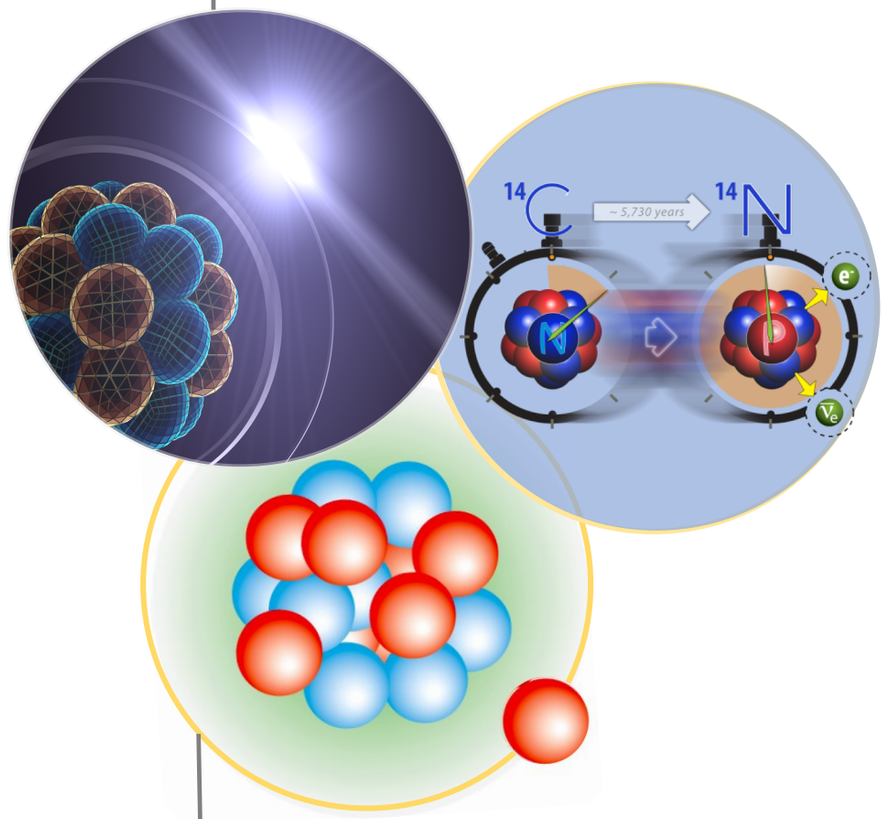
Open problems and challenges in ab initio descriptions of nuclei

Gaute Hagen
Oak Ridge National Laboratory



Chiral EFT: New Perspectives

INT, March 18th, 2025

U.S. DEPARTMENT OF ENERGY
NUCLEI
Nuclear Computational Low-Energy Initiative
STREAMLINE
SmarT Reduction and Emulation Applying Machine Learning In Nuclear Environments
OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Collaborators

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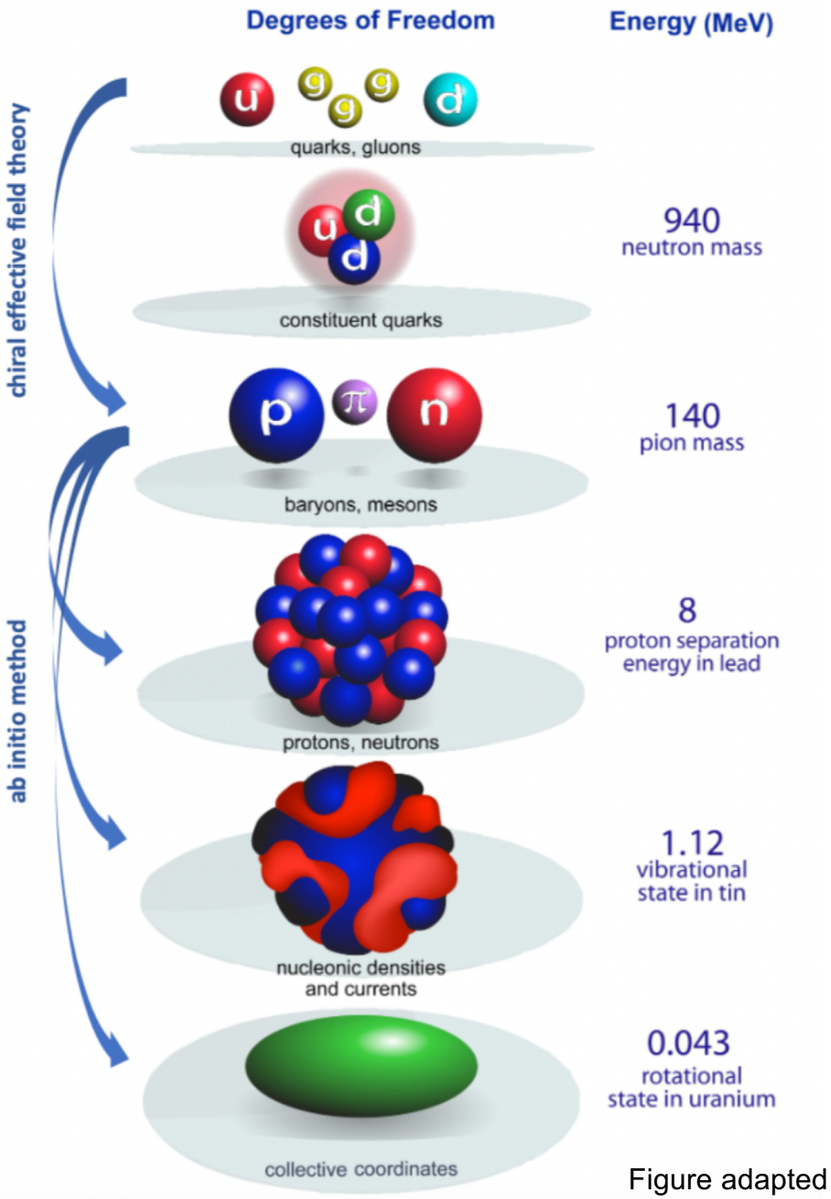
@ LSU: **Zhonghao Sun**

@ Chalmers: A. Ekström, C. Forssén

@ Mainz**:** S. Bacca, **Francesco Marino**, **J. E. Sobczyk, Weiguang Jiang**

@ WUSTL: **Sam Novario**

Multiscale physics of nuclei from ab-initio methods



What is ab initio in nuclear theory?

A. Ekström et al, Frontiers (2023)

"we interpret the ab initio method to be a systematically improvable approach for quantitatively describing nuclei using the finest resolution scale possible while maximizing its predictive capabilities"

- Nuclei exhibit multiple energy scales ranging from hundreds of MeV in binding energies to fractions of an MeV for low-lying collective excitations.
- Describing these different energy scales within a unified ab-initio framework from chiral interactions is a long-standing challenge

Figure adapted from Bertsch, Dean, Nazarewicz, SciDAC review (2007)

Solving the quantum many-nucleon problem

An exponentially hard problem to solve!

$$H|\Psi\rangle = E|\Psi\rangle$$

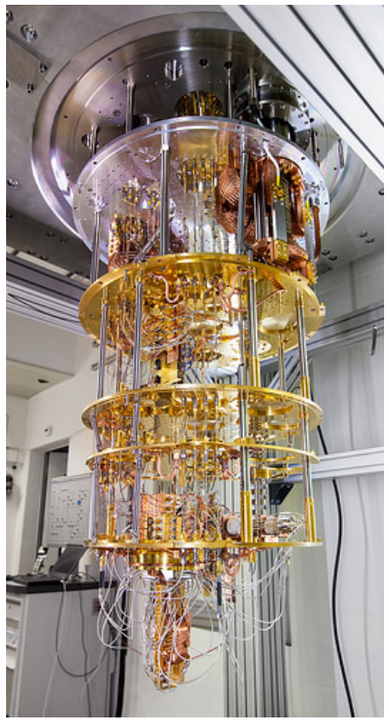
1.1 exaflops

Polynomial scaling

Systematically improvable approaches
with controlled approximations:
Coupled-cluster, IMSRG, Gorkov, SCGF,…

Emulators?

IBM Q Experience



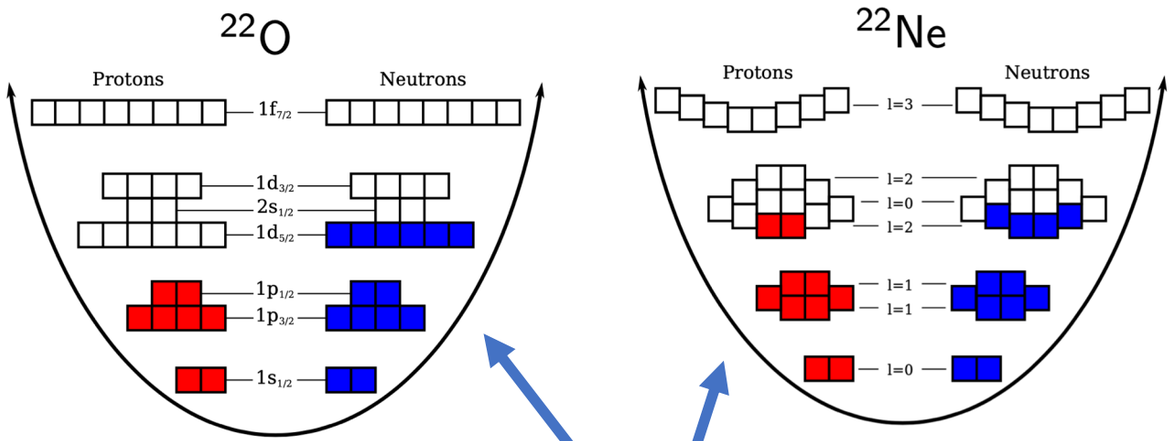
Fault tolerant quantum computing??

Coupled-cluster computations of nuclei

- Compute Hartree-Fock reference state: $W_0 + W_1 + W_2 + W_3$

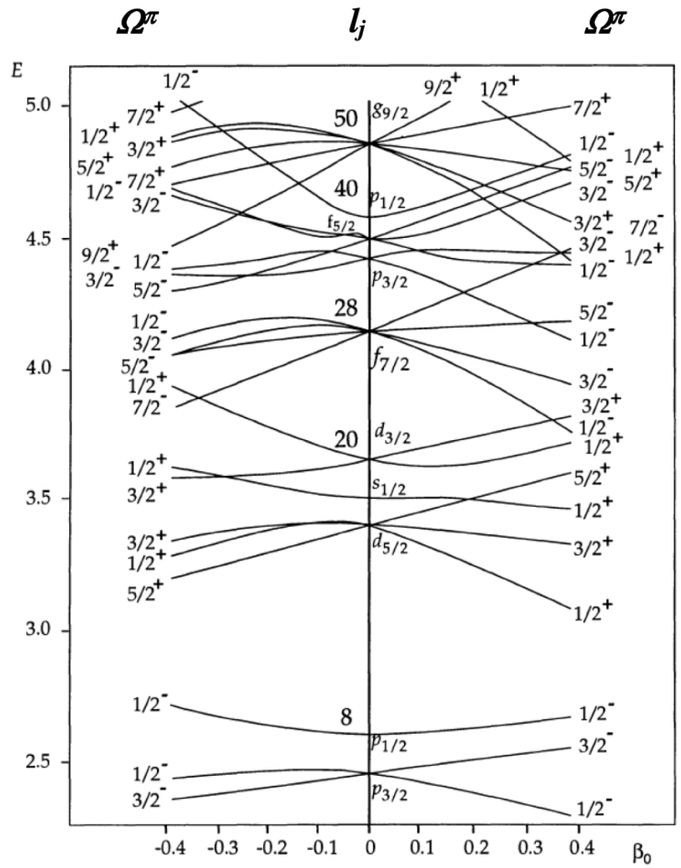
$$H = T - T_{\mathrm{CoM}} + V_{\mathrm{NN}} + V_{3\mathrm{N}}$$

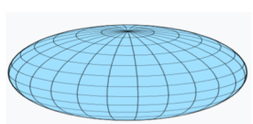
- Informs us about emergent breaking of symmetries

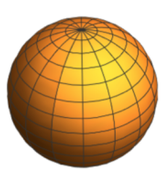


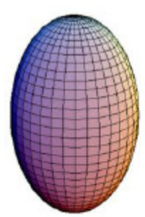
$$|\Psi\rangle = \Omega|\Phi\rangle$$

Wave-operator (includes many-body correlations)



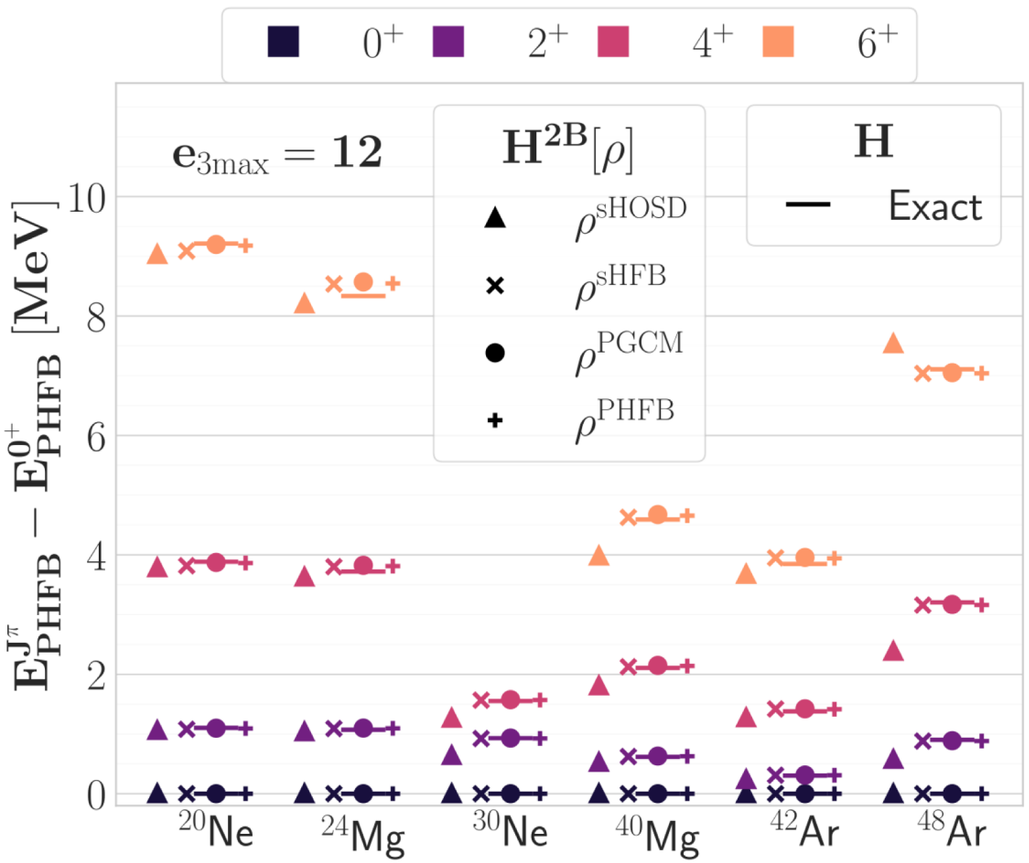




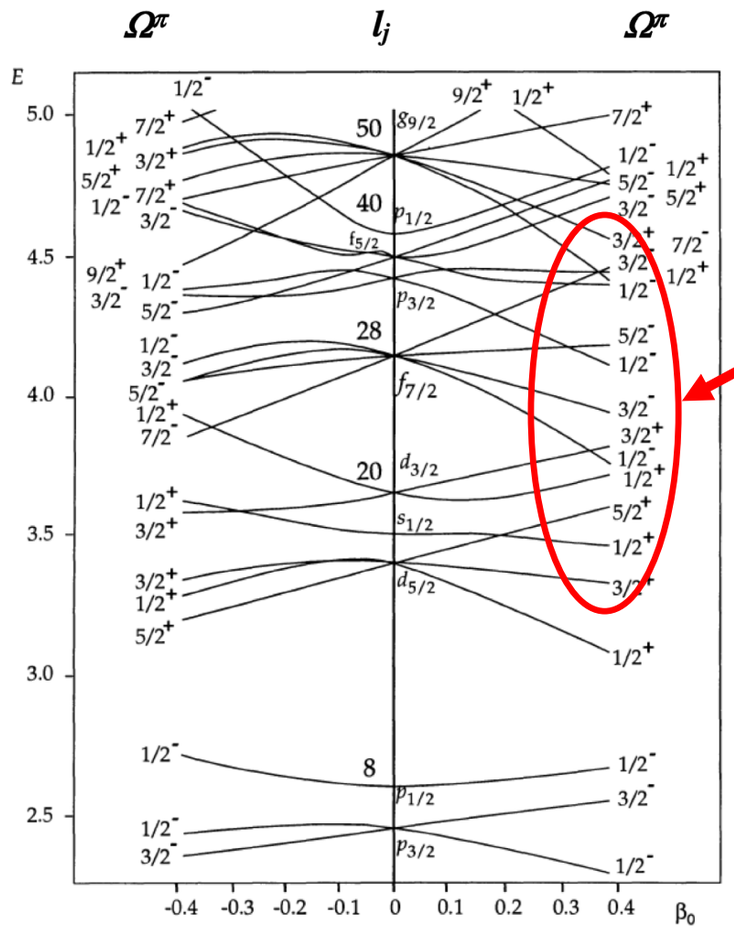


Inclusion of three-body forces

- The normal ordered 2-body approximation breaks rotational symmetry when normal-ordered with respect to a broken symmetry reference state
- Perform spherical HF with fractional filling to normal-order three-nucleon force



Mikael Frosini et al, Eur. Phys. J. A 57 (2021)



What is the correct spherical filling in very deformed nuclei?

Coupled-cluster computations of nuclei

- Include short-range correlations via coupled-cluster theory
  - Large contribution to total energy
  - Cost increases polynomial with mass

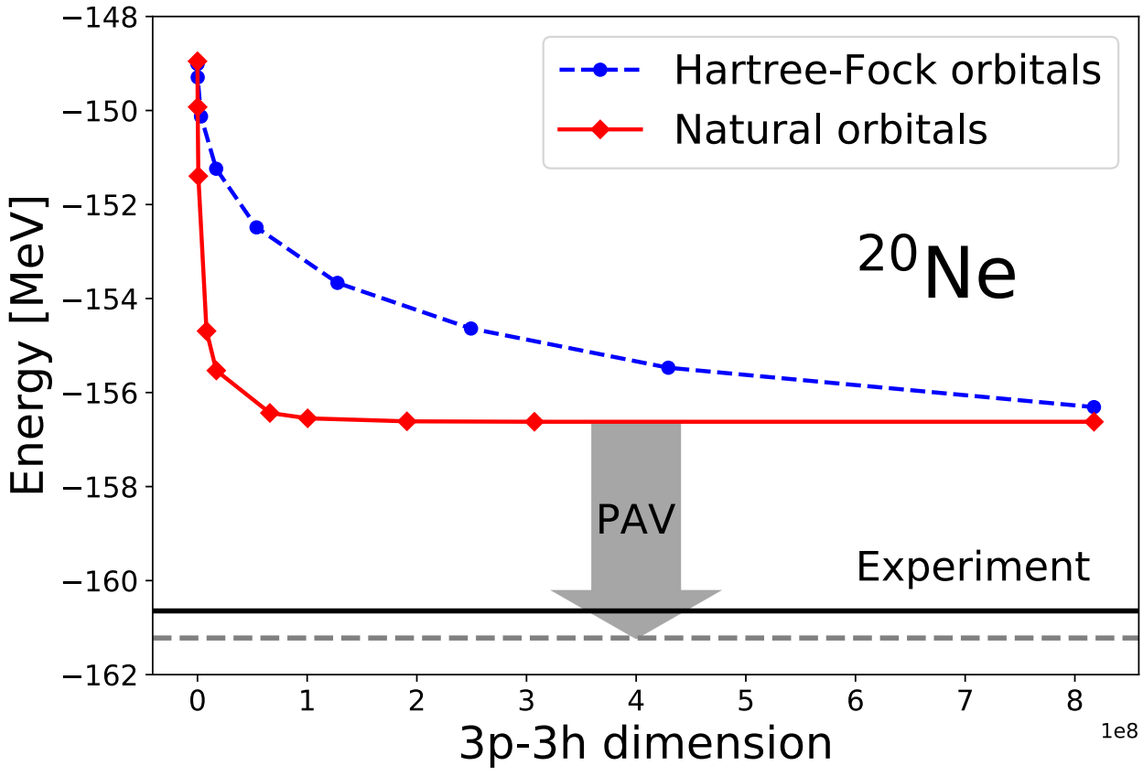
$$|\Psi\rangle = \Omega|\Phi_0\rangle = e^T|\Phi_0\rangle$$

$$T = T_1 + T_2 + \ldots$$

- Include long-range correlations via symmetry projections
  - Small contribution to total energy
  - Relevant for rotational bands and transition matrix elements

$$E^{(J)} = \frac{\langle\widetilde{\Psi}|P_J H|\Psi\rangle}{\langle\widetilde{\Psi}|P_J|\Psi\rangle}$$

S. J. Novario, et al PRC 102, 051303 (2020)



Total energy:

$$E = E_{\text{ref}} + \Delta E_{\text{CC}} + \delta E$$

Convergence of coupled-cluster method

$$C_1 = T_1,$$

$$C_2 = T_2 + \tfrac{1}{2}T_1^2,$$

$$C_3 = T_3 + T_1T_2 + T_1^3/3!,$$

$$C_4 = T_4 + T_2^2/2 + T_1T_3 + T_1^2T_2/2 + T_1^4/4!,$$

$$\vdots,$$

CCSD

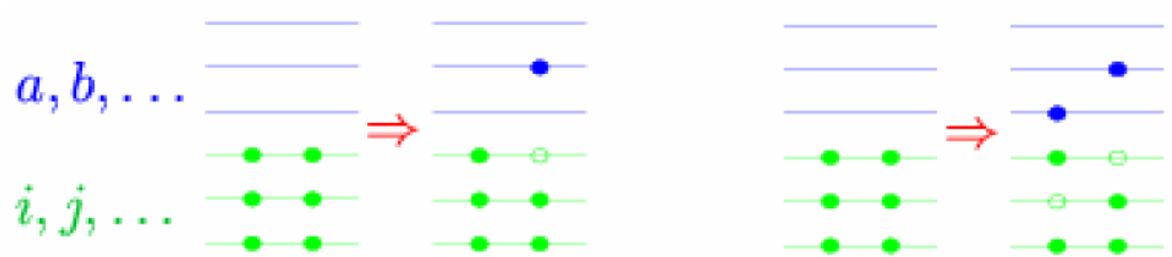
CCSDT

Exact CI:

$$|\Psi\rangle = \Omega|\Phi\rangle = (1 + \sum_{i=1}^{A} C_i)|\Phi\rangle$$

- CCSD captures most of the 3p3h and 4p4h excitations (scales as $n_o^2 n_u^4$)
- In order to describe α −cluster states need to include full quadruples (CCSDTQ) (scales $n_o^4 n_u^6$)

Correlations are *exponentiated* 1p-1h and 2p-2h excitations. Part of Ap-Ah excitations included!



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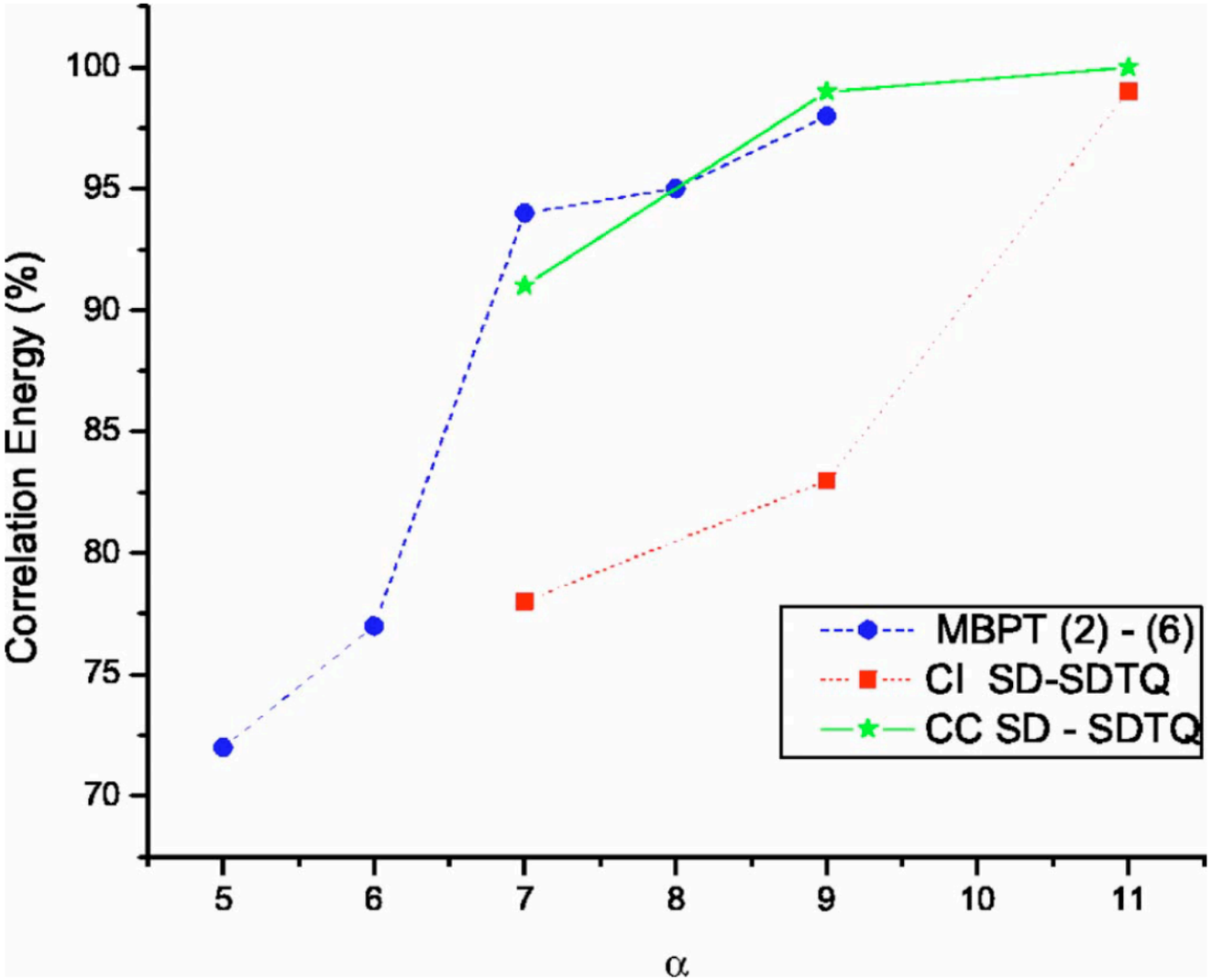
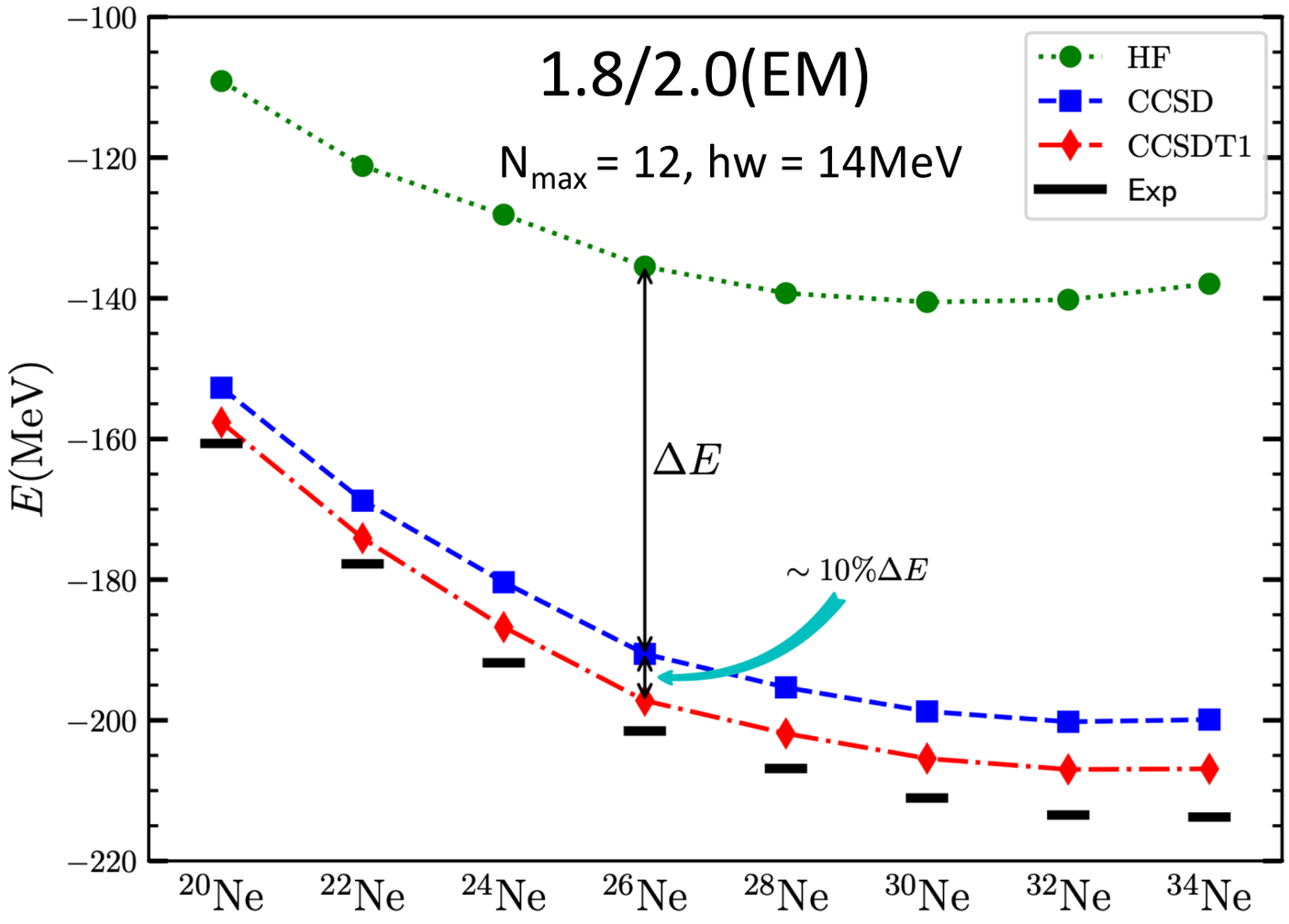


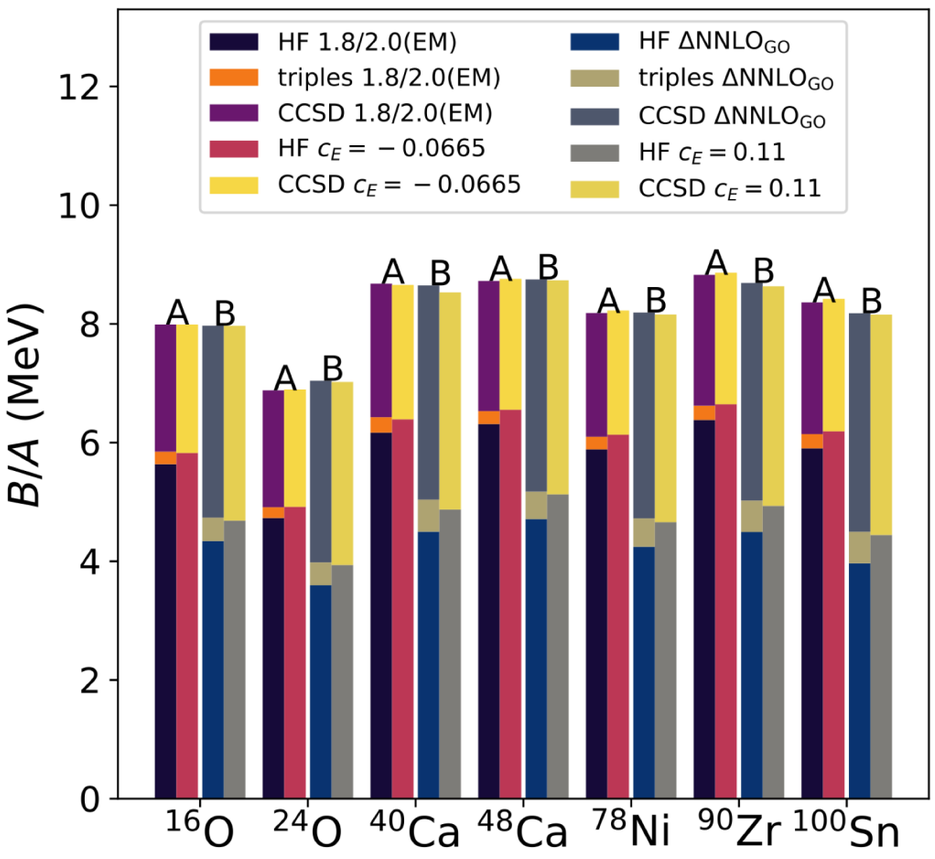
Bartlett & Musial Rev. Mod. Phys. (2007)

Convergence of coupled-cluster method



Zhonghao Sun et al, Phys. Rev. X **15**, 011028 (2025)

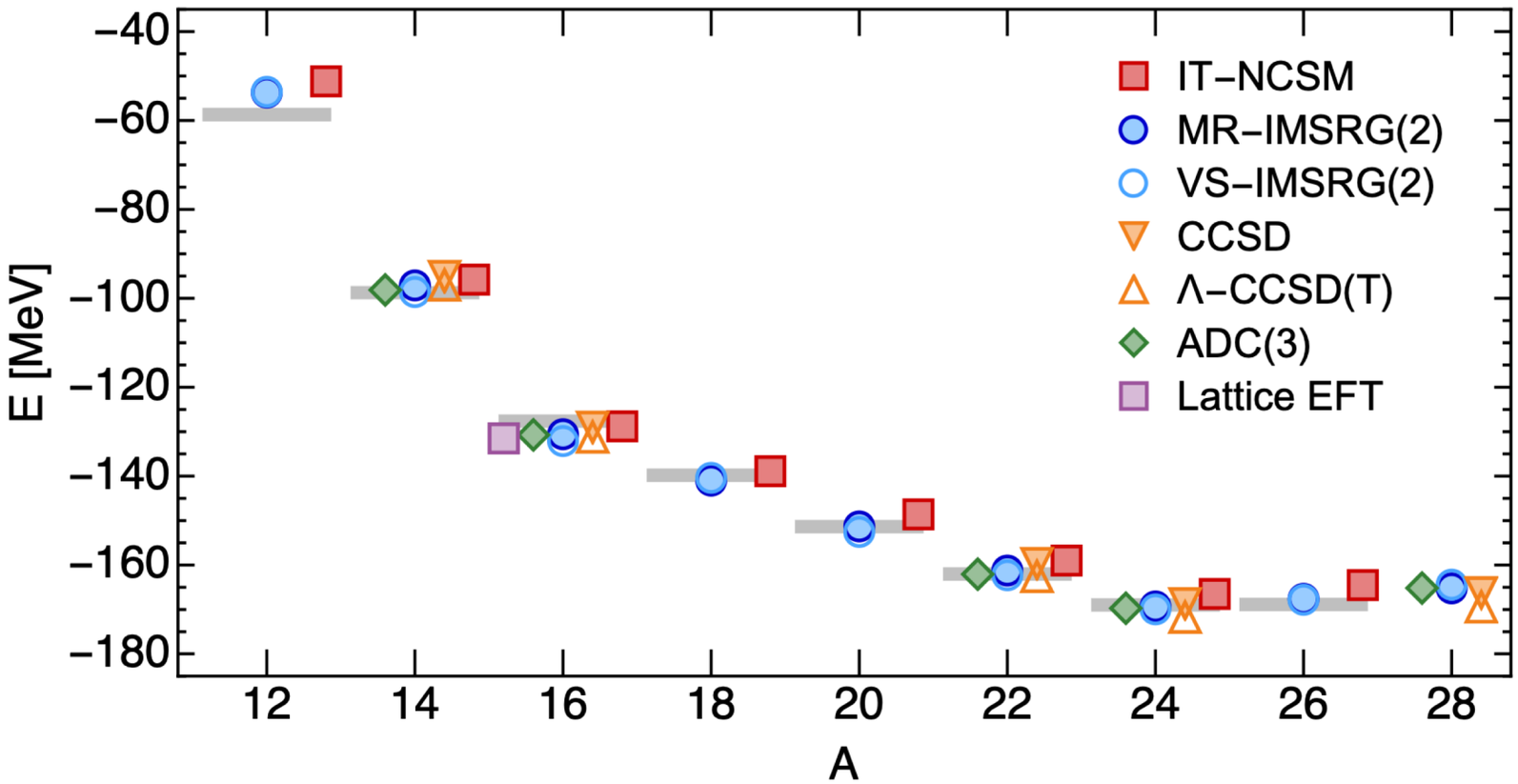
Triples excitations yield ~10% of CCSD correlation energy



Zhonghao Sun et al Phys. Rev. C **106**, L061302 (2022)

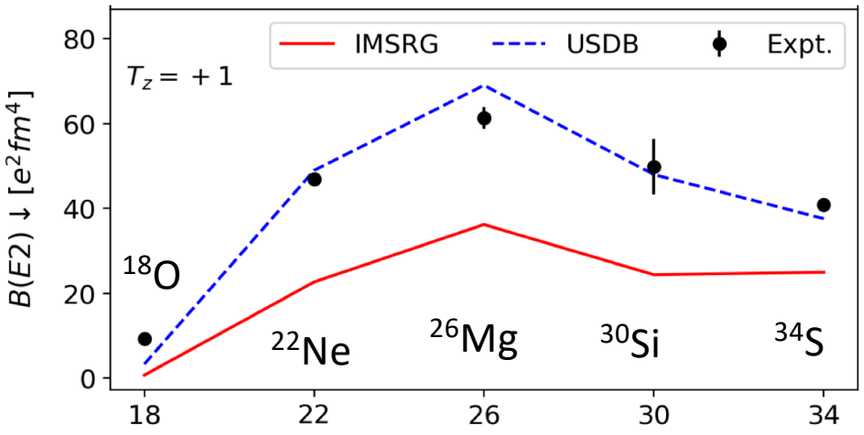
What precision/accuracy can we aim for in ab-initio modeling of nuclei?

Different many-body approaches agree with each for binding energies and radii
(challenges exist for transitions, isotope shifts, and deformed shapes)

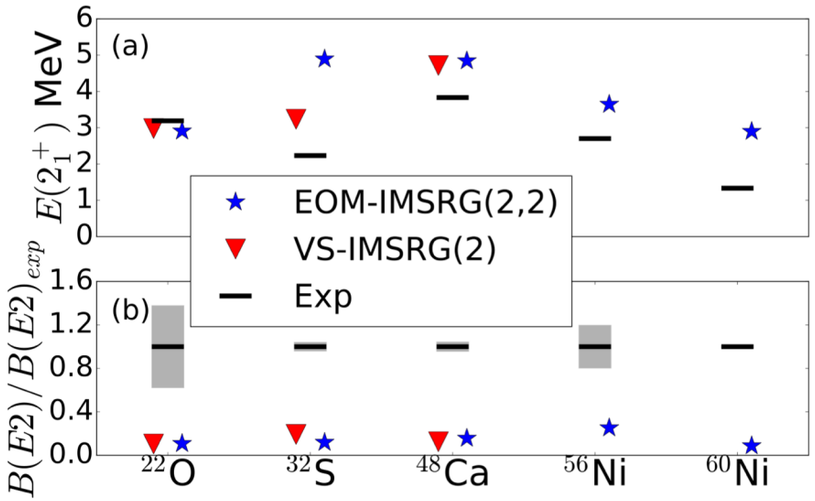


H. Hergert Front. Phys., (2020)

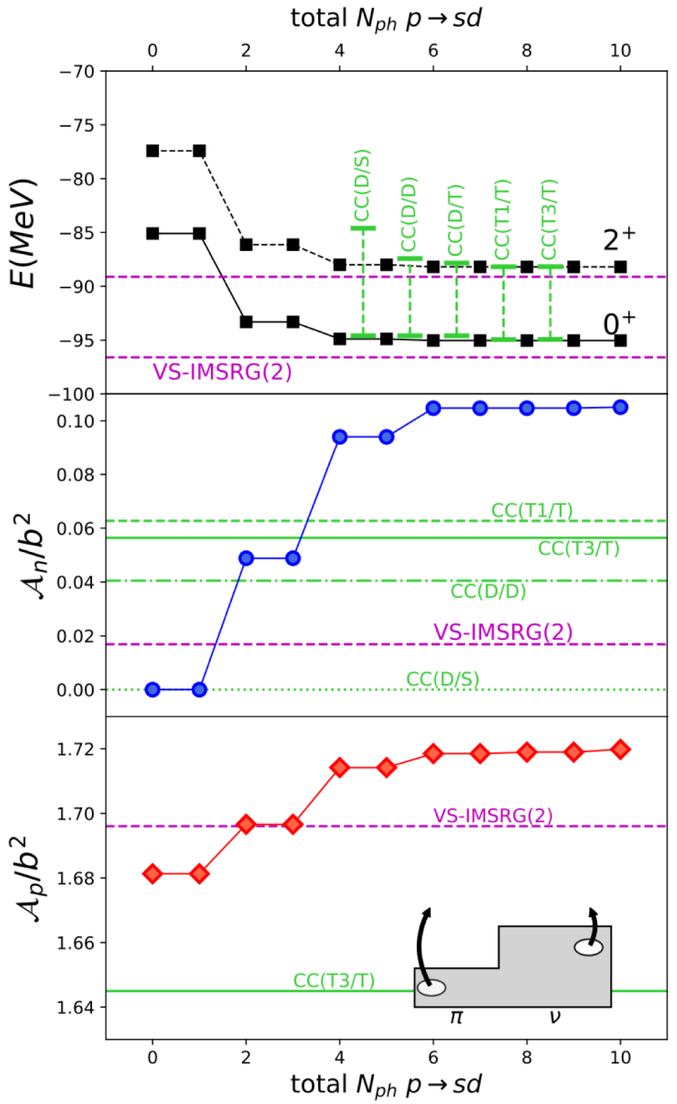
What precision/accuracy can we aim for in ab-initio modeling of nuclei?



S. R. Stroberg, et al PRC **105** 034333 (2022)



N. M. Parzuchowski, et al Phys. Rev. C 96, 034324 (2017)



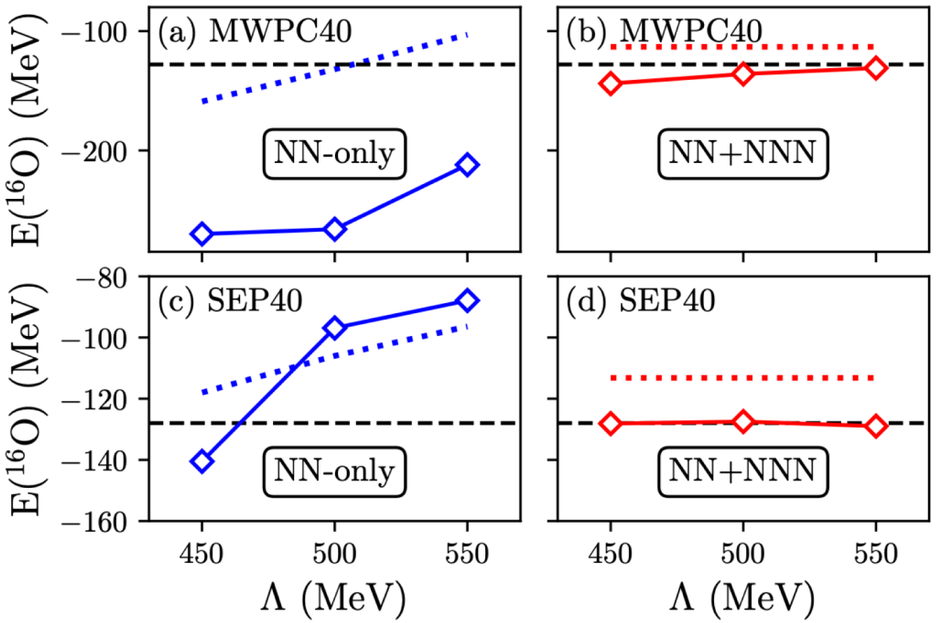
Electromagnetic transitions pose a significant challenge for polynomial scaling methods

How do we quantify uncertainties for observables that are sensitive to fine details in the wave function?

Application of modified Weinberg counting in nuclei

$$V_{\rm LO}^{\rm MWPC}(\mathbf{p},\mathbf{p}') = V_{\rm LO}^{\rm WPC}(\mathbf{p},\mathbf{p}') + (\tilde{C}_{^3P_0} + \tilde{C}_{^3P_2})pp'$$

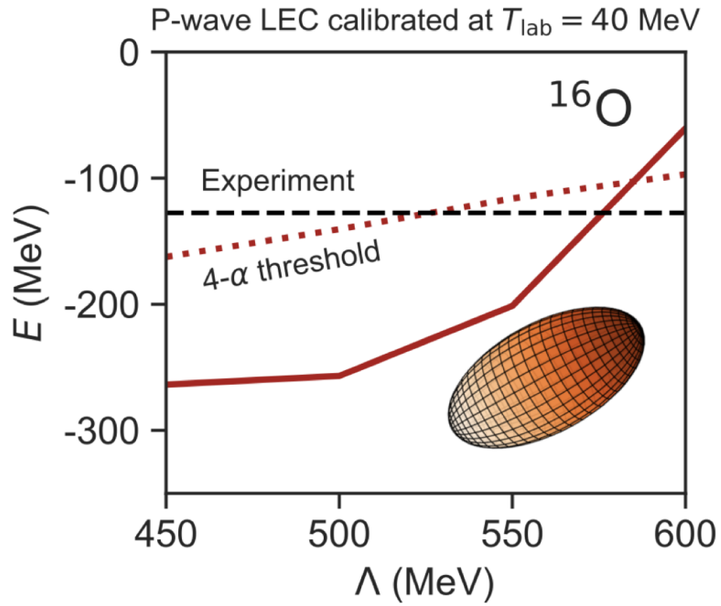
$$V_{\rm SEP}(p,p') = \frac{ym_N}{\sqrt{p^2+m_N\Delta}\sqrt{p'^2+m_N\Delta}}$$



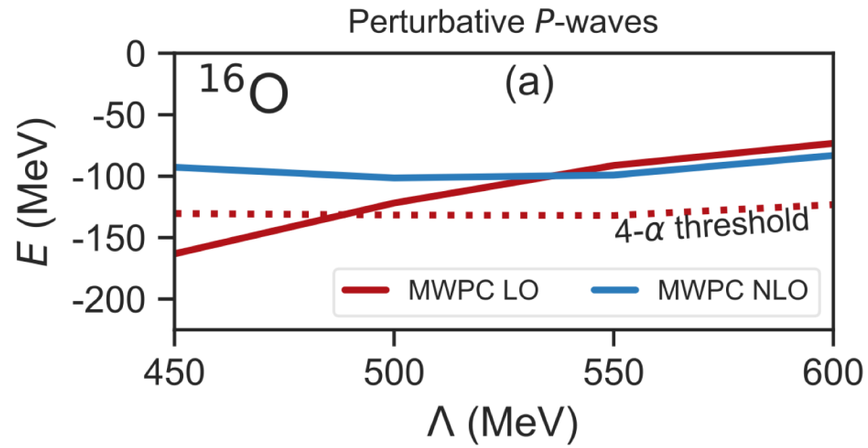
Inclusion of 3N at LO improves the description of ^{16}O
Initial results indicate that 4N forces are needed for heavier nuclei and this complicates many-body calculations

Yang, CJ., et al. Eur. Phys. J. A 59, 233 (2023)

See Jerry's talk tomorrow for more details

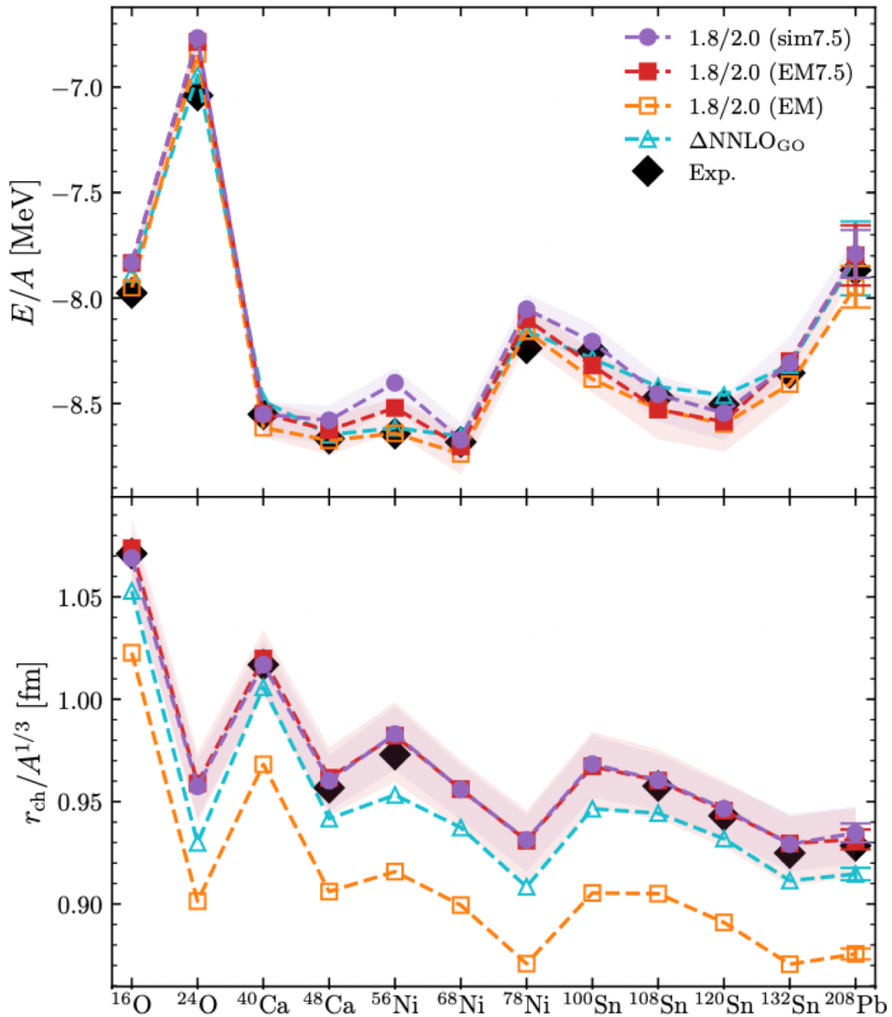


RG-invariant PCs in χEFT gives a deformed ground state at LO, which leaves small hope for a remedy from perturbative corrections.



C. -J. Yang, A. Ekström, C. Forssén, G. Hagen, Phys. Rev. C 103, 054304 (2021)

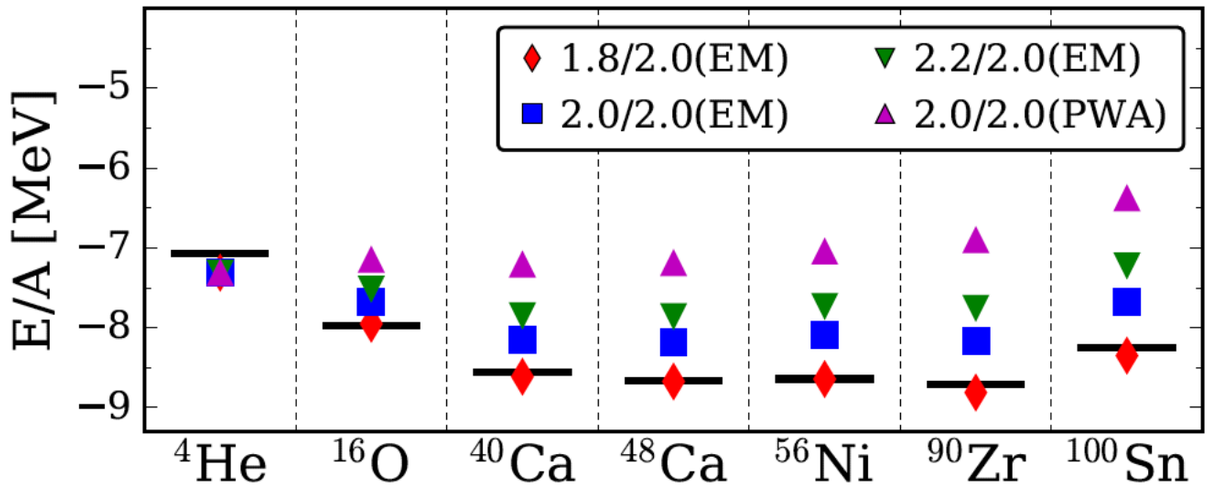
Some interaction models work “better” than others



P. Arthuis, K. Hebeler, A. Schwenk, arXiv:2401.06675 (2024)

Family of “magic” 1.8/2.0 (EM…)

- SRG evolve 2N force @ N3LO (Entem & Machleidt)
- Assume induced 3N can be absorbed into D and E contact terms
- Fit c_D and c_E to triton g.s. and ^{4}He radius using un-evolved 3N force @ N2LO
- Predict good binding energies and spectra across nuclear chart, even for ^{208}Pb

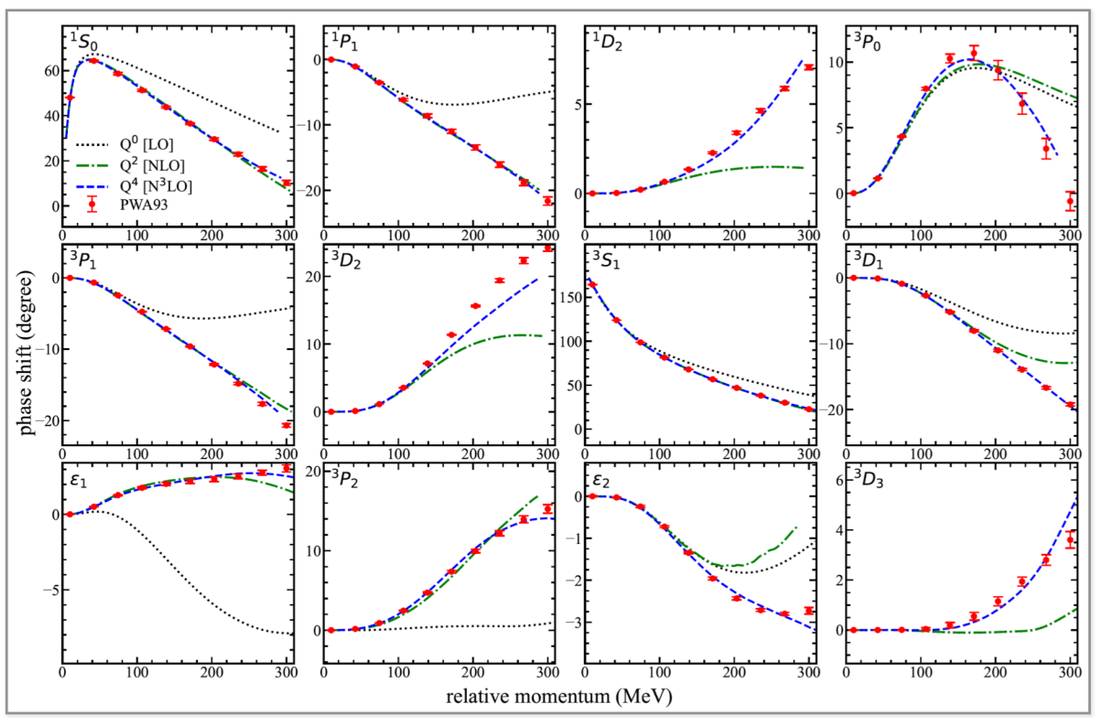


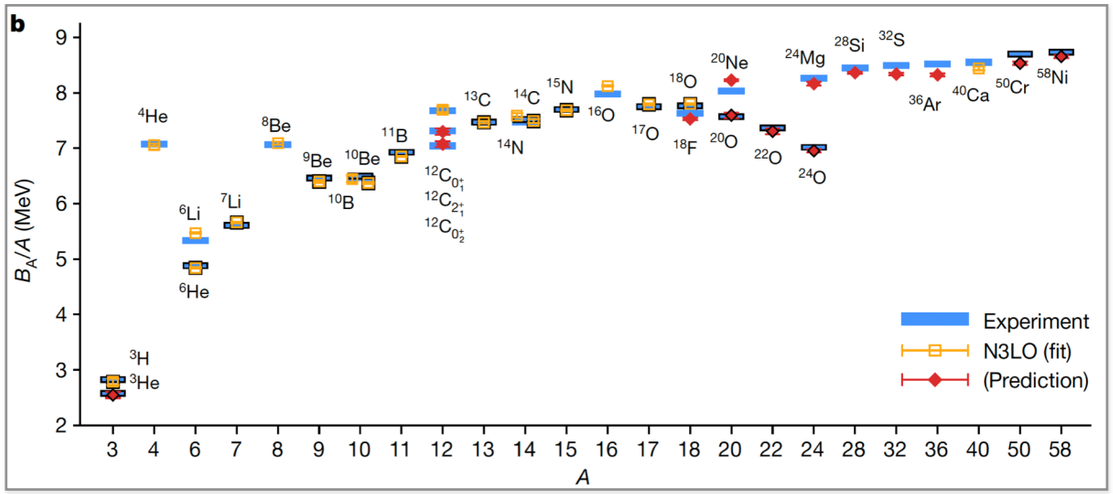
K. Hebeler *et al* PRC (2011).
T. Morris *et al*, PRL (2018).

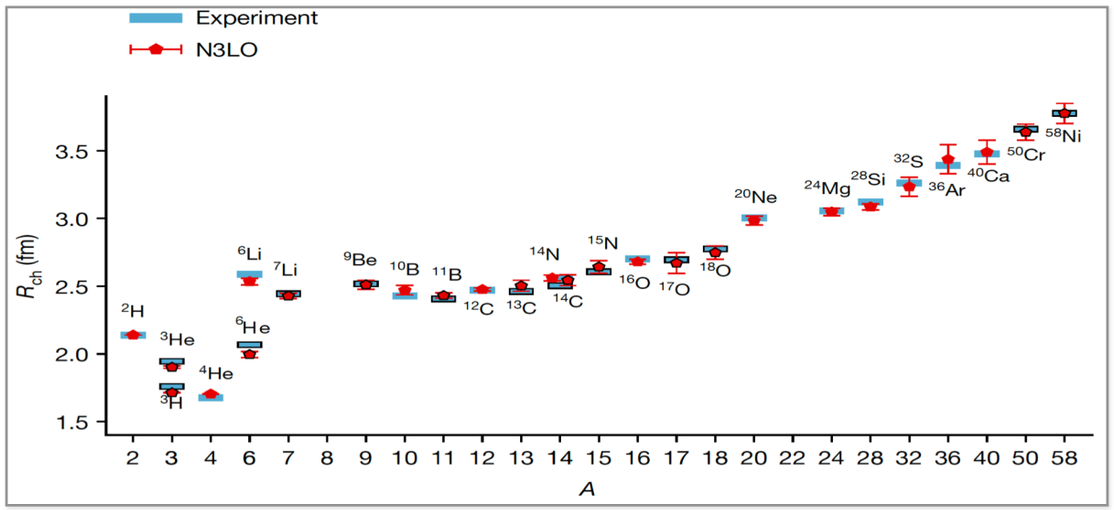
Some interaction models work “better” than others

Lattice EFT N^{3}LO

- 2NF@N3LO + 3NF@N2LO at fixed lattice spacing
- Six additional 3NF LECs adjusted to selected data
- Yield accurate binding energies and radii for a range of nuclei from A=2 to A=56 and infinite nuclear matter
- Challenging to use for other many-body methods

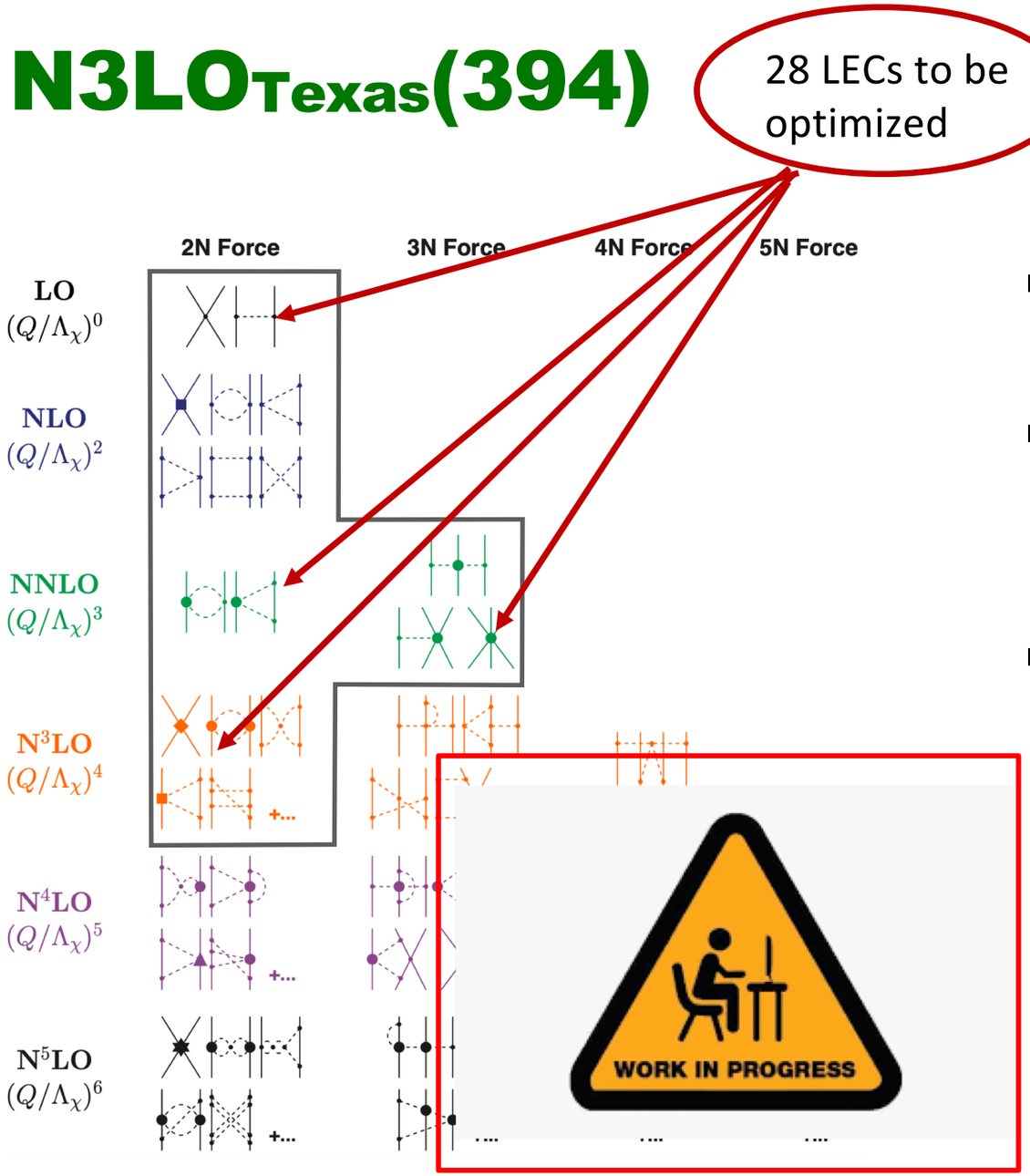






S Elhatisari, et al., Nature 630, 59 (2024)

N3LO$_{\text{Texas}}$(394)

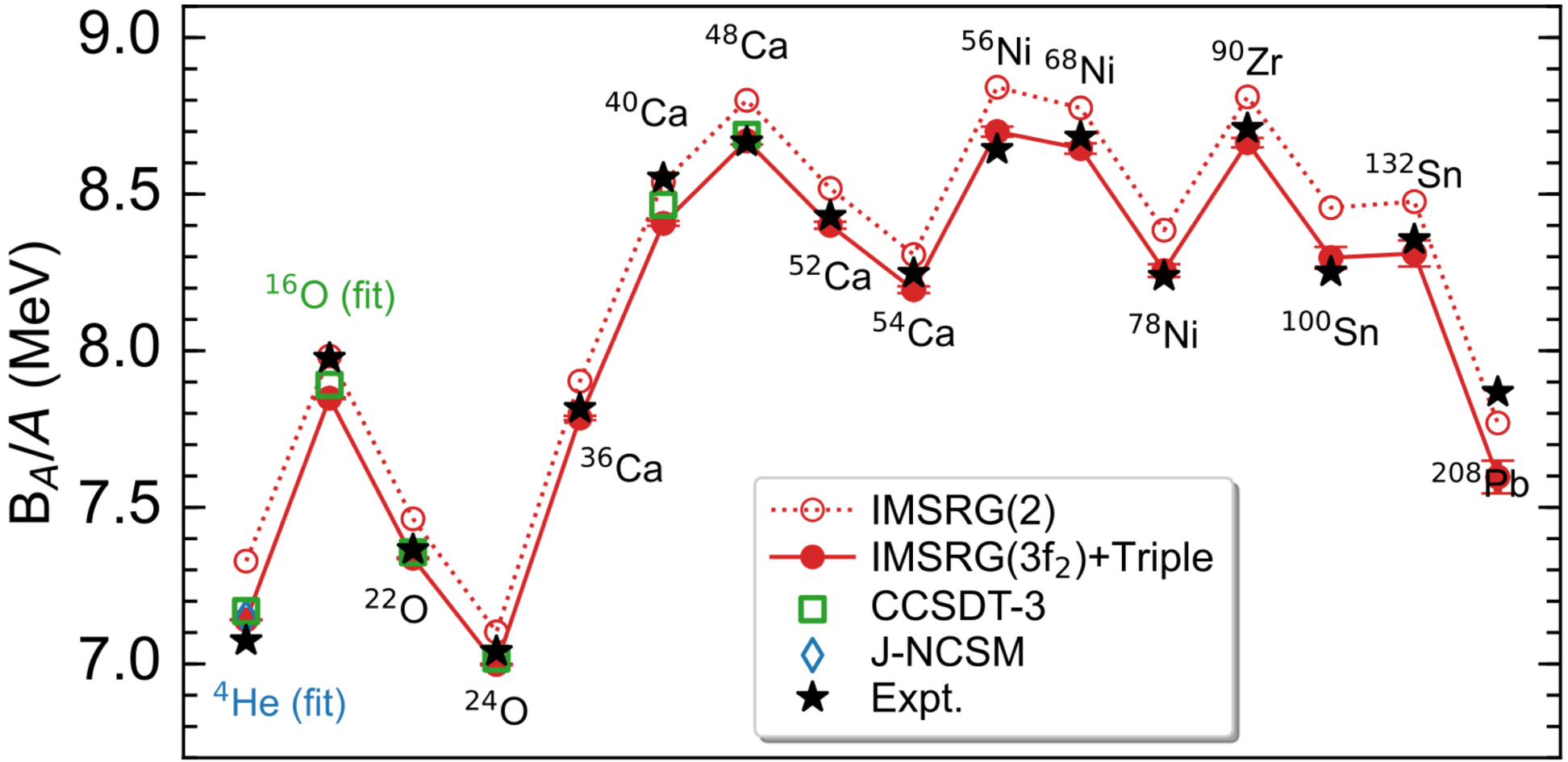


Optimization Strategy:

- Optimize a chiral interaction with NN at N3LO and 3NFs at N2LO
- Use high-fidelity few - and many-body emulators to efficiently evaluate observables in the objective function
- Observables included in the fit:
  - Scattering phase shifts
  - Scattering lengths and effective range
  - Deuteron properties,
  - ^{4}He binding energy and radius
  - ^{16}O binding energy and radius

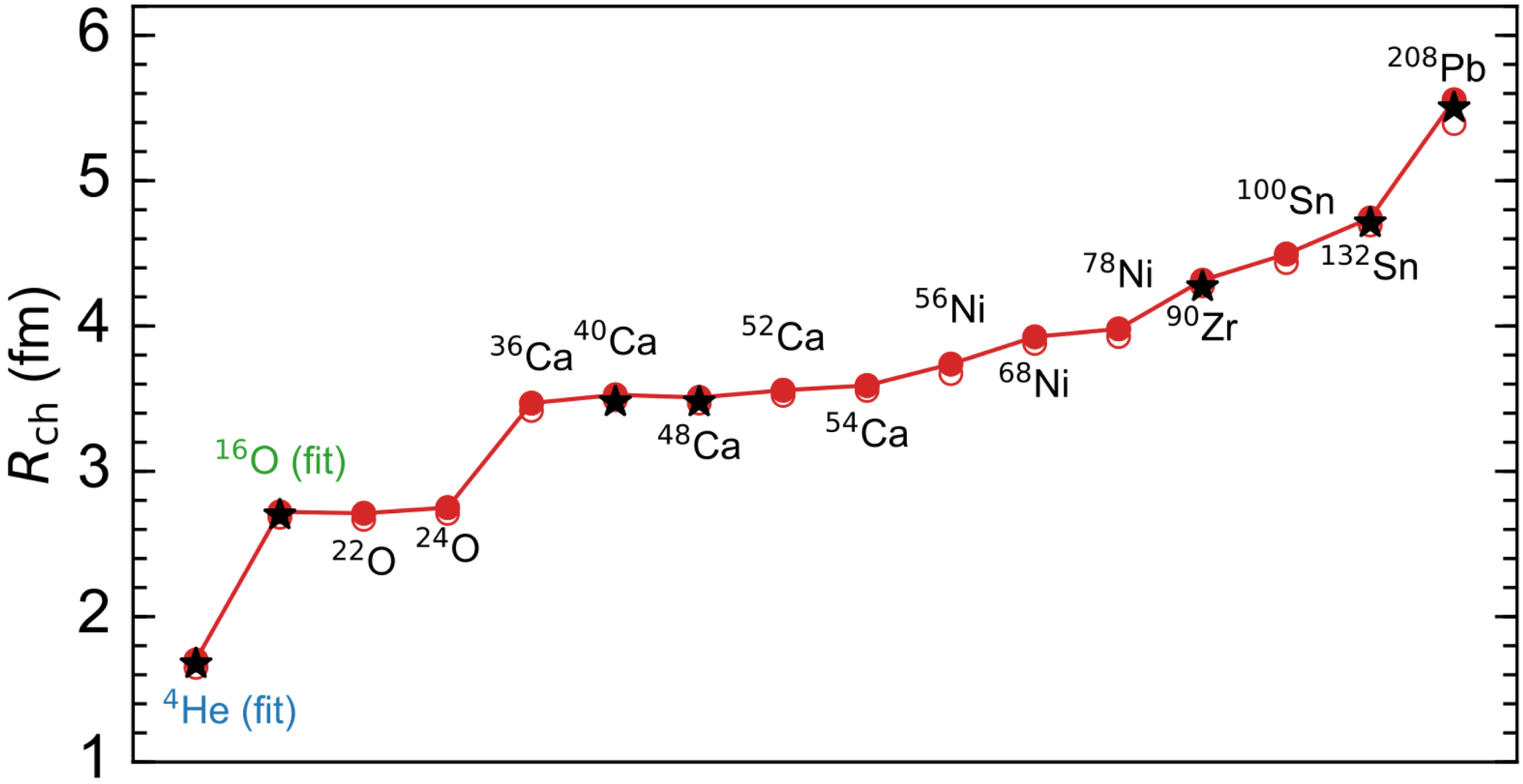
See Andreas' talk tomorrow for more details

Properties of light, medium mass and heavy nuclei



"IMSRG(3f2)+Triple" energies are extrapolated from N_{max} = 8, 10, 12, 14 with E_{3max} = 28
[B. C. He, S. R. Stroberg PRC 110, 044317 (2024)]
"IMSRG(2)" and all radii are calculated using N_{max}= 14 and E_{3max} = 28.
"CCSDT-3" results of ^{40}Ca and ^{48}Ca are extrapolated to infinite basis space from N_{max} = 8, 10, 12

Properties of light, medium mass and heavy nuclei

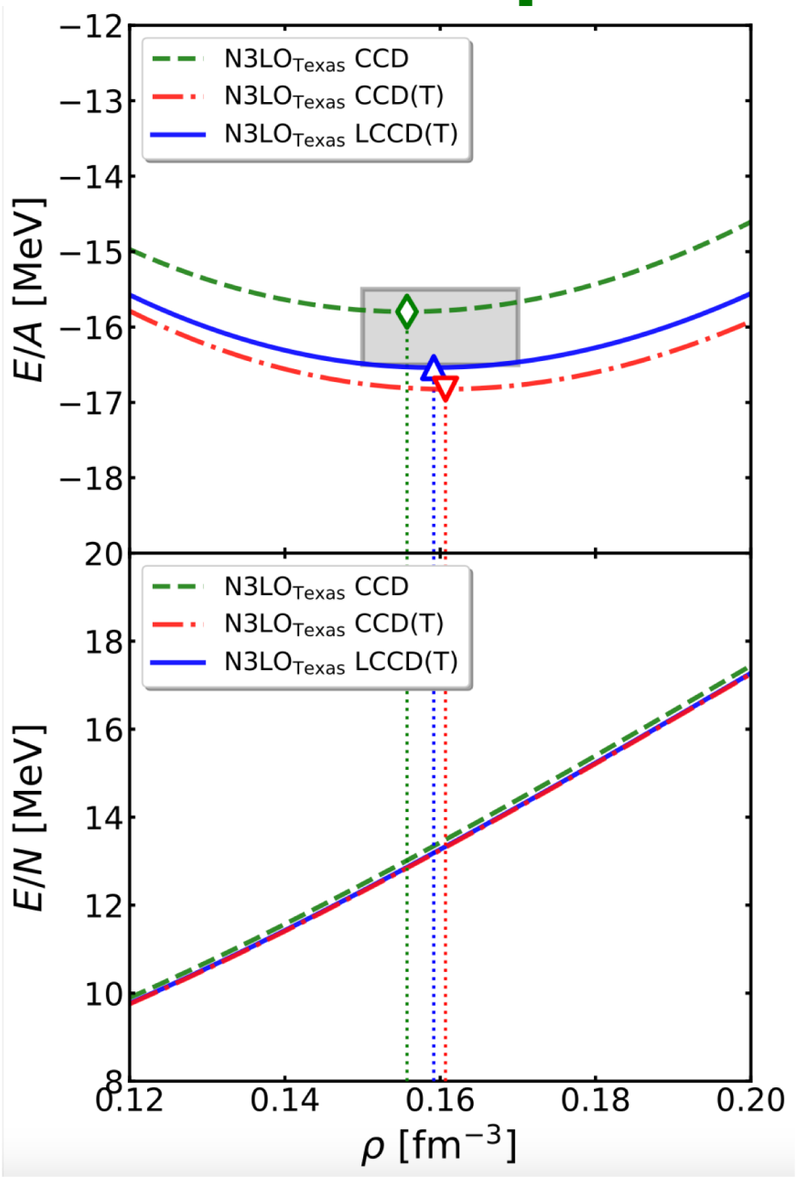


Spectra in selected closed shell nuclei

	EM1.8/2.0	ΔNNLO$_{\mathrm{GO}}$(394)	N^{3}LO$_{\mathrm{texas}}$(394)	Exp.
^{22}O 2_1^+	2.0	3.0(2)(1)	3.0(1)	3.20
^{24}O 2_1^+	4.3	3.9(2)(1)	3.2(1)	4.79
^{48}Ca 2_1^+	3.8	4.1(2)(1)	3.8(1)	3.83
^{78}Ni 2_1^+	2.5	–	3.1(3)	2.60

EOM-CCSD(T) results for N_{max} = 12, hw = 16MeV. The uncertainty comes from taking the difference to N_{max} = 10 results

Properties of neutron/nuclear matter

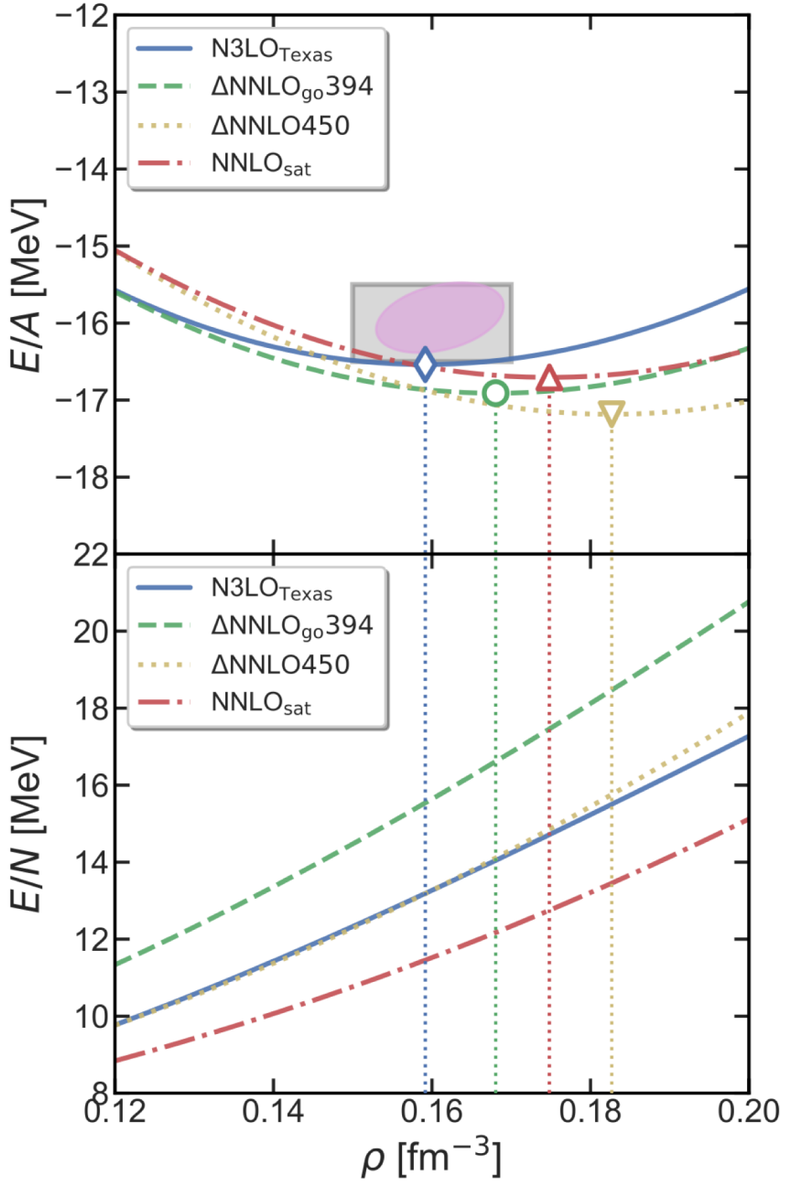


- Simulations used periodic boundary conditions

$$k_{n_i} = \frac{2\pi n_i}{L}, \quad n_i = 0, \pm 1, \ldots \pm n_{\max}, \quad i = x, y, z.$$

- 66 neutrons and protons, $n_{\max} = 4$
- Neutron matter well converged
- New development: Λ-CCD(T) for infinite nuclear matter

Properties of neutron/nuclear matter



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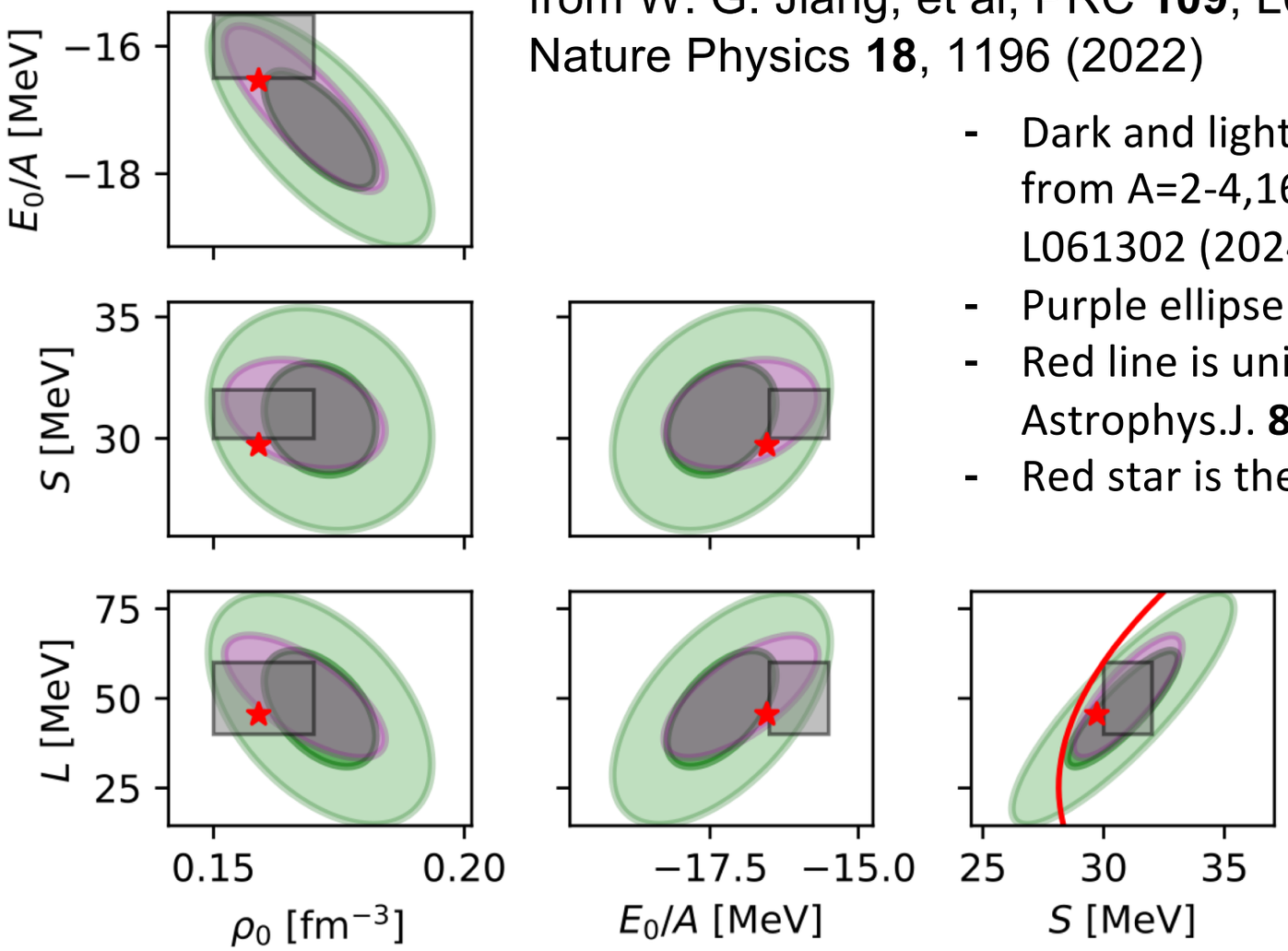
N3LO$_{Texas}$ results are compared with coupled cluster computations using different interactions [**Francesco Marino, Weiguang Jiang, Samuel J. Novario, Phys. Rev. C 110, 054322 (2024)**]

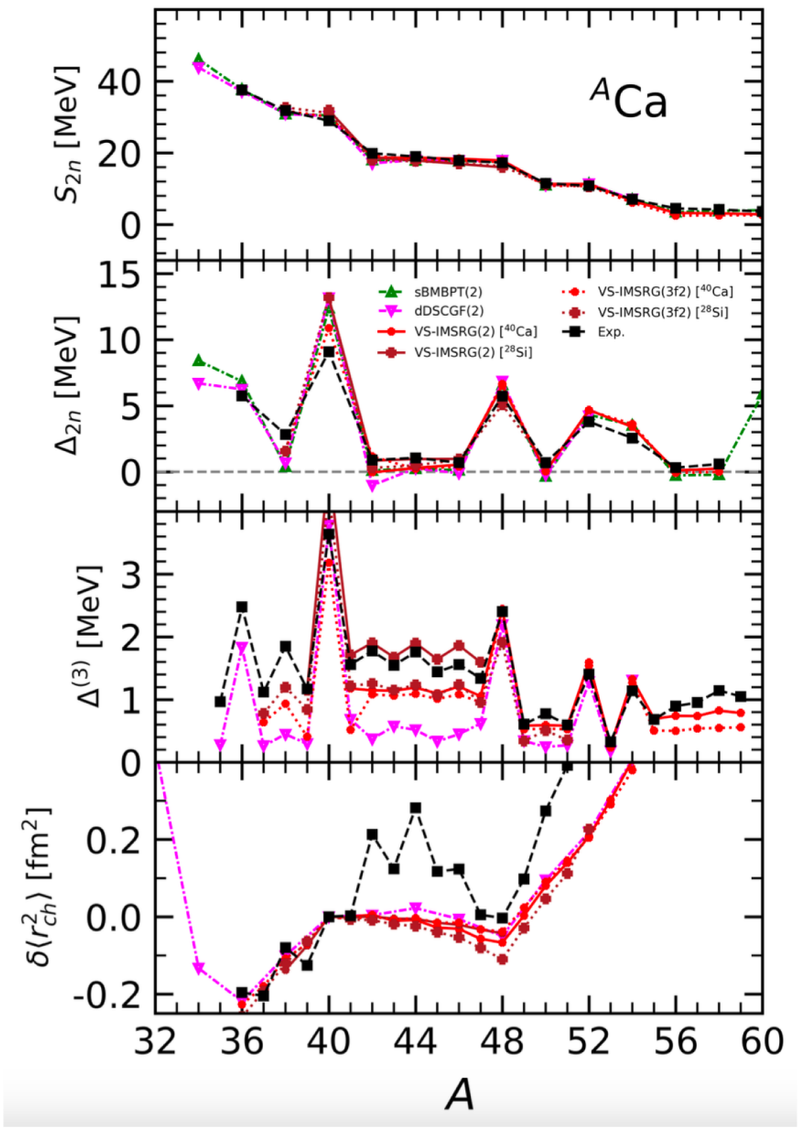
Properties of neutron/nuclear matter

PPD (Gaussian approximation) ellipses for NM saturation properties from W. G. Jiang, et al, PRC **109**, L061302 (2024) and from B. Hu et al, Nature Physics **18**, 1196 (2022)



- Dark and light green ellipses are "one- and two-sigma" from A=2-4,16 PPD [W. G. Jiang, et al, PRC 109, L061302 (2024)]
- Purple ellipse is “one sigma" from B. Hu et al, PPD
- Red line is unitary gas constraint for S vs L [I. Tews Astrophys.J. **848**, 105 (2017)]
- Red star is the N3LO$_{\text{Texas}}$ prediction

Where is the pairing gone?



A. Scalesi et al, unpublished

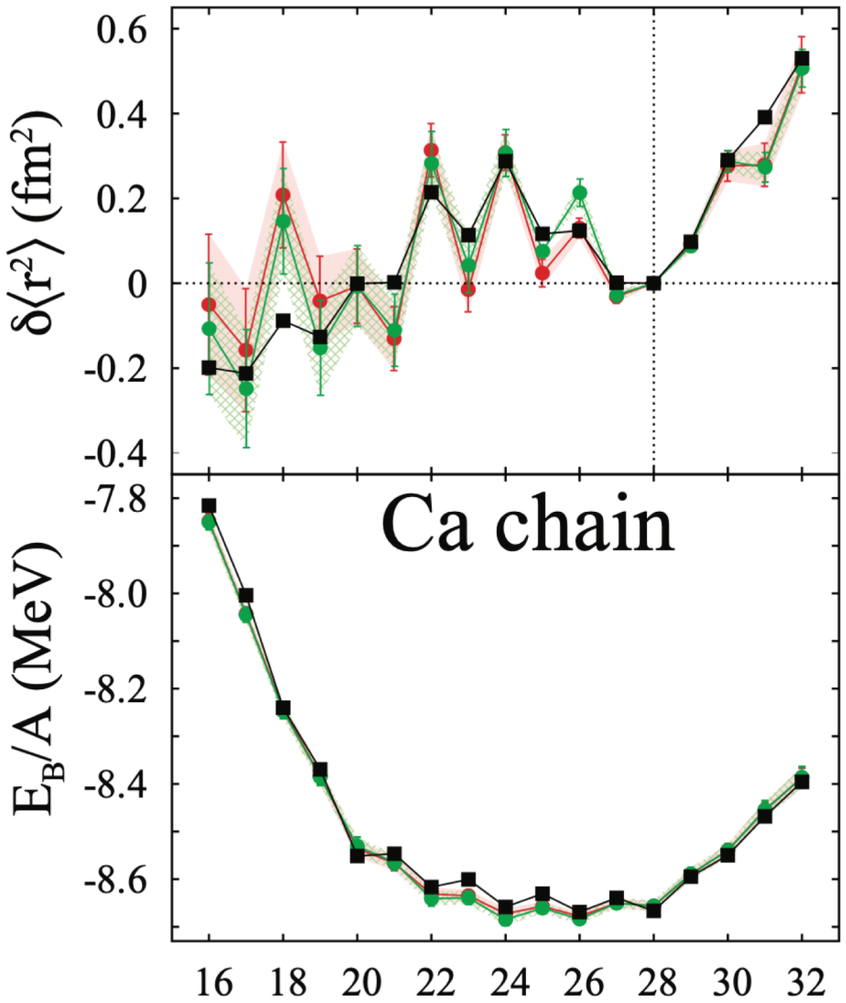
Fayans EDF
(density dependent
pairing functional)

Pairing

Ab initio computations
based on chiral EFT
interactions

A. Scalesi, et al Eur. Phys. J. A **60**, 209 (2024).

No Pairing



P-G Reinhard et al, J. Phys. G 51, 105101 (2024)

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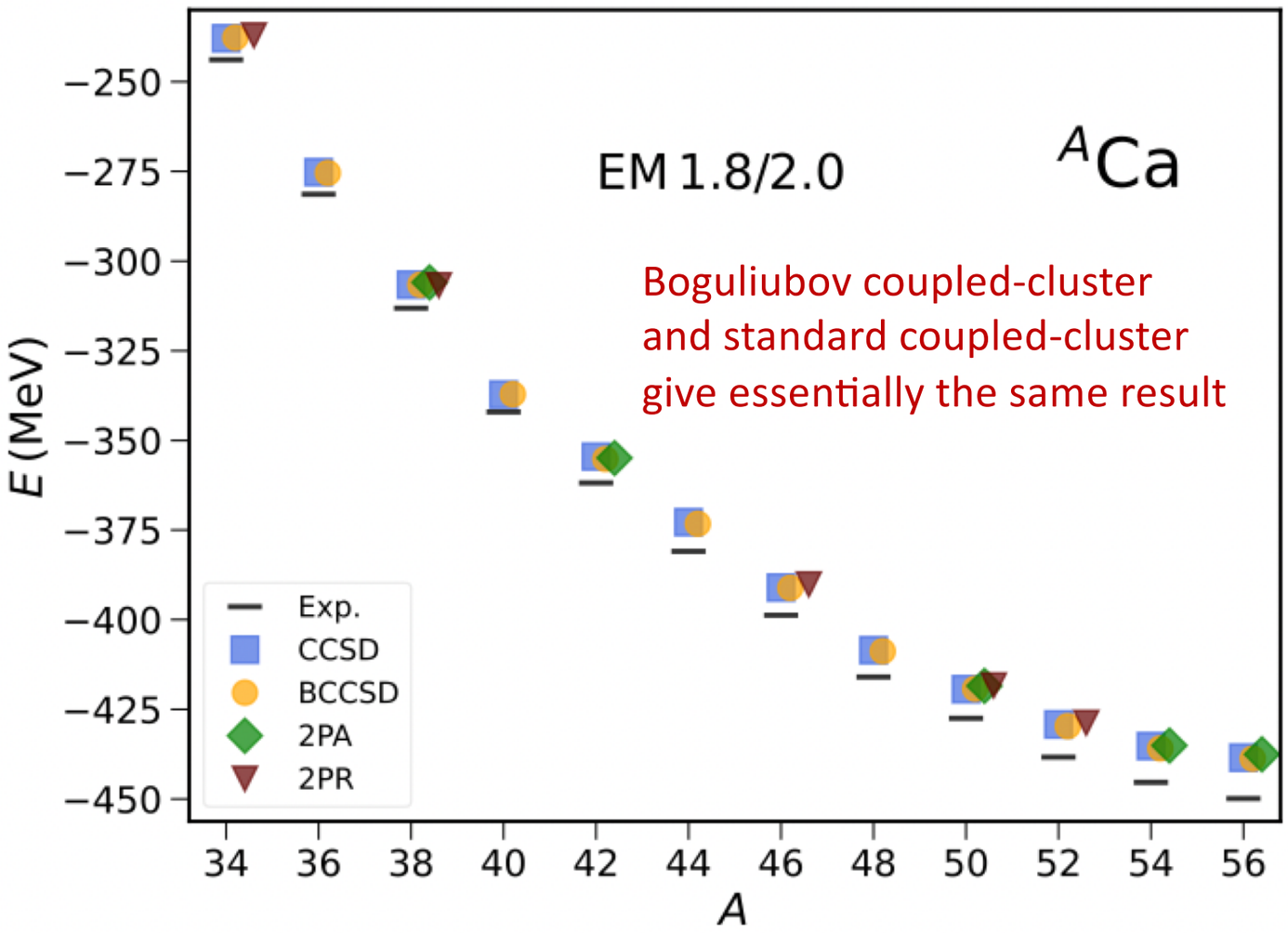
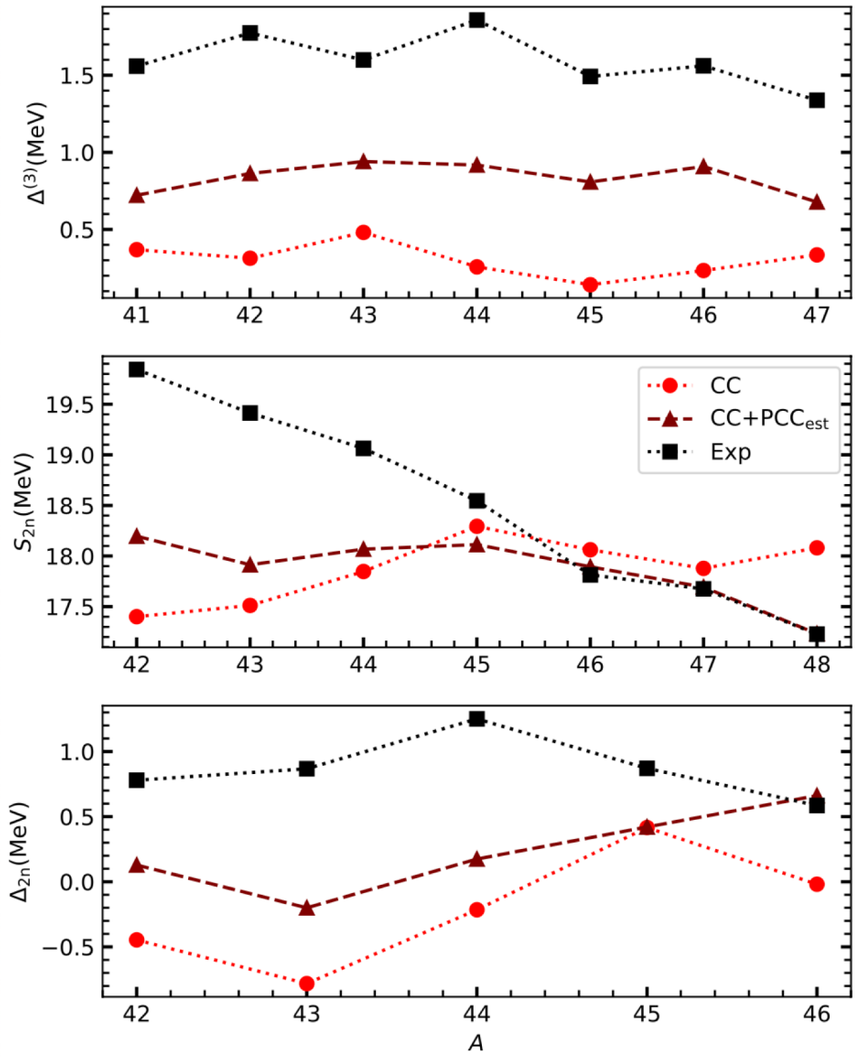


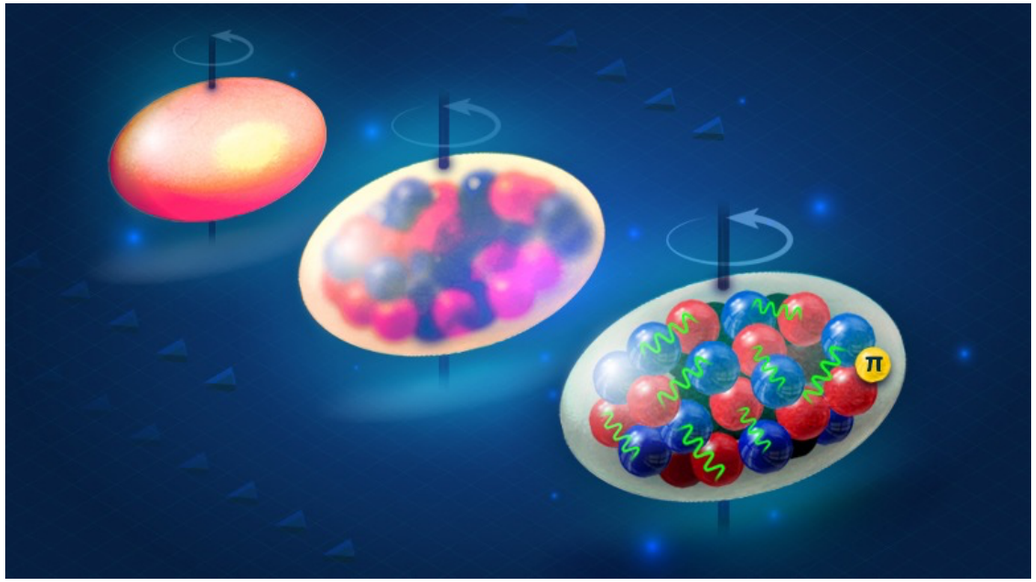
Francesco Marino, et al, arXiv:2410.19511 (2024)



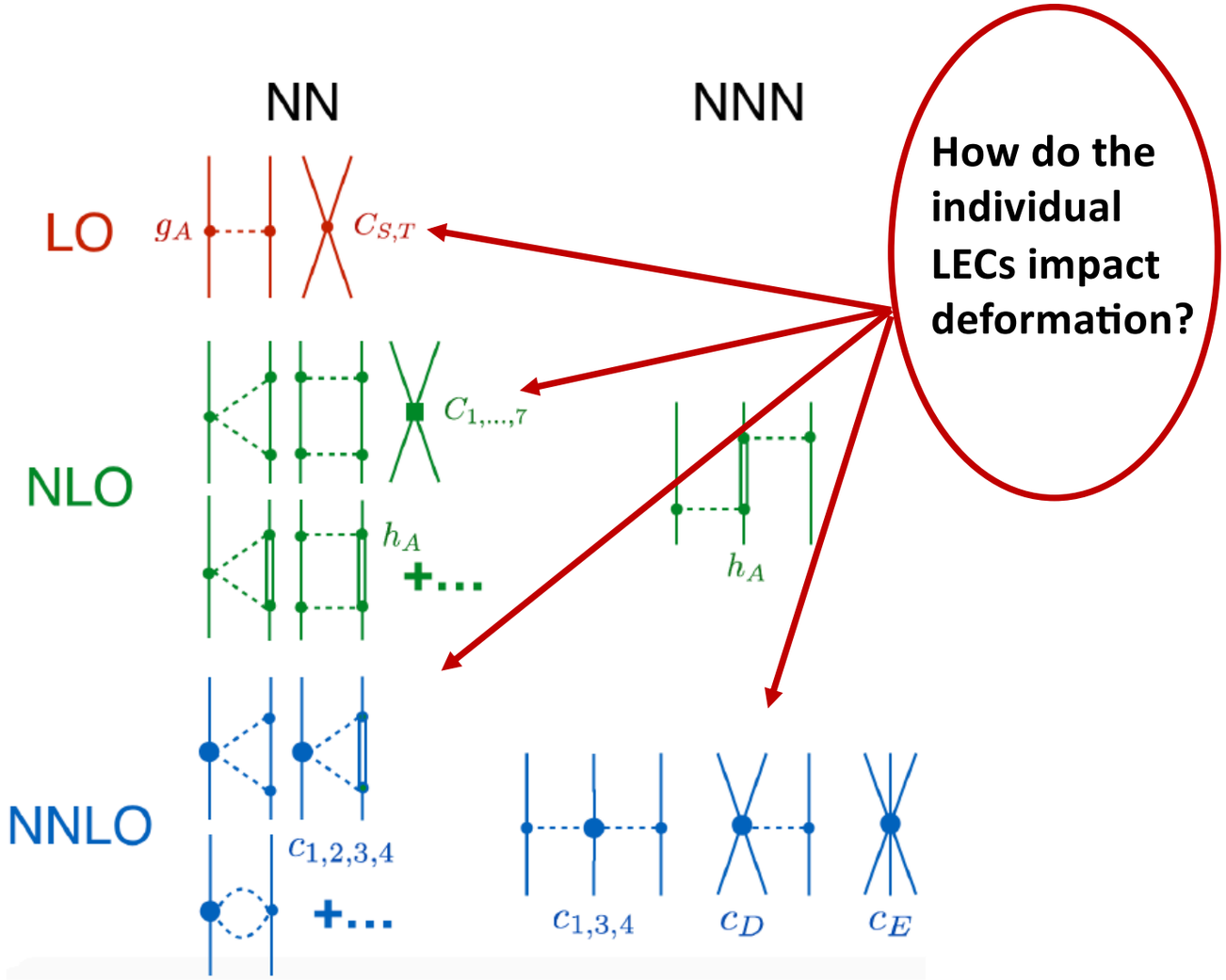
Zhonghao, et al, unpublished

What drives deformation in nuclei?

- 50's: surface vibrations of a liquid drop (Bohr/Mottelson)
- 60's: competition between pairing and quadrupole interactions from HFB calculations in two shells (Baranger/Kumar)
- 70's: isoscalar neutron-proton interactions dominate over isovector pairing from shell model (Federman/Pittel, Dufour/Zuker)



Nuclear deformation viewed at different resolution scales
Credit: Güneş Özcan/ORNL, U.S. Dept. of Energy

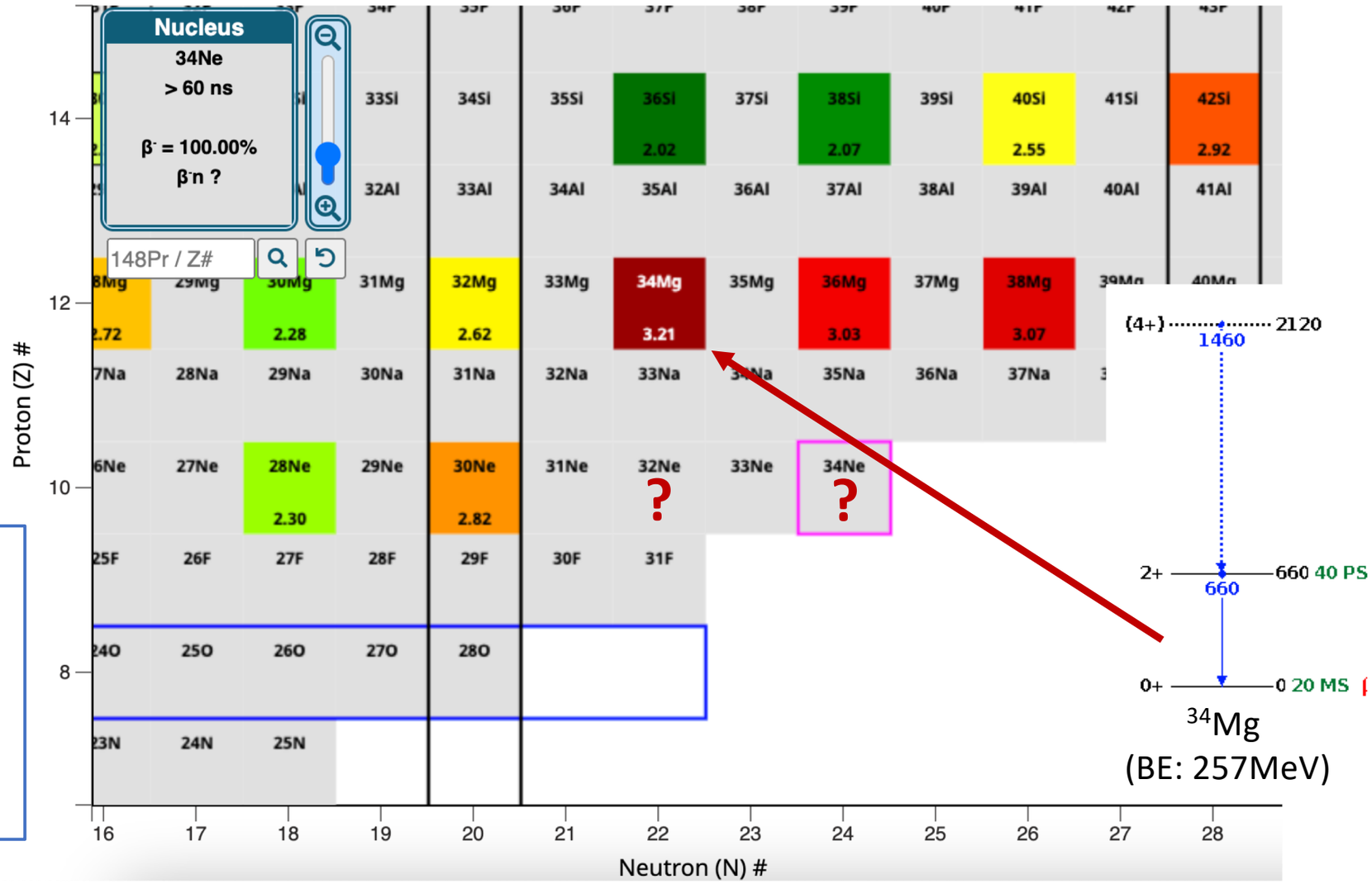


Neutron-rich nuclei beyond N = 20 are deformed

$$R_{4/2} \equiv \frac{E_{4^+}}{E_{2^+}}$$

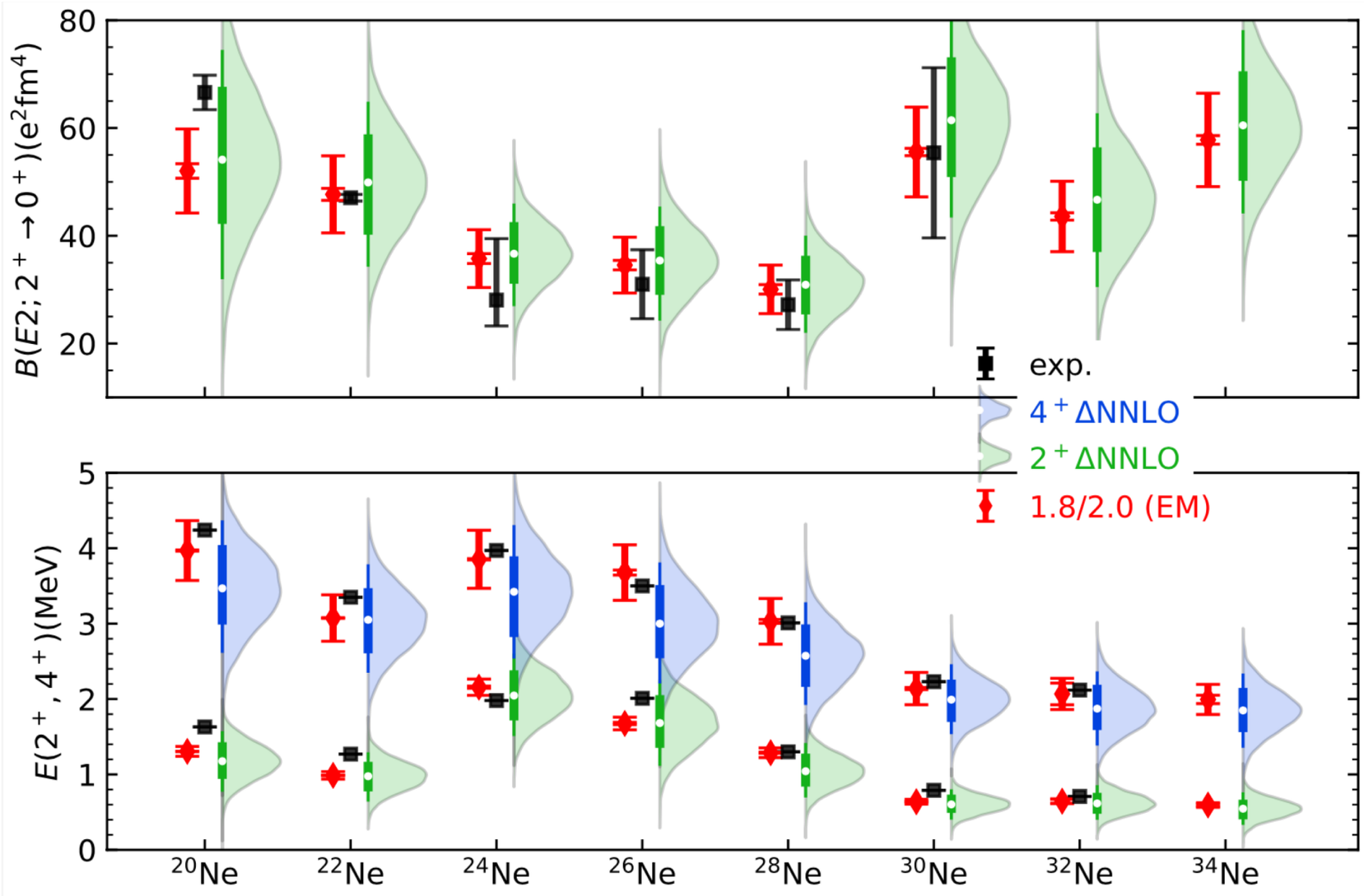
$R_{4/2} = 10/3$ for a rigid rotor

Simple picture: Spherical states (magic $N = 20$ number in the traditional shell model) coexist with deformed ground states



Poves & Retamosa (1987); Warburton, Becker, and Brown (1990); …

Collectivity in neon isotopes



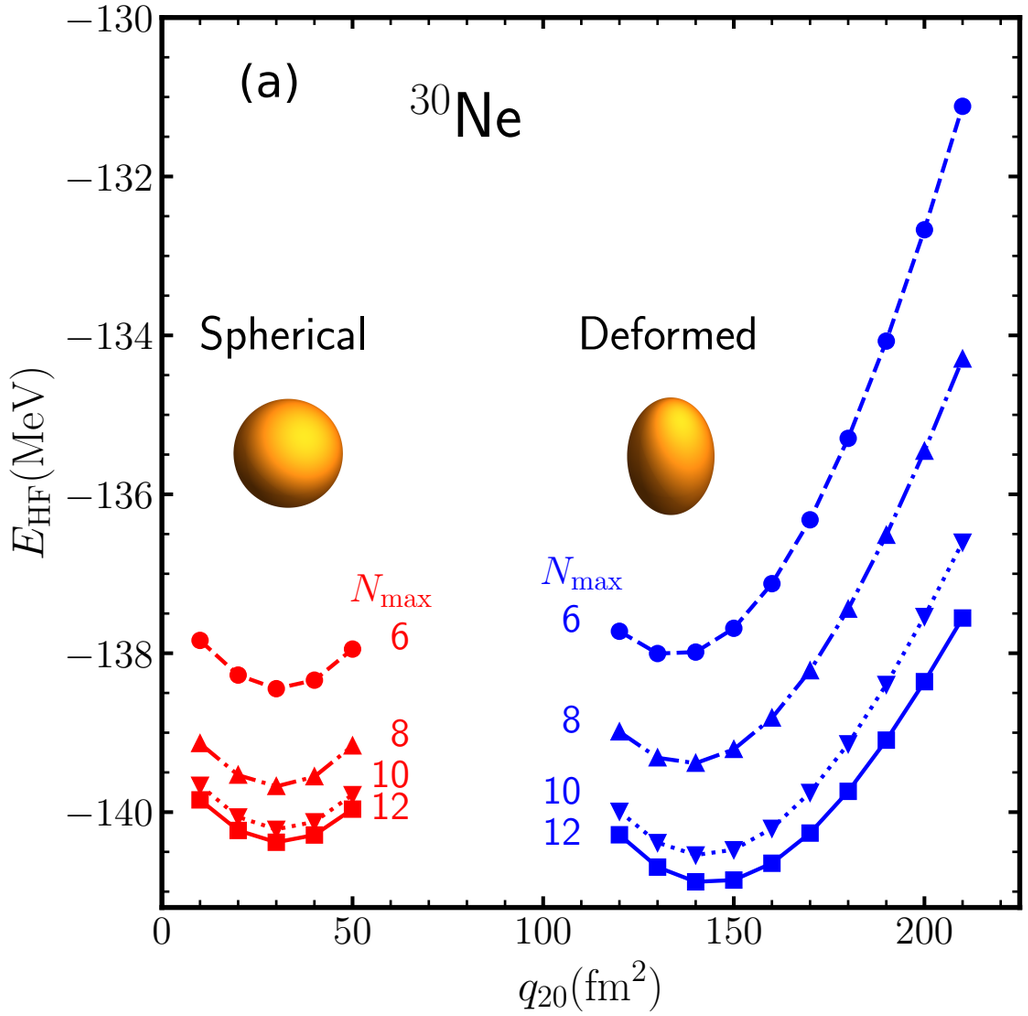
- Small energies reflect a large moment of inertia and a strong deformation
- Lack of pairing leads to larger moment of inertia
- Radii are underpredicted and leads to smaller moment of inertia
- Lucky interplay of these two effects leads to good agreement?

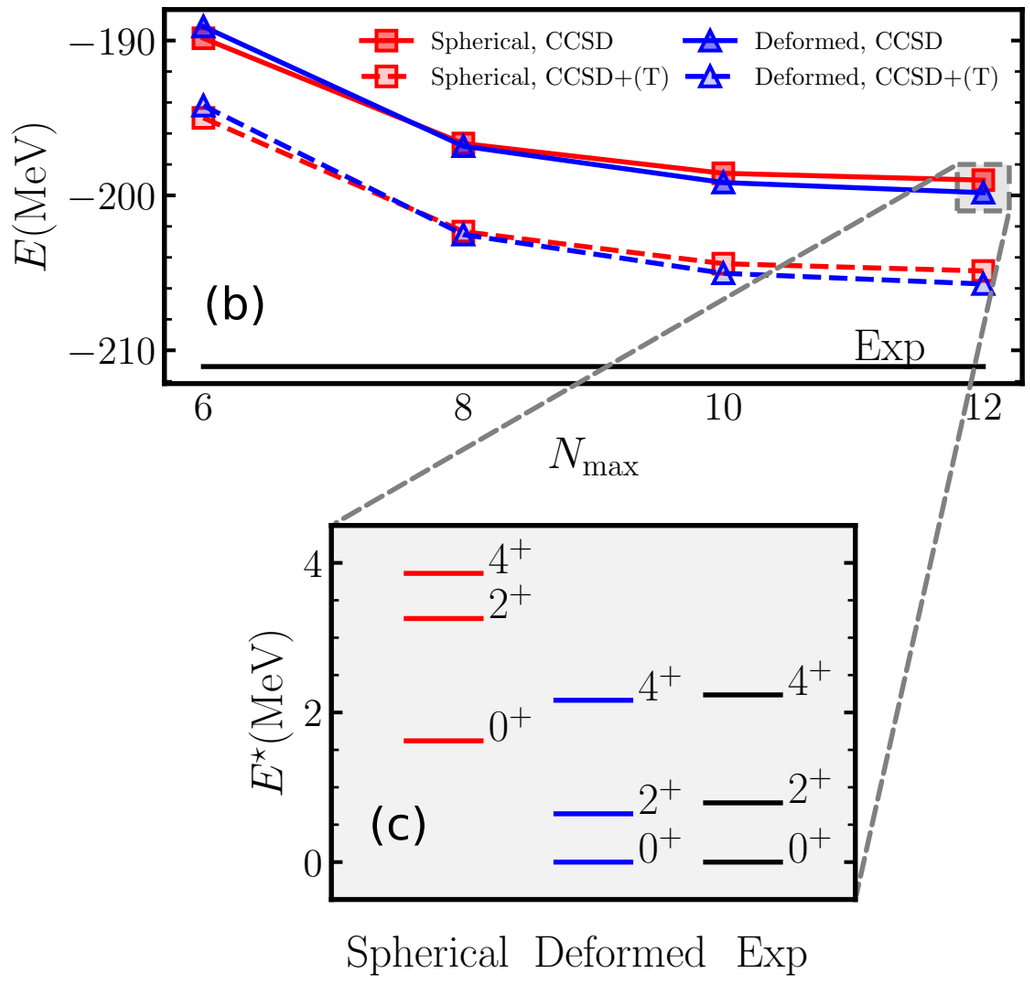
Ensemble of delta-full interactions from recent study of ^{28}O

Y. Kondo et al.,
Nature **620**, 965–970 (2023)

Zhonghao Sun, A. Ekstrom, C. Forssen, G. Hagen. G. R. Jansen, T. Papenbrock, Phys. Rev. X **15**, 011028 (2025)

Shape co-existence in ^{30}Ne





Zhonghao Sun, A. Ekstrom, C. Forssen, G. Hagen. G. R. Jansen, T. Papenbrock, Phys. Rev. X **15**, 011028 (2025)

Global sensitivity analysis

Sensitivity analysis addresses the question ‘How much does each model parameter contribute to the uncertainty in the prediction?’

Global methods deal with the uncertainties of the outputs due to input variations over the whole domain.

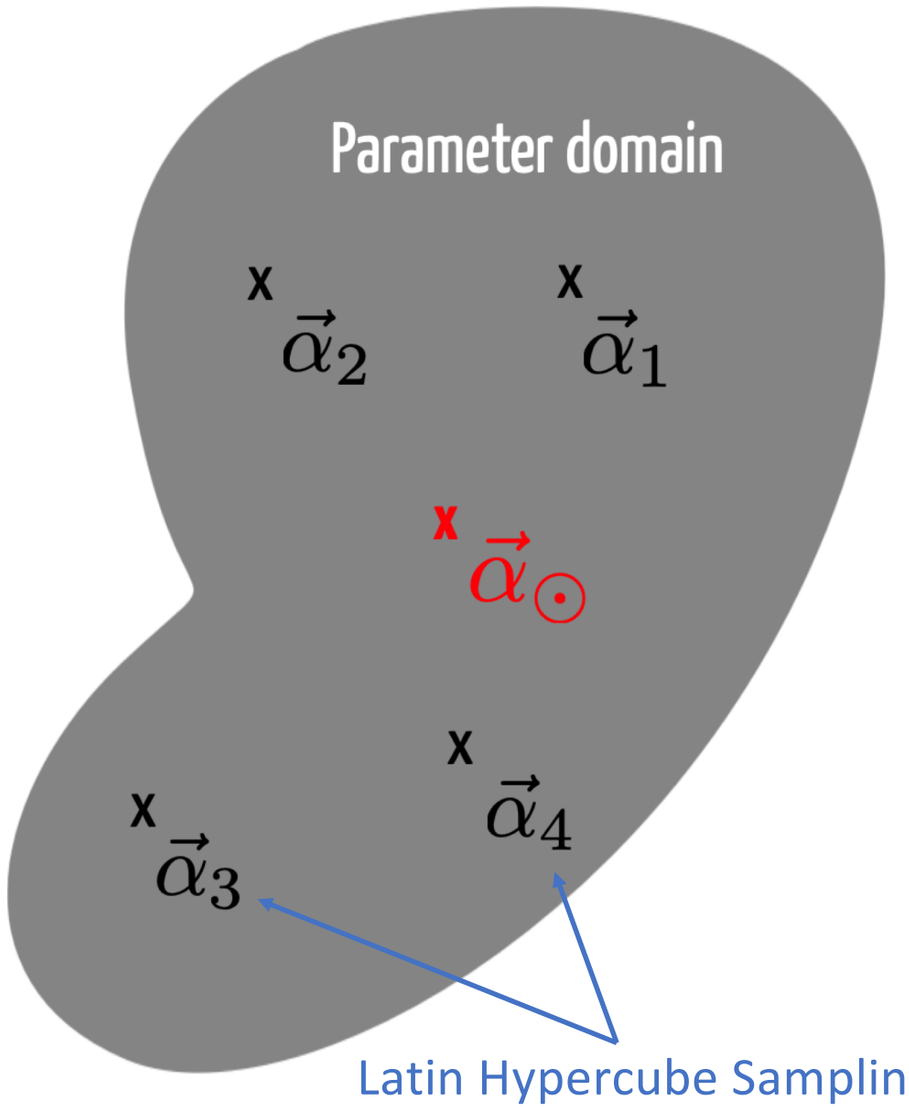
Computational bottleneck

A global sensitivity analyses of properties of atomic nuclei typically would require more than one million model evaluations

Sensitivity analysis of the radius and binding energy of ^{16}O

Andreas Ekström, Gaute Hagen PRL **123**, 252501 (2019)

Reduced order models for ab initio computations



- Eigenvector continuation method [Frame D. et al., Phys. Rev. Lett. 121, 032501 (2018), A. Ekström, G. Hagen PRL 123, 252501 (2019), S. König et al Phys. Lett. B 810 (2020) 135814]
- Write the Hamiltonian in a linearized form

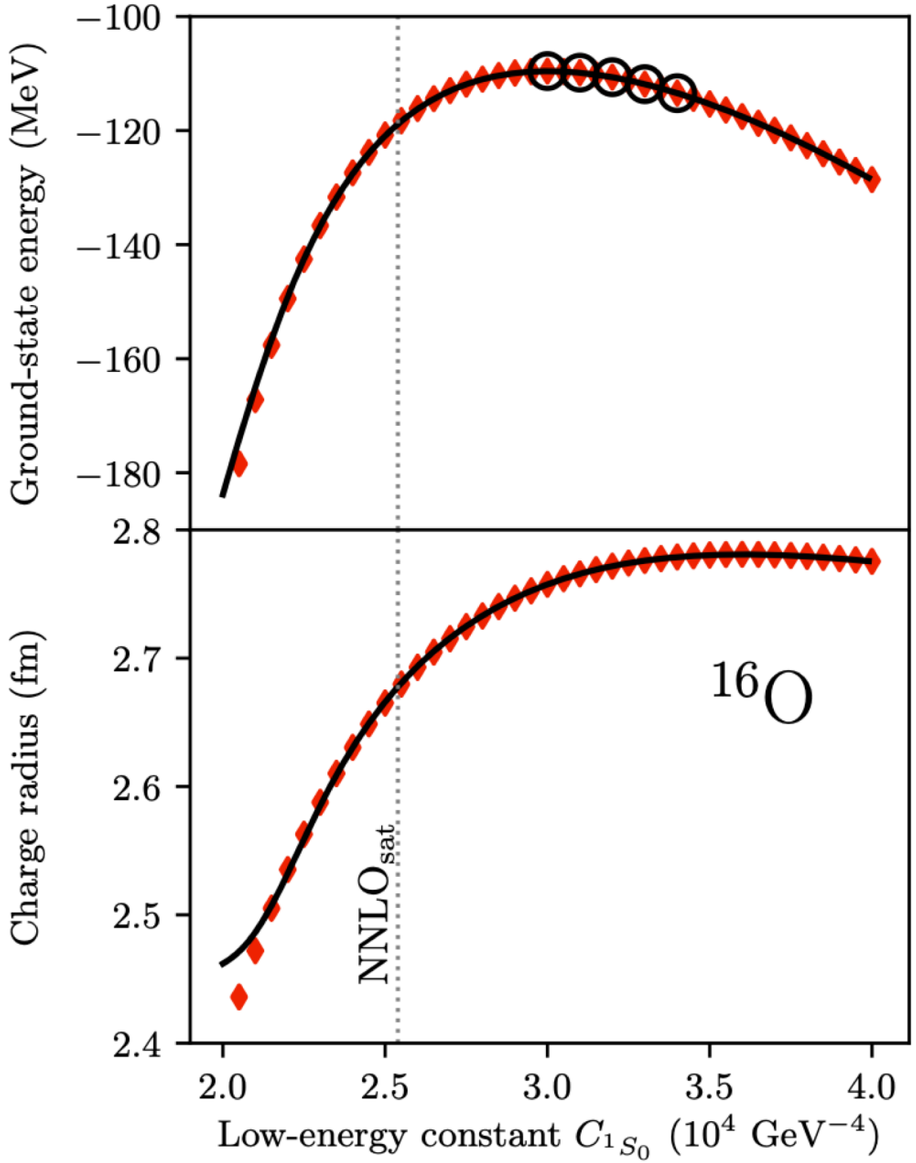
$$H(\vec{\alpha}) = h_0 + \sum_{i=1}^{N_{\mathrm{LECs}}=17} \alpha_i h_i$$

- Select "training points" (snap-shots) where we solve the exact problem
- Project a target Hamiltonian onto sub-space of training vectors and diagonalize the generalized eigenvalue problem

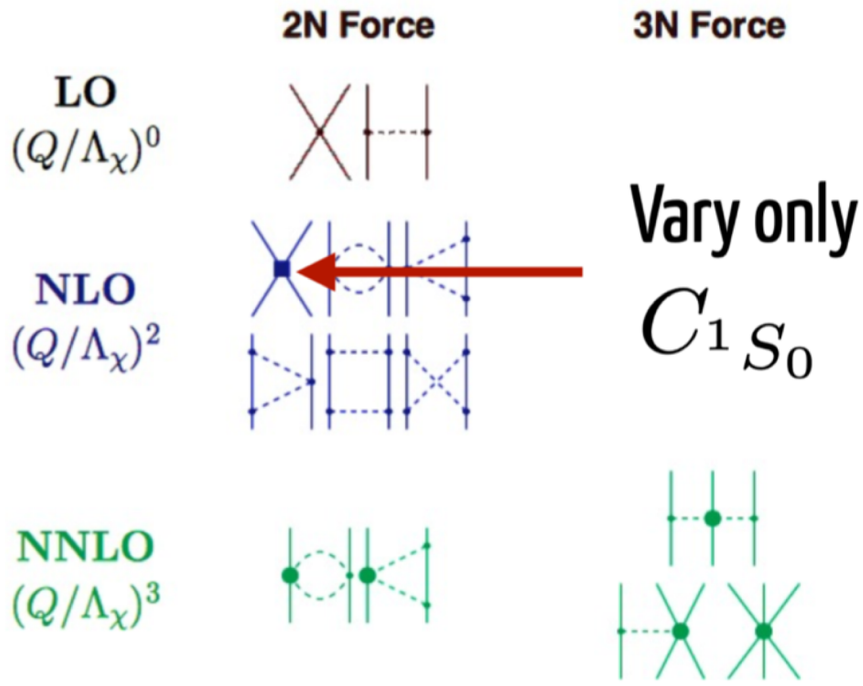
$$\mathbf{H}(\vec{\alpha}_\odot)\,\vec{c} = E(\vec{\alpha}_\odot)\,\mathbf{N}\,\vec{c}$$

Emulating ab-initio coupled-cluster calculations

Andreas Ekström, Gaute Hagen PRL **123**, 252501 (2019)

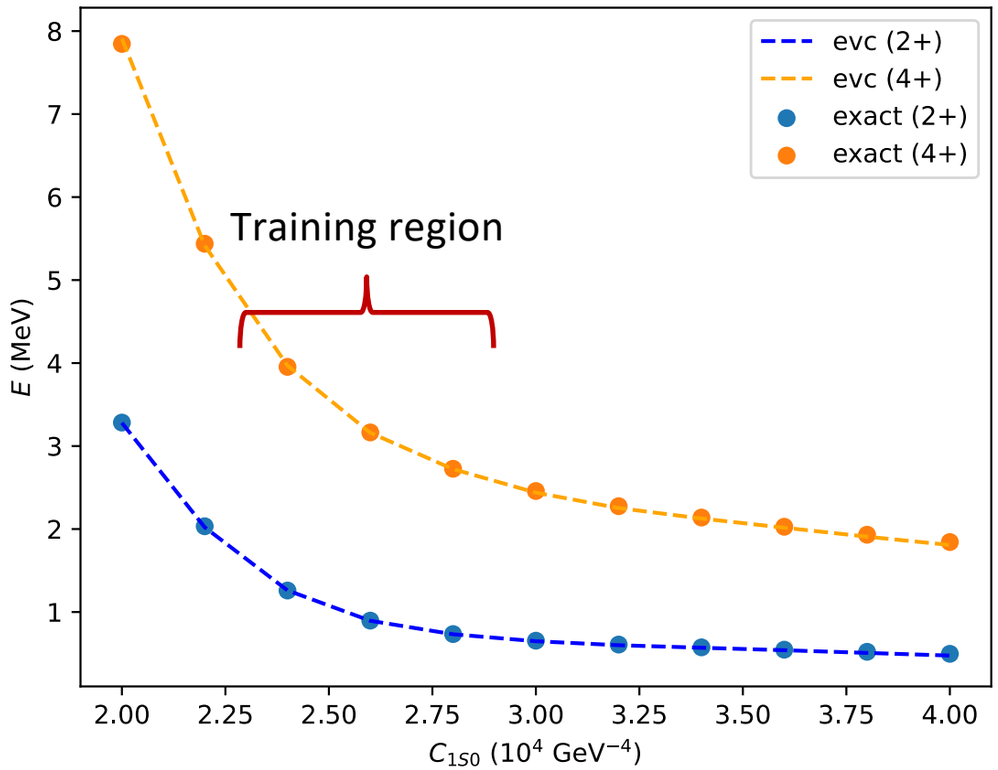


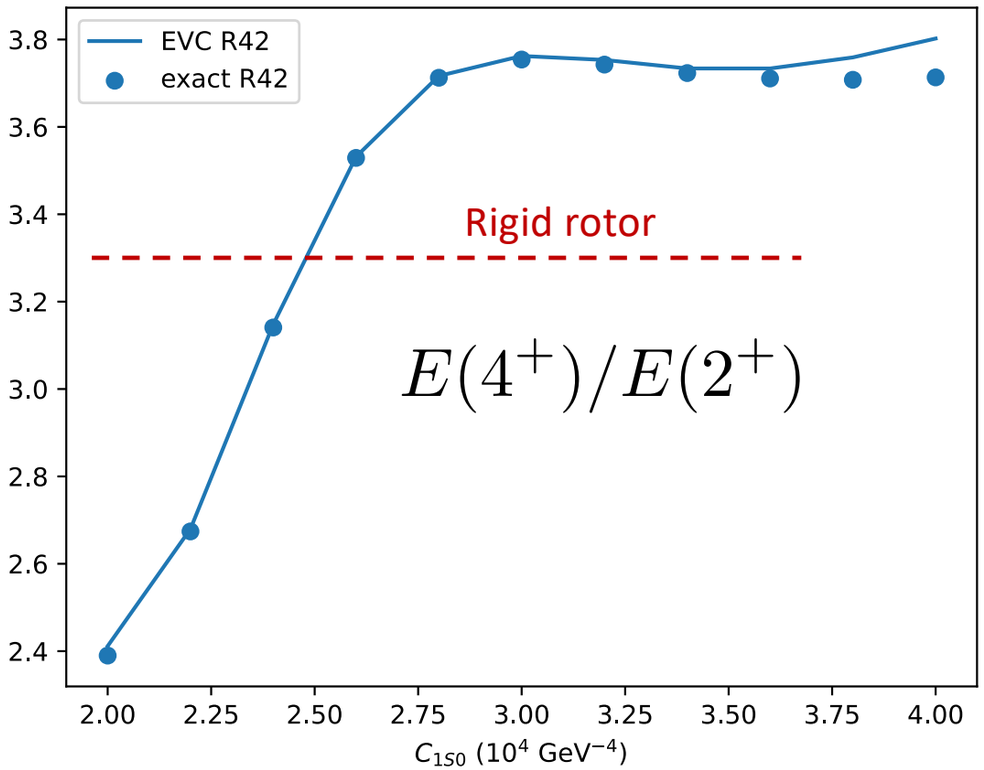
Exact coupled cluster calculations at the singles and doubles level



Emulating rotational structure of ^{20}Ne

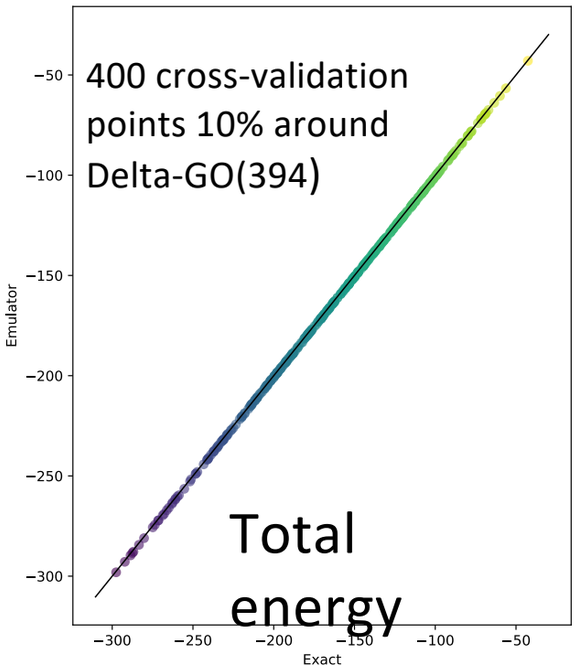
Varying only one parameter: $C_{^1S_0}$

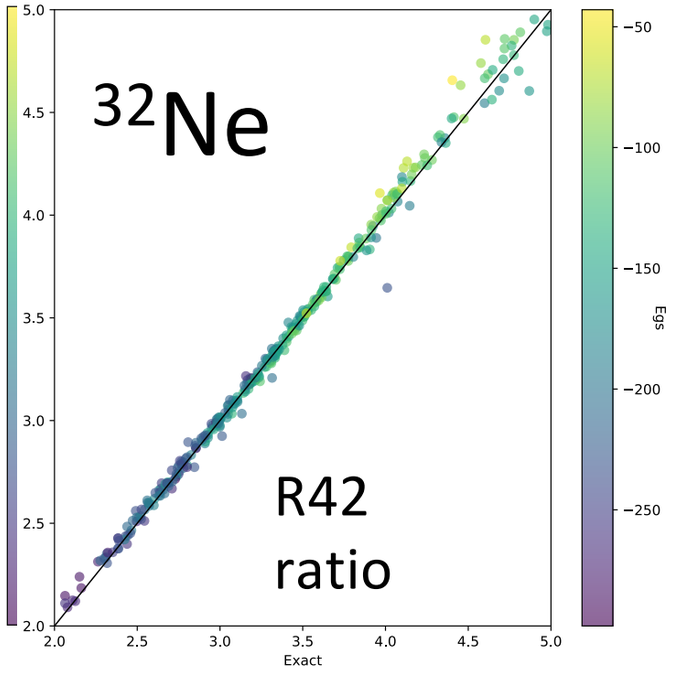




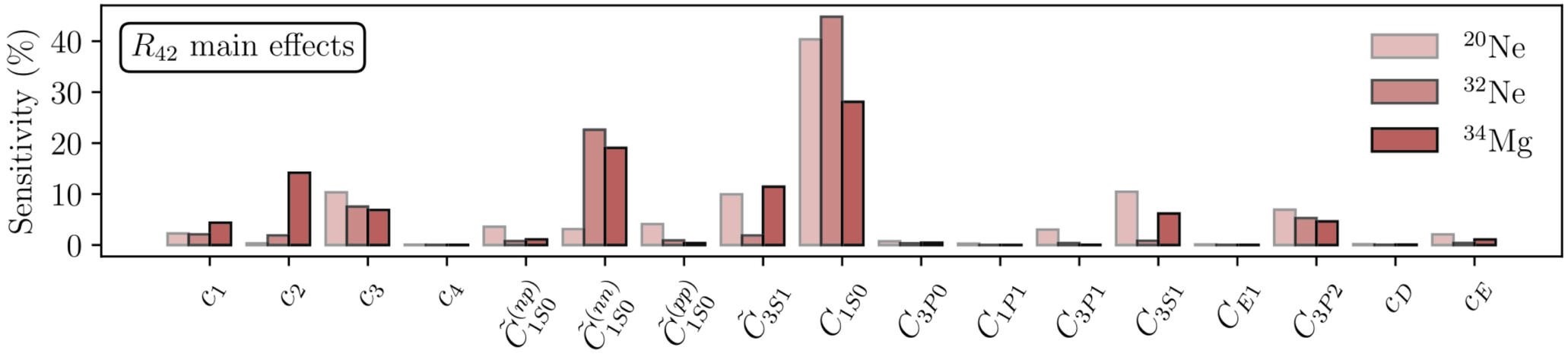
Zhonghao Sun, A. Ekstrom, C. Forssen, G. Hagen. G. R. Jansen, T. Papenbrock, Phys. Rev. X **15**, 011028 (2025)

Linking deformation to nuclear forces





- More than 50% of the deformation is driven by the S-wave contact part of the interaction
- Adding short-range repulsion increase deformation presumably by reducing pairing
- Increasing the pion-nucleon coupling strength also increases deformation, presumably by adding attraction in higher partial waves



Summary

- Few and many-body emulators allow for new optimization strategies
- Saturation properties are much improved by including ^{16}O in the fit
- Shape coexistence in ^{30}Ne and ^{32}Mg
- Much improved B(E2) values with no effective charges in ^{3x}Ne, ^{3x}Mg, ^{80}Zr
- Connected deformation to microscopic forces

What precision should/can we aim for with ab-initio methods?

Why do some interaction models work “better”?

Where is the pairing gone?

How can we test modified Weinberg power counting in nuclei?

How can we better assess the uncertainties?