\ \vdots \end{pmatrix}$$

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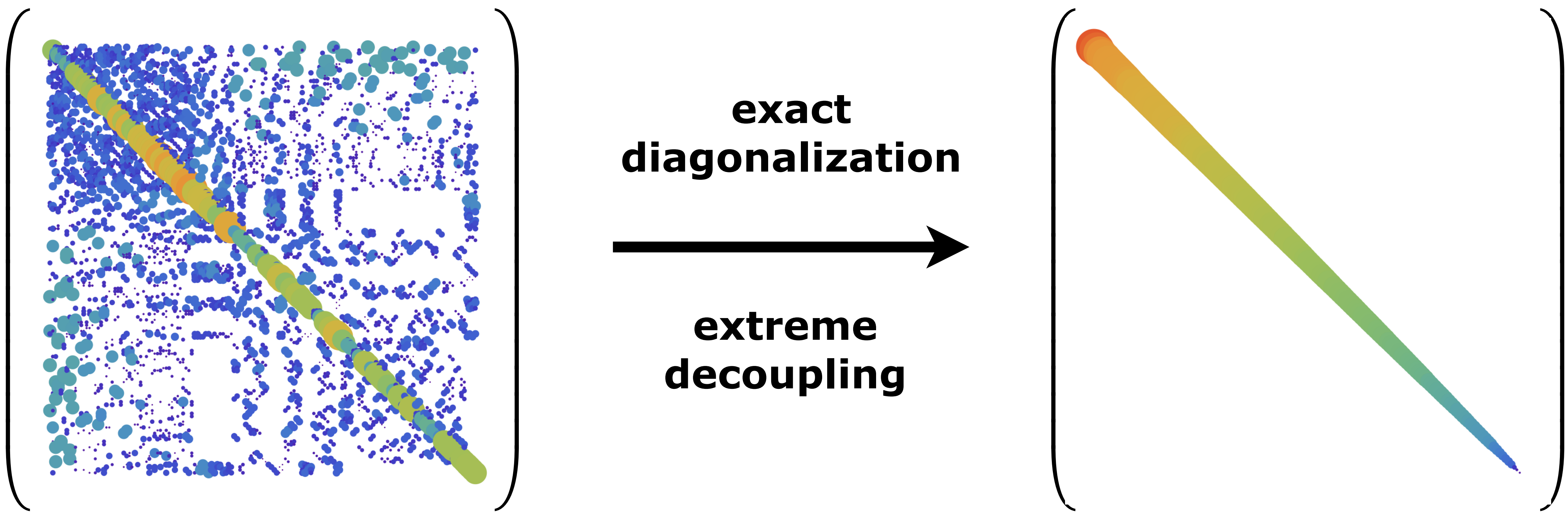
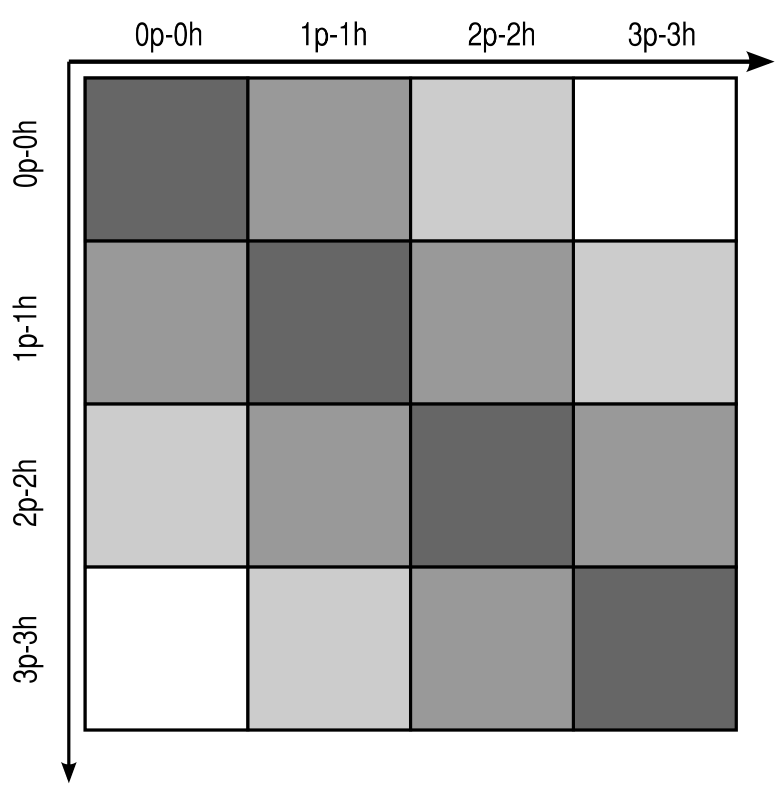


In-Medium SRG

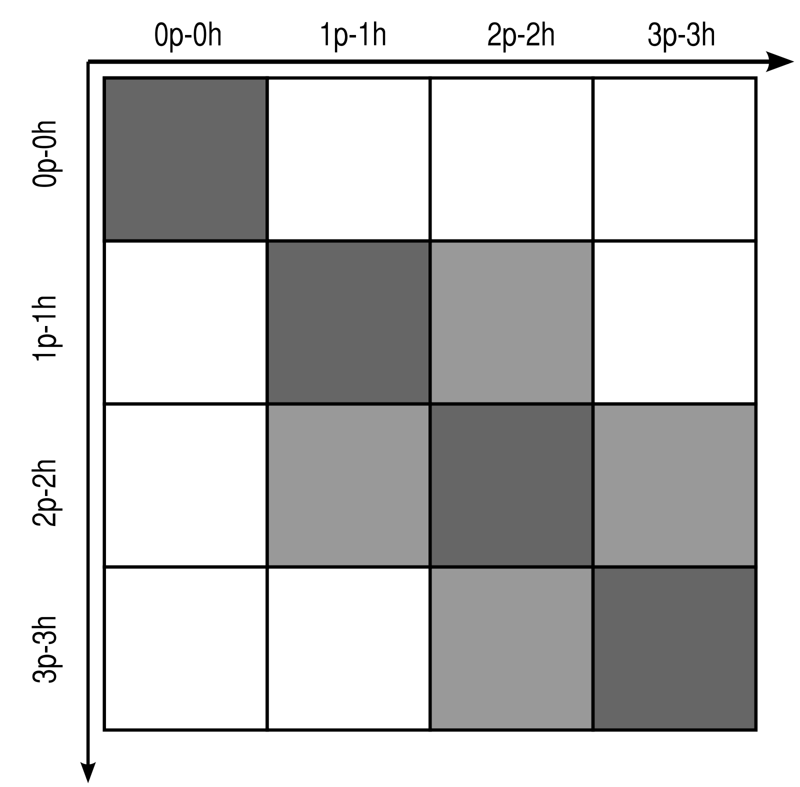
Tsukiyama, Bogner, Schwenk, Hergert,...

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



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

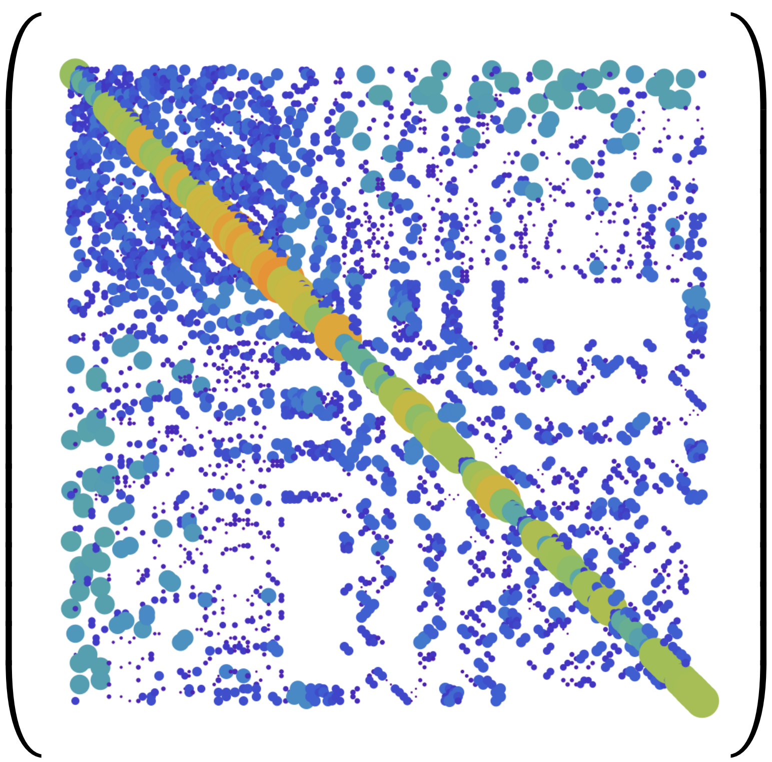


Multi-Reference In-Medium SRG

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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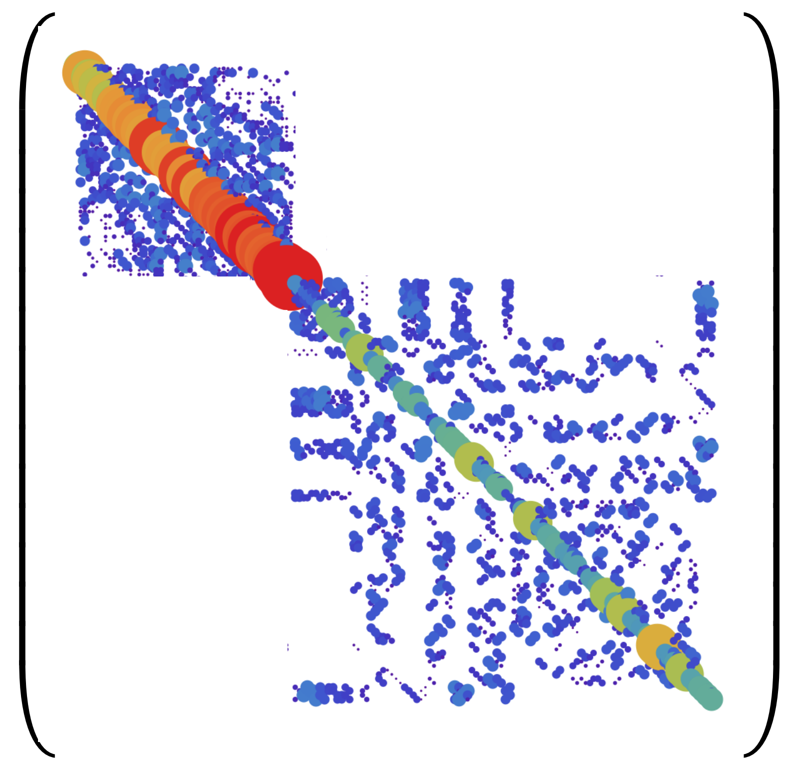
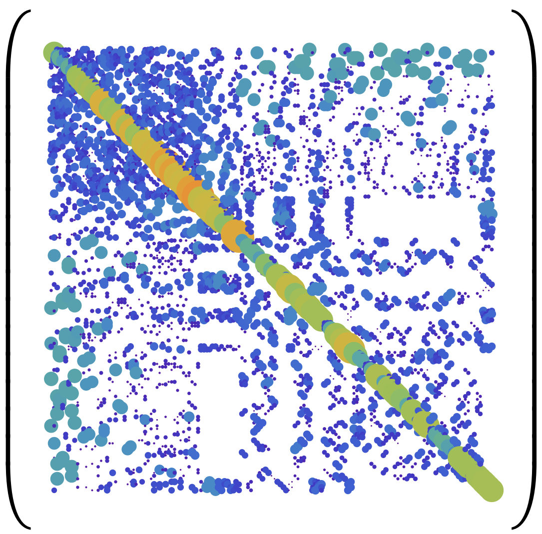
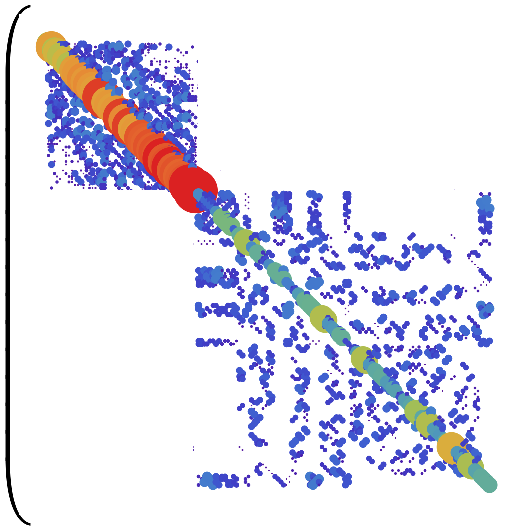


Multi-Reference In-Medium SRG

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

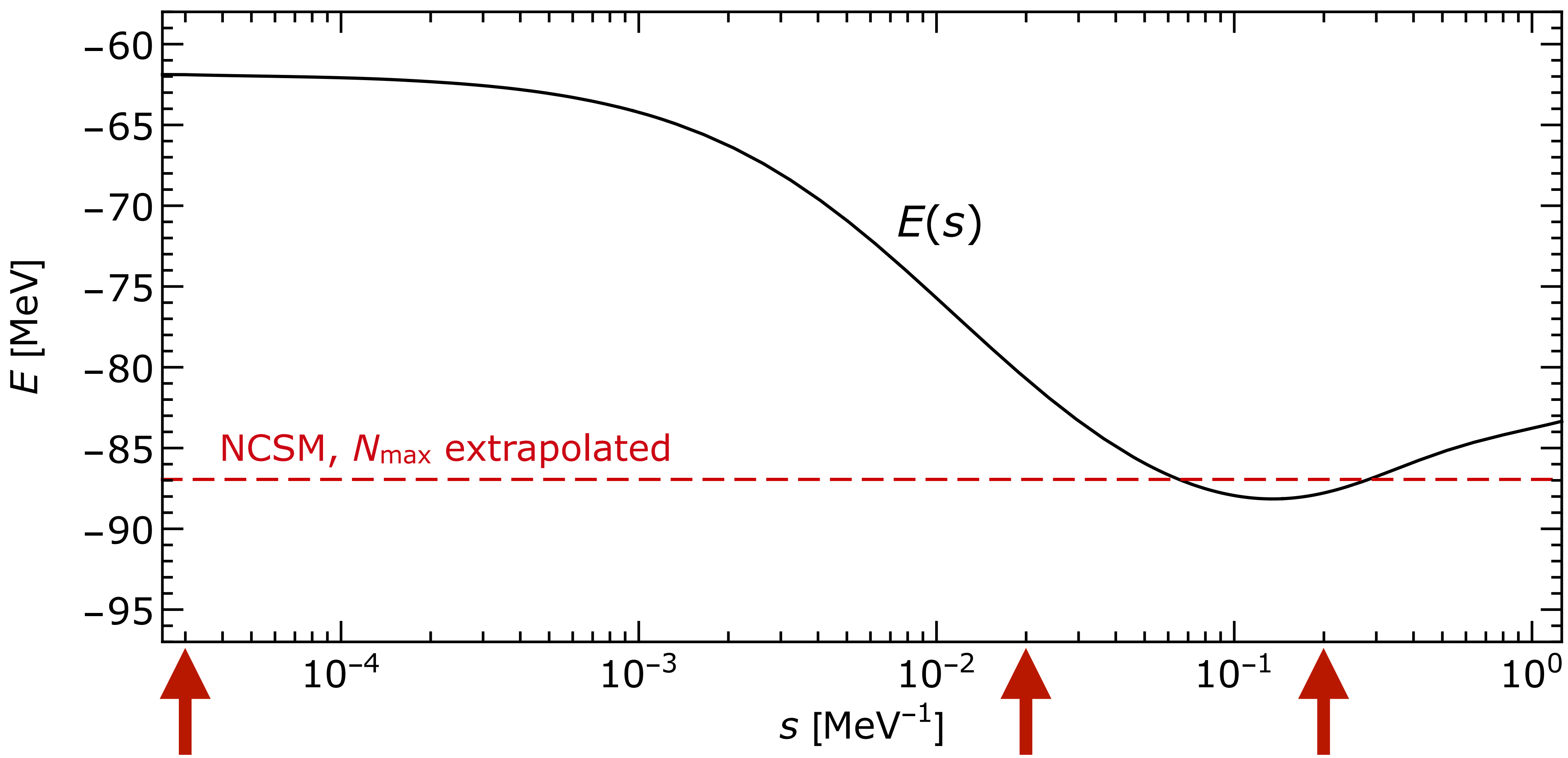
- IM-SRG evolution of multi-reference normal-ordered Hamiltonian and other operators
- decoupling of particle-hole excitations, i.e., pre-diagonalization in many-body space

NCSM
many-body solution

- use in-medium evolved Hamiltonian and operators for 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

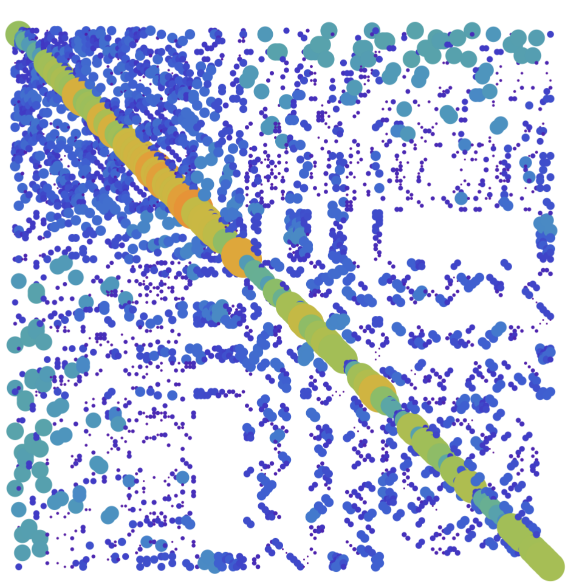
α=0.08 fm^4

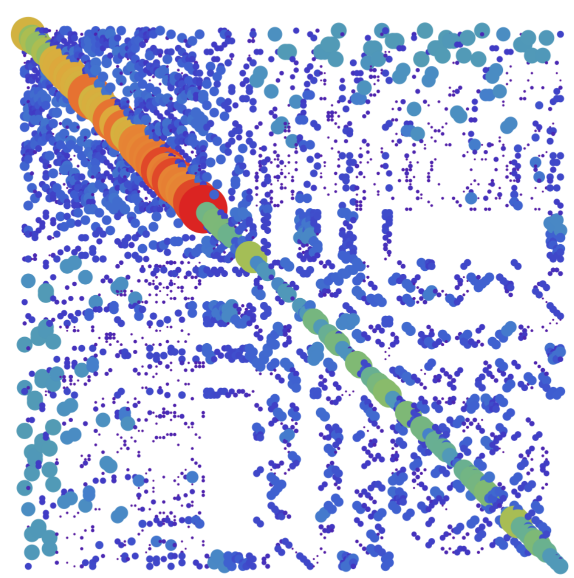
ħΩ=20 MeV

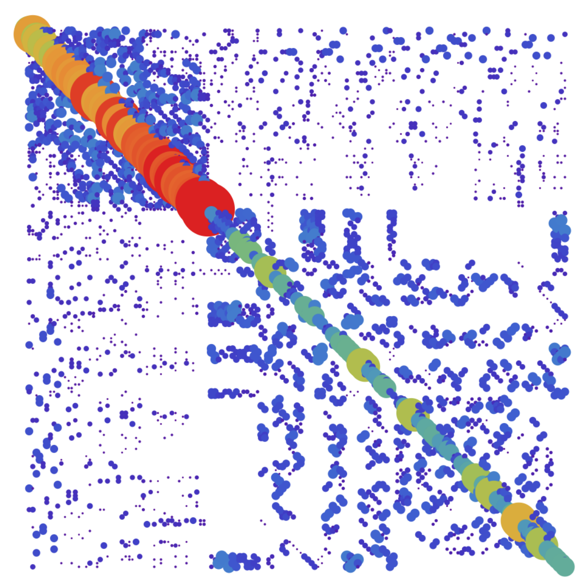
e_{max}=12

N_{max}=0 reference

HF basis



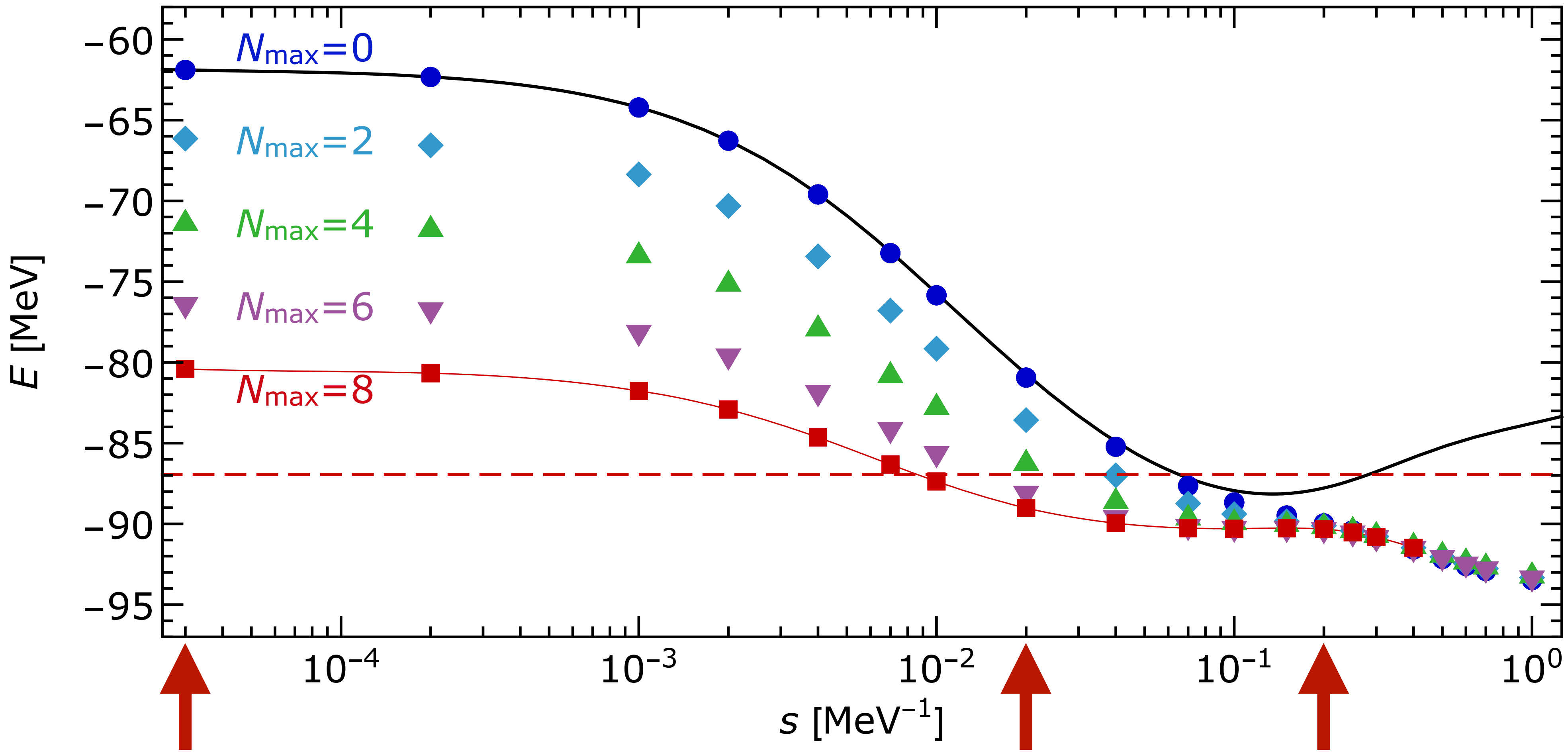




Hamilton matrix in N_{max}=2 space

In-Medium NCSM: Flow Evolution

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



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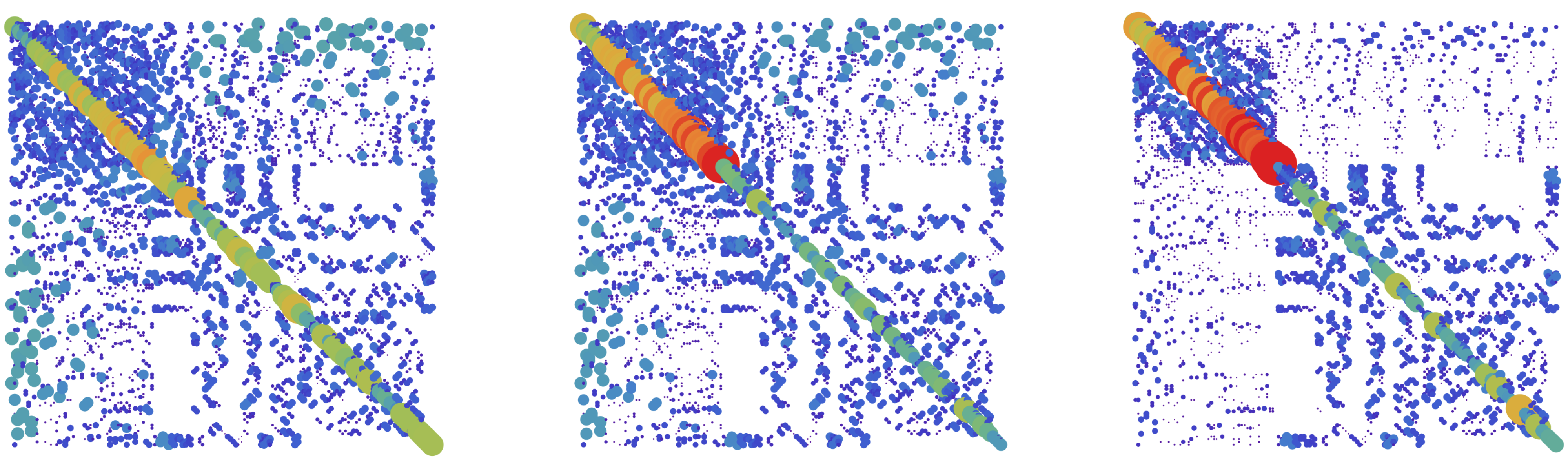

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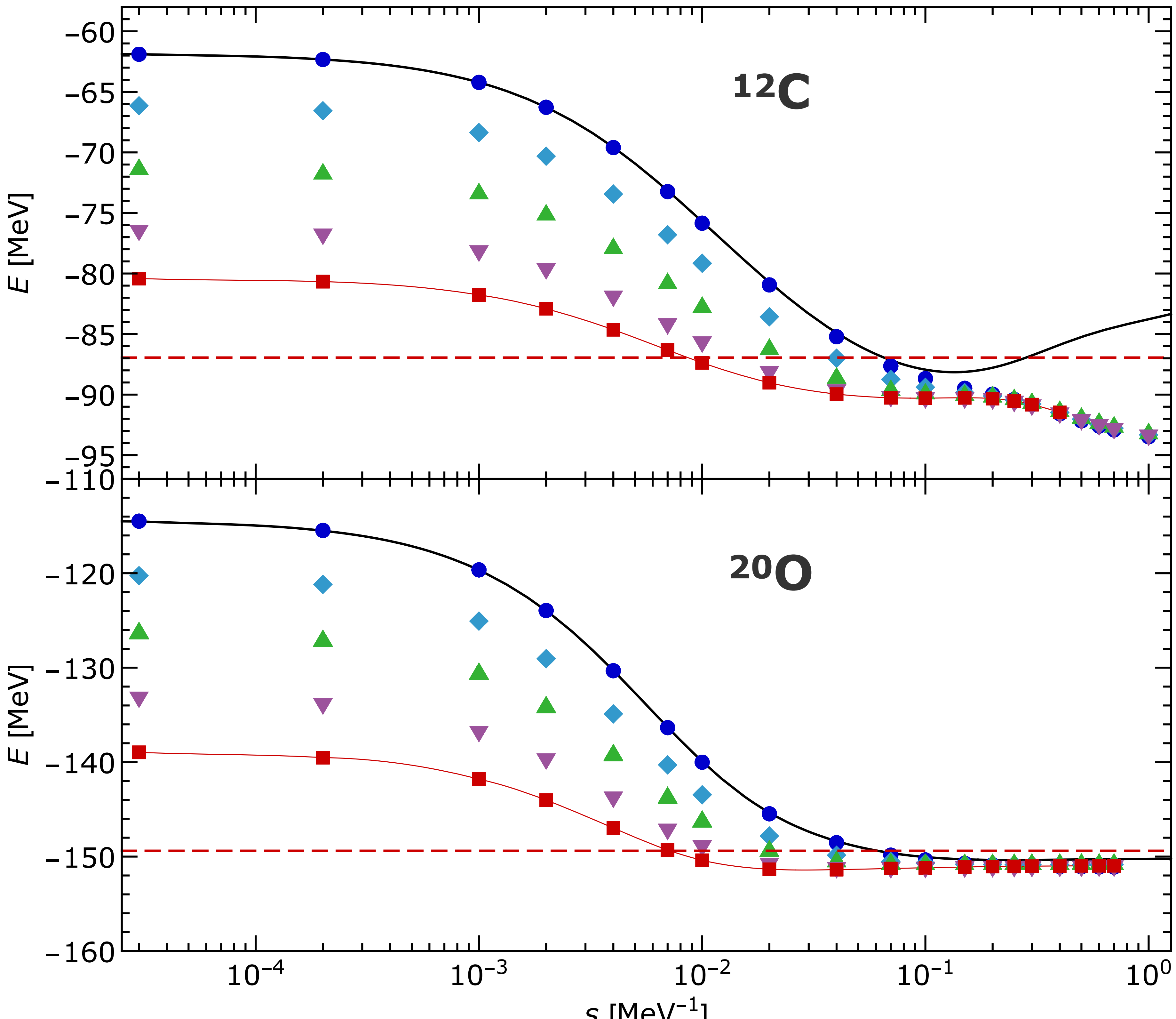


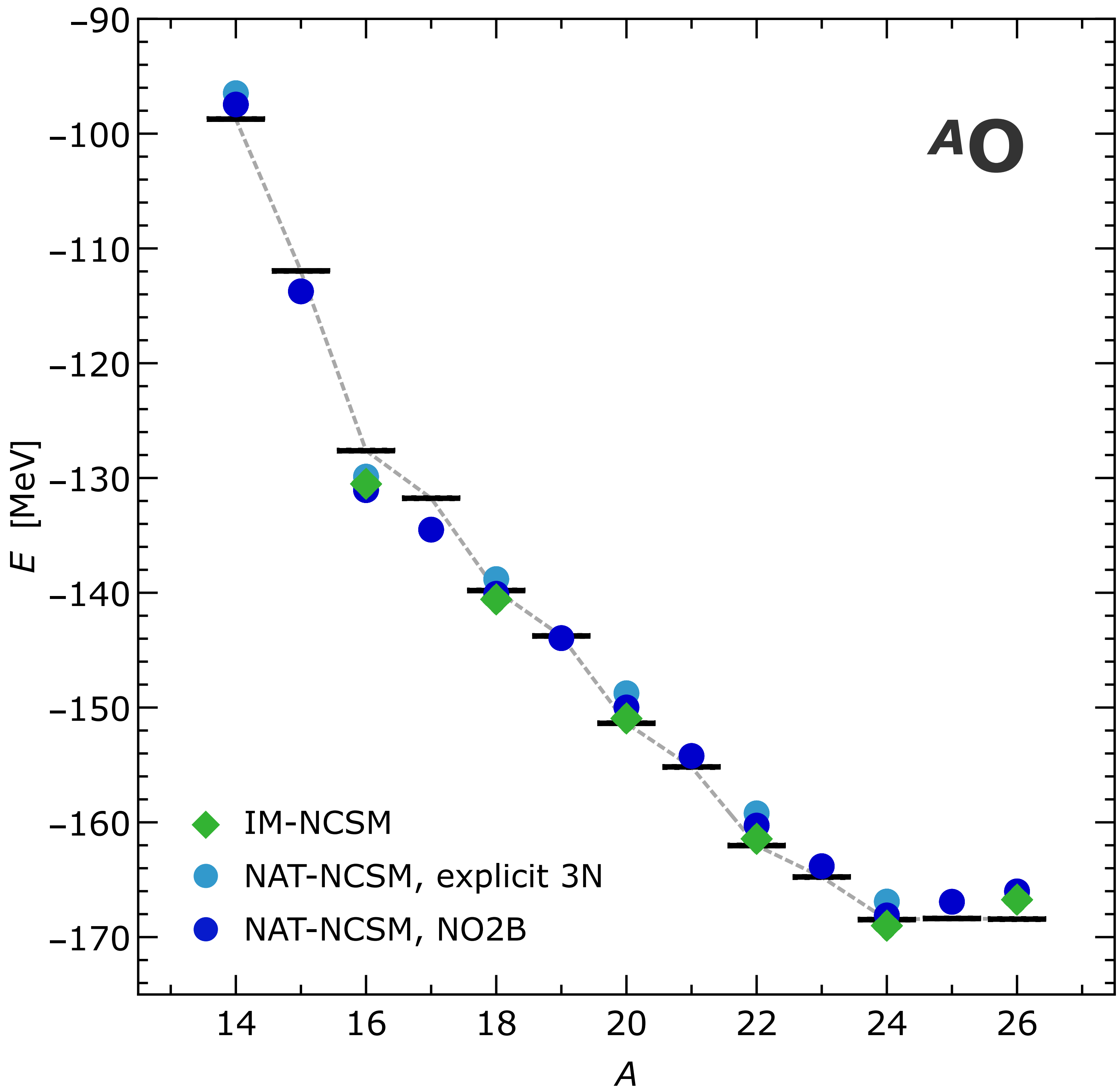
- NCSM convergence is drastically improved
- N_{max}=0 eigenvalues deviated from $E(s)$

chiral NN+3N
Λ_{3N}=400 MeV
α=0.08 fm⁴
ħΩ=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

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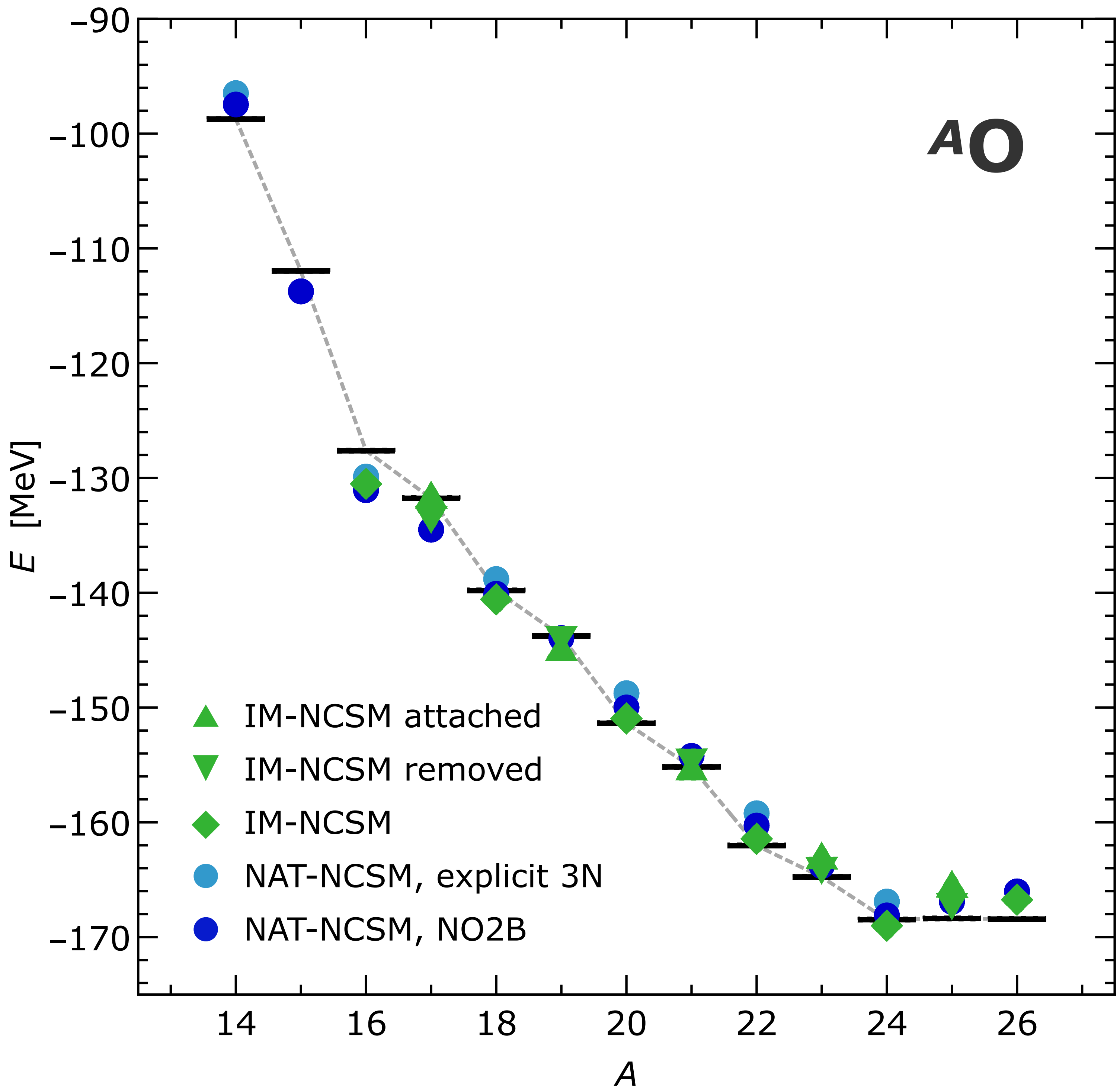
e_{max}=12

HF basis
N_{max}=0 reference

IM-NCSM: Oxygen Isotopes

Vobig, Mongelli, Roth; in prep.



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e_{max}=12

HF basis
N_{max}=0 reference

In-Medium NCSM: Refinements

Mongelli 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)

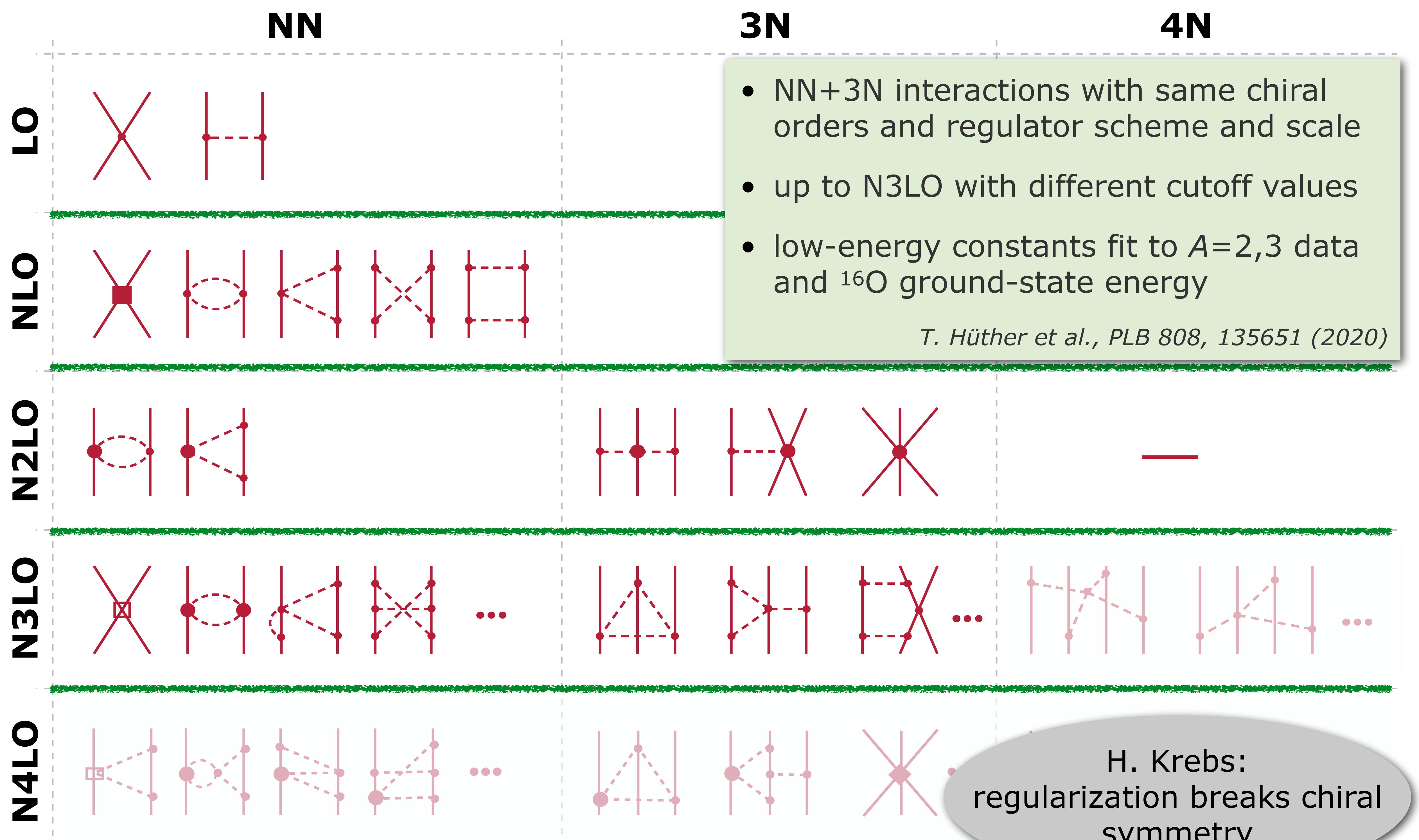
- probe accuracy of NO2B approximation by variation of flow parameter & reference space truncation

- **uncertainty quantification protocol:** perform IM-NCSM calculation for...
  - different reference space truncations: N_{max}^{ref} = 0, 2, 4
  - different flow parameters: s_{sat} , $s_{sat}/2$
  - different model-space truncations: N_{max} = 0, 2, 4, 6,...
  - different single-particle and 3N truncations: e_{max} , E_{3max}

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

Applications with Non-Local NN+3N Interactions

Family of Non-Local NN+3N Interactions



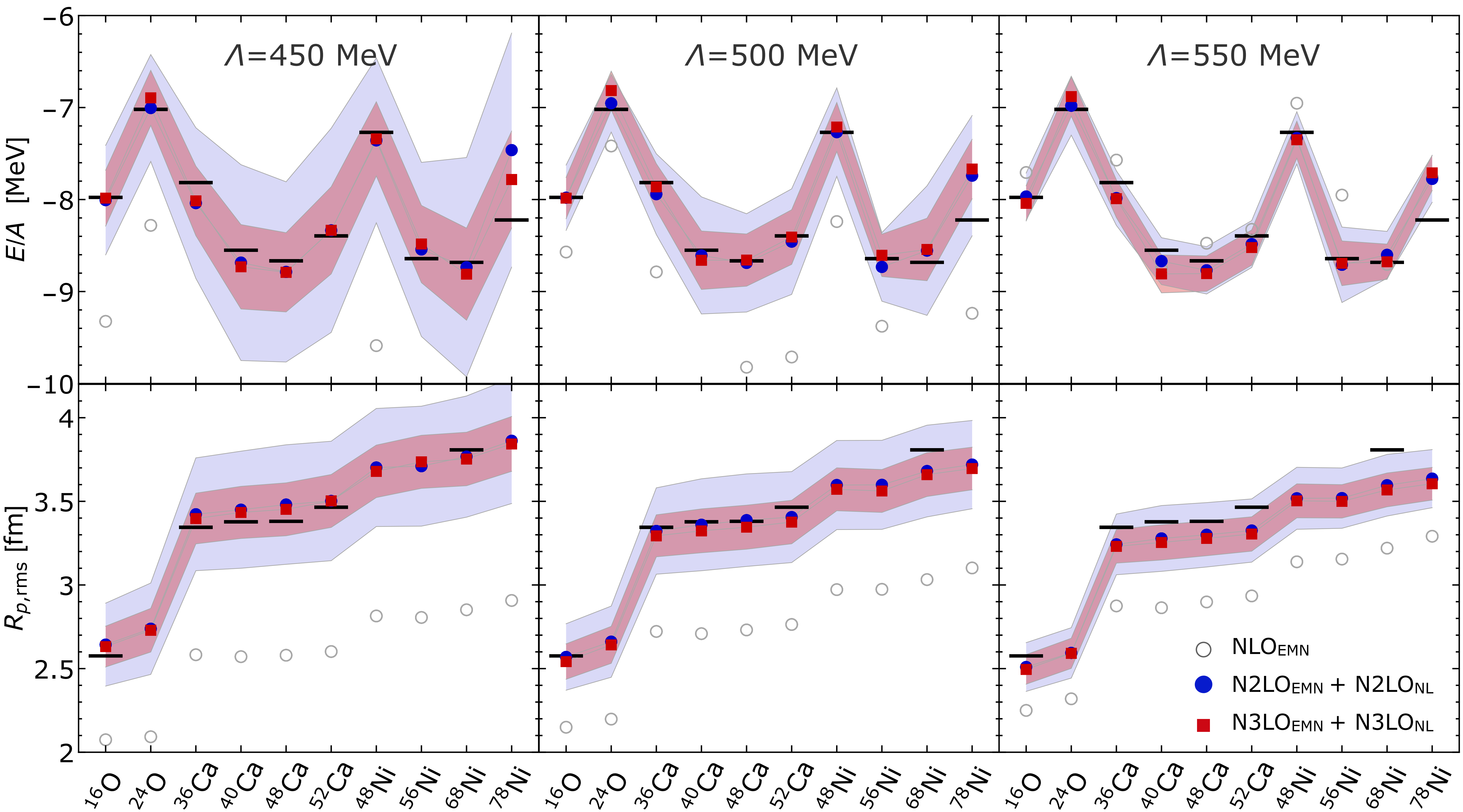
- NN+3N interactions with same chiral orders and regulator scheme and scale
- up to N3LO with different cutoff values
- low-energy constants fit to A=2,3 data and ^{16}O ground-state energy

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

H. Krebs: regularization breaks chiral symmetry

Medium-Mass Nuclei

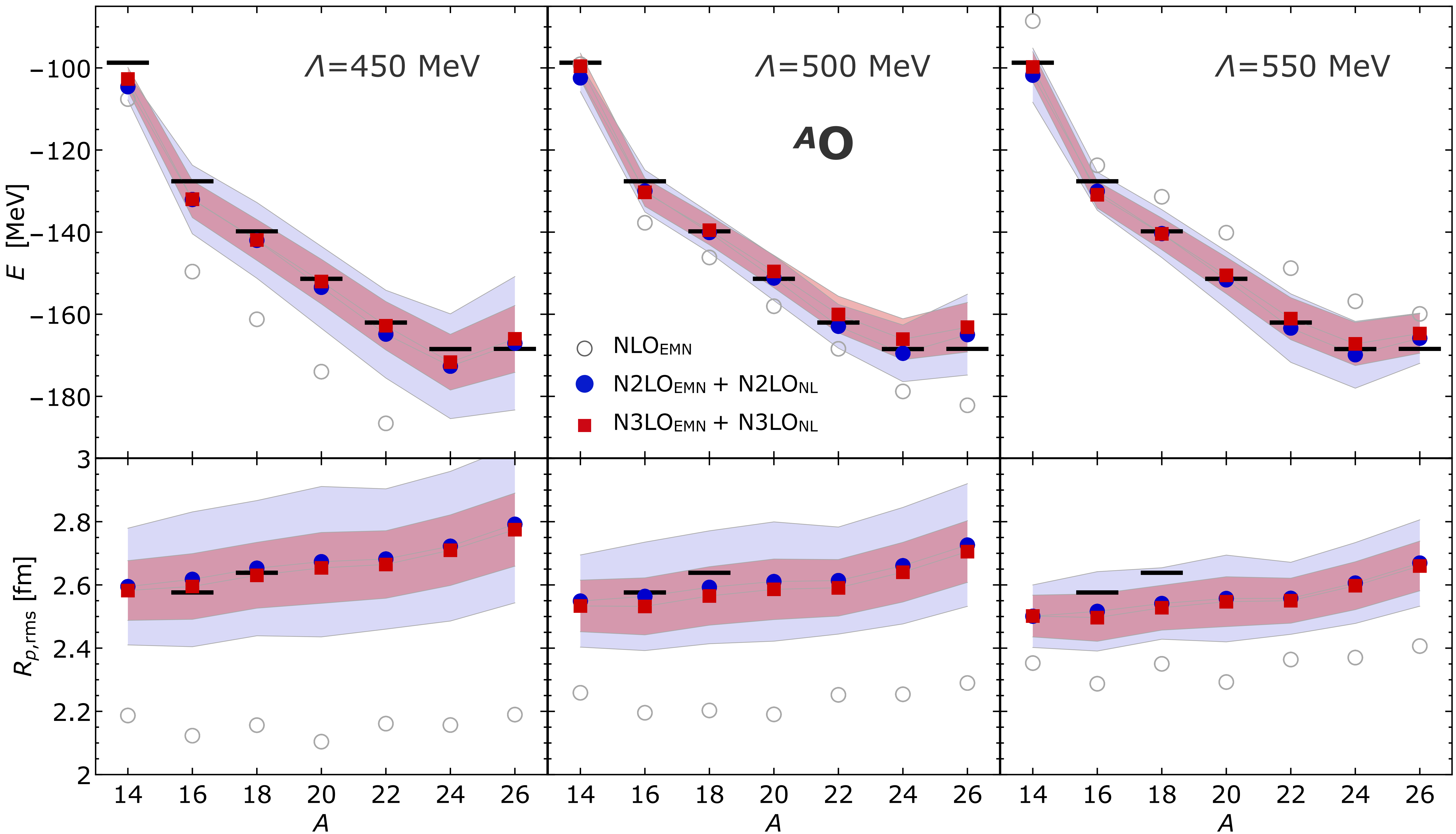
Hüther et al.; PLB 808, 135651 (2020)



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)



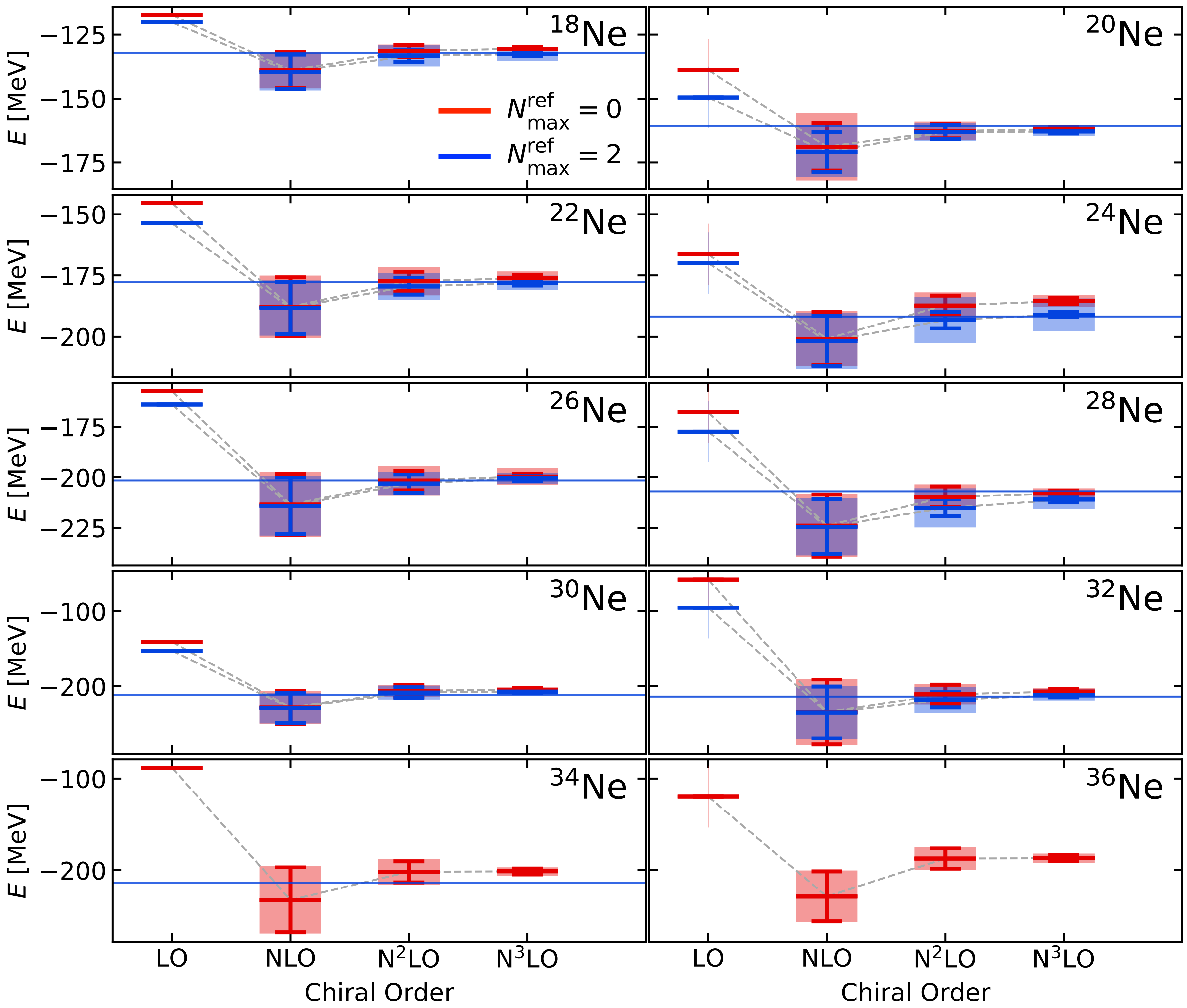
IM-NCSM, natural orbitals, $\hbar\Omega$=20 MeV, α=0.04 fm^4, e_{max}=12, E_{3max}=14, N_{ref}=2

error bands show interaction + many-body uncertainties

Applications: Neon Isotopes

Ground-State Energies

Frosini et al., EPJ A 58, 63 (2022), Mongelli et al., in preparation



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

Λ = 500 MeV
α = 0.04 fm⁴
ħΩ = 20 MeV
e_{max} = 12
NAT basis

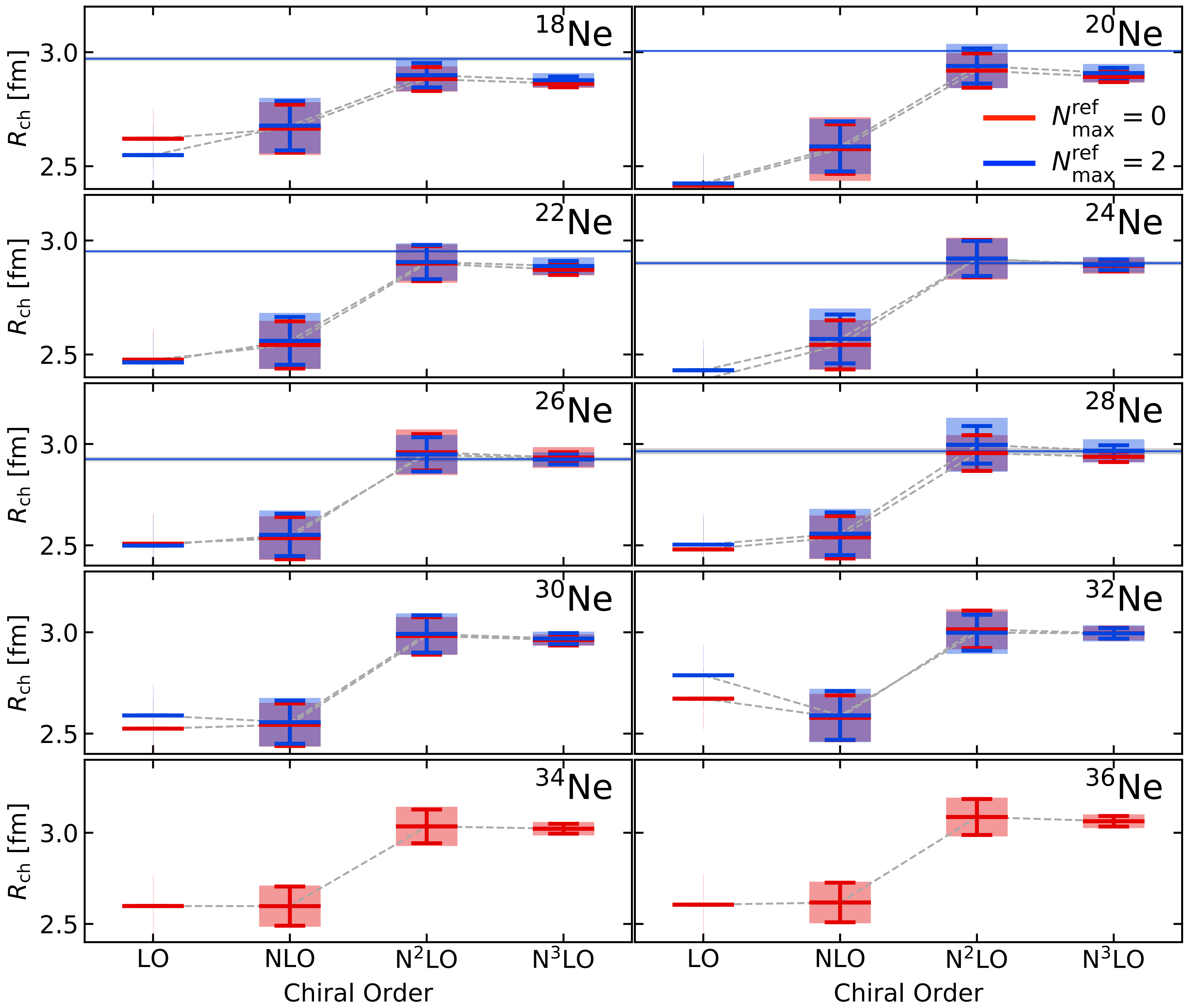
$N^{ref}_{max} = 0, 2$
$N_{max} = 4$

error bars:
68% interaction uncertainties

error bands:
interaction + many-body uncertainties

Charge Radii

Frosini et al., EPJ A 58, 63 (2022), Mongelli et al., in preparation



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

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

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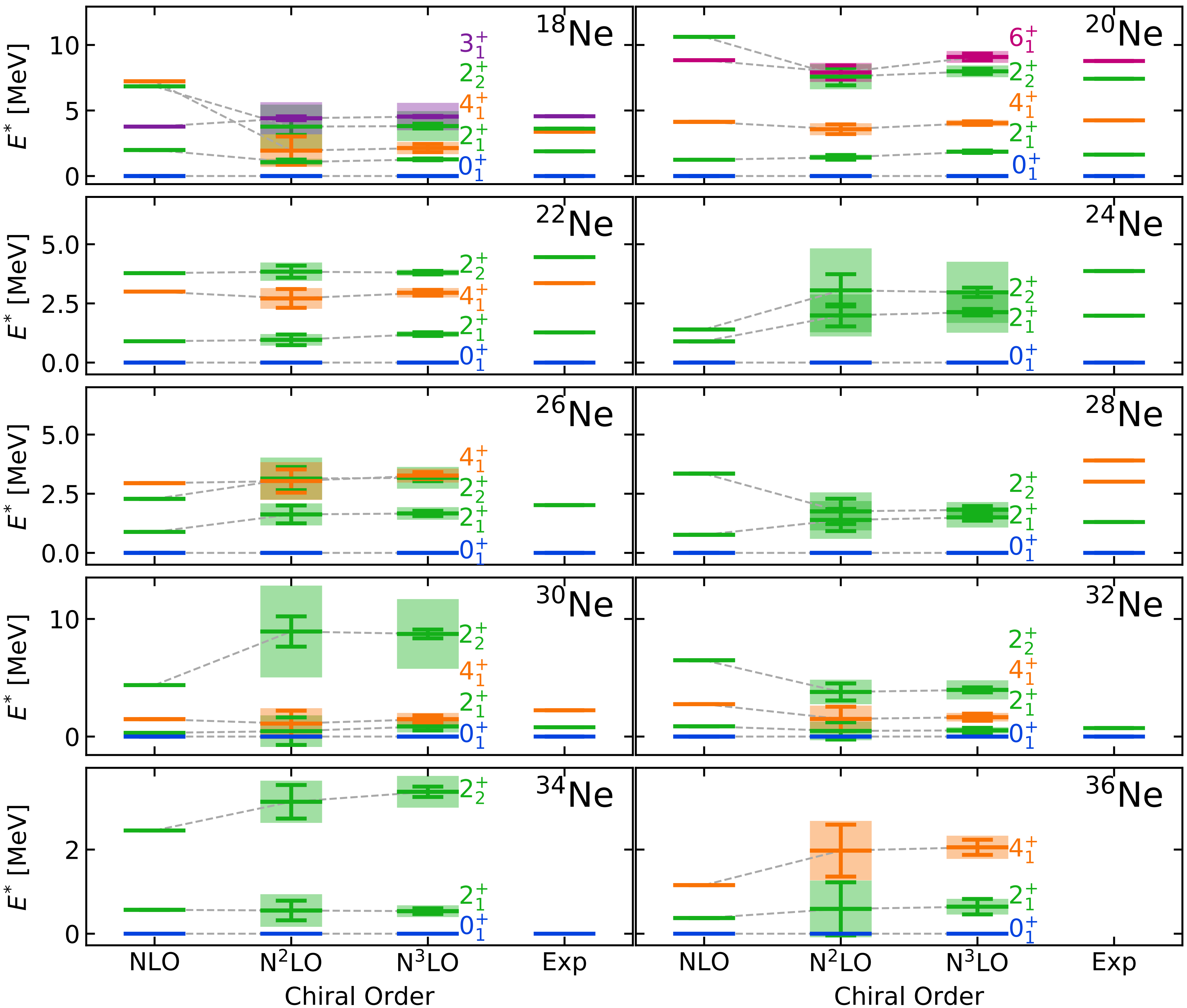
Excitation Energies

Frosini et al., EPJ A 58, 63 (2022), Mongelli et al., in preparation



- excellent description of excitation spectra

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

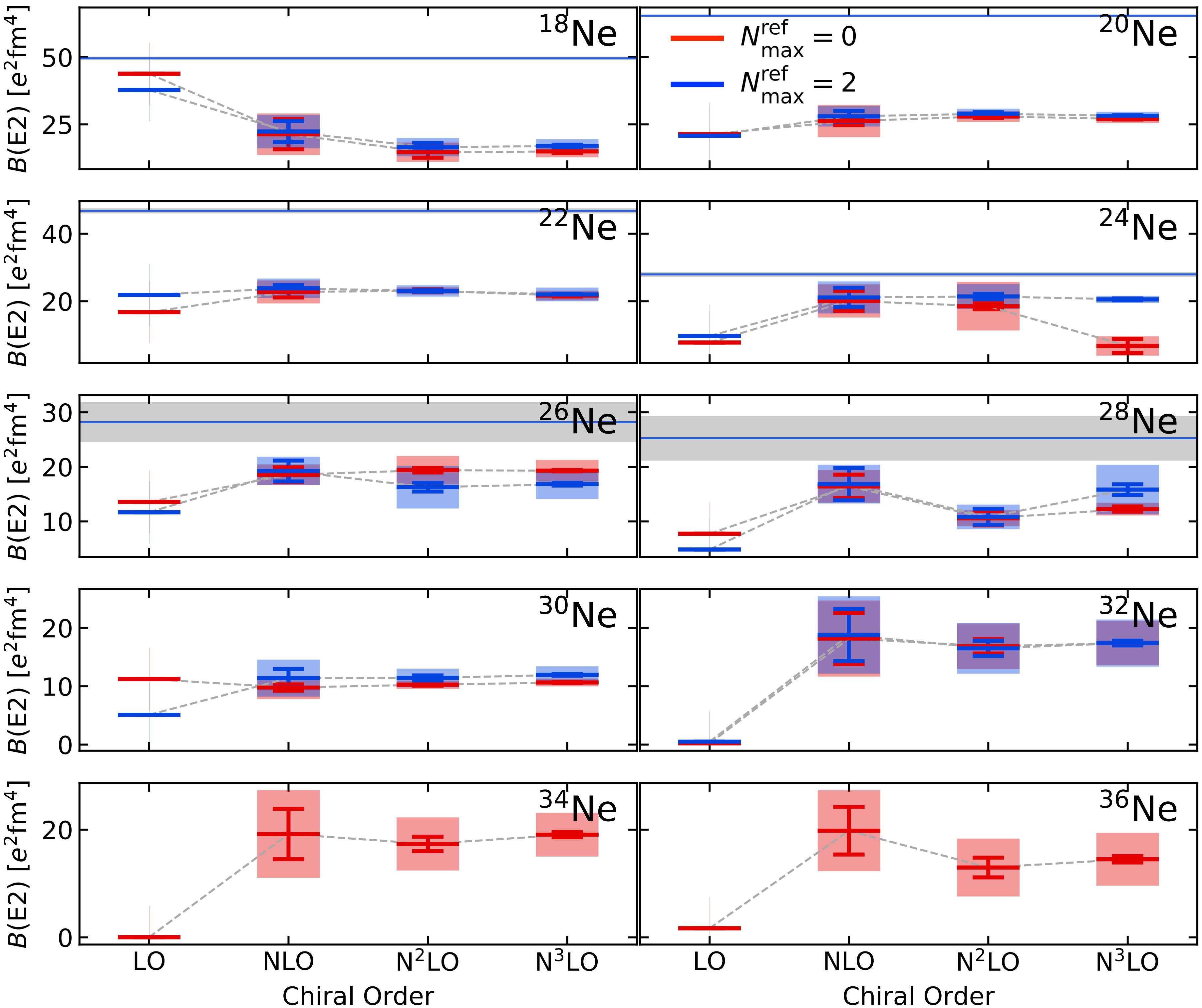
$N_{max}^{ref} = 2$
$N_{max} = 4$

error bars:
68% interaction uncertainties

error bands:
interaction + many-body uncertainties

B(E2, 2⁺ → 0⁺) Transition Strength

Frosini et al., EPJ A 58, 63 (2022), Mongelli et al., in preparation



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

similar problem in valence-space IM-SRG:
Stroberg et al., PRC 105, 034333 (2022)

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

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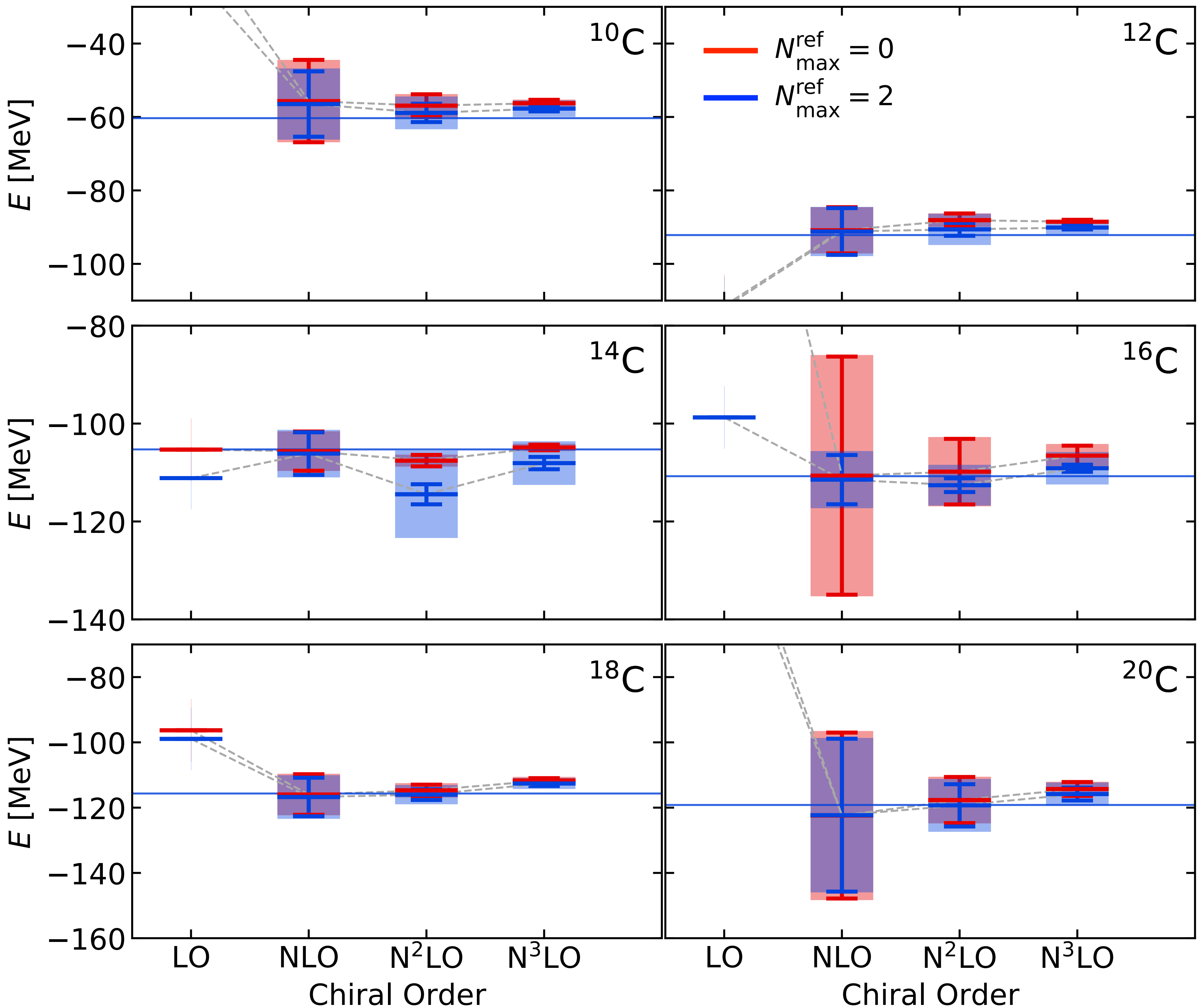
Back to Carbon Isotopes

Ground-State Energies

Mongelli et al., in preparation



- 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

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$N_{max} = 4$

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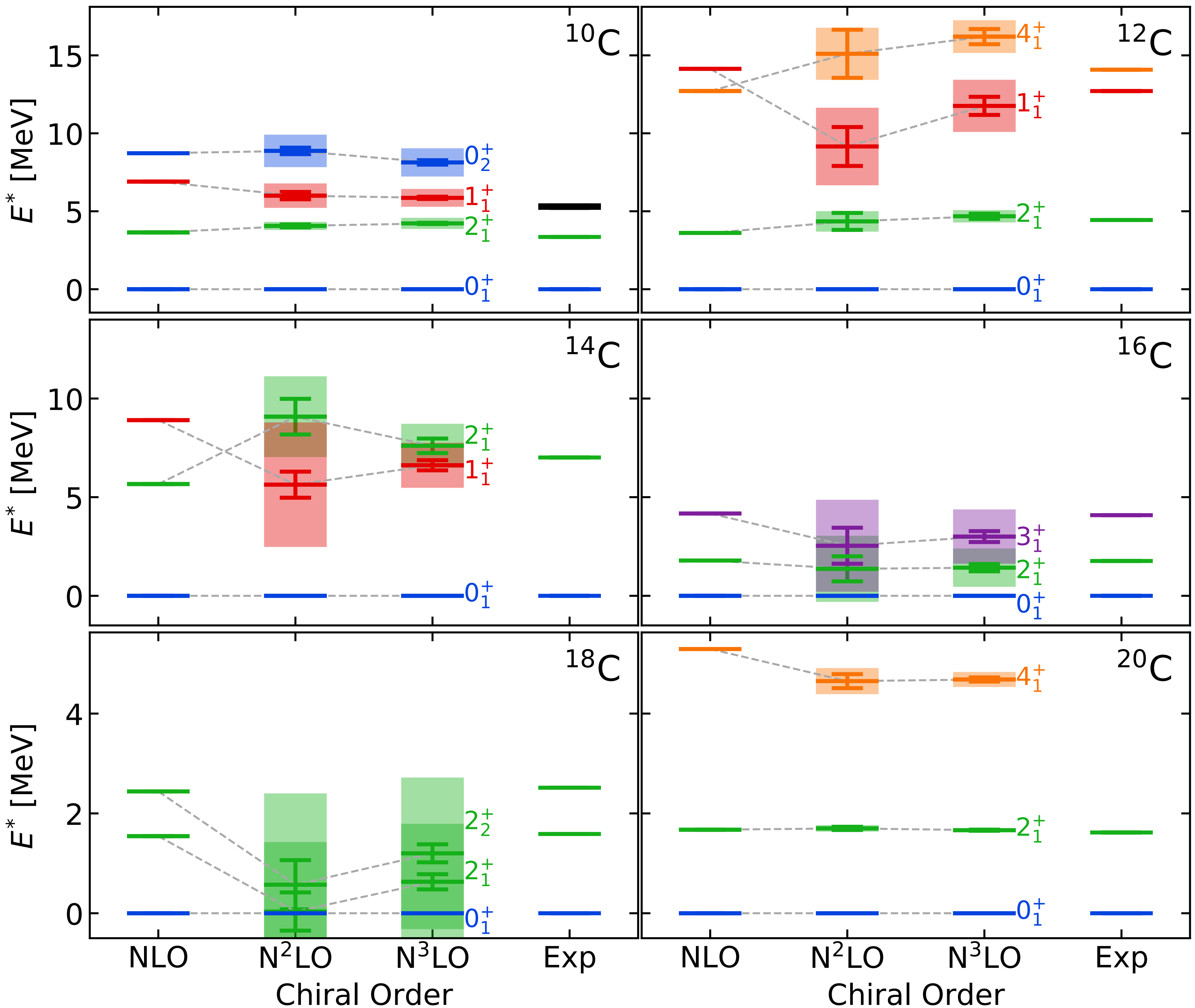
Excitation Spectra

Mongelli et al., in preparation



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

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

$N^{ref}_{max} = 2$
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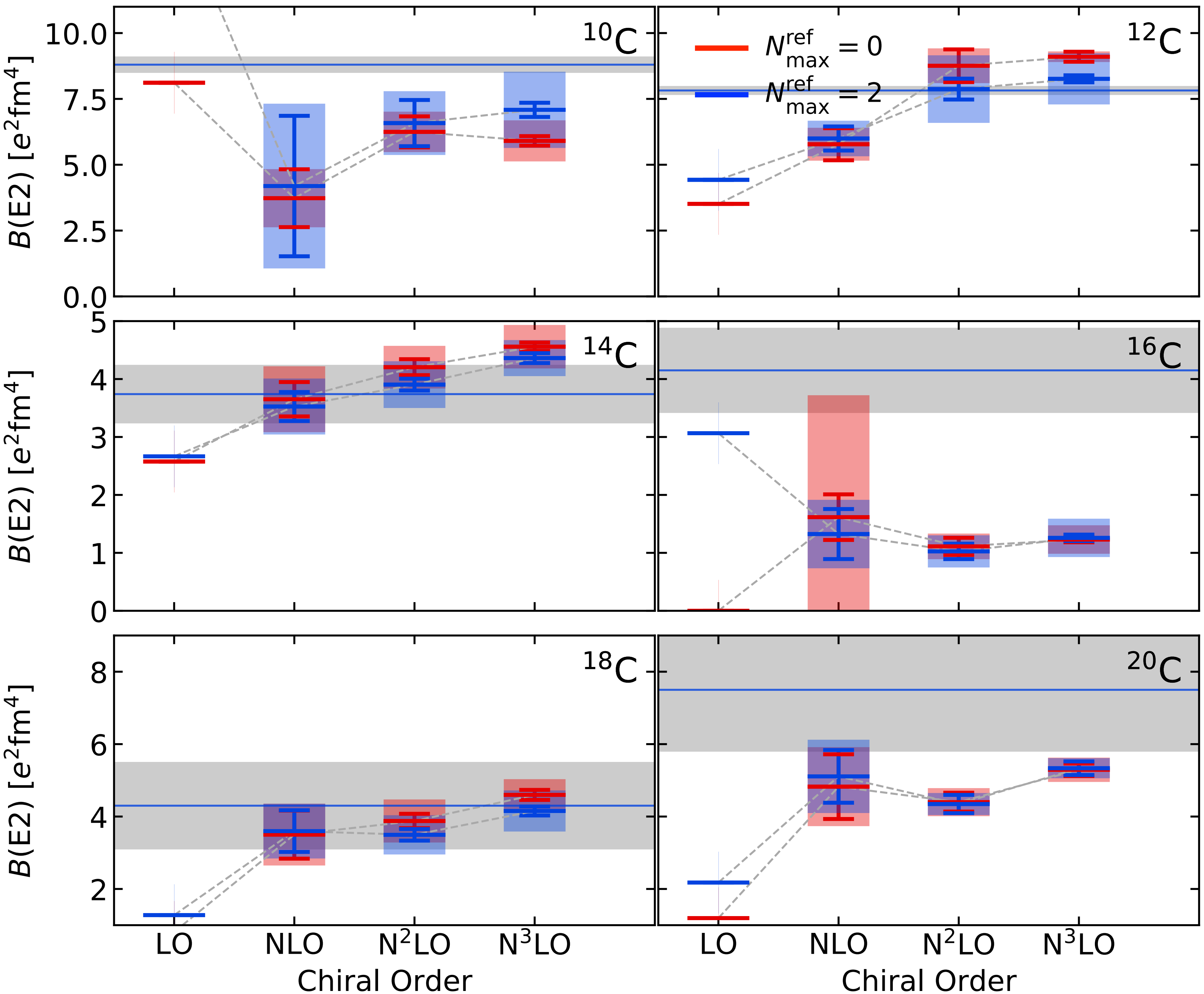
error bars:
68% interaction uncertainties

error bands:
interaction + many-body uncertainties

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

Mongelli et al., in preparation



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

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

$N^{ref}_{max} = 0, 2$
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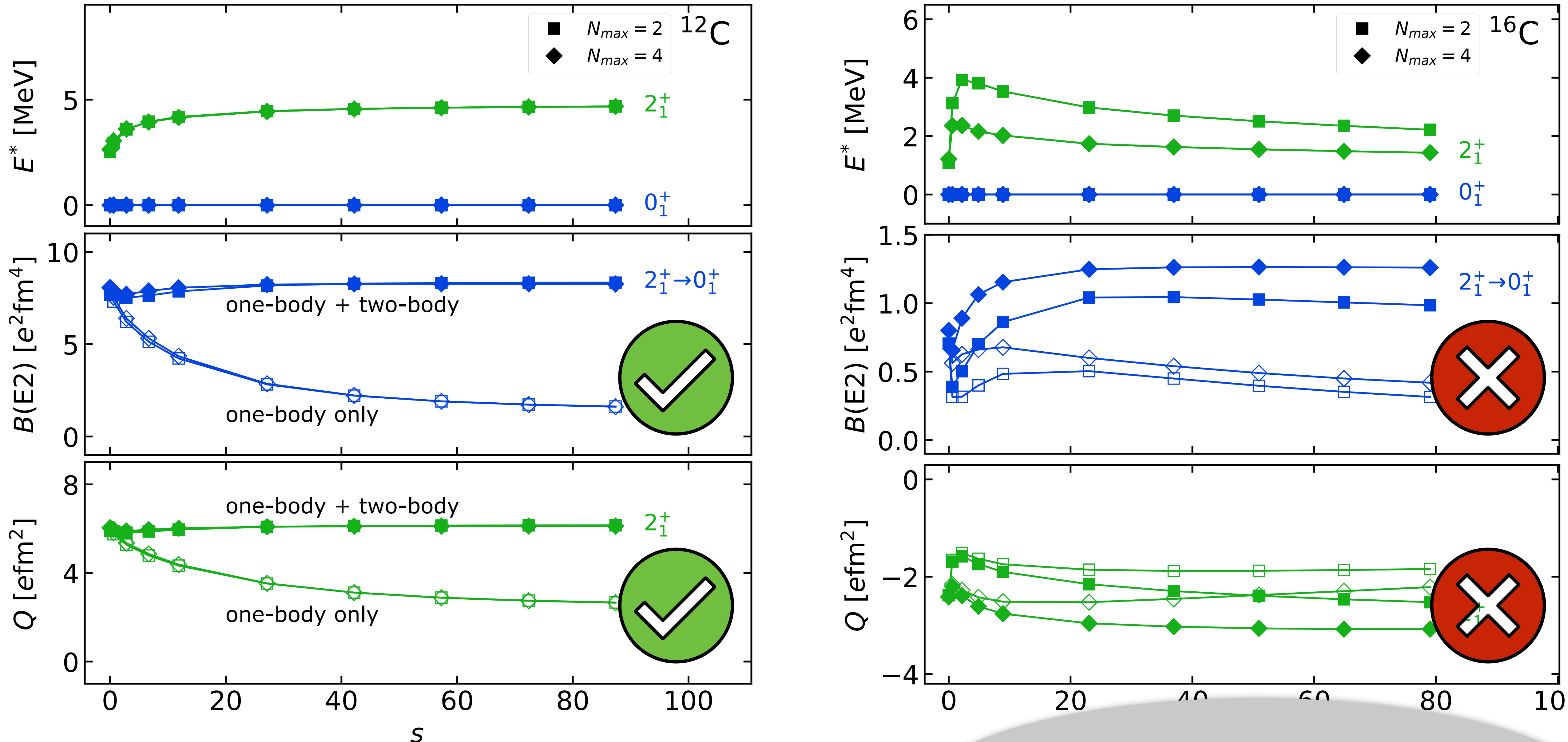
error bands:
interaction + many-body uncertainties

Hierarchy Inversion

Mongelli et al., in preparation



R. Stroberg & H. Hergert: "IM-SRG truncation error depends on reference"

- IM-SRG evolution of E2 operator generates ... contribution... what about three-body and be...
- 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/complete 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

- **thanks to my group and my collaborators**
  - P. Falk, K. Katzenmeier, M. Knöll, P. Lehnung, L. Mertes, T. Mongelli, J. Müller, L. Wagner, C. Wenz, T. Wolfgruber & K. Hebeler, A. Tichai
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  - T. Duguet & friends
    CEA Saclay
  - P. Navrátil
    TRIUMF, Vancouver
  - H. Hergert
    NSCL / Michigan State University
  - J. Vary, P. Maris
    Iowa State University
  - E. Epelbaum, H. Krebs & the LENPIC Collaboration
    Universität Bochum, ...

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Exzellente Forschung für Hessens Zukunft

HELMHOLTZ GEMEINSCHAFT

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