Hybrid Ab Initio Methods

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Ab Initio Methods

No-Core Shell Model

- solution of matrix eigenvalue problem in truncated many-body model space
- **flexibility:** all nuclei and all bound-state observables on the same footing
- **but:** limited by model-space convergence

In-Medium Similarity Renormalization Group

- decoupling ground-state from excitations through unitary transformation via flow equation
- **efficiency:** favorable scaling gives access to medium-mass nuclei
- **but:** limited to ground-state observables

Many-Body Perturbation Theory

- power-series expansion of energies and states
- **simplicity:** low-order contributions can be evaluated very easily and efficiently
- **but:** order-by-order convergence problematic

CC, SCGF, QMC, ...

Hybrid Ab Initio Methods

No-Core Shell Model

In-Medium Similarity Renormalization Group

Many-Body Perturbation Theory

CC, SCGF, QMC, ...

- complementarity of advantages and limitations of the different methods
- combine methods to overcome limitations
- expand reach in terms of observables, particle number or model-space size
- established example: CC-EOM
- target: spectroscopy of fully open-shell medium-mass nuclei

Hybrid Ab Initio Methods

IM-NCSM

No-Core Shell Model

In-Medium Similarity Renormalization Group

No-Core Shell Model

NCSM-PT

No-Core Shell Model

Many-Body Perturbation Theory

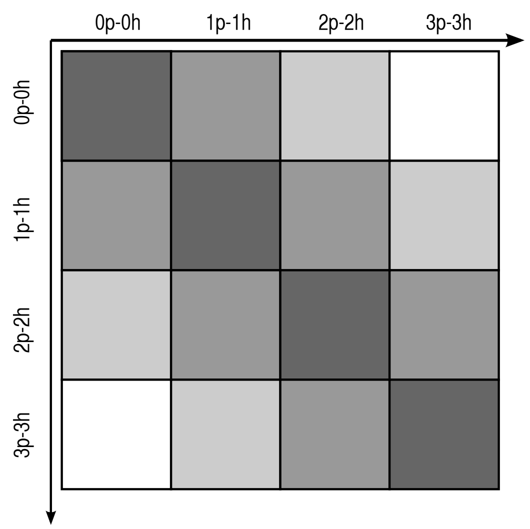
IM-NCSM:
Merging NCSM and IM-SRG

with E. Gebrerufael, K. Vobig, H. Hergert

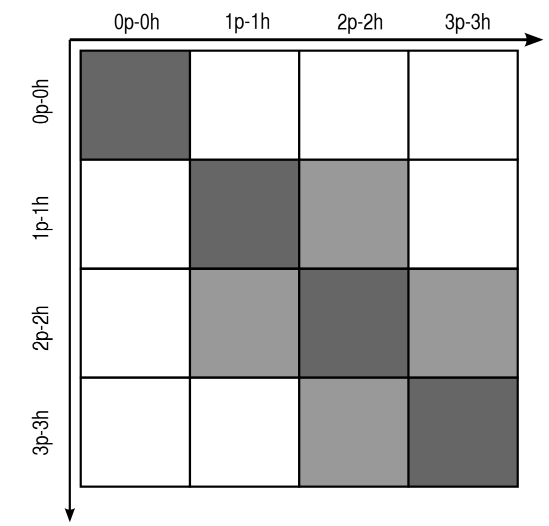
see poster by K. Vobig

In-Medium SRG

Tsukiyama, Bogner, Schwenk, Hergert,...



use SRG flow equations for normal-ordered Hamiltonian to decouple many-body reference state from excitations



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

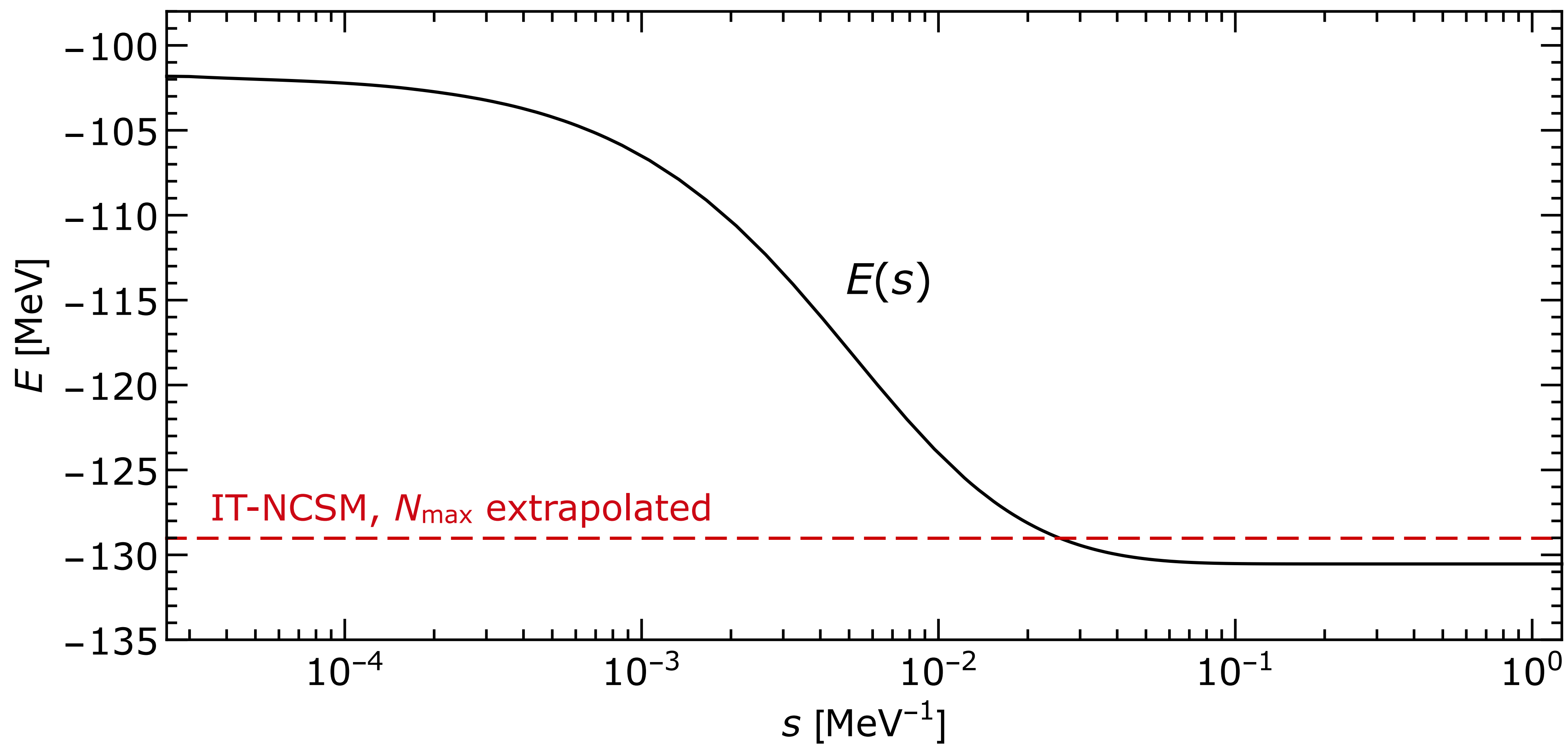
- Hamiltonian and generator in normal order with respect to single or multi-determinant reference state, omit residual three-body piece

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

- 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 SRG: Single Reference



^{16}O

chiral NN+3N

Λ_{3N}=400 MeV

α=0.08 fm^4

$\hbar\Omega$=20 MeV

e_{max}=12

N_{max}=0 reference

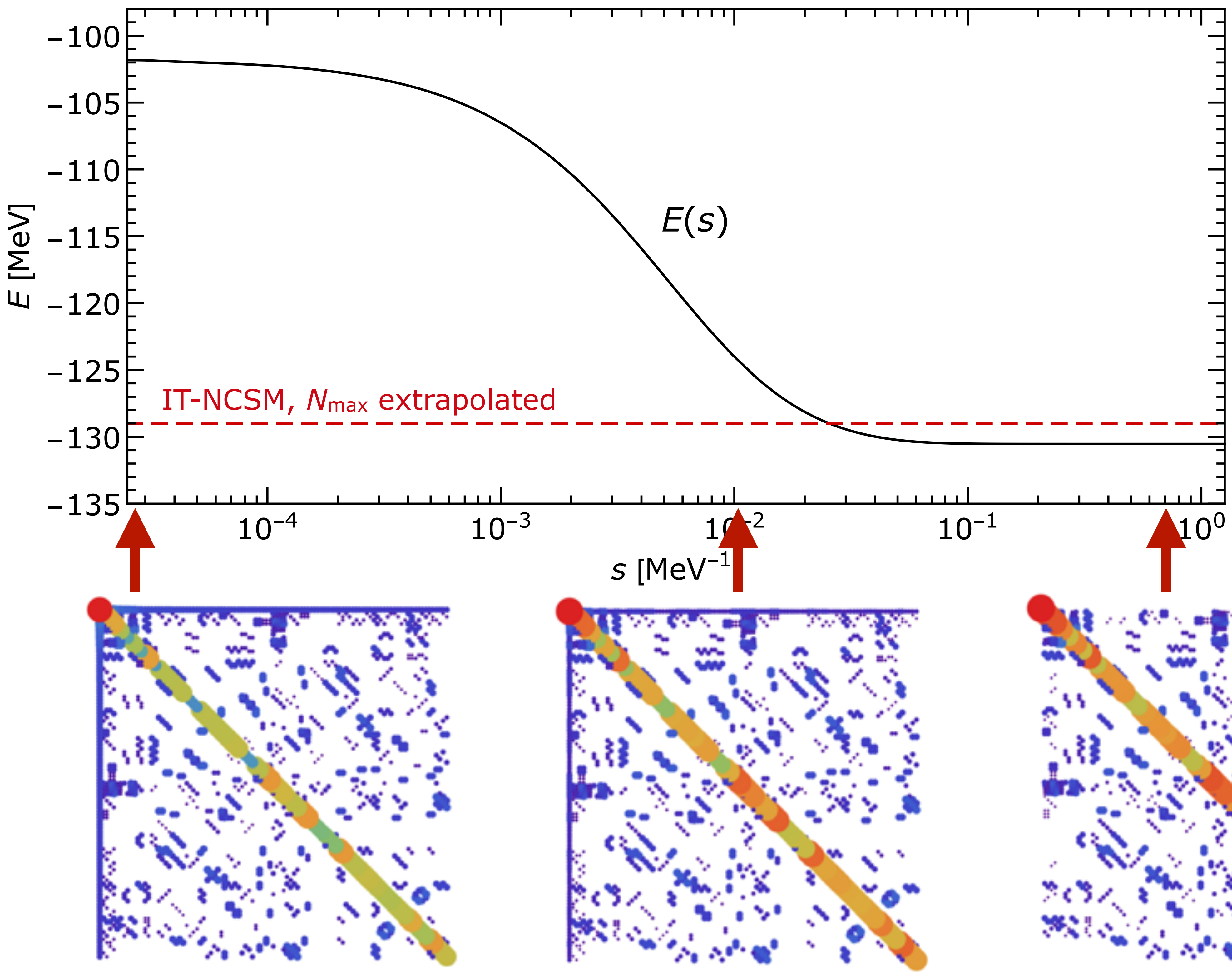
HF basis

- zero-body piece of the flowing Hamiltonian gives **ground-state energy** when full decoupling is reached

$$E(s) = \langle \Phi_{ref} | H(s) | \Phi_{ref} \rangle$$

- truncation of flow equations destroys unitarity, induced many-body terms

In-Medium SRG: Single Reference



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HF basis

Hamilton matrix in N_{max}=2 space

Merging NCSM and IM-SRG

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

IM-SRG:
Many-Body Decoupling

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

NCSM:
Observables

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

Merging NCSM and IM-SRG

NCSM:
Reference State

IM-SRG:
Many-Body Decoupling

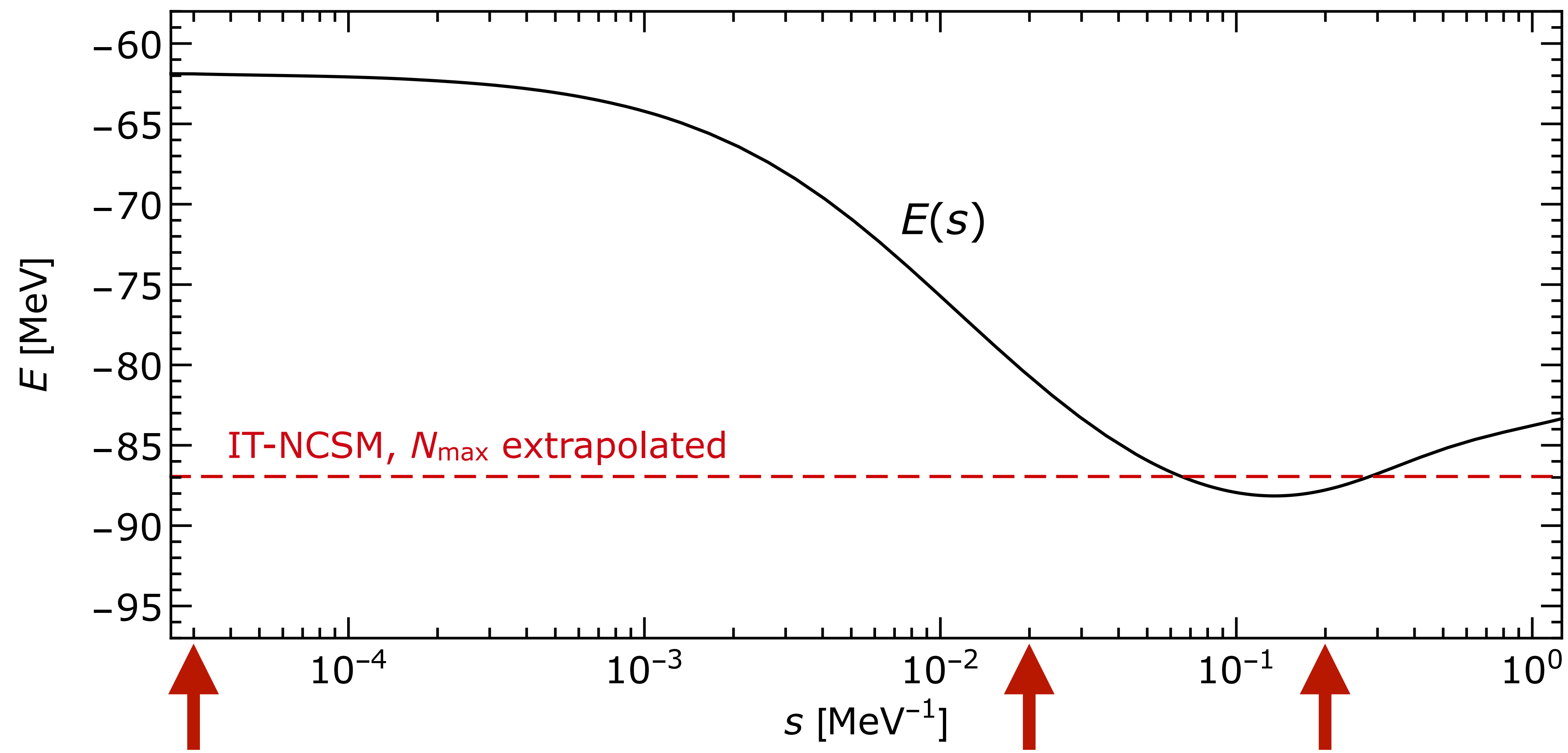
NCSM:
Observables

IM-NCSM is different from IM-SRG for valence-space interactions:

- build on explicit multi-reference formulation for nucleus of choice
- full no-core approach, all nucleons active
- all model-space truncations are converged

In-Medium SRG: Multi Reference

Gebrerufael et al., arXiv:1610.05254



^{12}C

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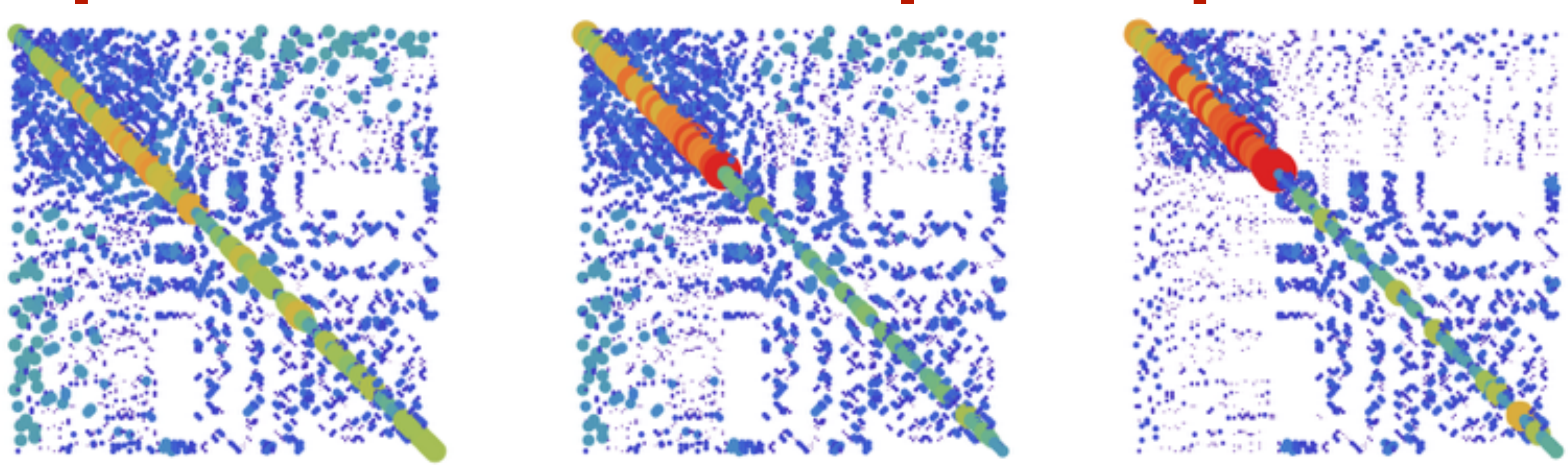

Hamilton matrix in N_{max}=2 space

In-Medium SRG: Multi Reference

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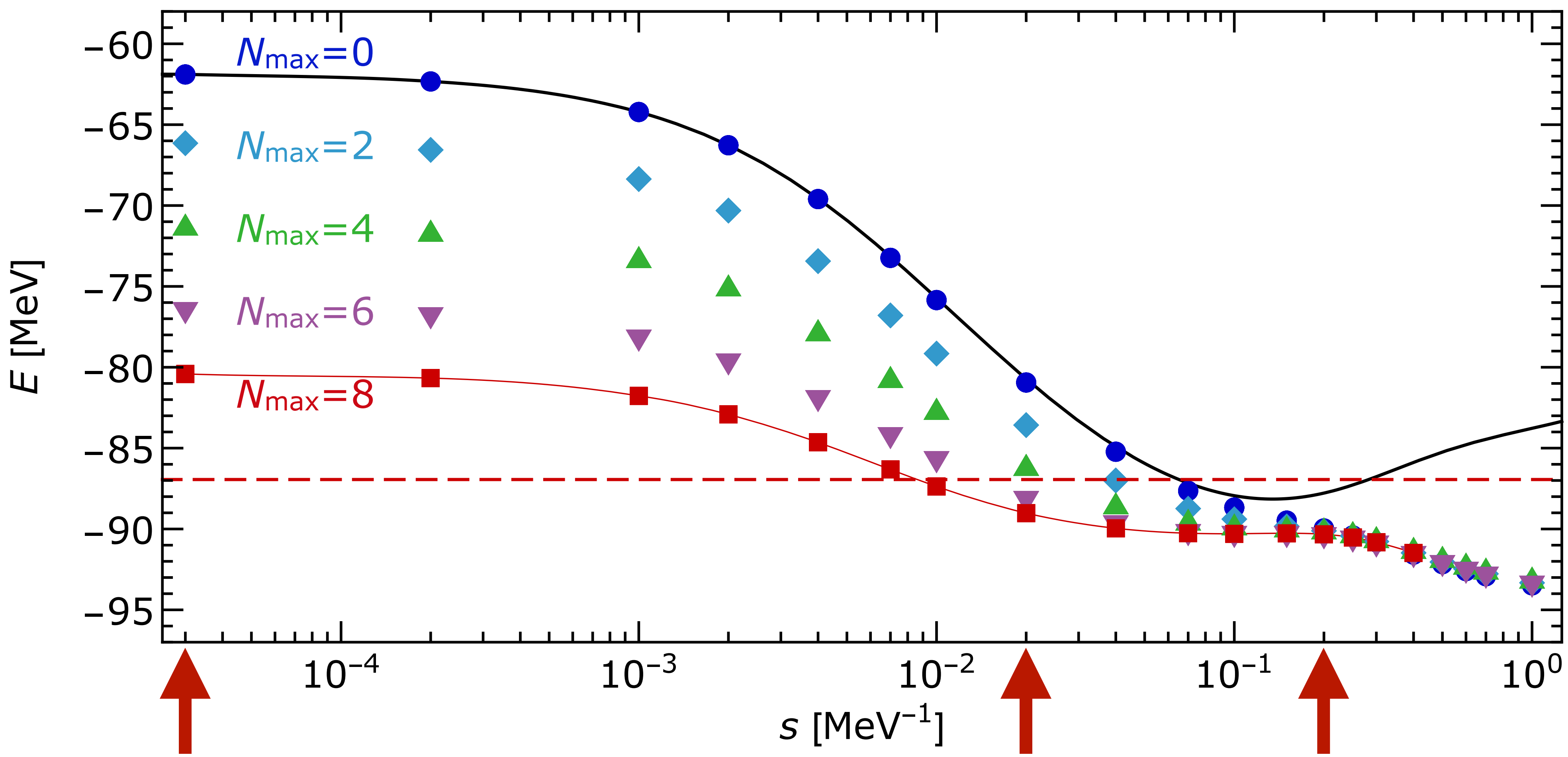

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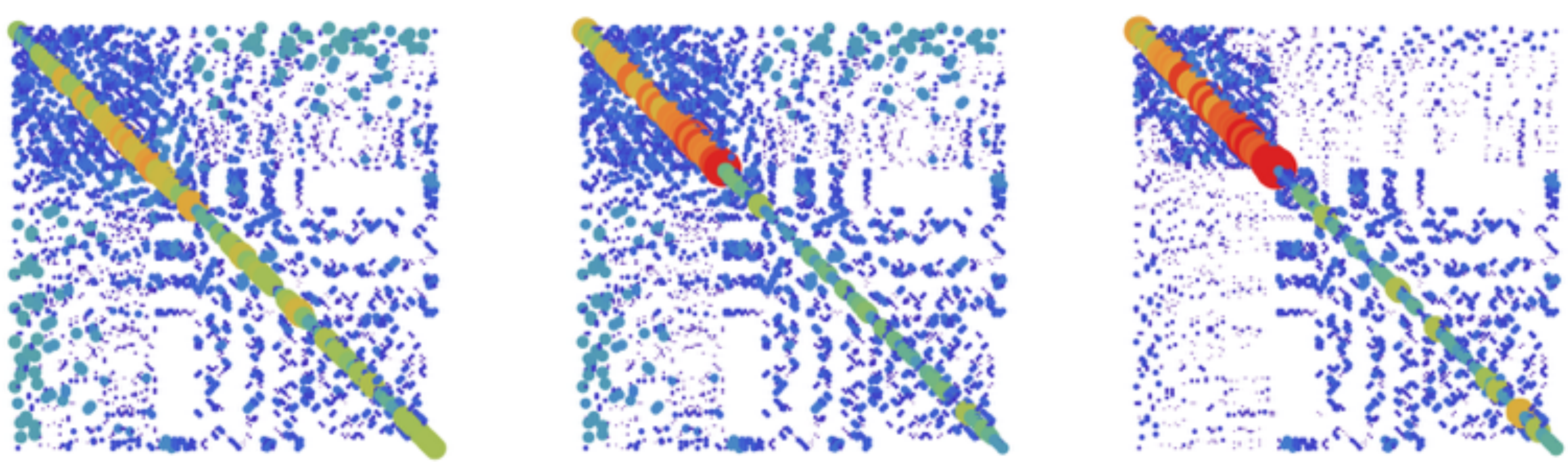
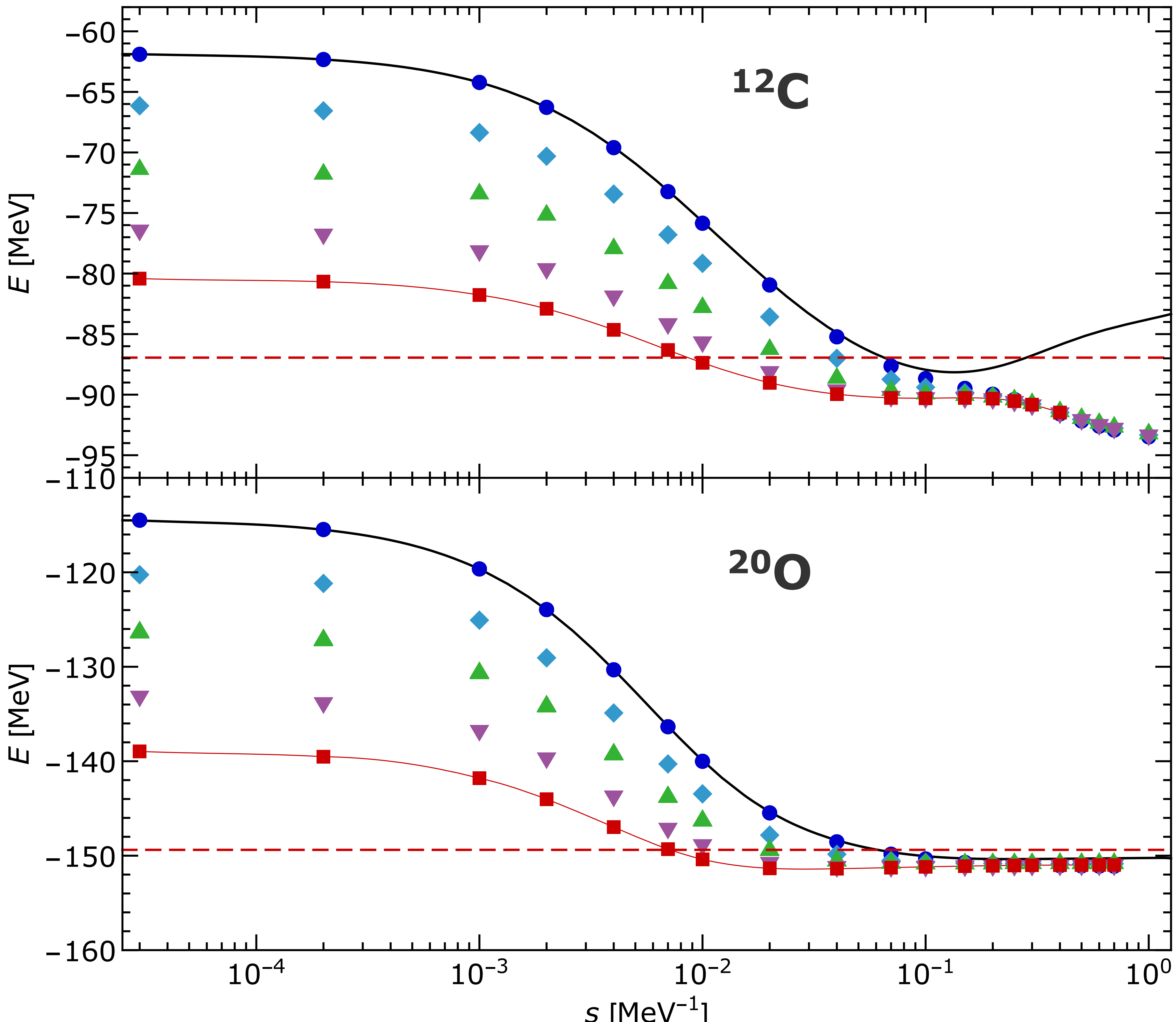


Hamilton matrix in N_{max}=2 space

Flow: Ground-State Energy

Gebrerufael et al., arXiv:1610.05254



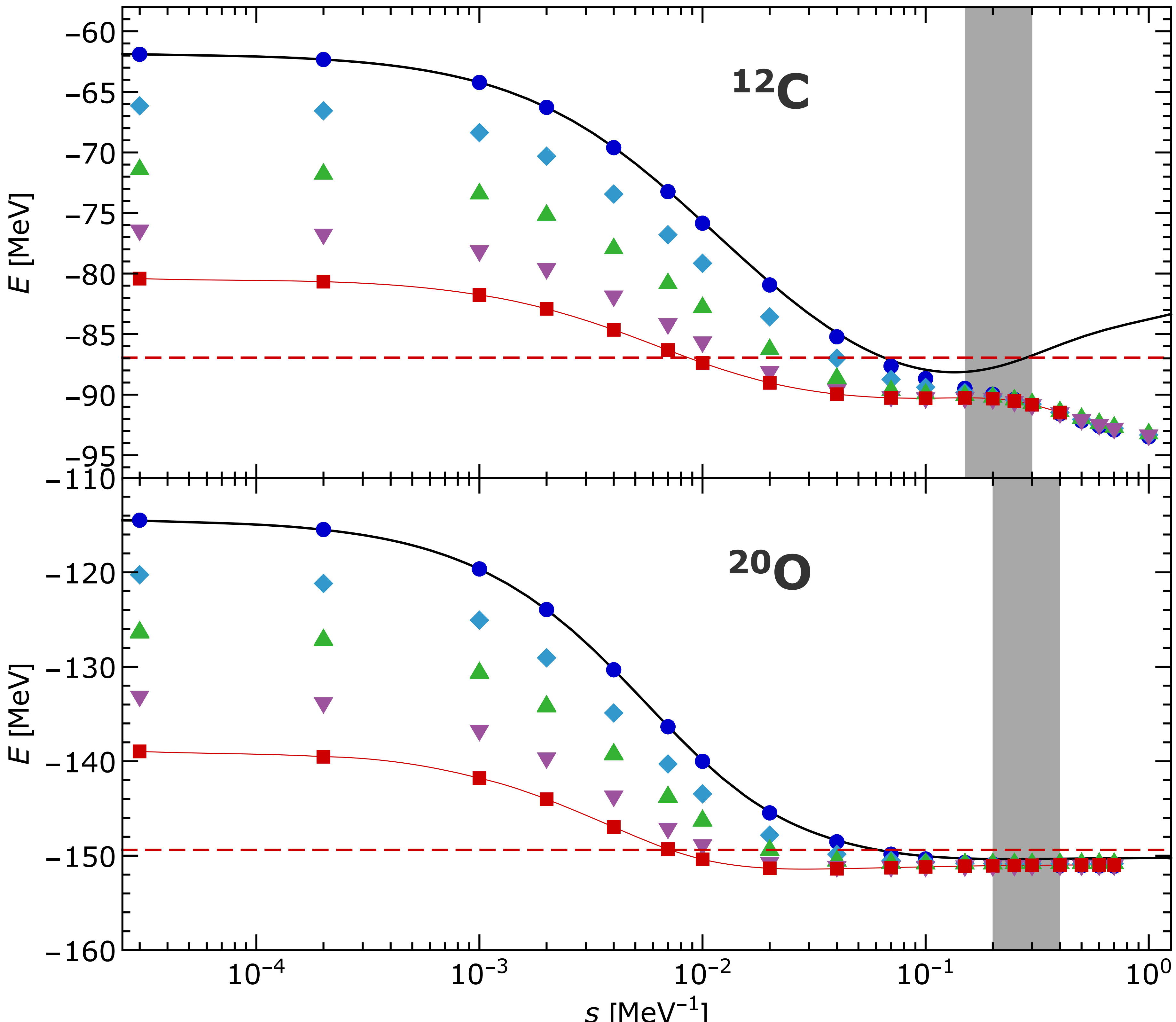
- NCSM convergence is drastically improved
- N_{max}=0 eigenvalues deviated from $E(s)$
- identify plateau in s before induced terms blow up

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

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

Flow: Ground-State Energy

Gebrerufael et al., arXiv:1610.05254



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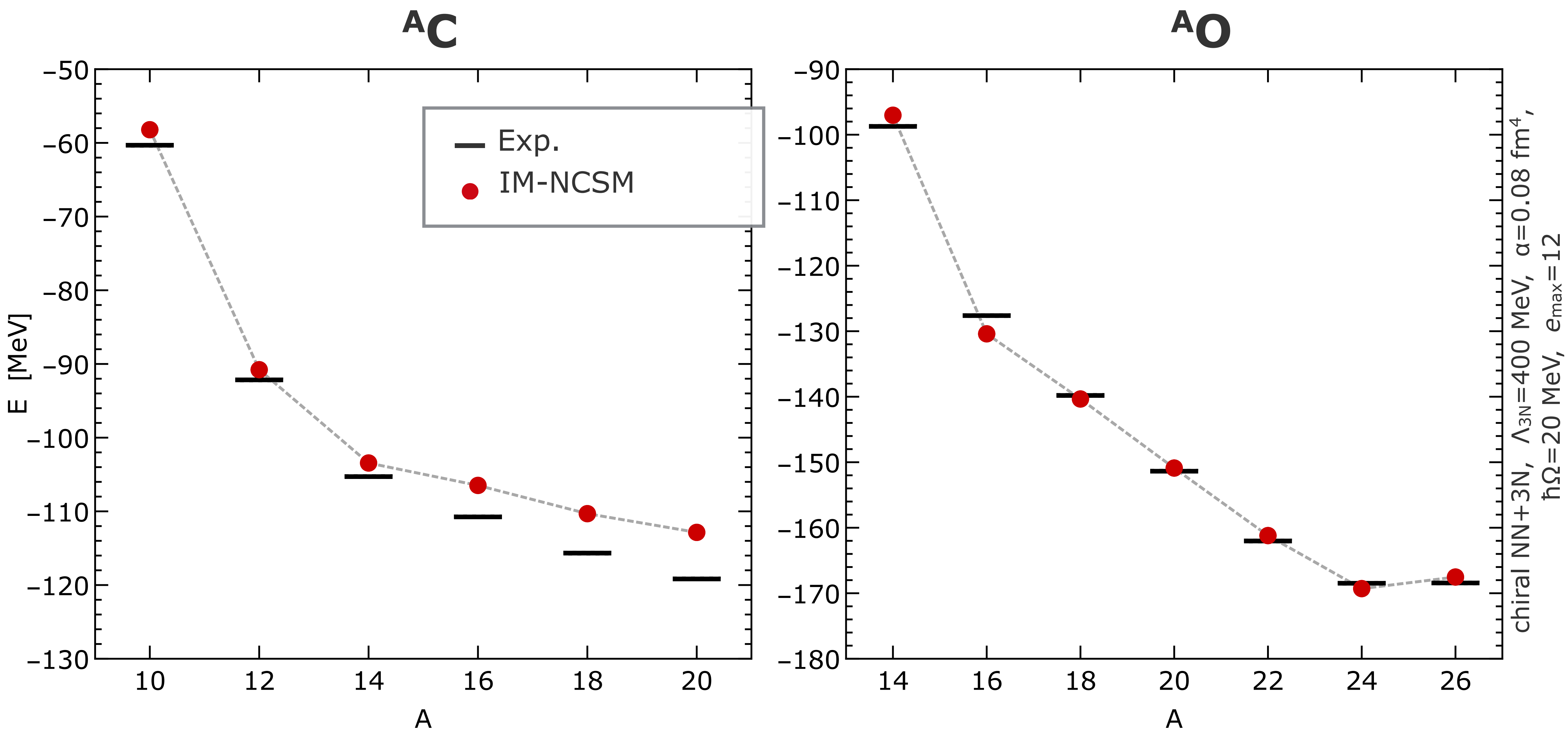
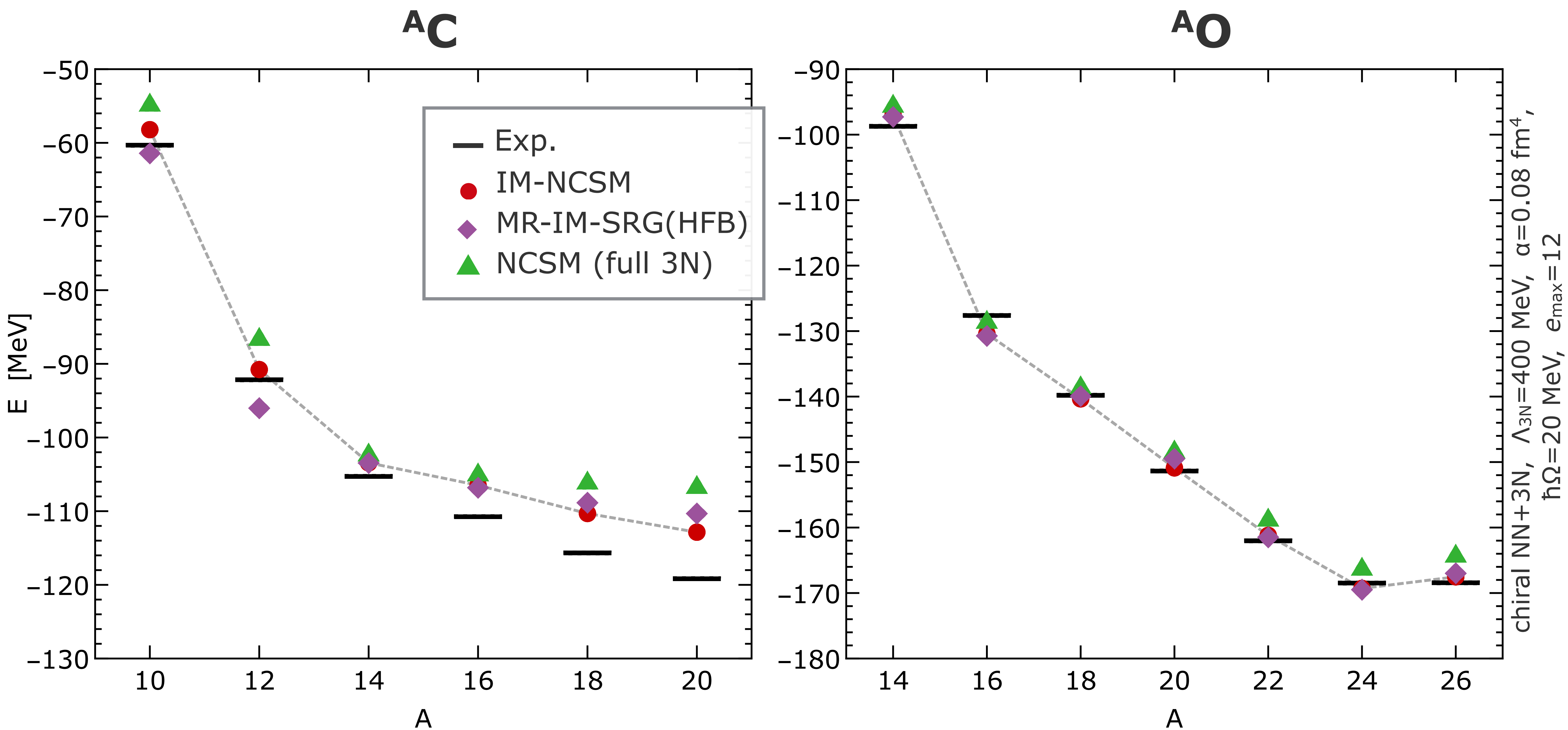
IM-NCSM: Ground-State Energies

Gebrerufael et al., arXiv:1610.05254



IM-NCSM: Ground-State Energies

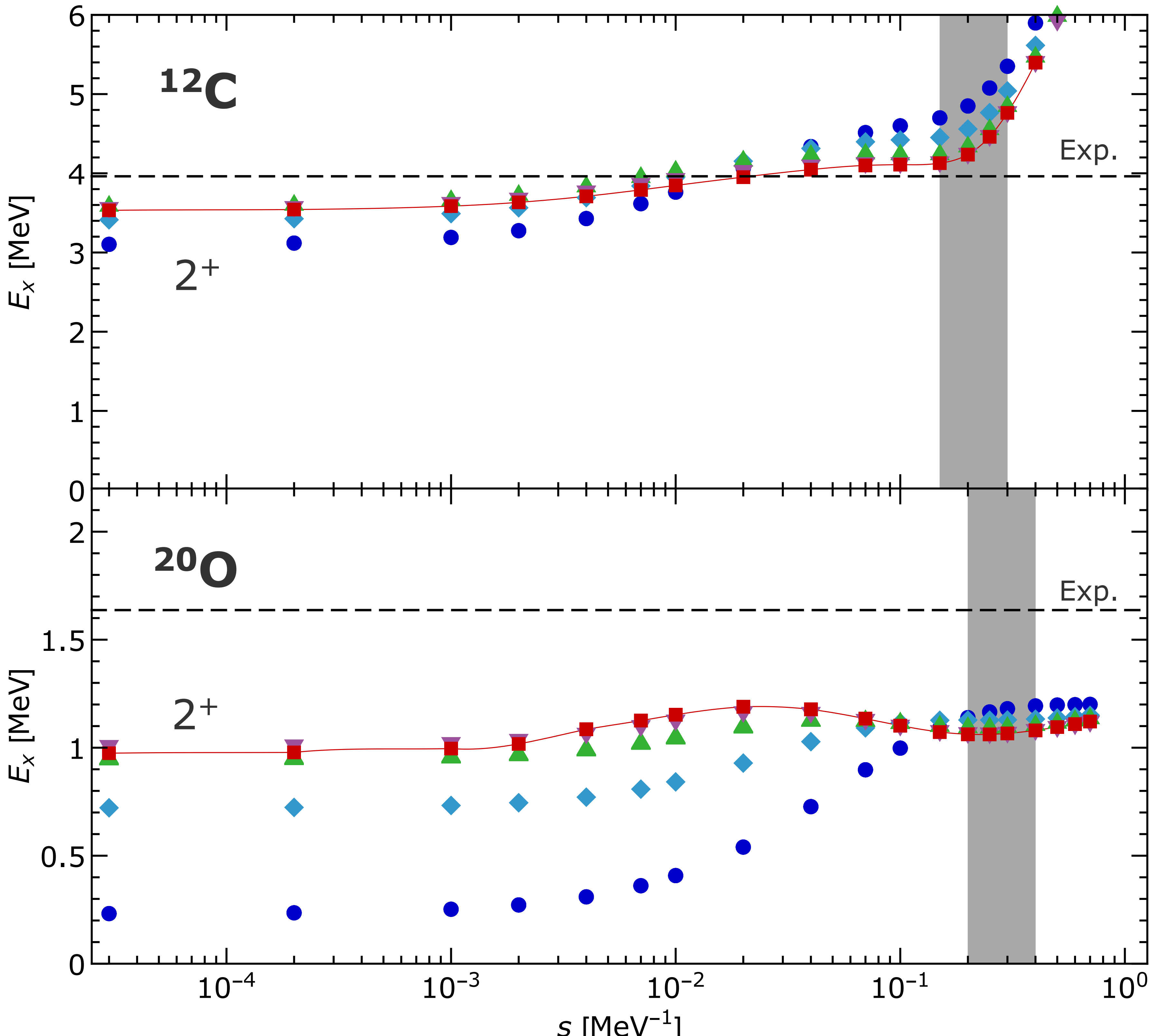
Gebrerufael et al., arXiv:1610.05254



- good agreement with NCSM within uncertainties expected from omission of normal-ordered many-body terms
- ^{12}C shows surprisingly large spread among methods

Flow: 2^+ Excitation Energy

Gebrerufael et al., arXiv:1610.05254



- excitation energies are less affected by flow evolution
- convergence from above in decoupled regime

chiral NN+3N

Λ_{3N}=400 MeV

α=0.08 fm^4

$\hbar\Omega$=20 MeV

e_{max}=12

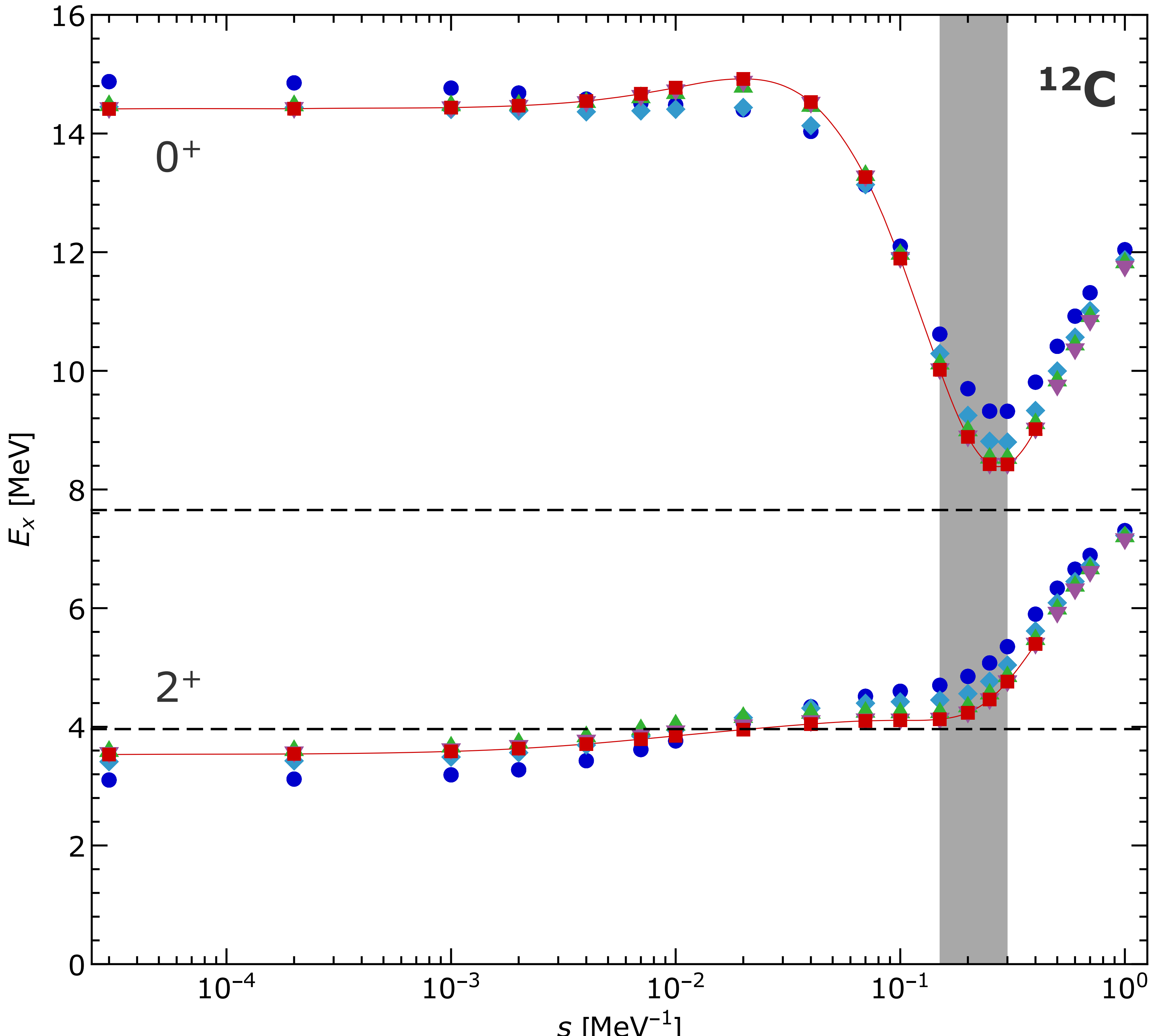
HF basis

N_{max}=0 reference state

N_{max}=0,2,4,6,8

Flow: 0^+ Excitation Energy

Gebrerufael et al., arXiv:1610.05254



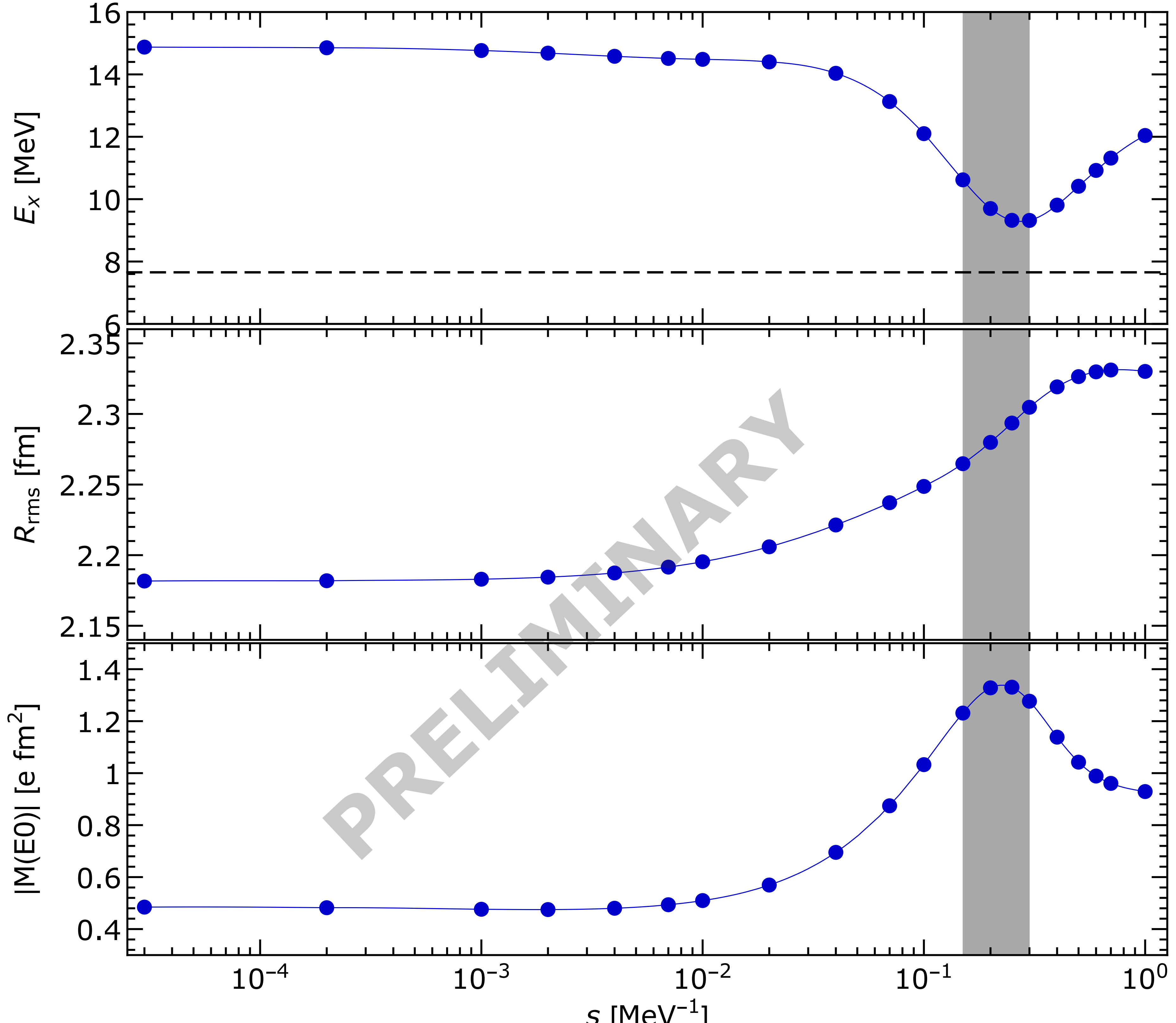
- excited 0^+ state behaves differently
- excitation energy drops by ~5 MeV in decoupling regime
- no stable result before induced many-body terms blow up

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

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

Flow: Signatures of Hoyle State

Gebrerufael et al., arXiv:1610.05254



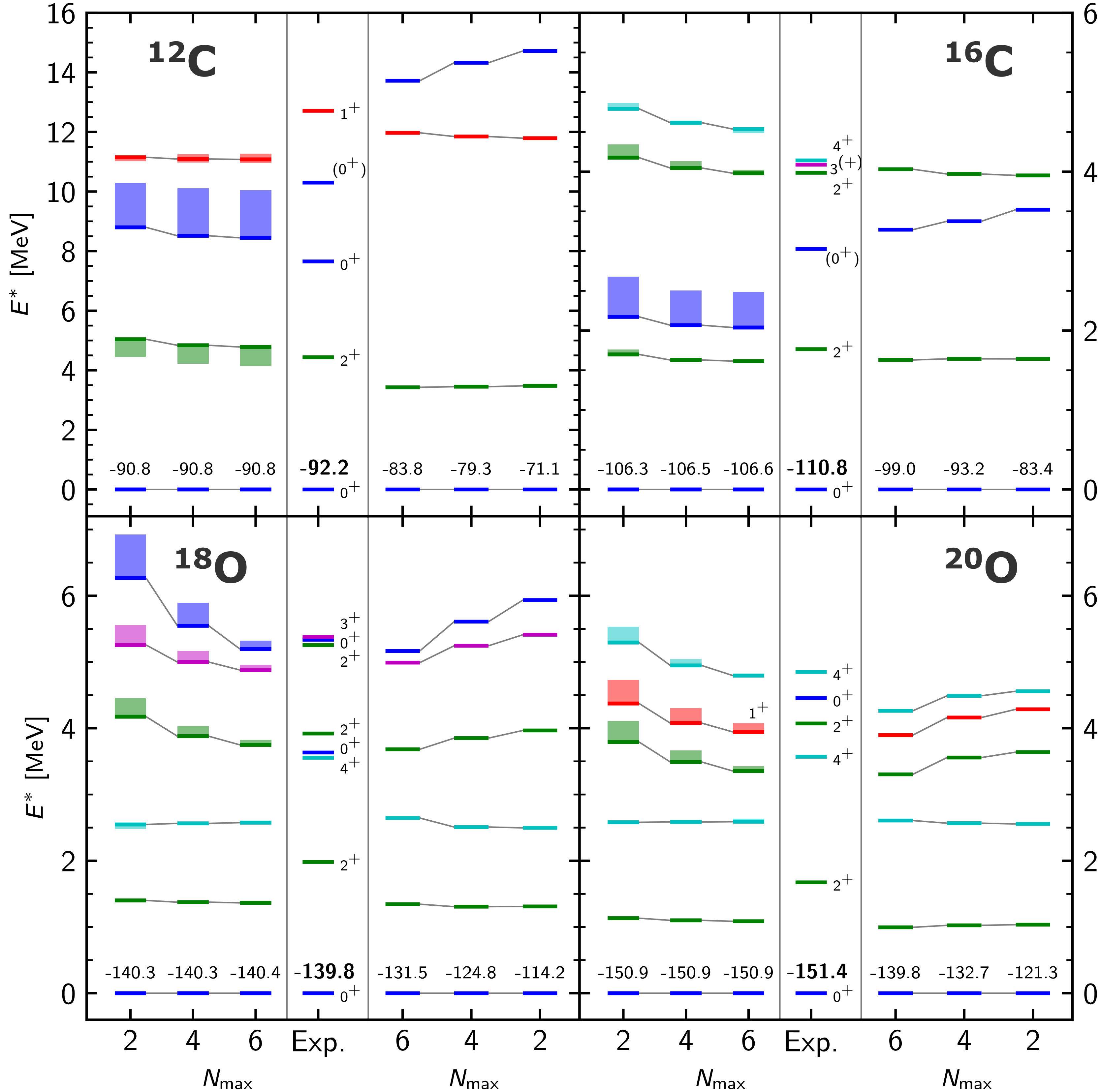
- trends are compatible with Hoyle-state interpretation
- need better control of induced many-body terms for quantitative statements

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

IM-NCSM: Excitation Spectra

Gebrerufael et al., arXiv:1610.05254



- IM-NCSM and direct NCSM in excellent agreement for converged states
- first excited 0^+ states in ^{12}C and ^{16}C differ

chiral NN+3N
Λ_{3N}=400 MeV
α=0.08 fm^4
$\hbar\Omega$=16 MeV
e_{max}=12
HF basis

NCSM-PT:
Merging NCSM with MBPT

with A. Tichai

Merging NCSM and MBPT

NCSM:
'Unperturbed' States

- eigenstates from NCSM at moderate N_{max} as unperturbed states
- access to all open-shell nuclei and systematically improvable

MBPT:
Convergence Booster

- multi-configurational MBPT at low orders for individual unperturbed states
- capture couplings in huge model-space through perturbative corrections

Multi-Configurational Perturbation Theory

Tichai et al., in prep.

- prior NCSM calculation: **reference or unperturbed state** is superposition of Slater determinants from reference space

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

- define partitioning and **unperturbed Hamiltonian**

$$\mathrm{H}_0 = \epsilon_{\text{ref}} \, |\Psi_{\text{ref}}\rangle\langle\Psi_{\text{ref}}| + \sum_{\nu \notin \mathcal{M}_{\text{ref}}} \epsilon_\nu \, |\Phi_\nu\rangle\langle\Phi_\nu|$$

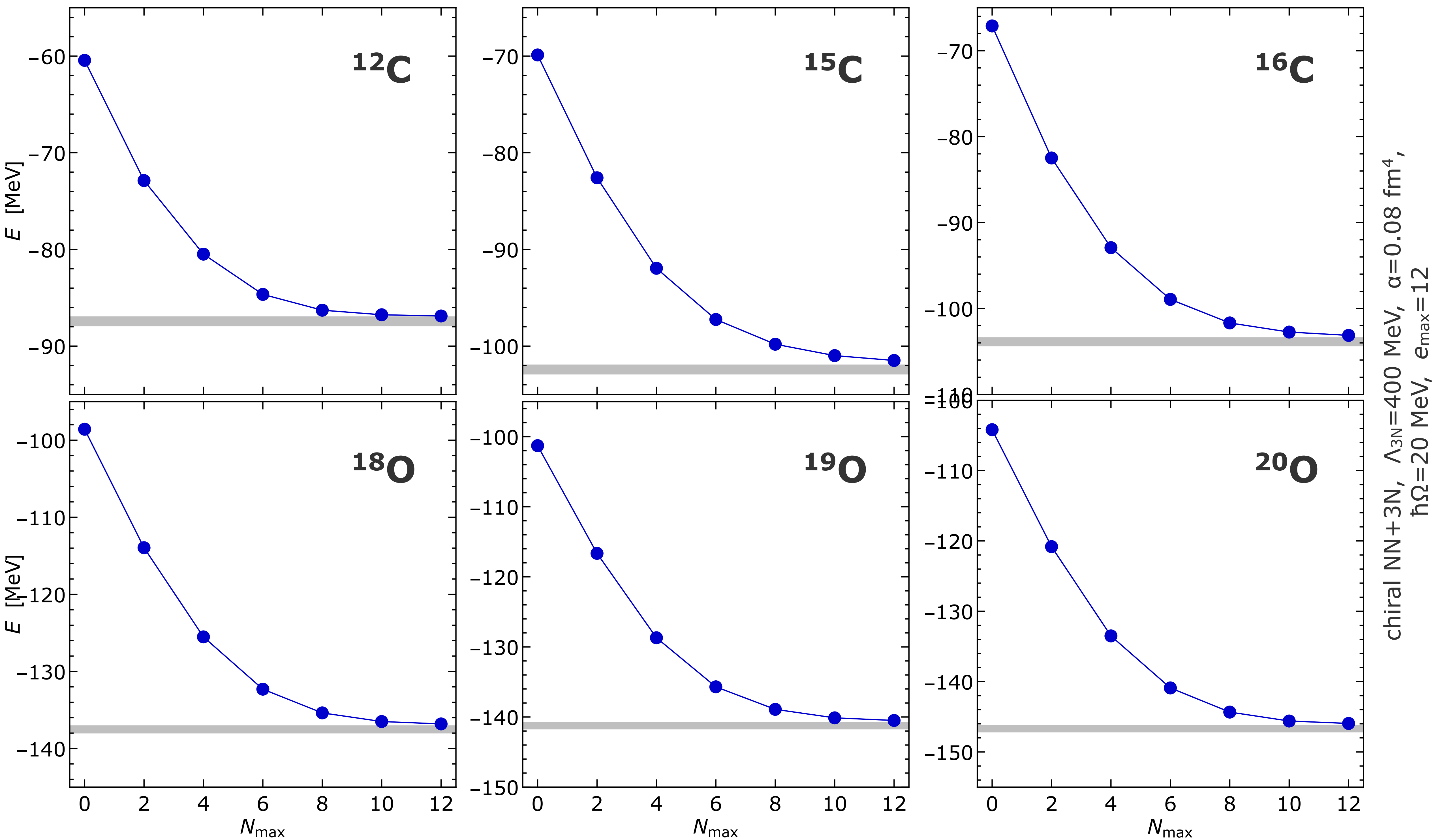
- evaluate **second-order correction** to the energy at many-body level

$$E^{(2)} = - \sum_{\nu \notin \mathcal{M}_{\text{ref}}} \frac{|\langle\Phi_\nu| \, \mathrm{H} \, |\Psi_{\text{ref}}\rangle|^2}{\epsilon_\nu - \epsilon_{\text{ref}}}$$

- use **m-scheme NCSM technology** and multi-reference normal-ordering to evaluate matrix elements for $E^{(2)}$

Ground-State Energies

Tichai et al., in prep.



Ground-State Energies

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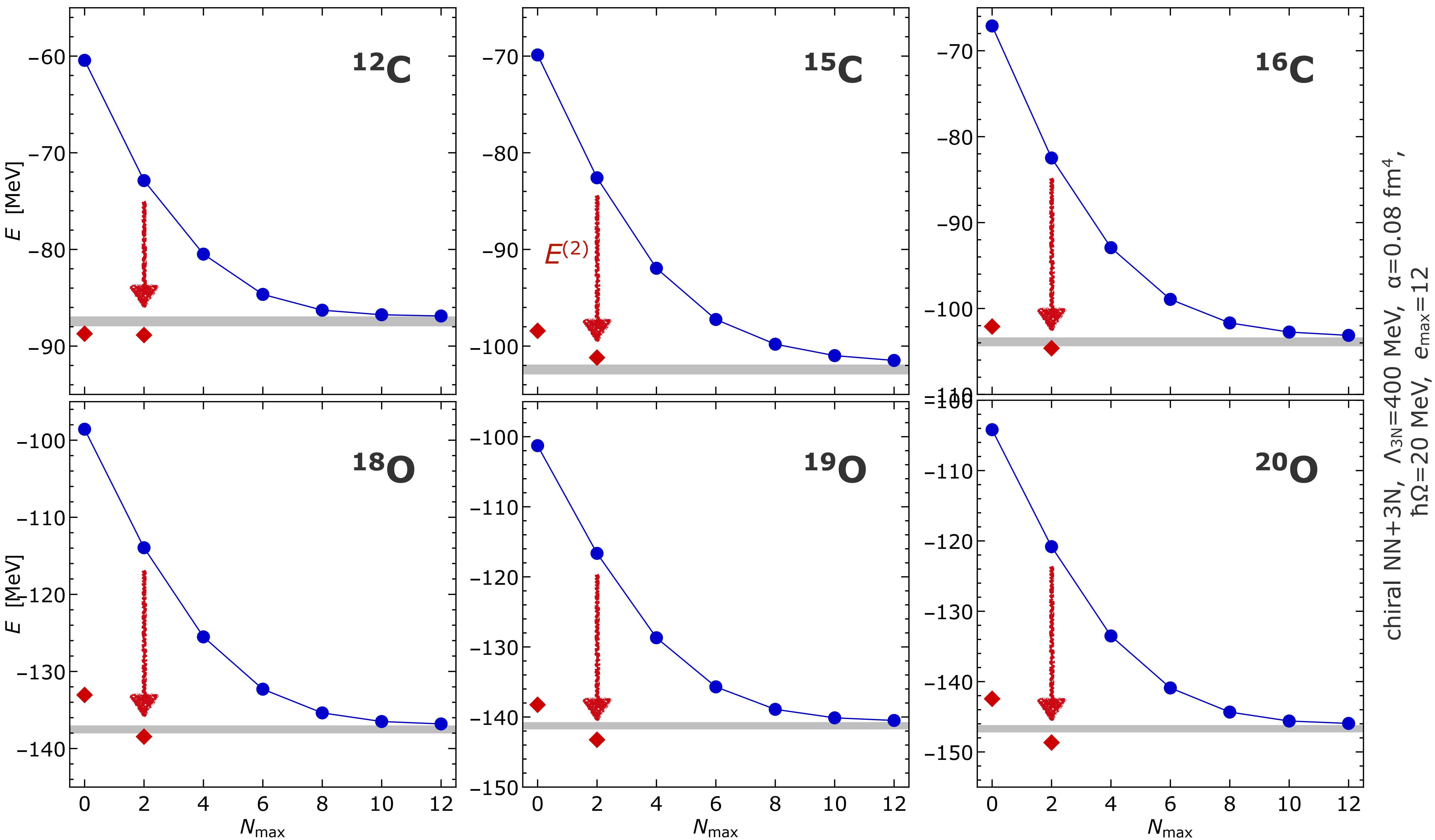
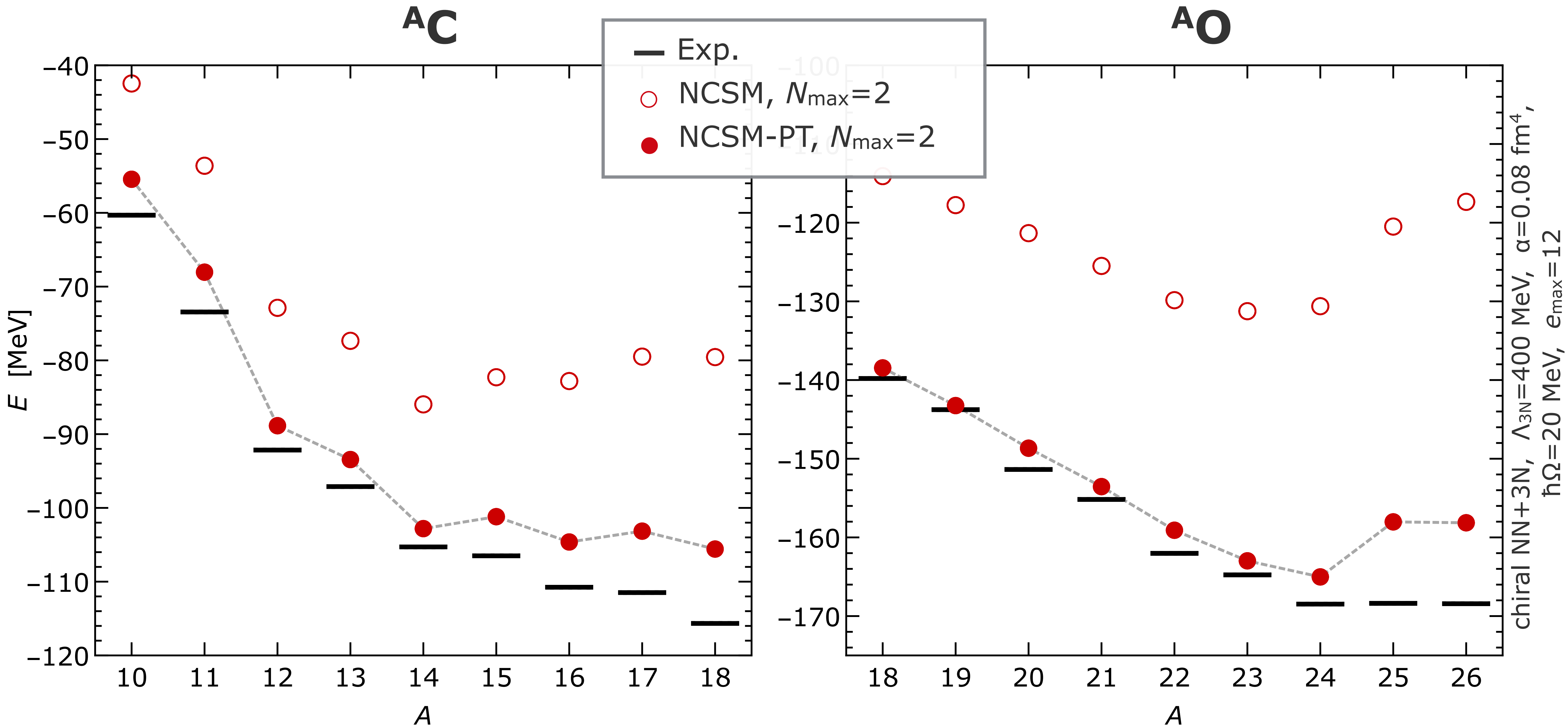


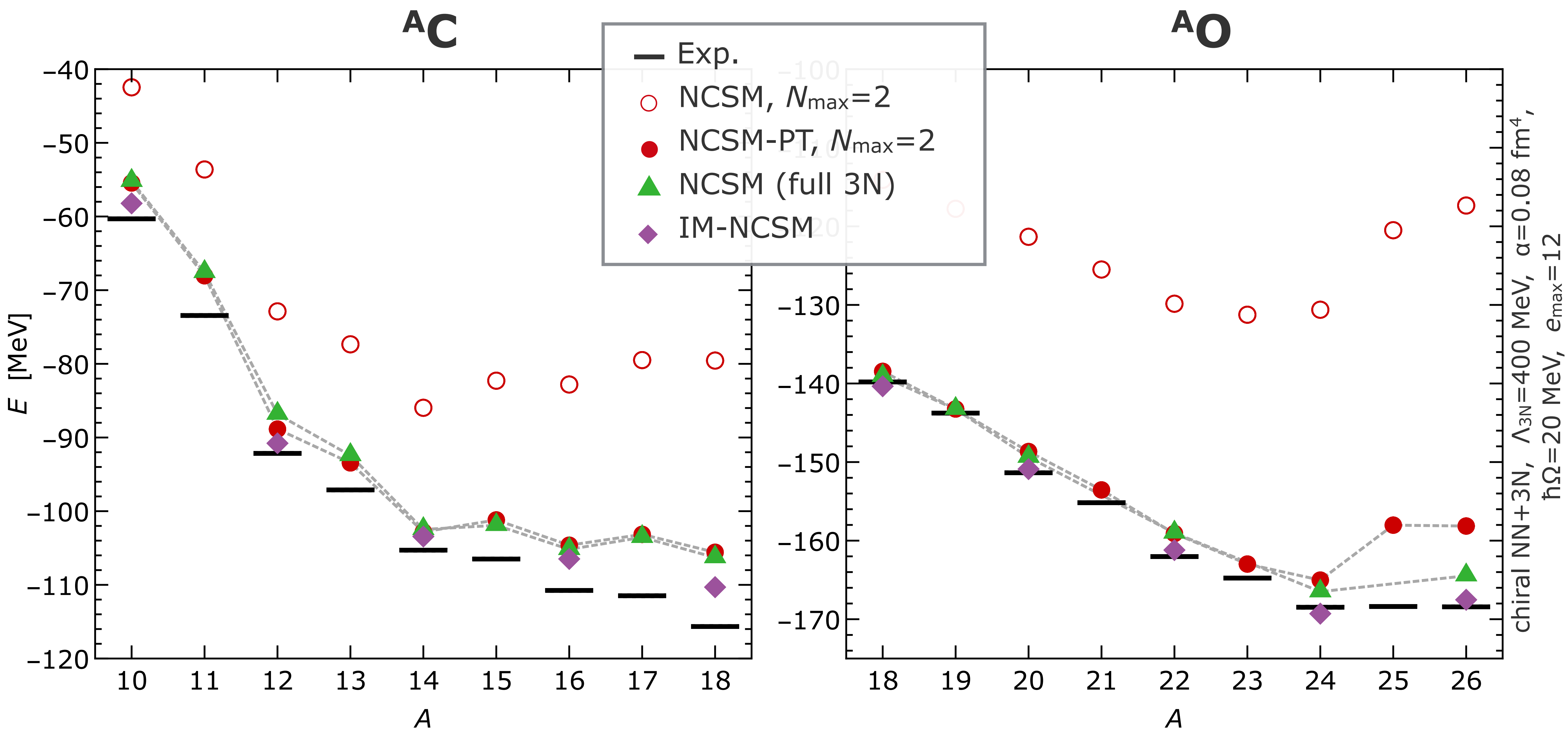
NCSM-PT: Ground-State Energies

Tichai et al., in prep.



NCSM-PT: Ground-State Energies

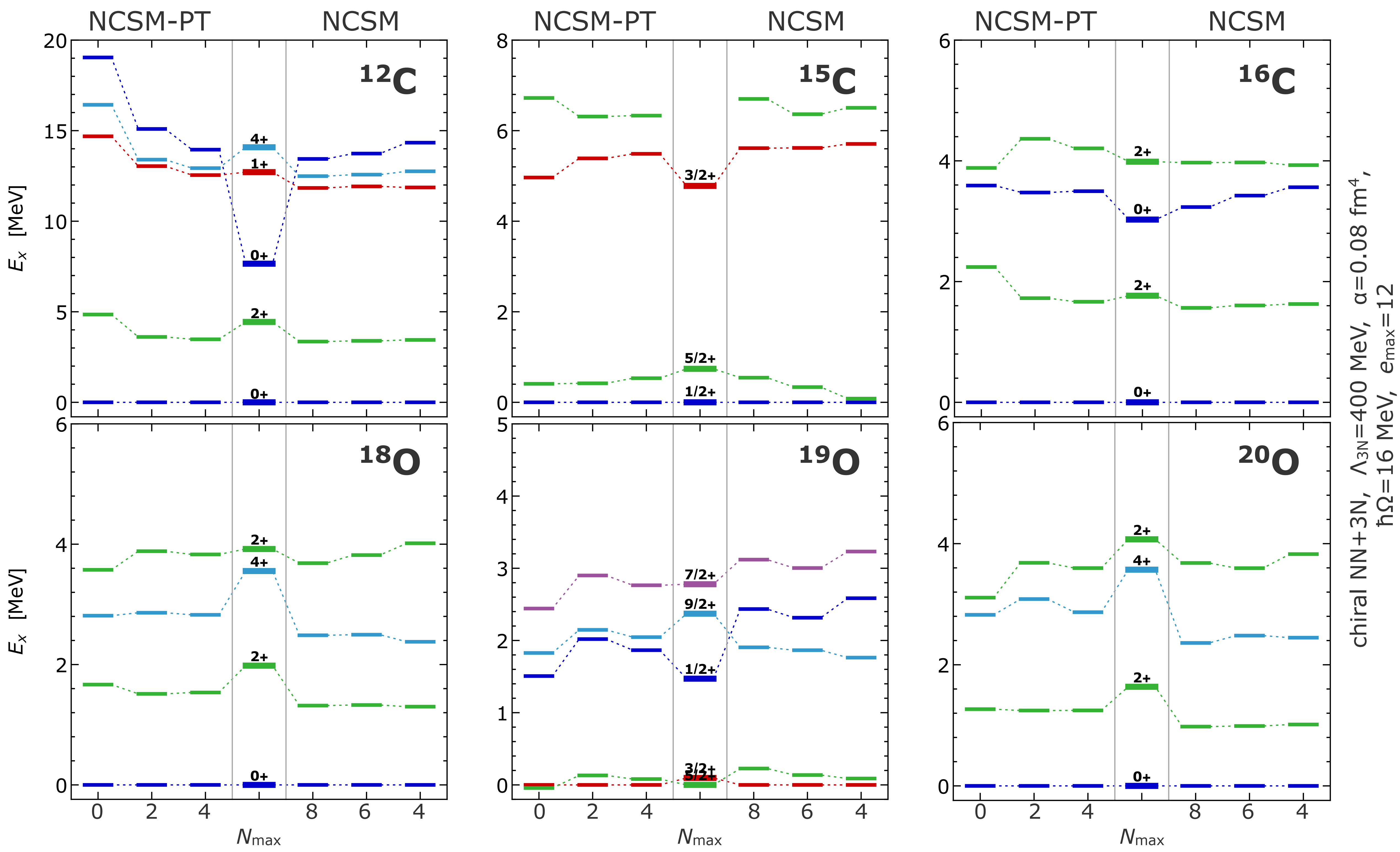
Tichai et al., in prep.



- excellent agreement with full NCSM except for nuclei beyond the drip line
- factor 1000 less CPU time for NCSM-PT compared to large-scale IT-NCSM

NCSM-PT: Excitation Spectra

Tichai et al., in prep.



Conclusions: Hybrid Ab Initio Methods

IM-NCSM

No-Core Shell Model

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In-Medium Similarity Renormalization Group

↓

No-Core Shell Model

NCSM-PT

No-Core Shell Model

↓

Many-Body Perturbation Theory

- ab initio access to ground and excited states of fully open-shell medium-mass nuclei
- 2-3 orders of magnitude less CPU time than IT-NCSM and very different computational characteristics

Epilogue

- **thanks to my group and my collaborators**
  - S. Alexa, E. Gebrerufael, T. Hüther, L. Mertes, S. Schulz, H. Spielvogel, C. Stumpf, A. Tichai, K. Vobig, R. Wirth
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