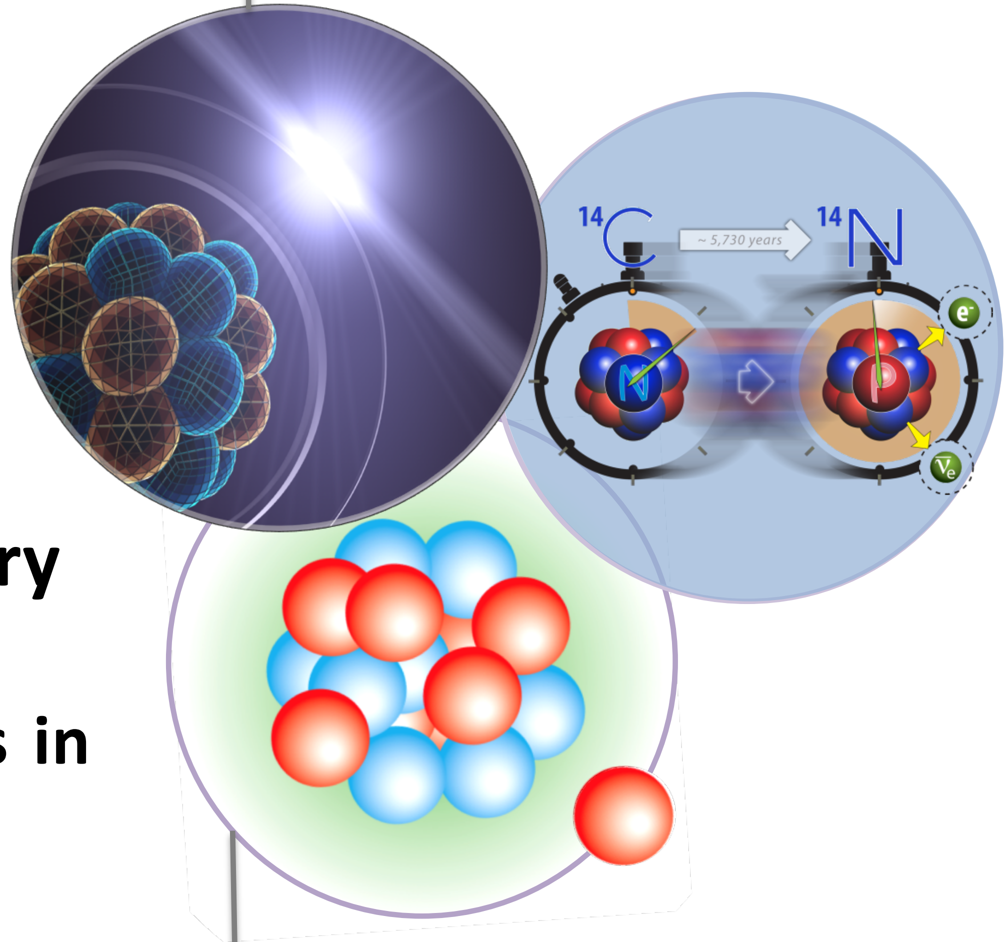
(Todays) Progress in coupled cluster compuations of atomic nuclei



Gaute Hagen
Oak Ridge National Laboratory

Progress in Ab Initio Techniques in Nuclear Physics

TRIUMF, February 26th, 2019

U.S. DEPARTMENT OF ENERGY

NUCLEI
Nuclear Computational Low-Energy Initiative

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Collaborators

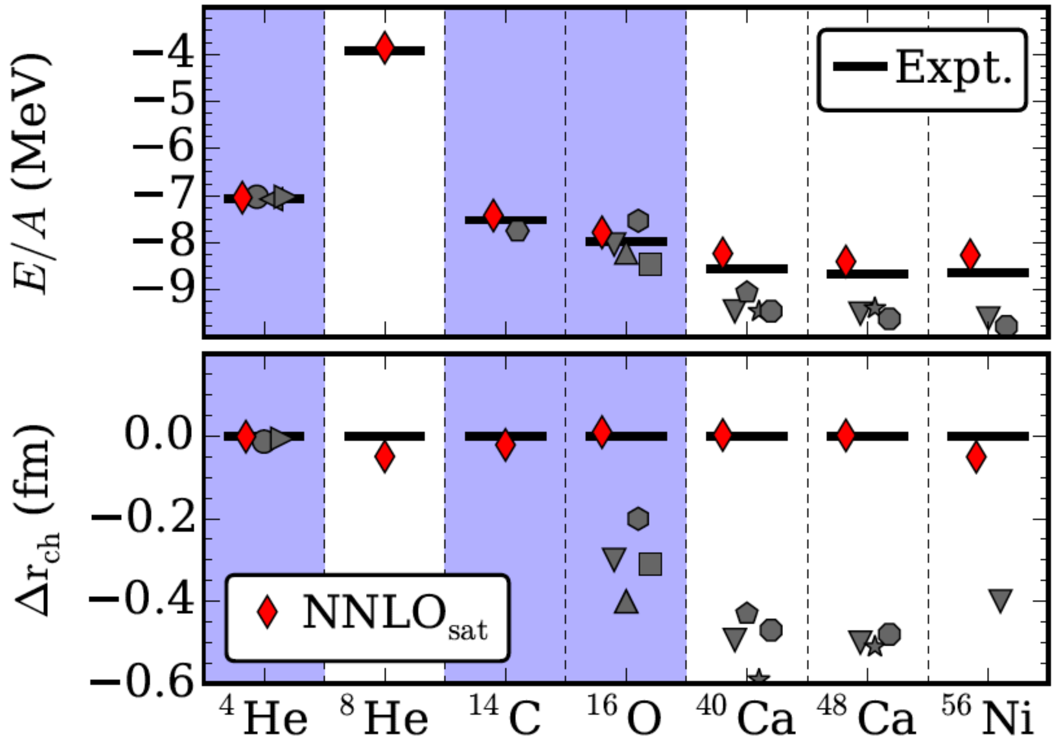
@ ORNL / UTK: G. R. Jansen, **T. Morris**, **S. J. Novario,** T. Papenbrock, **W. Jiang**

@ Chalmers: A. Ekström, C. Forssén

@ UNC: Jon Engel

@ TRIUMF: Peter Gysbers, Petr Navratil

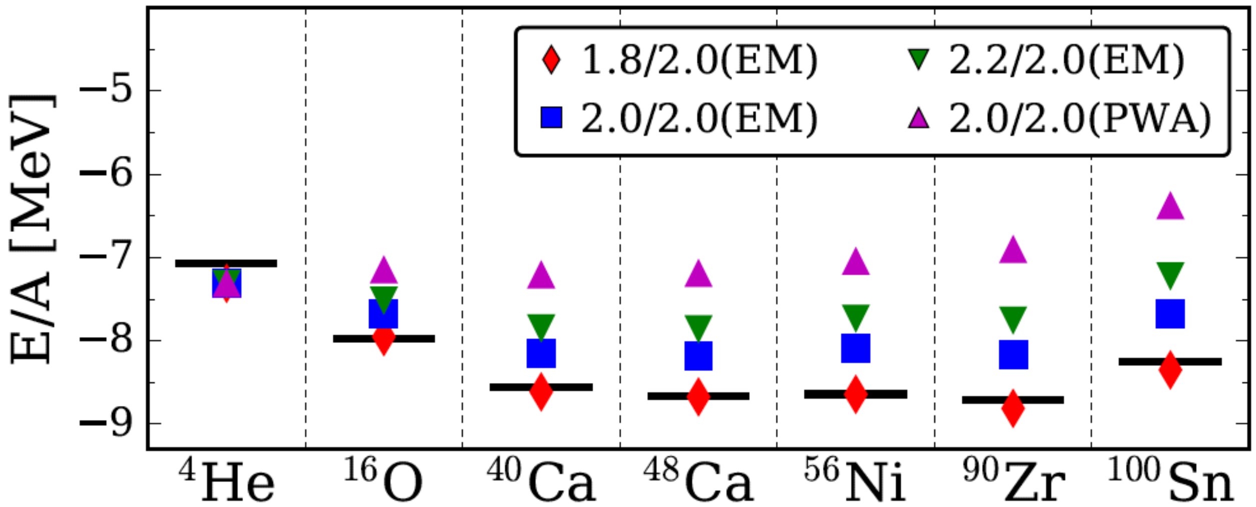
Pragmatists view of interactions from chiral EFT



NNLO$_{sat}$: Accurate radii and BEs

- Simultaneous optimization of NN and 3NFs
- Include charge radii and binding energies of ^{3}H, ^{3,4}He, ^{14}C, ^{16}O in the optimization
- Harder interaction: difficult to converge beyond ^{56}Ni

A. Ekström *et al*, Phys. Rev. C **91**, 051301(R) (2015).



1.8/2.0(EM): Accurate BEs

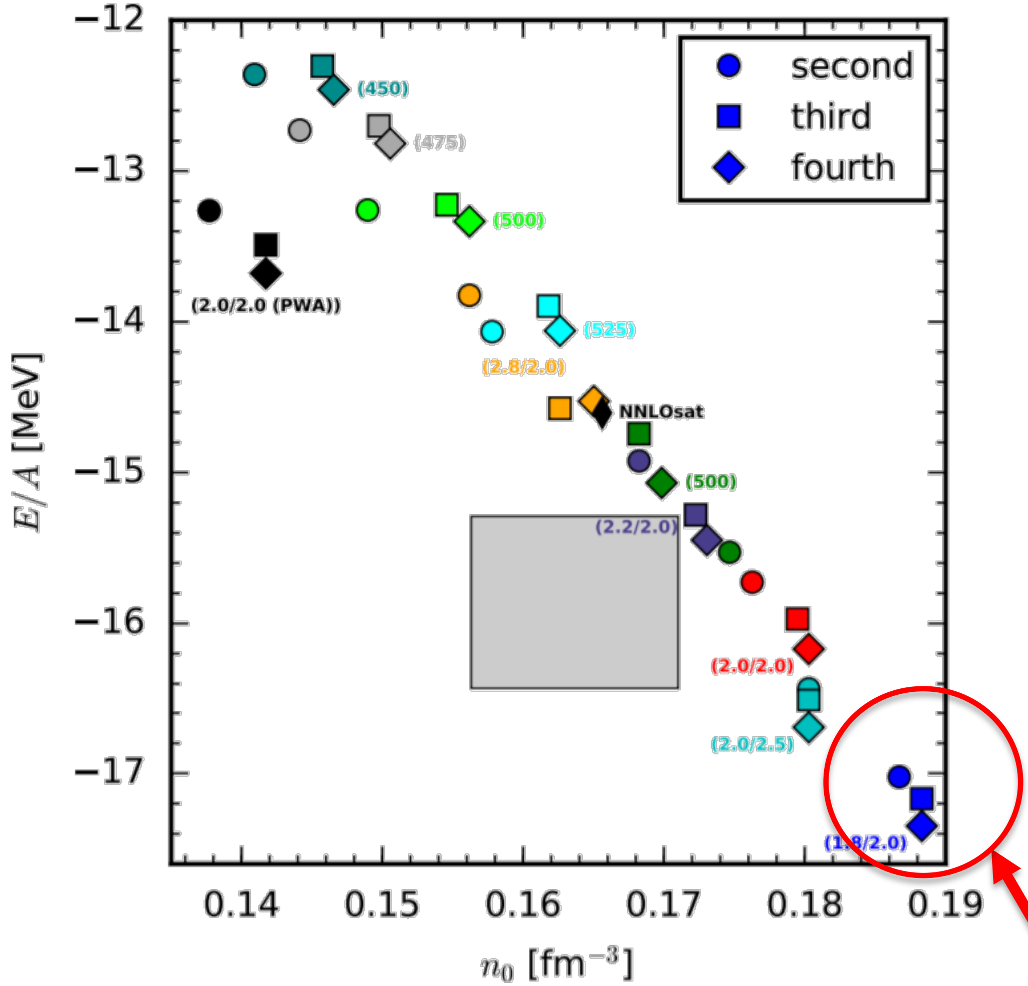
Soft interaction: SRG NN from Entem & Machleidt with 3NF from chiral EFT

K. Hebeler *et al* PRC (2011).

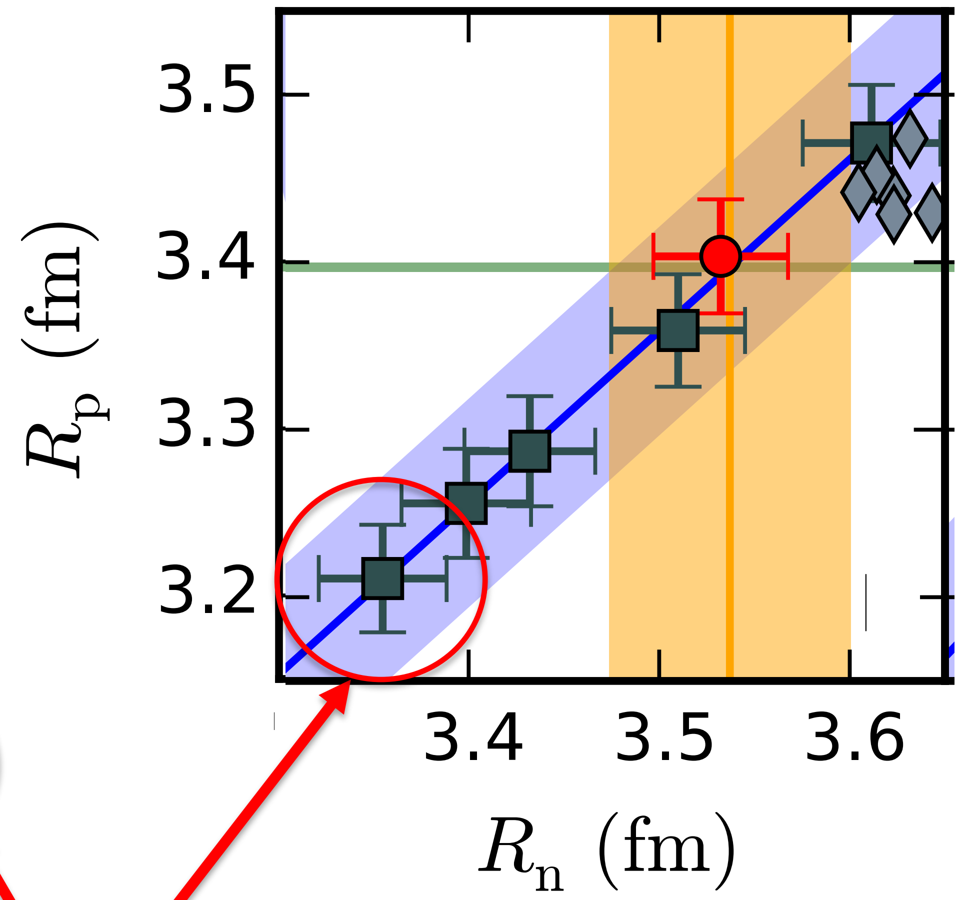
T. Morris *et al*, arXiv:1709.02786 (2017).

The 1.8/2.0 (EM) interaction

J. Simonis, et al , Phys. Rev. C 96, 014303 (2017).



G. Hagen *et al*, Nat. Phys. **12**, 186 (2016)

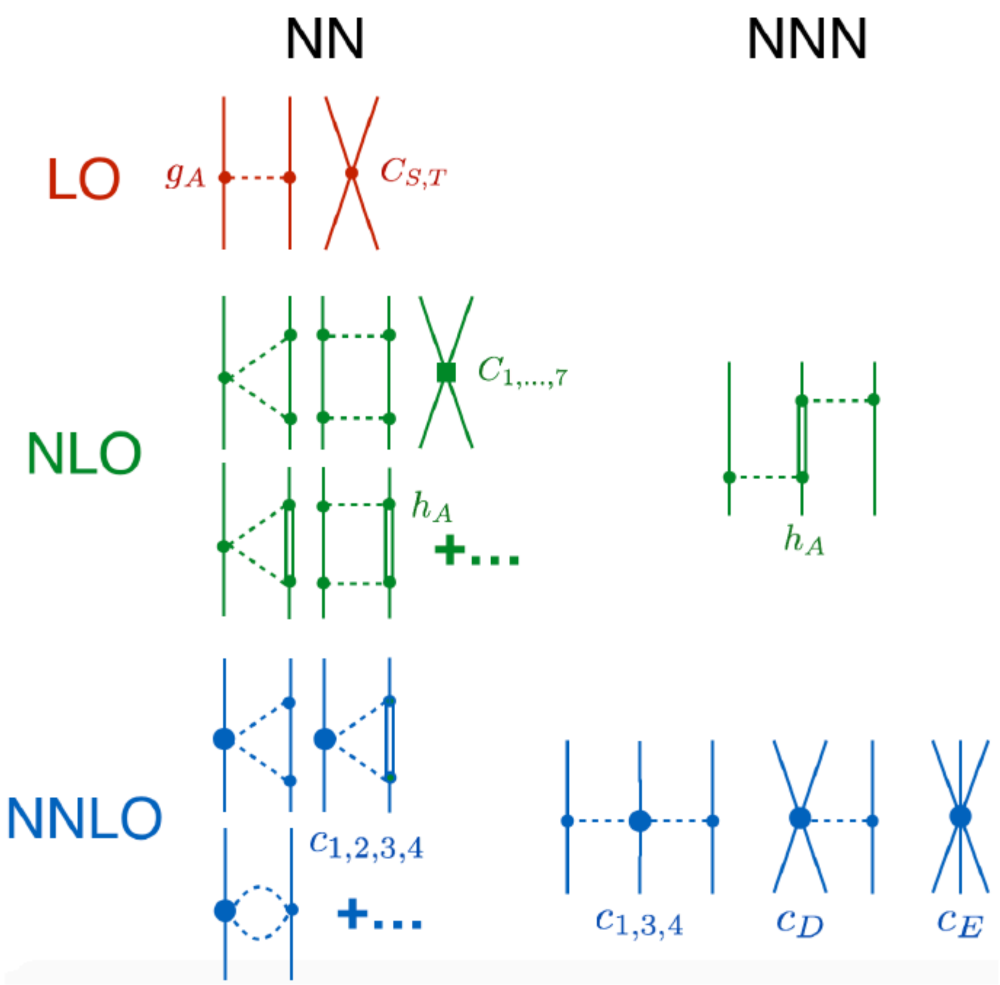


1.8/2.0 (EM) is great for binding energies and spectra.

Nuclear matter saturates at too high density → Radii too small

Role of delta isobars on nuclear saturation

A. Ekström, et al, Phys. Rev. C 97, 024332 (2018)



- Pion-nucleon LECs fixed from recent analysis based on Roy-Steiner equations
- Short ranged contacts fixed from NN scattering and ^{4}He BE and charge radius
- Estimate uncertainties at given order following Epelbaum, Krebs, Meissner (2015) and Furnstahl, Klco, Phillips (2015).

$$\sigma_X(\mathrm{NjLO}) = X_0 Q^{j+2} \max(|a_0|, |a_1|, \ldots, |a_{j+1}|)$$

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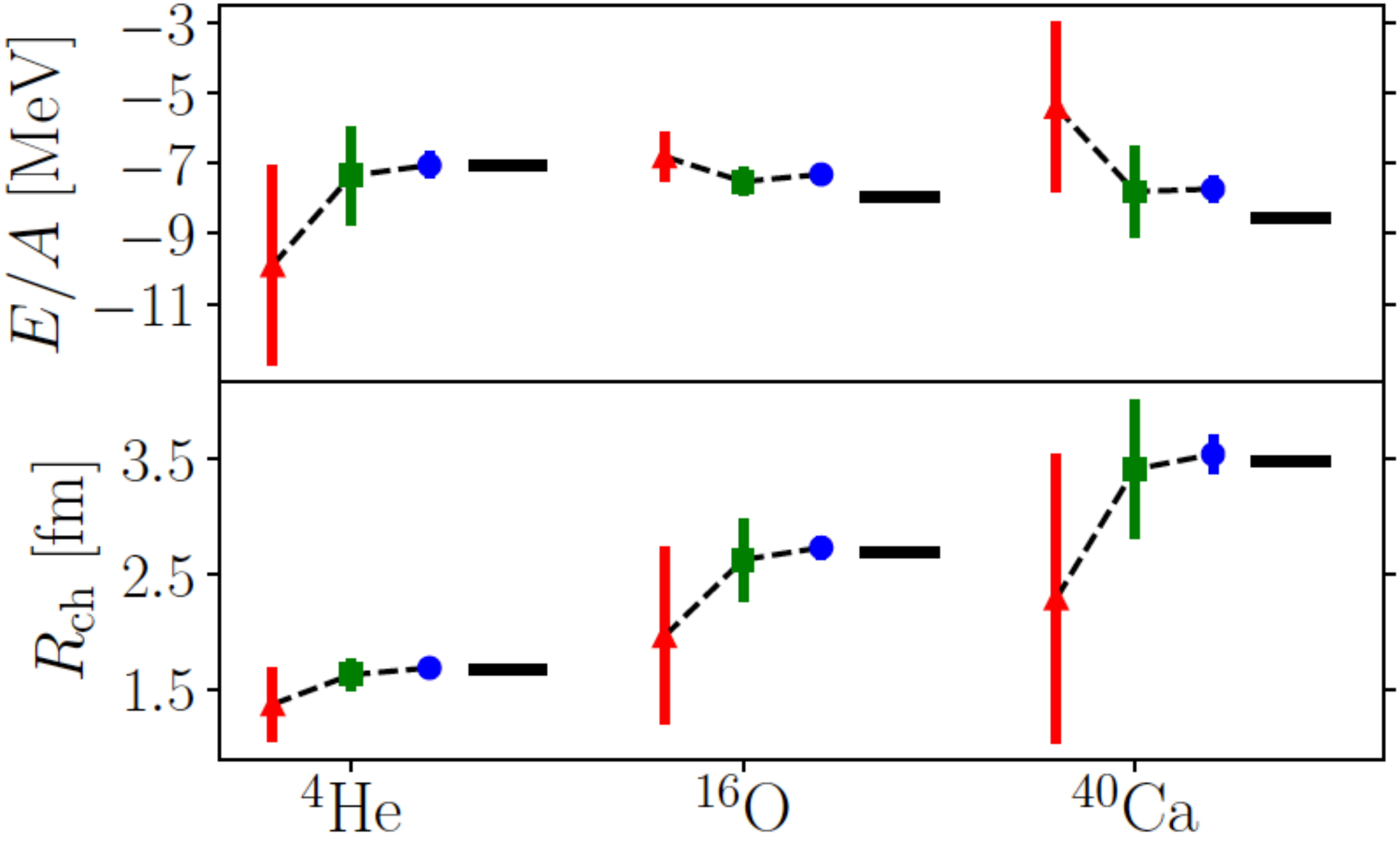

Role of delta isobars on nuclear saturation

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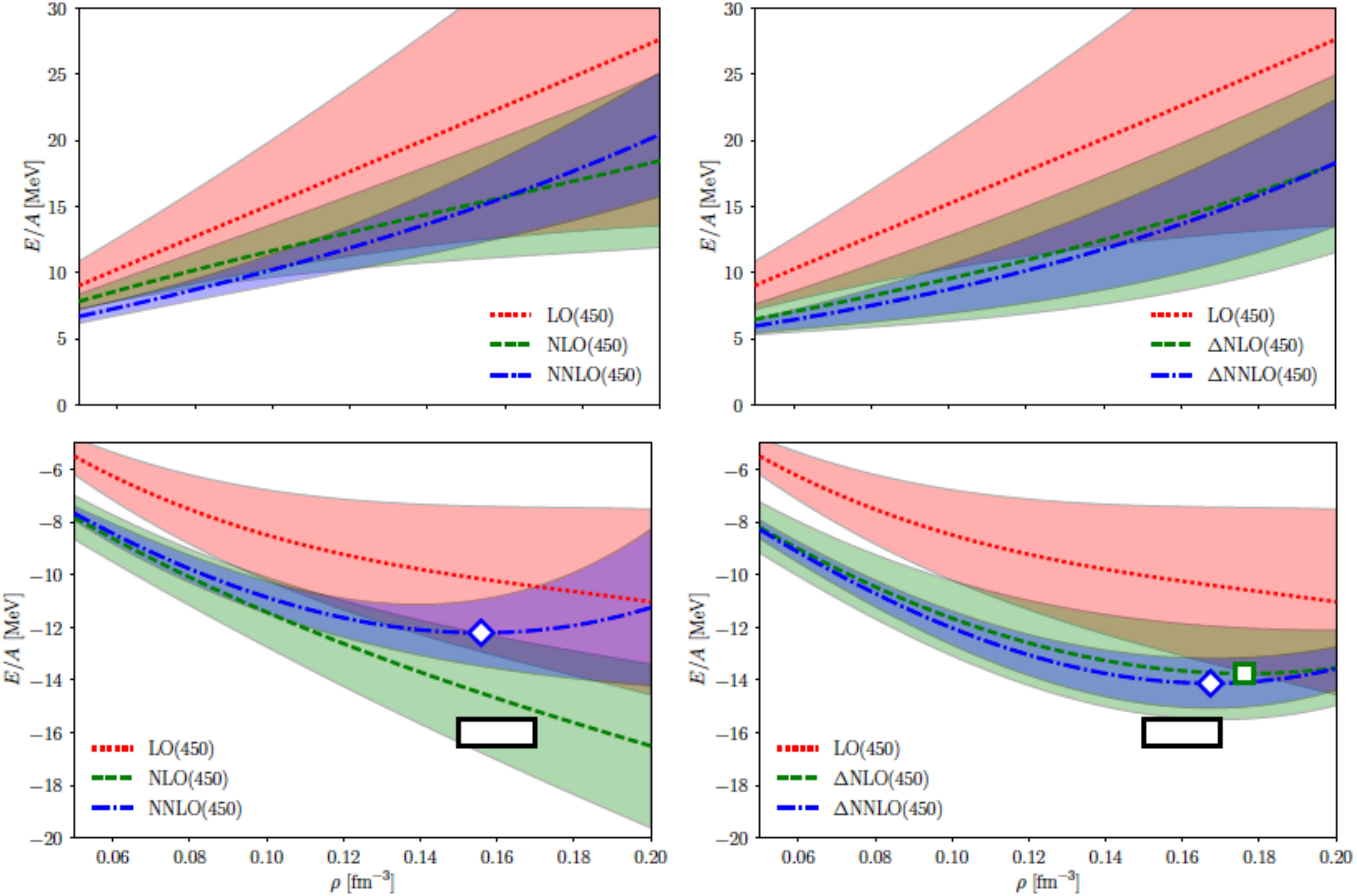
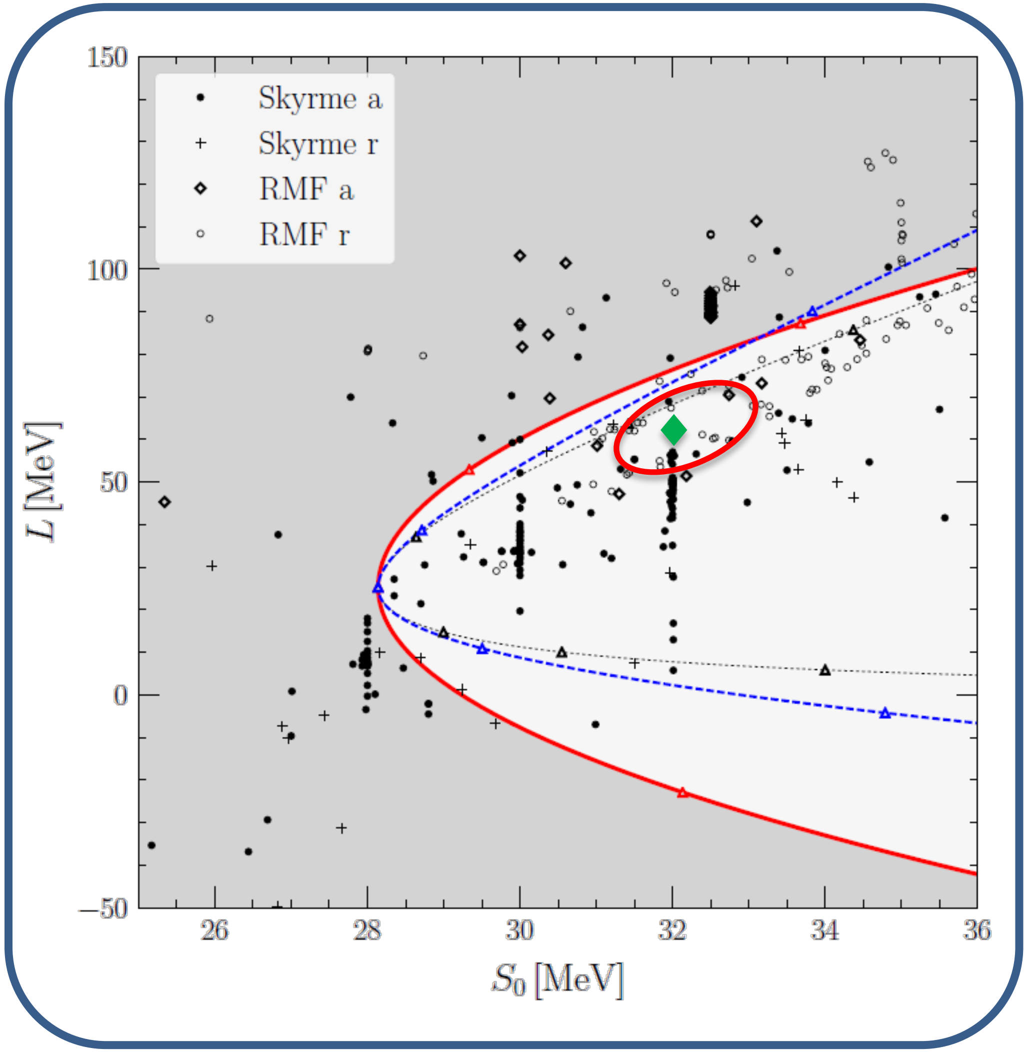


Optimization strategy

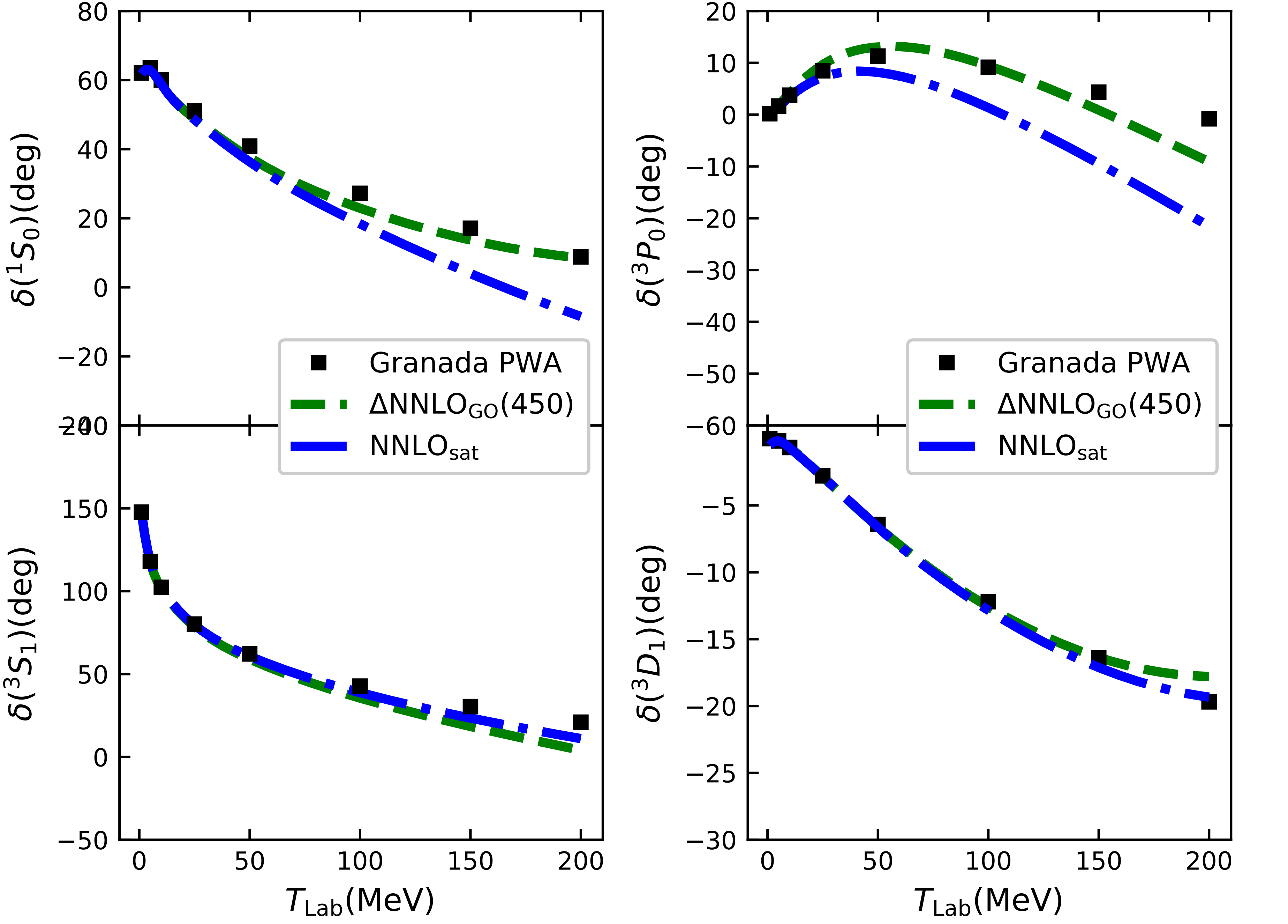


- Use the empirical saturation point of nuclear matter and constraints on symmetry energy and its slope
- Fit NN to phase shifts (up to 200MeV) and deuteron properties
- 3NF fixed to reproduce A = 3, 4 nuclei
- Informed by BE and radii in medium mass nuclei

Ingo Tews, et al. Symmetry parameter constraints from a lower bound on neutron-matter energy. The Astrophysical Journal, 848(2):105, 2017.

NNLO(450): S = 32MeV, L = 65MeV

Scattering phaseshifts

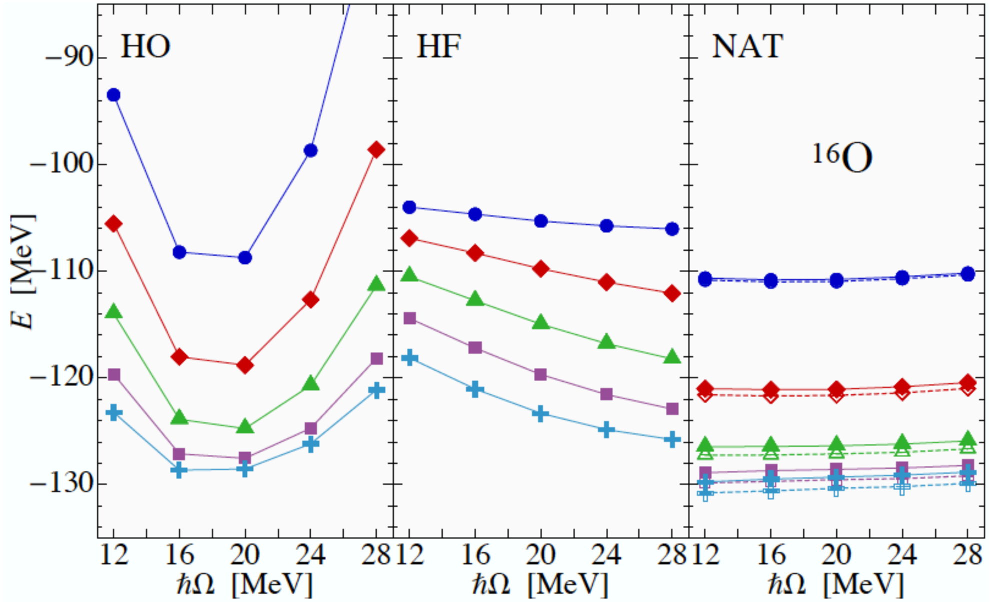


Light nuclei

TABLE I. Binding energies (E) in MeV, charge radii (R_{ch}) in fm, for ^{2,3}H and ^{3,4}He with ΔNNLO$_{GO}$(450), compared to experiment.

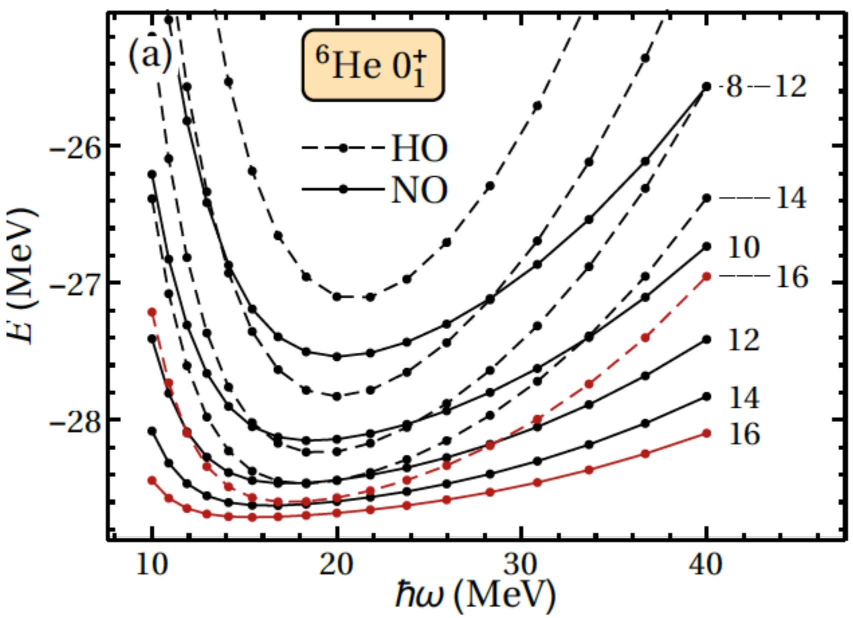
	ΔNNLO$_{GO}$(450)	Expt.
$E(^2\text{H})$	2.2358	2.2245
$R_{ch}(^2\text{H})$	2.1509	2.1421
P_D (^2H)	3.12	-
$Q(^2\text{H})$	0.267	0.27
$E(^3\text{H})$	8.4809	8.4818
$R_{ch}(^3\text{H})$	1.7801	1.7591
$E(^3\text{He})$	7.7162	7.7180
$R_{ch}(^3\text{He})$	2.0036	1.9661
$E(^4\text{He})$	28.2975	28.2957
$R_{ch}(^4\text{He})$	1.6960	1.6775

Natural orbitals in many-body approaches



A. Tichai, J. Müller, K. Vobig, R. Roth, arXiv:1809.07571 (2018).

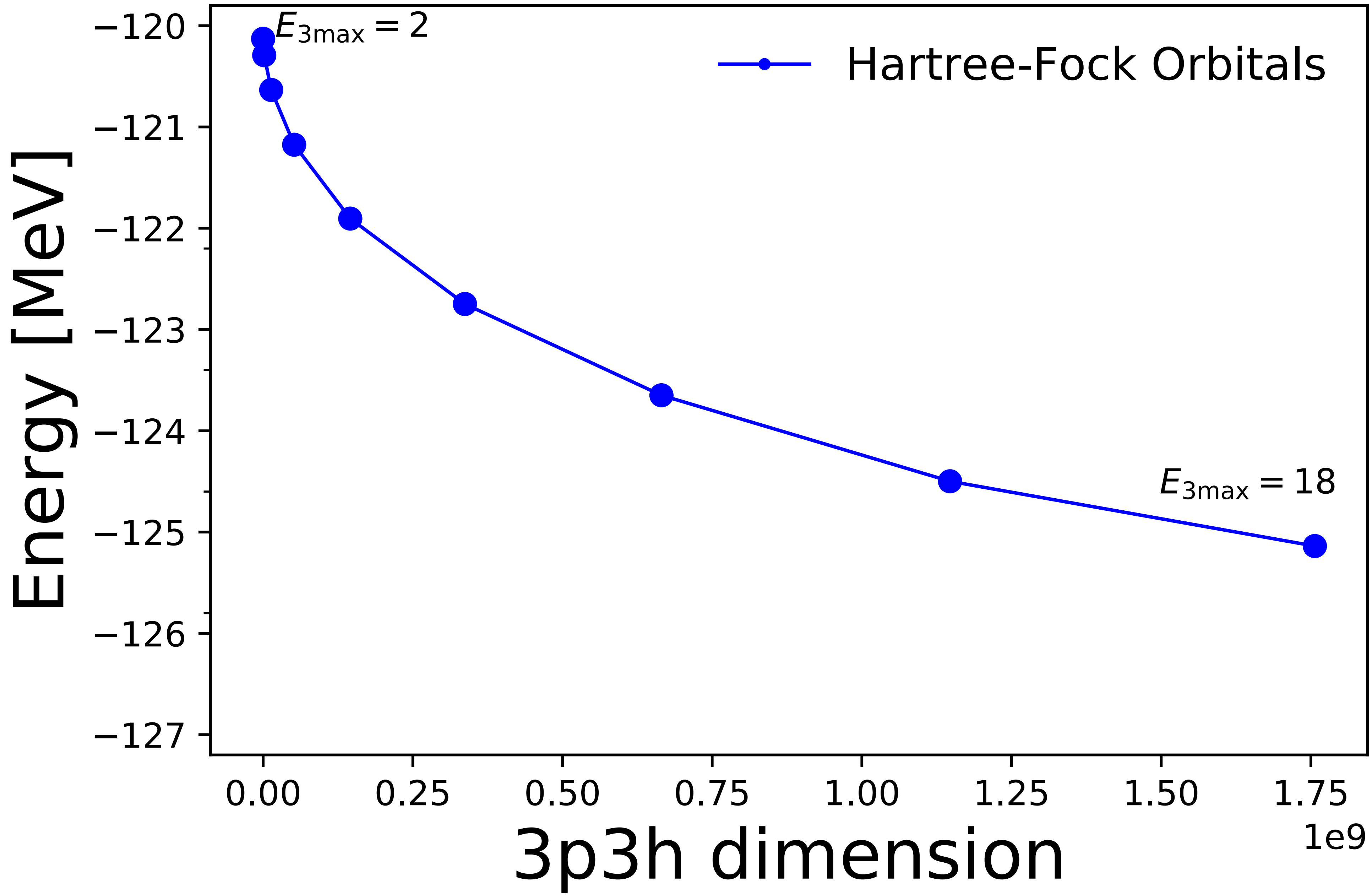
- NCSM with natural orbitals show significant improvement in convergence wrt model-space



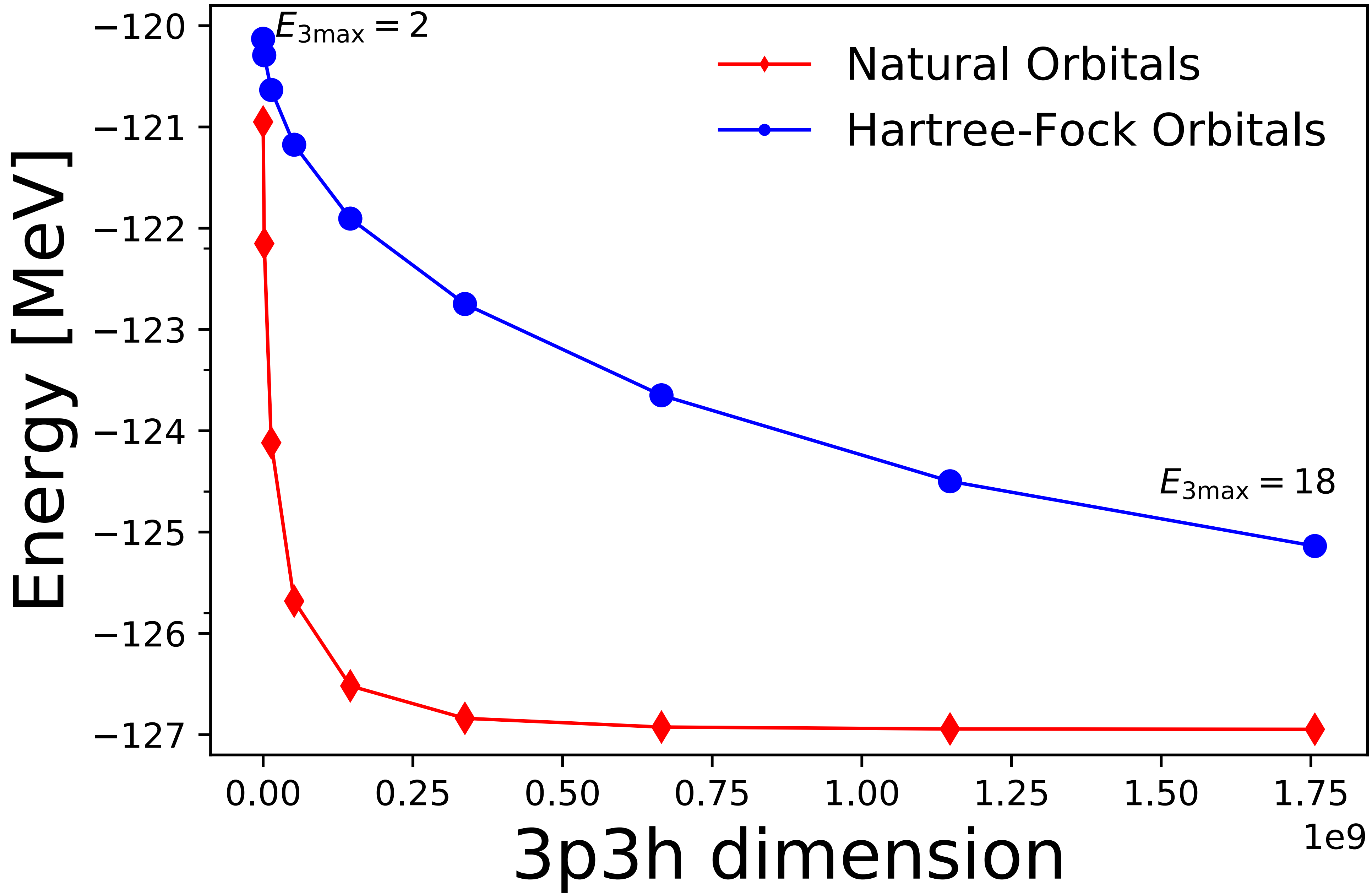
- We follow A. Tichai et al and construct natural orbitals from many-body perturbation theory
- Aim: explore convergence in higher order coupled-cluster approaches to nuclei

Ch. Constantinou, M. A. Caprio, J. P. Vary, P. Maris, Nucl. Sci. Tech. 28, 179 (2017)

16-O with natural orbitals



16-O with natural orbitals



Equation-of-motion with perturbative energy correction for excited states

Diagonalize $\overline{H} = e^{-T} H_N e^{T}$ via equation-of-motion technique:

$$R_\mu = \sum r_i^a \, p_a^\dagger n_i + \frac{1}{4}\sum r_{ij}^{ab} \, p_a^\dagger N_b^\dagger N_j n_i + \frac{1}{36}\sum r_{ijk}^{abc} \, p_a^\dagger N_b^\dagger N_c^\dagger N_k N_j n_i$$

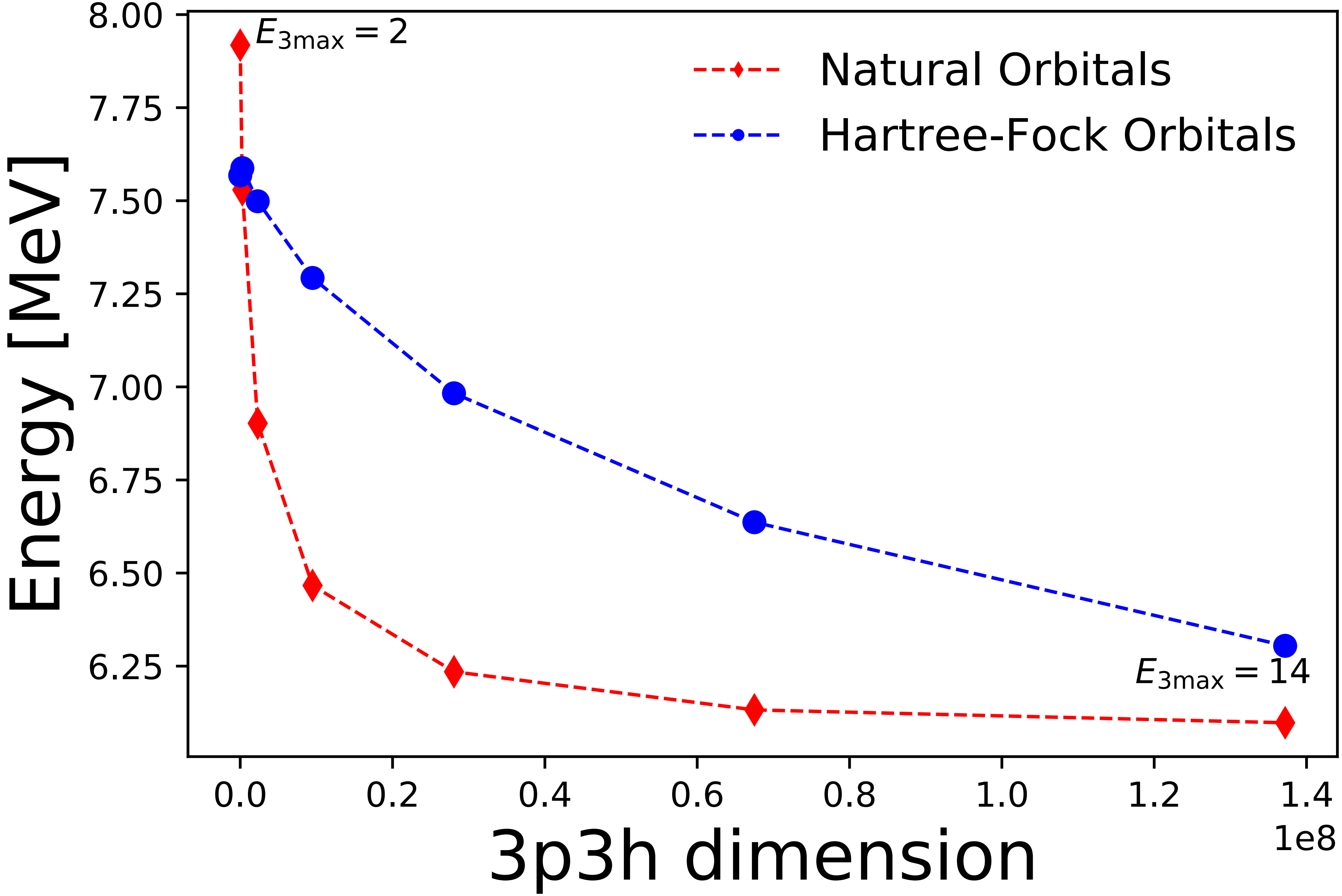
- Diagonalize in the P-space:

$$\tilde{E}_{pqr} = \tilde{e}_p + \tilde{e}_q + \tilde{e}_r \leq \tilde{E}_{3\max} \qquad \tilde{e}_p = |N_p - N_F|$$

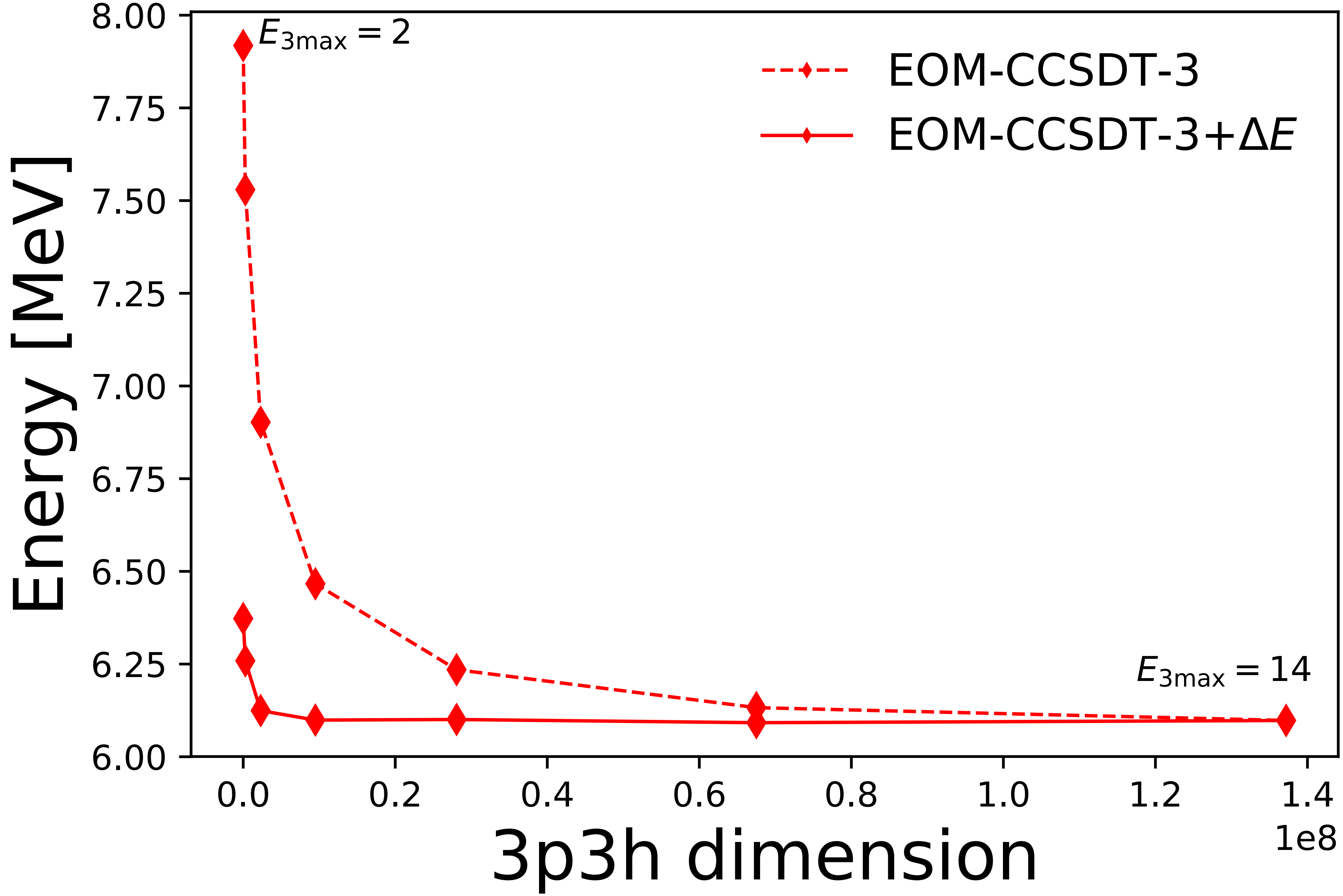
- Correct perturbatively for all excitations outside of P:

$$\Delta E_\mu = \langle \Phi_0 | L_\mu \overline{H}_{PQ} (E_\mu - \overline{H}_{QQ})^{-1} \overline{H}_{QP} R_\mu | \Phi_0 \rangle$$

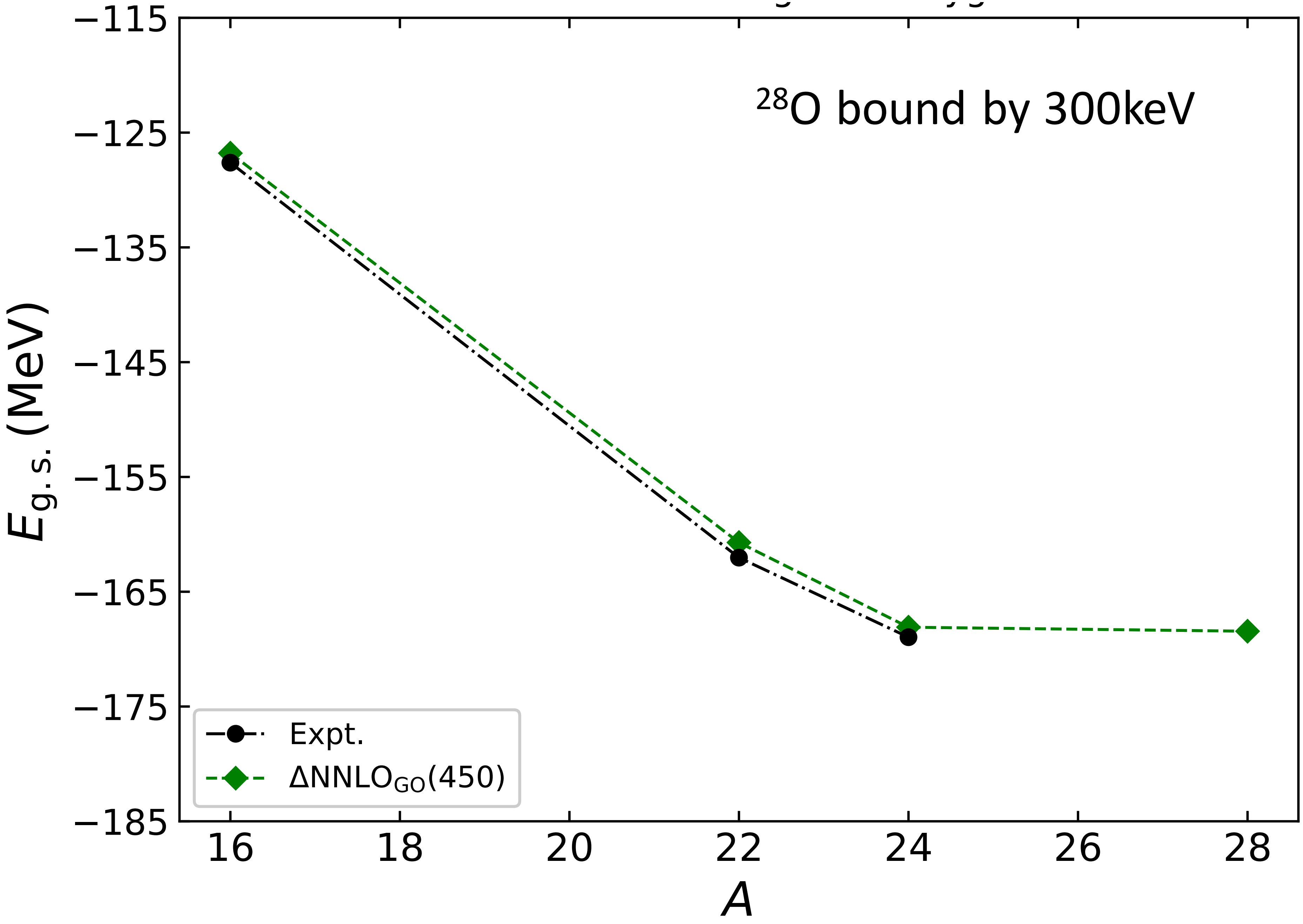
3^- state in 16-O



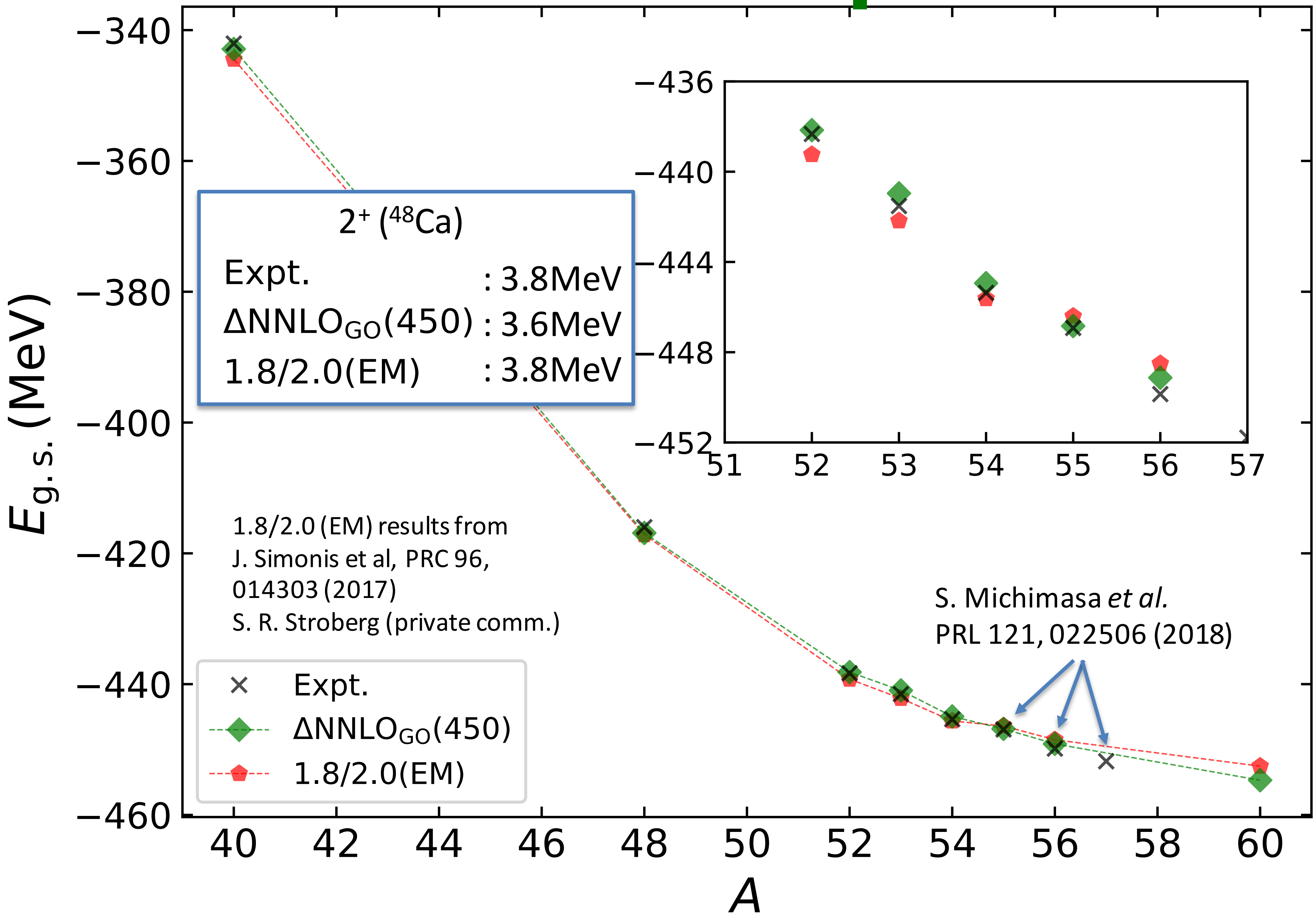
3^- state in 16-O



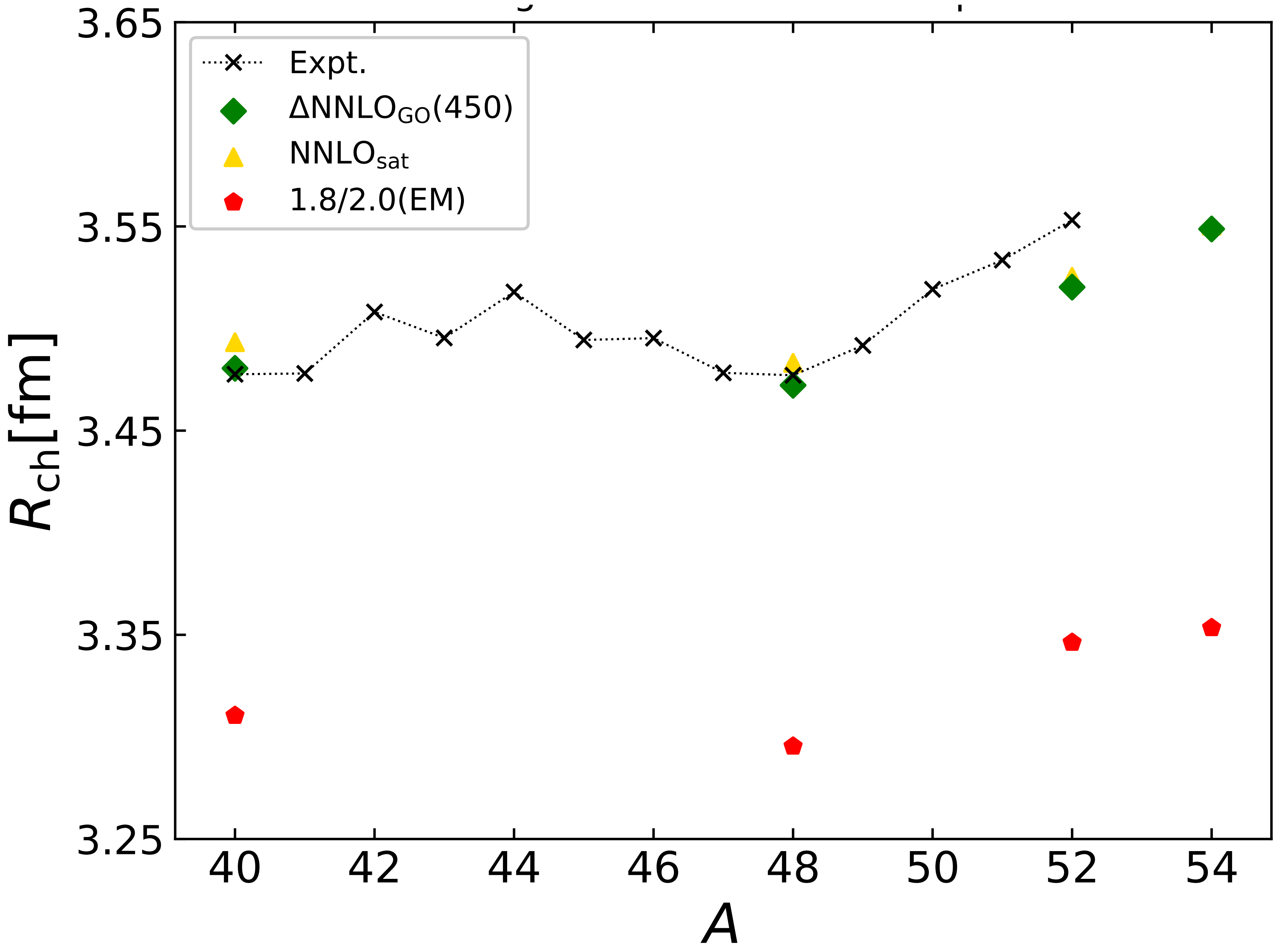
Oxygen isotopes



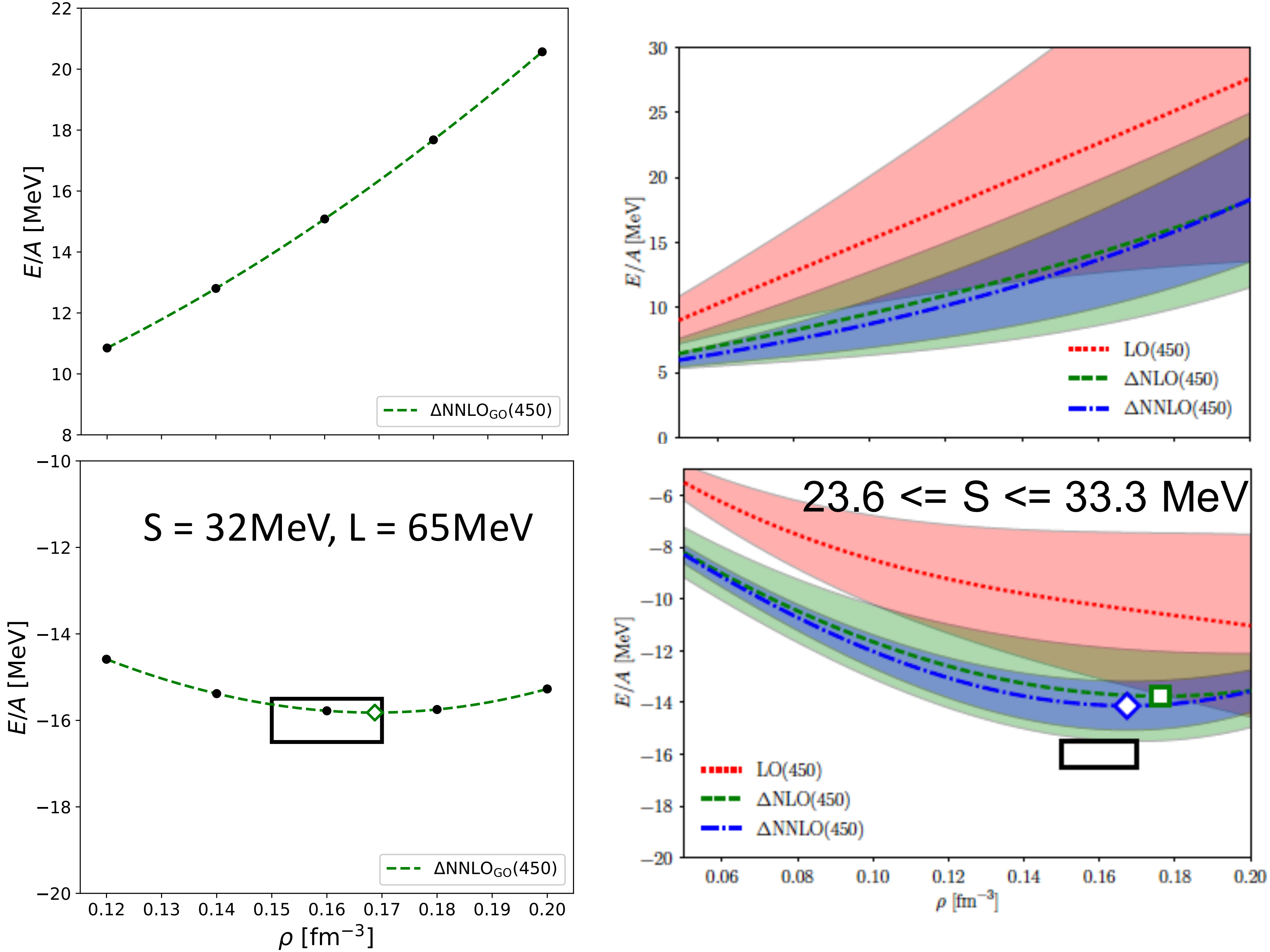
Calcium isotopes



Calcium isotopes



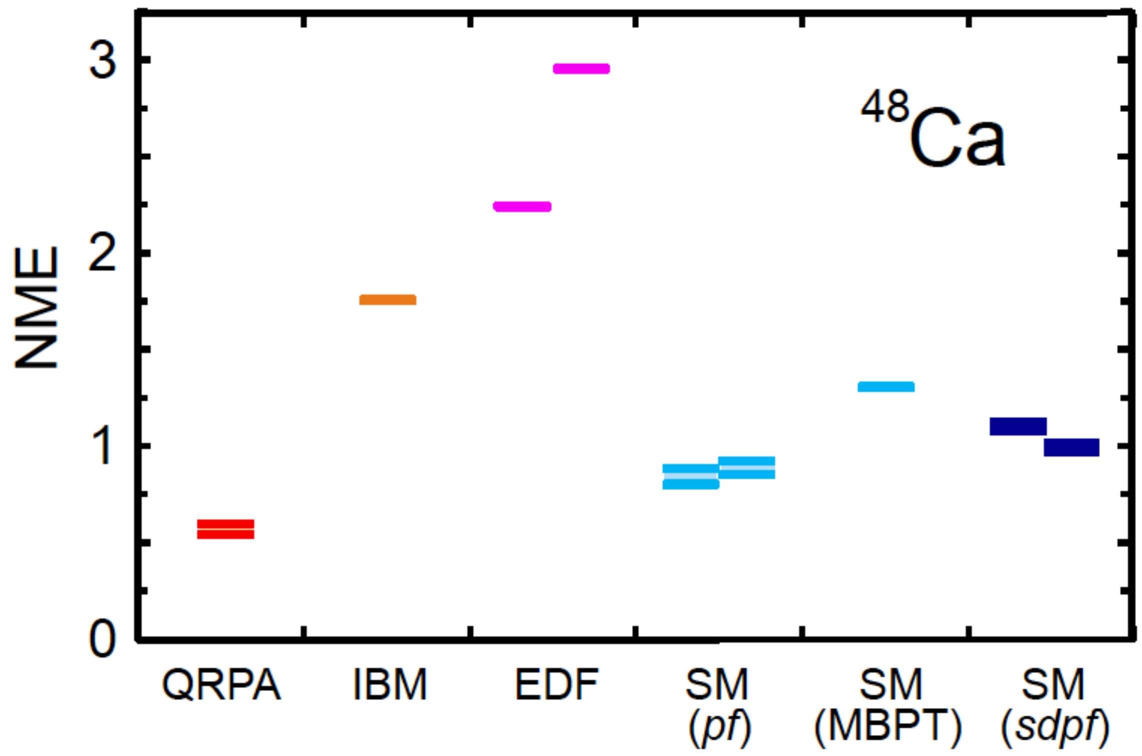
Nuclear/neutron matter at CCD(T)



Neutrinoless ββ-decay of ^{48}Ca

$$\left[T_{1/2}^{0\nu}\left(0_i^+ \rightarrow 0_f^+\right)\right]^{-1} = G^{0\nu}|M^{0\nu}|^2 \left(\frac{\langle m_{\beta\beta}\rangle}{m_e}\right)^2$$

0νββ



Nuclear matrix element for neutrinoless double beta decay in ^{48}Ca using different methods. From Y. Iwata et al, PRL (2016).

- The NME for 0νββ differ by a factor two to six depending on the method
- Need to determine the NME more precisely with quantified uncertainties
- What does ab-initio calculations add to this picture?

Neutrinoless ββ-decay of ^{48}Ca

$$|\langle^{48}\mathrm{Ti}|O|^{48}\mathrm{Ca}\rangle|^2 = \langle^{48}\mathrm{Ti}|O|^{48}\mathrm{Ca}\rangle\langle^{48}\mathrm{Ca}|O^\dagger|^{48}\mathrm{Ti}\rangle$$

Closure approximation with Gamow-Teller, Fermi and Tensor contributions:

$$M_{GT}^{0\nu} + \left(\frac{g_V}{g_A}\right)^2 M_F^{0\nu} + M_T^{0\nu}$$

The ground-state of ^{48}Ca is computed in the CCSD approximation:

$$\overline{H}_N|\Phi_0\rangle = E_0|\Phi_0\rangle,\ \ \overline{H}_N = e^{-T}H_N e^T,\ \ T = T_1 + T_2$$

The CC energy functional is expressed in term of left/right ground-states

$$\langle\Phi_0|(1+\Lambda)\overline{H}_N|\Phi_0\rangle = E_0,\ \ \langle\Phi_0|(1+\Lambda)|\Phi_0\rangle = 1.$$

$$\Lambda = \sum_{ia}\lambda_a^i a_a a_i^\dagger + \frac{1}{2}\sum_{ijab}\lambda_{ab}^{ij} a_b a_a a_i^\dagger a_j^\dagger$$

Neutrinoless ββ-decay of ^{48}Ca

^{48}Ti is computed using a double charge exchange equation of motion method with 2p2h and 3p3h excitations

$$\overline{H}_N R_\mu|\Phi_0\rangle = E_\mu R_\mu|\Phi_0\rangle$$

$$\langle\Phi_0|L_\mu \overline{H}_N = \langle\Phi_0|L_\mu E_\mu$$

$$R_\mu = \frac{1}{4}\sum_{ijab} r_{ij}^{ab} p_a^\dagger p_b^\dagger n_i n_j + \frac{1}{36}\sum_{ijkabc} r_{ijk}^{abc} p_a^\dagger p_b^\dagger N_c^\dagger N_k n_i n_j$$

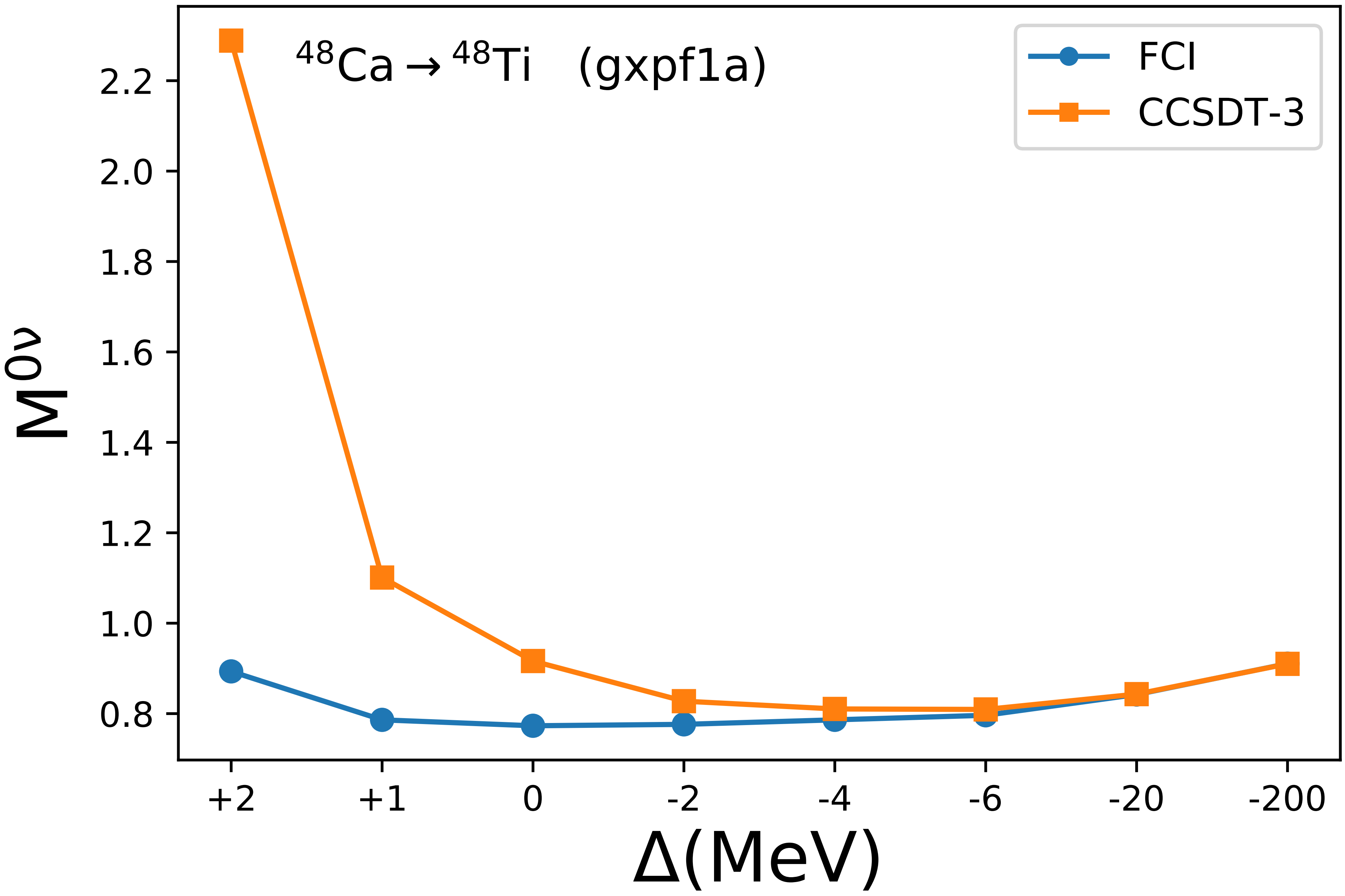
$$L_\mu = \frac{1}{4}\sum_{ijab} l_{ab}^{ij} p_b p_a n_i^\dagger n_j^\dagger + \frac{1}{36}\sum_{ijkabc} l_{abc}^{ijj} p_a p_b N_c N_k^\dagger n_i^\dagger n_j^\dagger$$

The Nuclear matrix element for 0νββ in ^{48}Ca is given by:

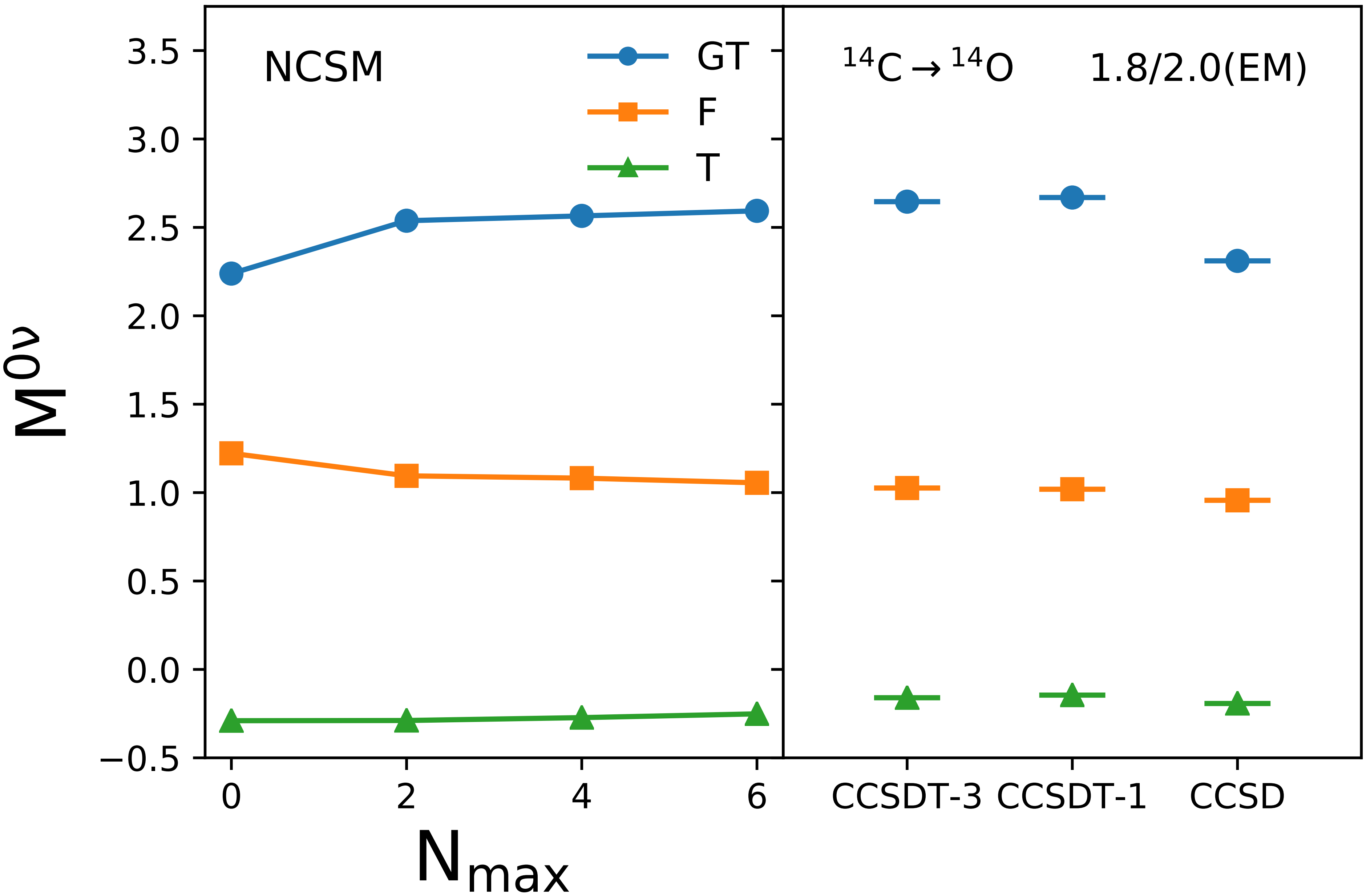
$$|\langle^{48}\mathrm{Ti}|O|^{48}\mathrm{Ca}\rangle|^2 = \langle^{48}\mathrm{Ti}|O|^{48}\mathrm{Ca}\rangle\langle^{48}\mathrm{Ca}|O^\dagger|^{48}\mathrm{Ti}\rangle$$

$$= \langle\Phi_0|L_0\overline{O}_N|\Phi_0\rangle\langle\Phi_0|(1+\Lambda)\overline{O^\dagger}_N R_0|\Phi_0\rangle$$

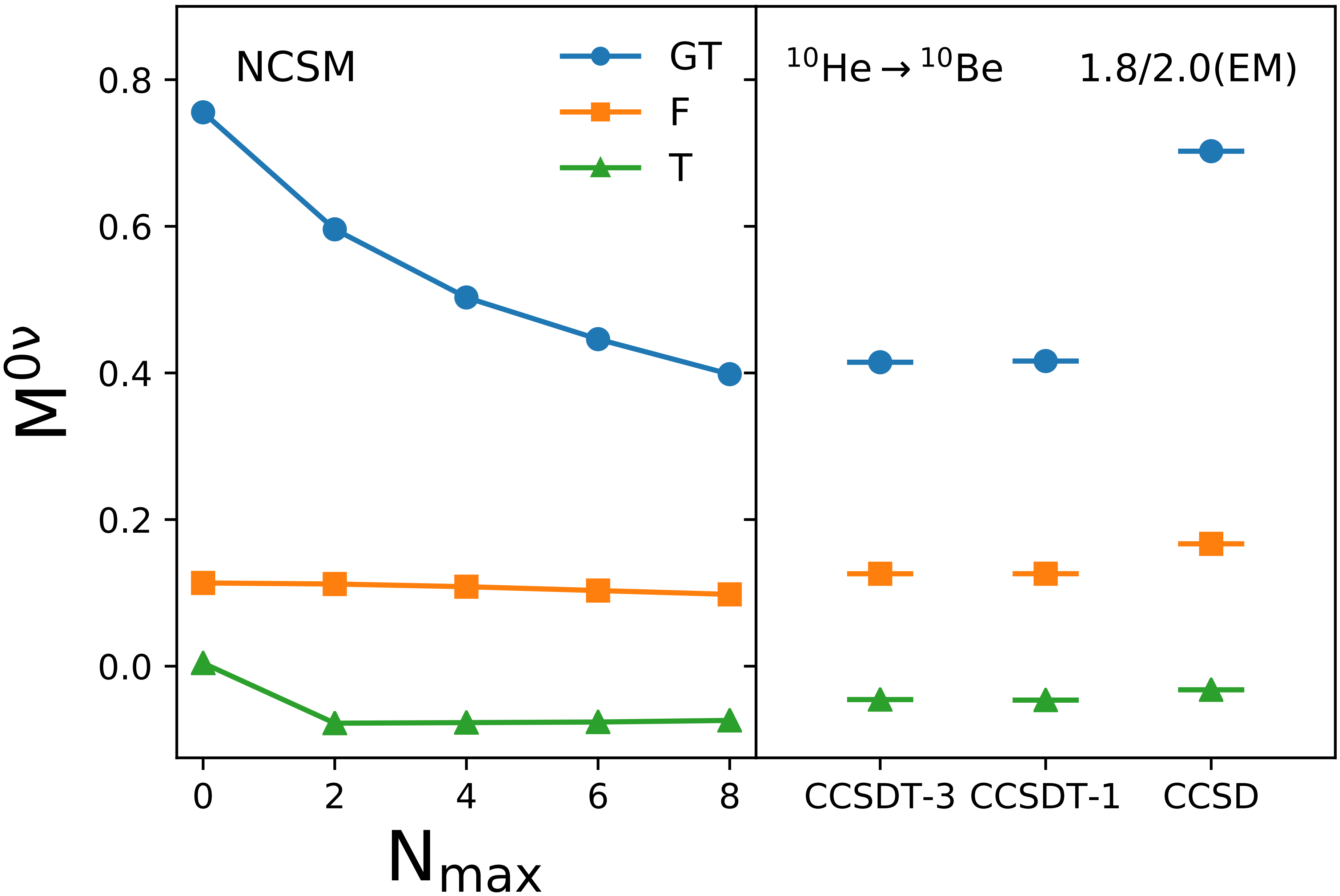
ββ-decay of ^{48}Ca with GXPF1A shell-model interaction



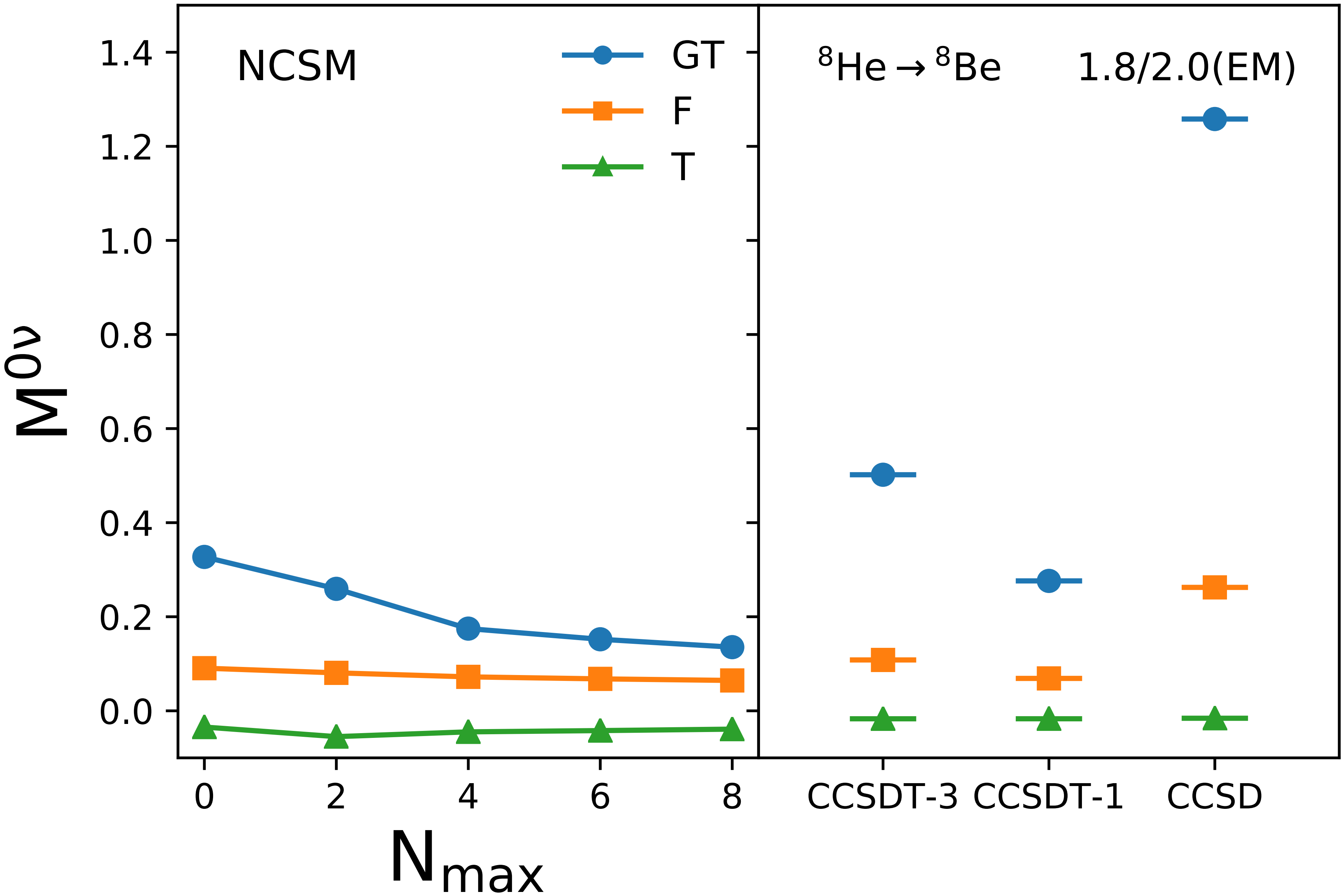
Benchmark between CC and NCSM in light nuclei



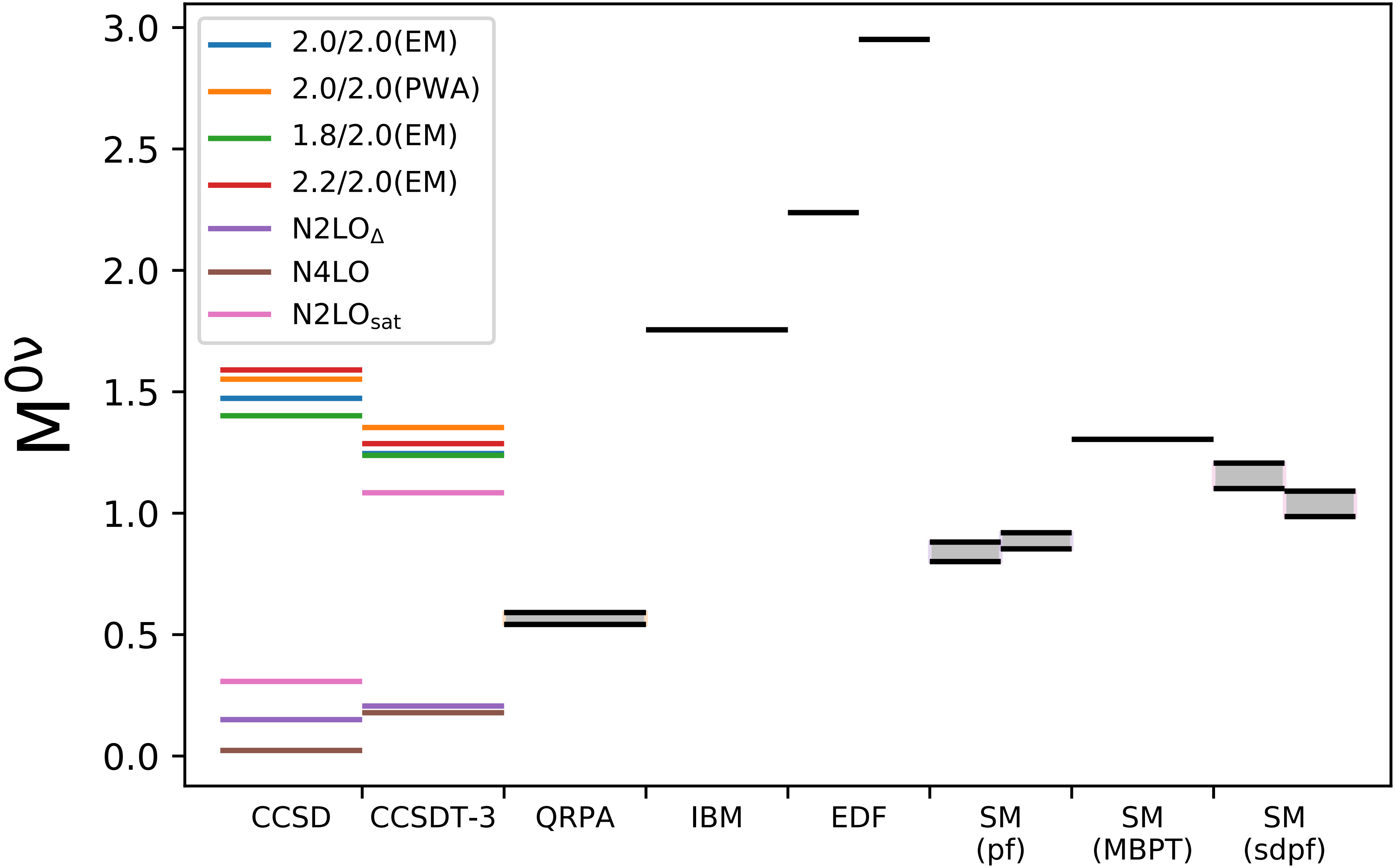
Benchmark between CC and NCSM in light nuclei



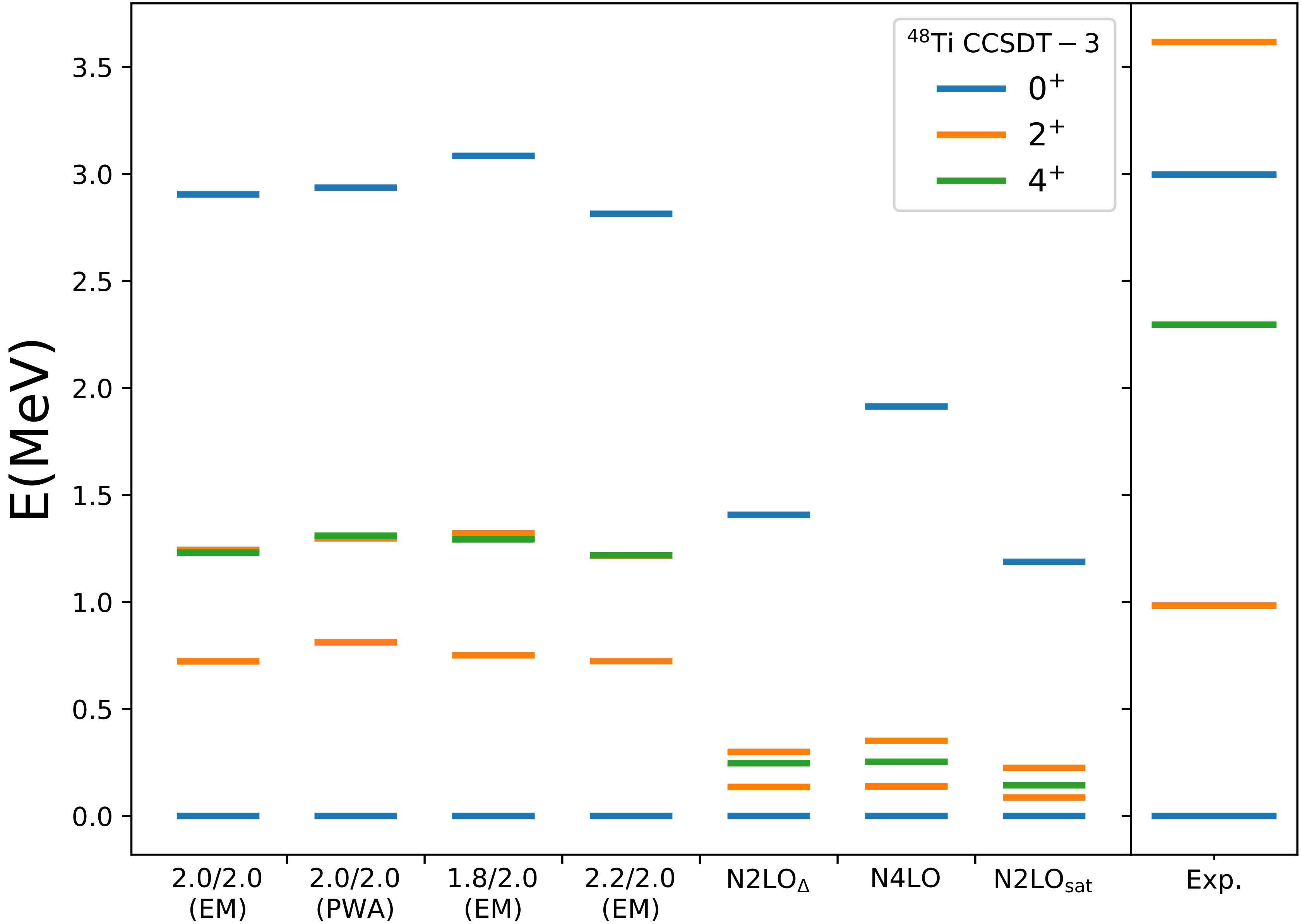
Benchmark between CC and NCSM in light nuclei



^{48}Ti from CR-EOM-CCSD(T)



^{48}Ti from CR-EOM-CCSD(T)



ββ-decay of ^{48}Ca

$$M^{2\nu} = \sum_{\mu} \frac{\langle 0_f^+ | O_{\mathrm{GT}} | 1_\mu^+ \rangle \langle 1_\mu^+ | O_{\mathrm{GT}} | 0_i^+ \rangle}{E_\mu - E_i + Q_{\beta\beta}/2}$$

$$= \langle 0_f^+ | O_{\mathrm{GT}} \frac{1}{H - E_i + Q_{\beta\beta}/2} O_{\mathrm{GT}} | 0_i^+ \rangle$$

$$= \langle \Phi_0 | L_0 \overline{O}_{\mathrm{GT}} \frac{1}{\overline{H} - E_i + Q_{\beta\beta}/2} \overline{O}_{\mathrm{GT}} | \Phi_0 \rangle$$

Lanczos continued fraction method

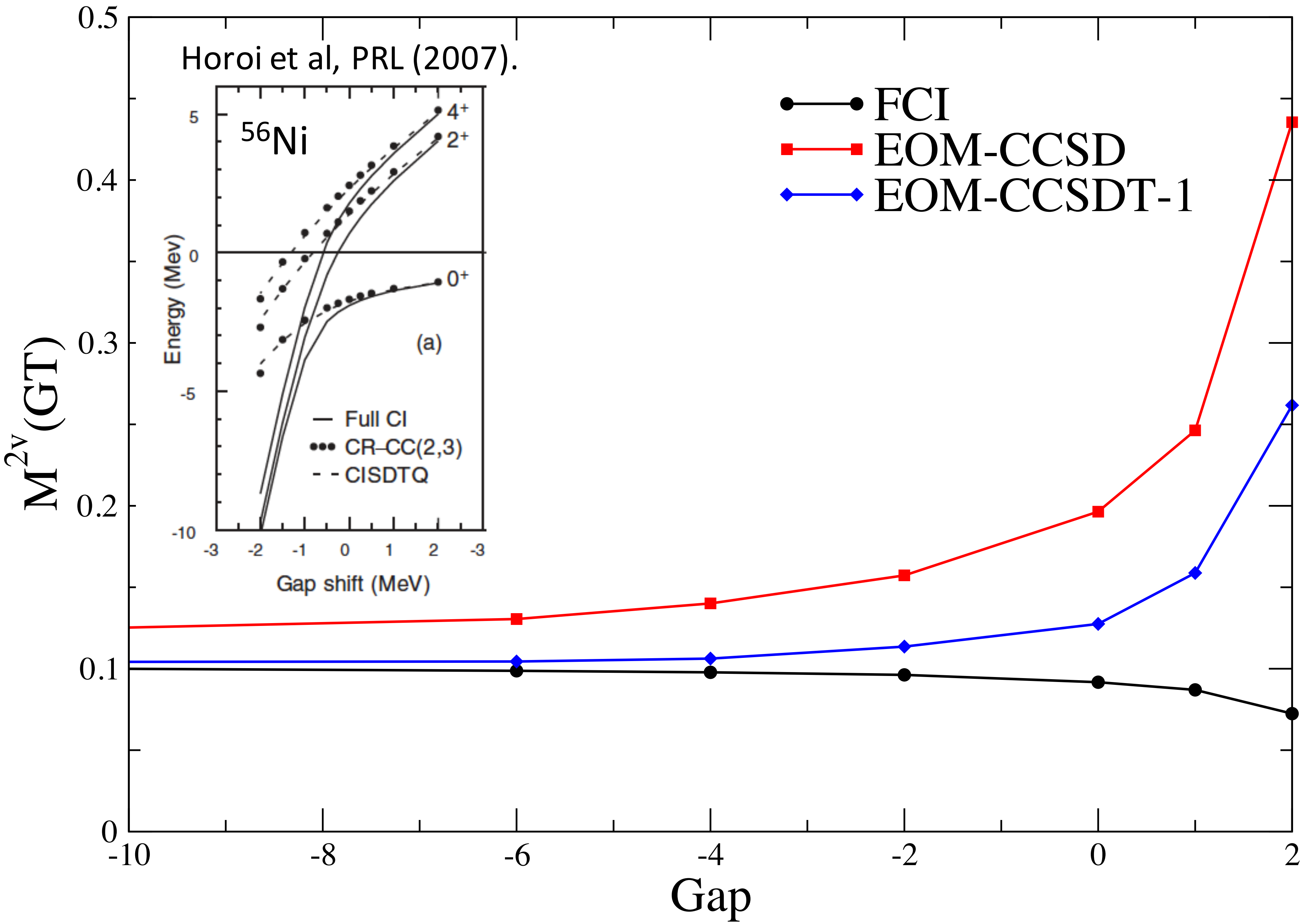
$$M^{2\nu} = \langle \Phi_0 | L_0 \overline{O}_{\rm GT} \frac{1}{\overline{H} - E_i + Q_{\beta\beta}/2} \overline{O}_{\rm GT} | \Phi_0 \rangle$$

Define left/right Lanczos pivots: $\langle \tilde{\nu}_0 | = \langle \Phi_0 | L_0 \overline{O}_{\rm GT} \quad | \nu_0 \rangle = \overline{O}_{\rm GT} | \Phi_0 \rangle$

$$M^{2\nu} = \langle \tilde{\nu}_0 | \nu_0 \rangle \left\{ \frac{1}{(a_0 - Q_{\beta\beta}/2) - \frac{b_0^2}{(a_1 - Q_{\beta\beta}/2) - \frac{b_1^2}{(a_2 - Q_{\beta\beta}/2) \; - \cdots}}} \right\}$$

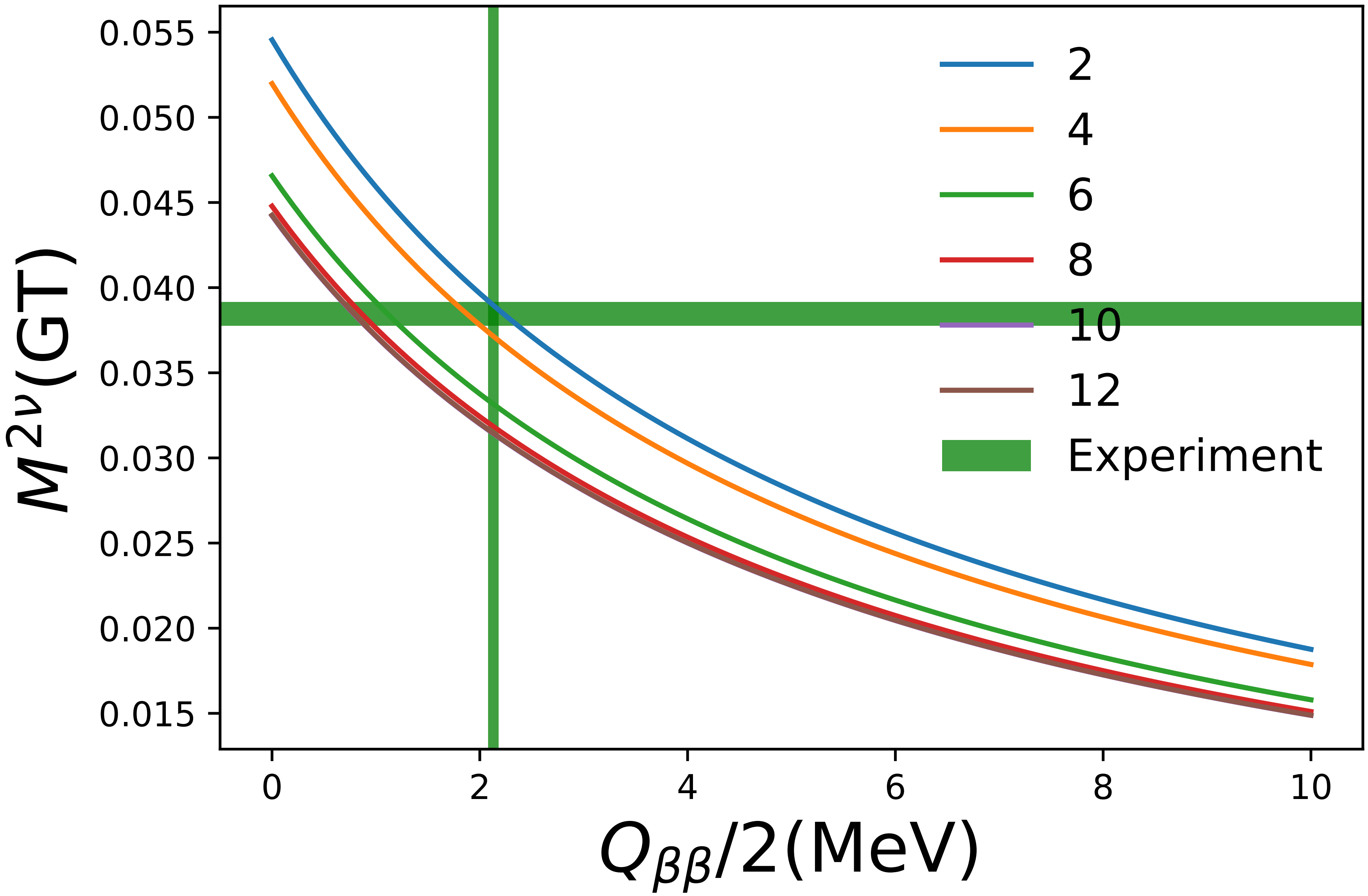
- Lanczos continued fraction method, see e.g. Engel, Haxton, Vogel PRC (1992), Haxton, Nollett, Zurek PRC (2005), Miorelli et al PRC (2016).
- Matrix element is converged to machine precision after ~10 iterations.
- Need more than 50 1^+ states converged in ^{48}Sc (300-400 Lanczos iterations) if we sum explicitly over intermediate states

ββ-decay of ^{48}Ca with GXPF1A shell-model interaction



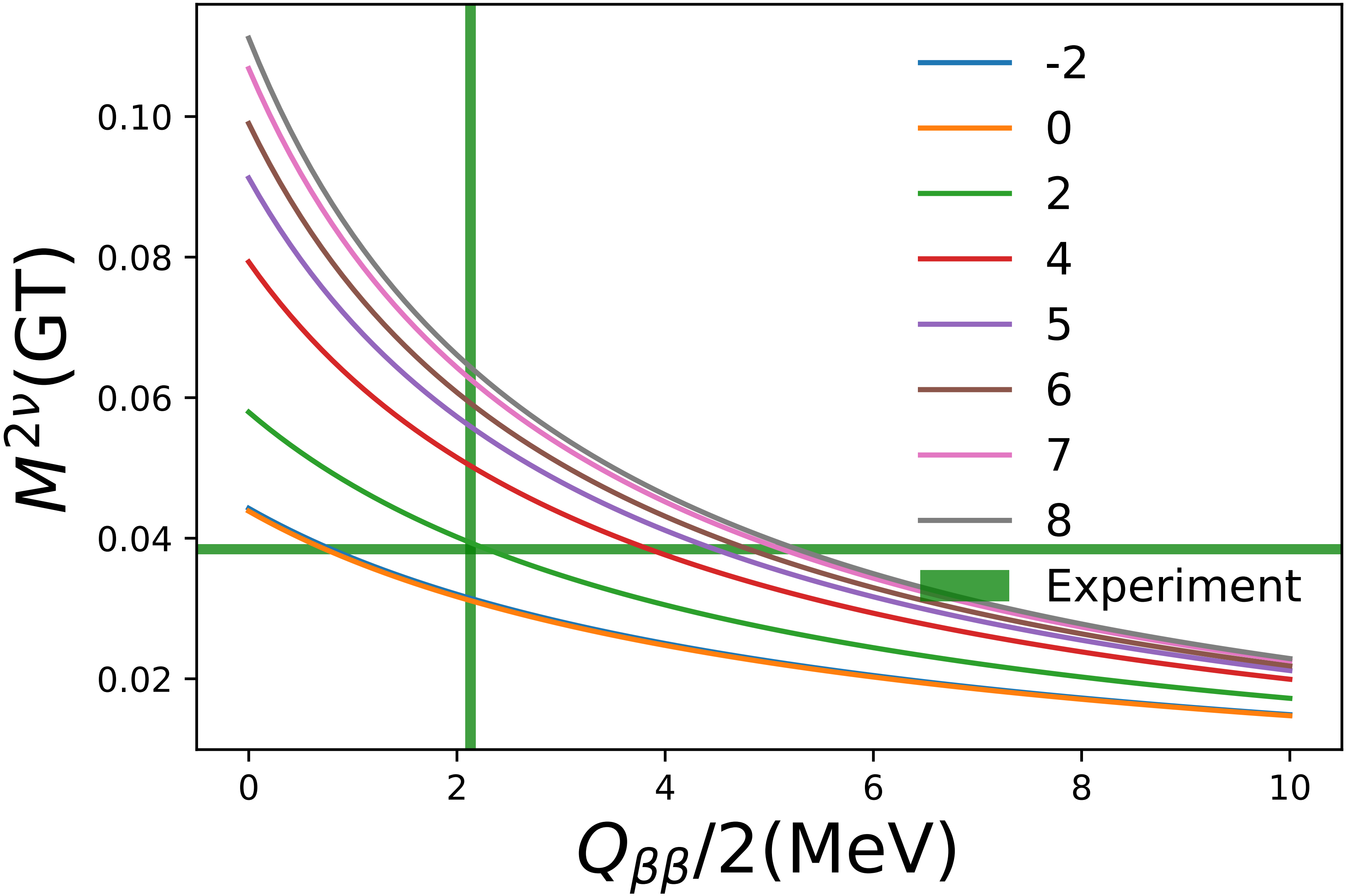
ββ-decay of ^{48}Ca

The role of 3p3h excitations in the ground-state of ^{48}Ti



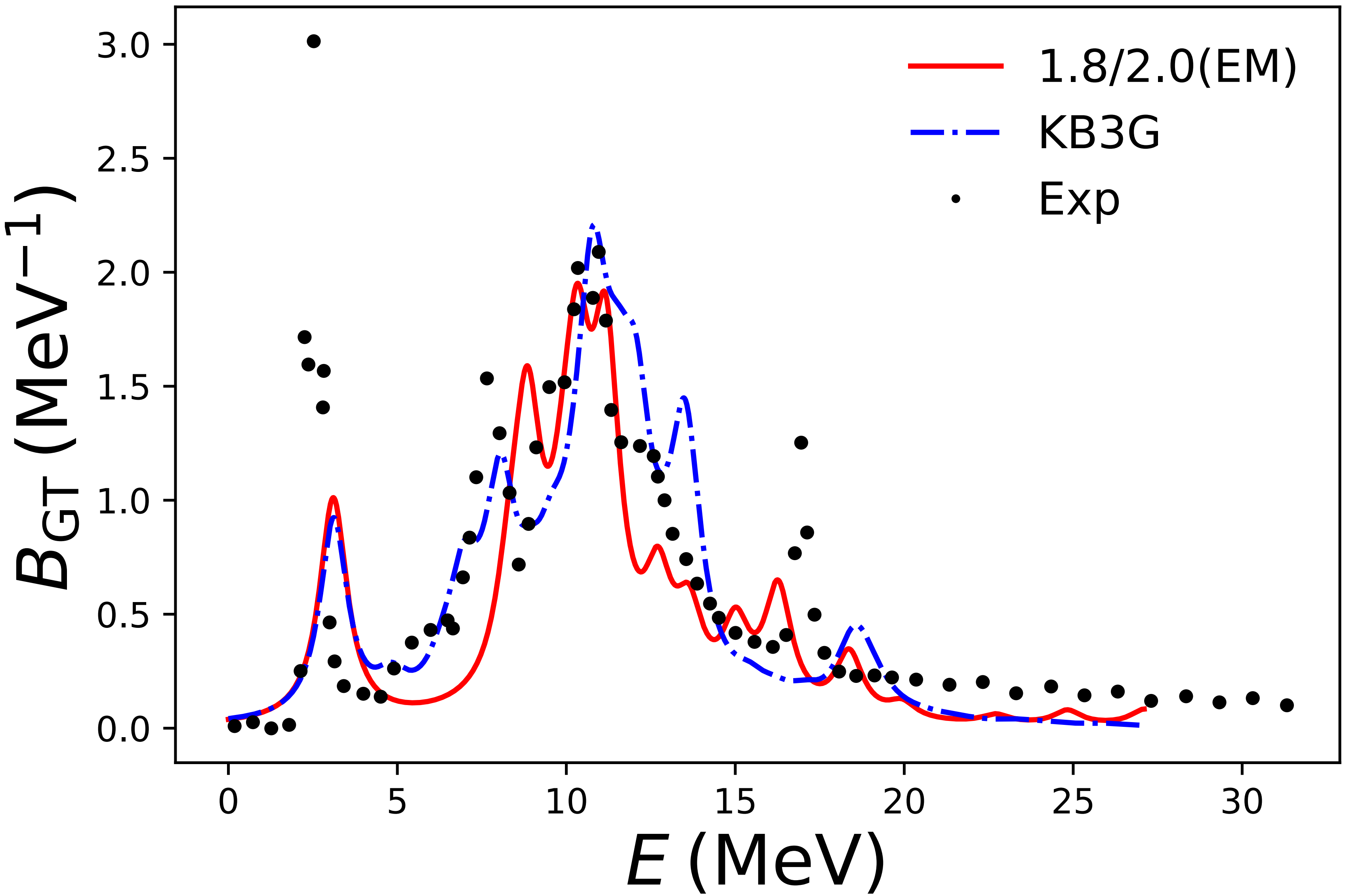
ββ-decay of ^{48}Ca

The role of 3p3h excitations in the intermediate 1^+ states of ^{48}Sc



Gamow-Teller strengths in ^{48}Ca

GT-strength computed using the Lanczos method and EOM-CCSDT-1
No 2BCs, strength function folded with a Lorentzian of width 0.5MeV.



Summary

- Optimized chiral interactions with explicit delta’s show significant improvement in description of light- and medium mass nuclei and infinite matter
- Natural orbitals offers a promising route to include higher order correlations in coupled-cluster computations
- First NME for $0\nu\beta\beta$ and $2\nu\beta\beta$ in ^{48}Ca from coupled-cluster calcualtions