New Horizons for the No-Core Shell Model

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No-Core Shell Model & Friends

No-Core Shell Model

- 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

- 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

No-Core Shell Model & Friends

No-Core Shell Model

In-Medium Similarity Renormalization Group

Many-Body Perturbation Theory

- complementarity of advantages and limitations of the different methods
- combine NCSM with other 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

Hybrid NCSM Methods

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

Natural-Orbital NCSM

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

Natural Orbitals from MBPT

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

- perform constrained **spherical Hartree-Fock calculation** to obtain unperturbed single-particle basis and ground state
- compute **MBPT corrections to HF ground state** up to second order

$$|\Psi^{(PT)}\rangle = |HF\rangle + |\Psi^{(1)}\rangle + |\Psi^{(2)}\rangle$$

- evaluate **one-body density matrix** with perturbed state up to second order

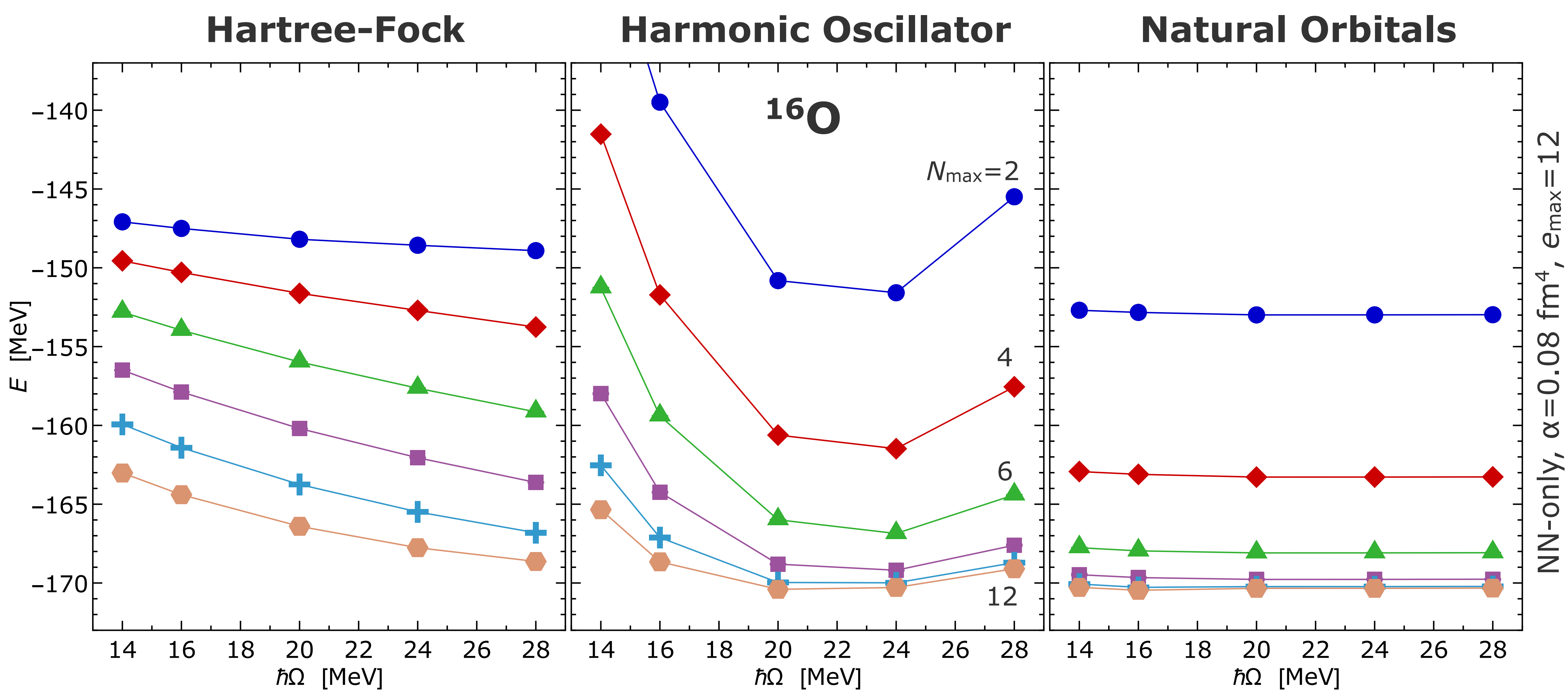
$$\rho^{(PT)}_{ij} = \rho^{(HF)}_{ij} + 2\rho^{(02)}_{ij} + \rho^{(11)}_{ij}$$

$$\rho^{(HF)}_{ij} = \langle HF|\, a^\dagger_i a_j \,|HF\rangle \,, \qquad \rho^{(02)}_{ij} = \langle HF|\, a^\dagger_i a_j \,|\Psi^{(2)}\rangle \,, \qquad \rho^{(11)}_{ij} = \langle \Psi^{(1)}|\, a^\dagger_i a_j \,|\Psi^{(1)}\rangle$$

- write density-matrix corrections in terms of **single-particle summations**, evaluation only takes minutes...
- solve **eigenvalue problem of one-body density matrix**, eigenvectors define expansion coefficients of natural-orbital single-particle states
- transform all input matrix elements to natural-orbital basis

NCSM Convergence: Energies

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



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

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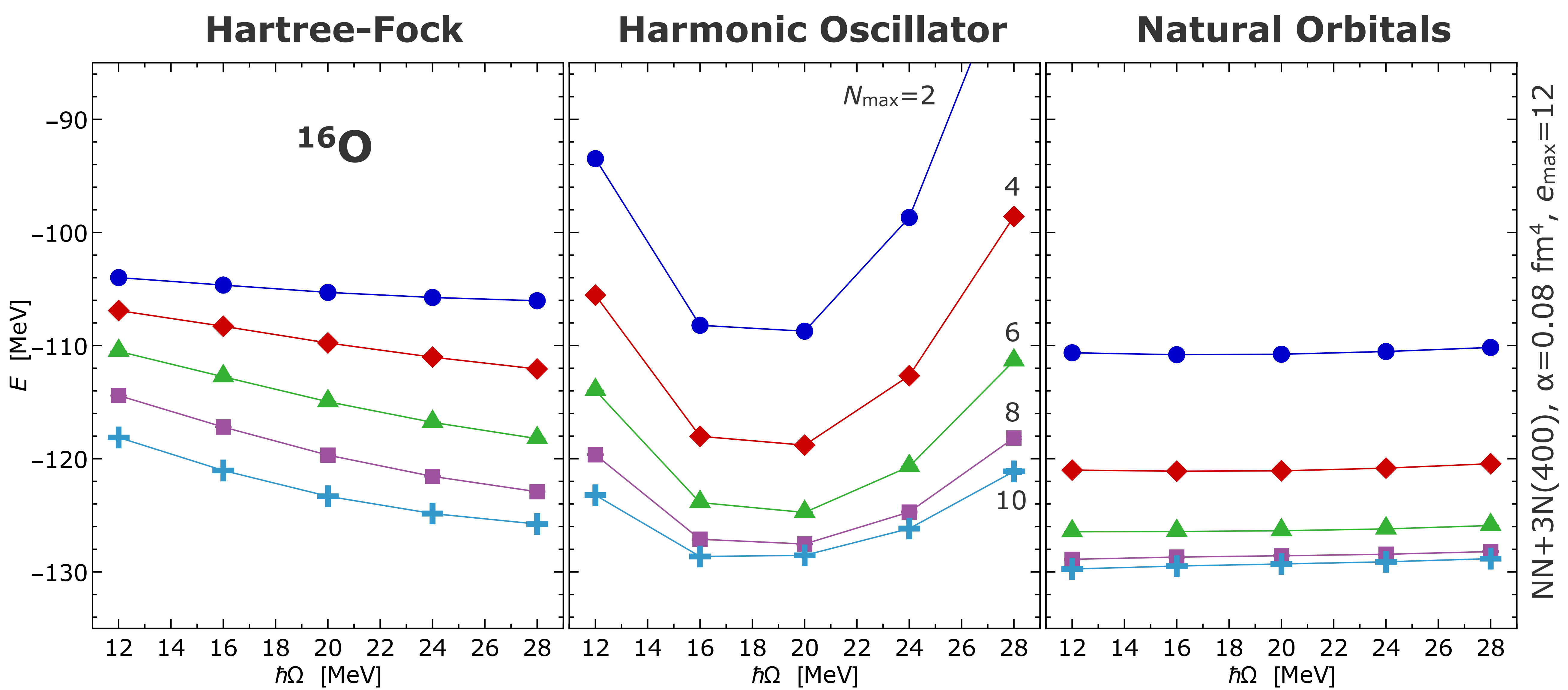

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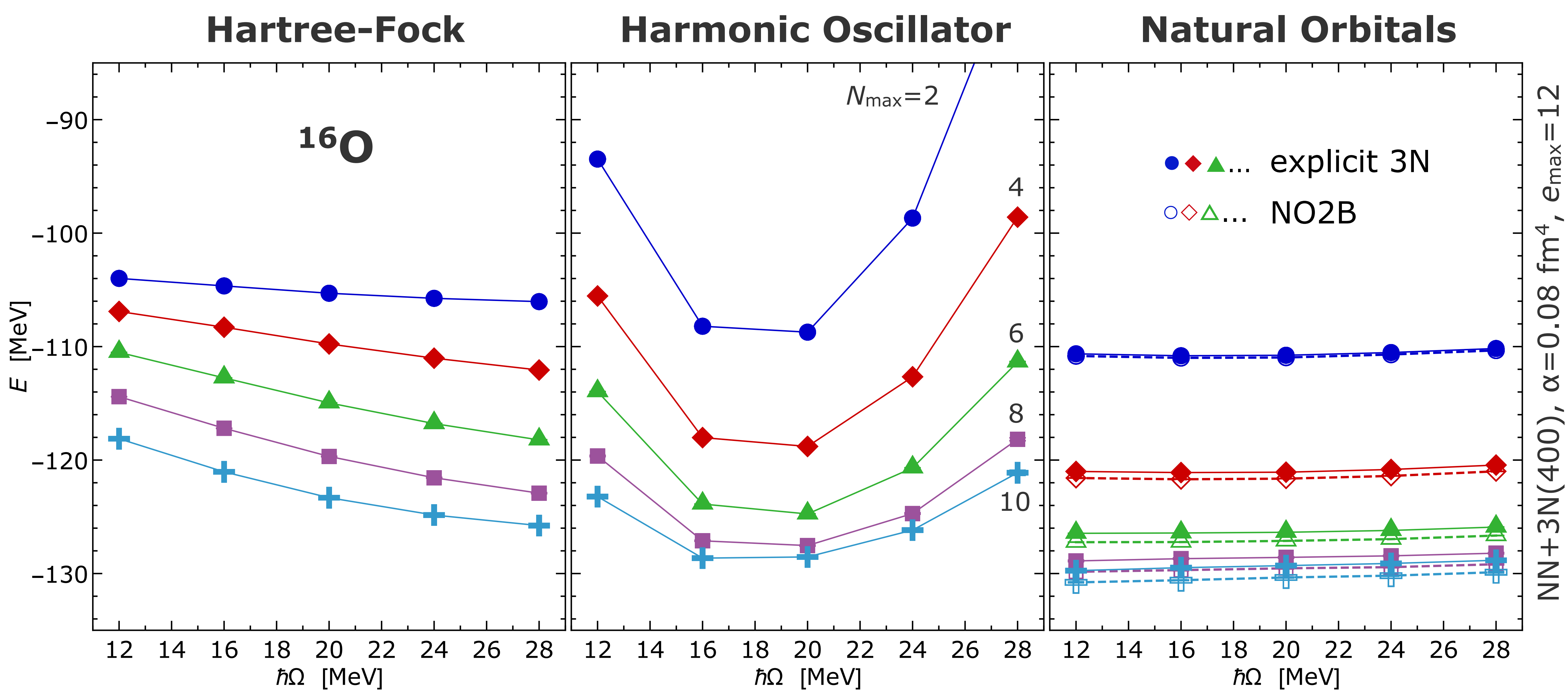

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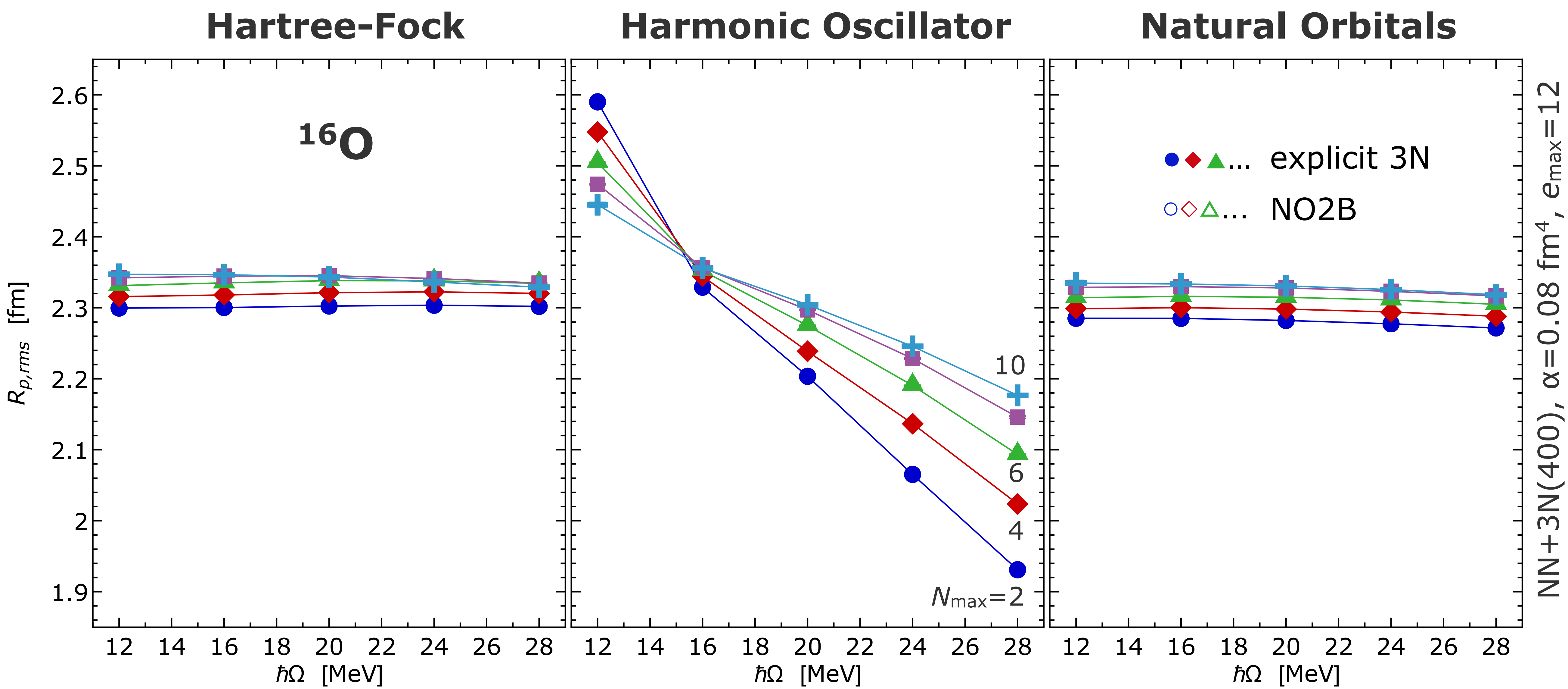
NCSM Convergence: Radii

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



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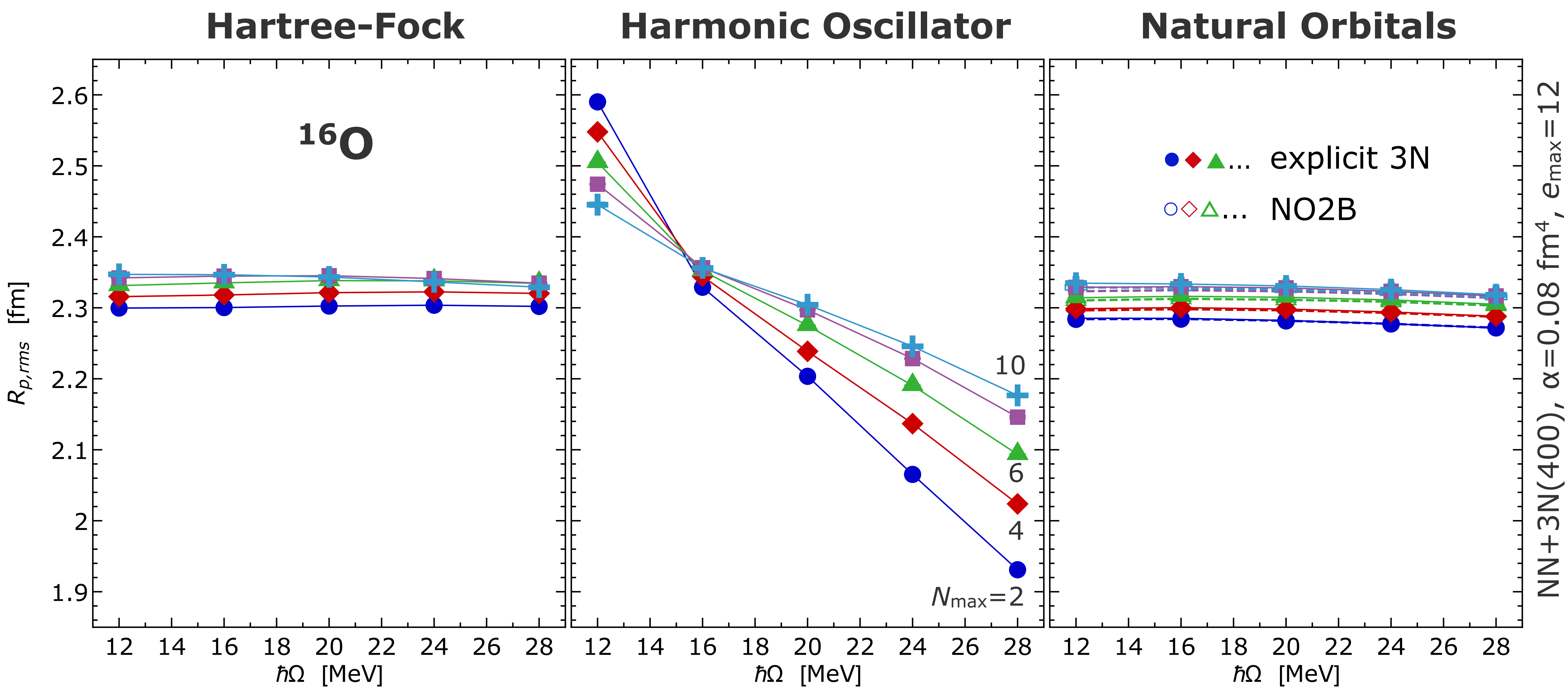

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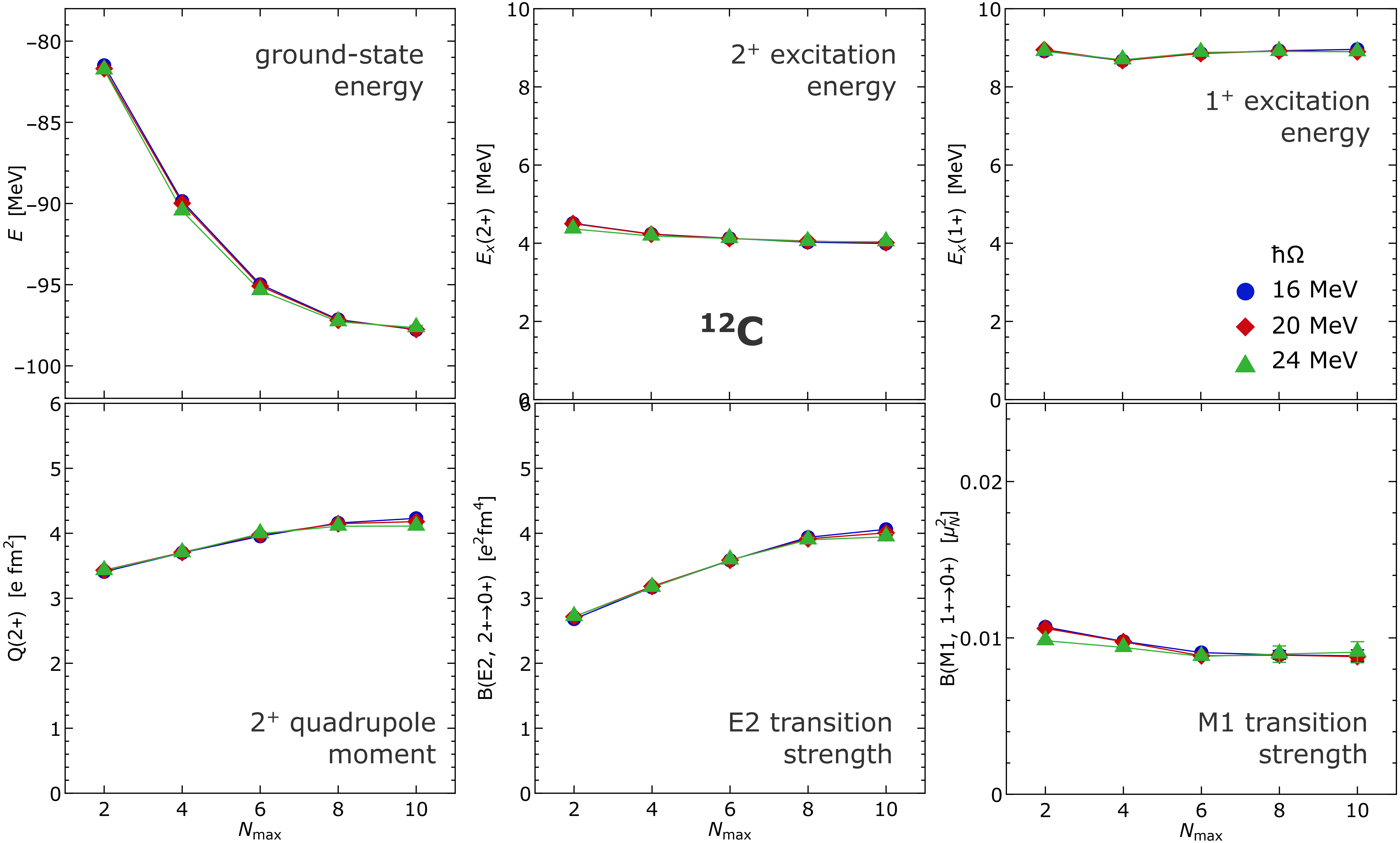
NCSM Convergence: Spectroscopy

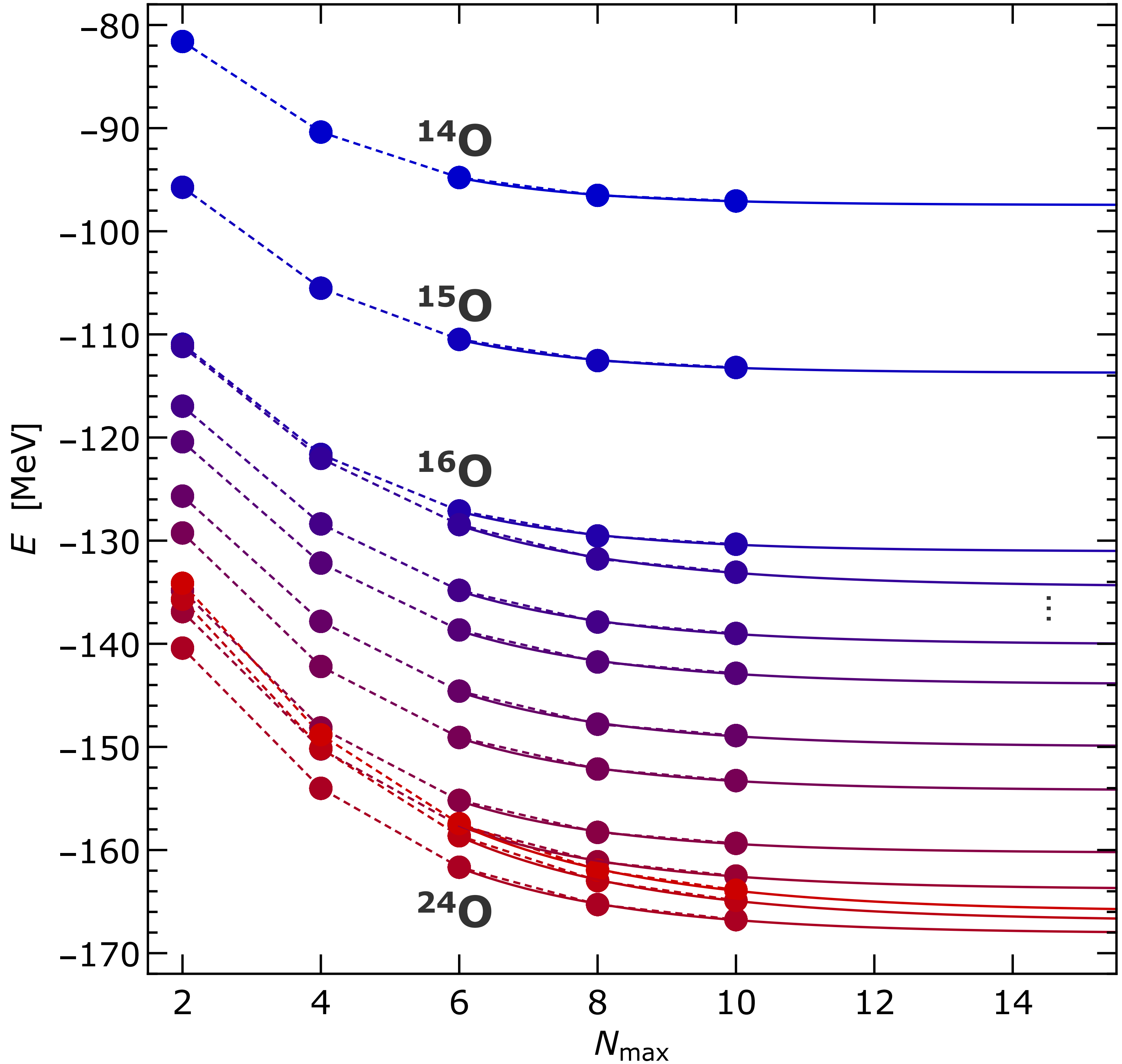
J. Müller, A. Tichai, K. Vobig, R. Roth, in prep.



NN+3N(500), α=0.08 fm^4, e_{max}=12

Oxygen Isotopes

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



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

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

Oxygen Isotopes

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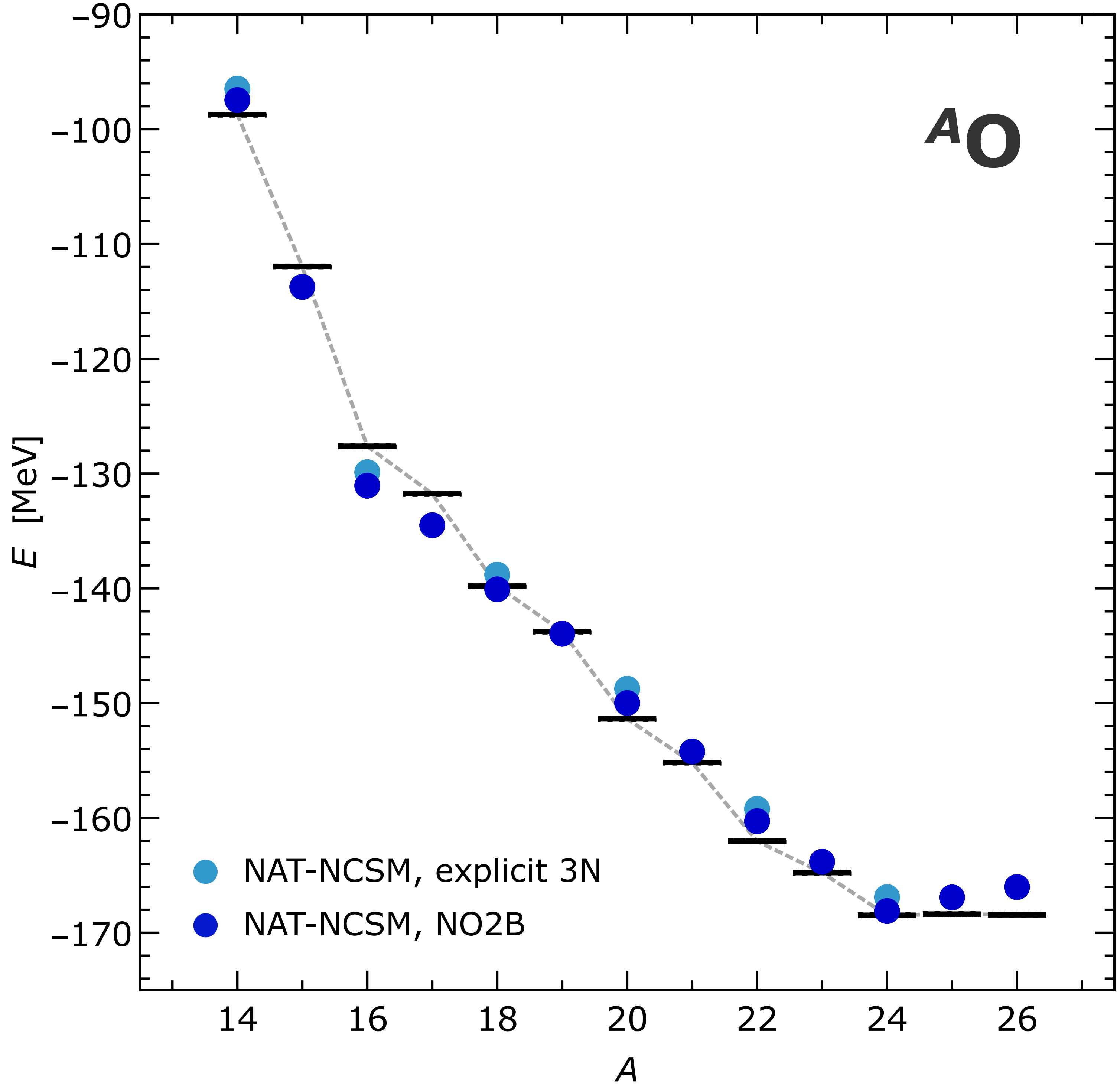

- excellent convergence with natural-orbital basis for all oxygen isotopes
- very good agreement with experimental systematics and dripline
- NO2B instead of explicit 3N causes ~1% overbinding

chiral NN+3N
Λ_{3N}=400 MeV
α=0.08 fm^4
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Perturbatively Improved NCSM

Perturbatively Improved NCSM

Tichai, Gebrerufael, Vobig, Roth; arXiv:1703.05664

NCSM
many-body solution

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

MBPT
convergence booster

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

Multi-Configurational Perturbation Theory

Tichai, Gebrerufael, Vobig, Roth; arXiv:1703.05664

- 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**

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

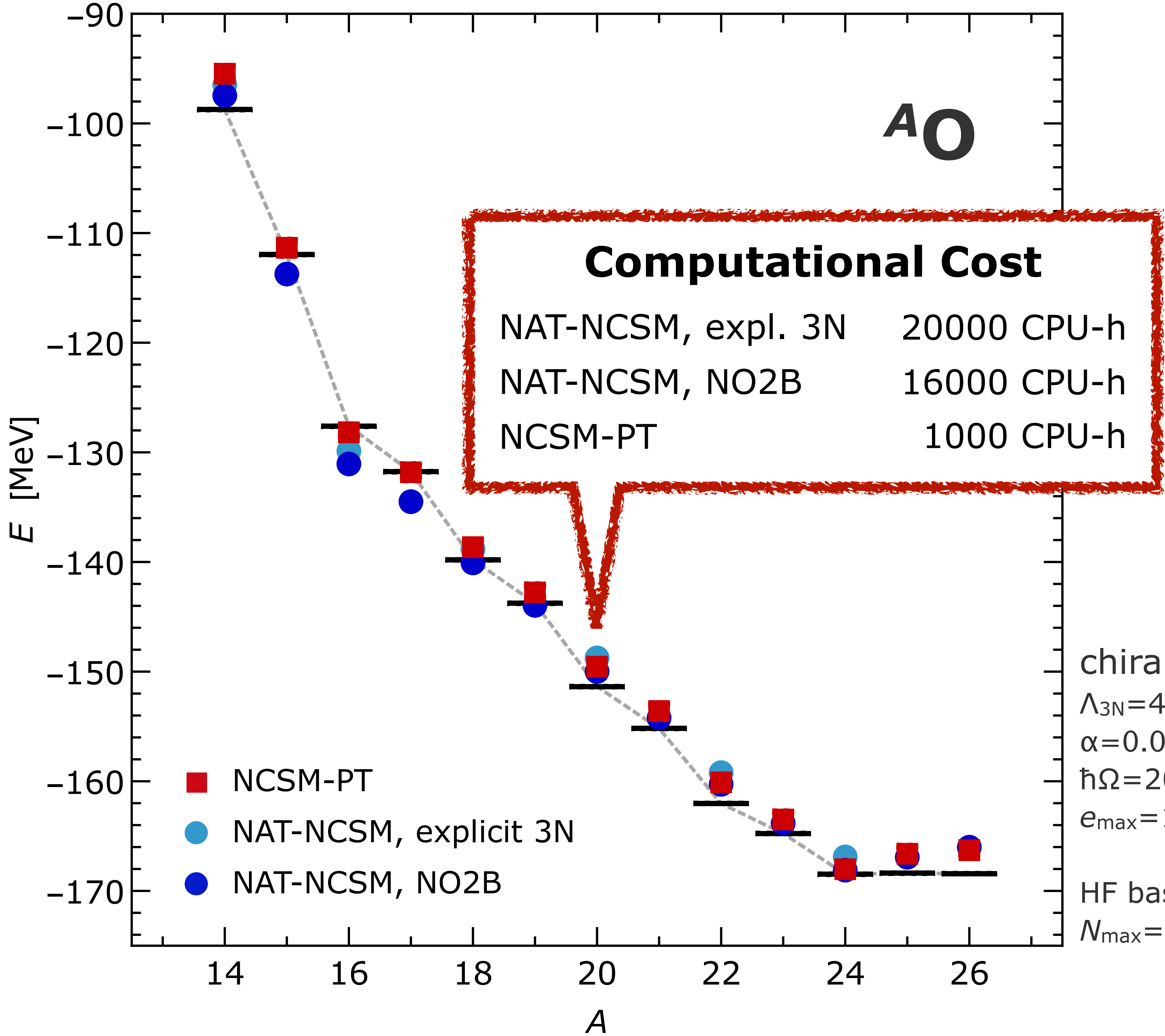
- evaluate **second-order correction** to the energy at many-body level

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

- reformulation in terms of **single-particle summations** gives access to very large model spaces

Oxygen Isotopes

Tichai, Gebrerufael, Vobig, Roth; arXiv:1703.05664



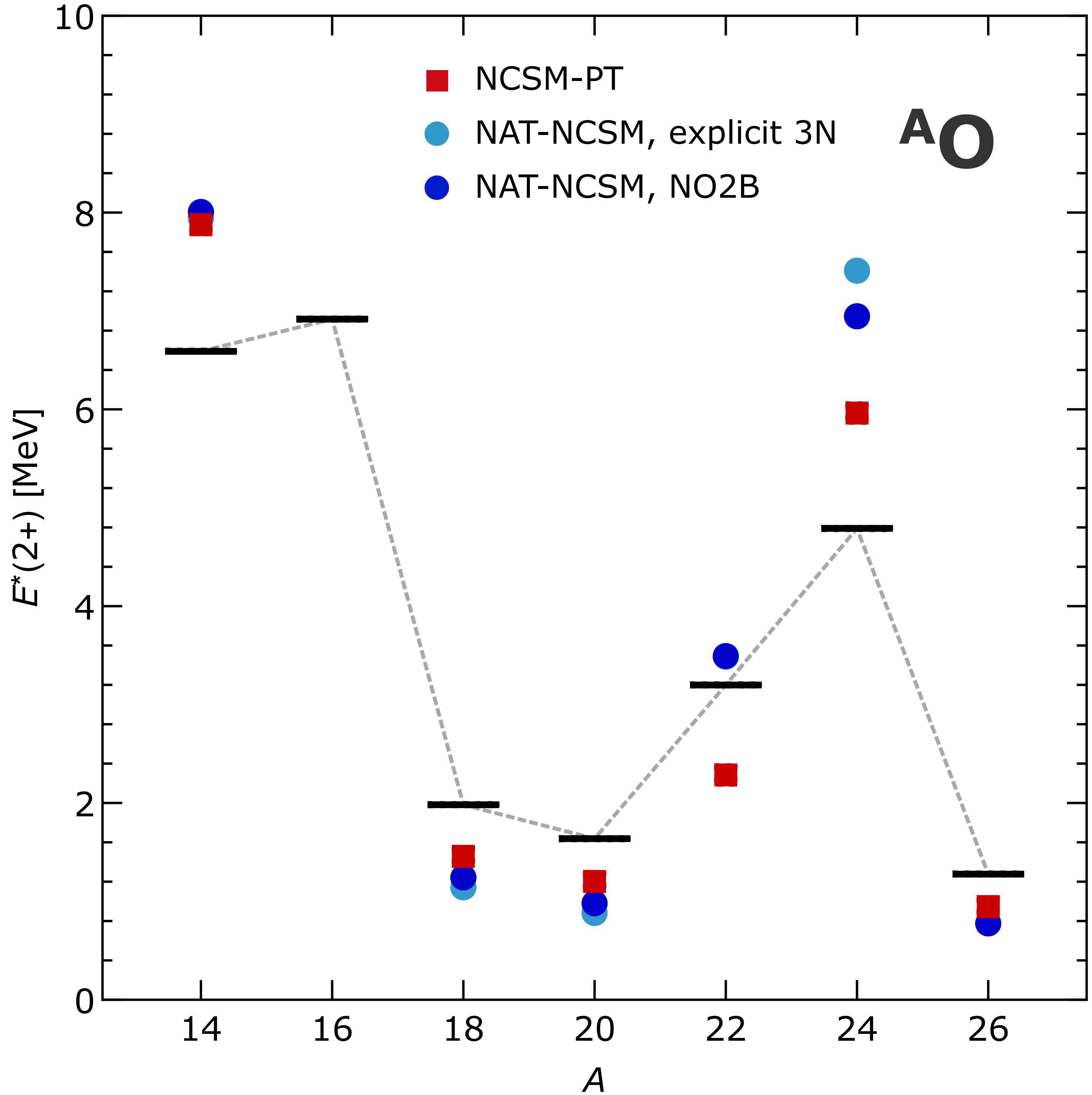
- excellent agreement with direct NCSM
- all isotopes are accessible due simple m-scheme implementation

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

Oxygen Isotopes: Excited 2^+ States

Tichai, et al.; in prep.



- all methods can treat excited states natively
- example: first 2^+ states in even oxygen isotopes
- excellent agreement among methods except for closed (sub-)shells ^{22}O, ^{24}O…

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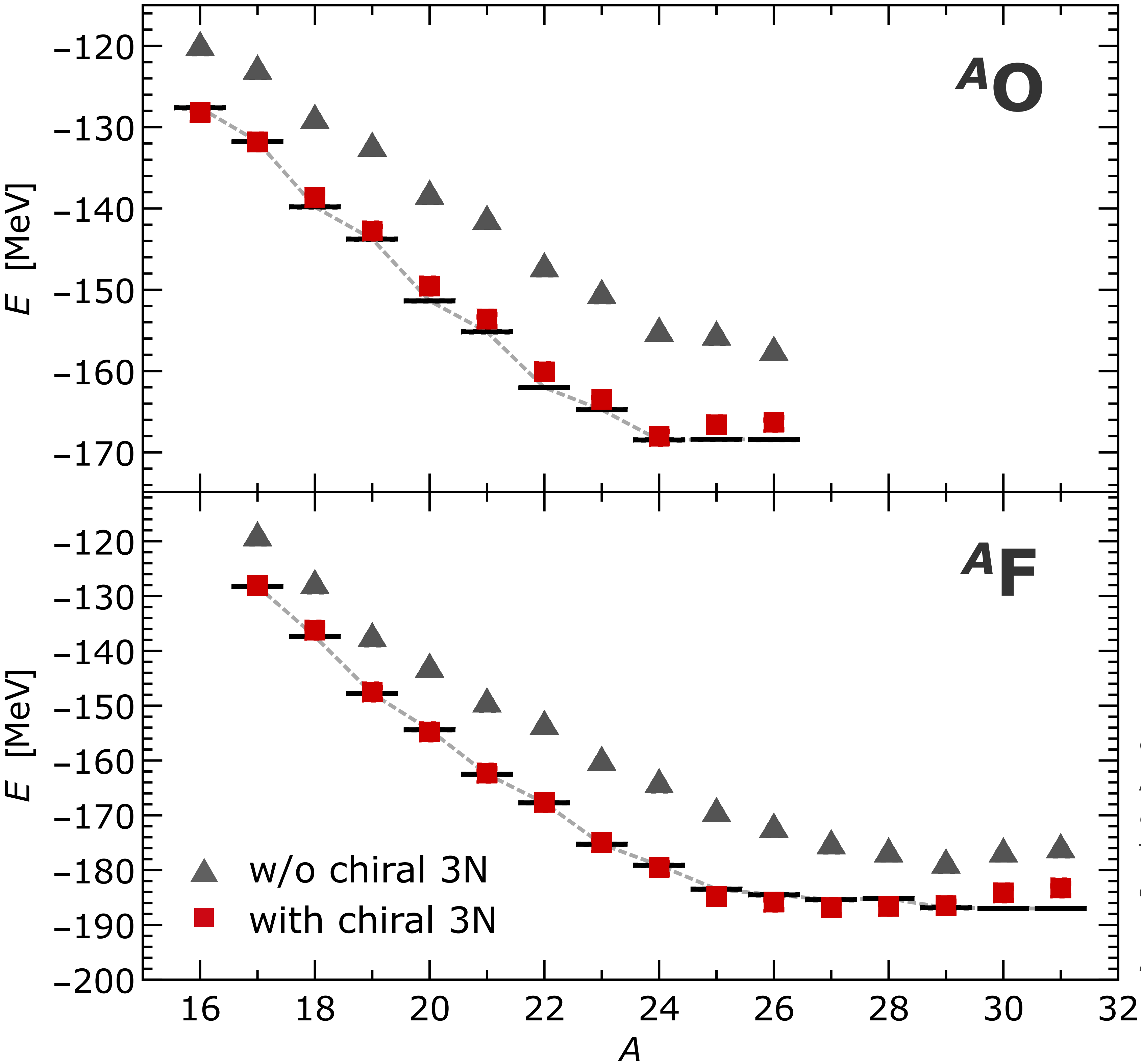
e_{max}=12

HF basis
N_{max}=2 reference

Exploring sd-Shell Phenomena

Tichai, Gebrerufael, Vobig, Roth; arXiv:1703.05664



- exploring sd-shell phenomena, e.g., oxygen anomaly
- low computational cost enables surveys with different interactions

NCSM-PT
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

In-Medium NCSM

In-Medium NCSM

NCSM
reference state

IM-SRG
decoupling

NCSM
many-body solution

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

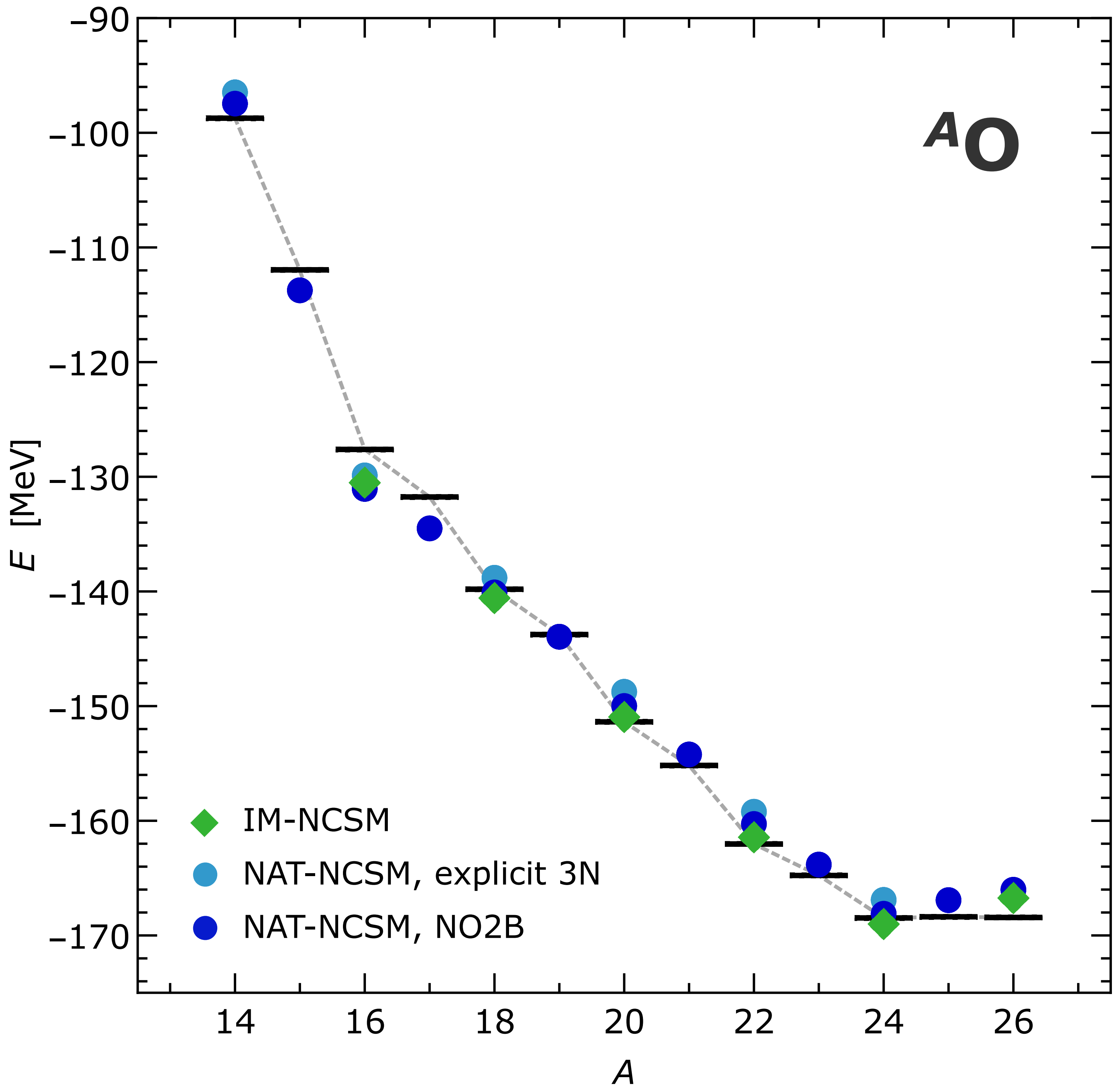
- IM-SRG evolutio… normal-ordered Hami… operators)
- decoupl… excitations, i.e., pre-… many-body space

talk by Klaus Vobig on Thursday

- use i… um evolved Hamiltonian for a subseq…nt NCSM calculation
- access to ground and excited states and full suite of observables

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

chiral NN+3N
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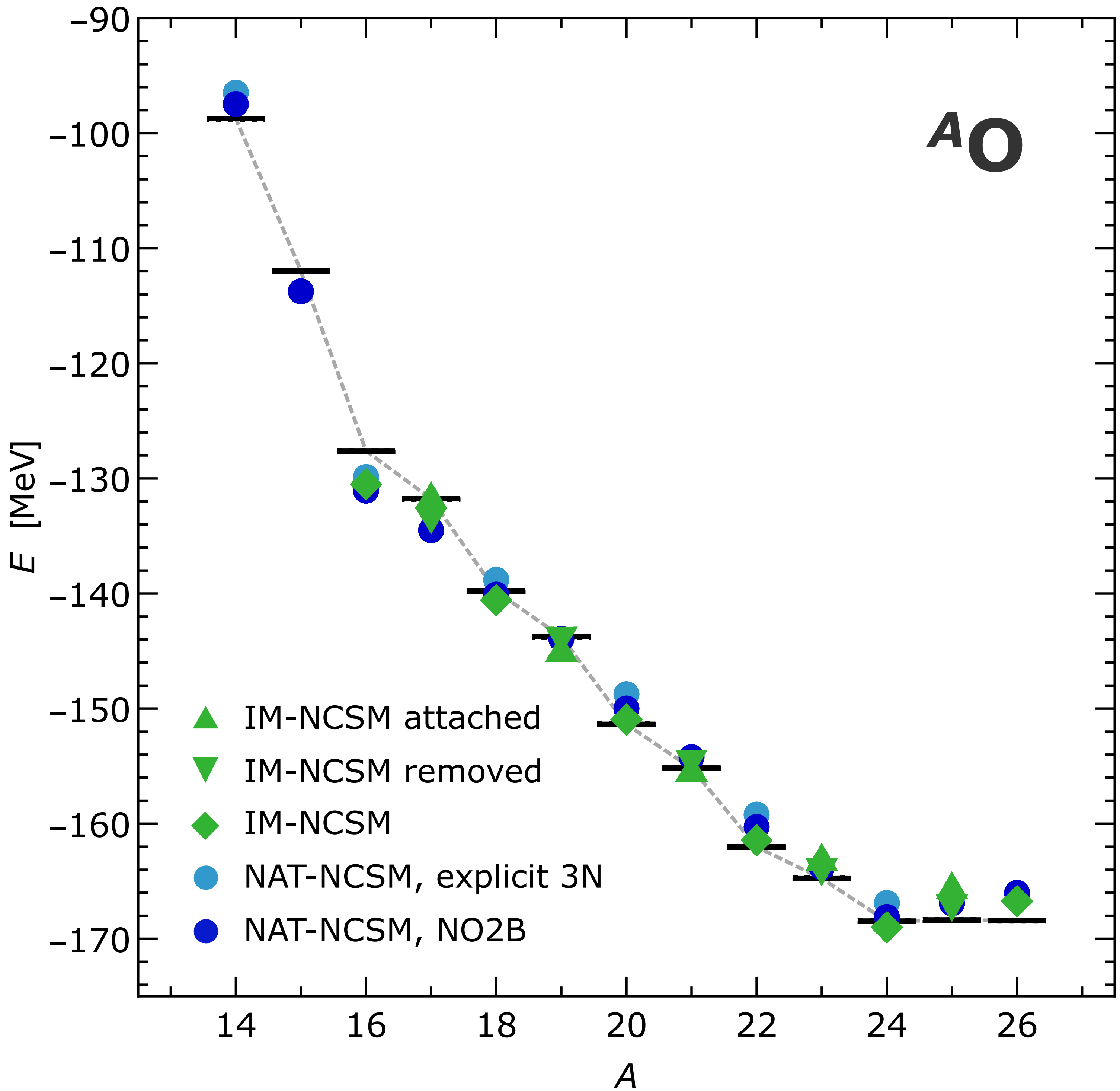
HF basis
N_{max}=0 reference

Oxygen Isotopes

Vobig, Gebrerufael, Roth; in prep.



- 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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α=0.08 fm^4
$\hbar\Omega$=20 MeV
e_{max}=12

HF basis
N_{max}=0 reference

Strength-Function NCSM

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 simplistic Lanczos iterations to generate strength distribution

Strength-Function NCSM

Stumpf, Wolfgruber, Roth; arXiv:1709.06840

- perform **NCSM calculation for ground state** $|E_0\rangle$
- prepare **pivot vector with transition operator**

$$|v_1\rangle = \mathcal{N}\, \mathrm{O}_\lambda\, |E_0\rangle \quad ; \quad \mathcal{N} = \langle E_0|\, \mathrm{O}_\lambda^\dagger \mathrm{O}_\lambda\, |E_0\rangle^{-1/2}$$

- perform **Lanczos algorithm** with Hamiltonian: obtain eigenvectors $|E_n\rangle$ as superposition of Lanczos vectors

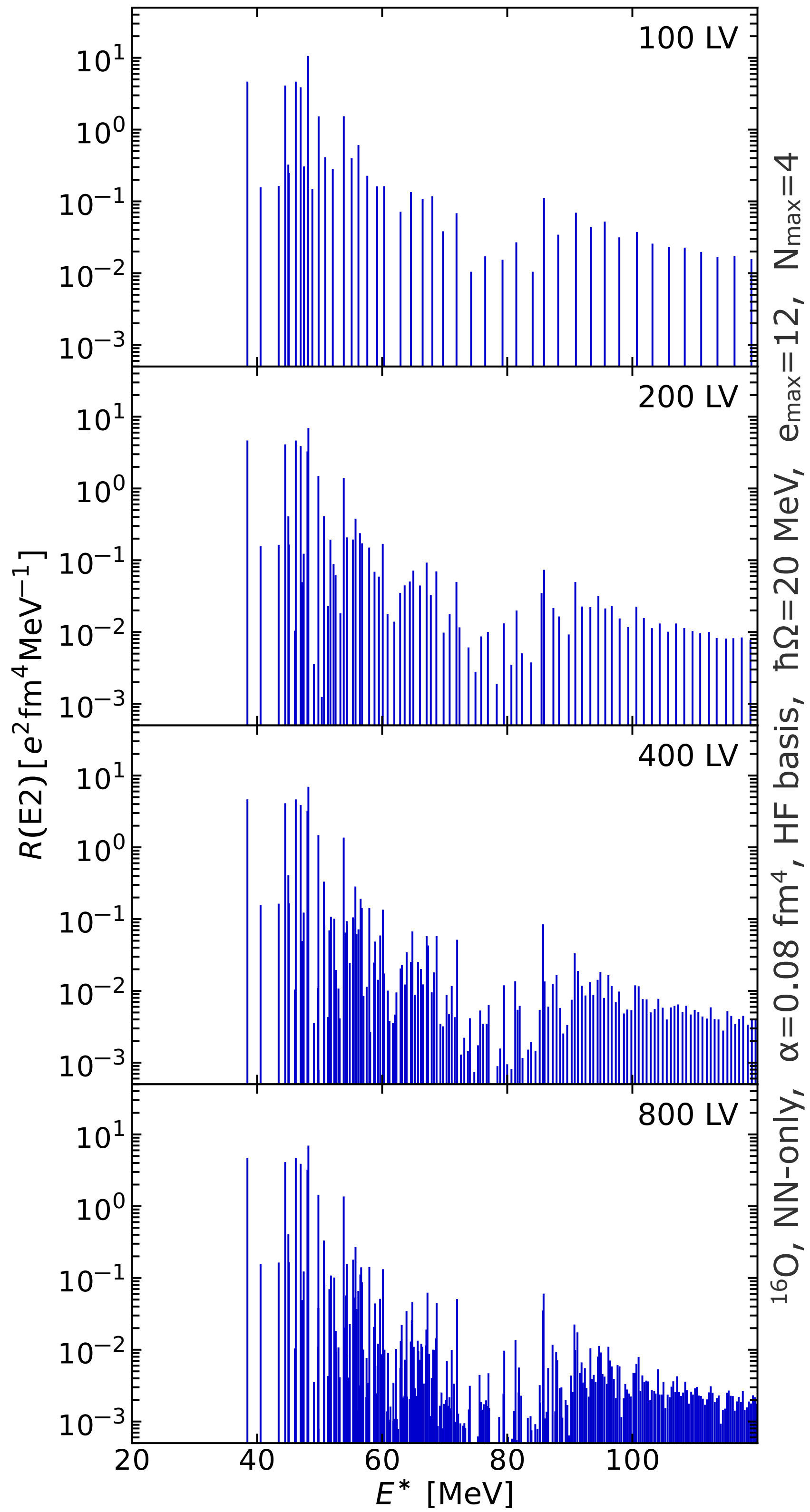
$$|E_n\rangle = \sum_{i=1}^{I} C_i^{(n)}\, |v_i\rangle$$

- first coefficient provides **transition matrix element**

$$C_1^{(n)} = \langle v_1 | E_n\rangle = \mathcal{N}\, \langle E_0|\, \mathrm{O}_\lambda\, |E_n\rangle$$

- construct **discrete strength distribution**

$$R(E\lambda, E^*) = \sum_n |\langle E_0 || \mathrm{O}_\lambda || E_n\rangle|^2\, \delta(E^* - (E_n - E_0))$$

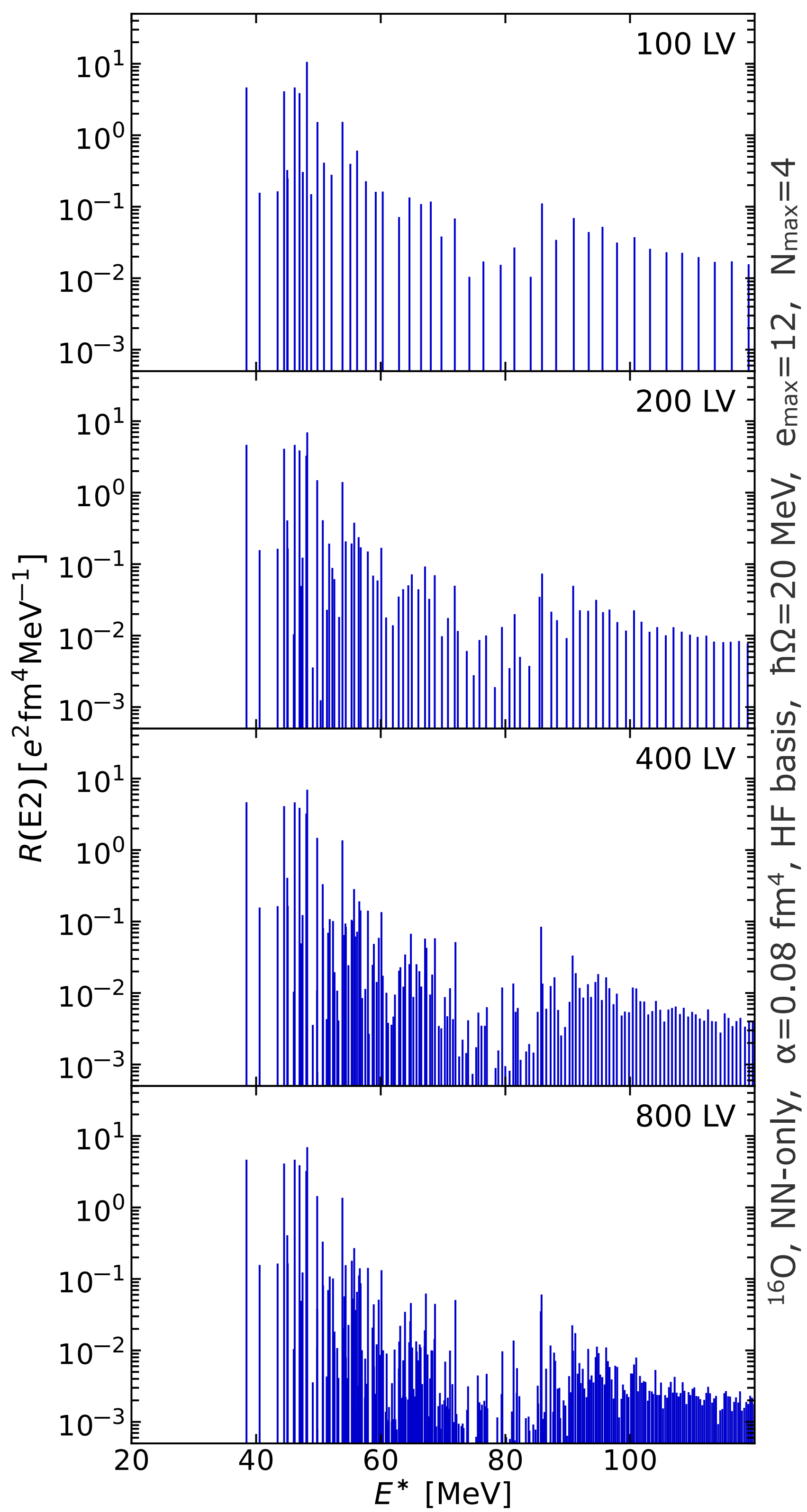


Strength-Function NCSM

Stumpf, Wolfgruber, Roth; arXiv:1709.06840

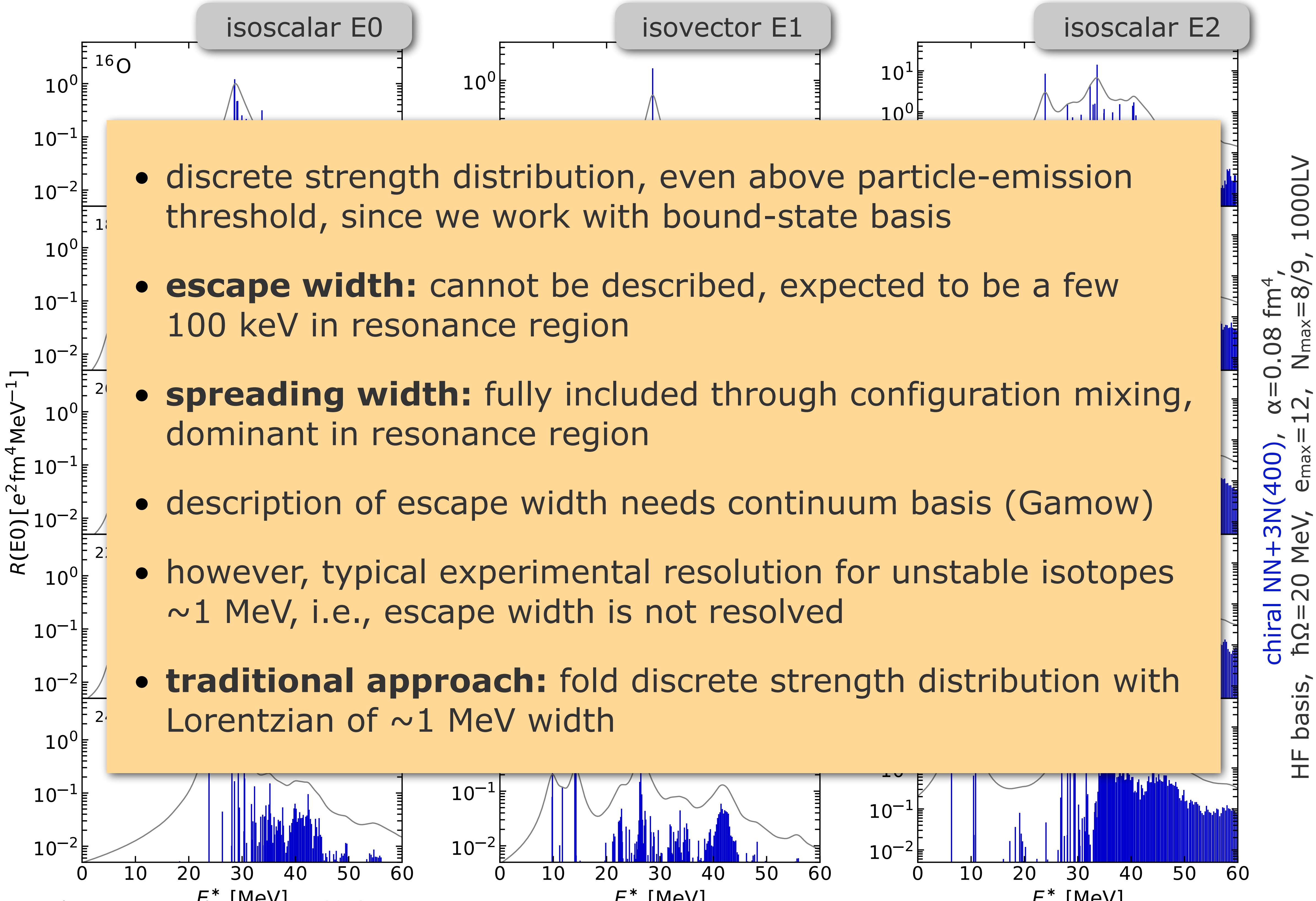
ab initio approach to strength distributions with many advantages

- works with simplest Lanczos algorithm (no reorthogonalization, Lanczos vectors discarded)
- same computational reach as regular NCSM
- no ad-hoc truncations, convergence in N_{max} and Lanczos iterations can be demonstrated explicitly
- full convergence of individual transitions in the relevant energy regime after ~800 iterations
- full access to fine structure of giant resonances
- full access to below-threshold features



Discrete Strength Distribution

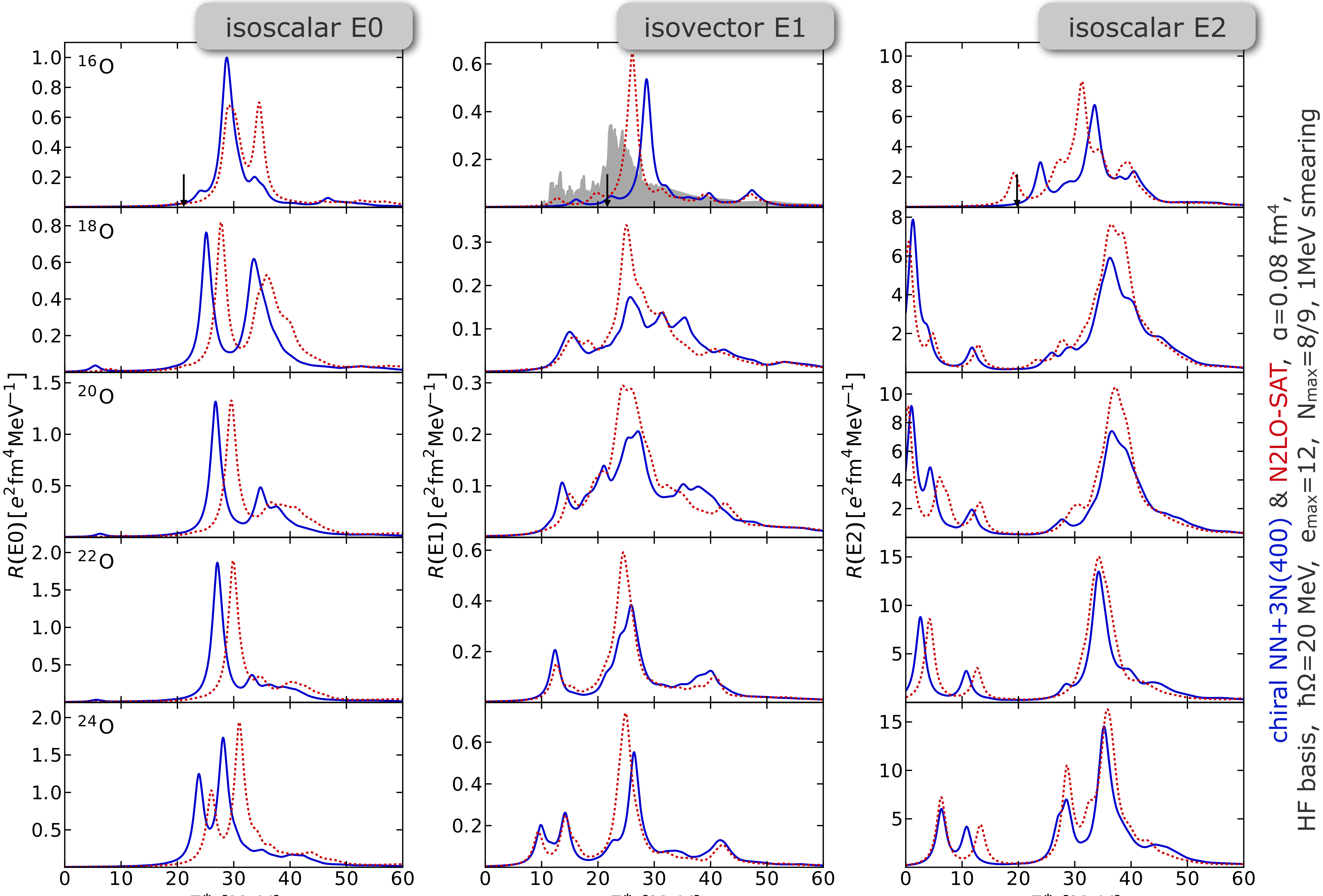
Stumpf, Wolfgruber, Roth; arXiv:1709.06840



- discrete strength distribution, even above particle-emission threshold, since we work with bound-state basis
- **escape width:** cannot be described, expected to be a few 100 keV in resonance region
- **spreading width:** fully included through configuration mixing, dominant in resonance region
- description of escape width needs continuum basis (Gamow)
- however, typical experimental resolution for unstable isotopes ~1 MeV, i.e., escape width is not resolved
- **traditional approach:** fold discrete strength distribution with Lorentzian of ~1 MeV width

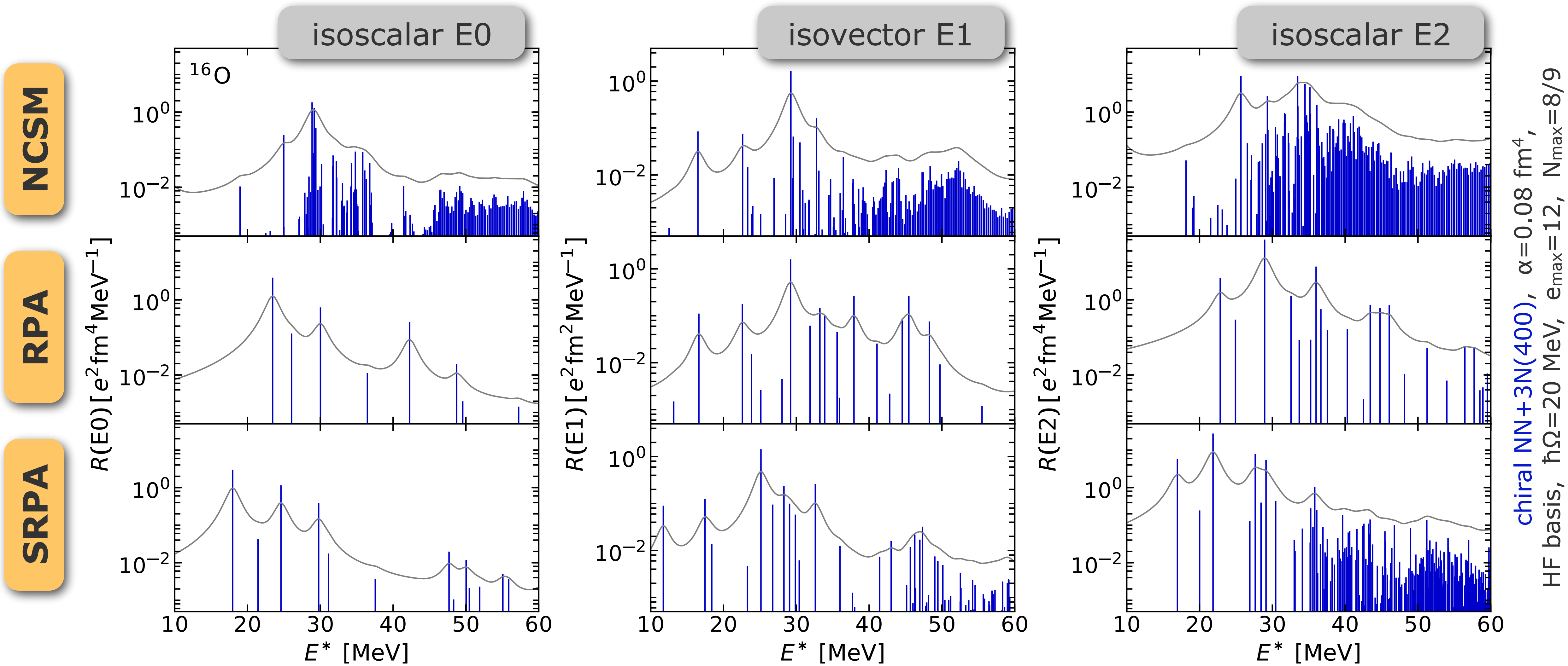
Strength Distribution

Stumpf, Wolfgruber, Roth; arXiv:1709.06840



Comparison with RPA and SRPA

Stumpf, Wolfgruber, Roth; arXiv:1709.06840



- collective excitations traditionally described in RPA or SRPA
- RPA (1p1h) cannot describe fragmentation, therefore, go to SRPA (2p2h)
- NCSM shows much more fine structure than SRPA and resolves notorious problem with pathological SRPA energy-shifts

Conclusions

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

- 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, HORSE,...

Epilogue

- **thanks to my group and my collaborators**
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    CEA Saclay
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    TRIUMF, Vancouver
  - H. Hergert
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    Iowa State University
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