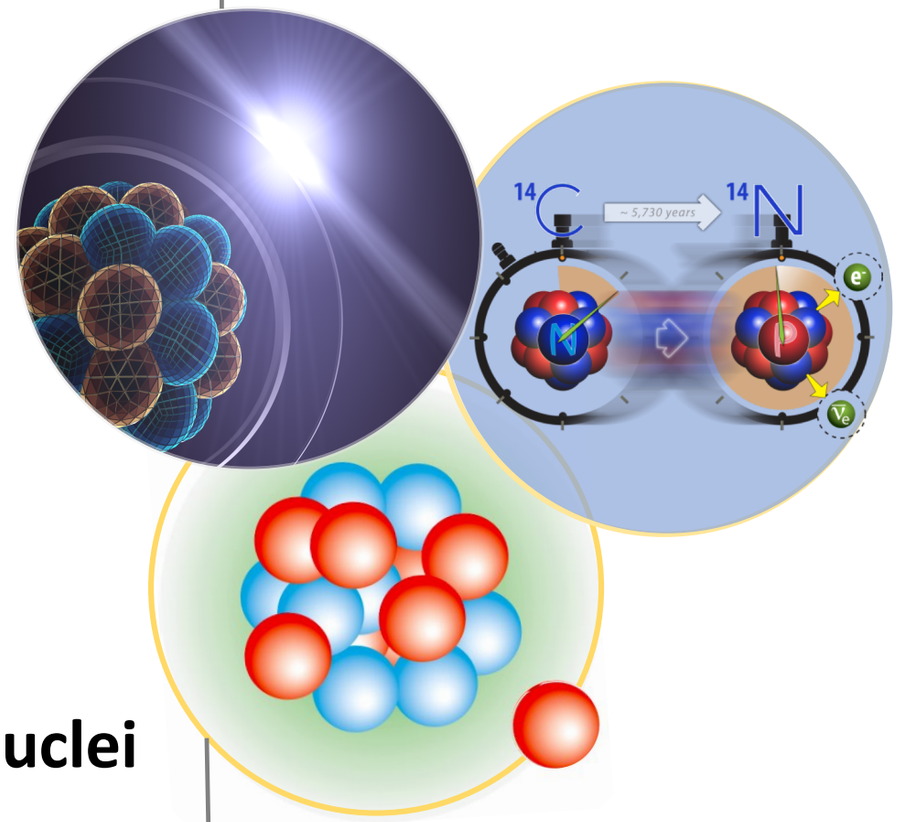
Coupled-cluster computations of deformed nuclei

Gaute Hagen
Oak Ridge National Laboratory

Hirschegg 2026 - Challenges in effective field theory descriptions of nuclei

Hirschegg, January 19th, 2026



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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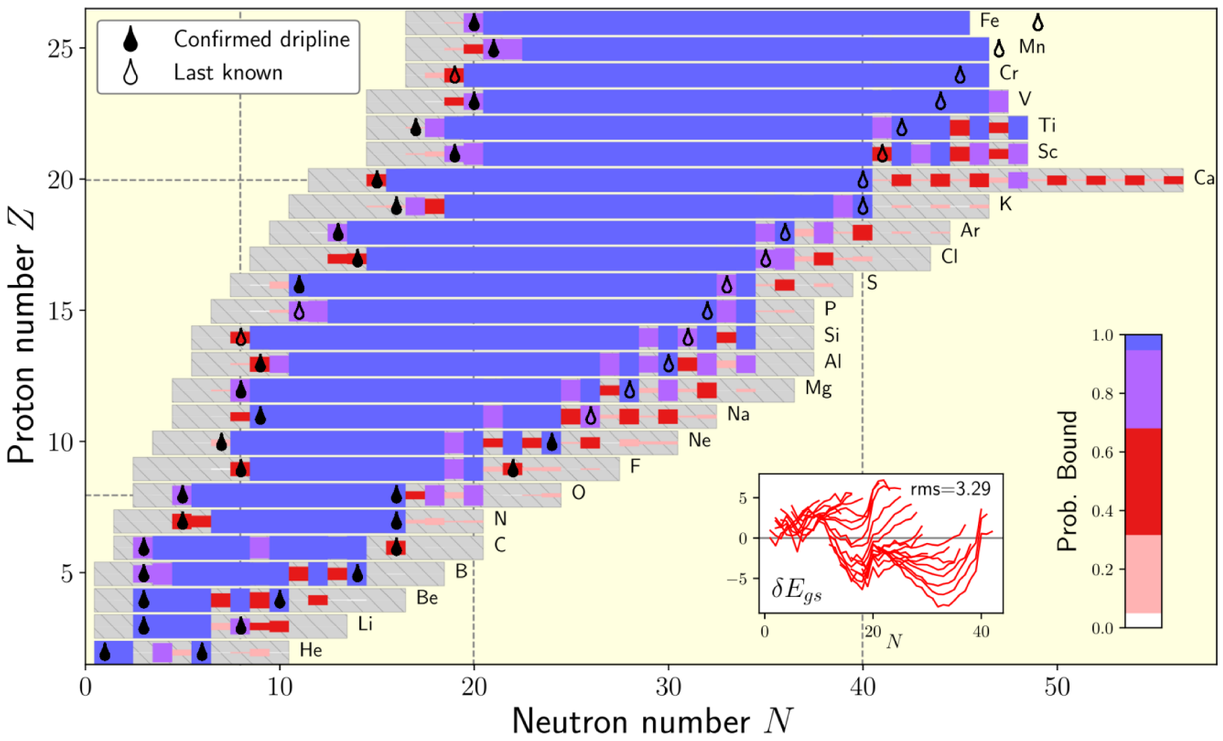
@ Notre Dame: **Zhonghao Sun**

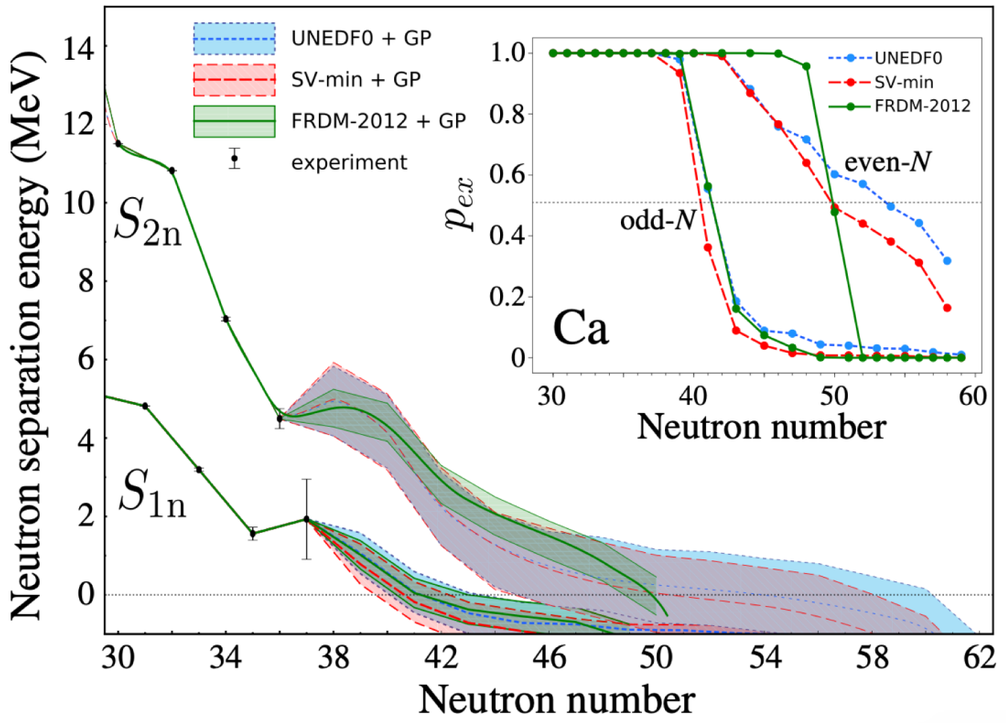
@ Chalmers: A. Ekström, C. Forssén, **A. Scalesi**, J. E. Sobczyk

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

The dripline in calcium isotopes



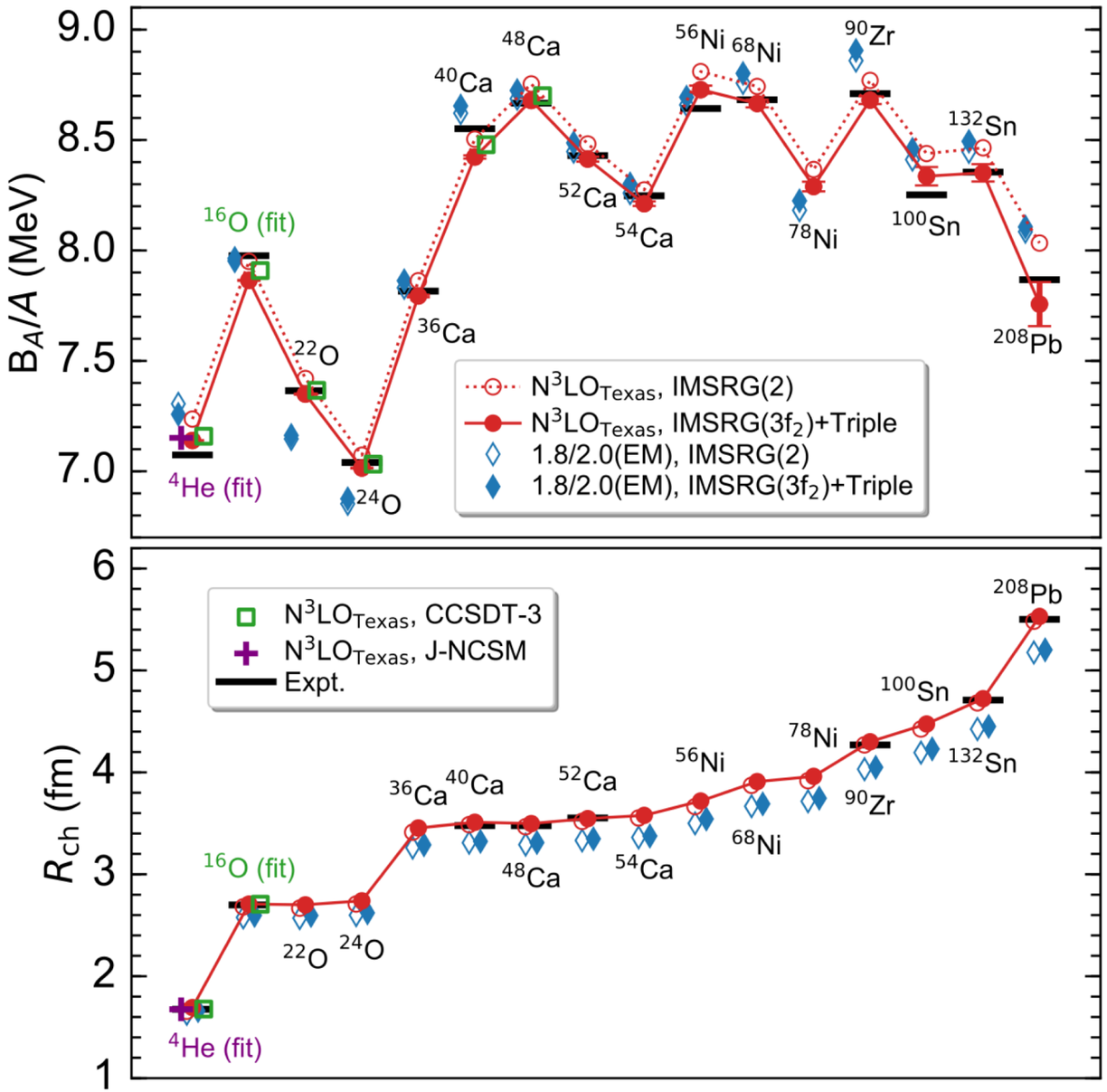
S. R. Stroberg et al, Phys. Rev. Lett. **126**, 022501 (2021)



Leo Neufcourt, et al, PRL **122** 062502 (2019)

- Existing data, energy density functional and relativistic mean field calculations suggest the dripline extends well beyond ^{60}Ca
- Ab initio computations sets the dripline closer to ^{60}Ca

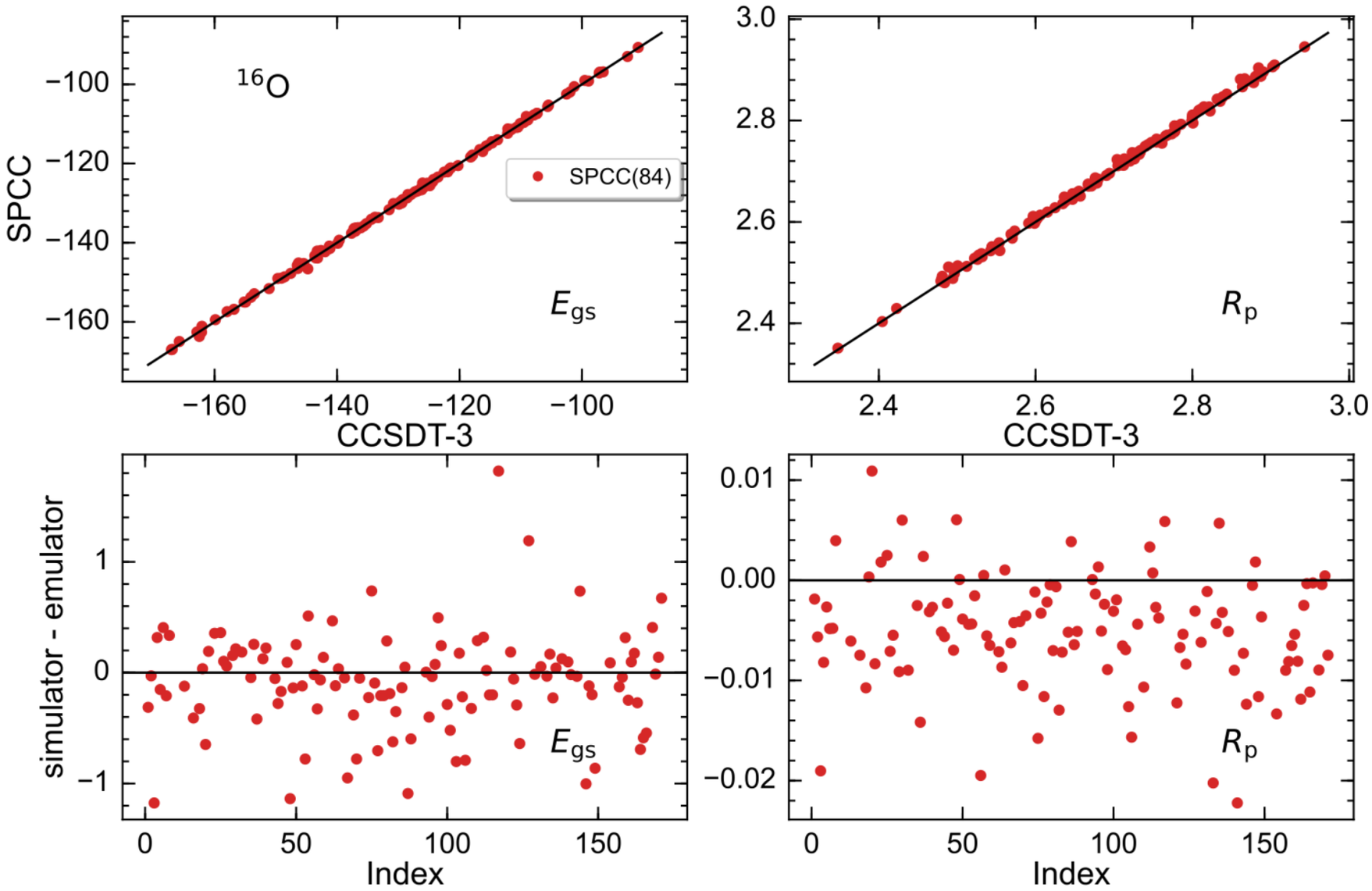
The dripline in calcium isotopes



- Optimized a new chiral interaction with NN at N3LO and 3NFs at N2LO
- Use few - and many-body emulators to efficiently evaluate 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

Baishan Hu et al, arXiv:2512.11723 (2025)

The dripline in calcium isotopes



Baishan Hu et al, arXiv:2512.11723 (2025)

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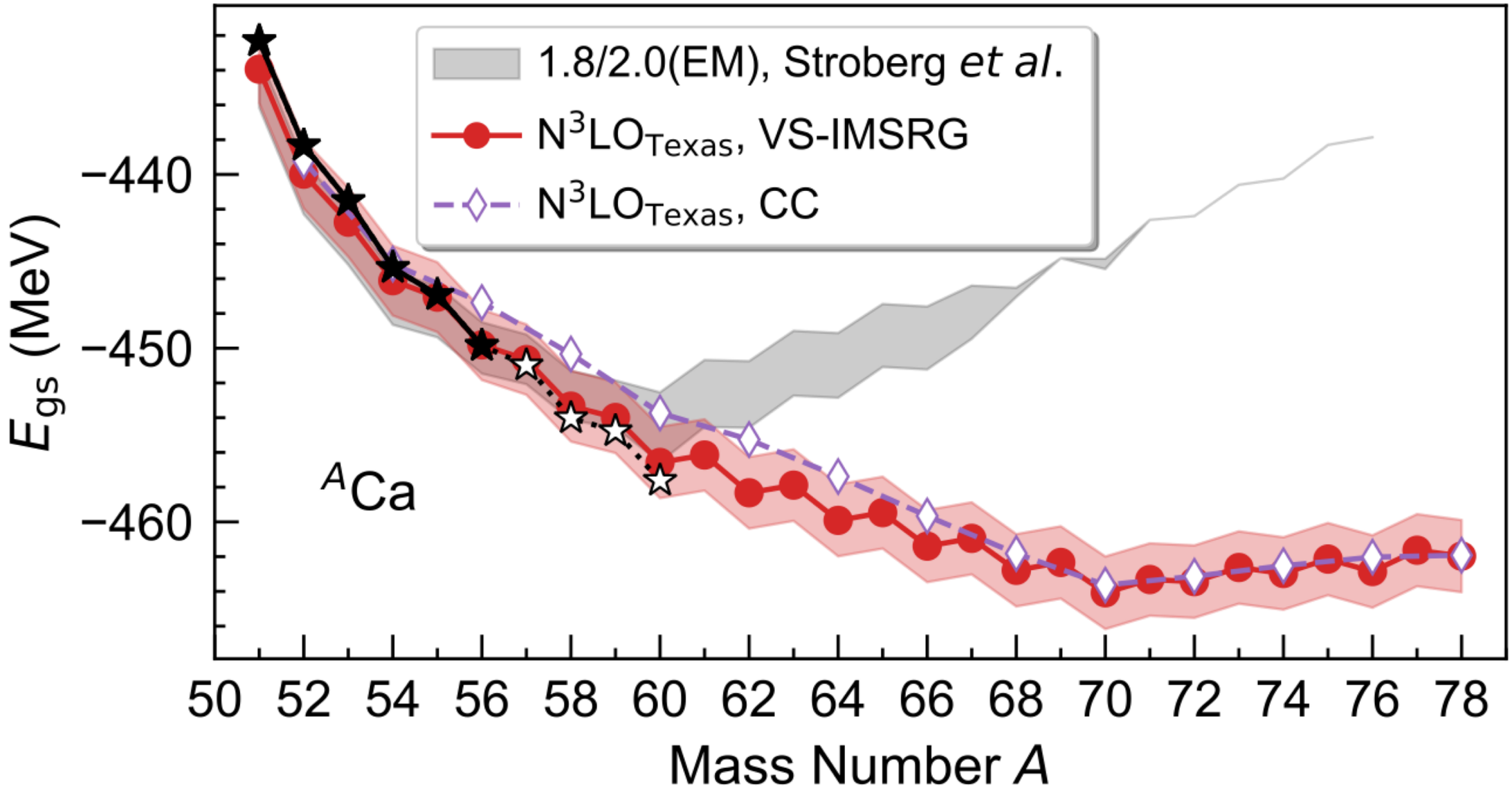
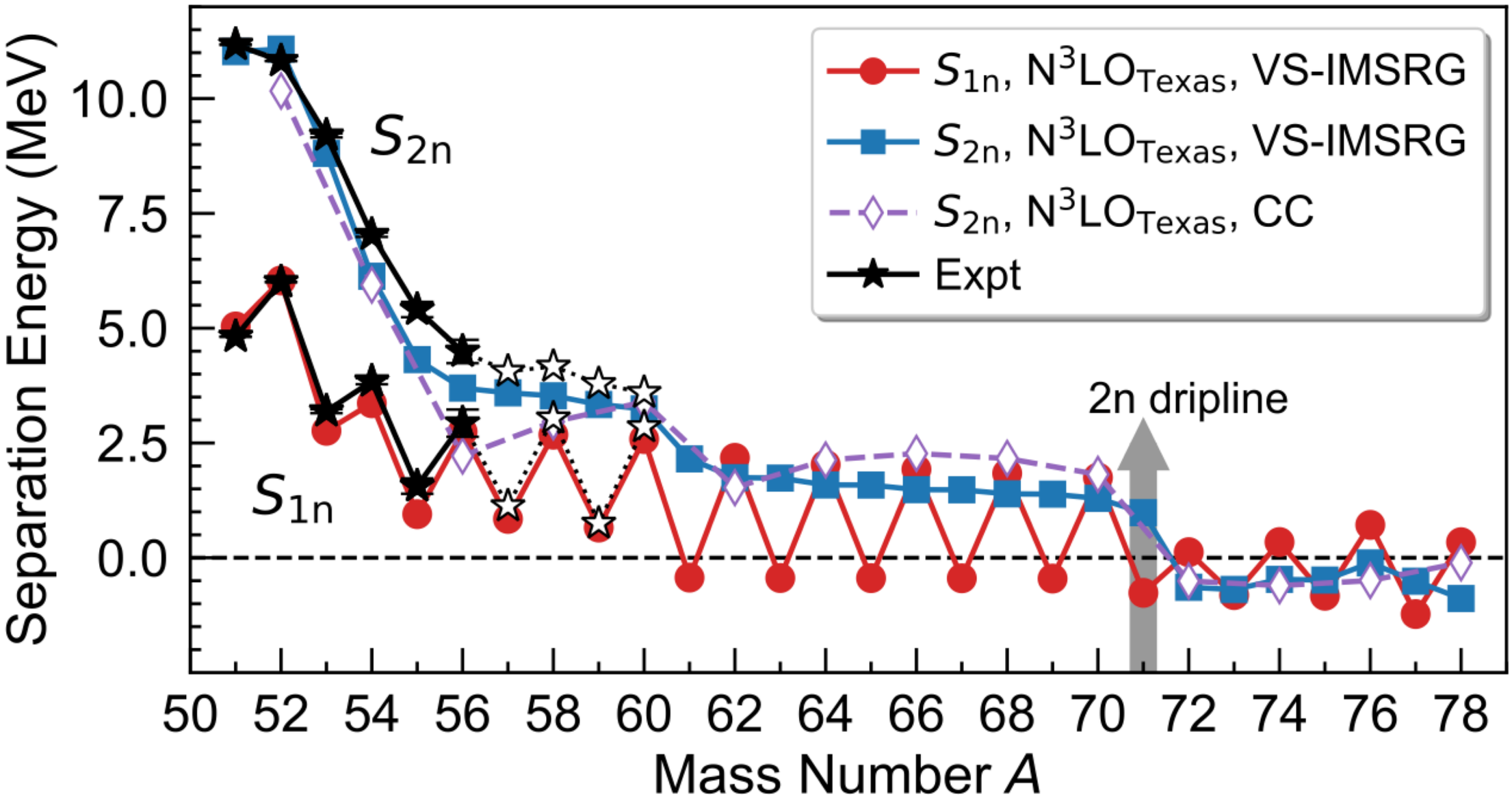
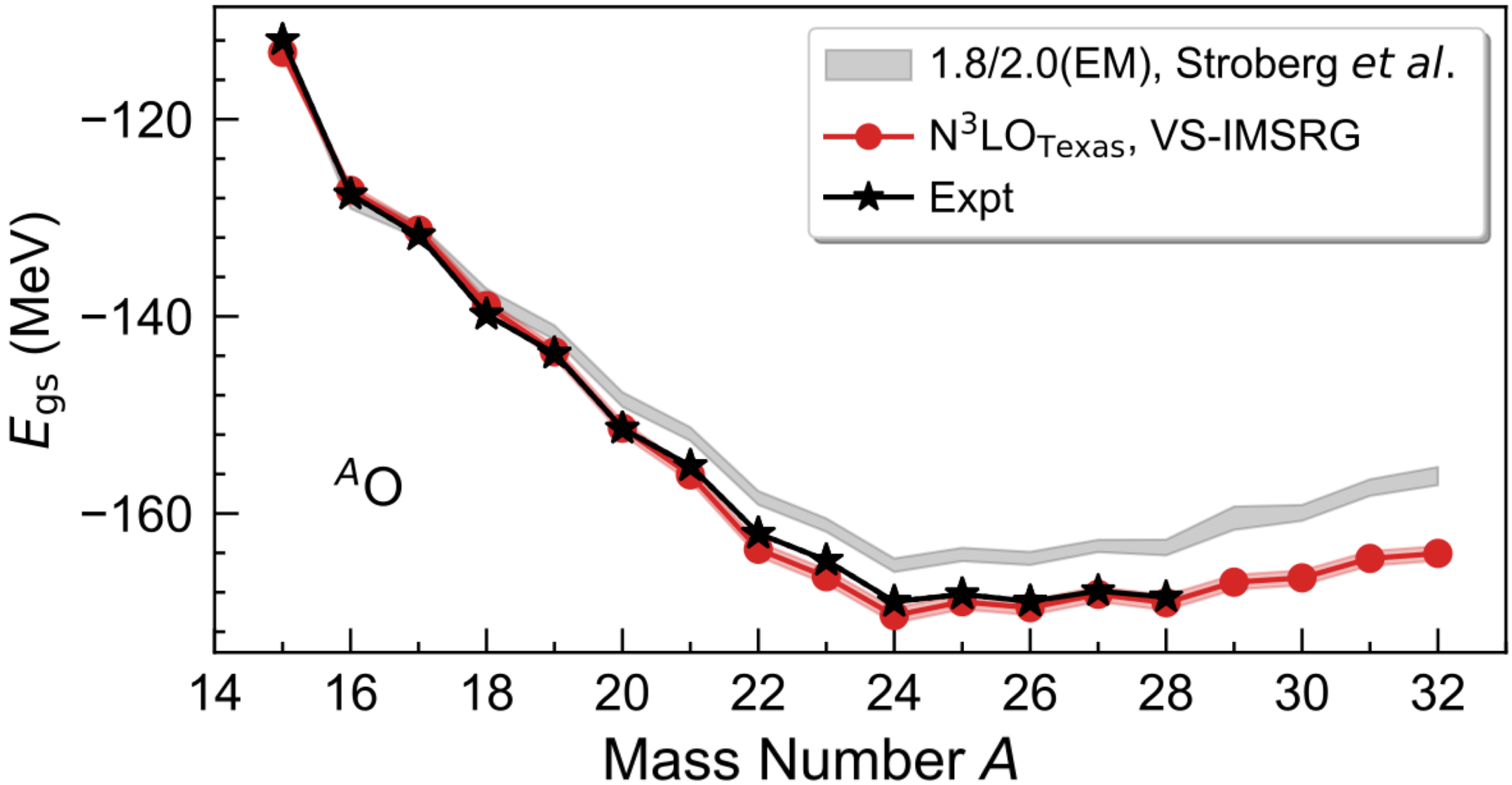


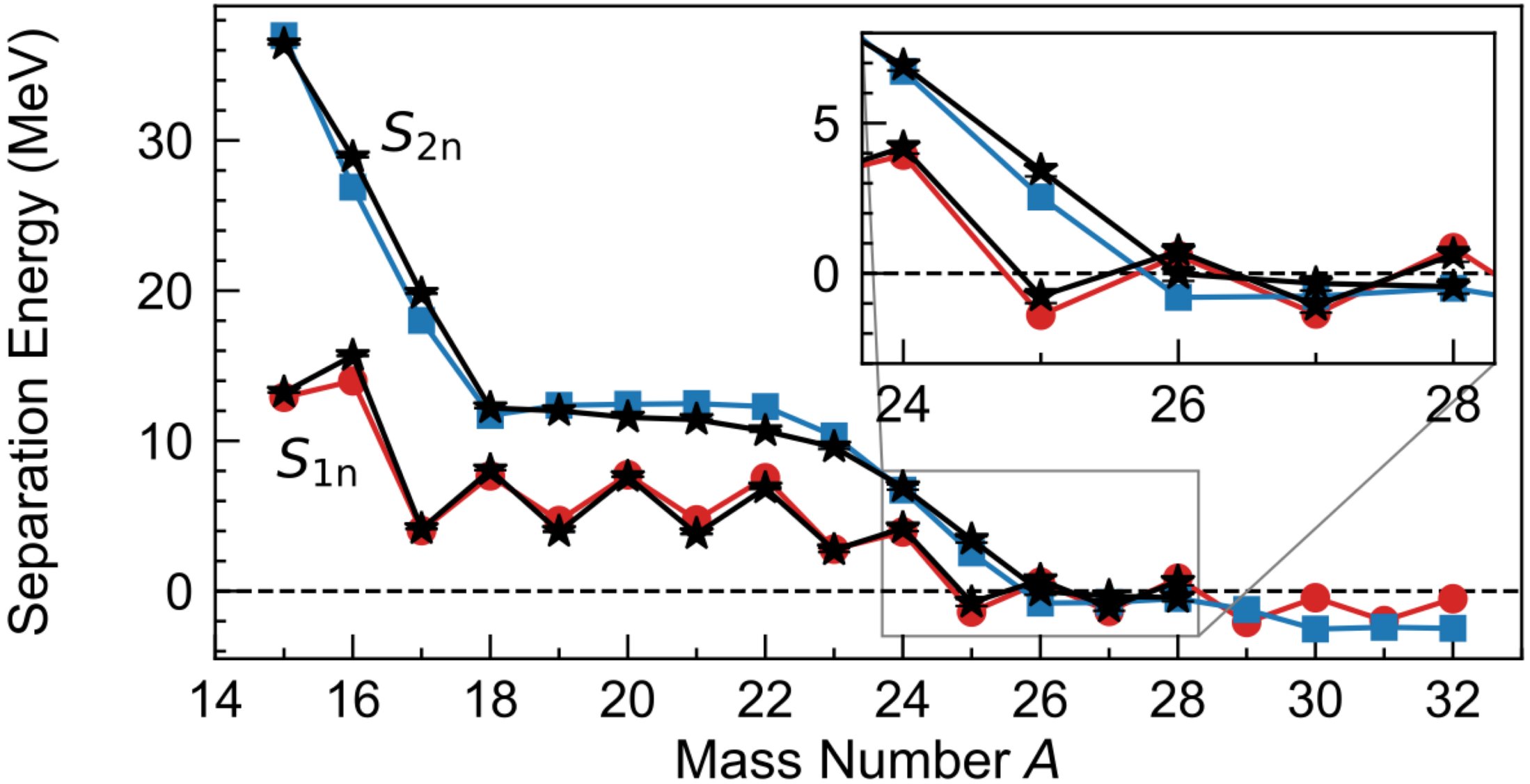
The dripline in calcium isotopes



The dripline in oxygen isotopes



The dripline in oxygen isotopes

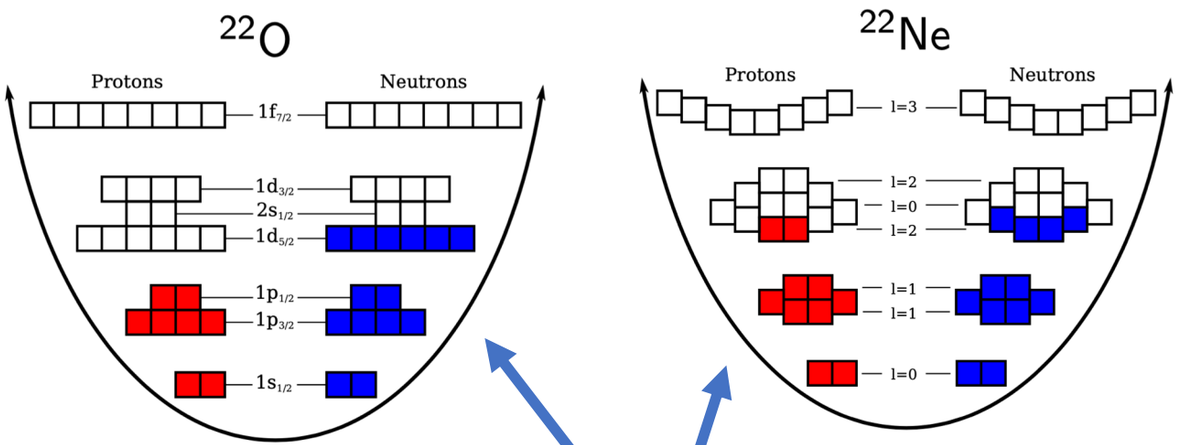


Coupled-cluster computations of nuclei

- Compute Hartree-Fock reference state: $W_0 + W_1 + W_2 + \cancel{W_3}$

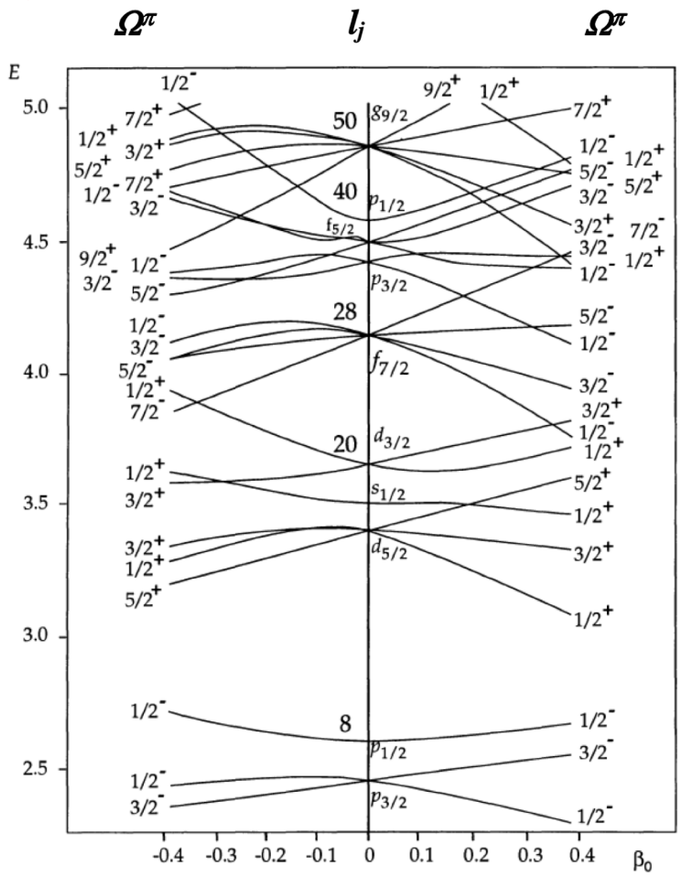
$$H = T - T_{\mathrm{CoM}} + V_{\mathrm{NN}} + V_{\mathrm{3N}}$$

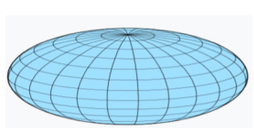
- Informs us about emergent breaking of symmetries

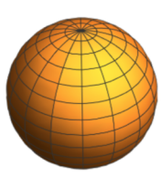


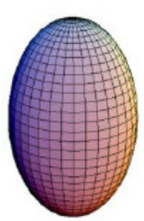
$$|\Psi\rangle = \Omega|\Phi\rangle$$

Wave-operator (includes many-body correlations)



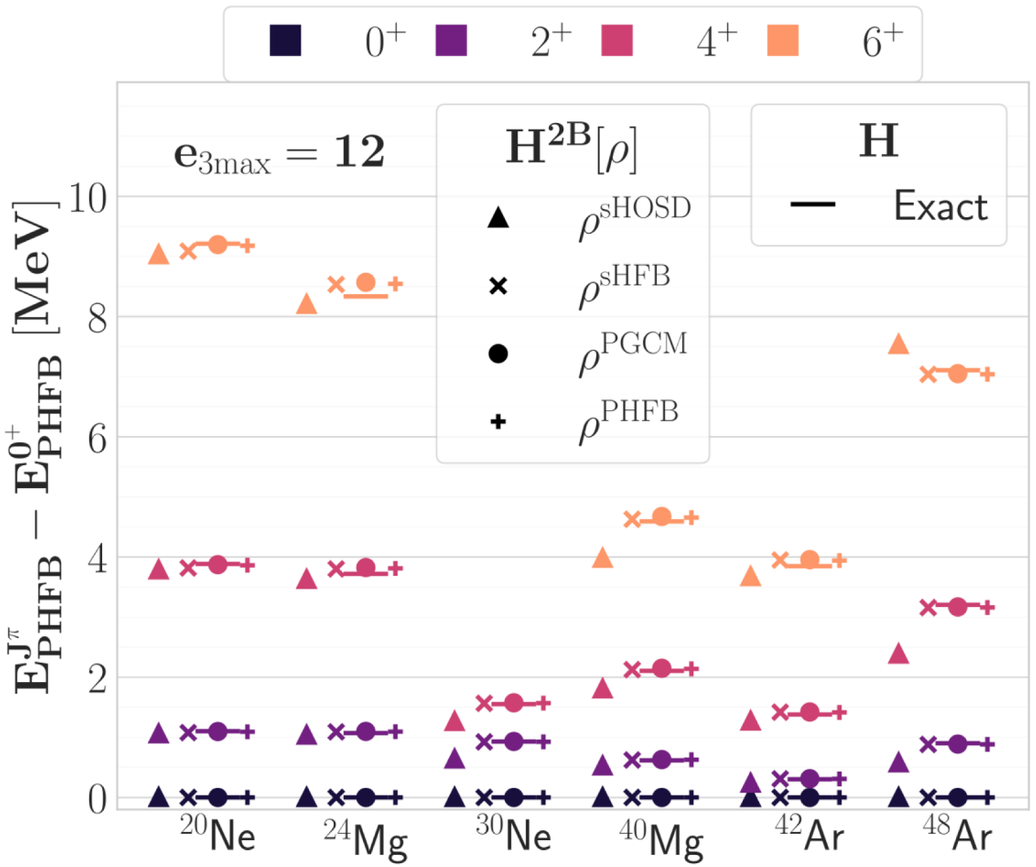


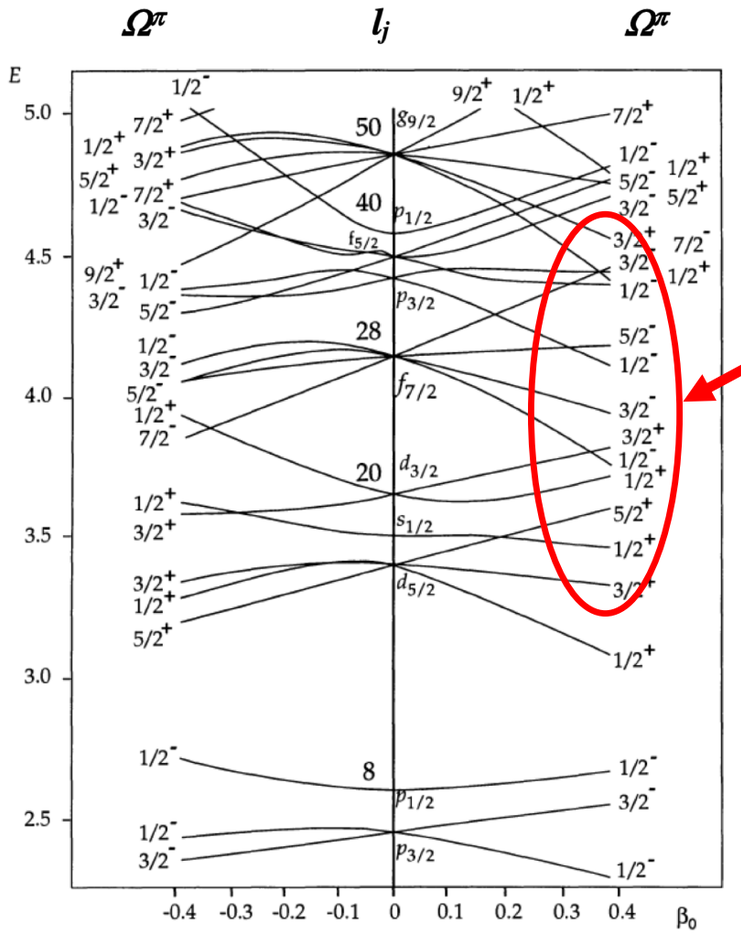




Inclusion of three-body forces

- 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





What is the correct spherical filling in very deformed nuclei?

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

Coupled-cluster computations of deformed nuclei

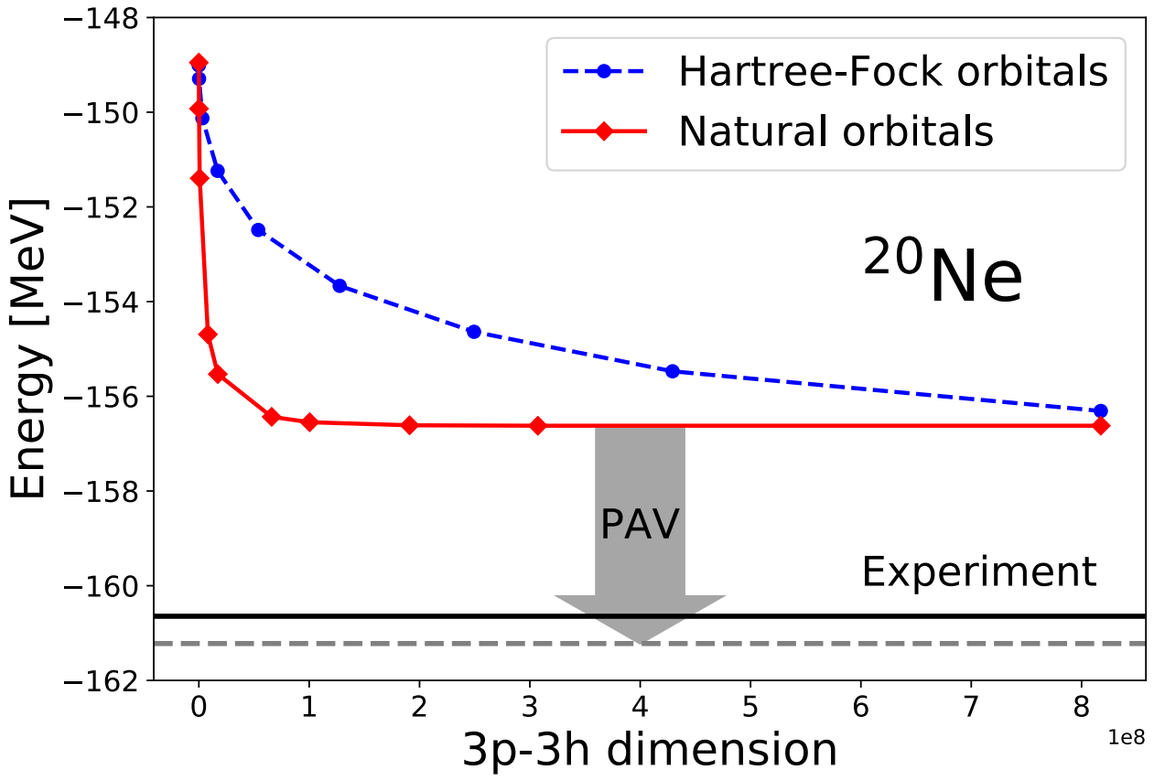
- Include short-range correlations via coupled-cluster theory
  - Large contribution to total energy
  - Cost increases polynomial with mass

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

- 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:

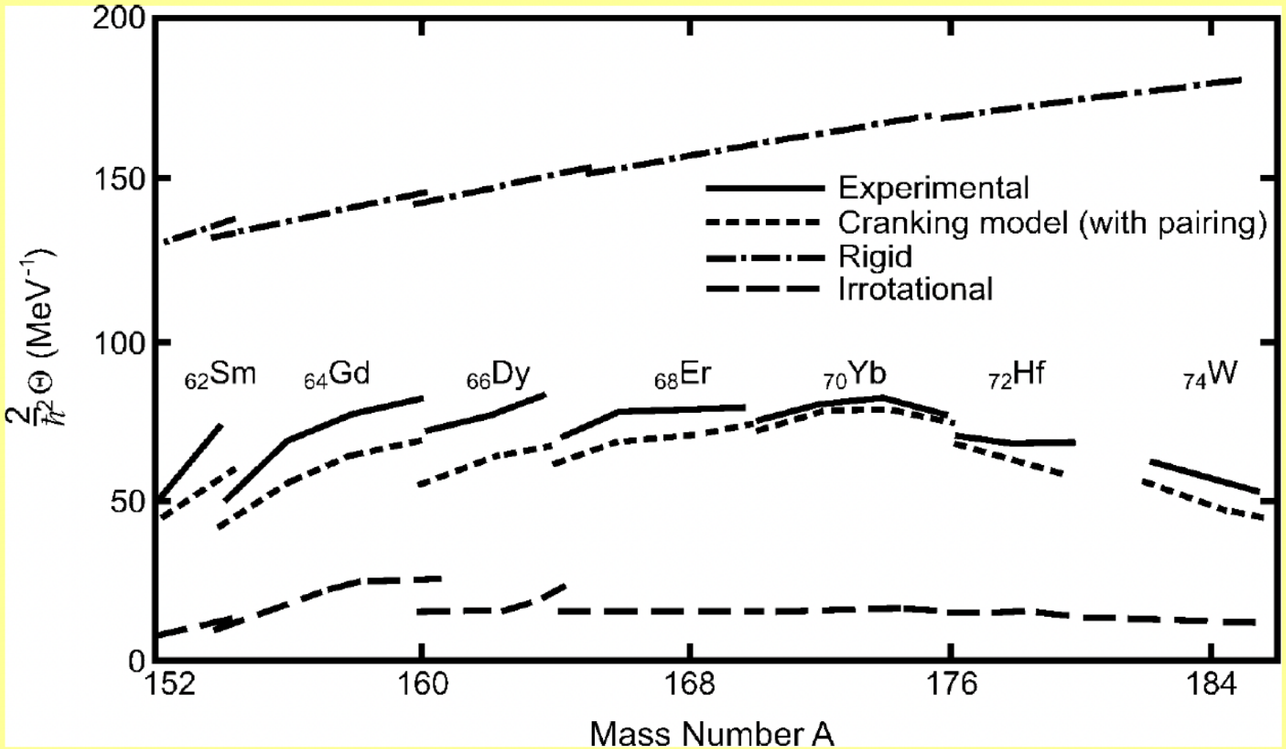
$$E = E_{\text{ref}} + \Delta E_{\text{CC}} + \delta E$$

The role of pairing on rotational bands

(v) Moment of inertia: extracted from level spacing in rotational bands

$$E = \frac{\hbar^2}{2\Theta} J(J+1)$$

deviates about a factor of two from the rigid rotor values.



- $\Theta_{irrot} < \Theta_{exp} < \Theta_{rigid}$
- Pairing correlations have a dramatic influence on collective modes.

Superfluidity reduces moments of inertia

Clearly visible in rotational bands, which are less compressed than what is expected from a rotating deformed liquid drop (no superfluid component)

Stretching of rotational bands

Rotational stretching: Moment of inertia increases with increasing spin

- Energy levels are lower than expected from $E(I) = \frac{I(I+1)}{2C_0}$
- Reflected in data: EFT at next-to-leading order $E(I) = \frac{I(I+1)}{2C_0} - \frac{C_2}{4C_0^4}[I(I+1)]^2$

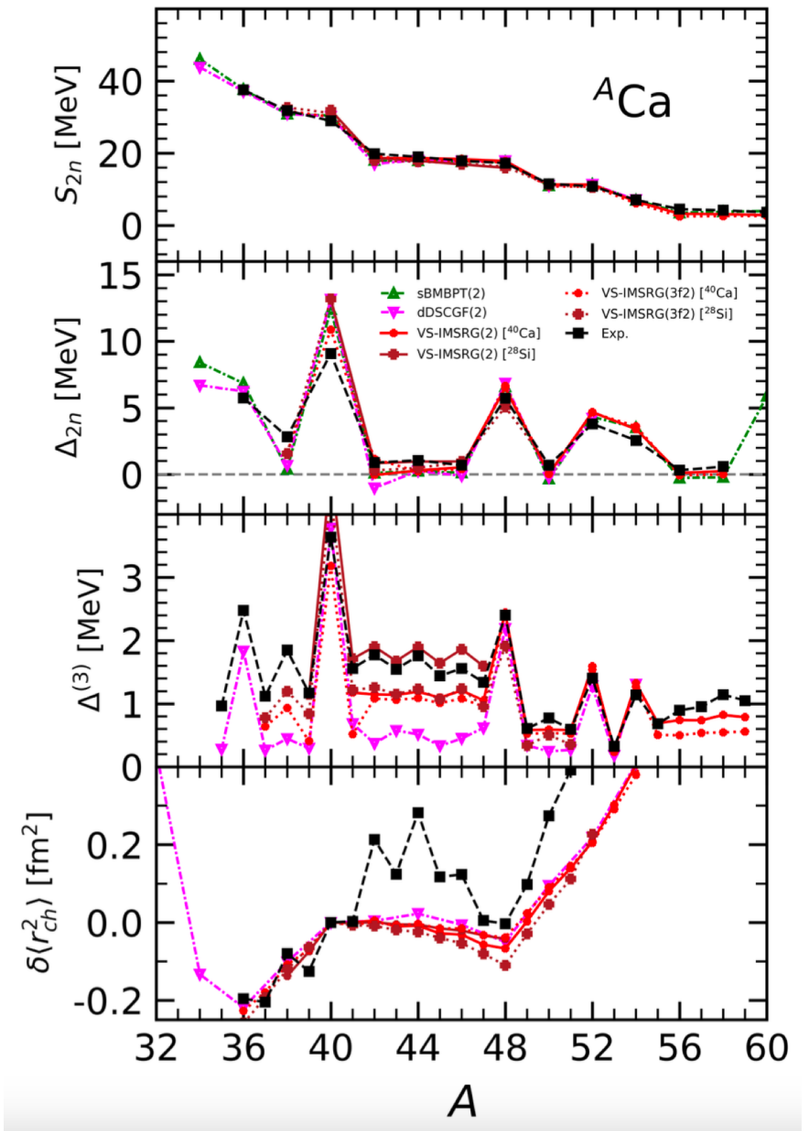
System	C_2/C_0^3
N_2	0.000 006
H_2	0.0015
^{236}U	0.0011
^{174}Yb	0.0010
^{168}Er	0.0010
^{166}Er	0.0020
^{162}Dy	0.0017
^{154}Sm	0.0033
^{188}Os	0.012
^{154}Gd	0.013
^{152}Sm	0.013
^{150}Nd	0.017

Rotors from molecules to deformed nuclei exhibit rotational stretching because $C_2 > 0$

What does ab initio calculations of deformed nuclei say?

Coello Perez & Papenbrock, Phys Rev C (2015)

Where is the pairing gone?



A. Scalesi et al, unpublished (2026)

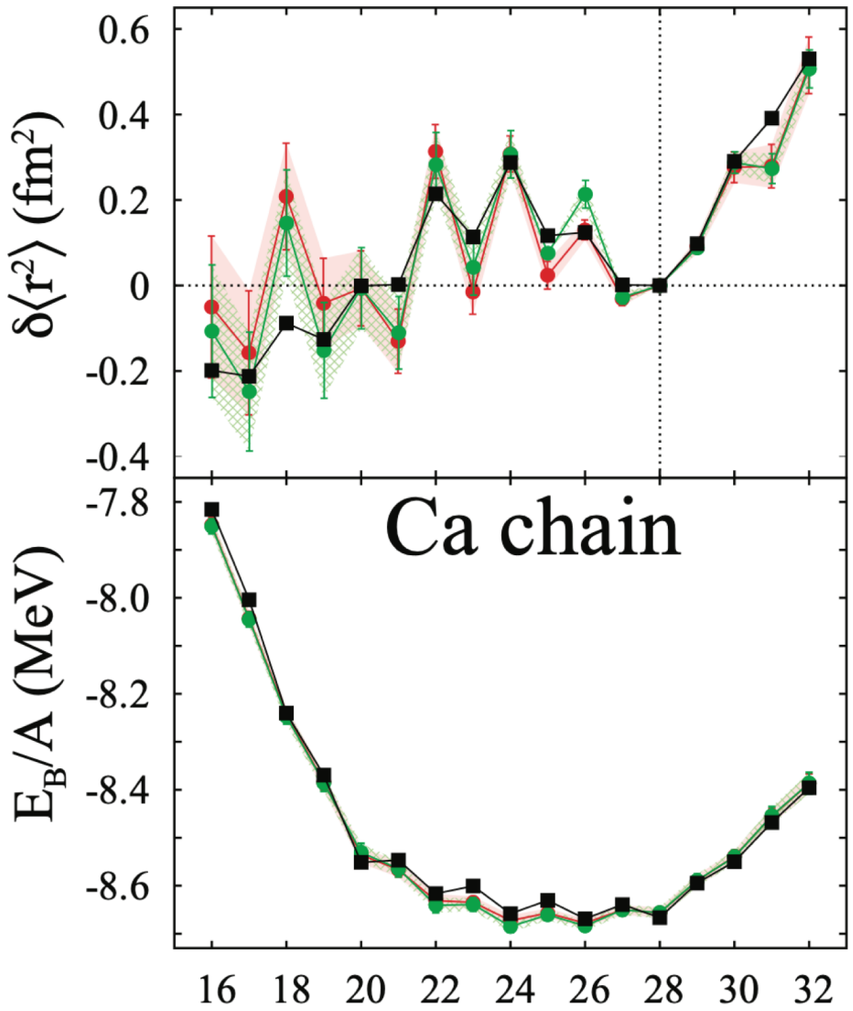
Fayans EDF
(density dependent
pairing functional)

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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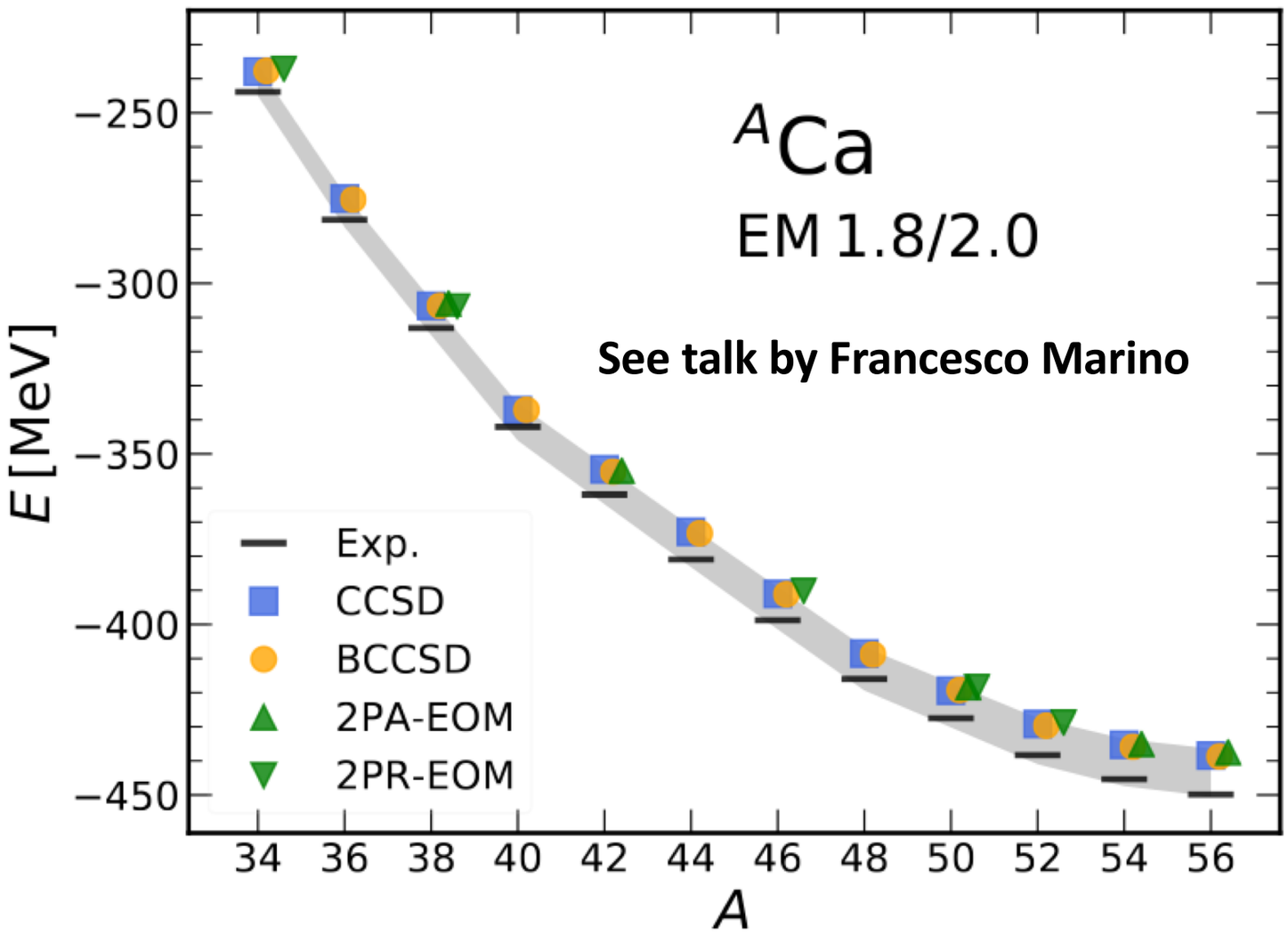
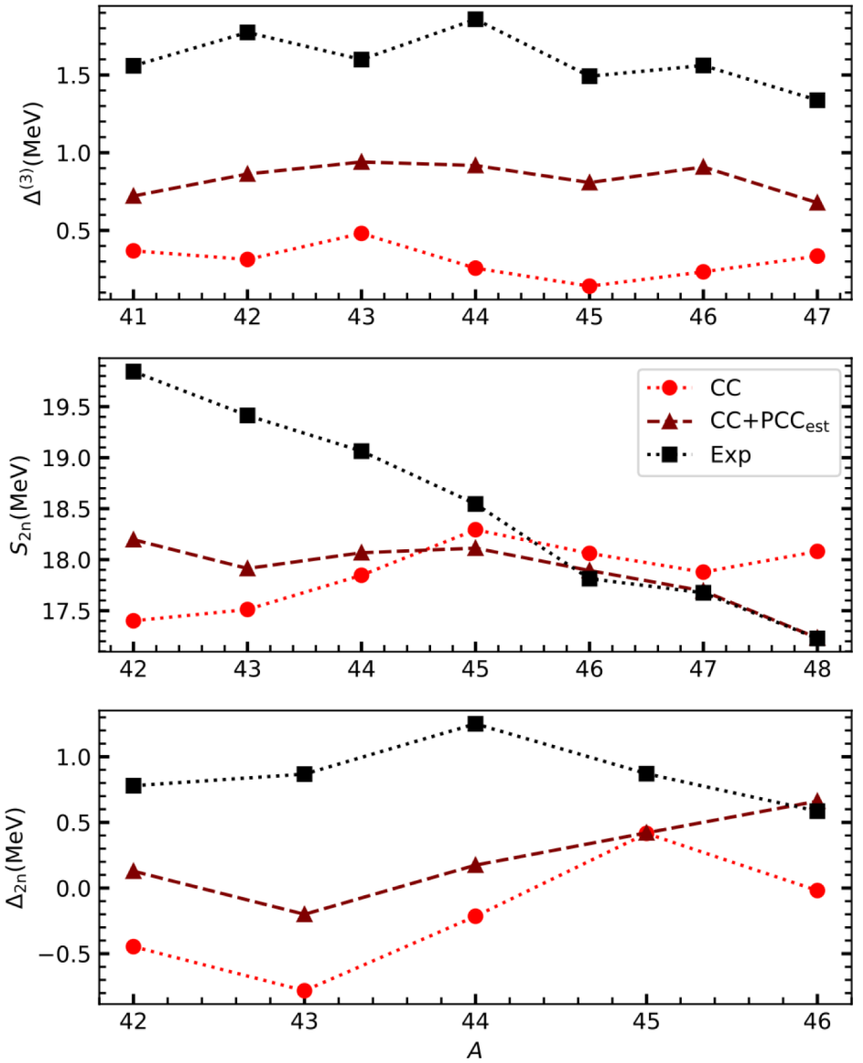
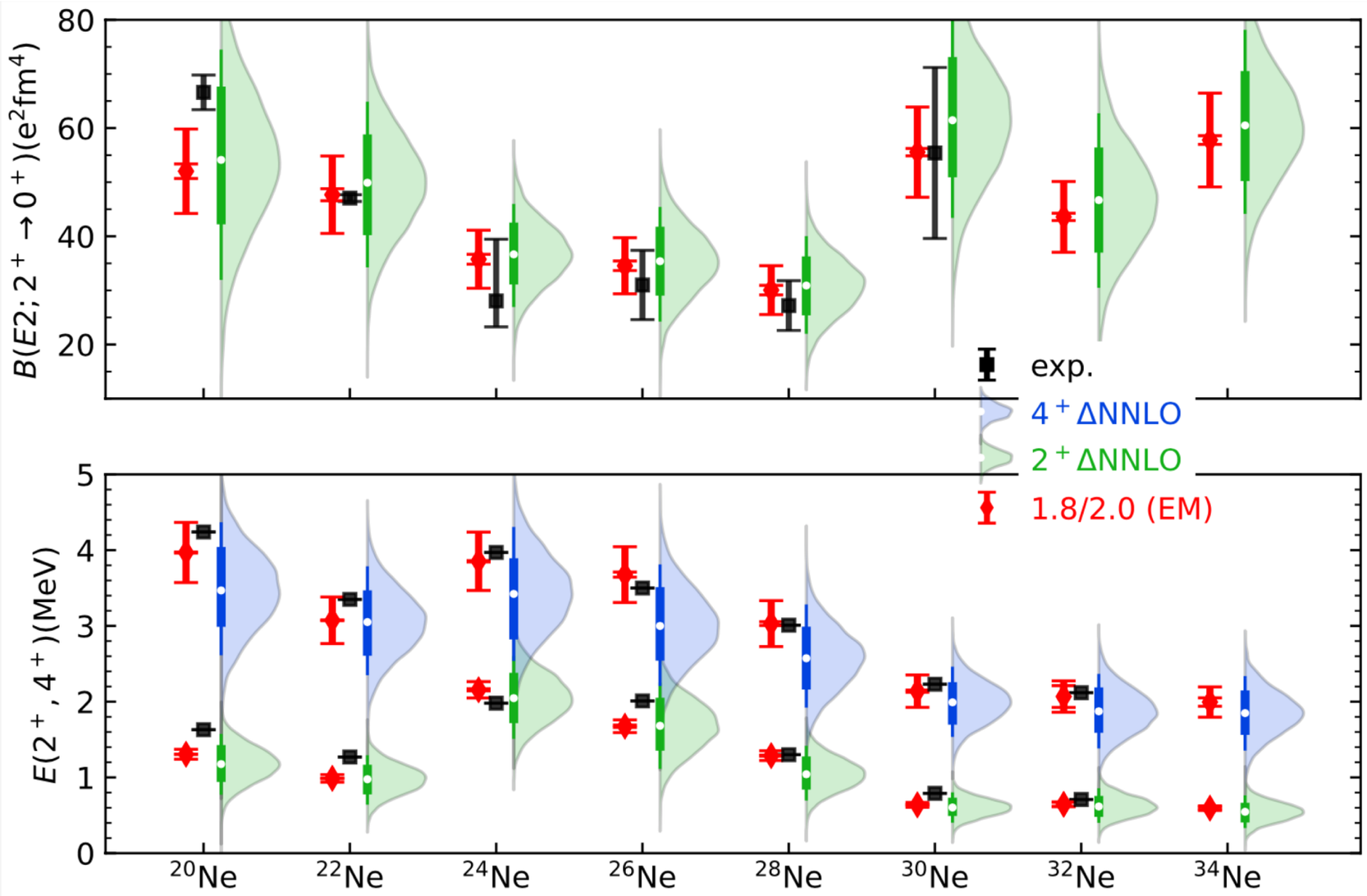


Francesco Marino et al. arXiv:2512.17311 (2025)



Zhonghao, et al, unpublished

Pairing puzzle for ab initio rotational bands



1.8/2.0 (EM) has too small radii

- Moment of inertia too small
- Rotational bands should have too large spacings compared to data

However, the spacings are fine when compared to data

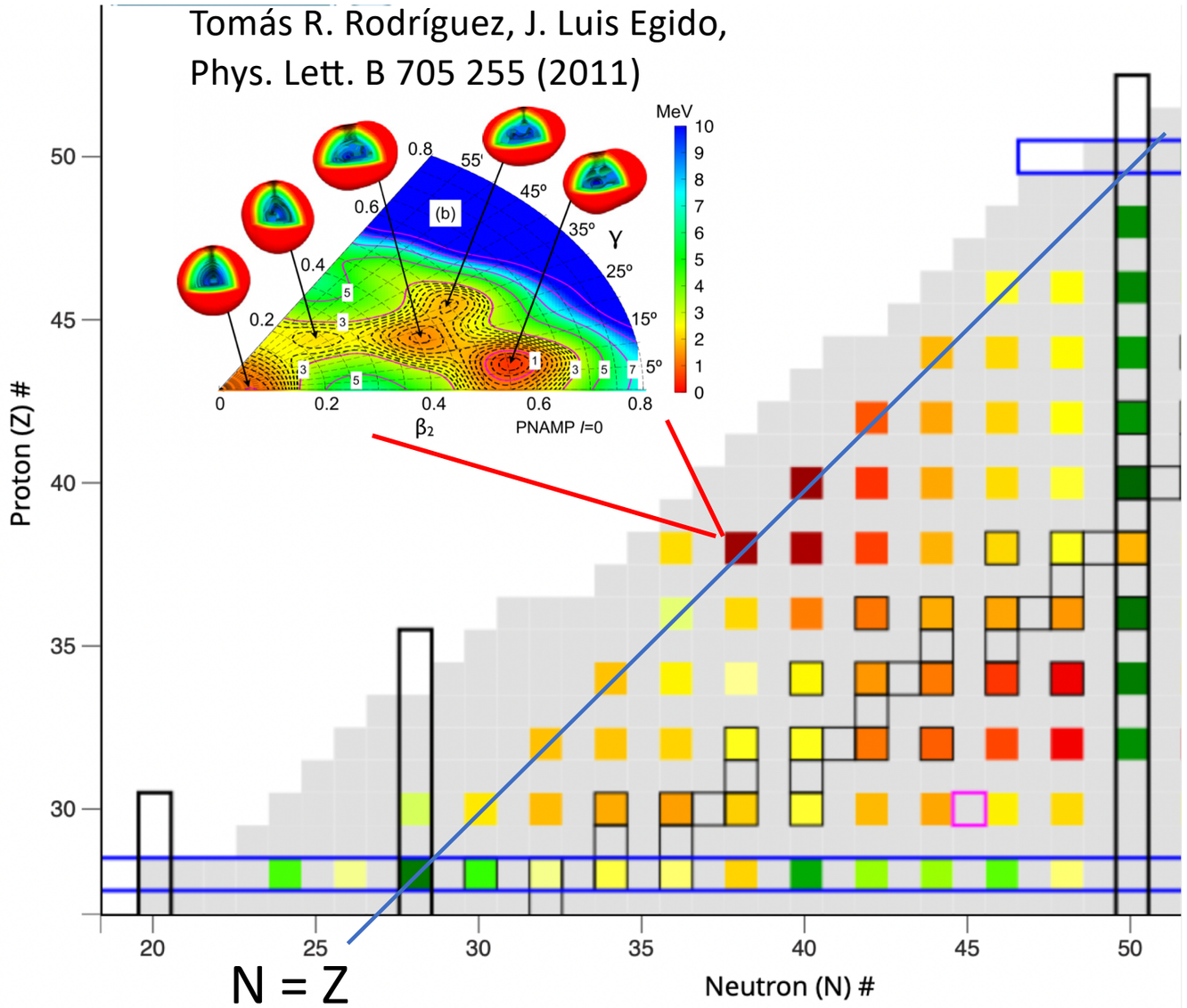
- Is the absence of superfluidity (which would increase moments of inertia) compensated by the too small radii???

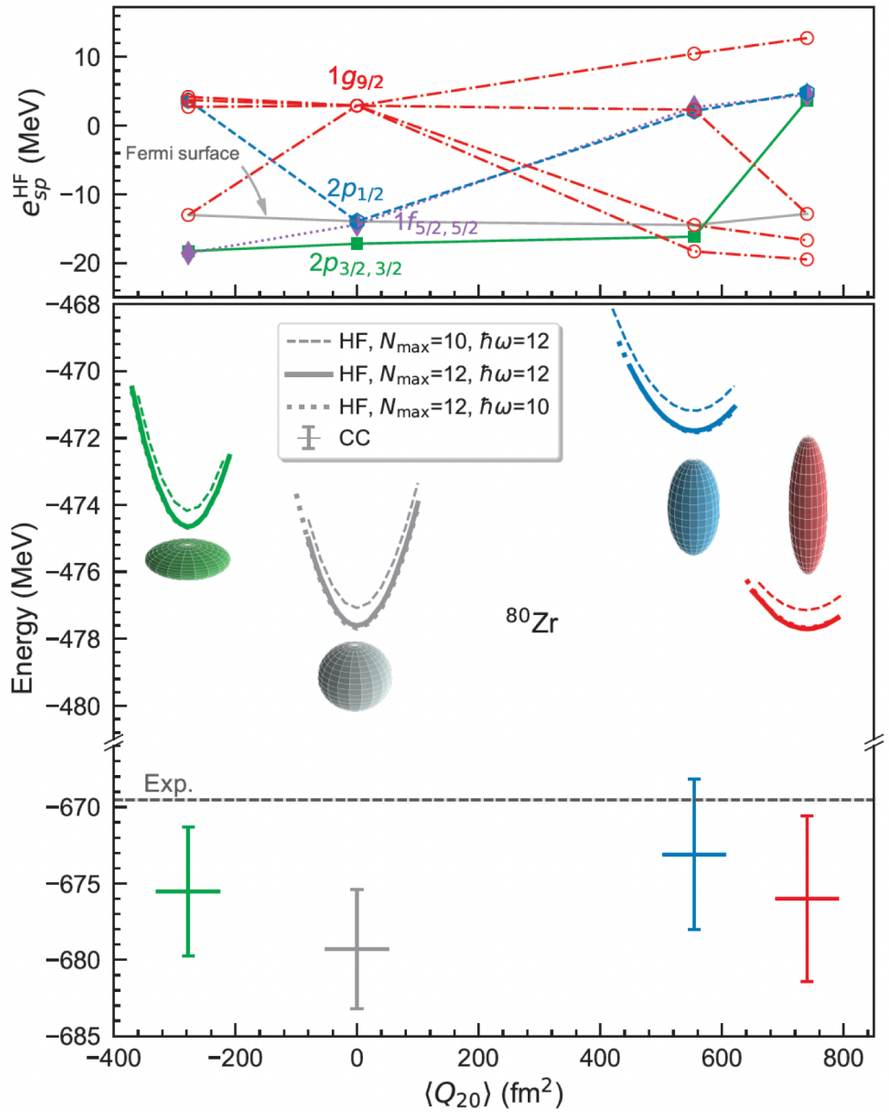
Ensemble of delta-full interactions from recent study of ^{28}O
Y. Kondo et al.,
Nature **620**, 965–970 (2023)

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

Strongly deformed nuclei around ^{80}Zr

Tomás R. Rodríguez, J. Luis Egido,
Phys. Lett. B 705 255 (2011)

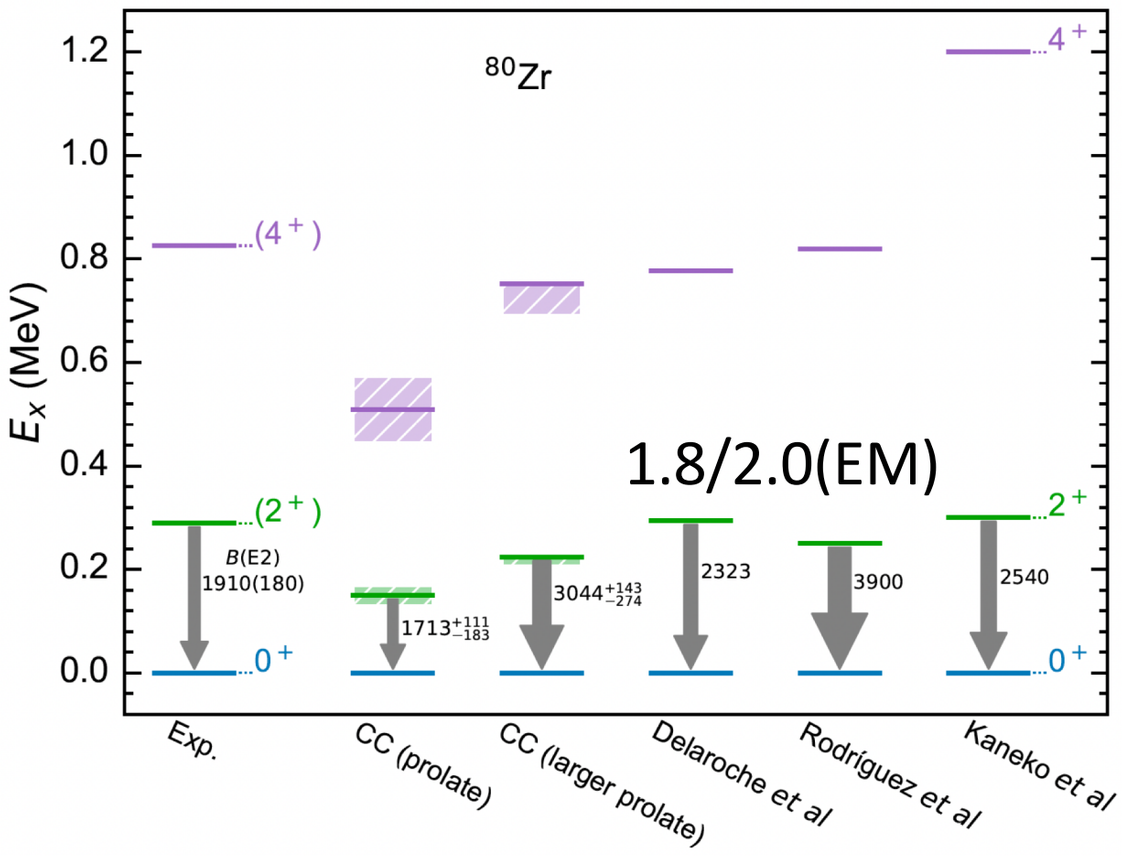




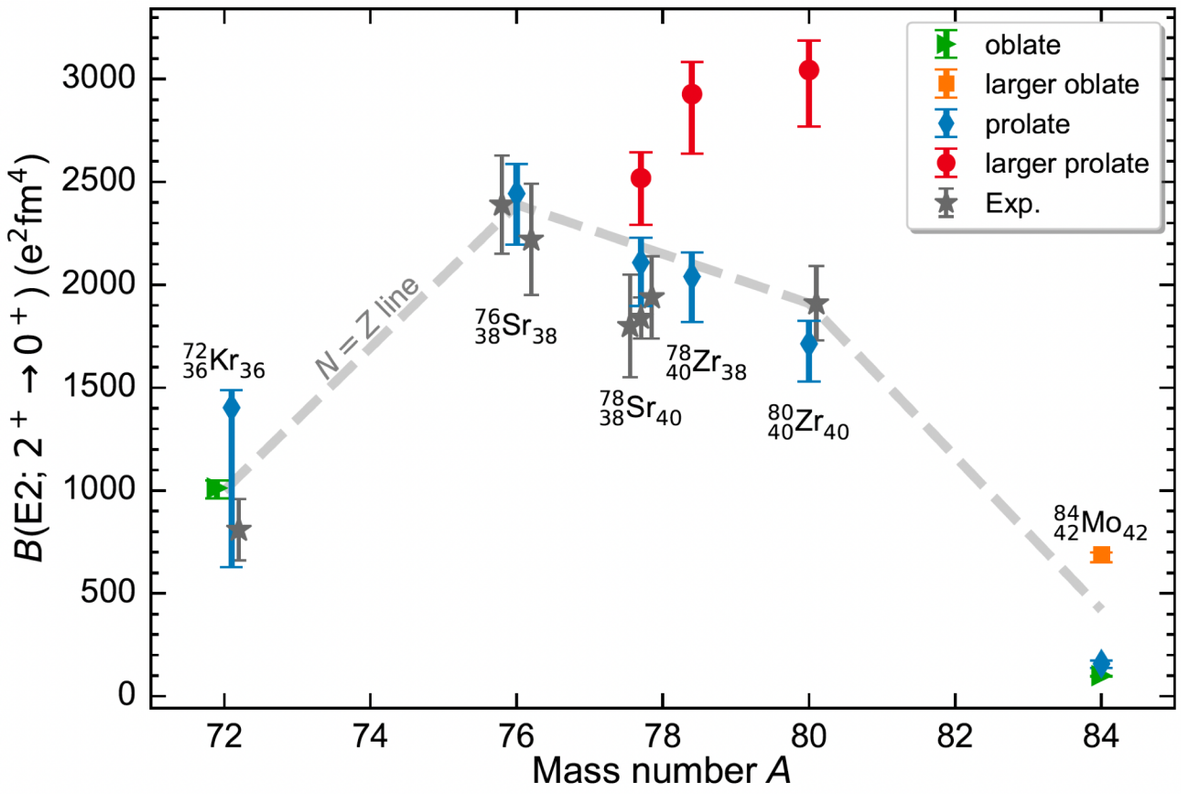
Baishan Hu, Zhonghao Sun, G. Hagen, T. Papenbrock.
Phys. Rev. C **110**, L011302 (2024)

Strongly deformed nuclei around ^{80}Zr

Spectrum prefers larger prolate shape



$B(E2)$ prefers prolate band

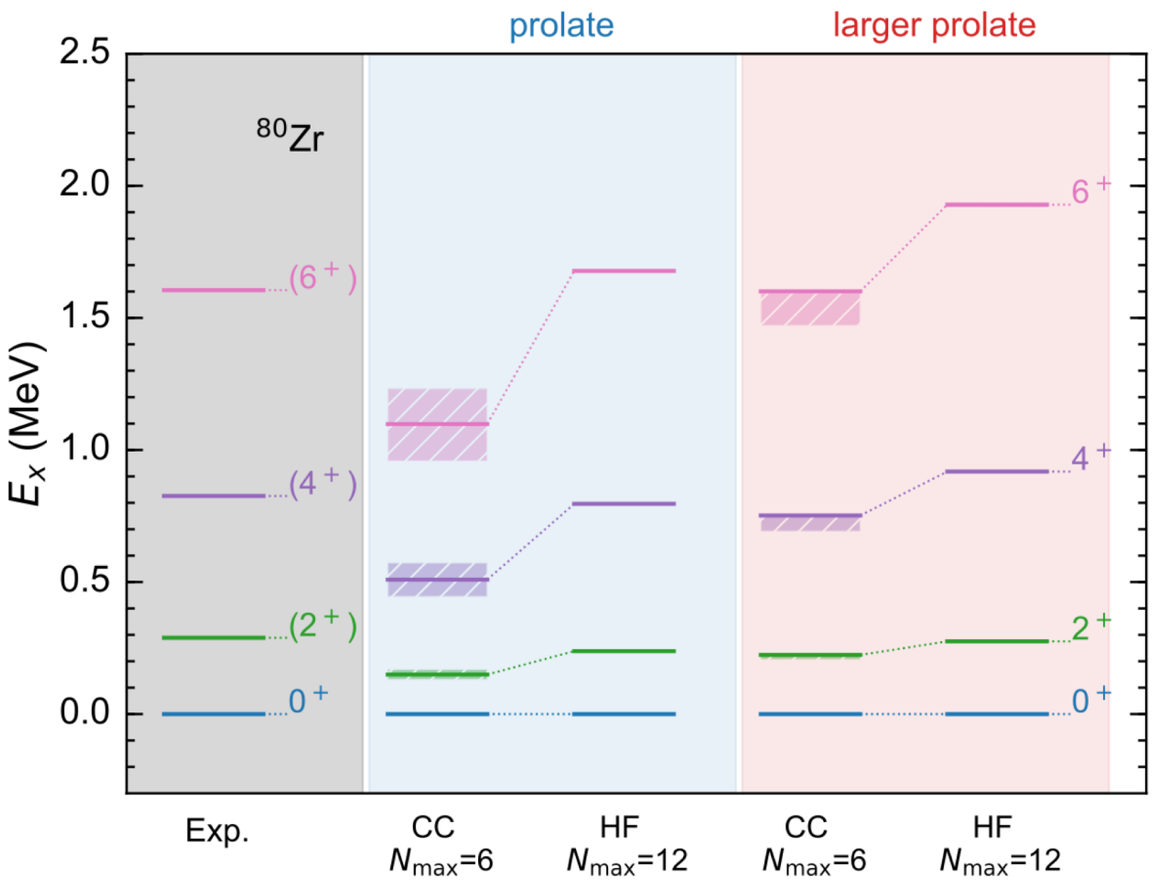


Baishan Hu, Zhonghao Sun, G. Hagen, T. Papenbrock. Phys. Rev. C **110**, L011302 (2024)

Ab initio rotational stretching

The verdict is still out in ab initio computations?

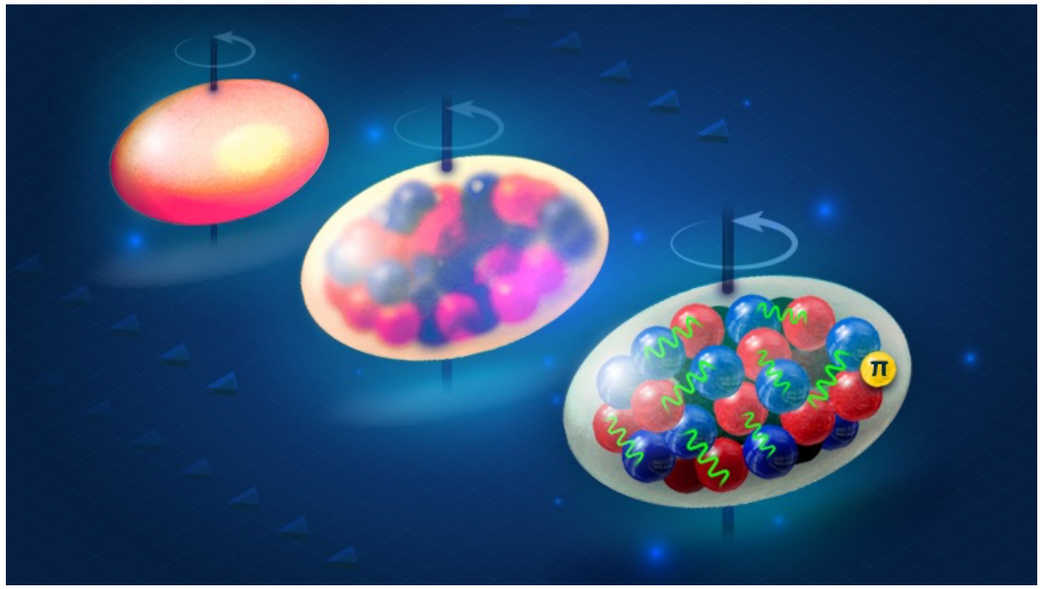
- Projection after variation would probably not yield much rotational stretching
  - GCM could perhaps remedy this
  - Projection after variation at spin-dependent deformations could remedy this



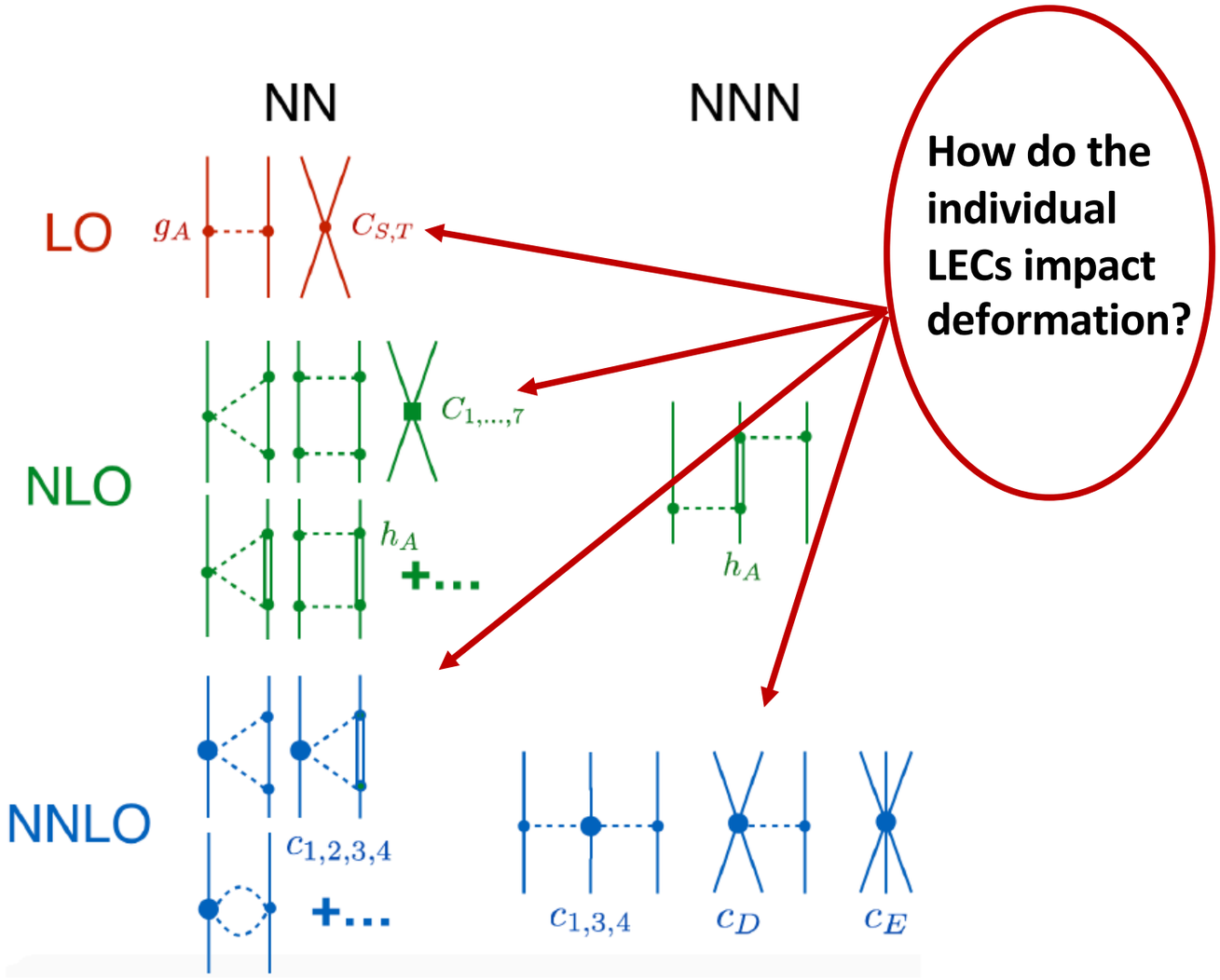
Lack of rotational stretching in coupled-cluster with projection after variation
[Hu, Sun, Hagen, Papenbrock, Phys Rev C (2024)]

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



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.

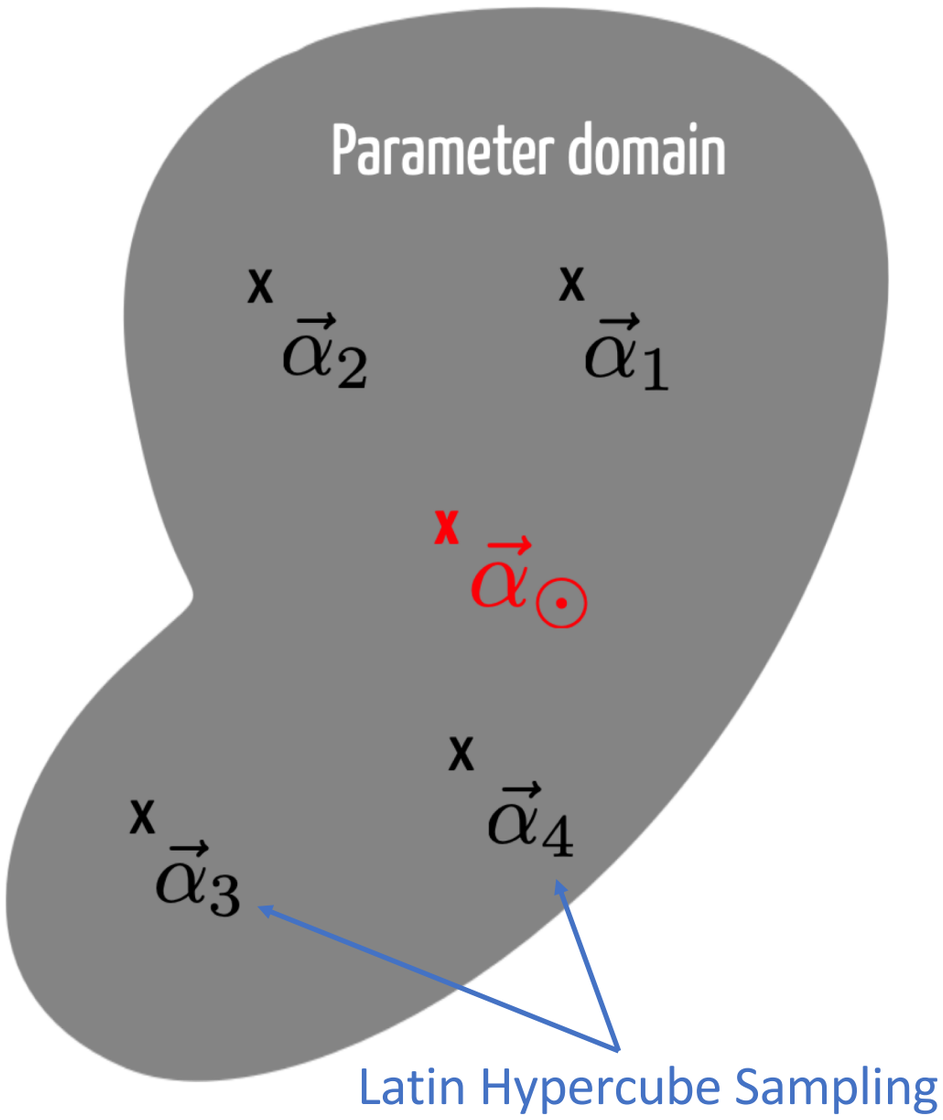
Computational bottleneck

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

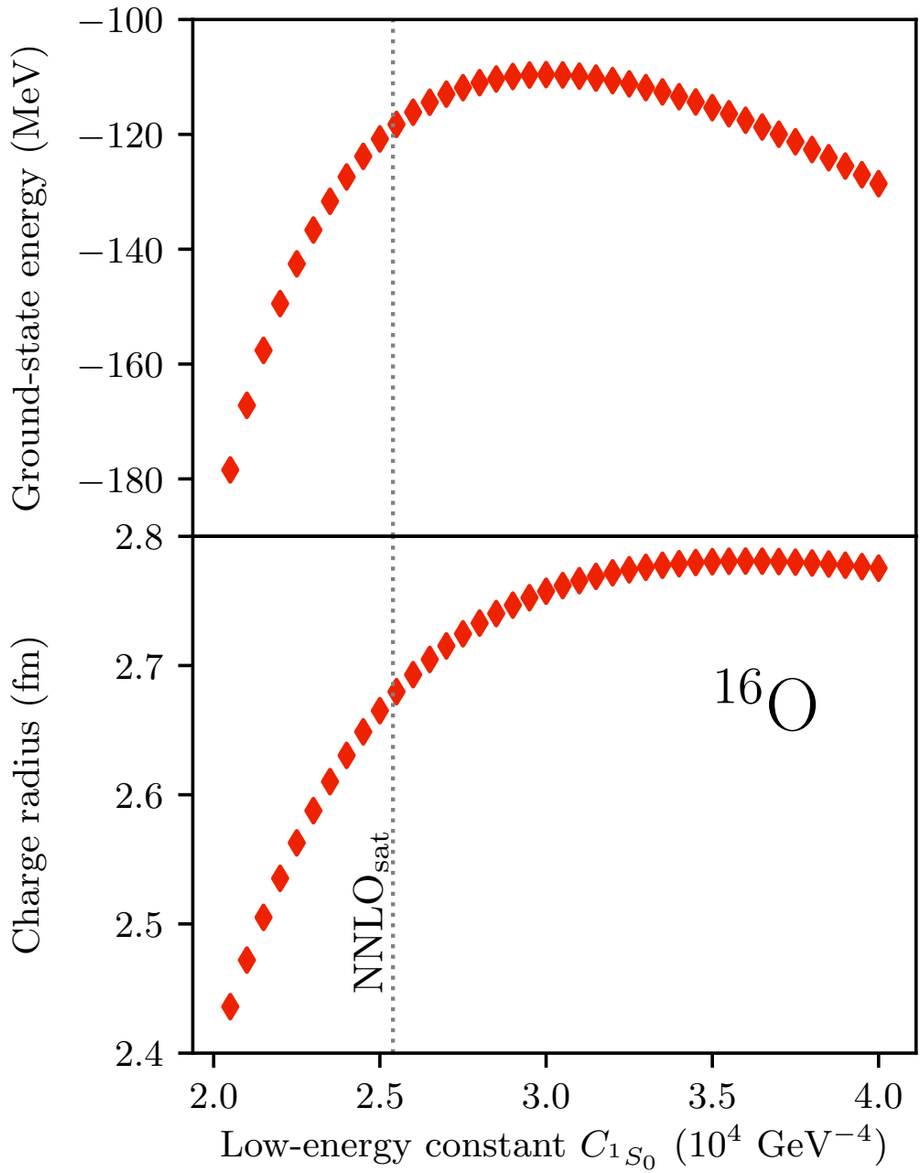
$$H(\vec{\alpha}) = h_0 + \sum_{i=1}^{N_{\mathrm{LECs}}=17} \alpha_i h_i$$

- 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

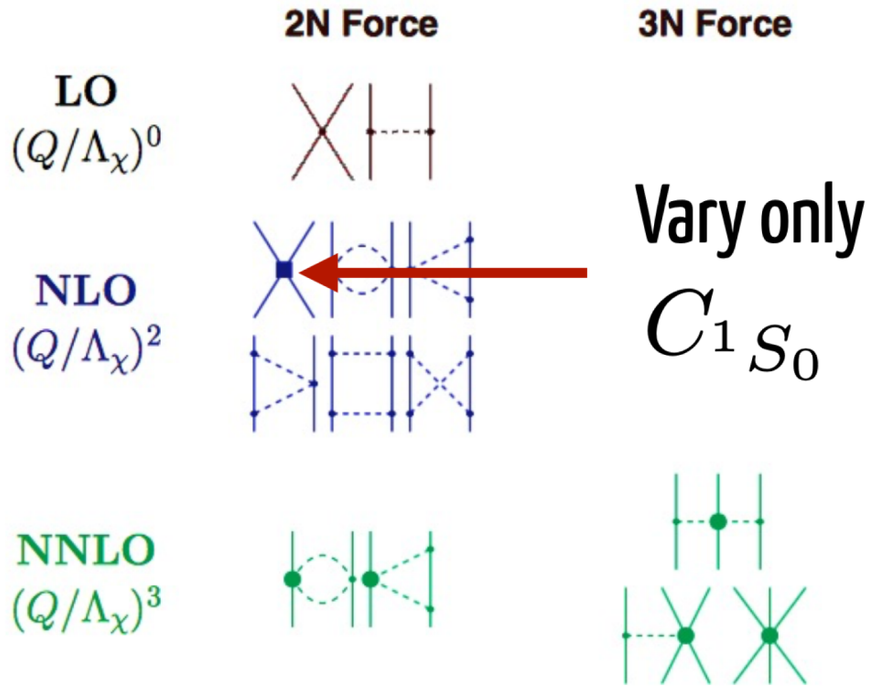
$$\mathbf{H}(\vec{\alpha}_\odot)\,\vec{c} = E(\vec{\alpha}_\odot)\,\mathbf{N}\,\vec{c}$$

Emulating ab-initio coupled-cluster calculations

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



Exact coupled cluster calculations at the singles and doubles level



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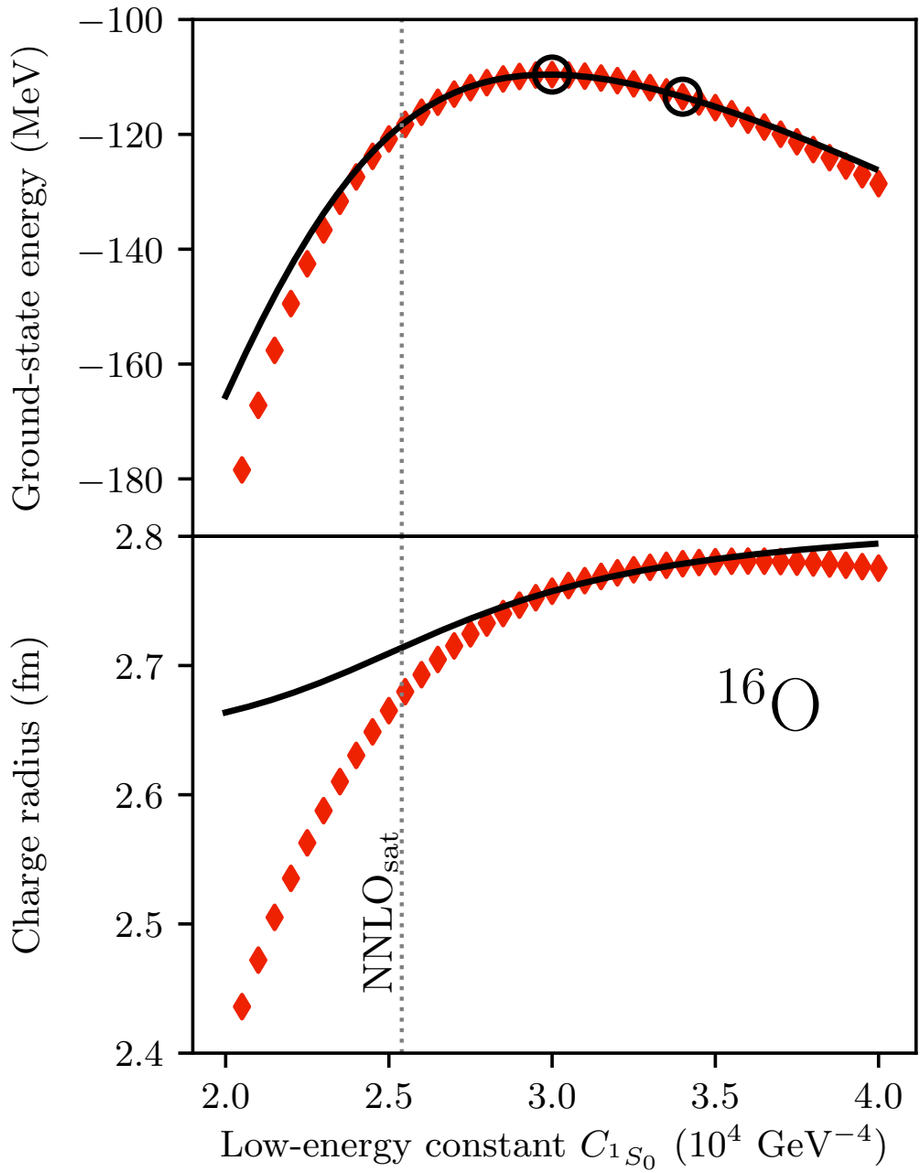
Andreas Ekström, Gaute Hagen PRL **123**, 252501 (2019)



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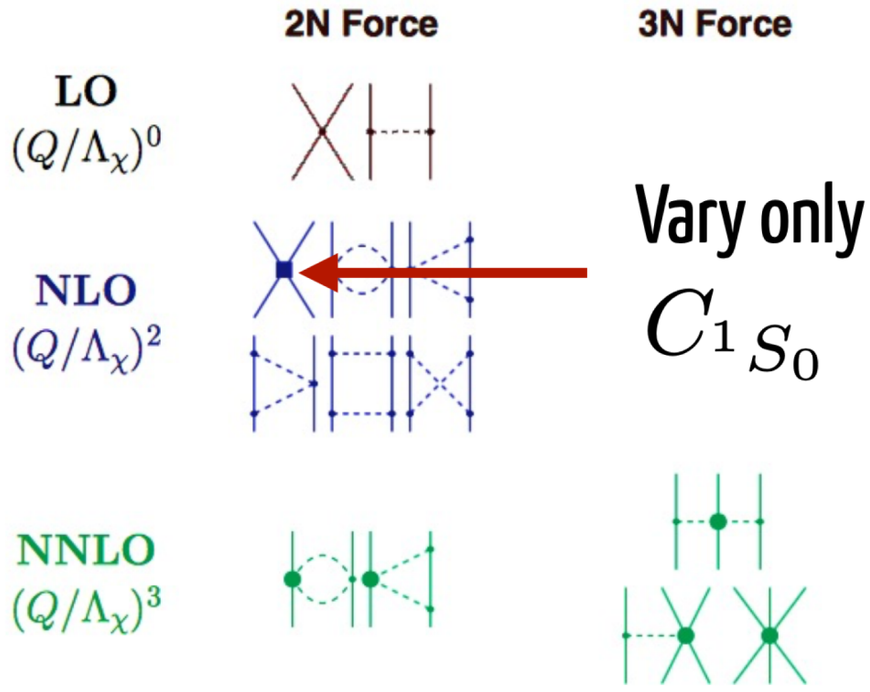

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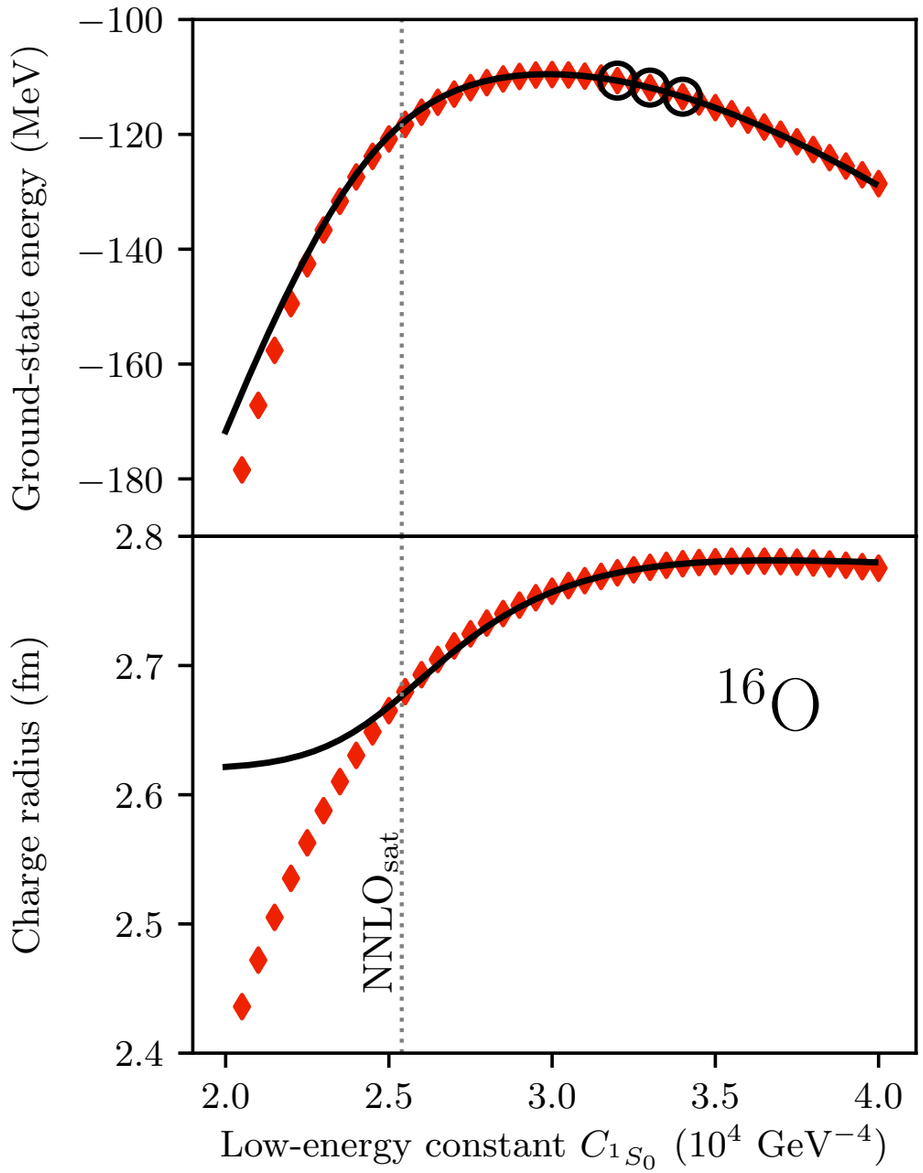

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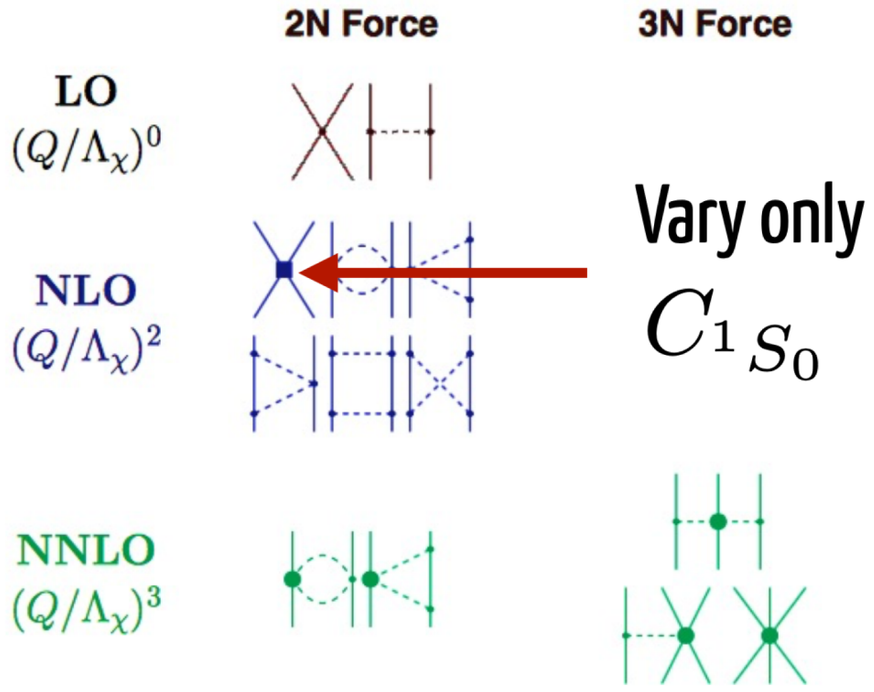

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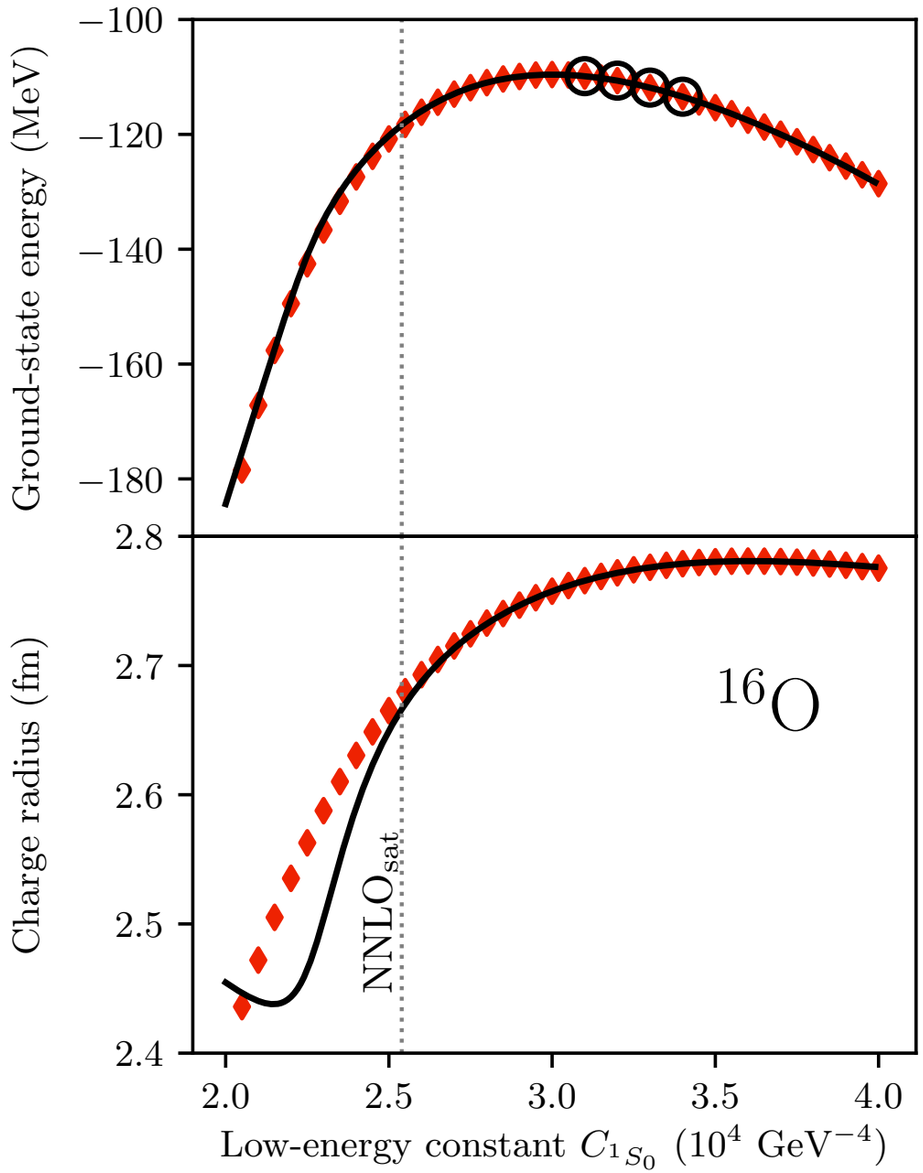

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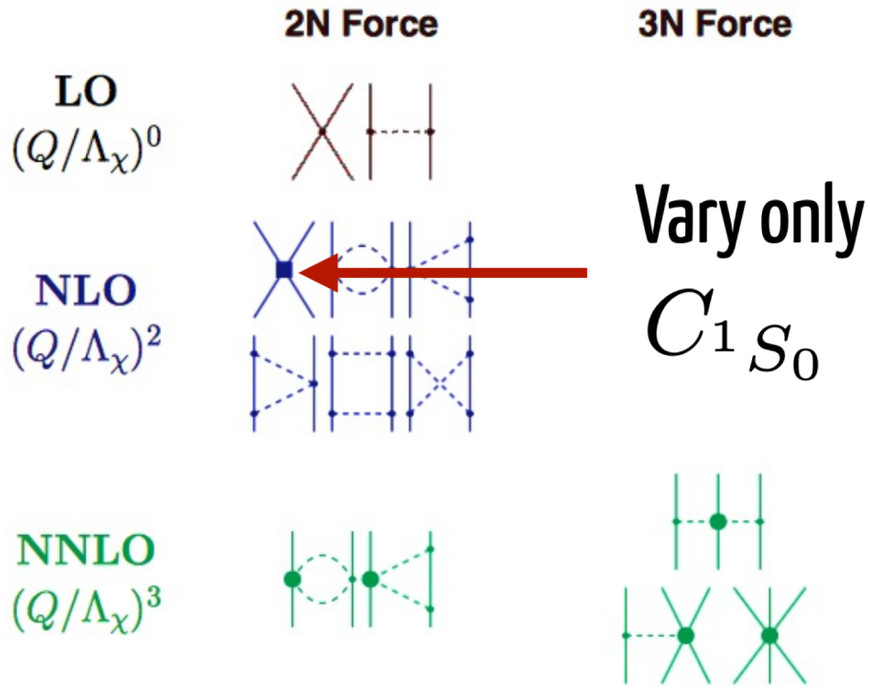
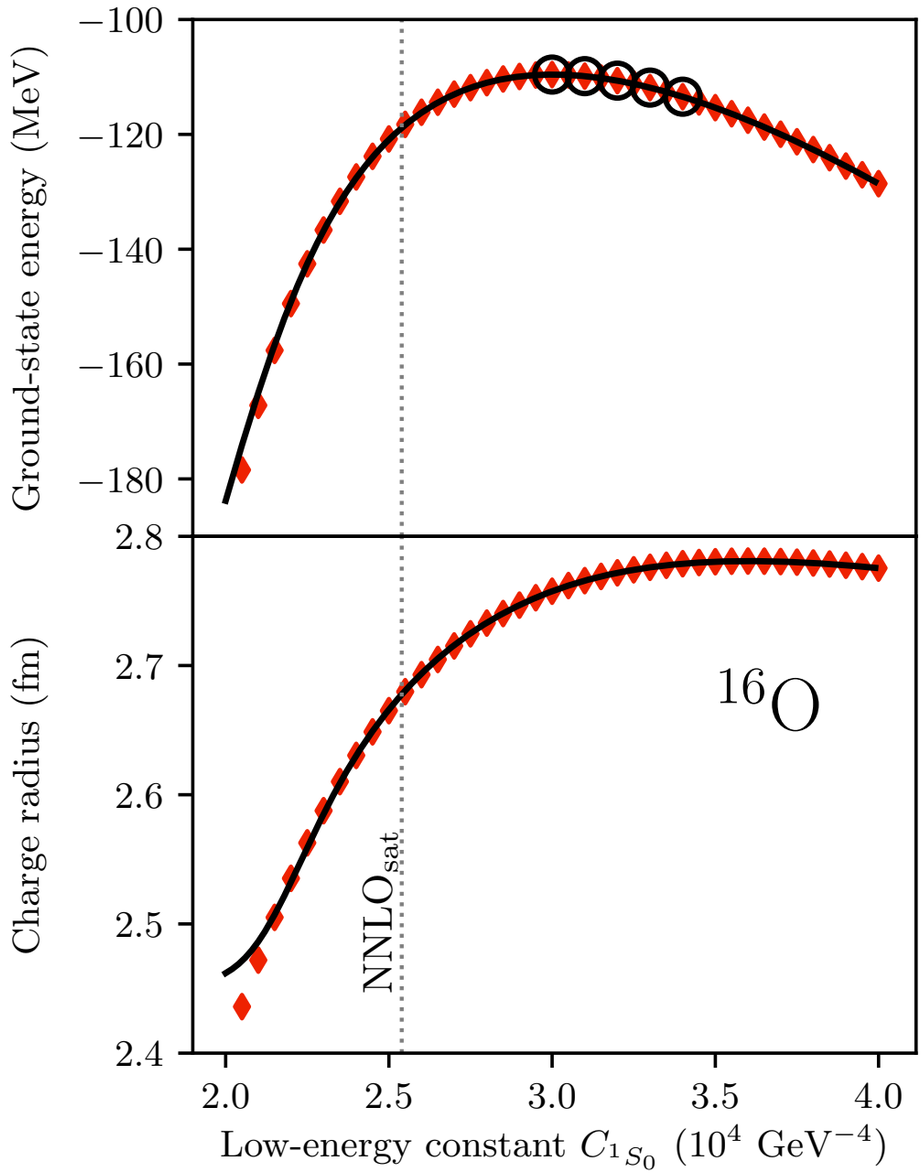
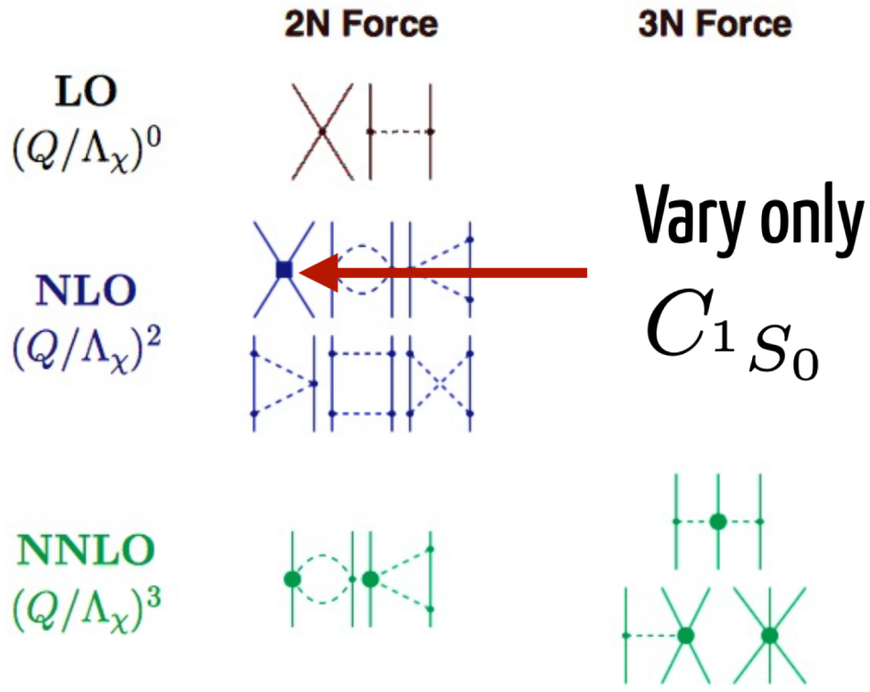


Emulating ab-initio coupled-cluster calculations

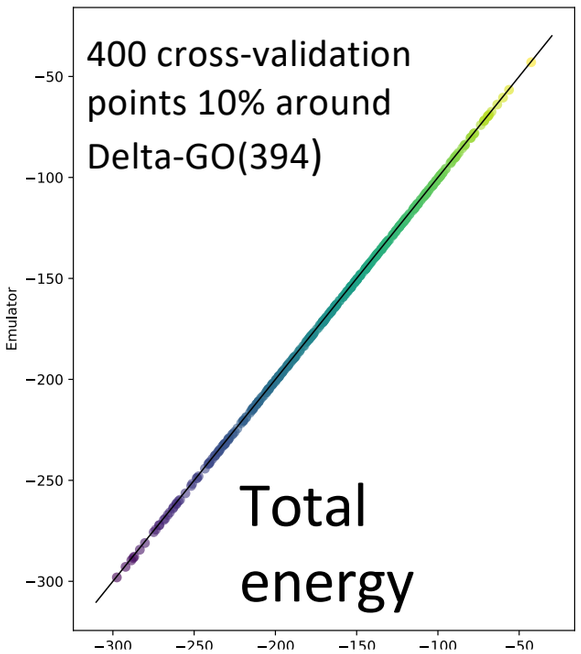
Andreas Ekström, Gaute Hagen PRL **123**, 252501 (2019)

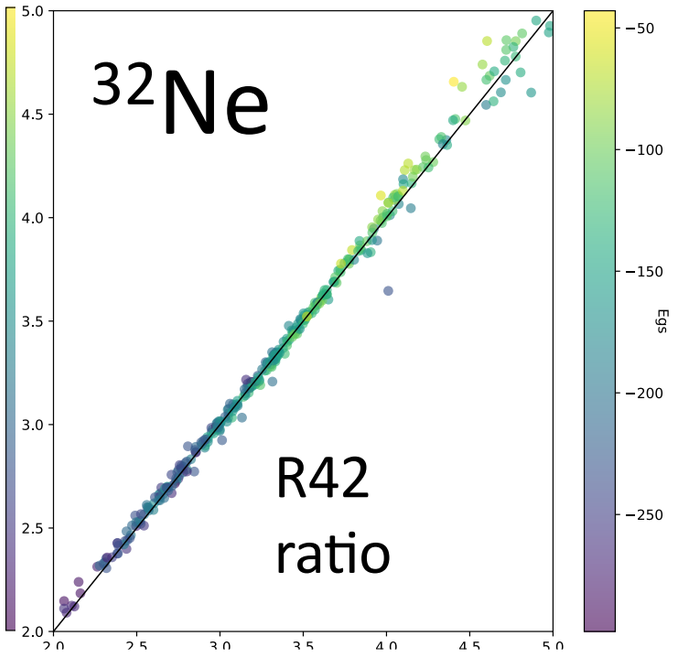


Exact coupled cluster calculations at the singles and doubles level

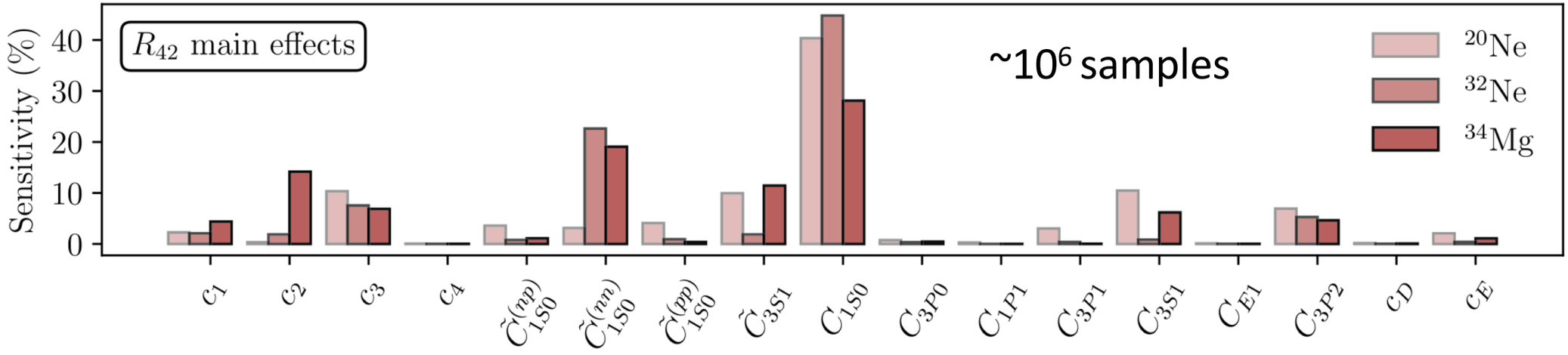


Linking deformation to nuclear forces



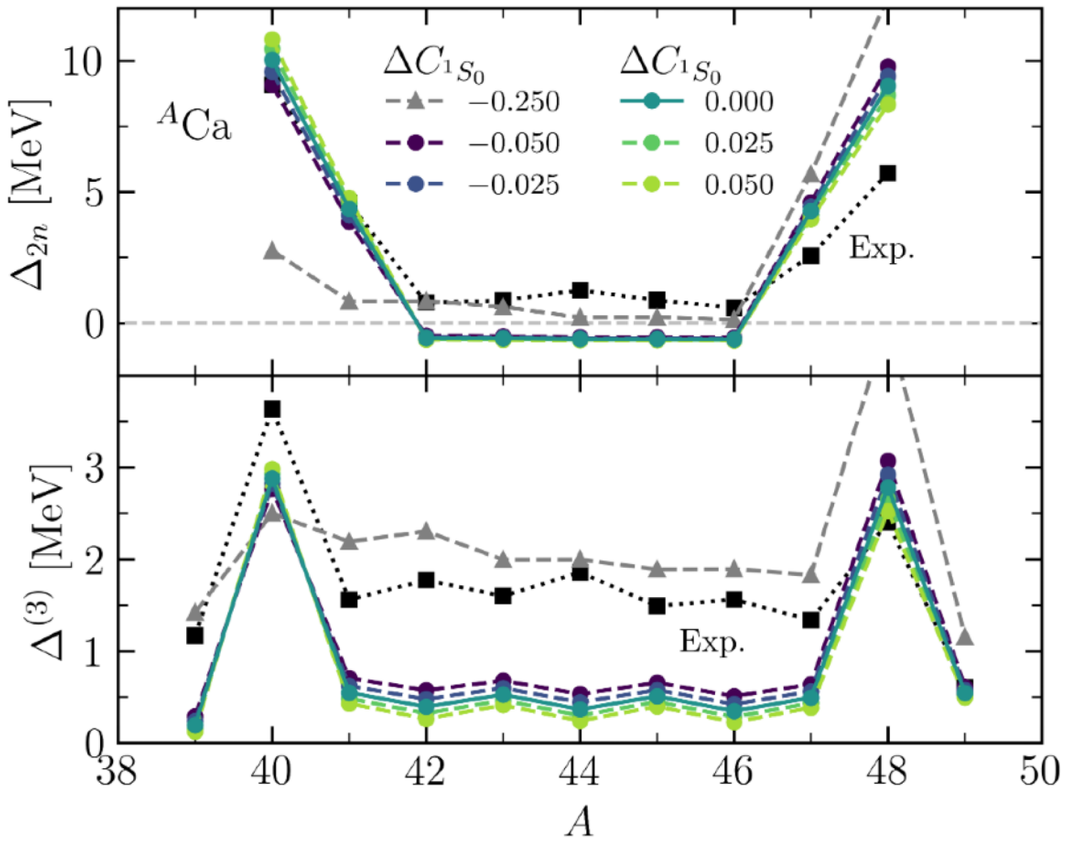


- More than 50% of the deformation is driven by the S-wave contact part of the interaction
- Adding short-range repulsion increase deformation presumably by reducing pairing
- Increasing the pion-nucleon coupling strength also increases deformation, presumably by adding attraction in higher partial waves



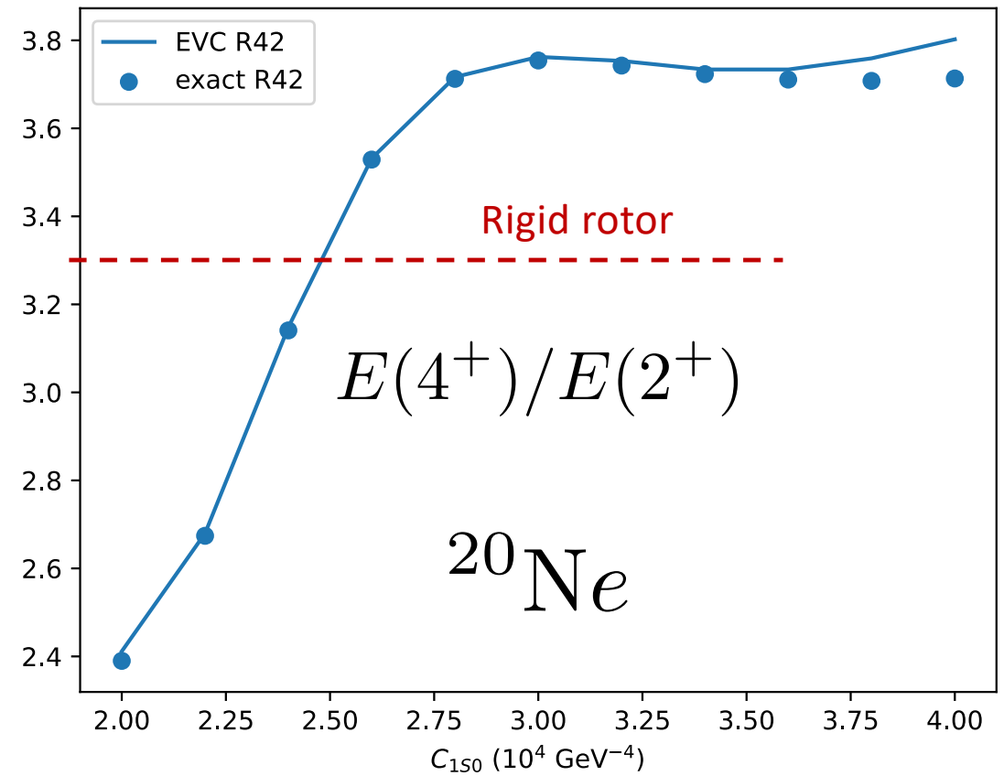
Linking deformation to nuclear forces

Varying only one parameter C_{1S_0}



Two neutron shell gap and three point difference in calcium isotopes

A. Scalesi, et al in preparation (2026)

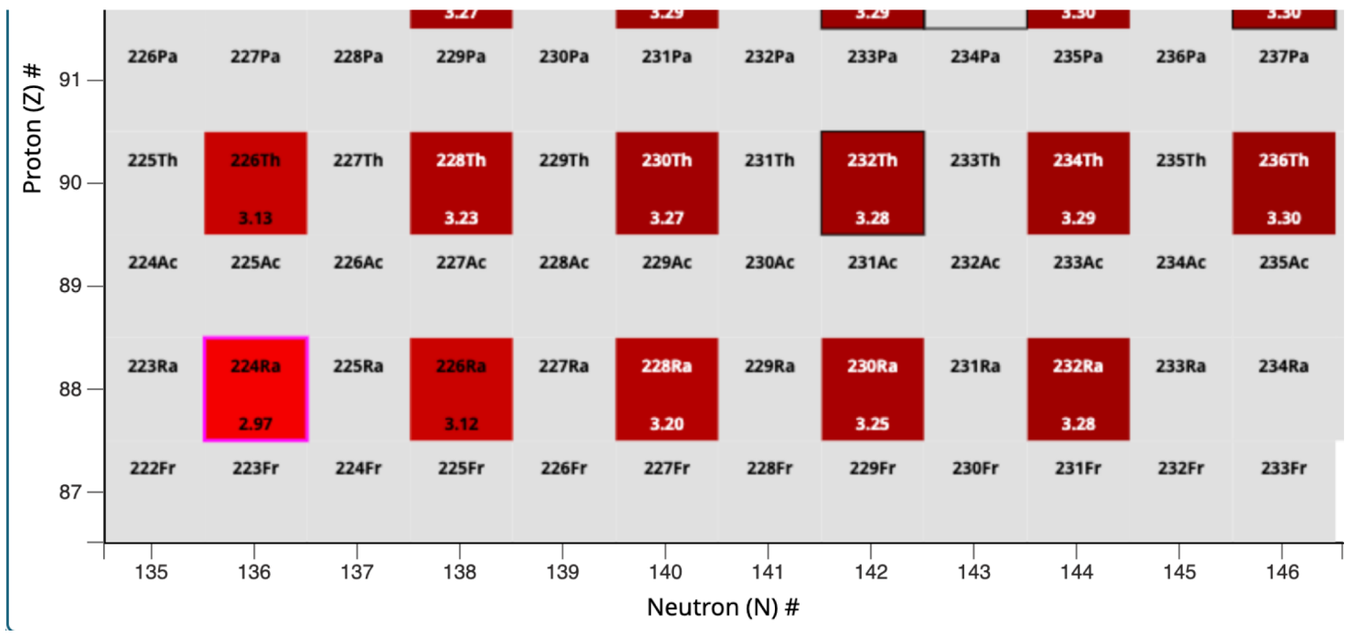


Decreasing the s-wave contact strength leads to increased pairing and reduced deformation

Towards ab-initio description of Schiff moments

Computation of Schiff moment in ^{225}Ra relevant for EDM searches in atoms and molecules. Schiff moment is particularly sensitive to octupole deformation

$$S \equiv \langle \Psi_0 | \hat{S}_0 | \Psi_0 \rangle \approx \sum_{i \neq 0} \frac{\langle \Psi_0 | \hat{S}_0 | \Psi_i \rangle \langle \Psi_i | \hat{V}_{PT} | \Psi_0 \rangle}{E_0 - E_i} + \text{c.c.},$$



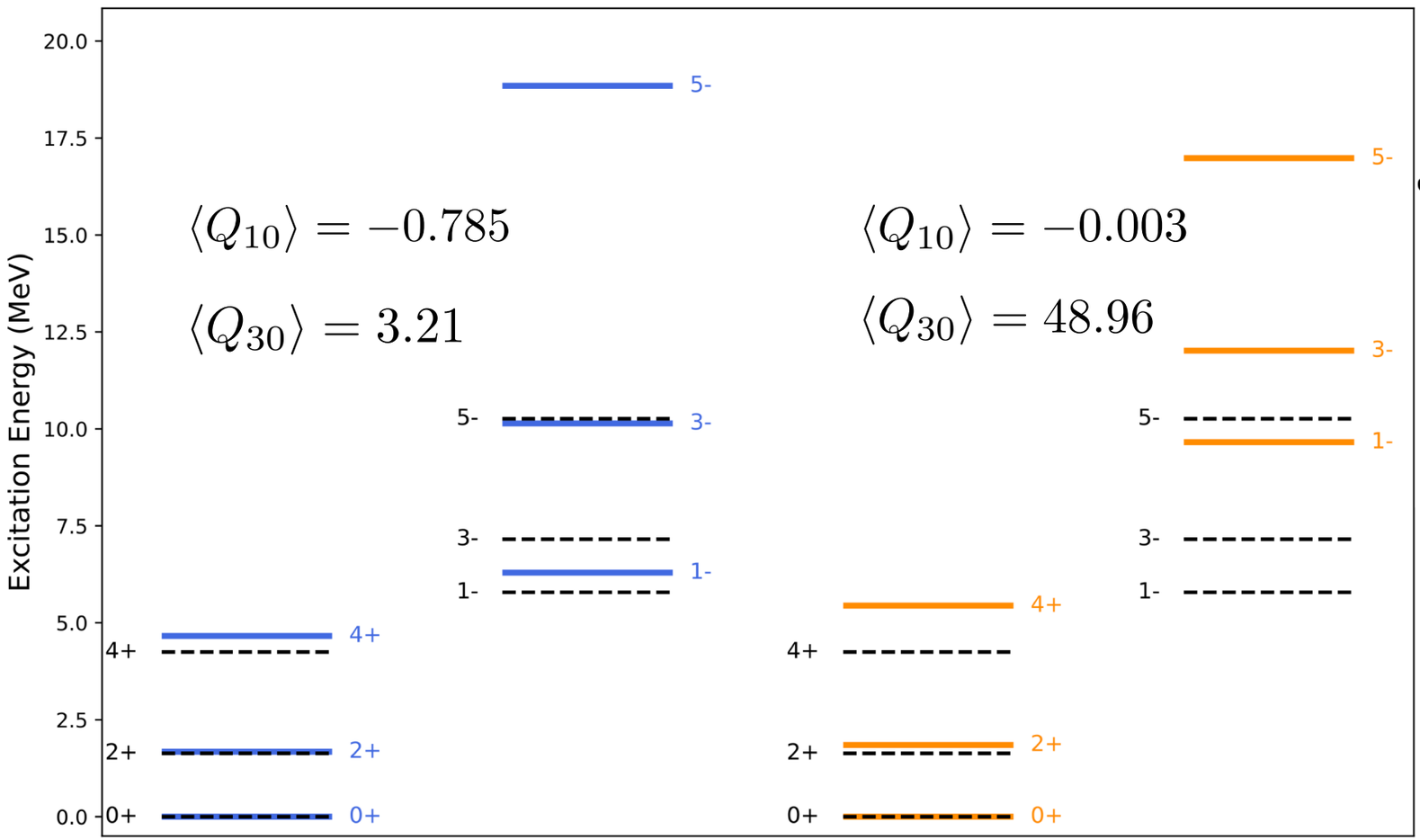
Nature 2013,
octupole deformed ^{220,224}Ra

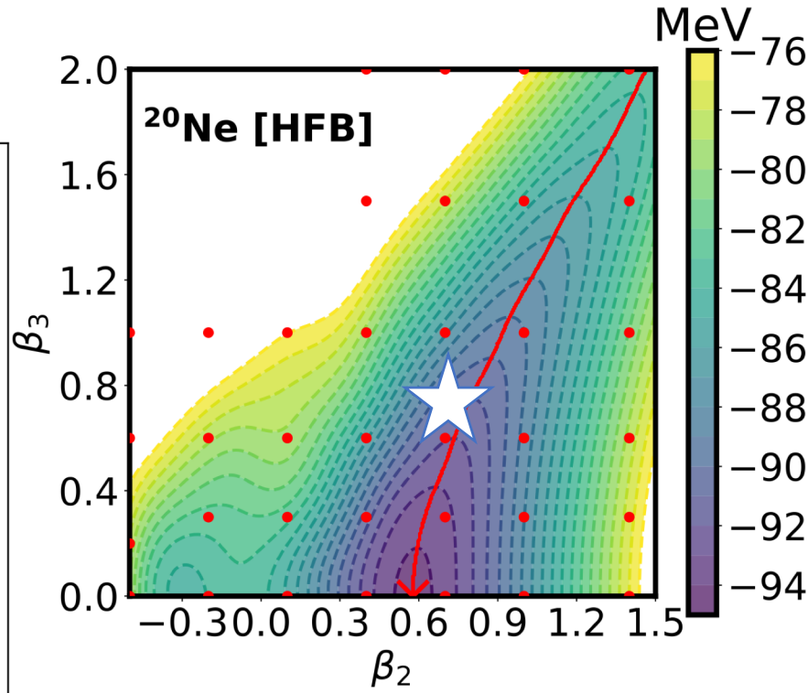
½+ and ½- parity doublet in ^{225}Ra differ by only 50keV

Explicit symmetry breaking as a tool

CCSD -149.43 MeV

CCD -147.79 MeV





M. Frosini et al, EPJA, **58**, 63 (2022)

Constrained HF:

$$\langle Q_{10} \rangle = 0$$

$$\langle Q_{30} \rangle = 50$$

Explicit symmetry breaking as a tool

$$H'(\vec{\lambda}) = H_{2b} - \sum_{i=1}^{n} \lambda_i Q_i$$

The coupled-cluster bi-variational energy functional:

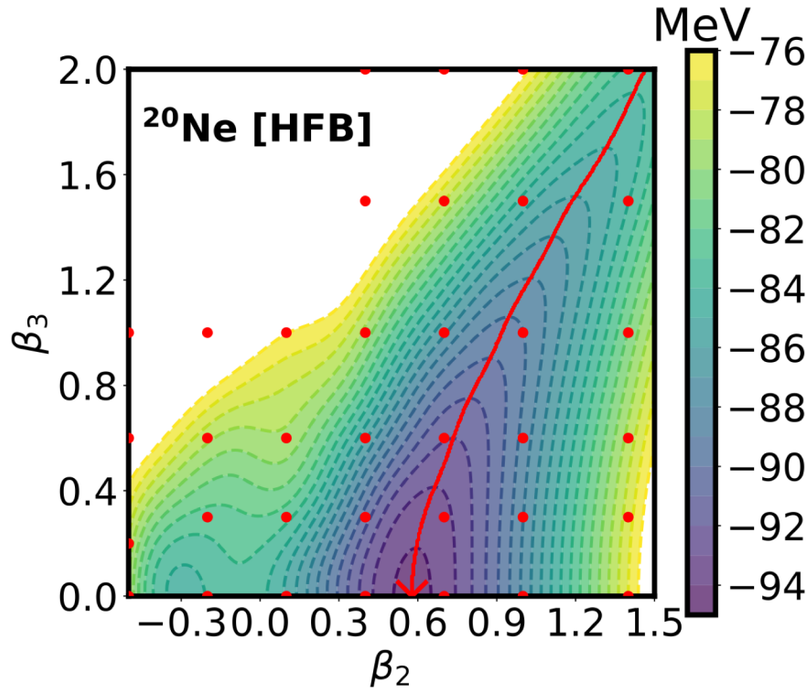
$$E'(T, \Lambda, \vec{\lambda}) = \langle \Phi_0 | (1 + \Lambda) \overline{H'}(\vec{\lambda}) | \Phi_0 \rangle$$

Finding the stationary solution implies:

$$\frac{\partial E'(T, \Lambda, \vec{\lambda})}{\partial T} = 0, \frac{\partial E'(T, \Lambda, \vec{\lambda})}{\partial \Lambda} = 0$$

Under the condition that the constraints are fulfilled:

$$\langle Q_{i0} \rangle = \langle \Phi_0 | (1 + \Lambda) \overline{Q}_{i0} | \Phi_0 \rangle = q_{i0}$$



M. Frosini et al, EPJA, **58**, 63 (2022)

With the solutions for $T, \Lambda, \vec{\lambda}$ we compute the energy:

$$E = \langle \Phi_0 | (1 + \Lambda) \overline{H}_{2b} | \Phi_0 \rangle \qquad E^{(J^\pi)} = \frac{\langle \Phi_0 | (1 + \Lambda) e^{-T} P^J P^\pi H_{2b} e^T | \Phi_0 \rangle}{\langle \Phi_0 | (1 + \Lambda) e^{-T} P^J P^\pi e^T | \Phi_0 \rangle}$$

Constrained sub-space Coupled-Cluster

$$H'(\lambda_1, \lambda_2, \lambda_3) = H_{2b} - \lambda_1 Q_1 - \lambda_2 Q_2 - \lambda_3 Q_3$$

Choose a small set of training points (snapshots)

Project the Hamiltonian onto sub-space of snapshots and diagonalize the generalized eigenvalue problem

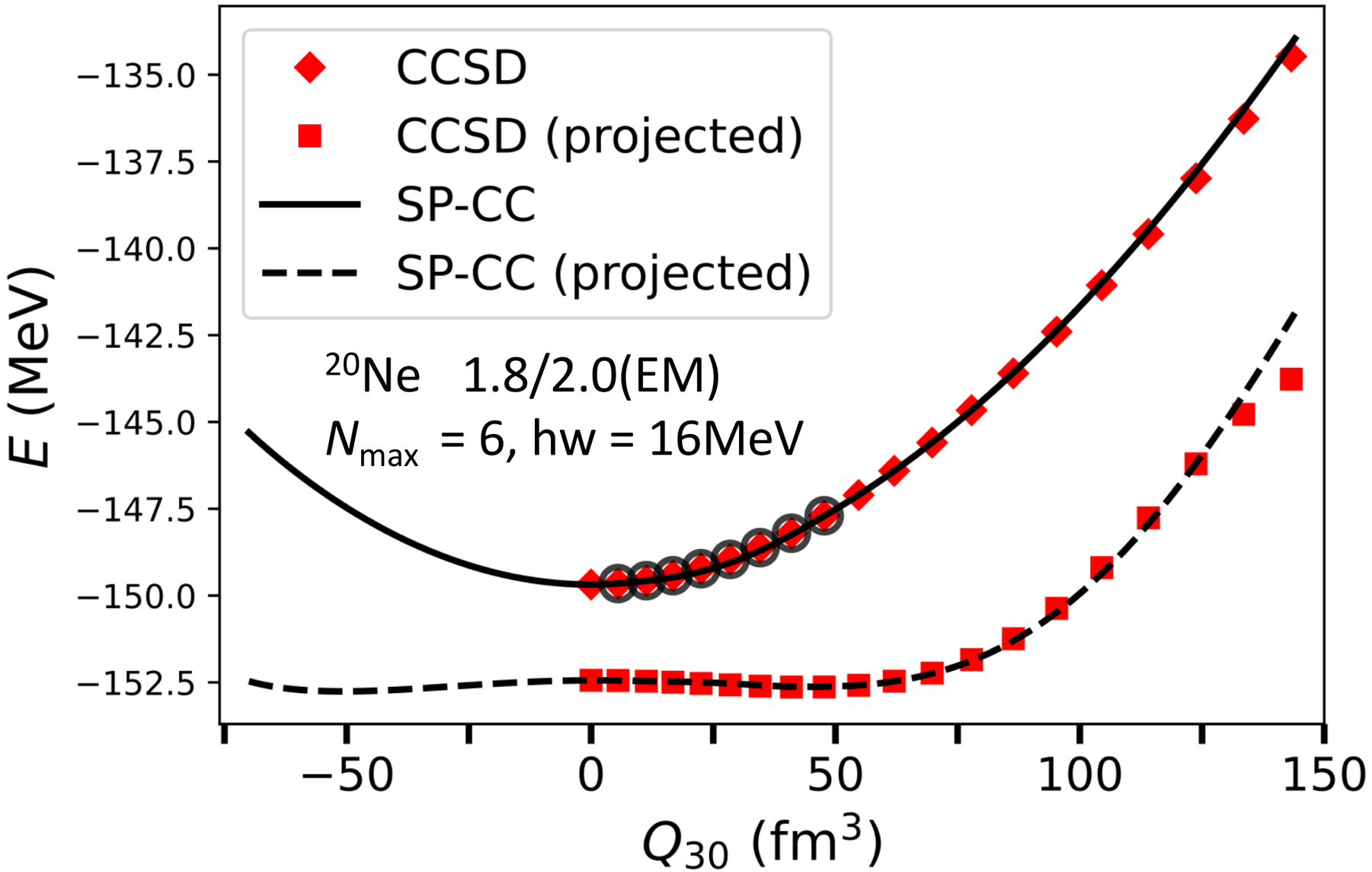
$$\left\{ \langle \Phi_0 | (1 + \Lambda_i) e^{-T_i}, \; e^{T_i} | \Phi_0 \rangle \right\}$$

Project $H_{2b}, Q_{i0}, H_{2b} P^{\pi} P^{J}$ onto sub-space

Solve the non-linear least-squares problem in the sub-space:

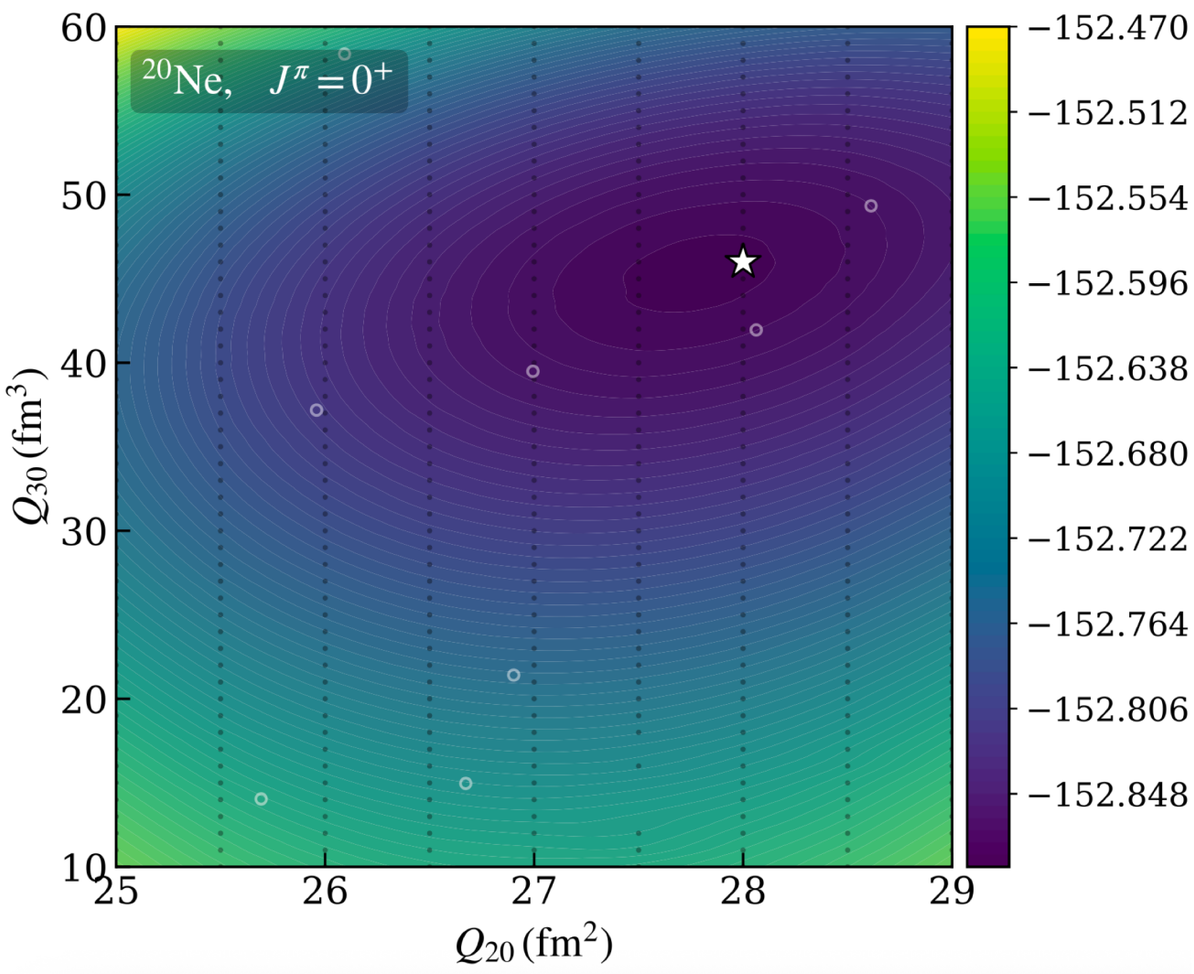
$$\min_{\vec{\lambda}} \left\{ \sum_{i=1}^{3} w_i (\langle Q_{i0}(\vec{\lambda}) \rangle - q_{i0})^2 \right\}.$$

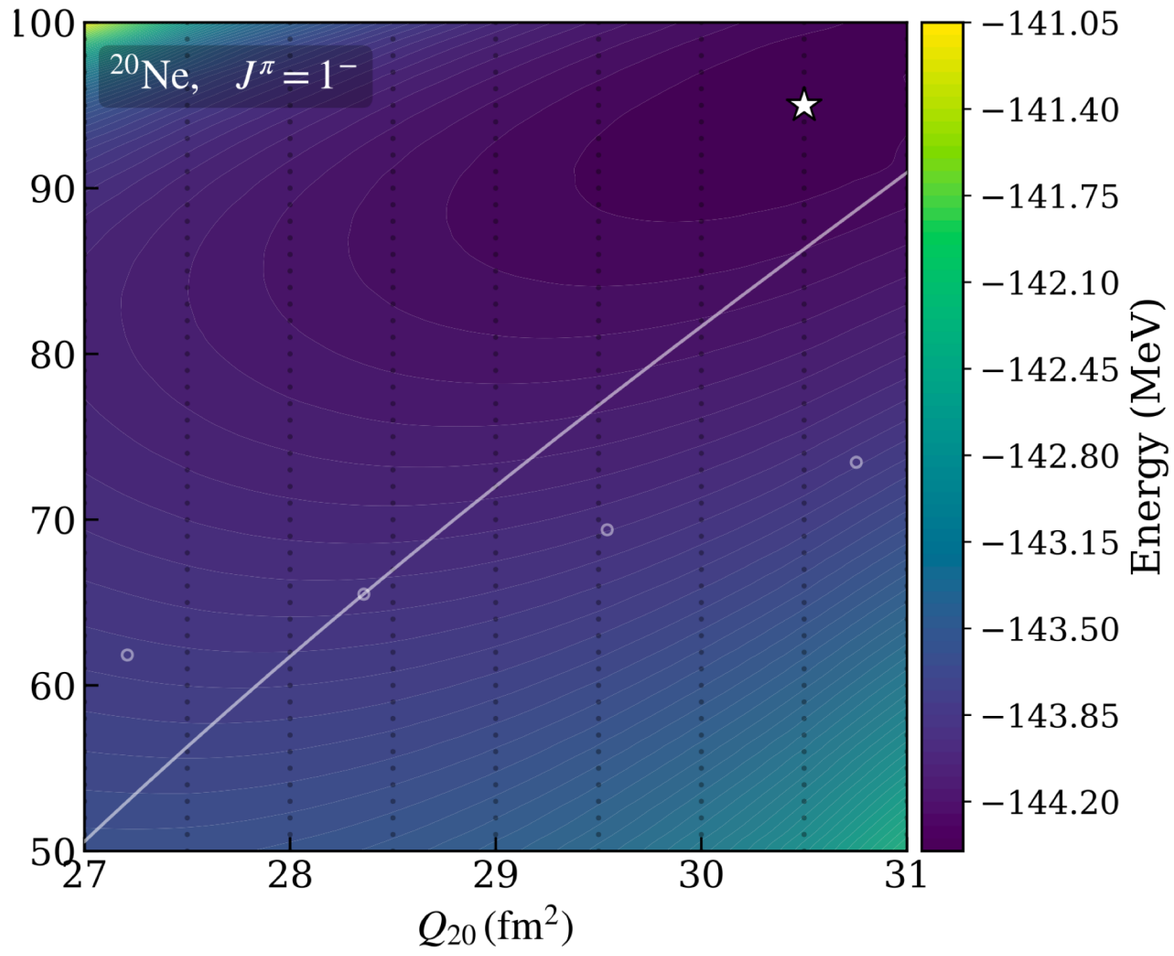
Constrained sub-space Coupled-Cluster



Constrained sub-space Coupled-Cluster

1.8/2.0(EM), N_{max} = 6, hw = 16MeV





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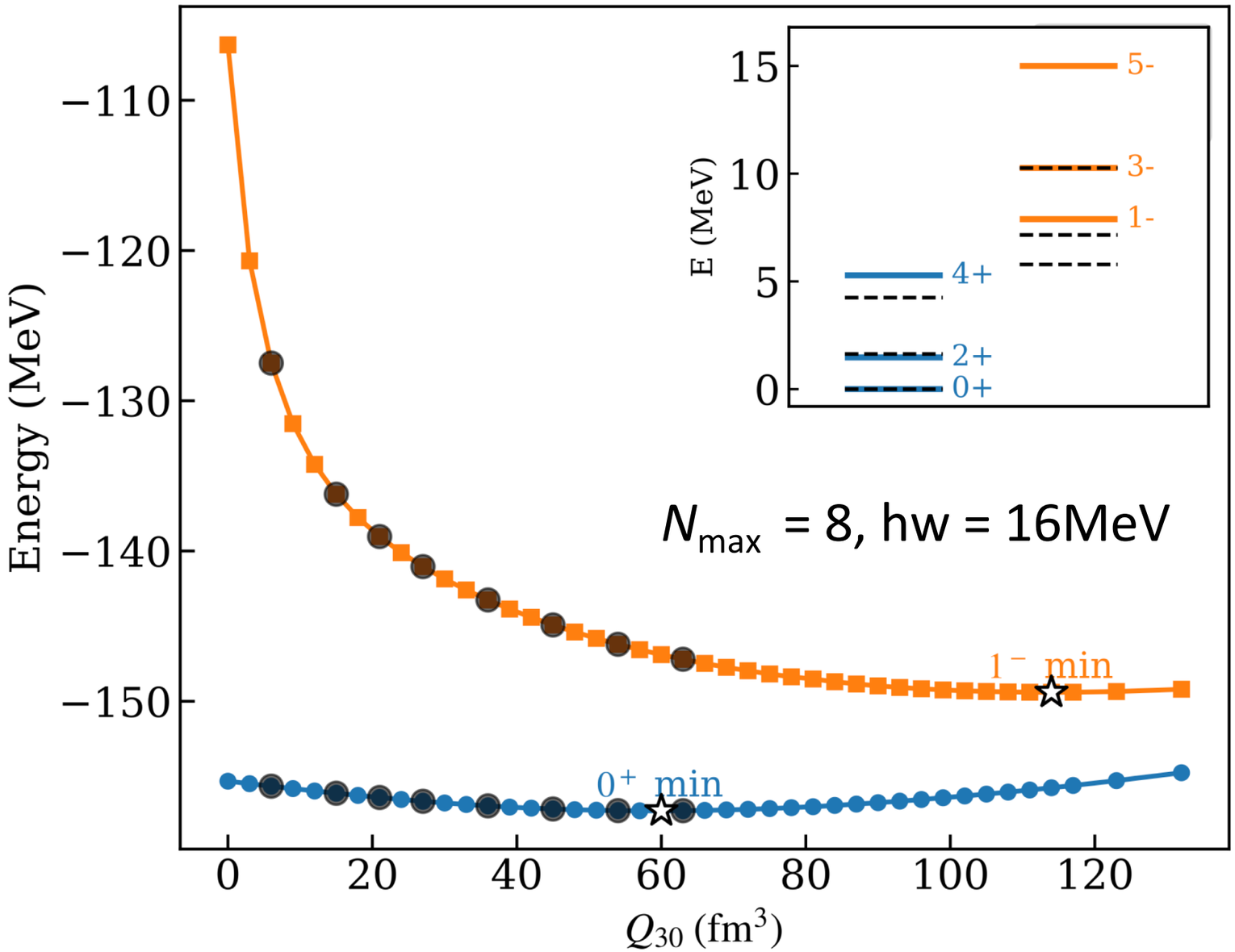

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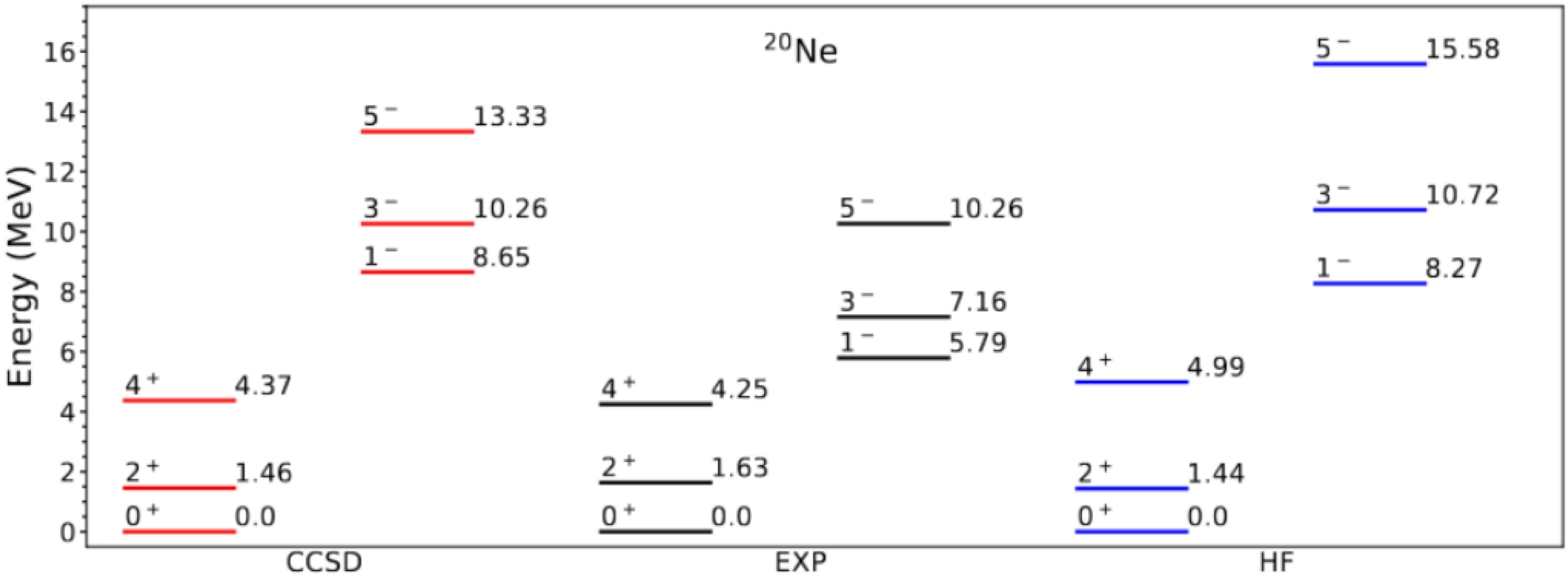

Summary

Breaking and restoring symmetries

Exploits separation of scale between collective and specific UV physics

Conceptually simple & computationally affordable

- Rotational bands well reproduced. Is the absence of superfluidity (which would increase moments of inertia) compensated by the too small radii???
- Much improved B(E2) values with no effective charges in ^{3x}Ne, ^{3x}Mg, ^{80}Zr
- Connected deformation to microscopic forces
- Constrained coupled-cluster for octupole deformed nuclei
- Dripline extends to 70Ca from a new chiral interaction