

Momentum of inertia of ground-state rotational bands in mid-mass nuclei: can one account for its increase with spin without explicitly breaking $U(1)$ symmetry?

Gaute Hagen

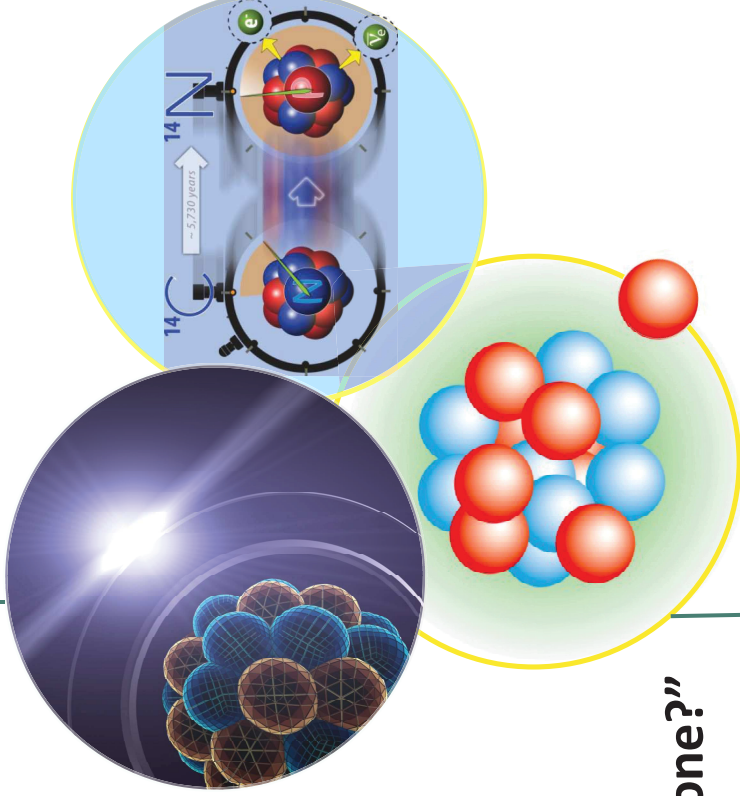
Oak Ridge National Laboratory

ESNT workshop: “Ab initio many-body calculations: where has the nuclear pairing gone?”

CEA/Saclay, May 15th, 2025



ENERGY
NUCLEI
Nuclear Computational Low-Energy Initiative



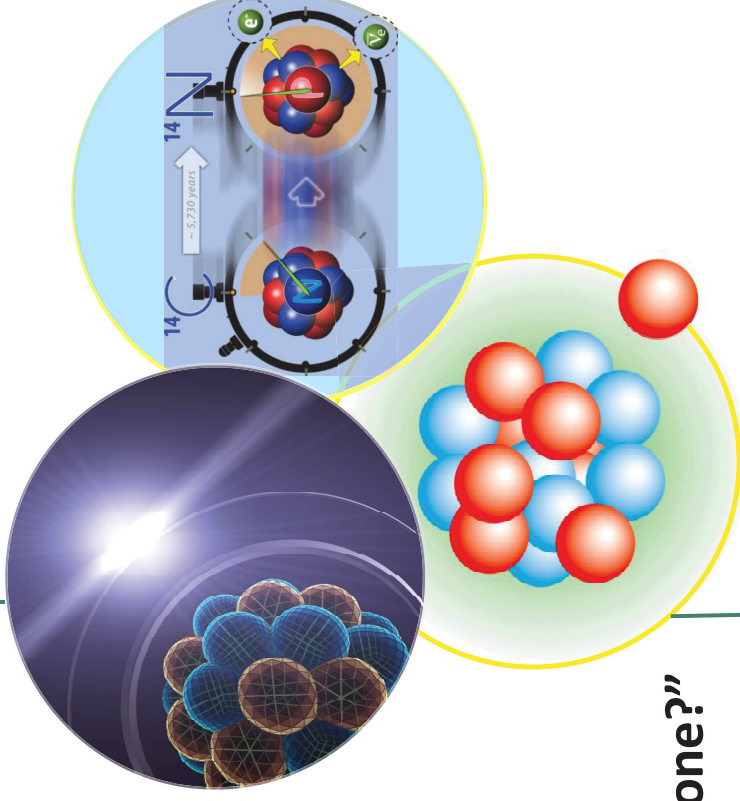
Coupled-cluster computation of deformed nuclei

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ESNT workshop: “Ab initio many-body
calculations: where has the nuclear pairing gone?”

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Collaborators

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Gustav Jansen, **Thomas Papenbrock**

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@ LSU: **Zhonghao Sun**

@ Chalmers: **A. Ekström**, **C. Forssén**, **Alberto Scalesi**

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

@ WUSTL: **Sam Novario**

The role of pairing on rotational bands

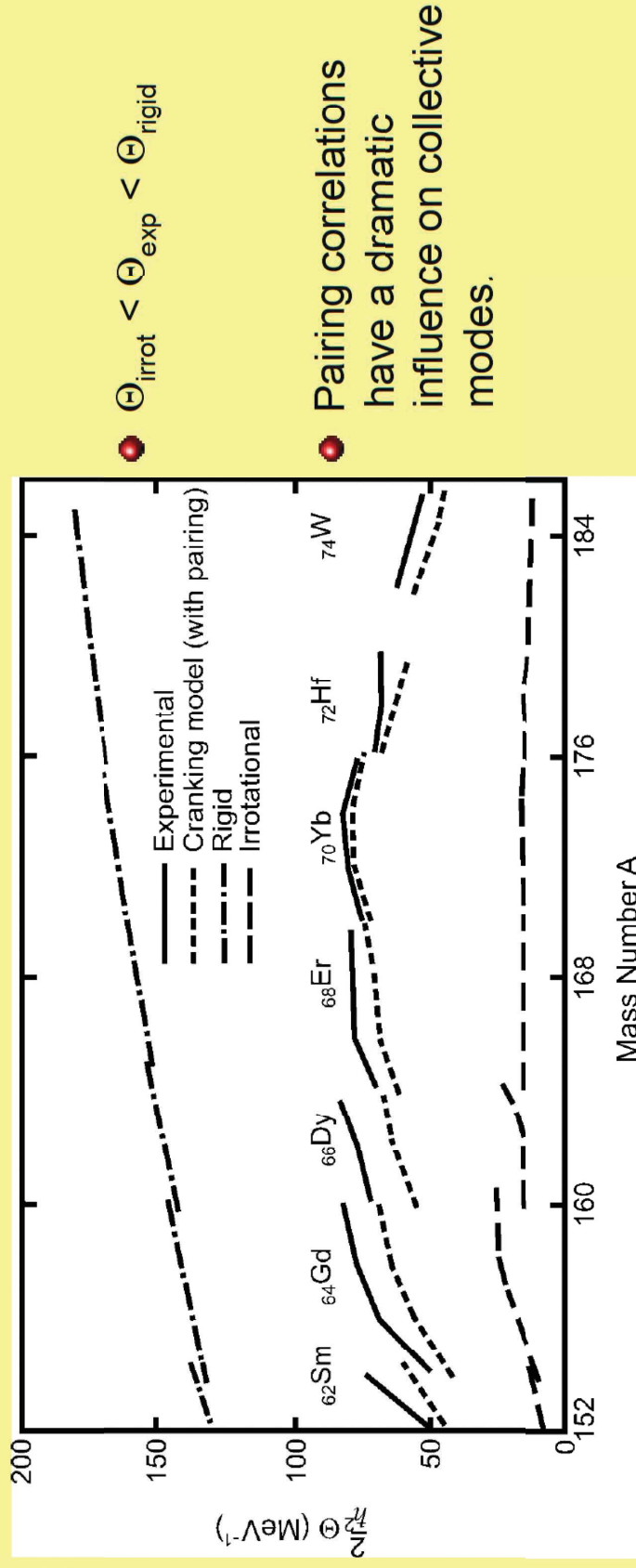
(v) Moment of inertia: extracted from level spacing in rotational bands

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

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

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?

Multiscale physics of nuclei from ab-initio methods

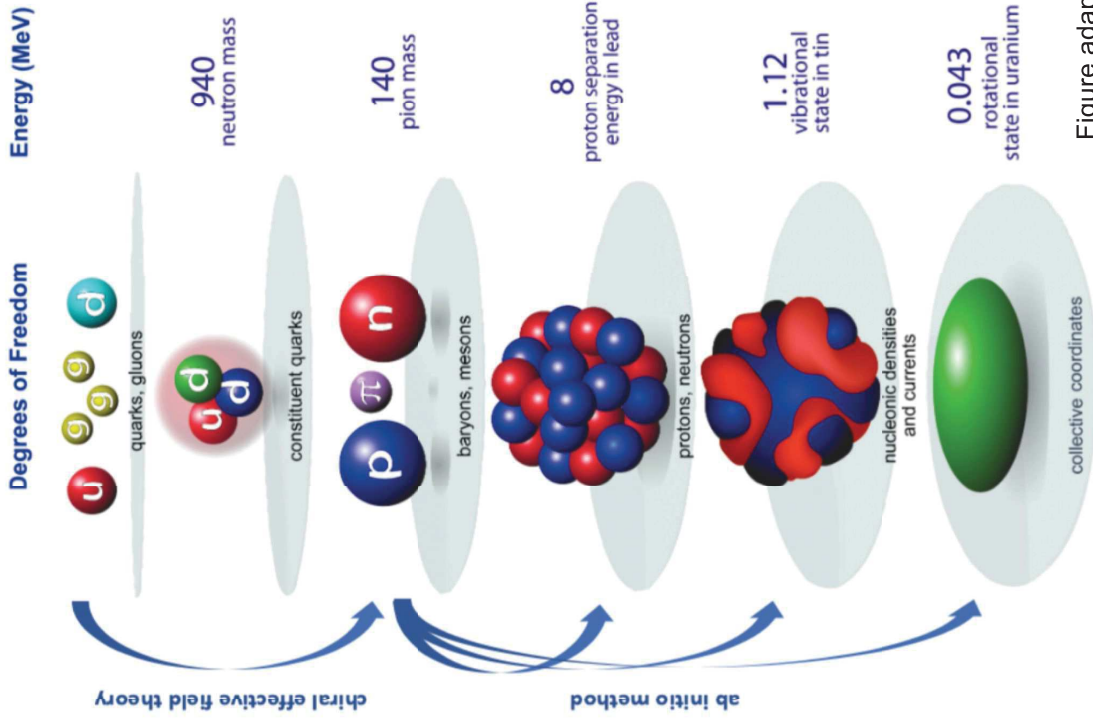


Figure adapted from Bertsch, Dean, Nazarewicz, SciDAC review (2007)

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

Solving the quantum many-nucleon problem

An exponentially hard problem to solve!

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

1.1 exaflops



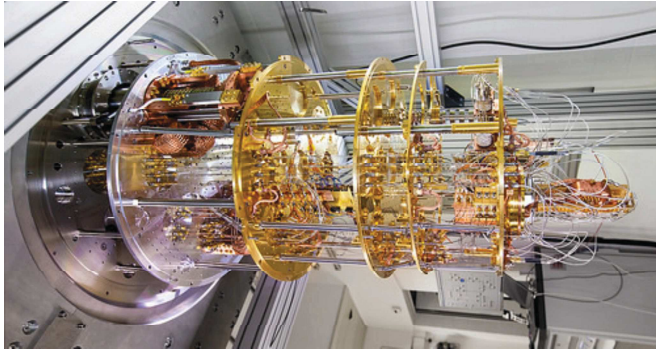
Systematically improvable approaches
with controlled approximations:
Coupled-cluster, IMSRG, Gorkov, SCGF,...



Emulators?



IBM Q Experience



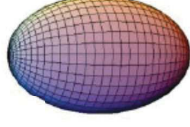
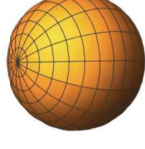
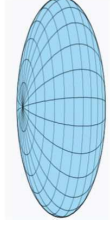
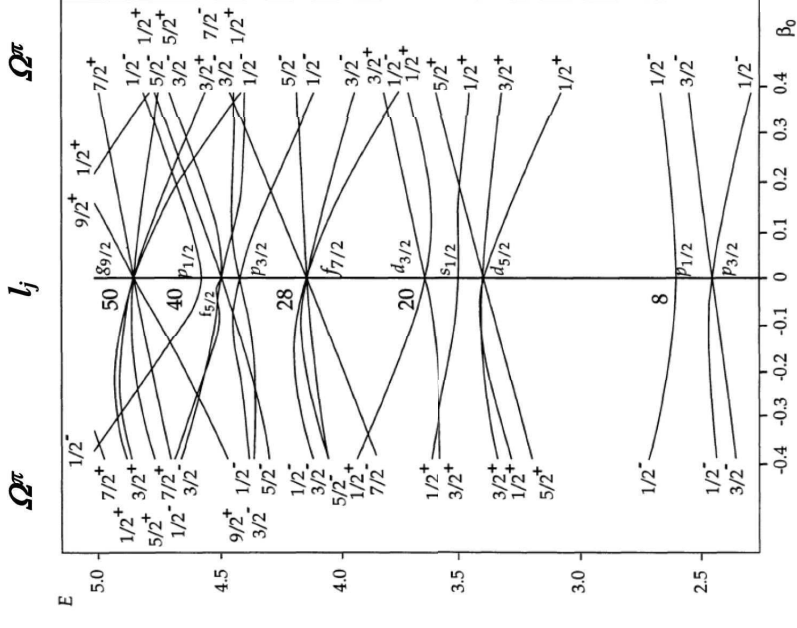
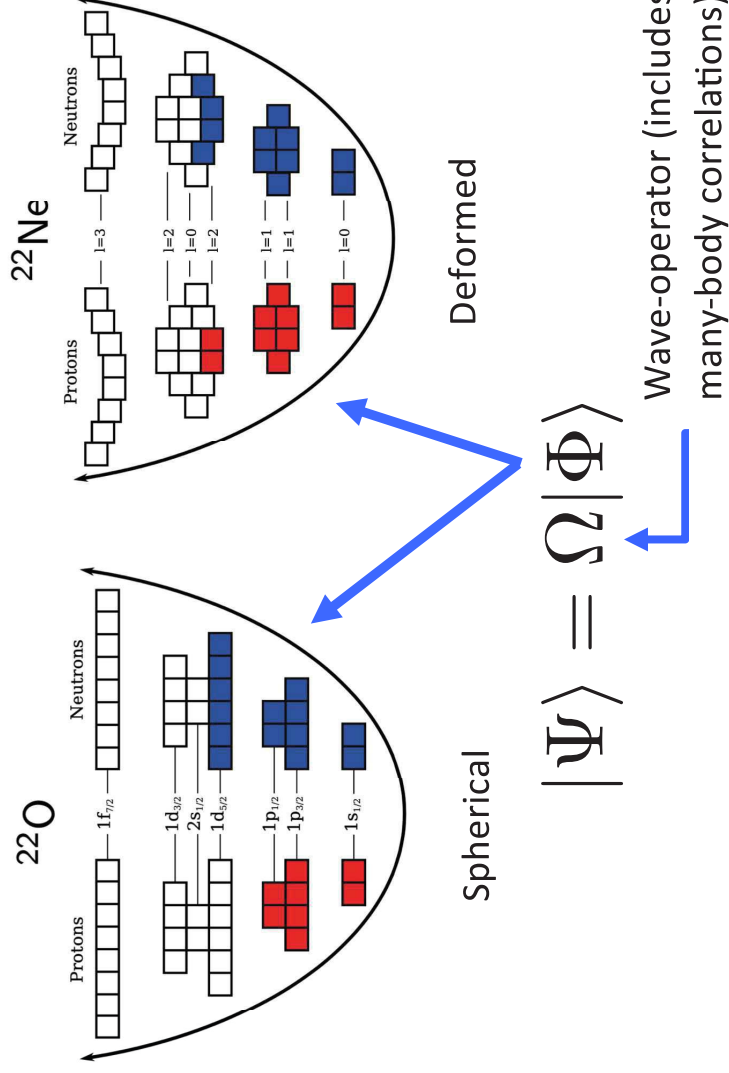
Fault tolerant quantum computing??

Coupled-cluster computations of nuclei

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

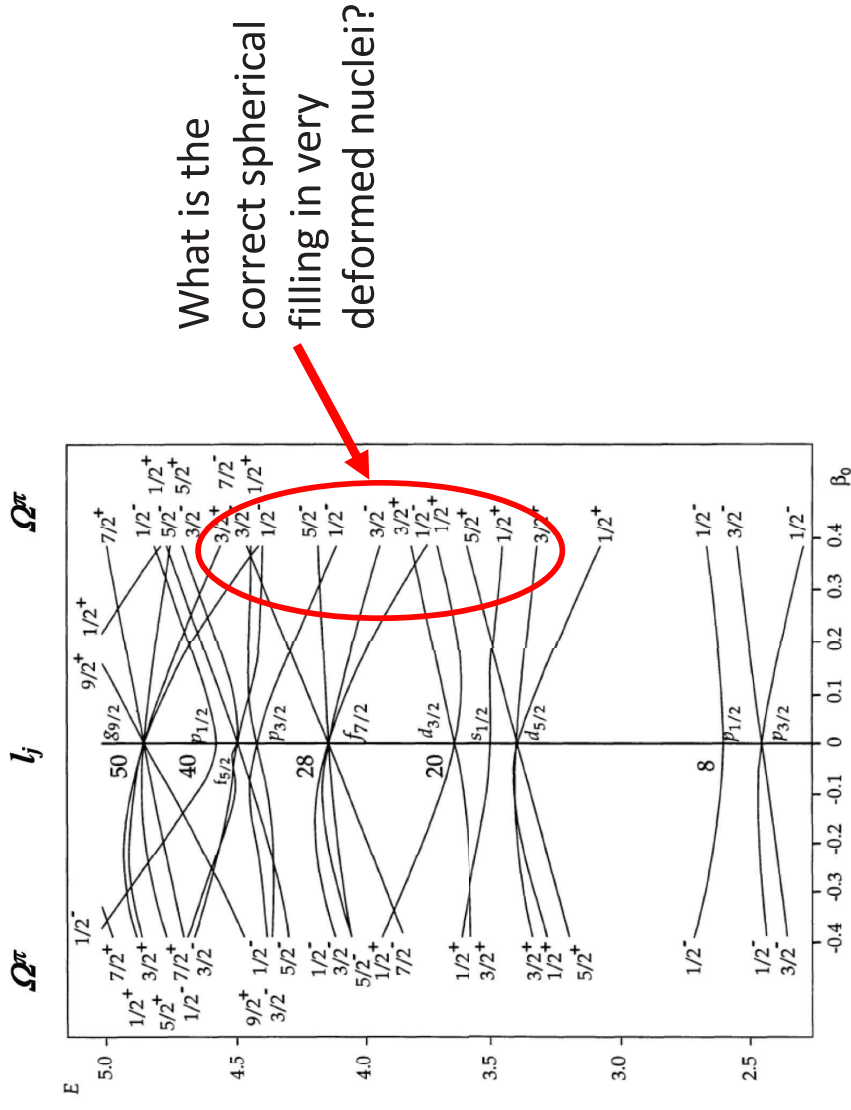
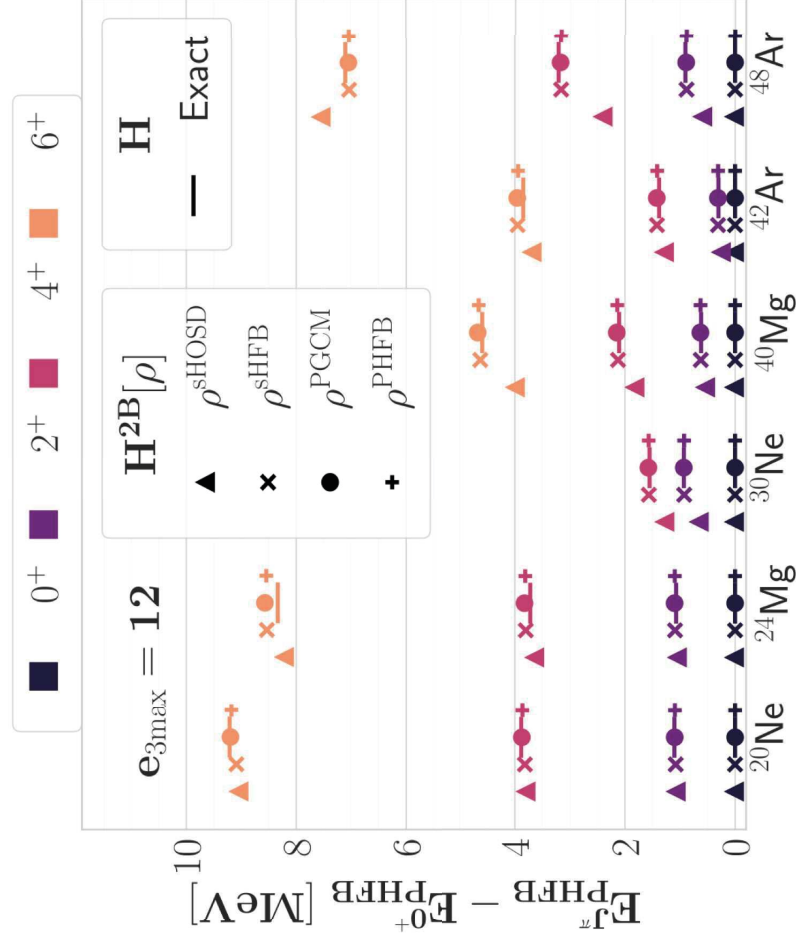
$$H = T - T_{\text{CoM}} + V_{\text{NN}} + V_{3\text{N}}$$

- Informs us about emergent breaking of symmetries



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

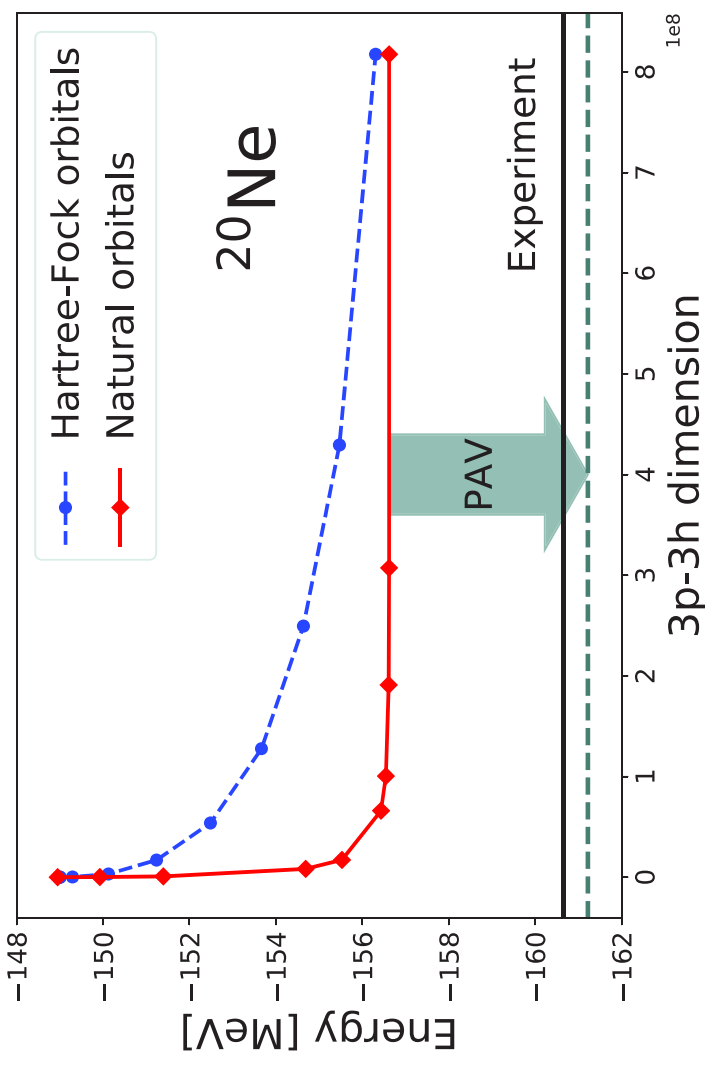
$$|\Psi\rangle = \Omega|\Phi_0\rangle = e^T|\Phi_0\rangle$$

$$T = T_1 + T_2 + \dots$$

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

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

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



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

Total energy:

Convergence of coupled-cluster method

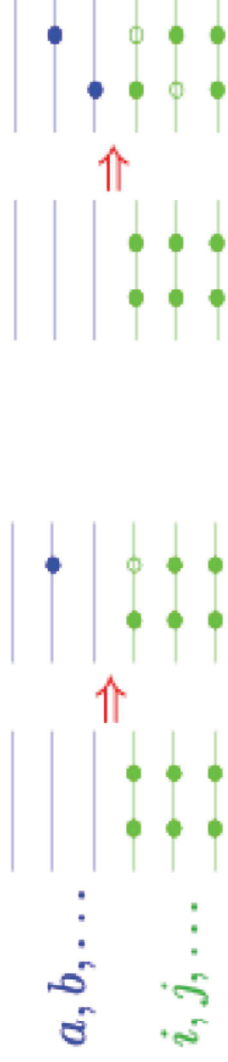
$$\begin{aligned}
 C_1 &= T_1, \\
 C_2 &= T_2 + \frac{1}{2}T_1^2, \\
 C_3 &= T_3 + T_1T_2 + \frac{T_1^3}{3!}, \\
 C_4 &= T_4 + \frac{T_2^2}{2} + T_1T_3 + \frac{T_1^2T_2}{2} + \frac{T_1^4}{4!}, \\
 &\vdots,
 \end{aligned}$$

Exact CI:

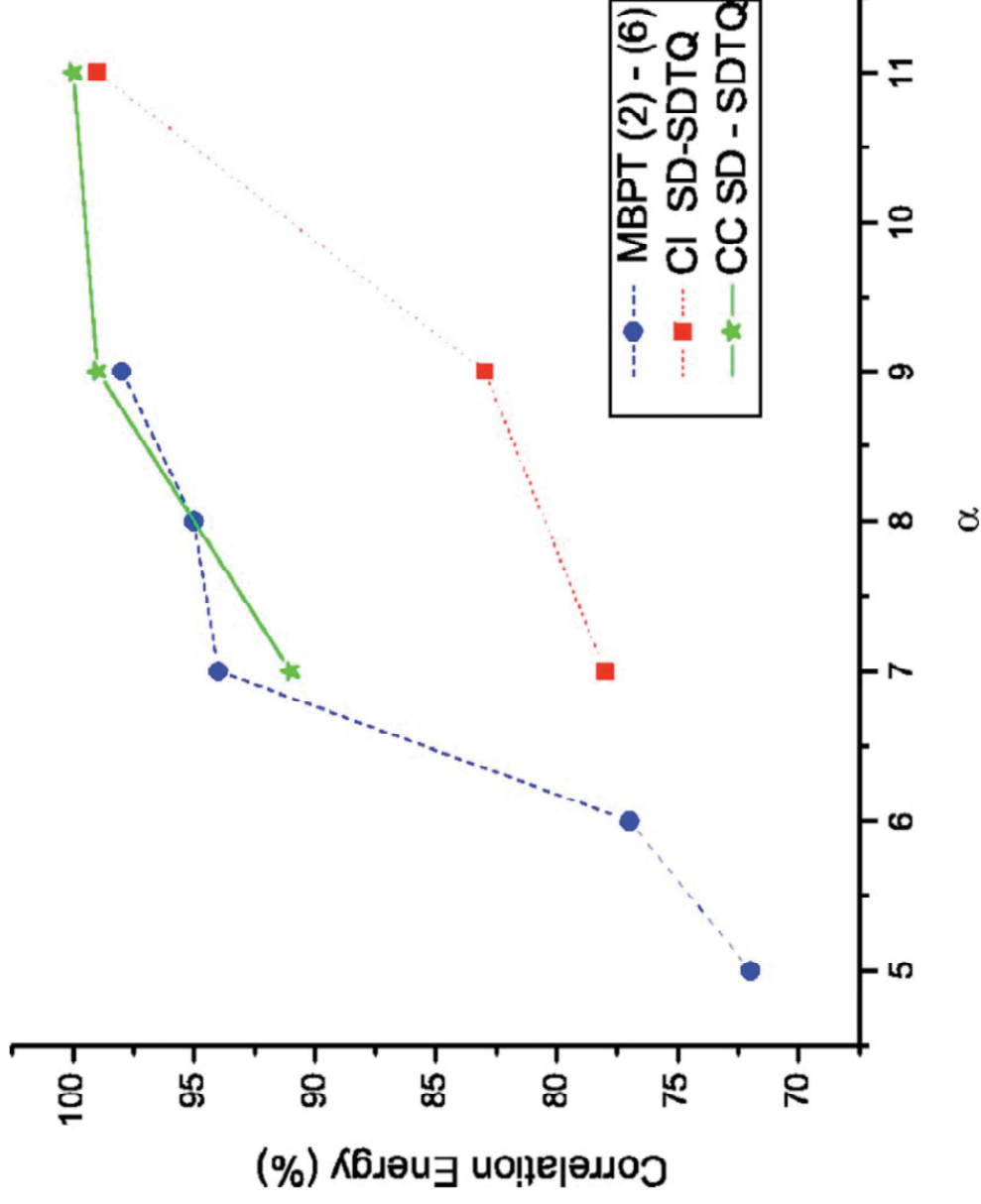
$$|\Psi\rangle = \Omega|\Phi\rangle = \left(1 + \sum_{i=1}^A C_i\right)|\Phi\rangle$$

- 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 $n_o^4 n_u^6$)

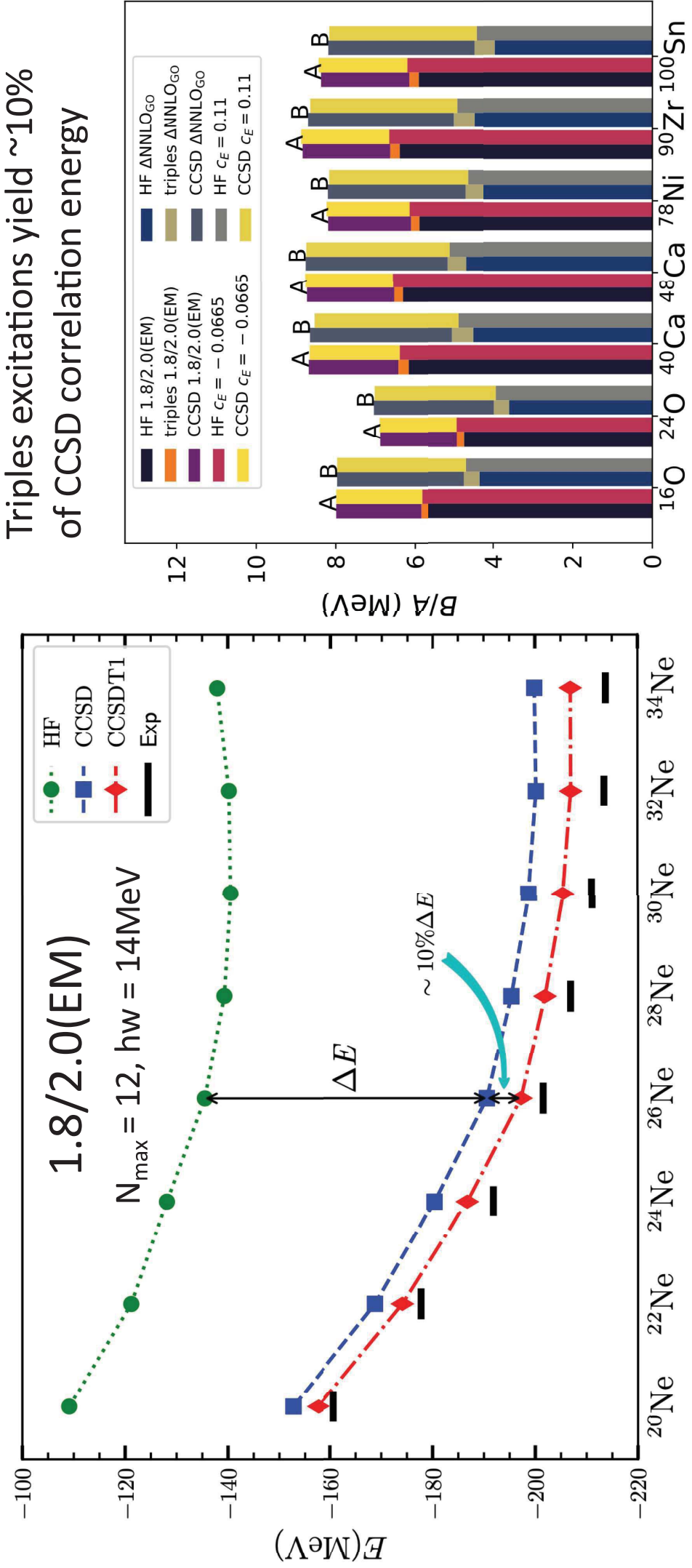
Correlations are exponentiated 1p-1h and 2p-2h excitations. Part of Ap-Ah excitations included!



Convergence of coupled-cluster method



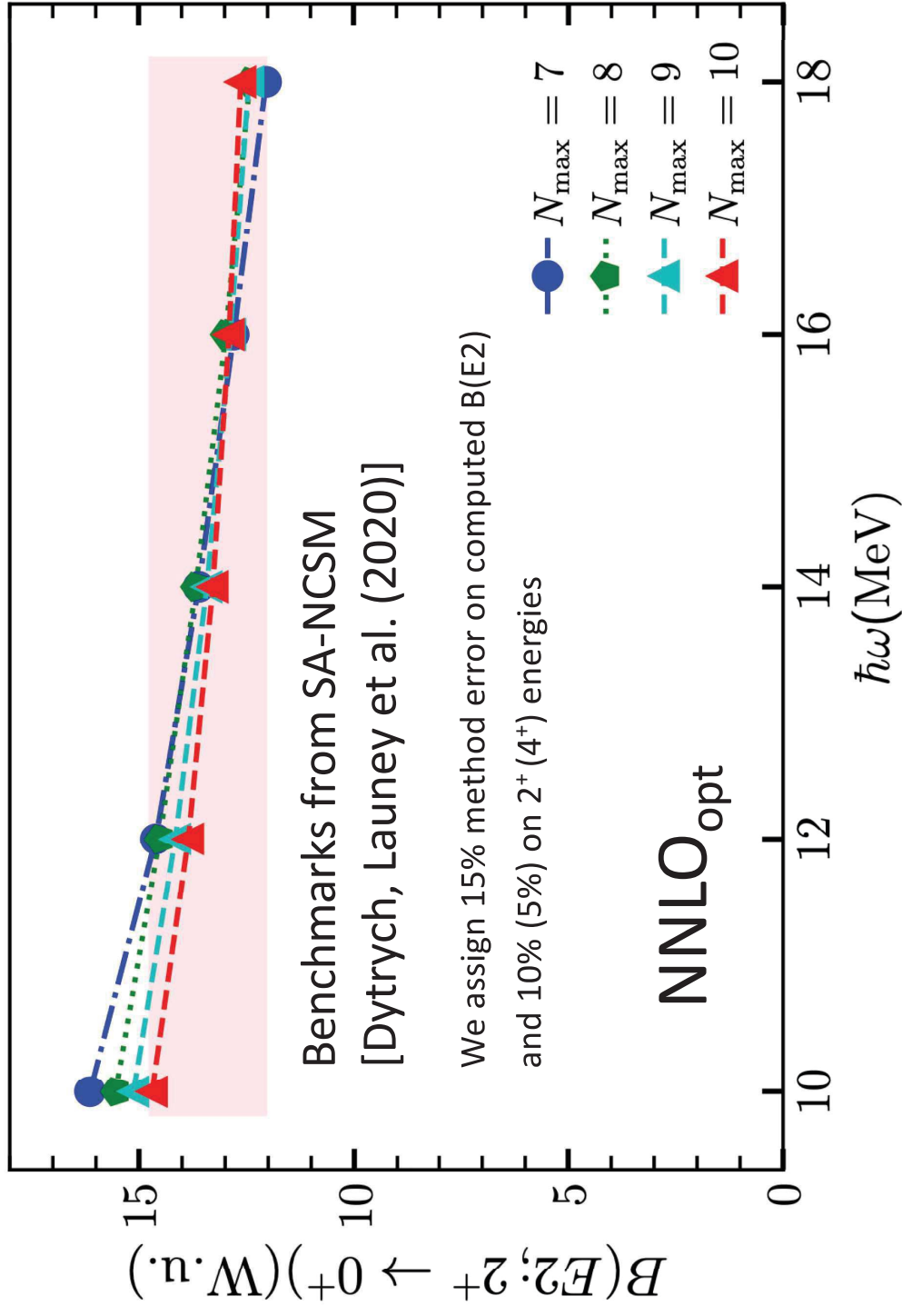
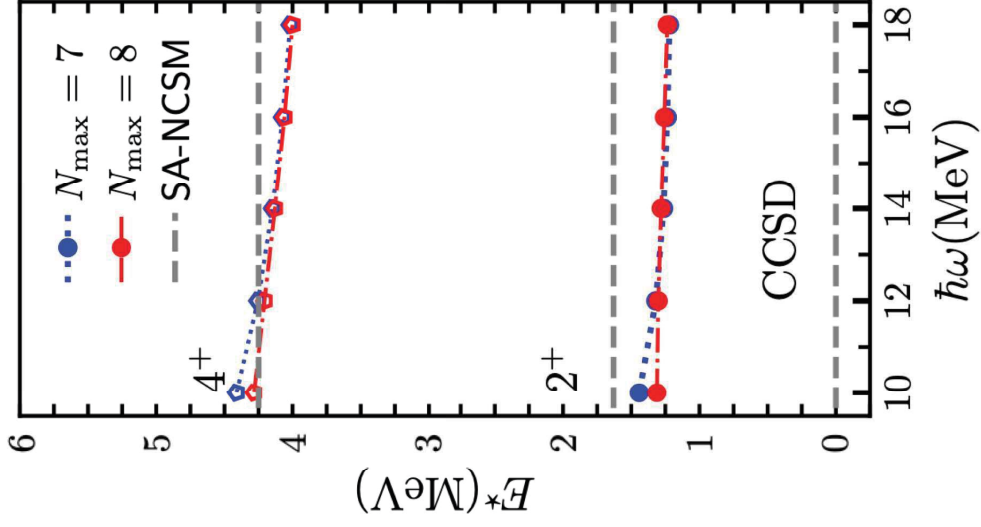
Convergence of coupled-cluster method



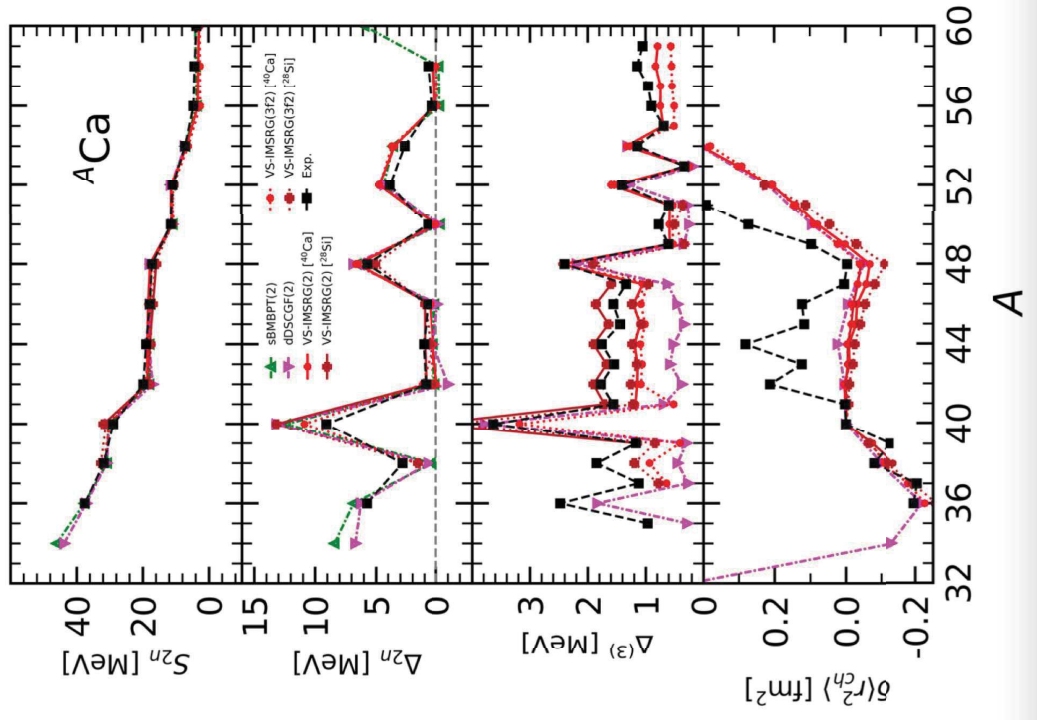
Zhonghao Sun et al, Phys. Rev. X **15**, 011028 (2025)

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

Benchmarks with SA-NCSM in ^{20}Ne



Where is the pairing gone?

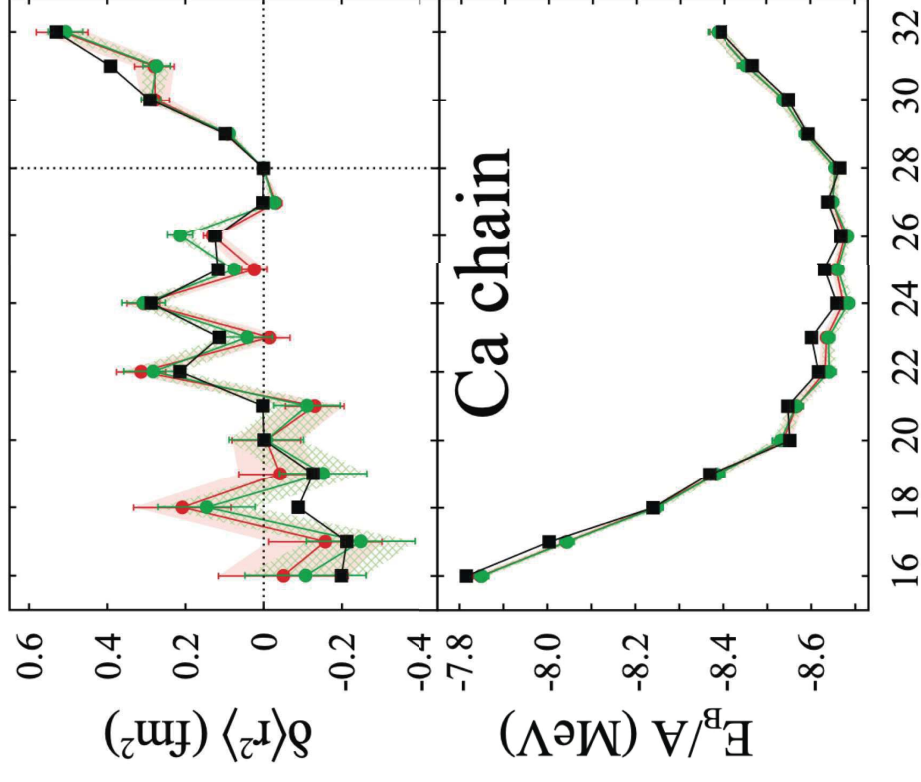
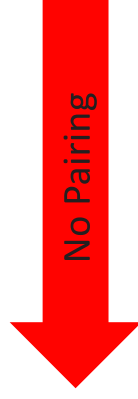


Fayans EDF
(density dependent
pairing functional)



Ab initio computations
based on chiral EFT
interactions

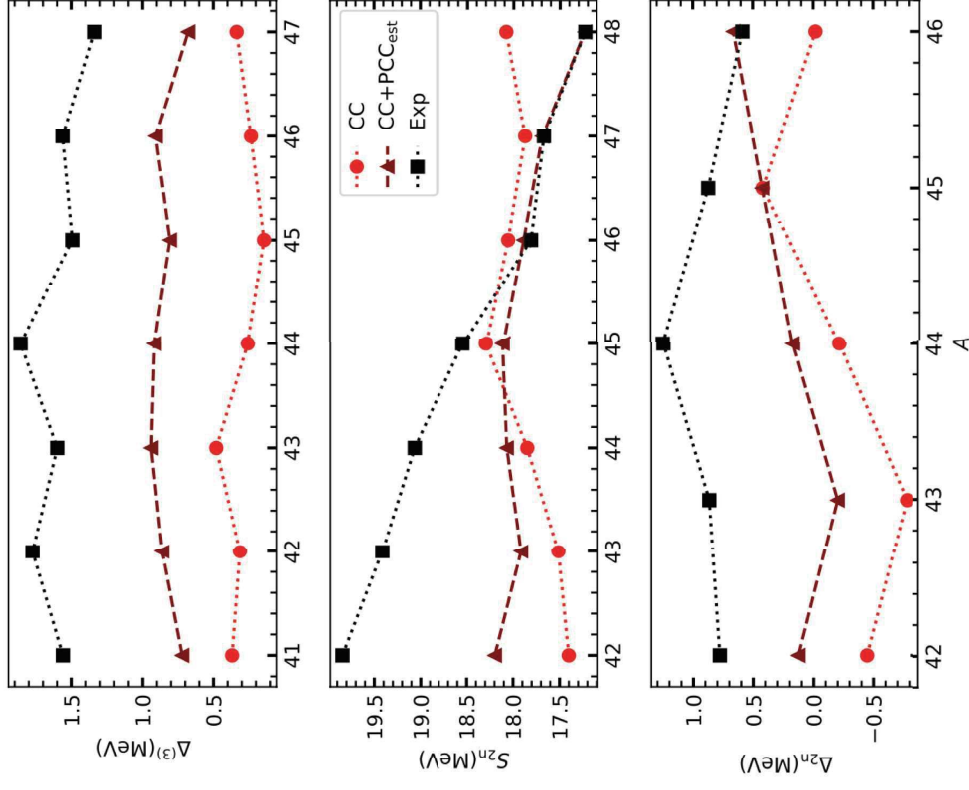
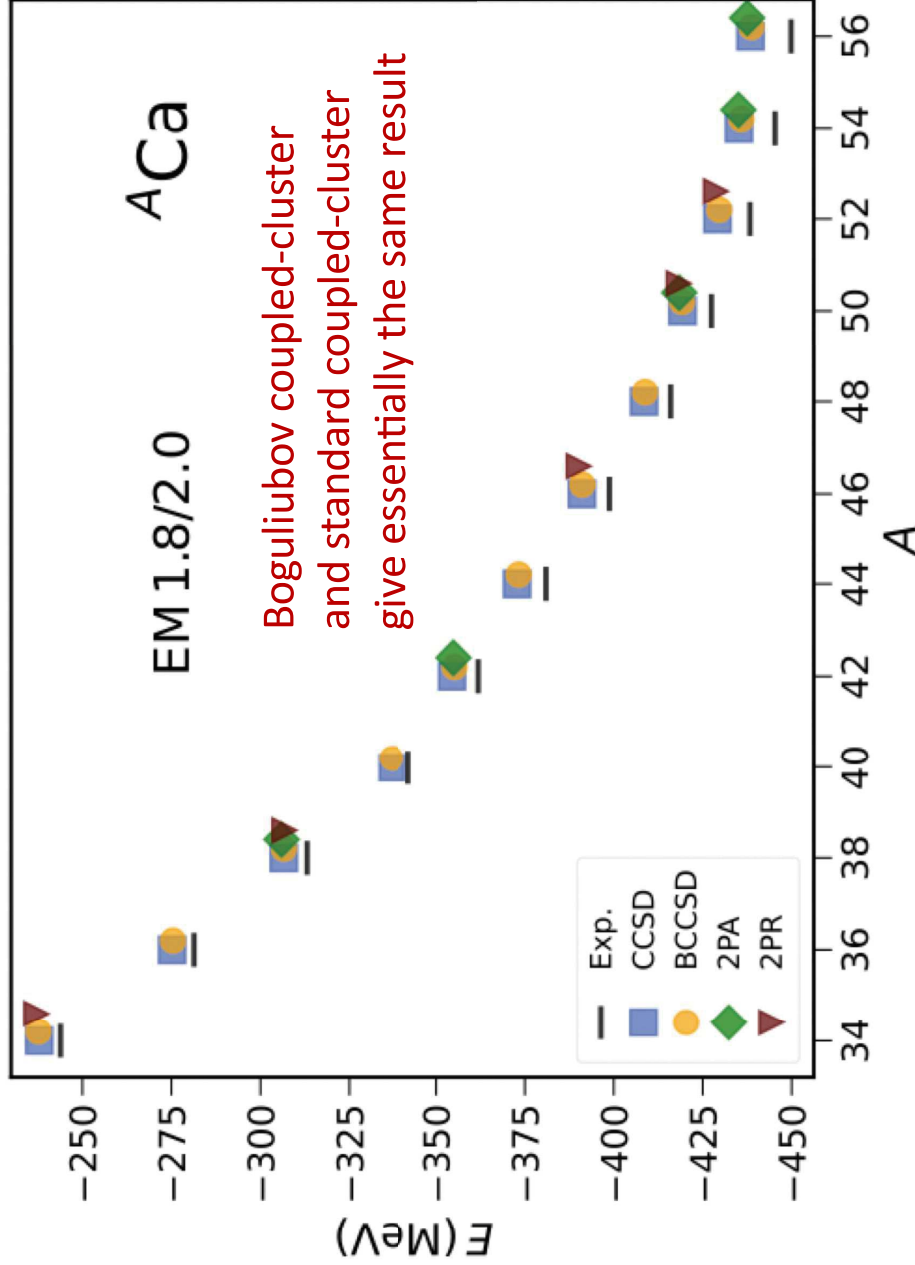
A. Scalesi, et al Eur. Phys. J. A 60,
209 (2024).



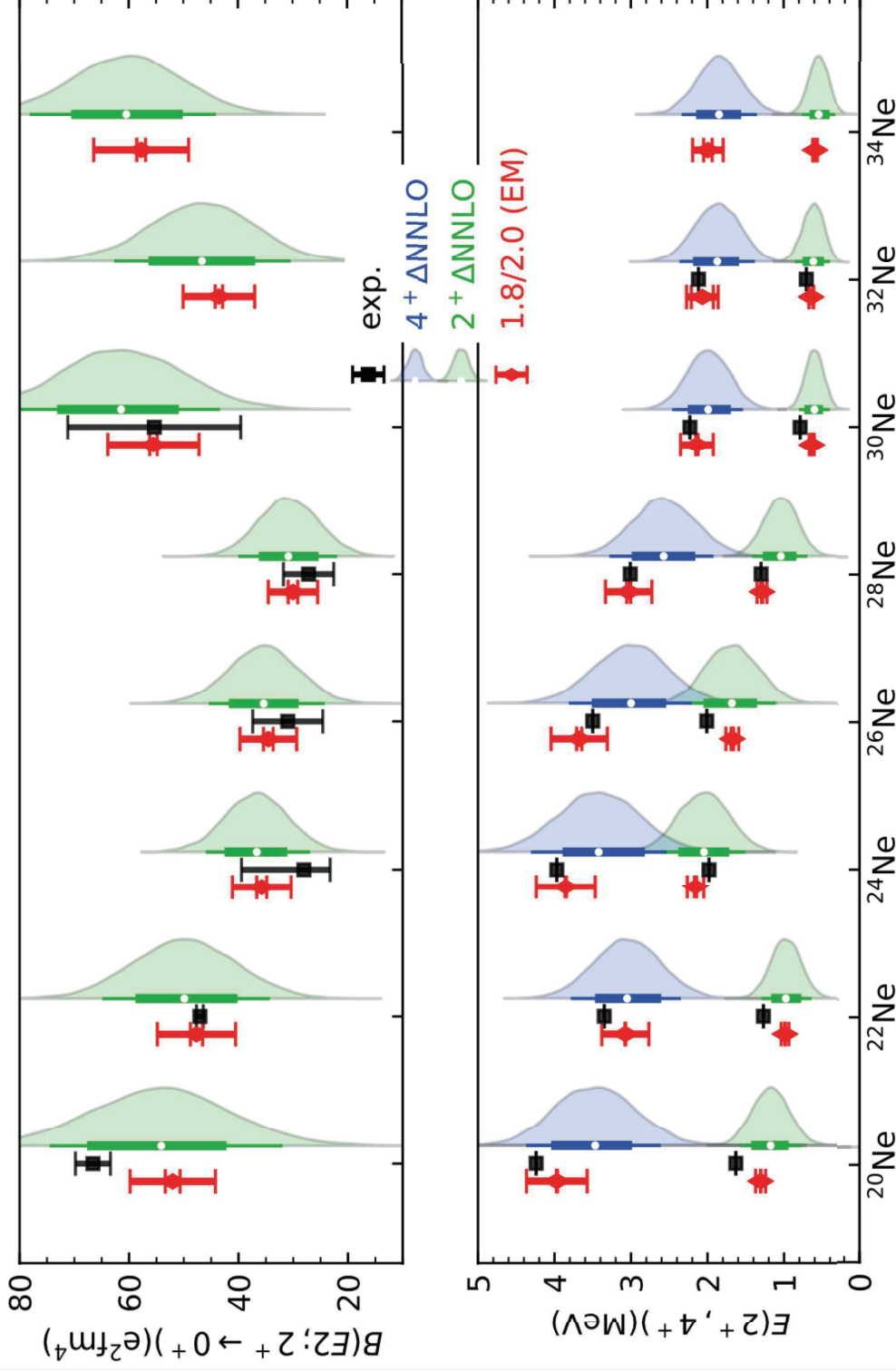
P-G Reinhard et al, J. Phys. G 51, 105101 (2024)

A. Scalesi et al, unpublished (2025)

Where is the pairing gone?



Pairing puzzle for ab initio rotational bands



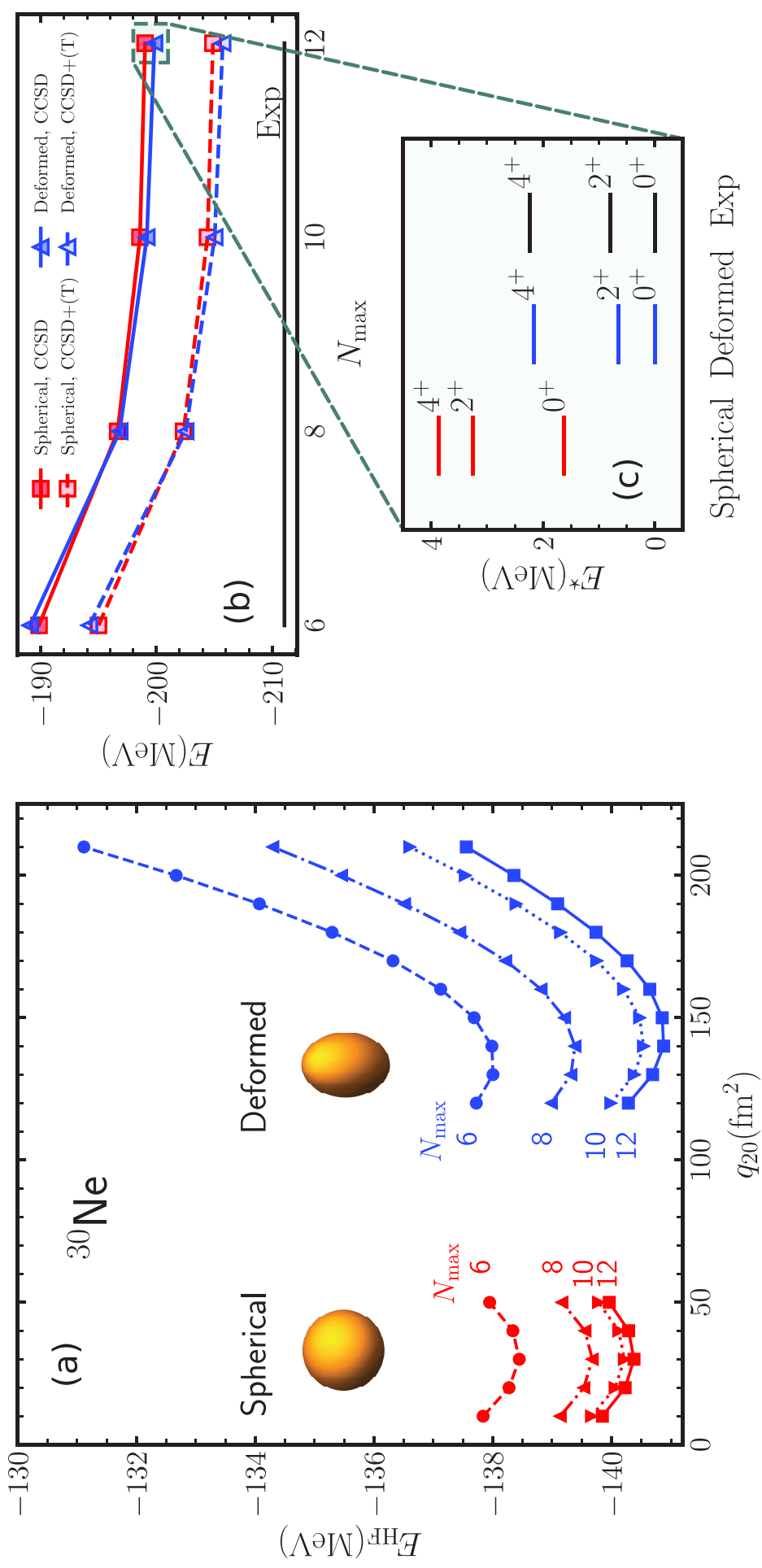
- 1.8/2.0 (EM) has too small radii
- Moment of inertia too small
 - Rotational bands should have too large spacings compared to data

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???

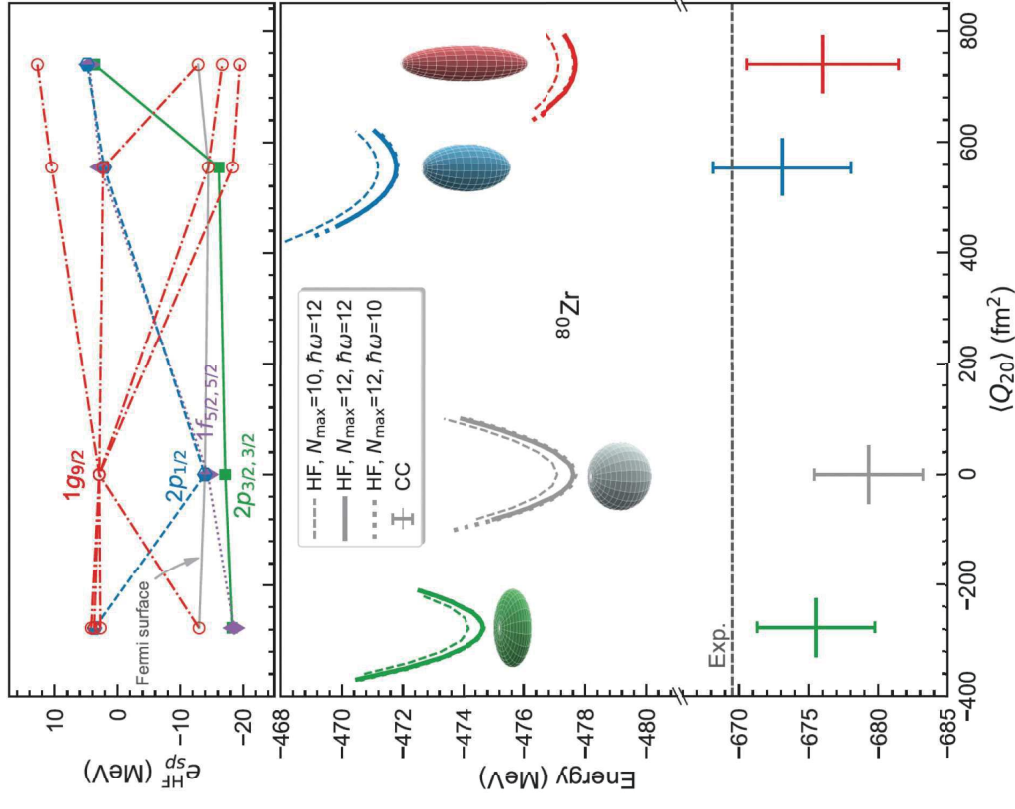
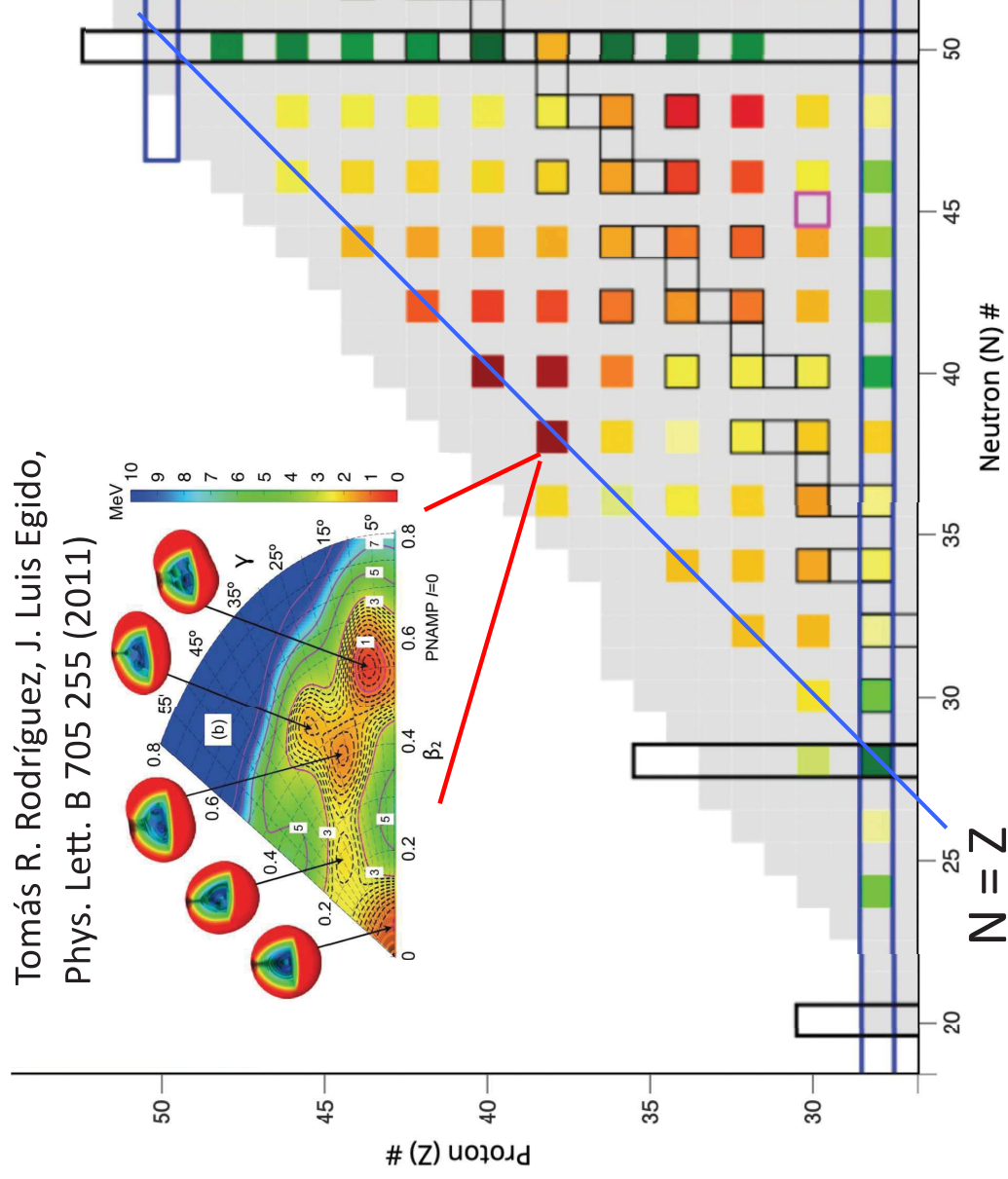
Ensemble of delta-full interactions from recent study of ^{28}O
Y. Kondo et al.,
Nature **620**, 965–970 (2023)

Pairing puzzle for ab initio rotational bands



Strongly deformed nuclei around ^{80}Zr

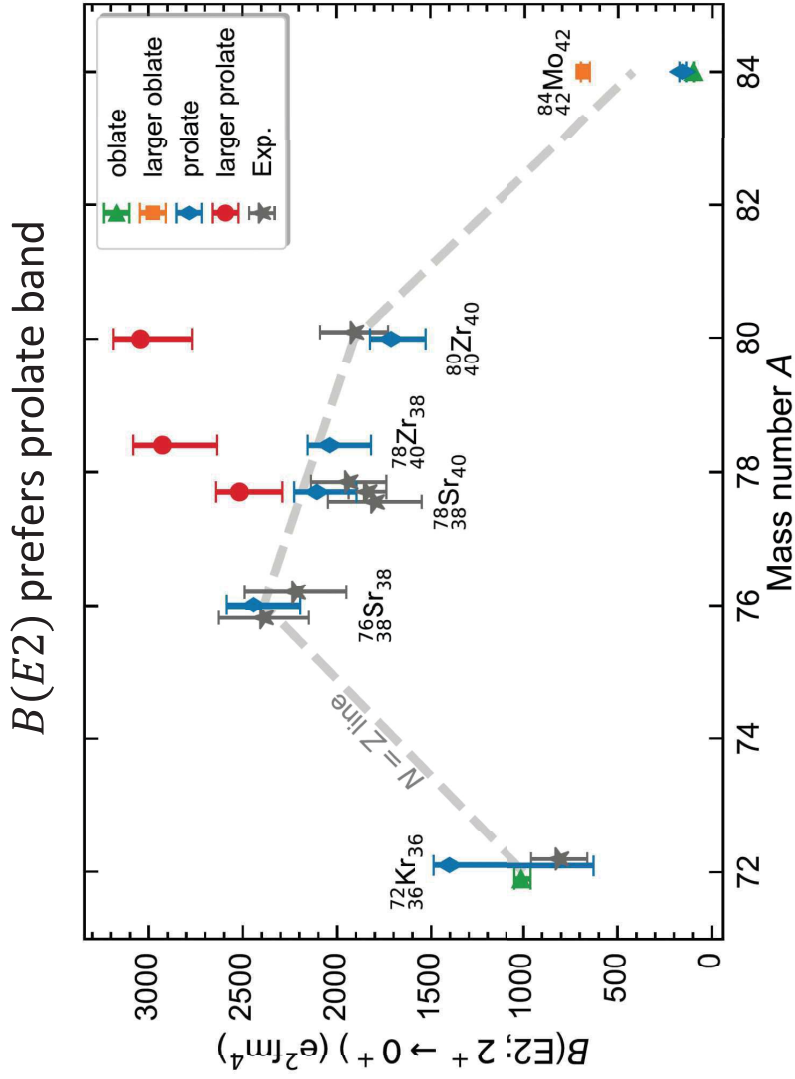
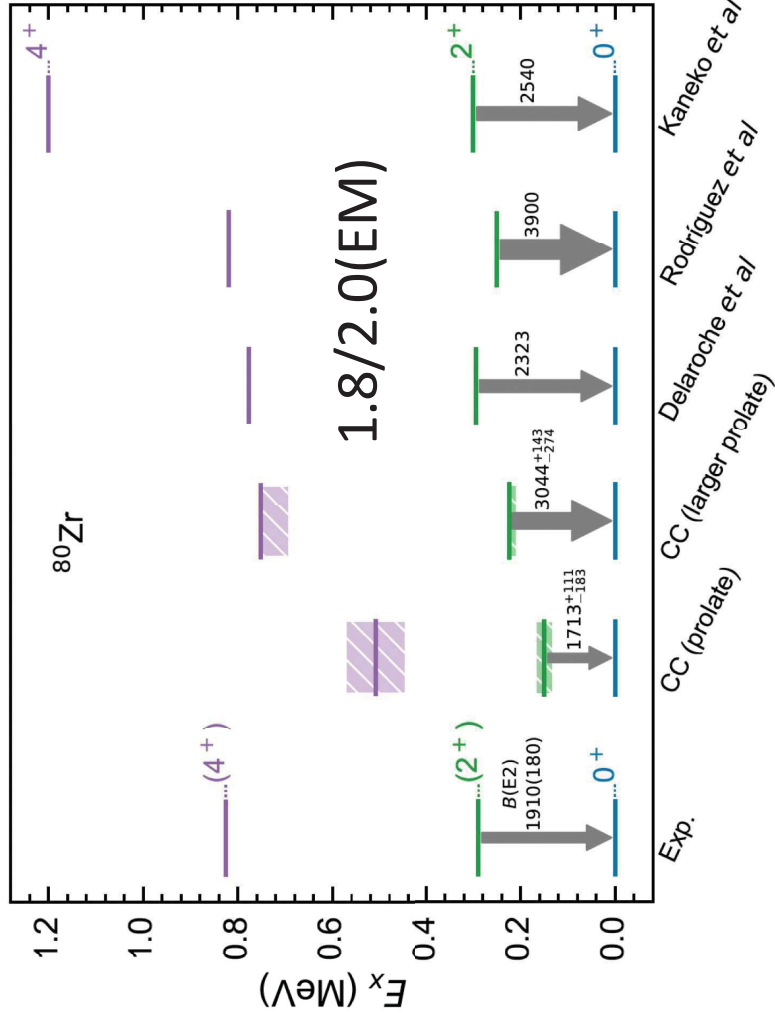
Tomás R. Rodríguez, J. Luis Egido,
Phys. Lett. B 705 255 (2011)



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

Coupled-cluster computations of strongly deformed nuclei around ^{80}Zr

Spectrum prefers larger prolate shape

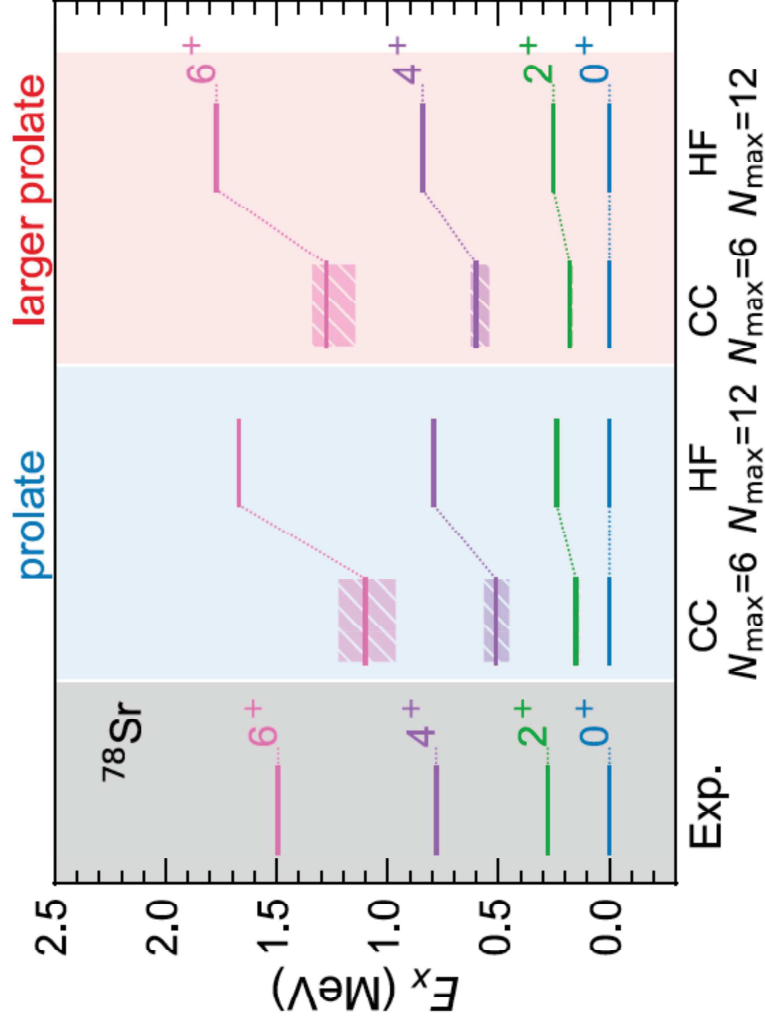


Baishan Hu, Zhonghao Sun, G. Hagen, T. Papenbrock. Phys. Rev. C **110**, L011302 (2024)

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

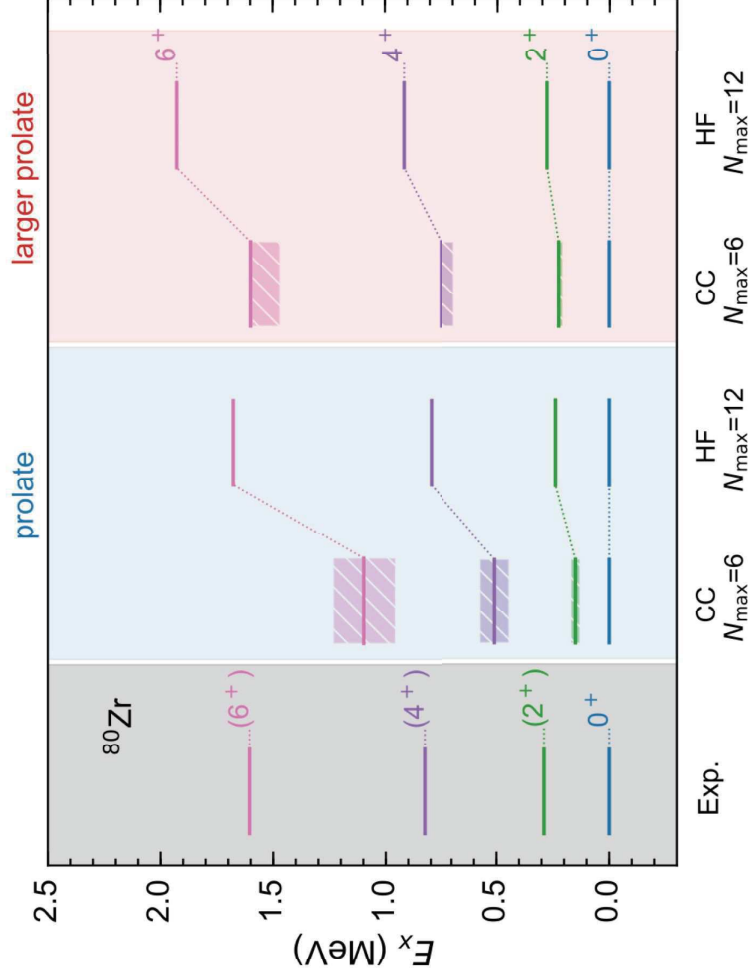


Lack of rotational stretching in coupled-cluster with projection after variation
[Hu, Sun, Hagen, Papenbrock, Phys Rev C (2024)]

Ab initio rotational stretching

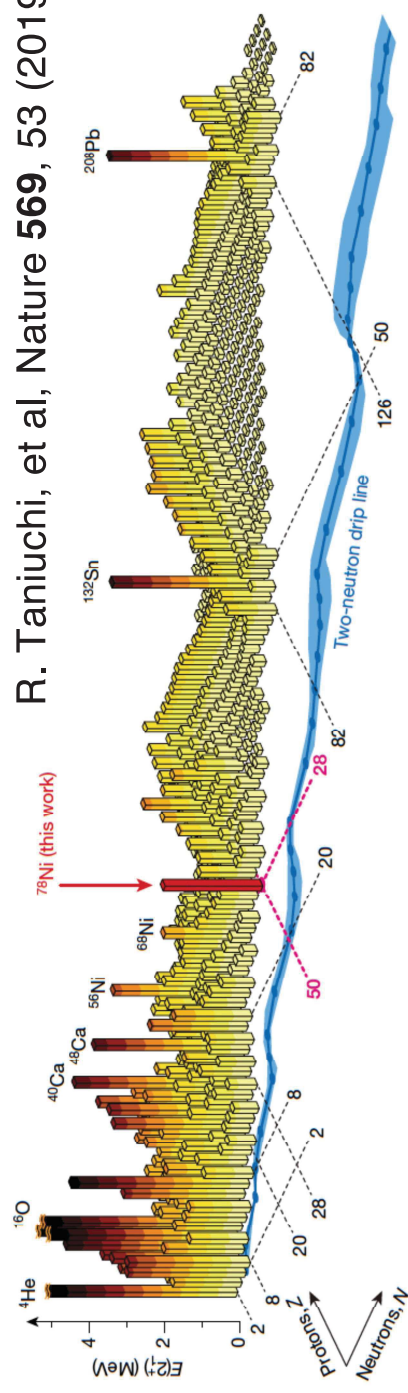
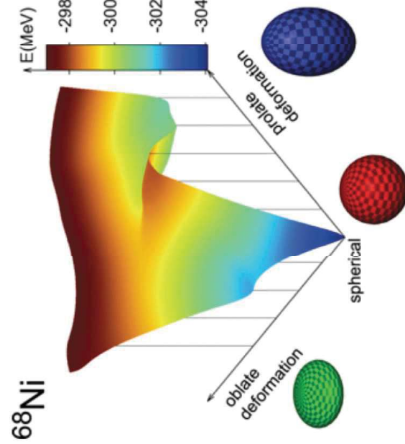
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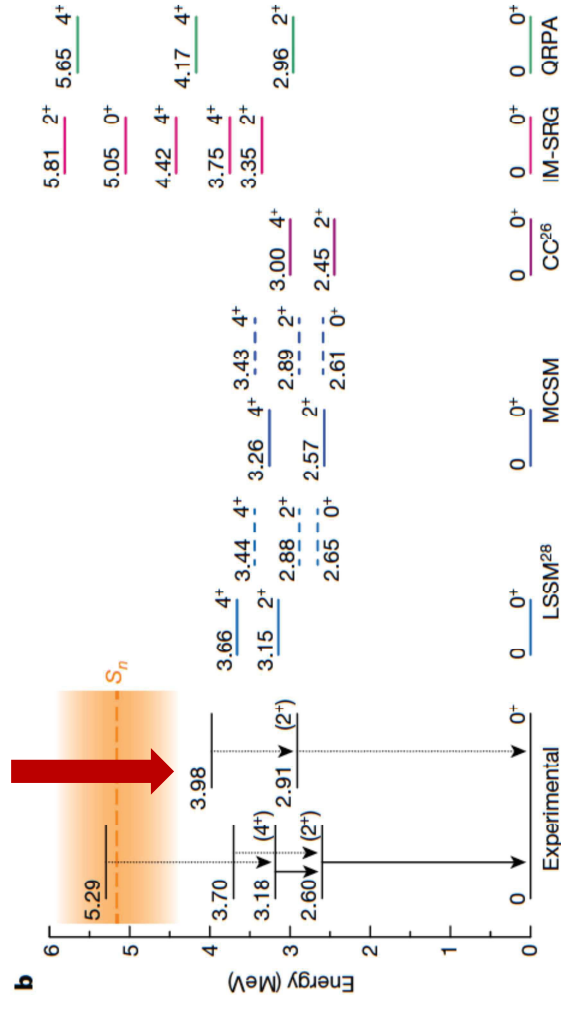
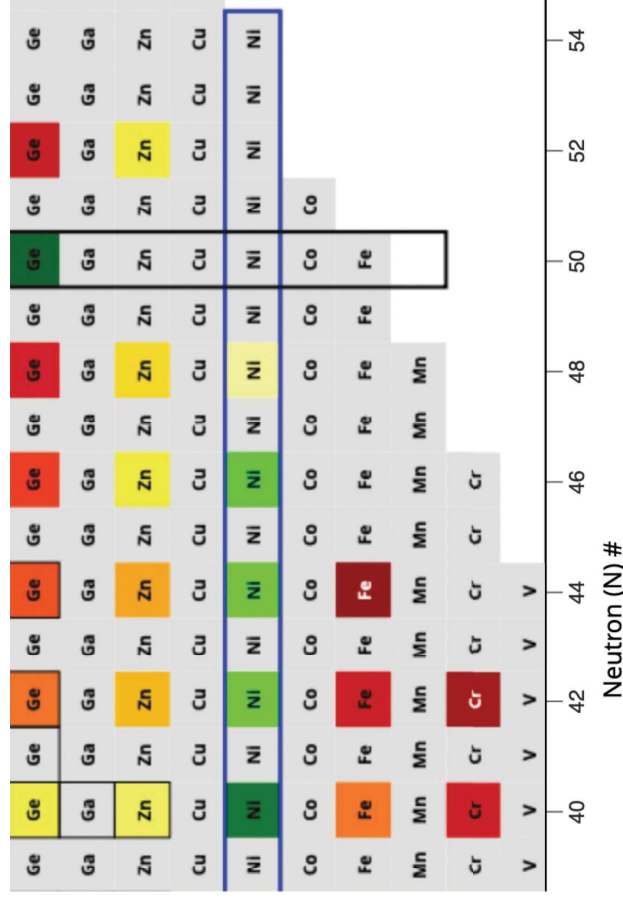
Lack of rotational stretching in coupled-cluster with projection after variation
[Hu, Sun, Hagen, Papenbrock, Phys Rev C (2024)]

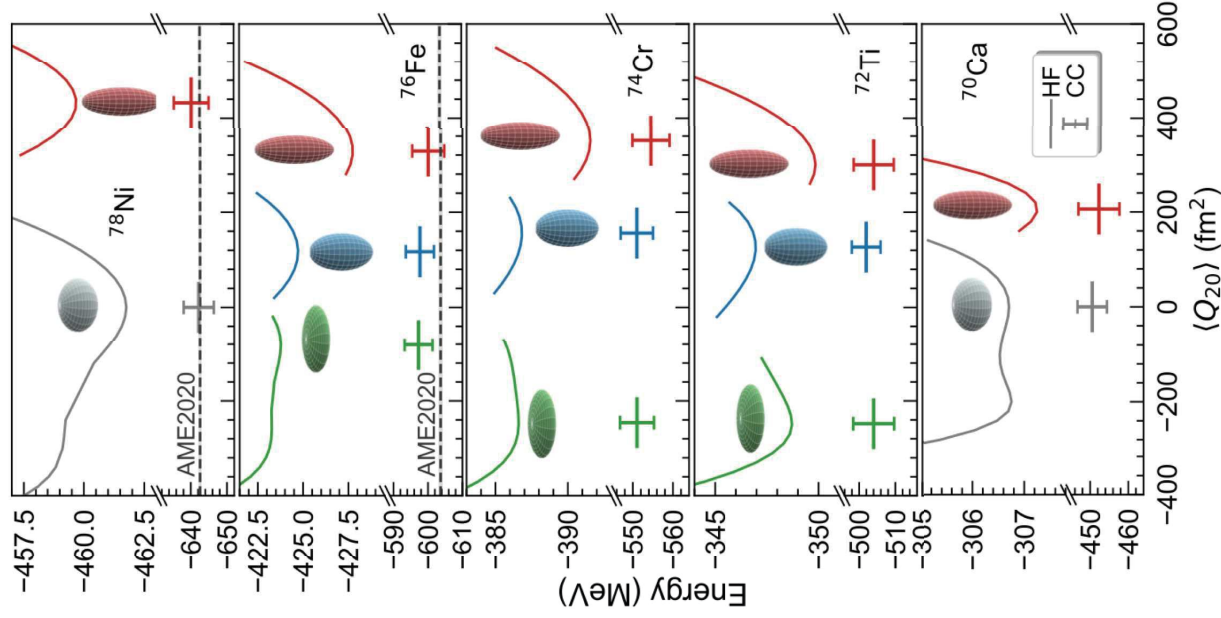
Deformation “south” of ^{78}Ni

⁶⁸Ni

T Otsuka and Y Tsunoda *J. Phys. G* **43** 024009 (2016)

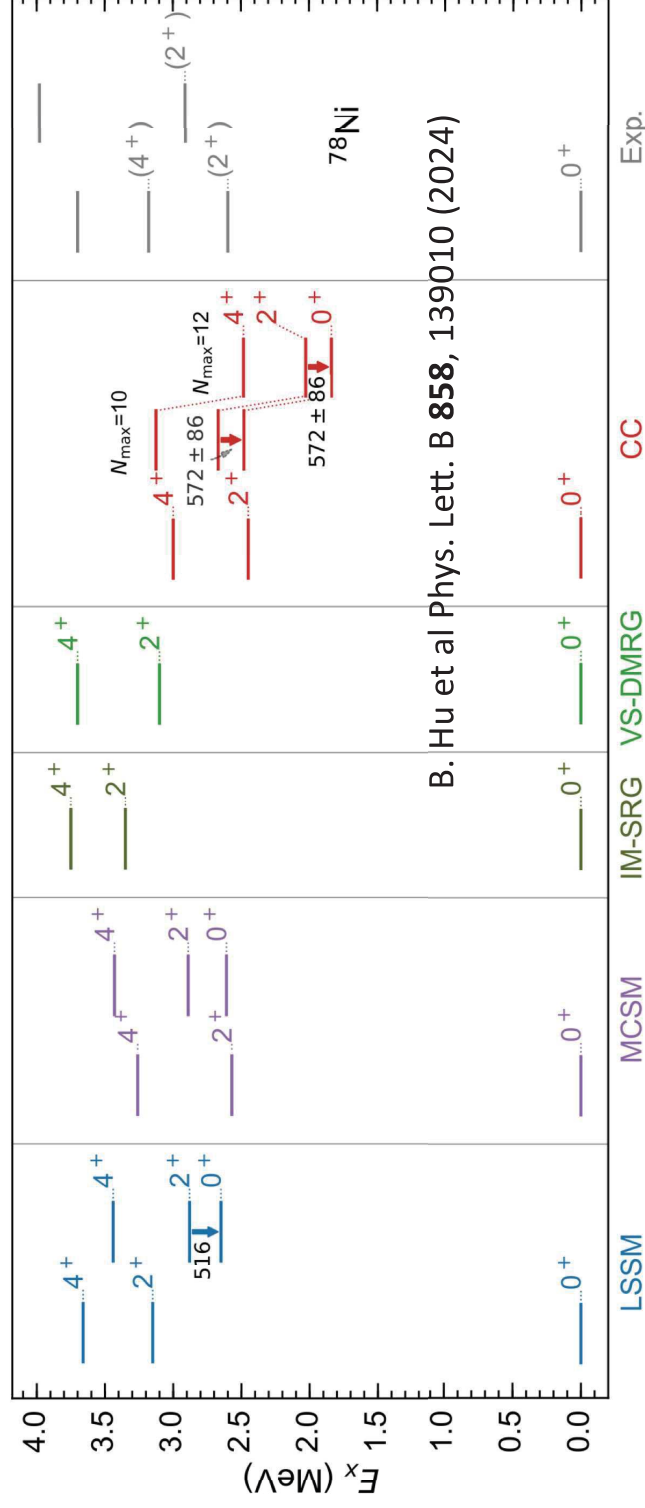
Deformed band?
Where is the band head?





Deformation “south” of ⁷⁸Ni

- Erosion of the magic number $N = 50$ toward ⁷⁰Ca manifested by onset of deformation in the ground-states
- For ⁷⁸Ni we predict a low-lying rotational band consistent with recent data and other



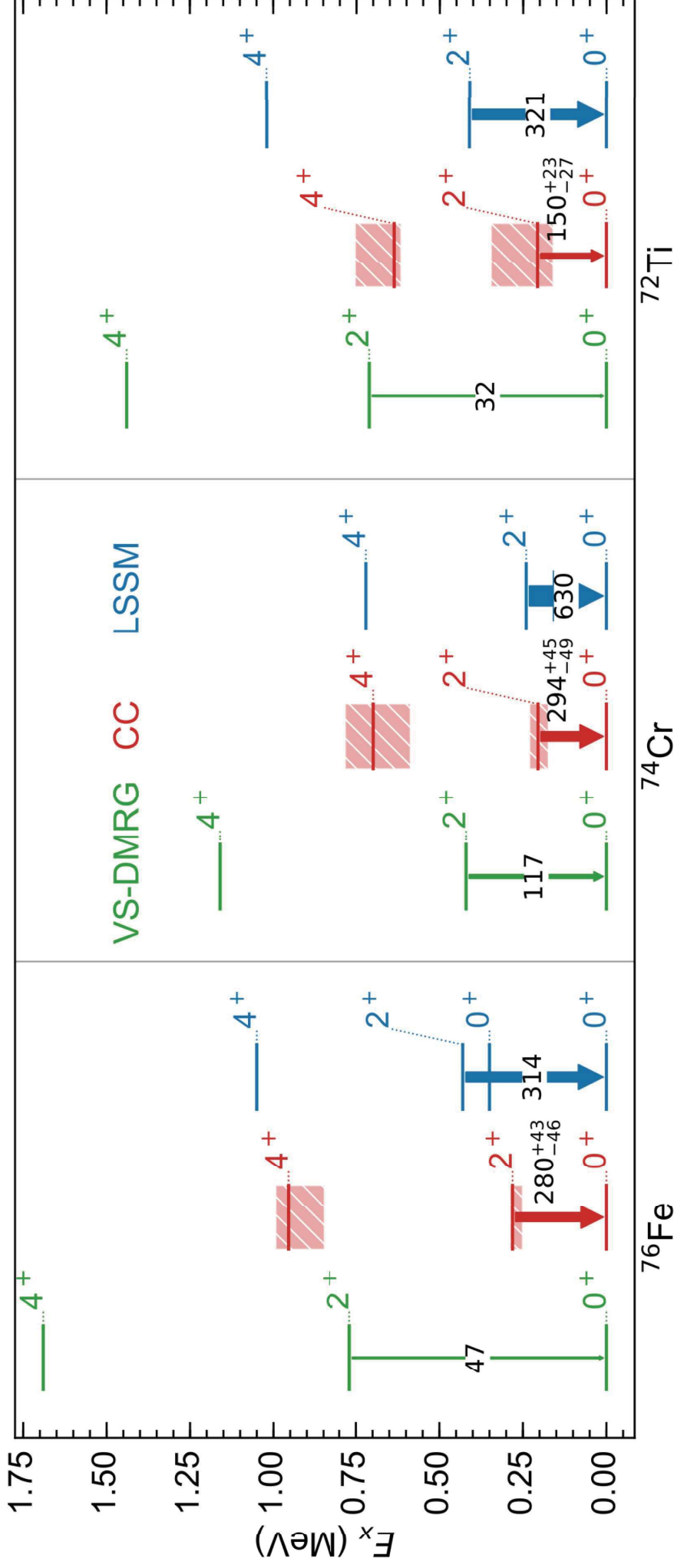
VS-DMRG: A. Tichai, et al, PLB **855**, 138841 (2024)

MCSM: R. Taniuchi, et al, Nature **569**, 53 (2019)

LSSM: F. Nowacki, et al, PRL **117**, 272501 (2016)

Deformation “south” of ^{78}Ni

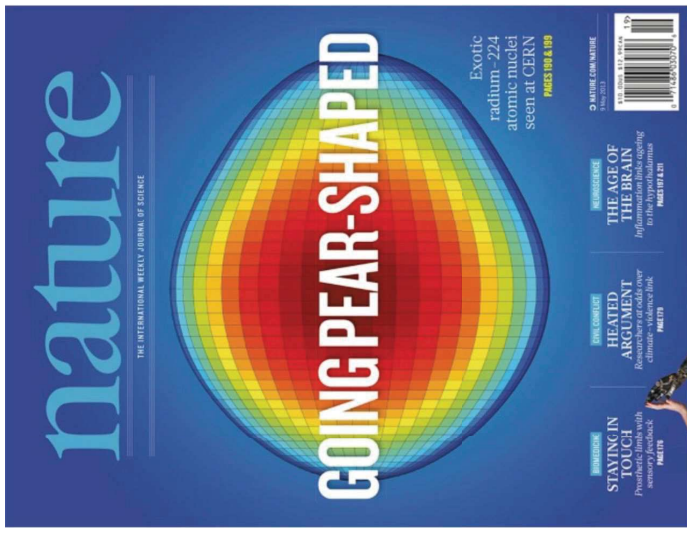
spectra largely agree with shell-model results within our uncertainty estimates



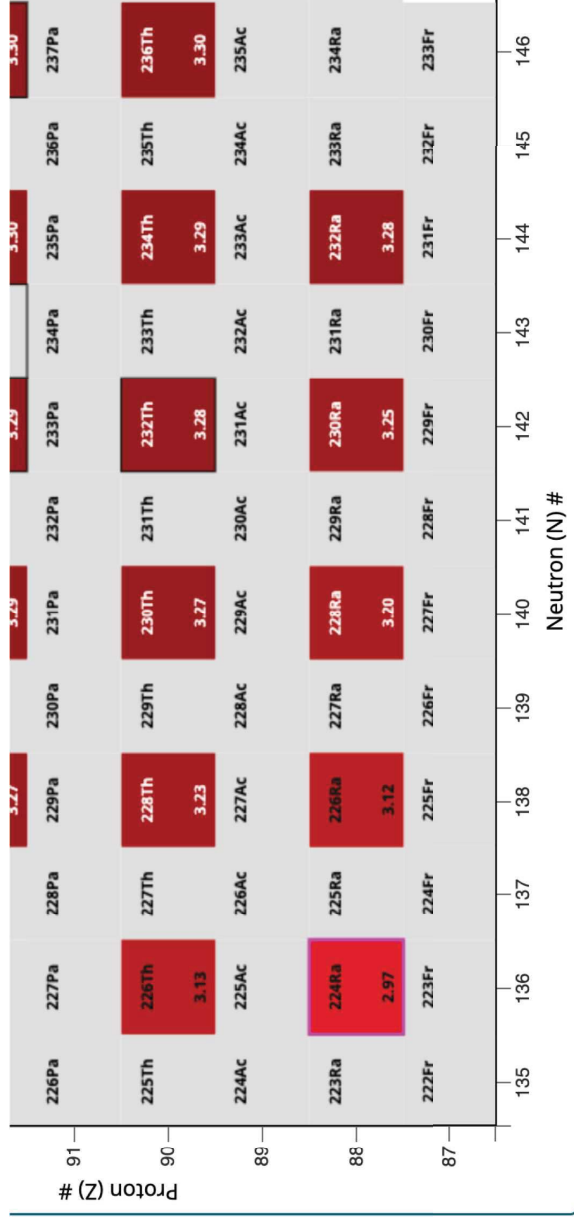
Towards ab-initio description of Schiff moments

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

Nature 2013,
octupole deformed $^{220,224}\text{Ra}$



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



$\frac{1}{2}^+$ and $\frac{1}{2}^-$ parity doublet in ^{225}Ra
differ by only 50keV

Constrained Coupled-Cluster $\Psi = e^T \phi$

$$H'(\lambda_1^{\text{AL}}, \lambda_3) = H_{2b} - \lambda_1^{\text{AL}} Q_1 - \lambda_3 Q_3$$

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:

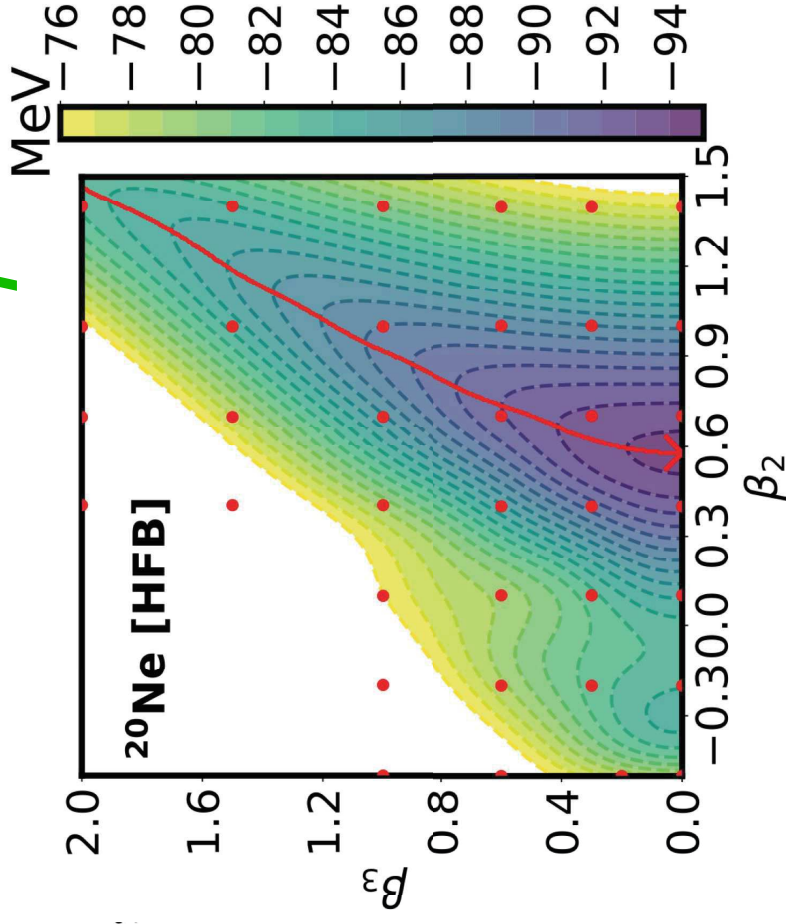
$$\frac{\partial E'(T, \Lambda, \vec{\lambda})}{\partial T} = 0, \quad \frac{\partial E'(T, \Lambda, \vec{\lambda})}{\partial \Lambda} = 0.$$

Under the condition that the constraints are fulfilled:

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

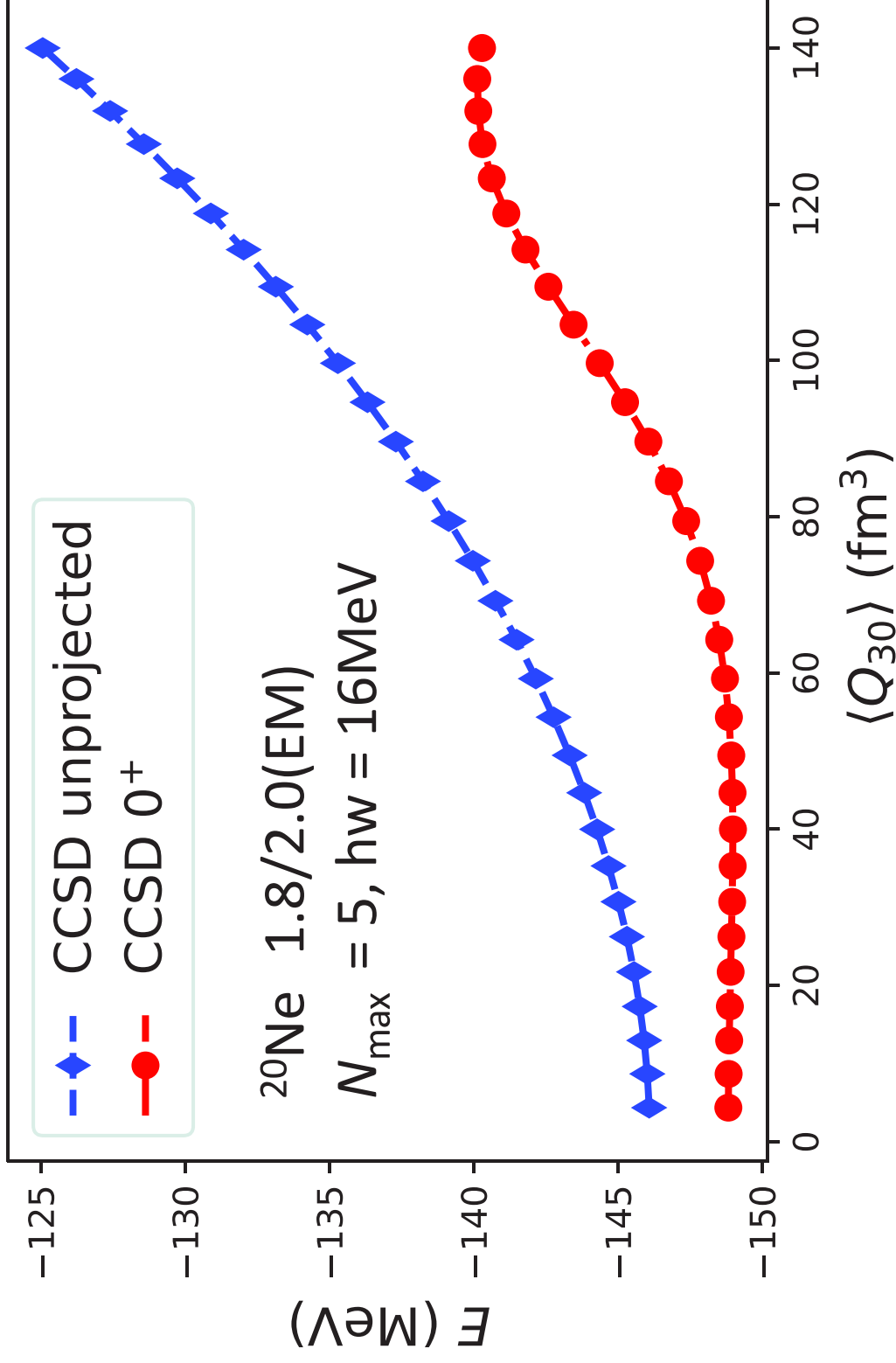
With the solutions for $T, \Lambda, \vec{\lambda}$ we compute the energy:

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




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

Constrained Coupled-Cluster $\Psi = e^T \phi$



Constrained sub-space Coupled-Cluster

$$H'(\lambda_1^{\text{AL}}, \lambda_3) = H_{2b} - \lambda_1^{\text{AL}} Q_1 - \lambda_3 Q_3.$$


Choose a small set of training points (snapshots)

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

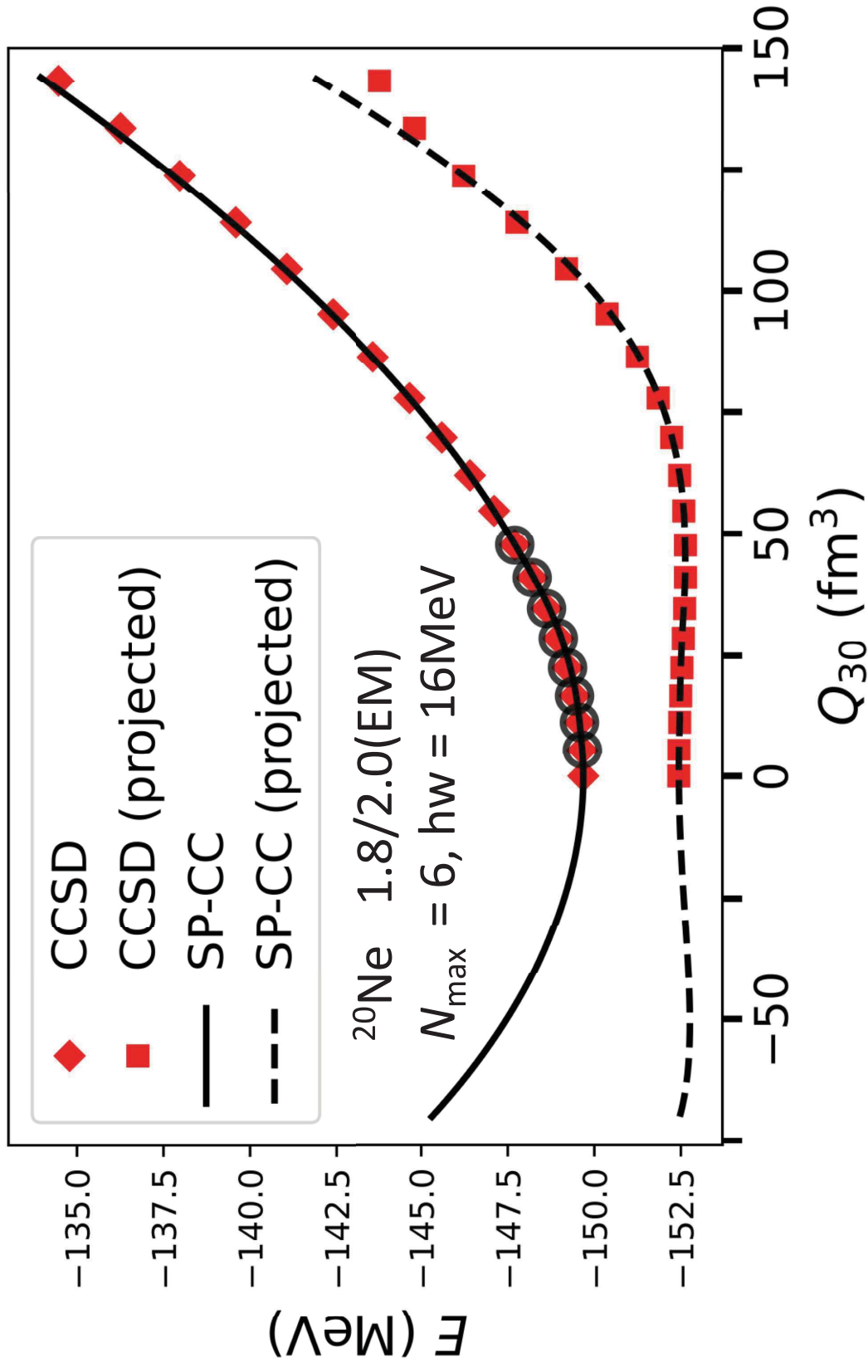
$$\left\{ \langle \Phi_0 | (1 + \Lambda_i) e^{-T_i}, e^{T_i} | \Phi_0 \rangle \right\}$$

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:

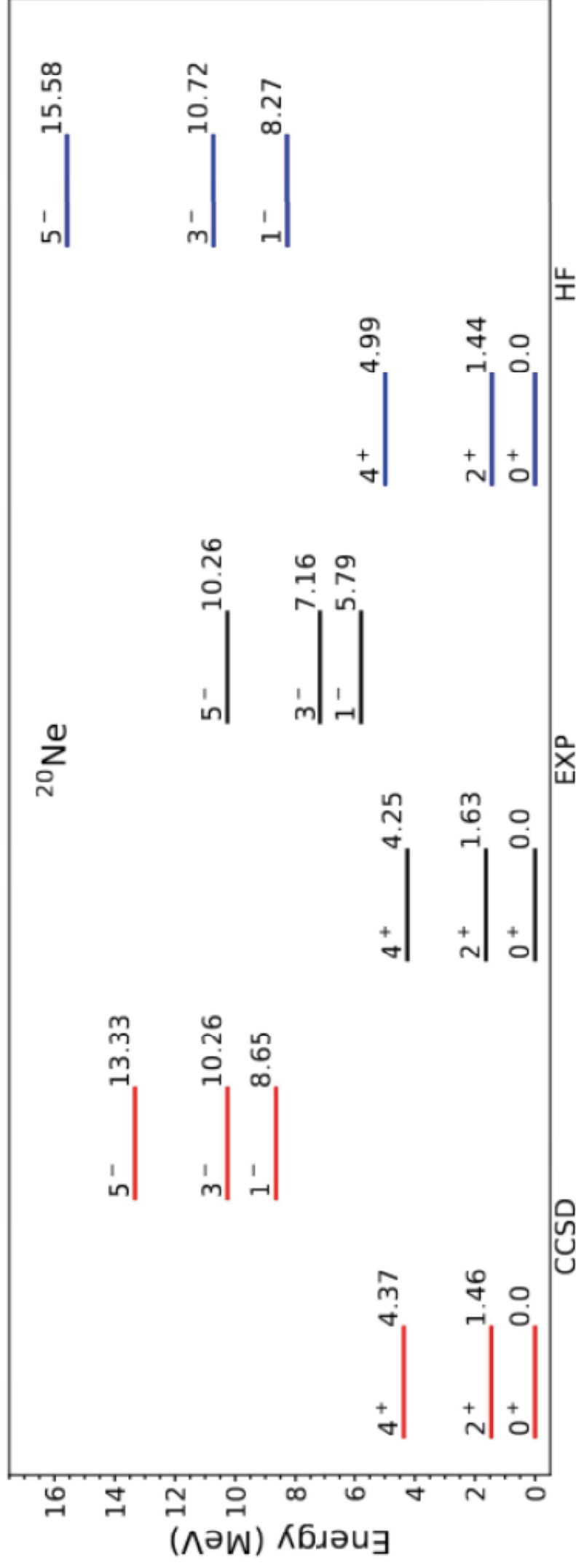
$$\min_{\lambda_1, \lambda_3} \left\{ (\langle Q_{10} \rangle - q_{10})^2 + (\langle Q_{30} \rangle - q_{30})^2 \right\}$$

Constrained sub-space Coupled-Cluster



Constrained sub-space Coupled-Cluster

$$1.8/2.0(\text{EM}) \ N_{\text{max}} = 6, \ h\omega = 16\text{MeV}$$



Summary

Rotational bands well reproduced. Is the absence of superfluidity (which would increase moments of inertia) compensated by the too small radii???

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

Constrained coupled-cluster for octupole deformed nuclei

Constrained sub-space coupled-cluster dramatically reduces the computational cost and is a promising tool for heavier nuclei