New Horizons in Ab Initio Theory...

...from an NCSM Perspective

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Ab Initio Methods

No-Core Shell Model

Navratil, Dytrych, Otsuka

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

In-Medium Similarity Renormalization Group

Hergert

- 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, LEFT, MC, ...

Hagen, Barbieri, Lee, Papenbrock

Ab Initio Methods

No-Core Shell Model

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Many-Body Perturbation Theory

CC, SCGF, LEFT, MC, ...

Hagen, Barbieri, Lee, Papenbrock

- 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
- target: spectroscopy of fully open-shell medium-mass nuclei

Natural-Orbital NCSM

J. Müller, A. Tichai, K. Vobig, R. Roth, in prep.

MBPT
basis optimization

- construct HF basis in large single-particle space
- compute perturbative corrections to one-body density matrix up to second order
- determine natural orbitals from one-body density matrix and transform matrix elements

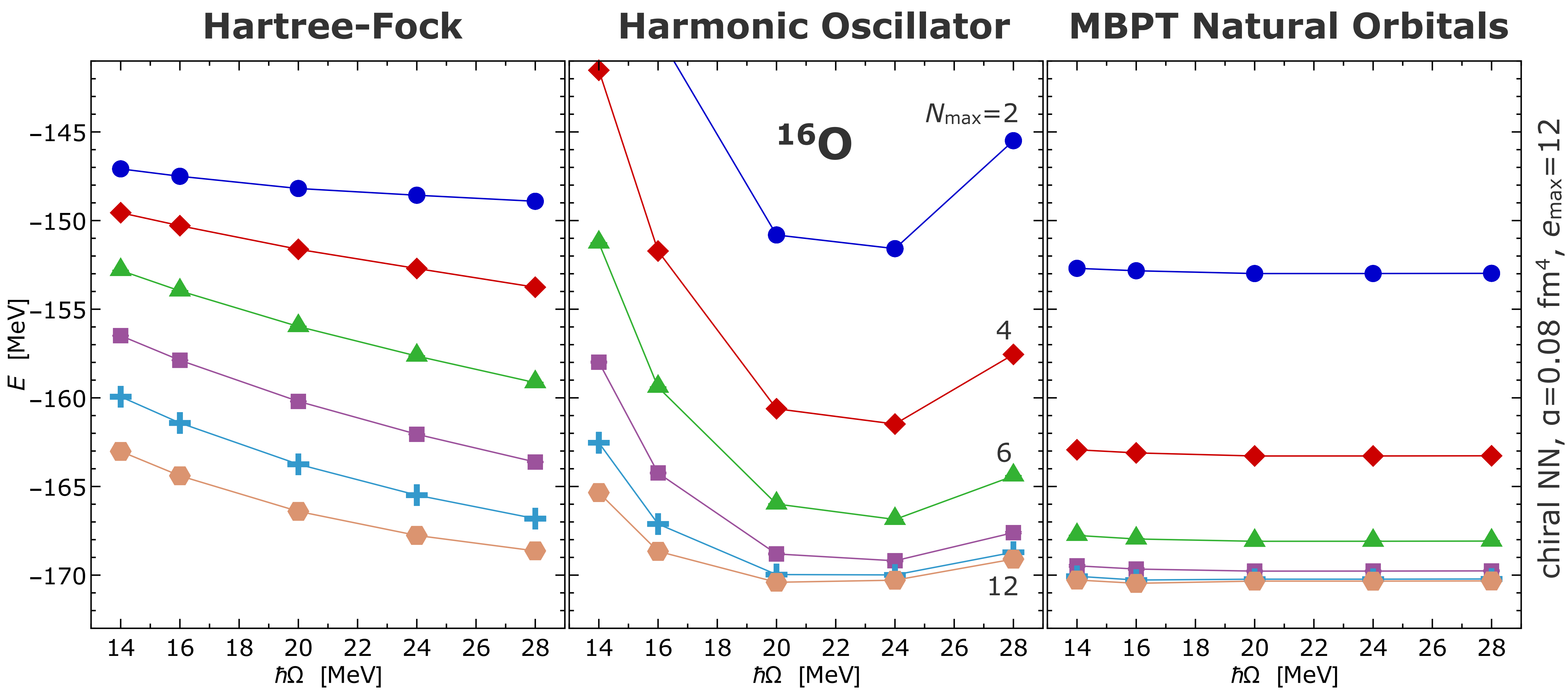
NCSM
many-body solution

- NCSM calculation with natural-orbital basis
- use importance truncation for large spaces and heavier nuclei (optional)
- use normal-order two-body approximation to include 3N interactions (optional)

cf. work of Ch. Constantinou, M. A. Caprio, J. P. Vary, P. Maris
on construction of natural-orbital basis from NCSM solutions

Basis Choice & NCSM Convergence

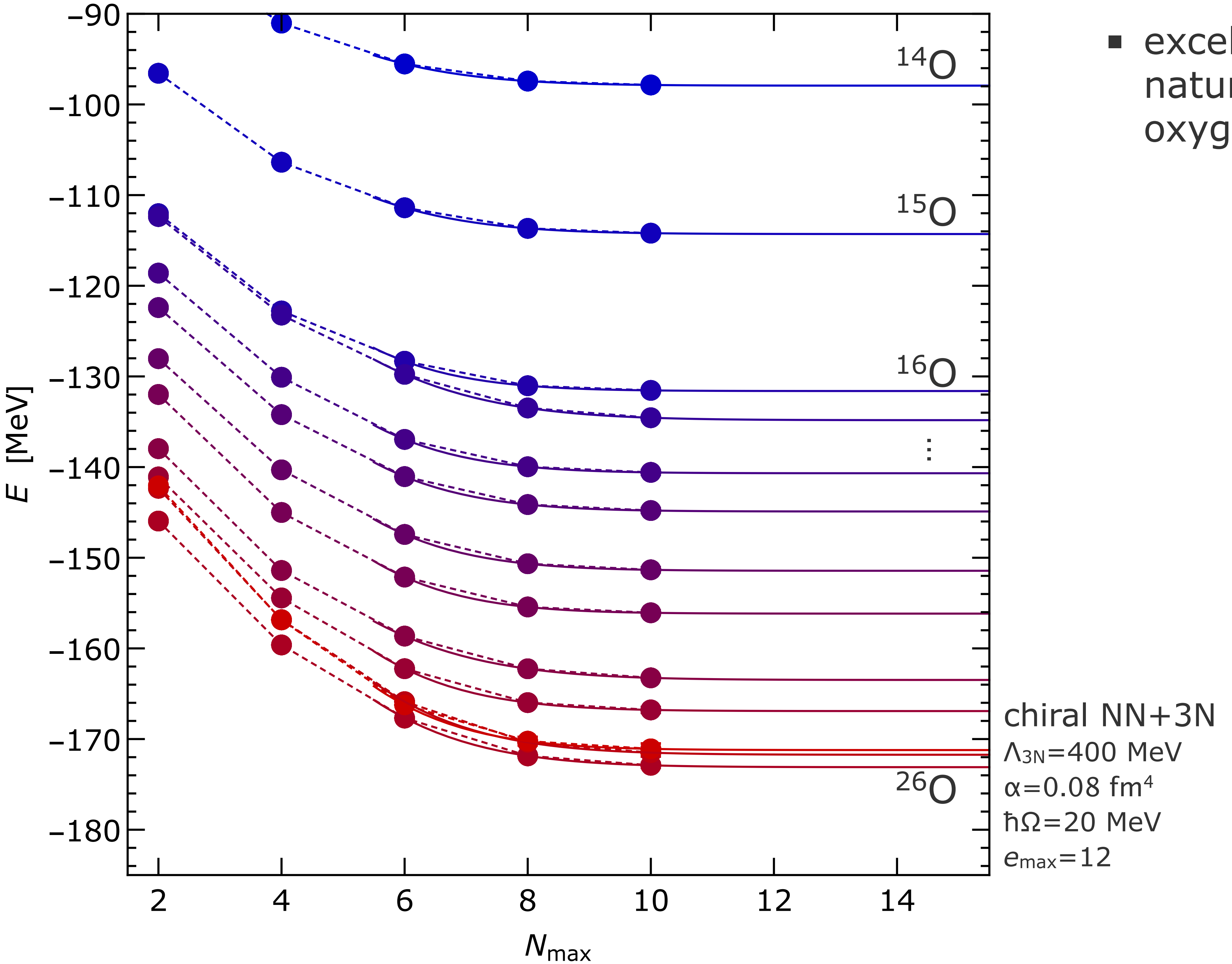
J. Müller, A. Tichai, K. Vobig, R. Roth, in prep.



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

Oxygen Isotopes

J. Müller, A. Tichai, K. Vobig, R. Roth, in prep.



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

Oxygen Isotopes

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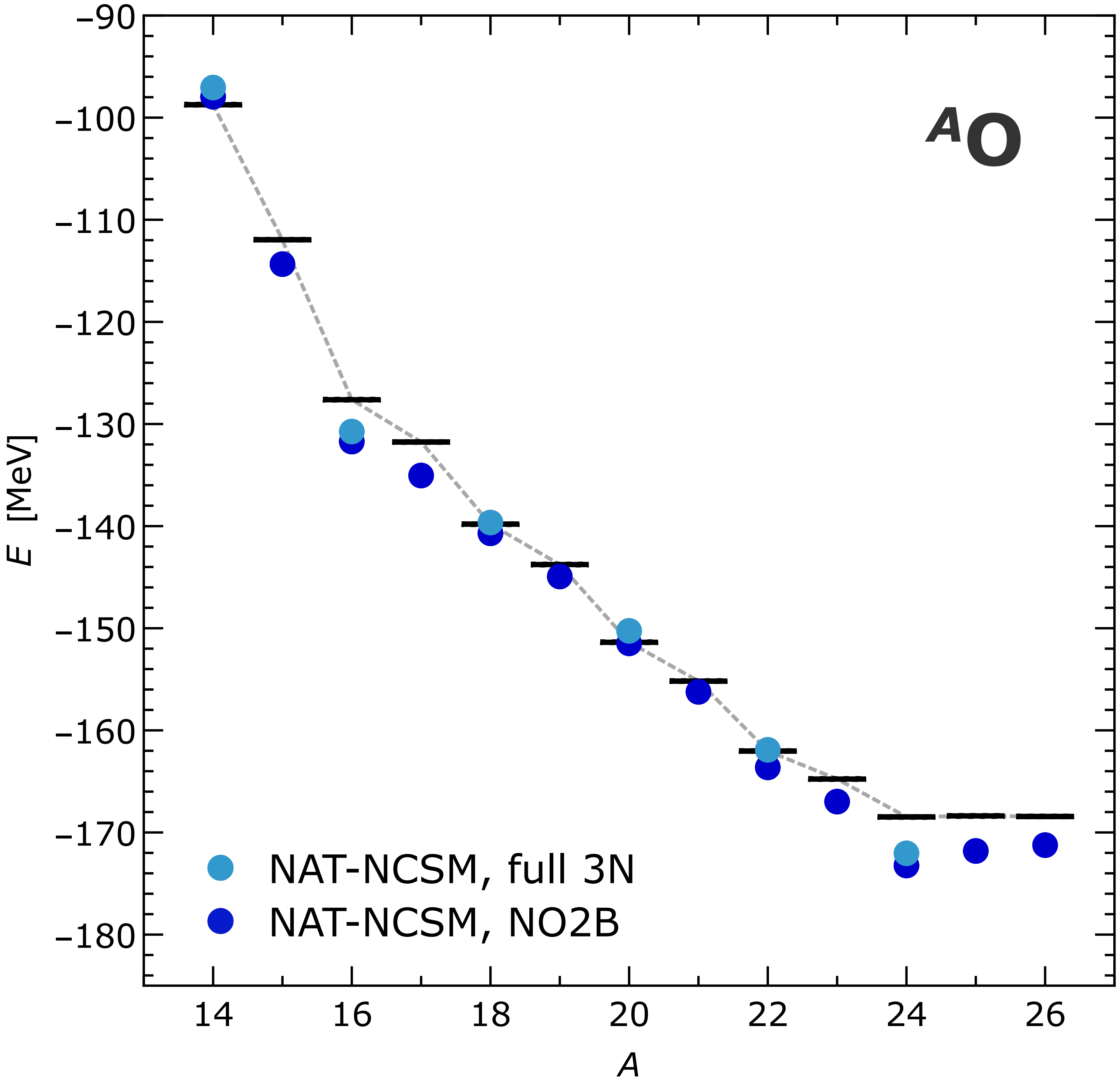


- excellent convergence with natural-orbital basis for all oxygen isotopes
- good agreement with experimental systematics and dripline
- normal-ordered two-body approx. instead of full 3N causes ~1% overbinding

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

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

IM-SRG
decoupling

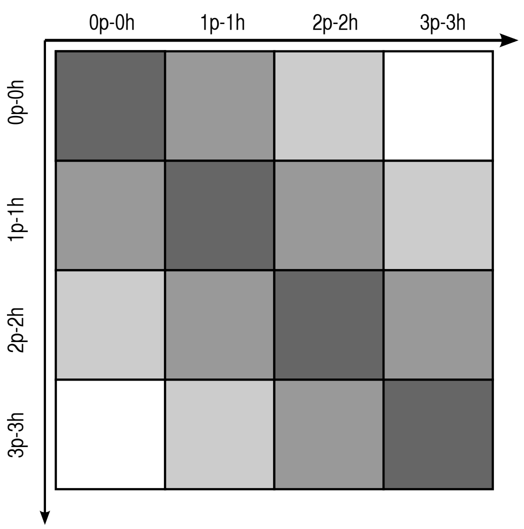
- IM-SRG evolution of multi-reference normal-ordered Hamiltonian (and other operators)
- decoupling of particle-hole excitations, i.e., pre-diagonalization in many-body space

NCSM
many-body solution

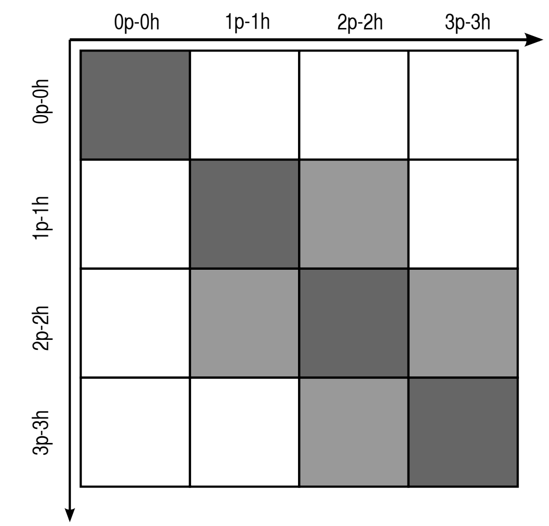
- use in-medium evolved Hamiltonian for a subsequent NCSM calculation
- access to ground and excited states and full suite of observables

In-Medium 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

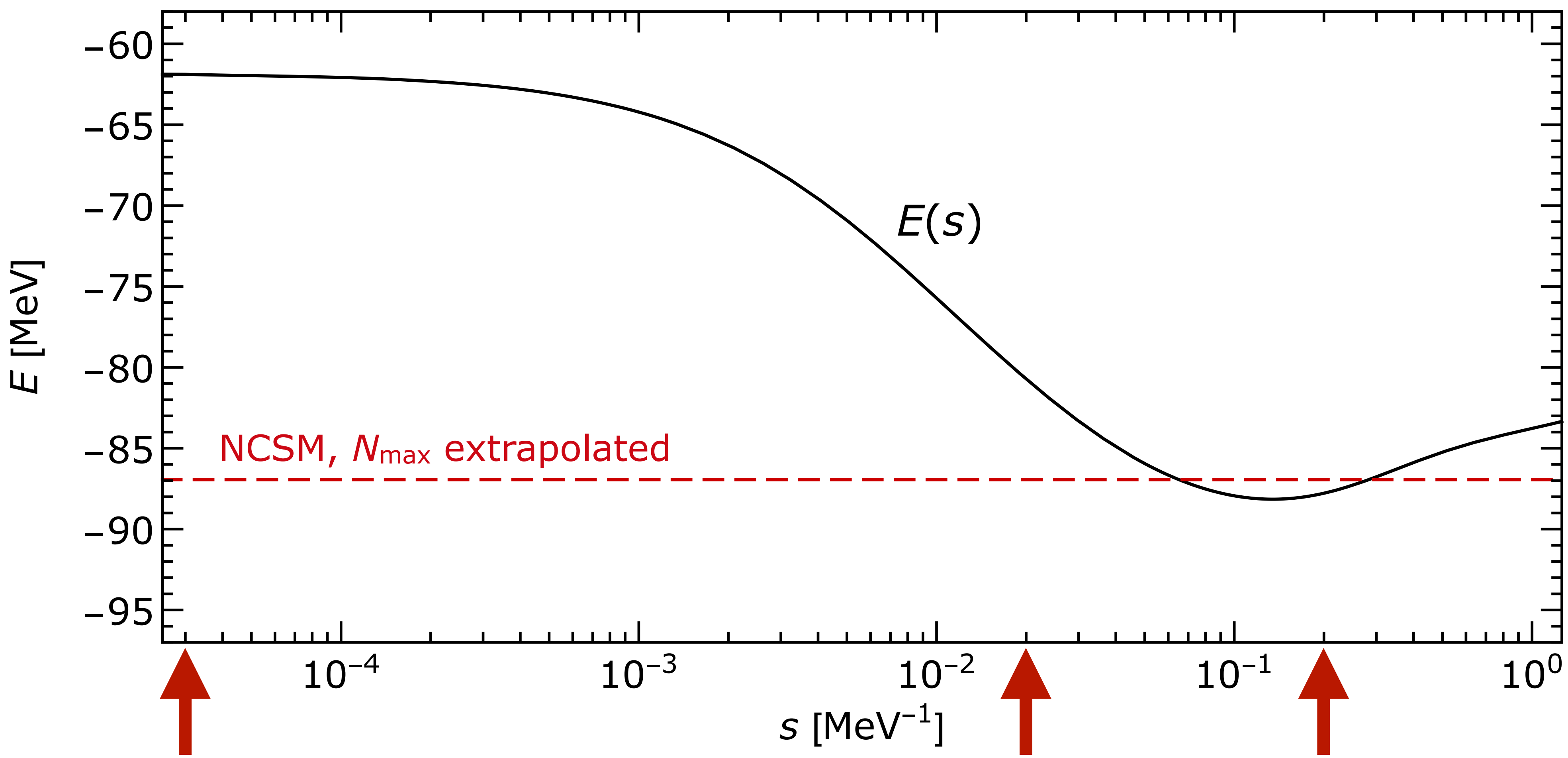
$$H(s) = E(s) + \sum_{ij} f^i_j(s)\, \tilde{A}^i_j + \frac{1}{4}\sum_{ijkl}\Gamma^{ij}_{kl}(s)\, \tilde{A}^{ij}_{kl} + \frac{1}{36}\sum_{ijklmn} W^{ijk}_{lmn}(s)\, \tilde{A}^{ijk}_{lmn}$$

- 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: Multi Reference

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

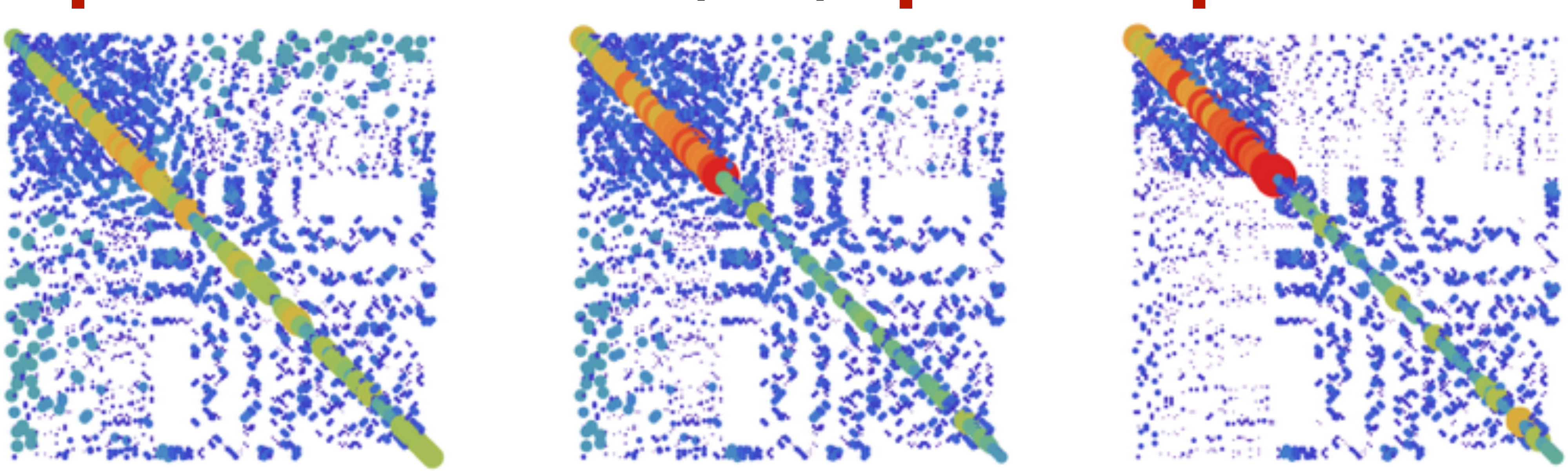


^{12}C

chiral NN+3N

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

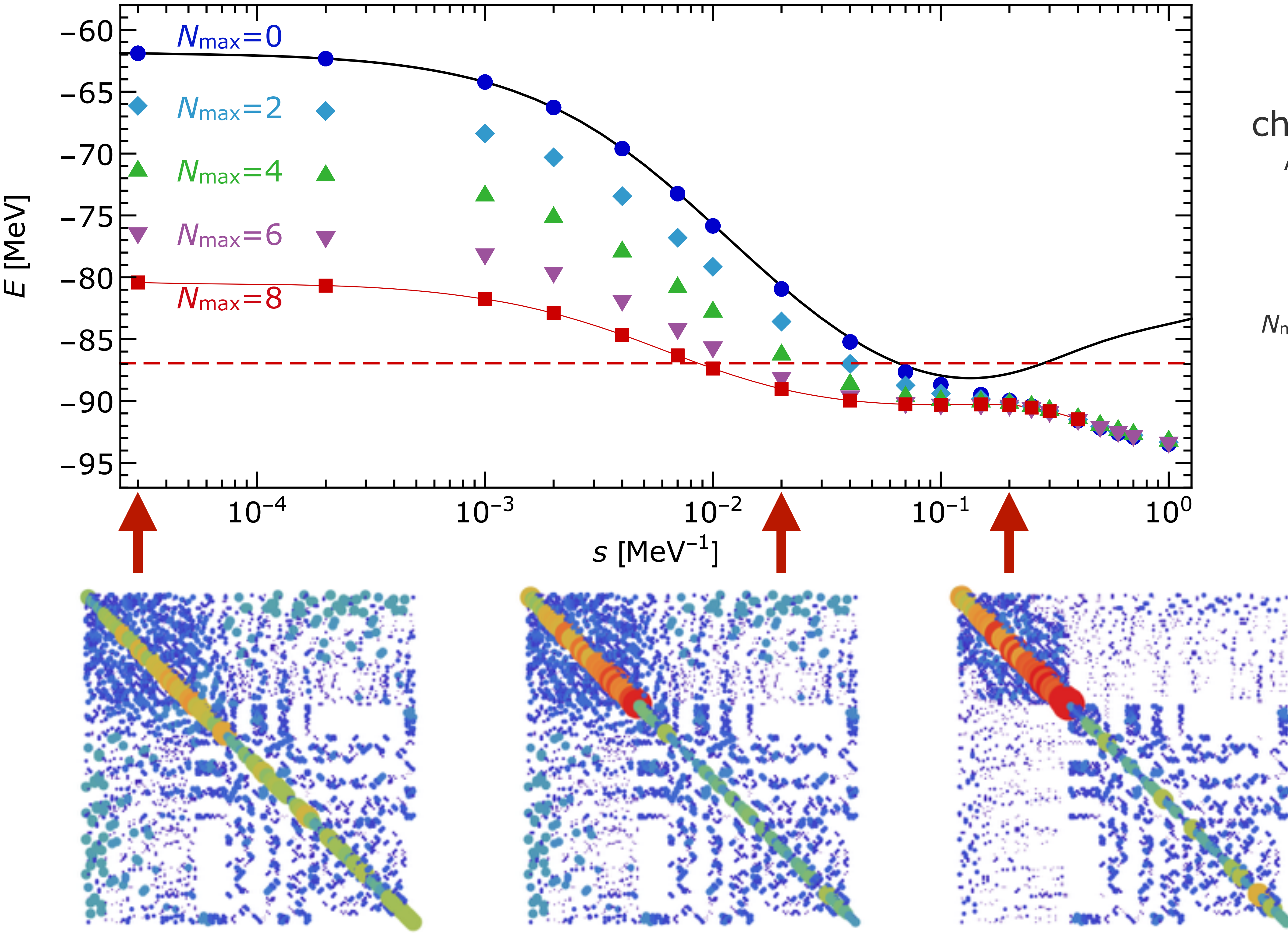
N_{max}=0 reference
HF basis



Hamilton matrix in N_{max}=2 space

In-Medium SRG: Multi Reference

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

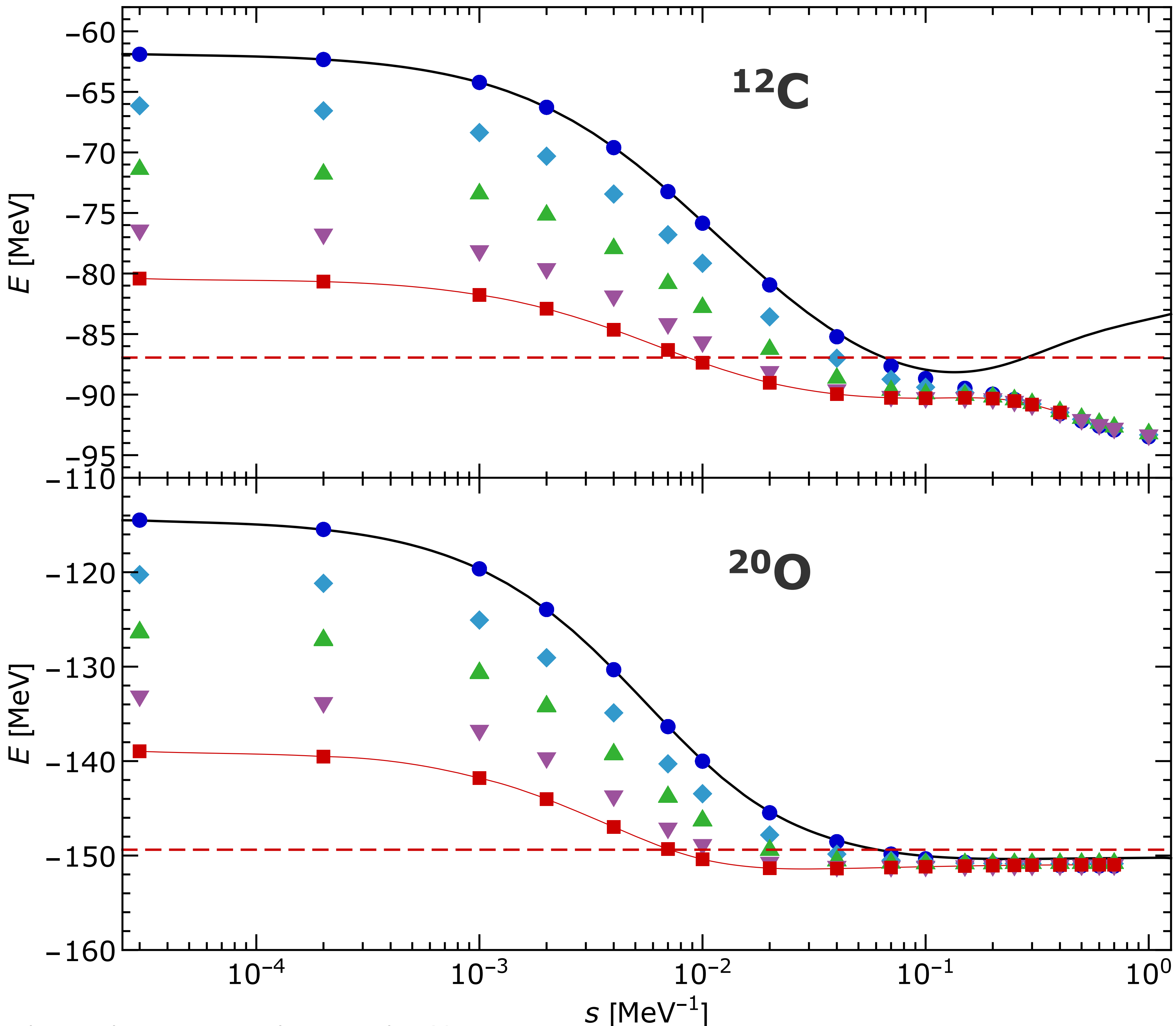
N_{max}=0 reference

HF basis

Hamilton matrix in N_{max}=2 space

Flow: Ground-State Energy

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



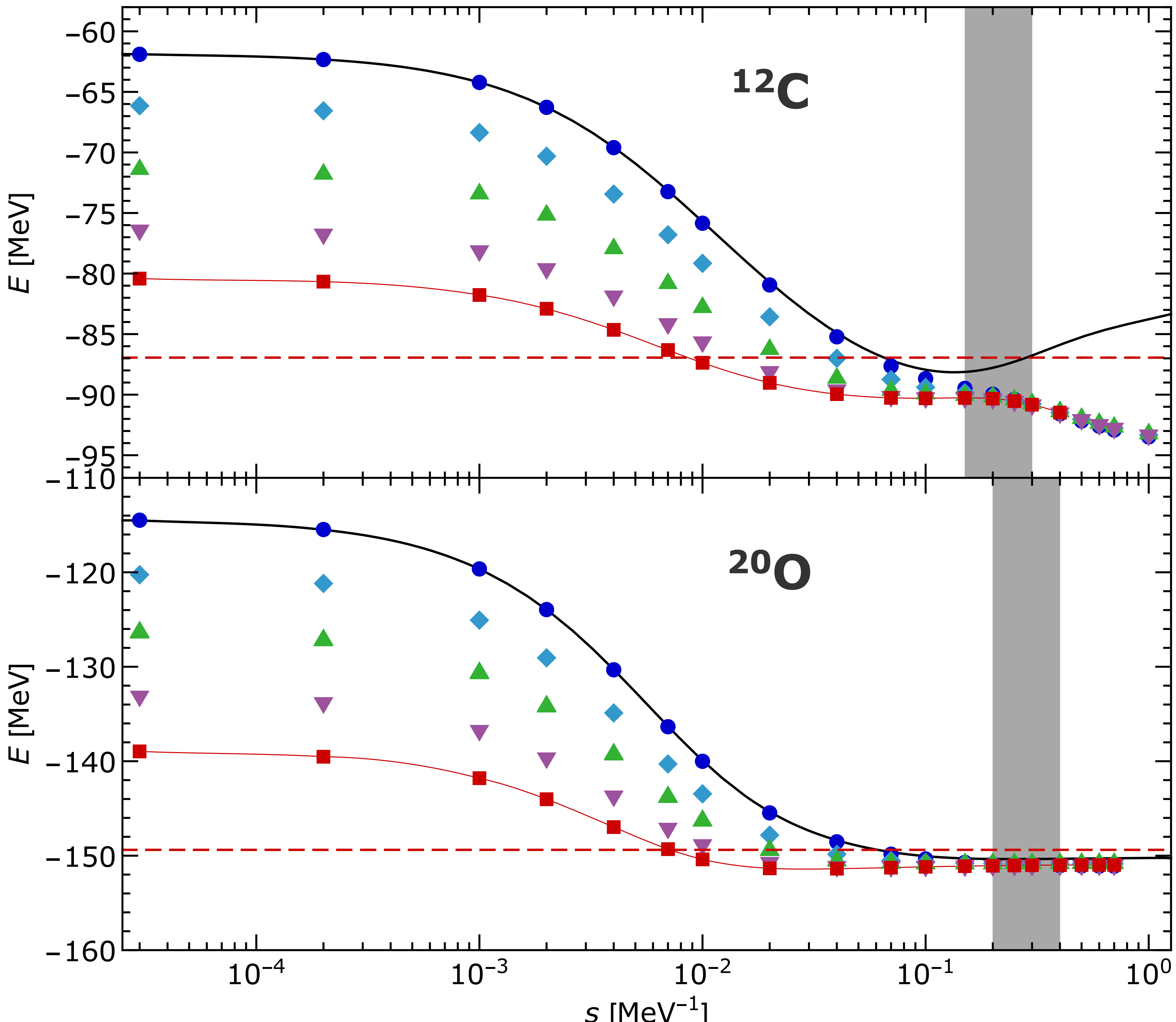
- NCSM convergence is drastically improved
- N_{max}=0 eigenvalues deviated from $E(s)$

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



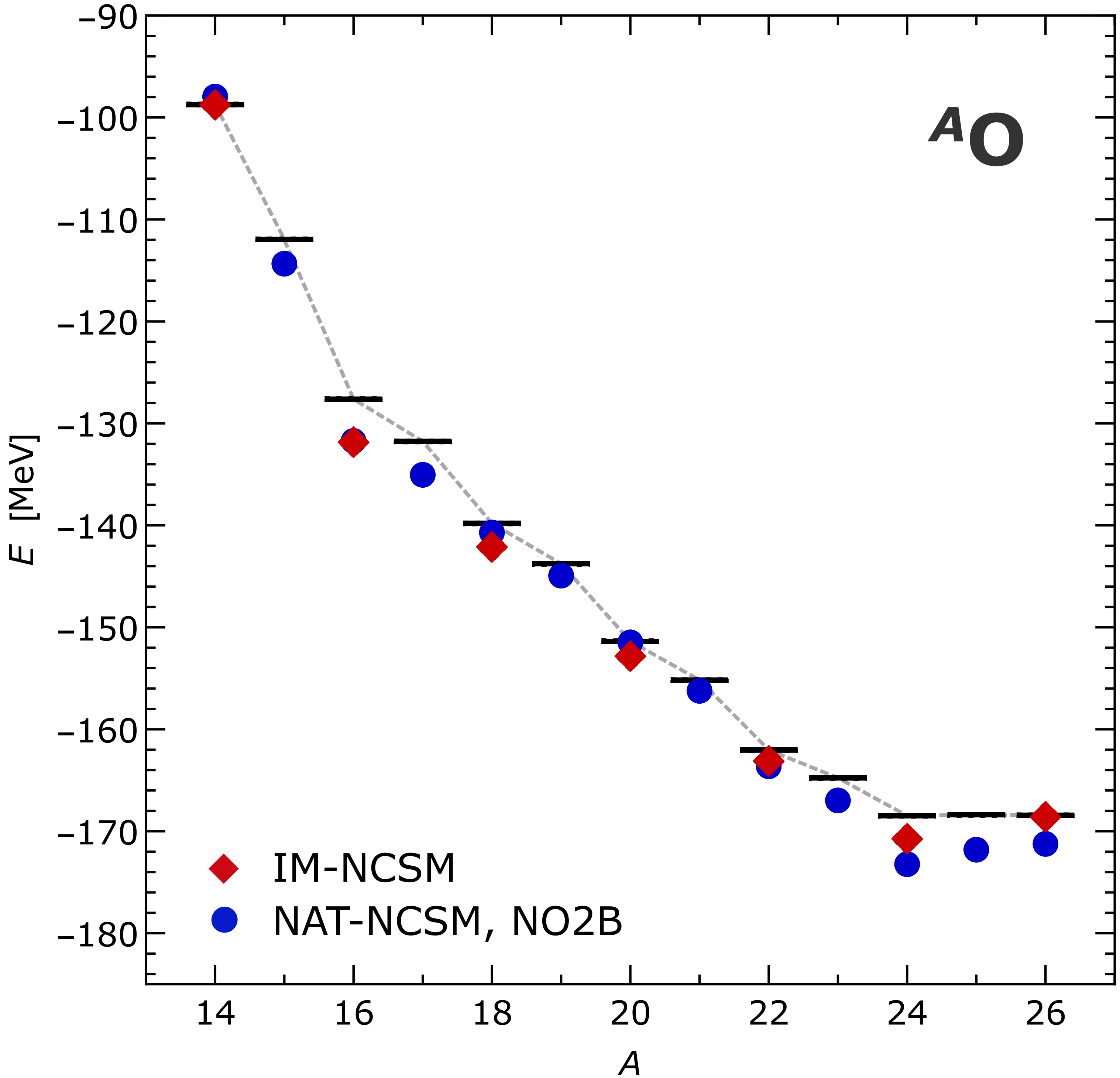
- NCSM convergence is drastically improved
- N_{max}=0 eigenvalues deviated from $E(s)$
- determine energy from flow-parameter region before induced terms become significant

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

Oxygen Isotopes

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



- excellent agreement with direct NCSM; slightly larger deviations from ^{24}O on
- IM-SRG evolution limited to J=0 reference states and thus even-mass isotopes

chiral NN+3N

Λ_{3N}=400 MeV

α=0.08 fm^4

$\hbar\Omega$=20 MeV

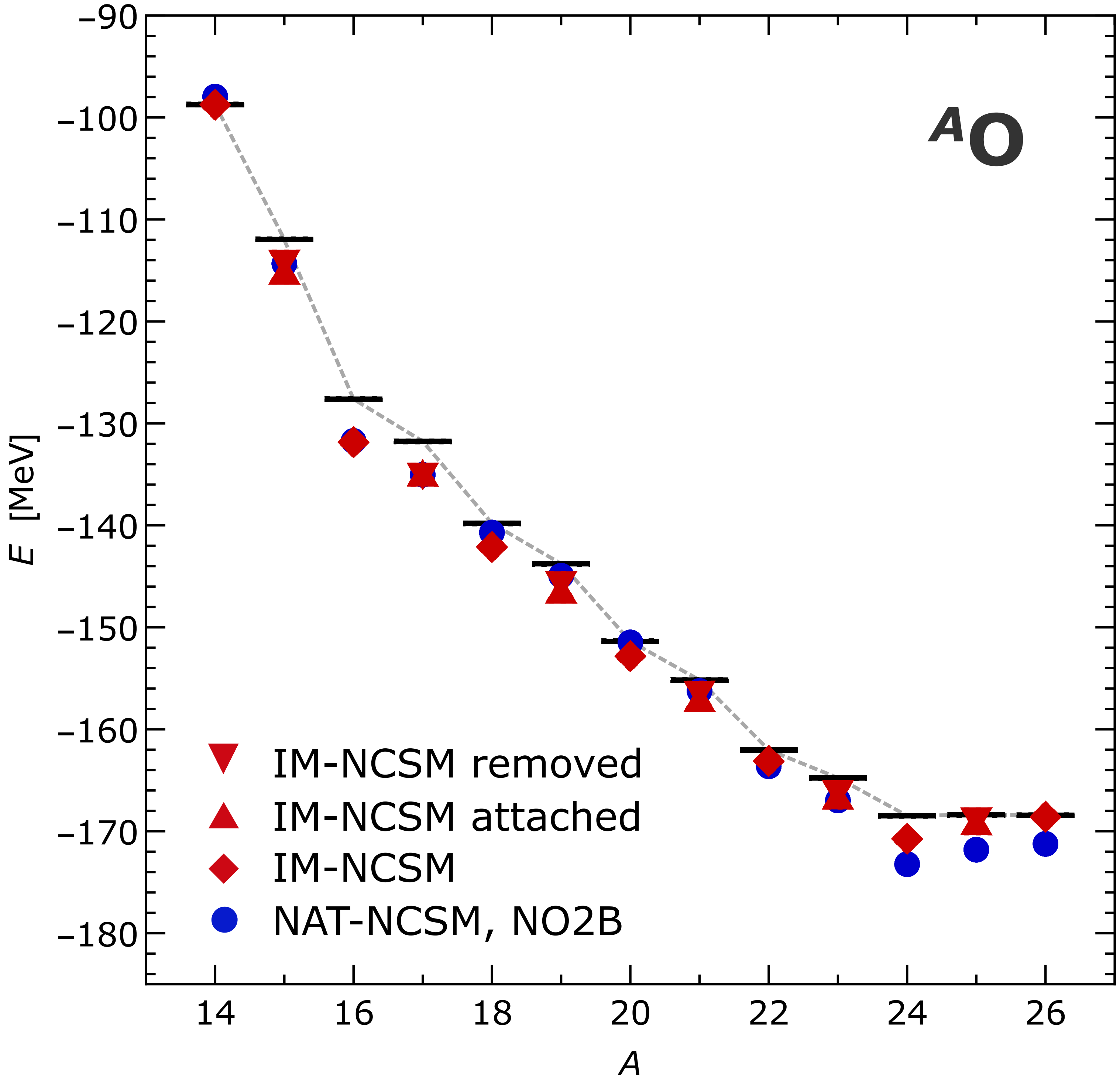
e_{max}=12

HF basis

N_{max}=0 reference

Oxygen Isotopes

Vobig, Gebrerufael, Roth; in prep.



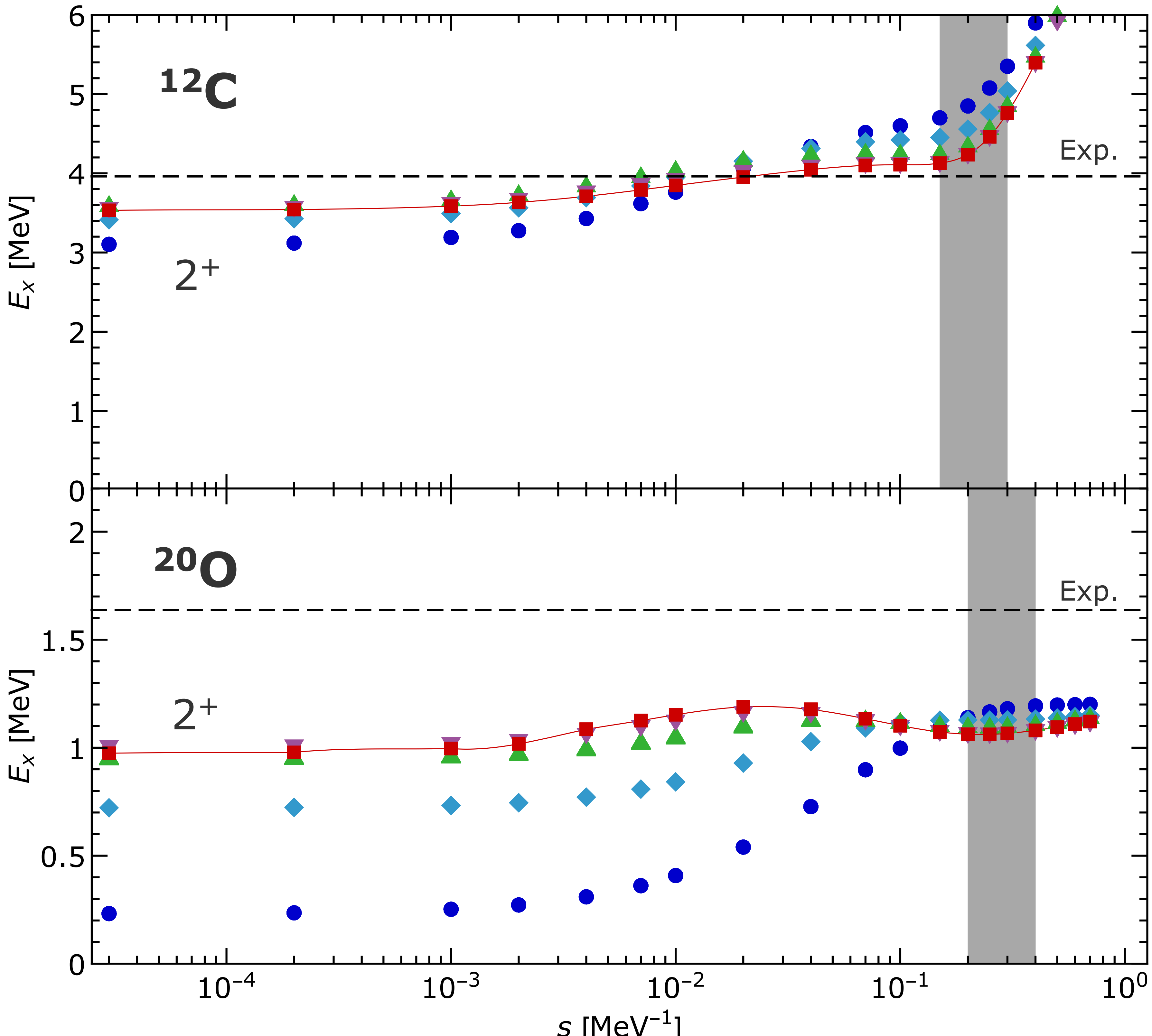
- excellent agreement with direct NCSM; slightly larger deviations from ^{24}O on
- IM-SRG evolution limited to J=0 reference states and thus even-mass isotopes
- odd-mass nuclei via simple particle attachment or removal in final NCSM run

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

HF basis
N_{max}=0 reference

Flow: 2^+ Excitation Energy

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



- 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

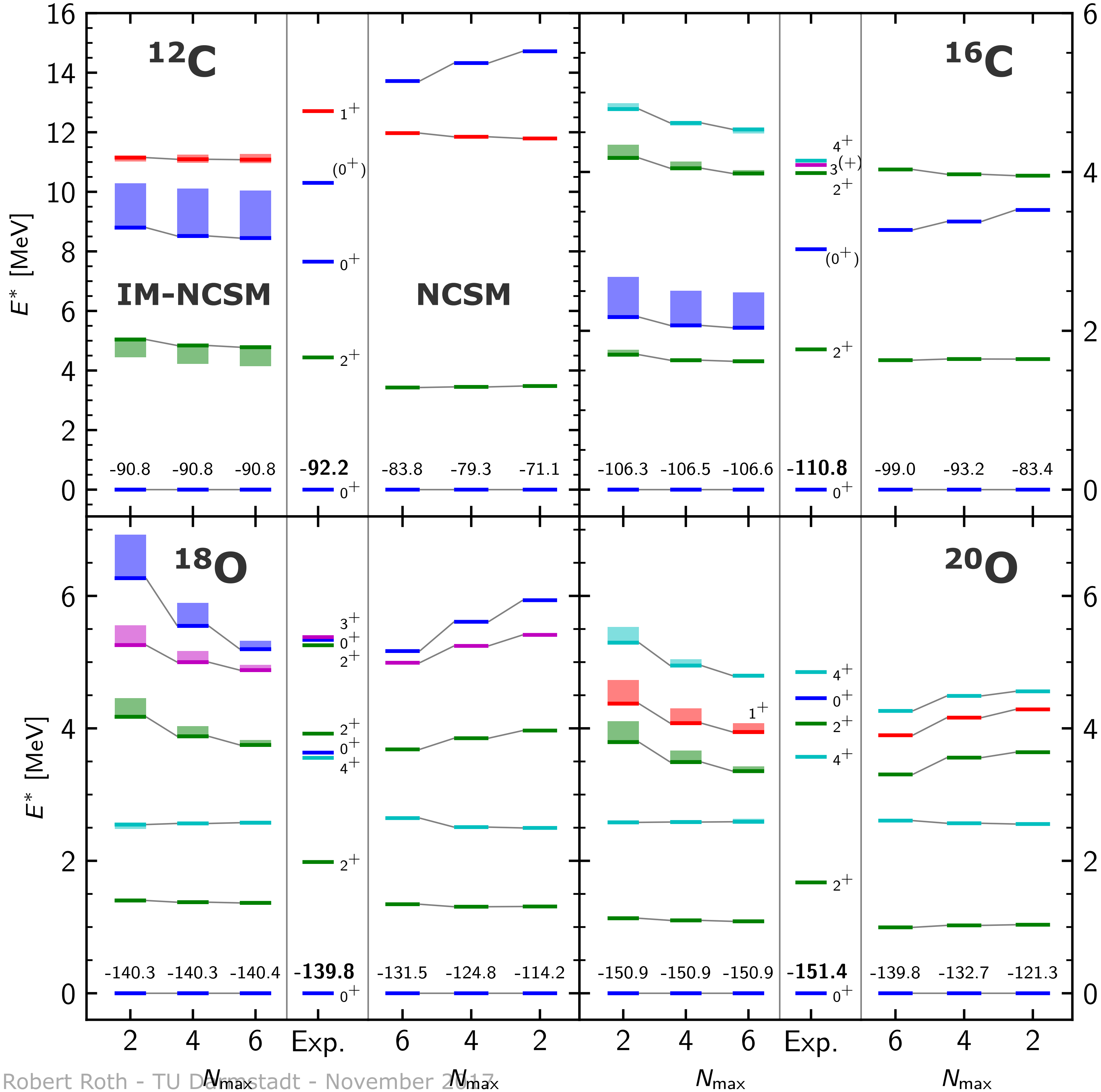
HF basis

N_{max}=0 reference state

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

IM-NCSM: Excitation Spectra

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



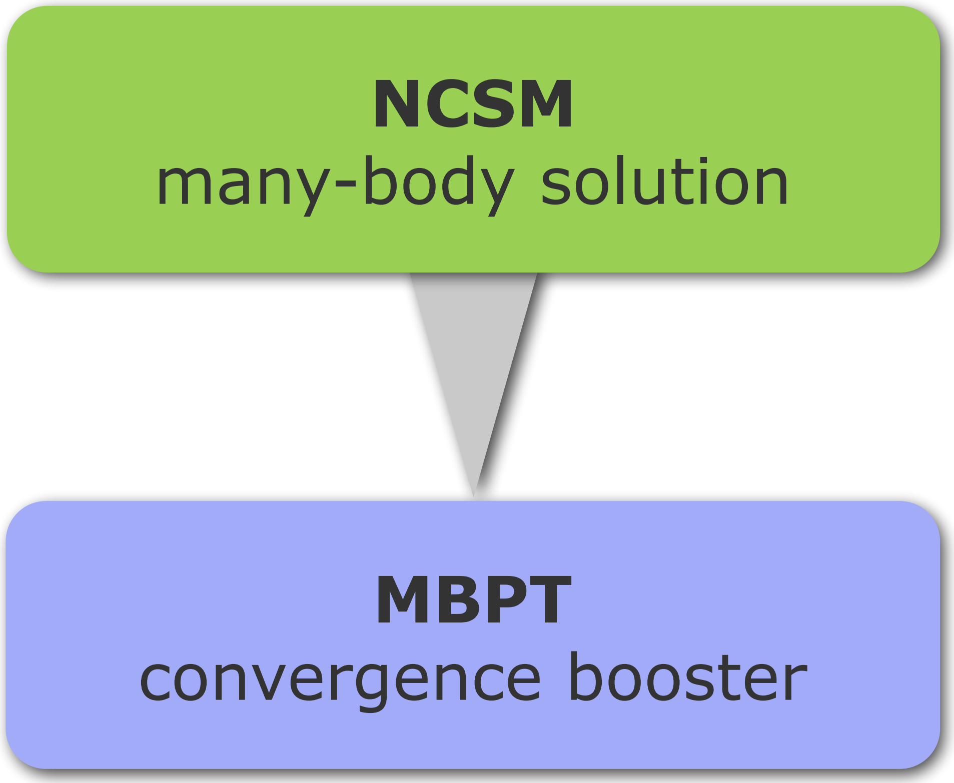
- IM-NCSM and direct NCSM in excellent agreement for converged states
- first excited 0^+ states in ^{12}C and ^{16}C differ

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

HF basis
N_{max}=0 reference

Perturbatively Improved NCSM

Tichai, Gebrerufael, Vobig, Roth; arXiv:1703.05664

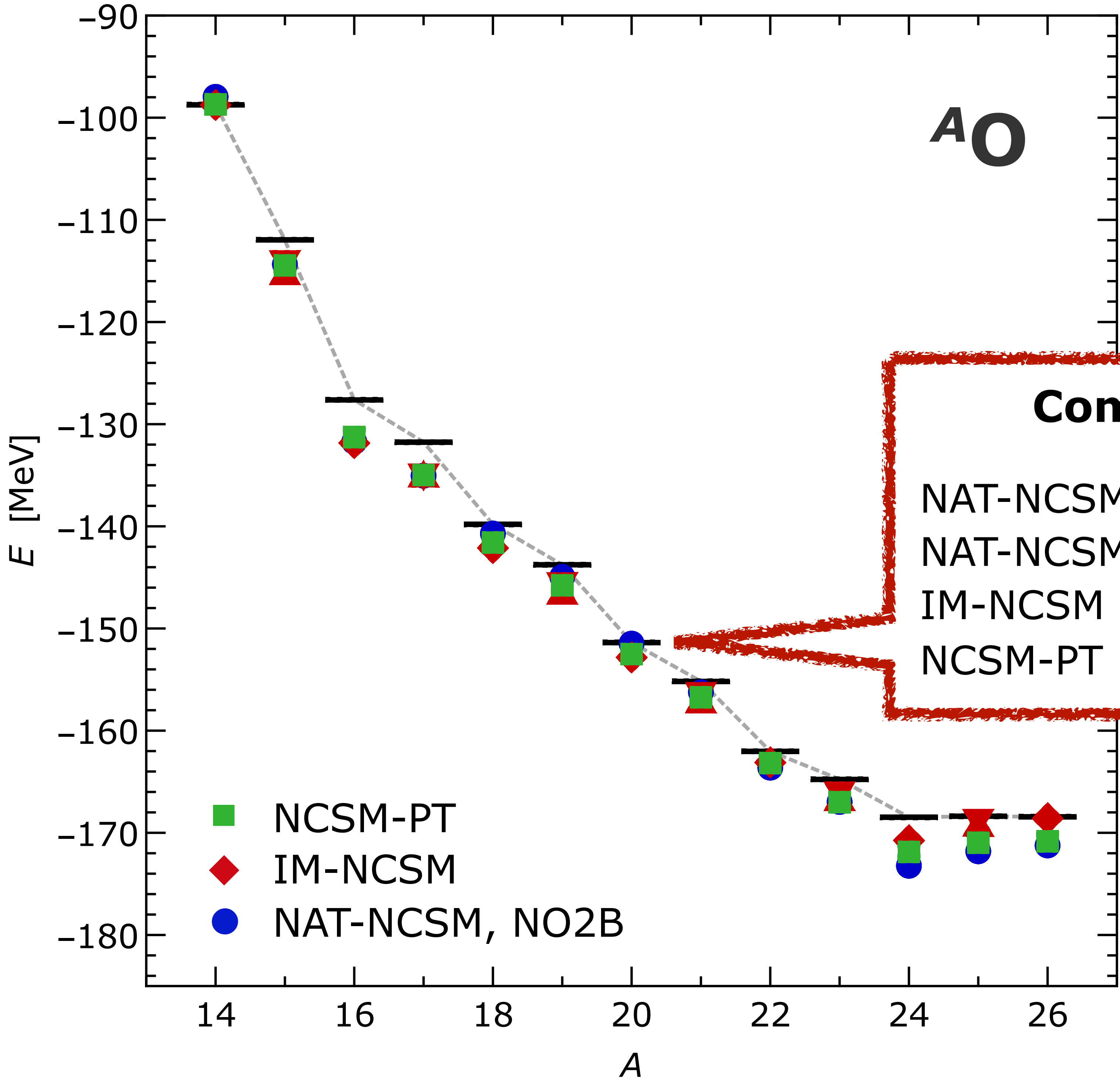


- eigenstates from NCSM at small N_{max} as unperturbed states
- access to all open-shell nuclei and systematically improvable

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

Oxygen Isotopes

Tichai, Gebrerufael, Vobig, Roth; arXiv:1703.05664



- excellent agreement with direct NCSM and IM-NCSM
- all isotopes are accessible due simple m-scheme implementation

Computational Cost

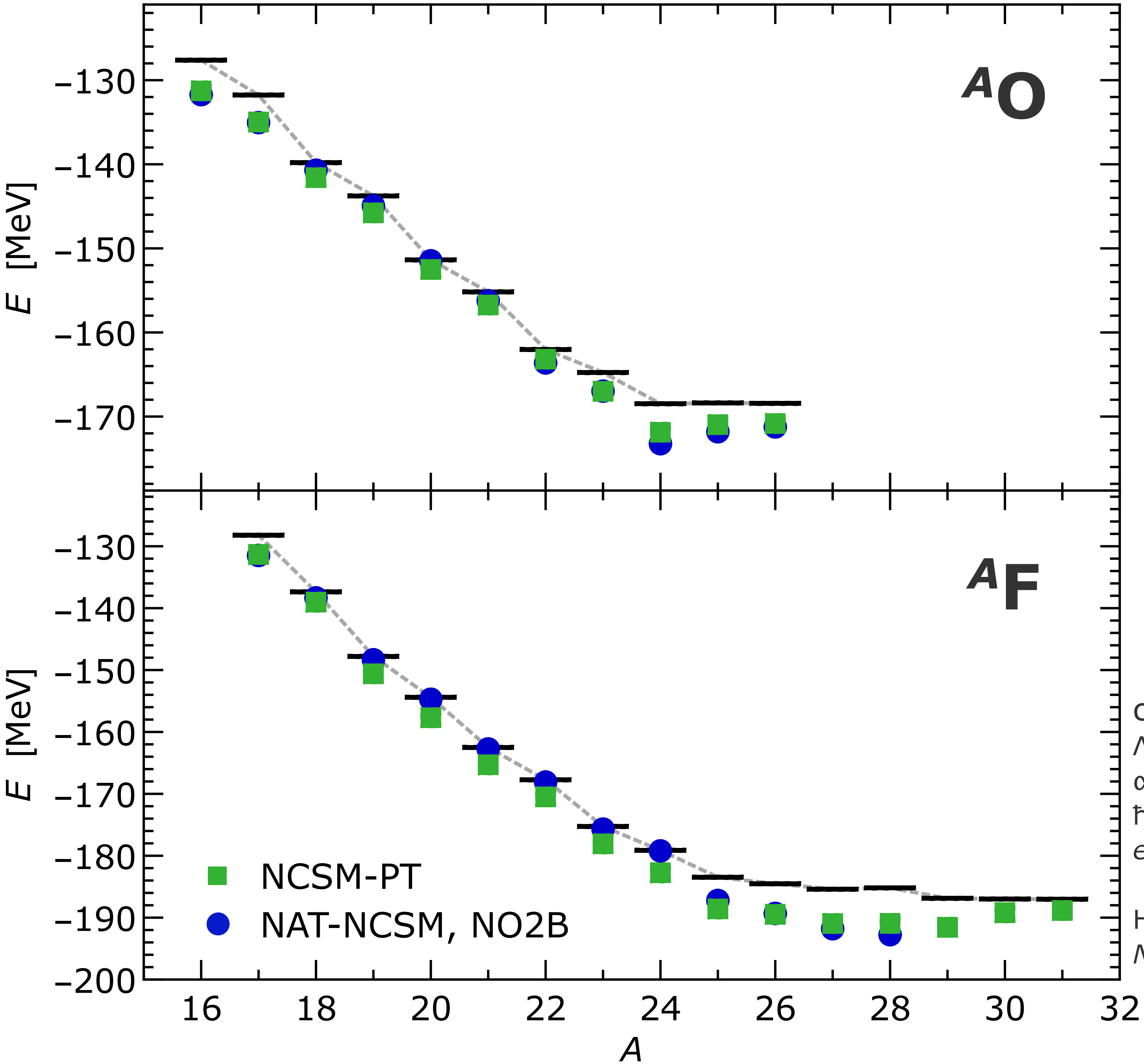
NAT-NCSM, full 3N	20000 CPU-h
NAT-NCSM, NO2B	16000 CPU-h
IM-NCSM	2500 CPU-h
NCSM-PT	1000 CPU-h

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

HF basis
N_{max}=2 reference

Exploring sd-Shell Phenomena

Tichai, Gebrerufael, Vobig, Roth; in prep.



- exploring sd-shell phenomena: oxygen anomaly and island of inversion

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

HF basis
N_{max}=2 reference

Strength-Function NCSM

Stumpf, Wolfgruber, Roth; arXiv:1709.06840

NCSM
ground state

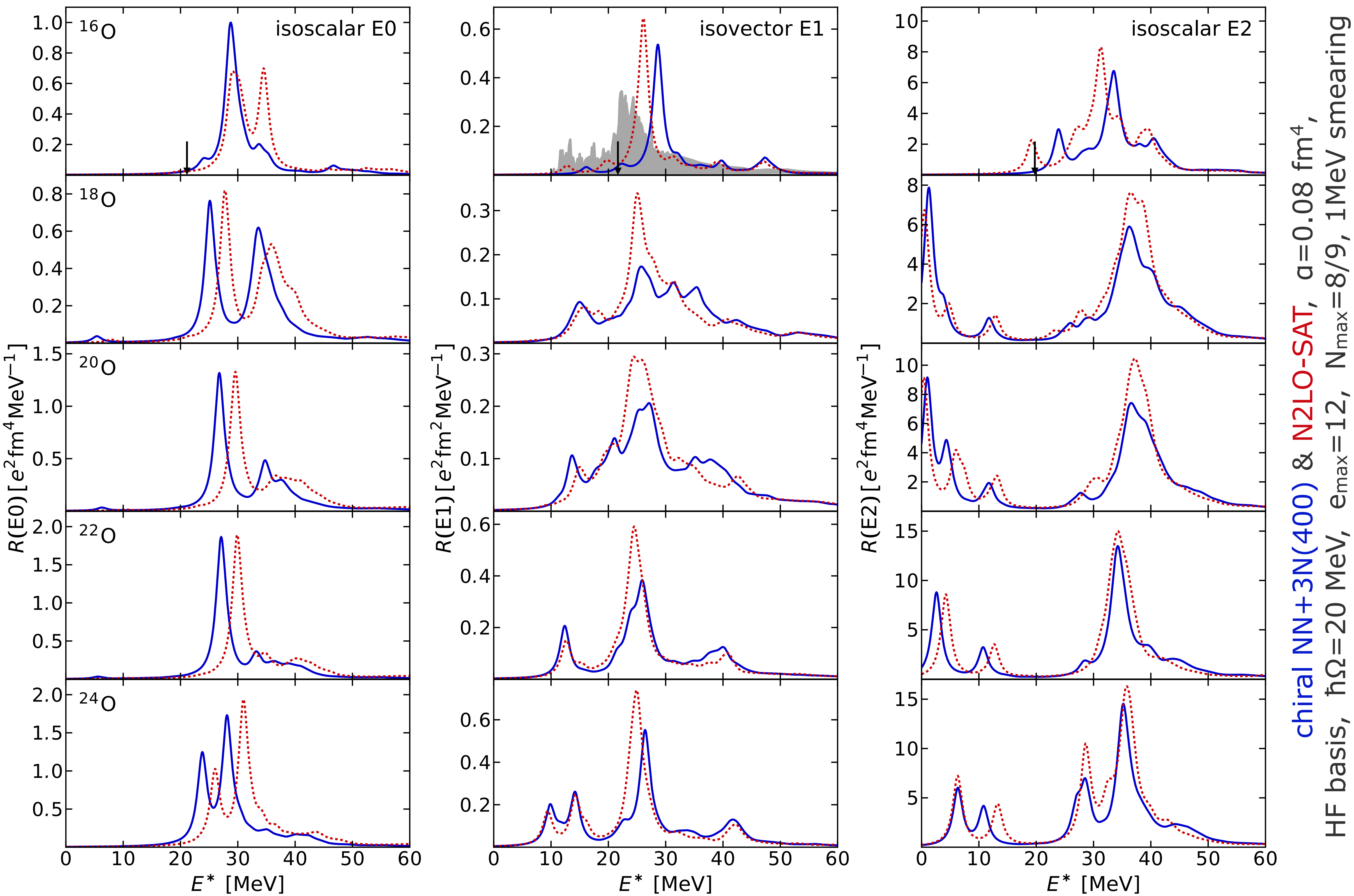
- regular NCSM calculation for ground state for a range of N_{max} truncations
- access to all open-shell nuclei

NCSM
strength distribution

- prepare pivot vector by applying transition operator to ground-state vector
- use Lanczos strength-function method to generate strength distribution

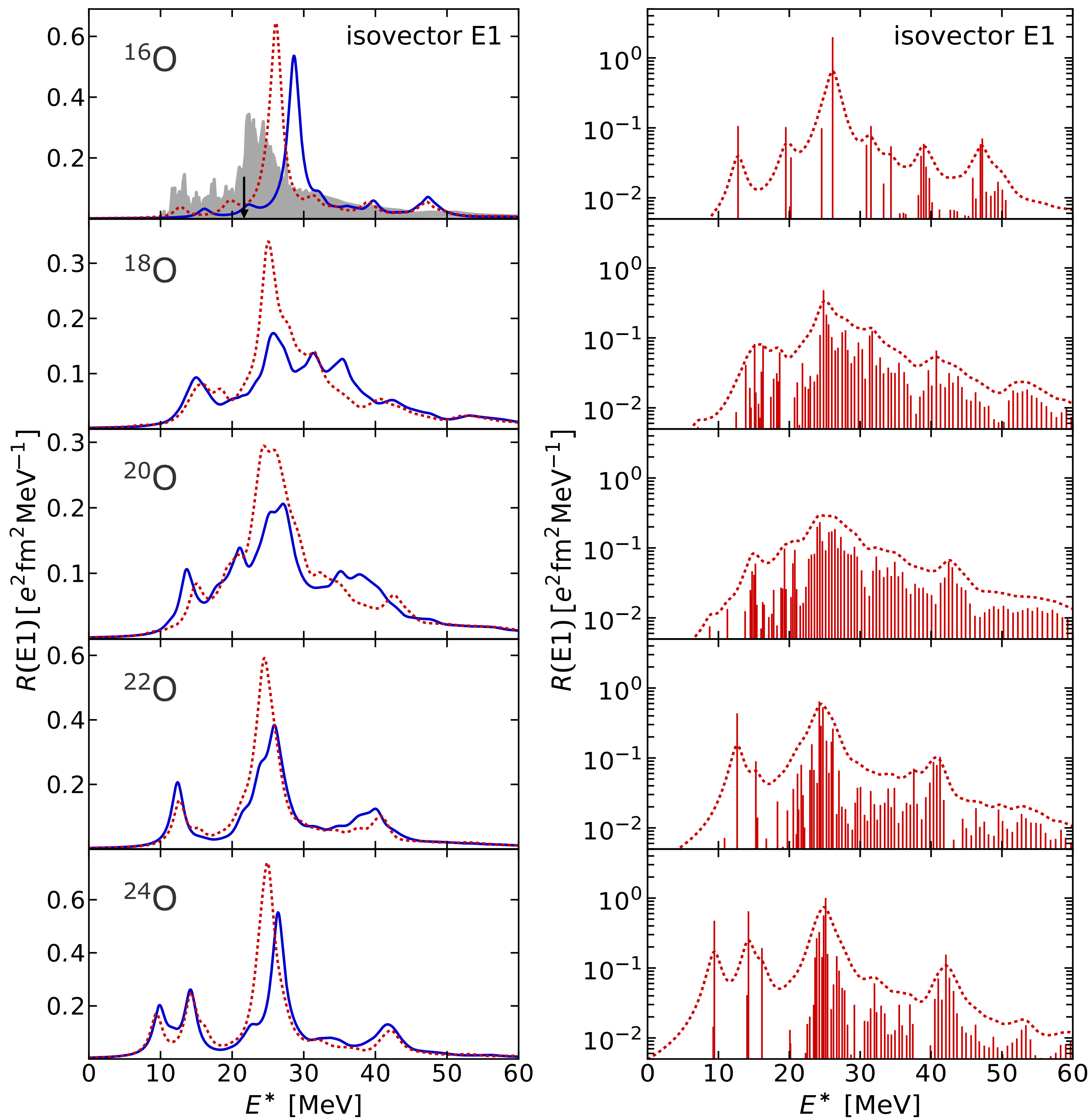
Strength-Function NCSM

Stumpf, Wolfgruber, Roth; arXiv:1709.06840



Strength-Function NCSM

Stumpf, Wolfgruber, Roth; arXiv:1709.06840



- strength distributions are fully converged
- account for low-lying strength around threshold, fragmentation, fine structure
- structural changes with increasing neutron number
- eliminate notorious problems with RPA or Second RPA

chiral NN+3N(400)
N2LO-SAT
α=0.08 fm^4
$\hbar\Omega$=20 MeV
e_{max}=12
HF basis
N_{max}=8/9

Conclusions

NAT-NCSM	IM-NCSM	NCSM-PT	SF-NCSM
MBPT basis optimization	**NCSM** reference state	**NCSM** many-body solution	**NCSM** ground state
NCSM many-body solution	**IM-SRG** decoupling	**MBPT** convergence booster	**NCSM** strength distribution
	NCSM many-body solution		

- development of new ab initio methods still going strong
- hybrids built on the NCSM enable comprehensive access to ground and excited states of arbitrary open-shell nuclei
- mass reach:
  A≲30 if large $N_{\max}$ is needed: NAT-NCSM, SF-NCSM
  A≲70 if small $N_{\max}$ is sufficient: IM-NCSM, NCSM-PT
- more hybrids: NCSM with Continuum **[see Petr Navratil's talk]**

Epilogue

- **thanks to my group and my collaborators**
  - S. Alexa, D. Derr, E. Gebrerufael, A. Geißel, T. Hüther, L. Mertes, J. Müller, S. Schulz, C. Stumpf, A. Tichai, K. Vobig, R. Wirth
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