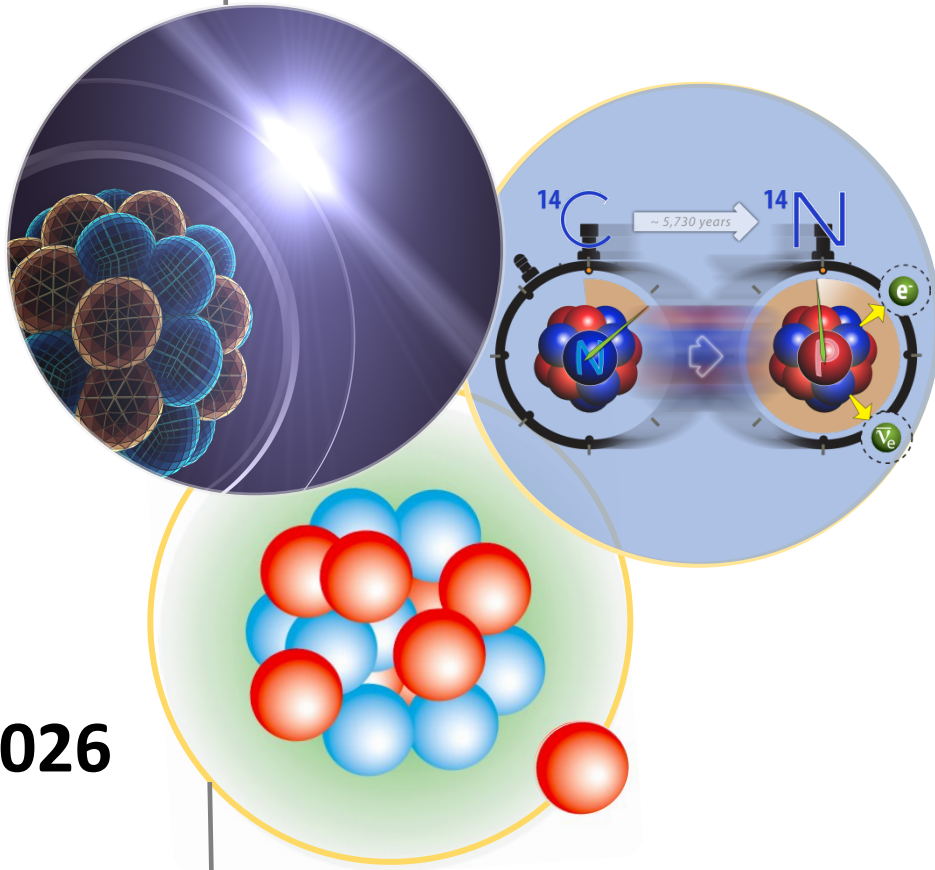


Ab initio nuclear theory: status and roadmap

Gaute Hagen
Oak Ridge National Laboratory

EMMI Workshop: Light-Ion Collisions 2026

Heidelberg, September 21st, 2026



NUCLEI
Nuclear Computational Low-Energy Initiative

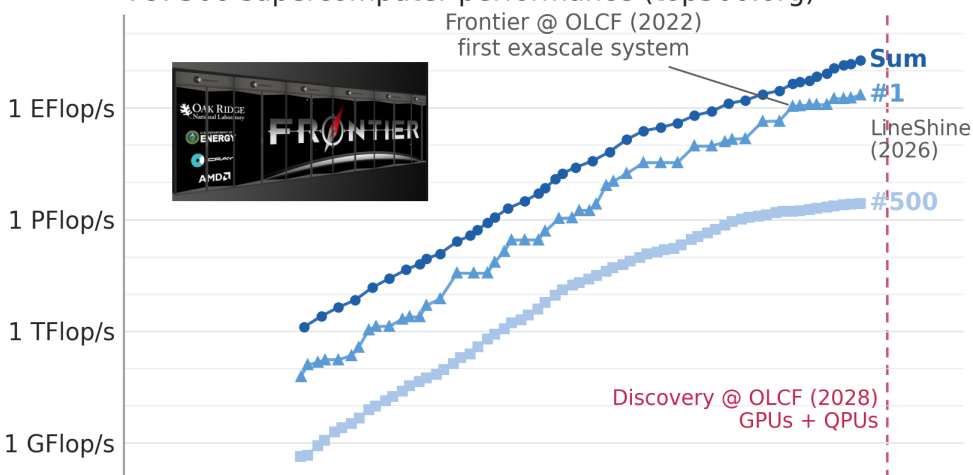


 **OAK RIDGE NATIONAL LABORATORY**
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

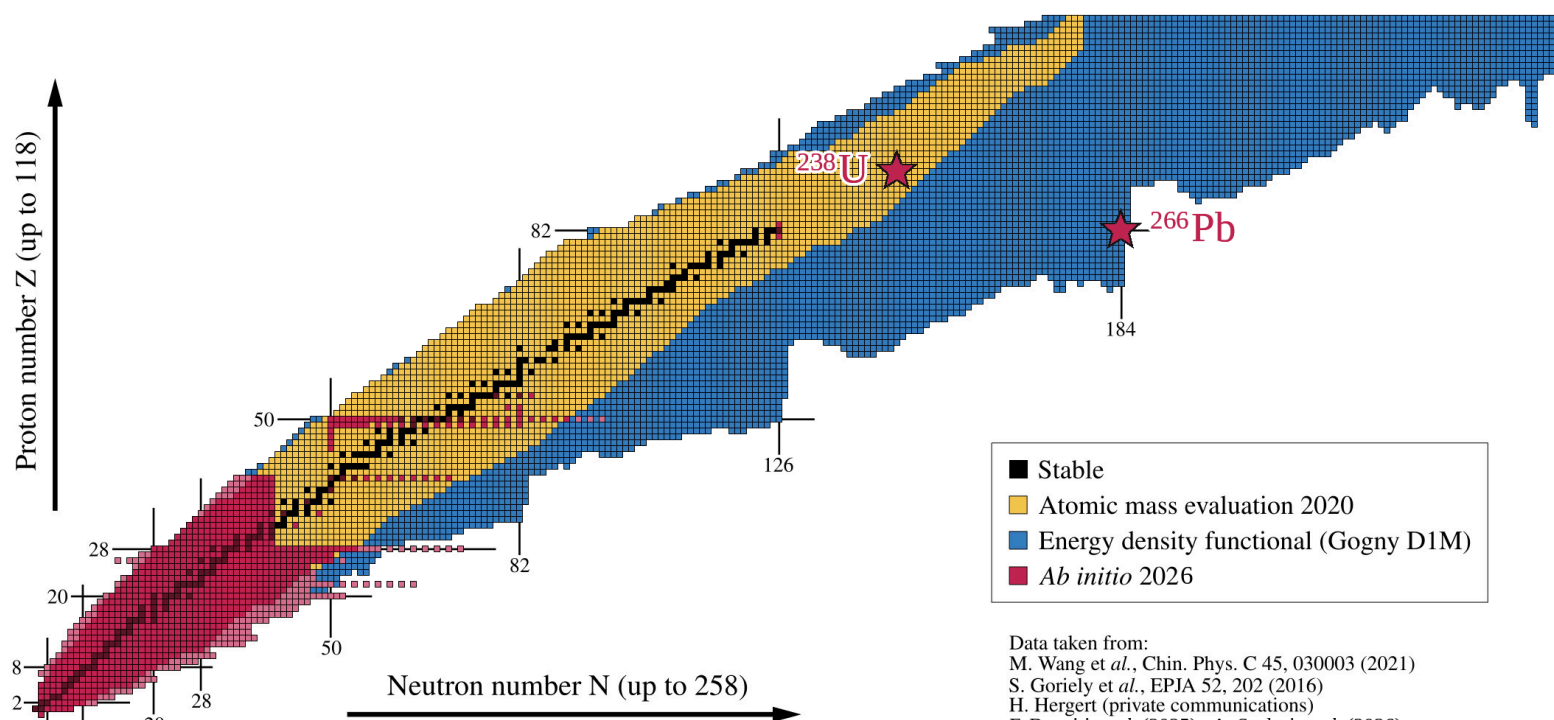
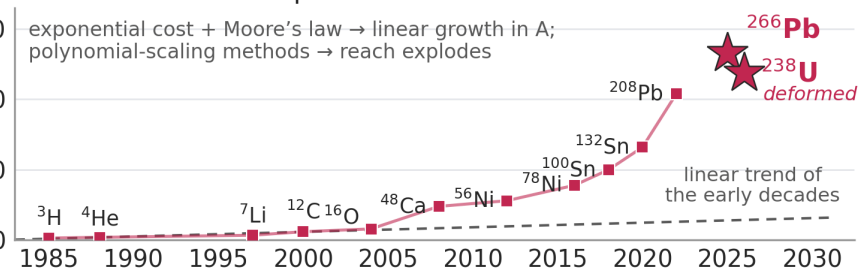
Trend in realistic ab-initio calculations

- A lot of progress in recent years because of ideas from EFT and the renormalization group
- Computational methods with polynomial cost (coupled clusters 😊 **quantum computing** 🤔)
- Ever-increasing computer power? Frontier (2022, first exascale) → Discovery @ OLCF (2028: GPUs + QPUs)
- **2025–26 highlights: ^{266}Pb (N = 184) and deformed ^{238}U — the heaviest nuclei computed from first principles**

TOP500 supercomputer performance (top500.org)



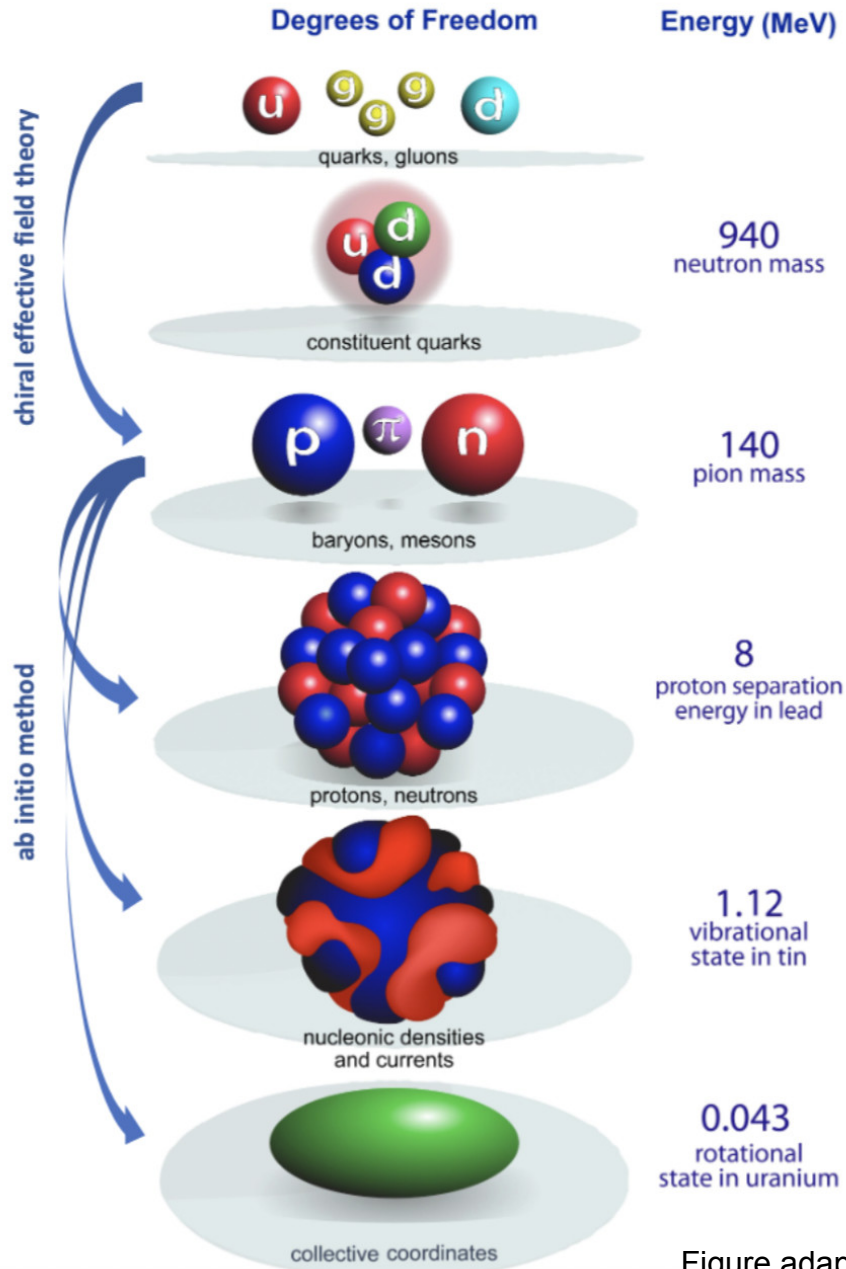
Heaviest nuclei computed ab initio



Data taken from:
M. Wang *et al.*, Chin. Phys. C 45, 030003 (2021)
S. Goriely *et al.*, EPJA 52, 202 (2016)
H. Hergert (private communications)
F. Bonaiti *et al.* (2025); A. Scalesi *et al.* (2026)

Nuclear chart courtesy of B. Bally

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

Interactions from chiral effective field theory

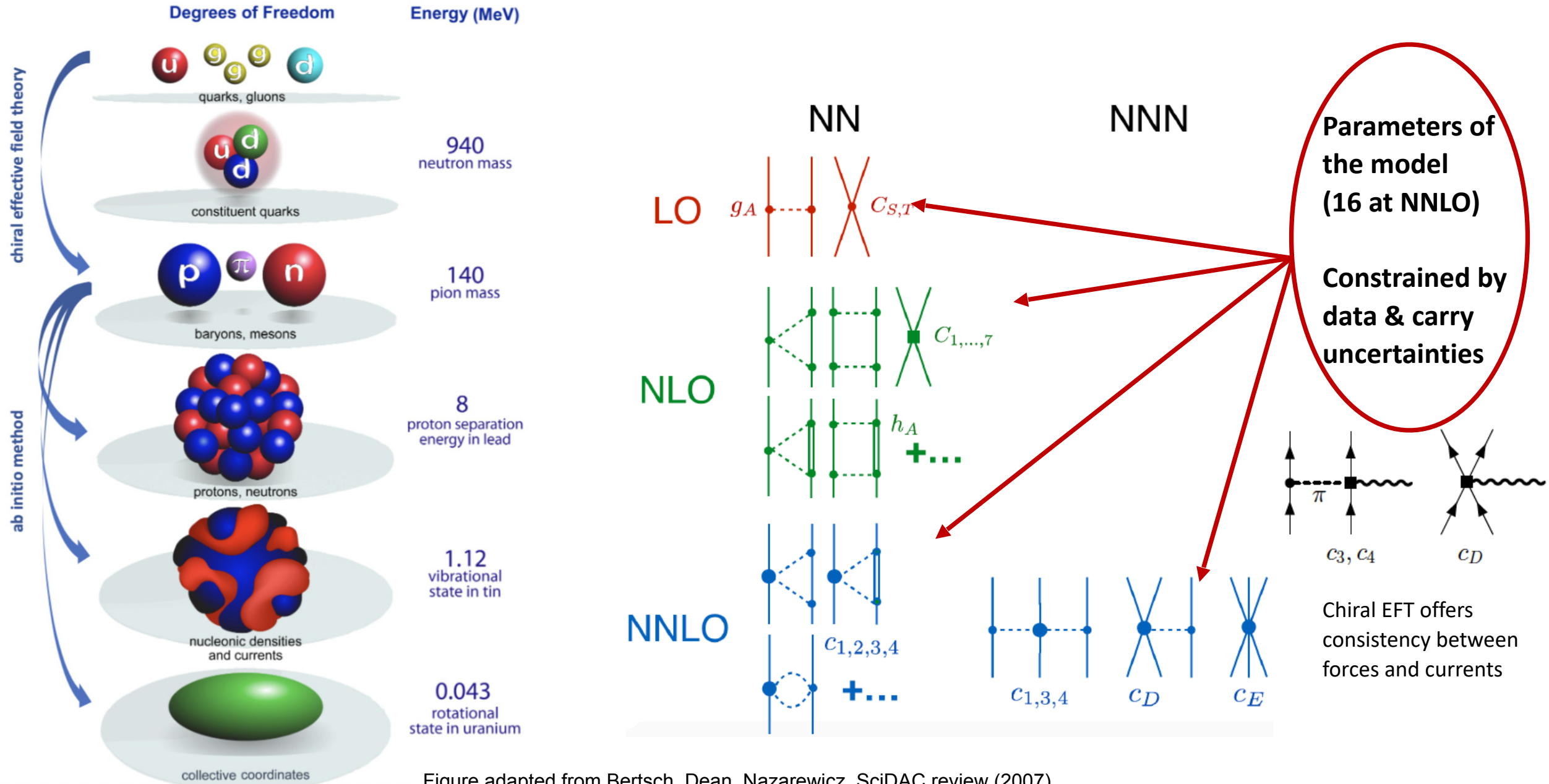
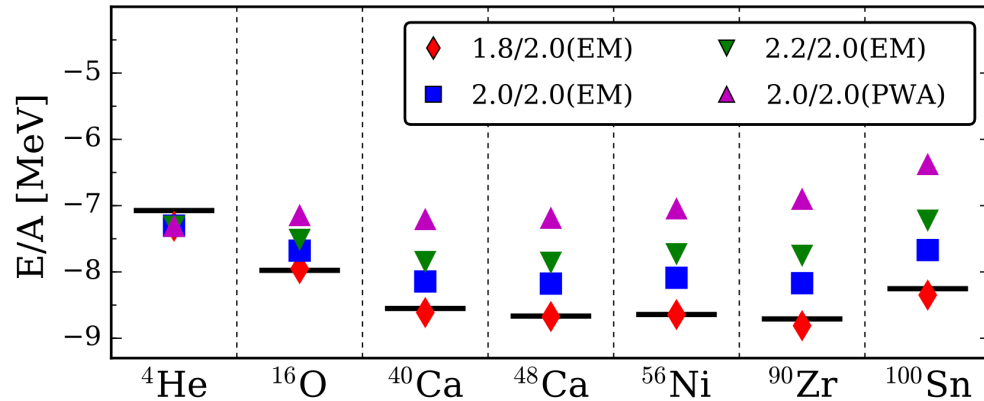


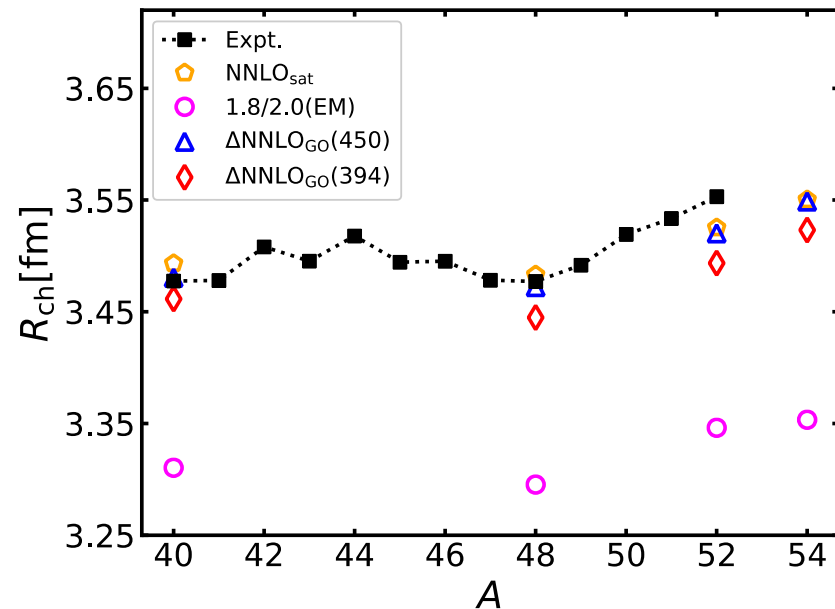
Figure adapted from Bertsch, Dean, Nazarewicz, SciDAC review (2007)

Some interactions work “better” than others

Radii and binding energies are very sensitive to small changes in the interactions – finetuning problem

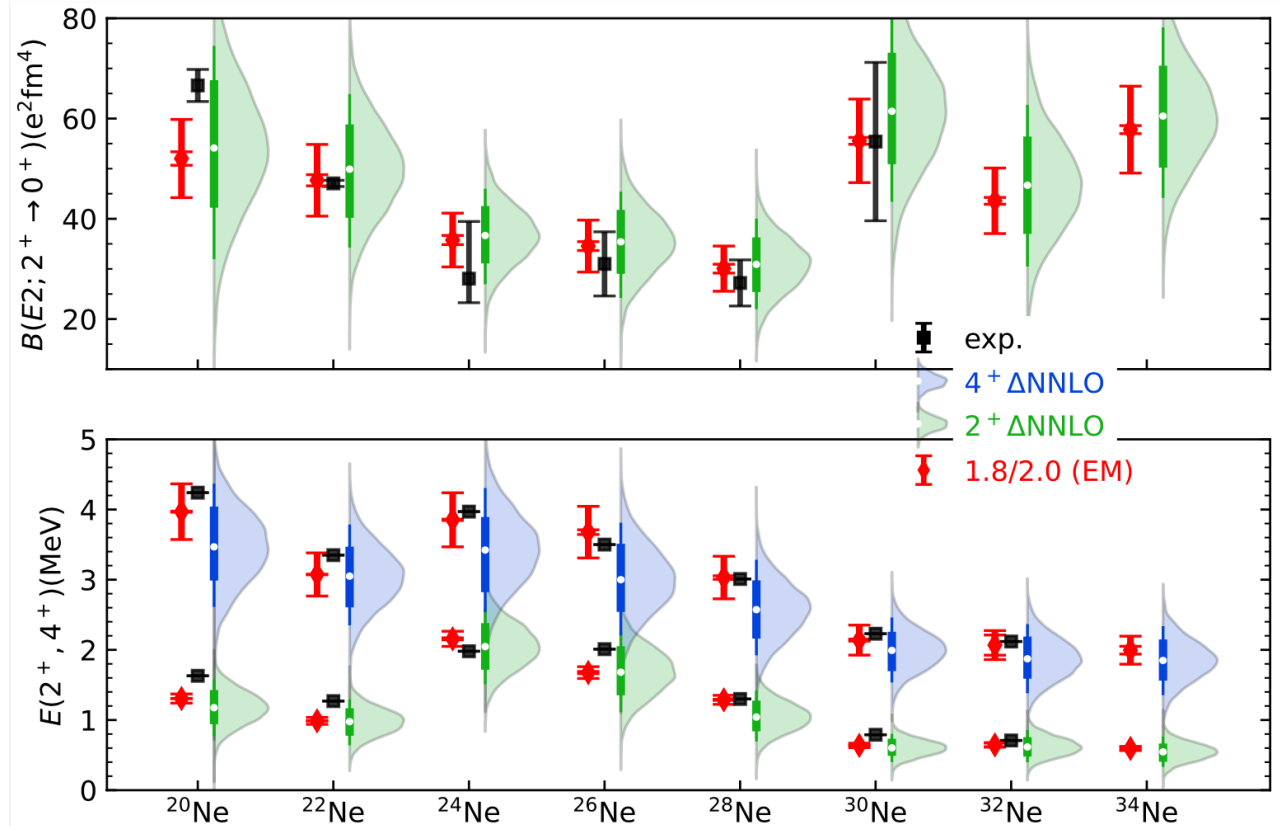


T. Morris et al, Phys. Rev. Lett. 120, 152503 (2018)



W. G. Jiang, et al., Phys. Rev. C 102, 054301 (2020)

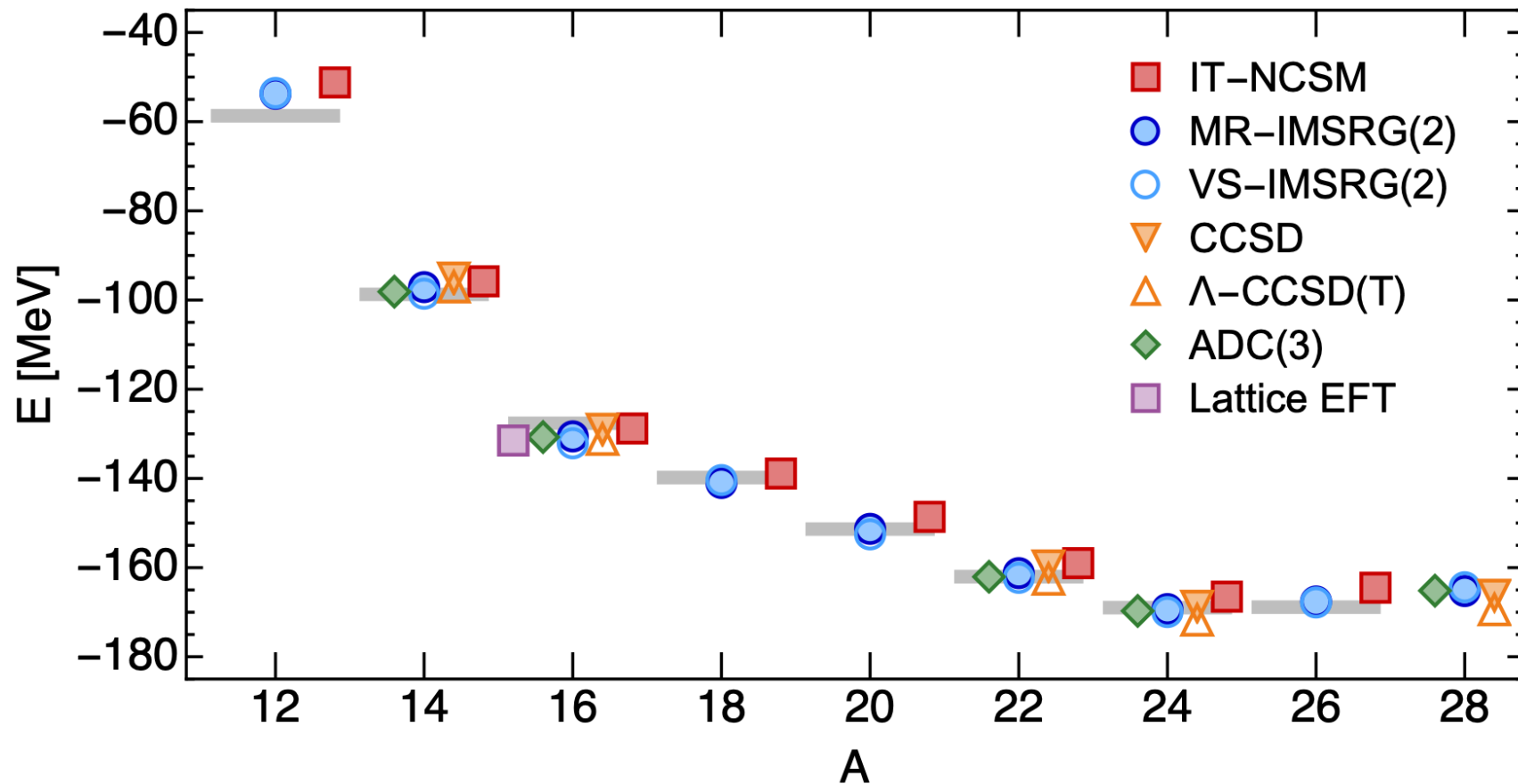
Good reproduction of excited states and transitions in neon



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

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)



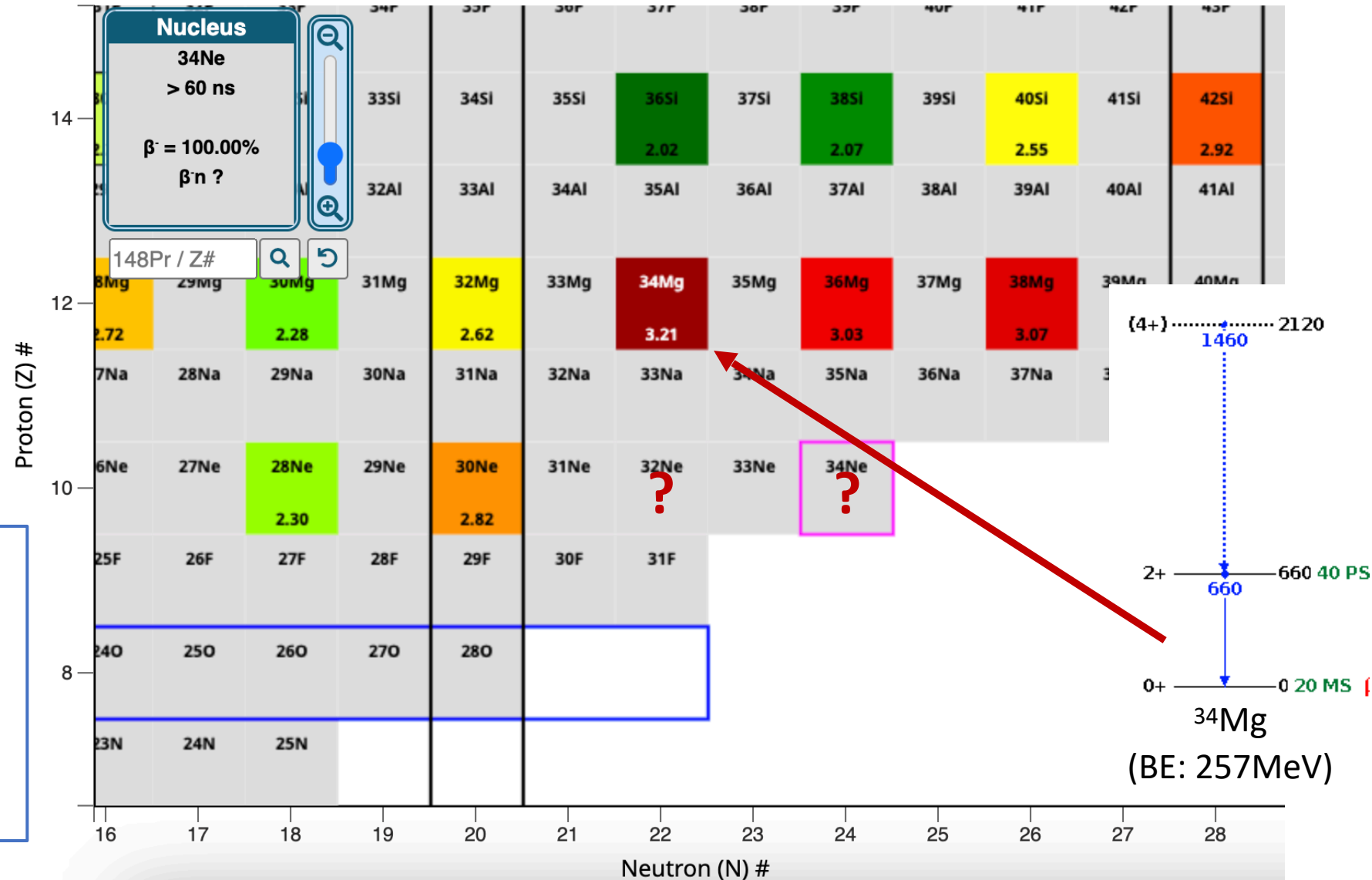
H. Hergert Front. Phys., (2020)

Neutron-rich nuclei beyond N = 20 are deformed

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

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

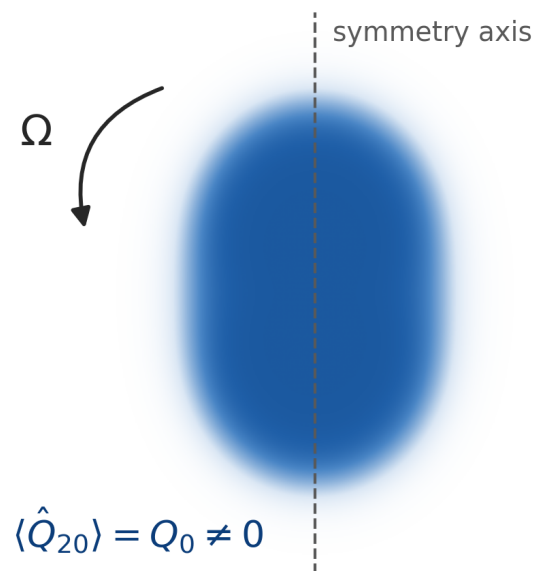
Simple picture: Spherical states (magic $N = 20$ number in the traditional shell model) coexist with deformed ground states



What do we mean by a deformed nucleus?

Intrinsic frame

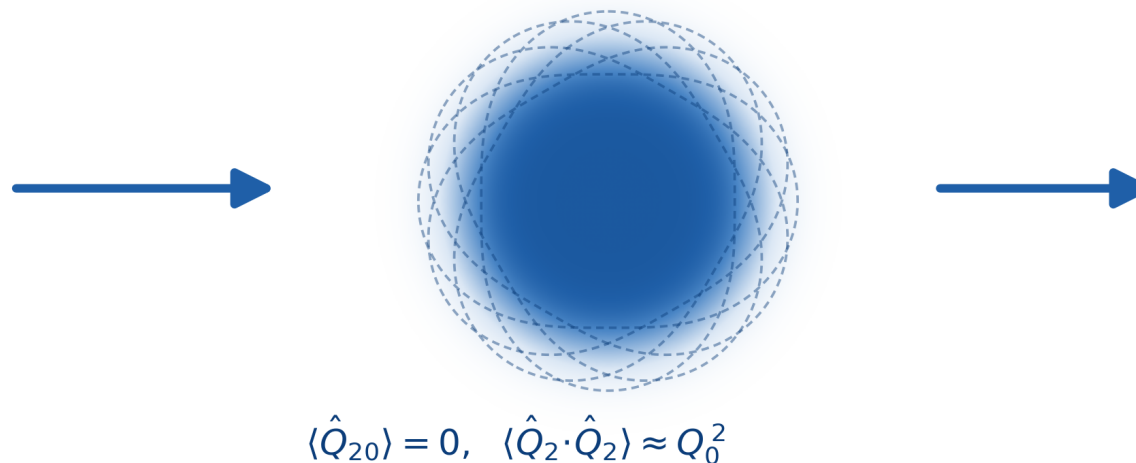
*symmetry-broken state
not an observable*



$$|\Psi\rangle = e^{\hat{T}}|\Phi\rangle = \sum_J c_J |\Psi^J\rangle$$

Laboratory frame

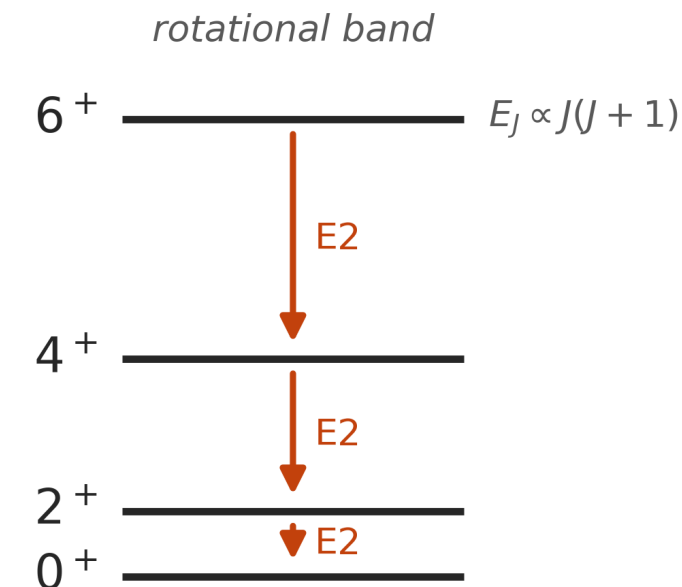
*projected $J = 0$ ground state
spherical*



$$|\Psi^{J=0}\rangle \propto \int d\Omega \hat{R}(\Omega) |\Psi\rangle$$

Observables

*signatures of the
intrinsic deformation*



$$E_J = \langle \tilde{\Psi} | \hat{H} \hat{P} | \Psi \rangle / \langle \tilde{\Psi} | \hat{P} | \Psi \rangle$$

$$\langle \delta \epsilon_\ell^2 \rangle \equiv \langle \delta \epsilon_\ell^2 \rangle^{1b} + \langle \delta \epsilon_\ell^2 \rangle^{2b}$$

- There is no timescale associated with symmetry projection
- One can not take an instantaneous snapshot of the intrinsic shape

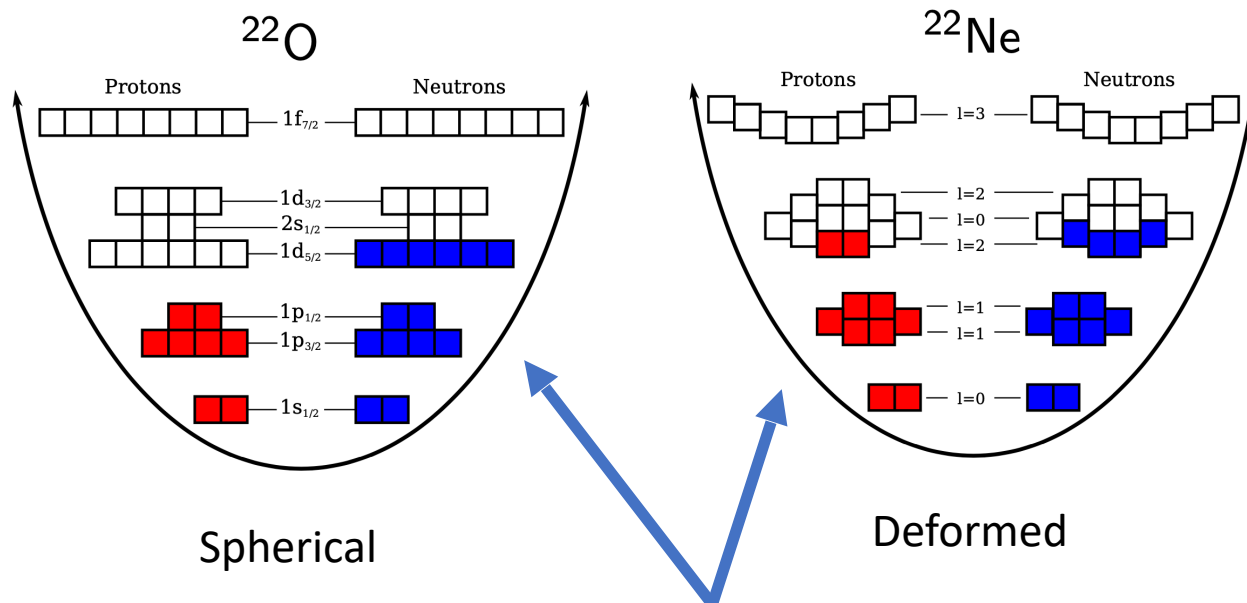
T. Duguet et al, Phys. Rev. Lett. **135**, 182301 (2025)
S. Bofos et al, Phys. Lett. B **879**, 140649 (2026)

Coupled-cluster computations of deformed nuclei

- Compute Hartree-Fock reference state:

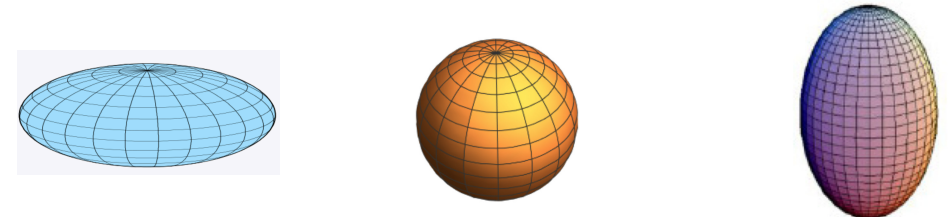
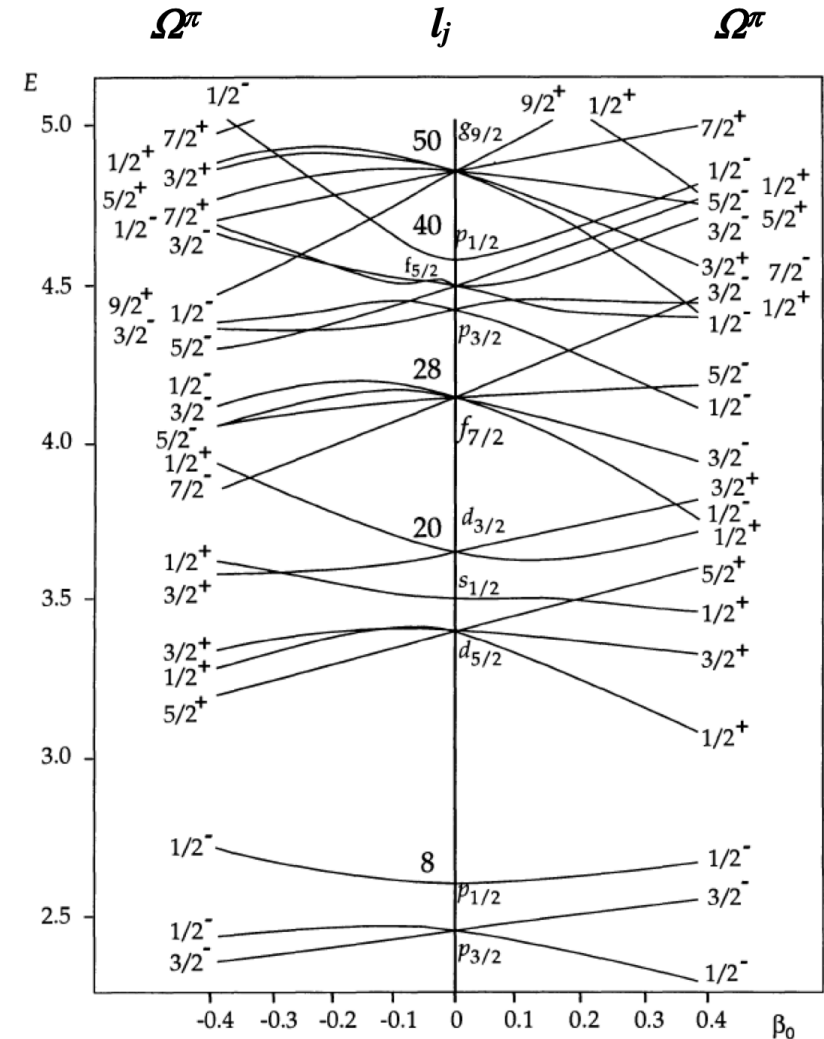
$$H = T - T_{\text{CoM}} + V_{\text{NN}} + V_{3\text{N}}$$

- Informs us about emergent breaking of symmetries



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

Wave-operator (includes many-body correlations)



Coupled-cluster computations of deformed nuclei

- Include short-range correlations via coupled-cluster theory

- Large contribution to total energy
- Cost increases polynomial with mass

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

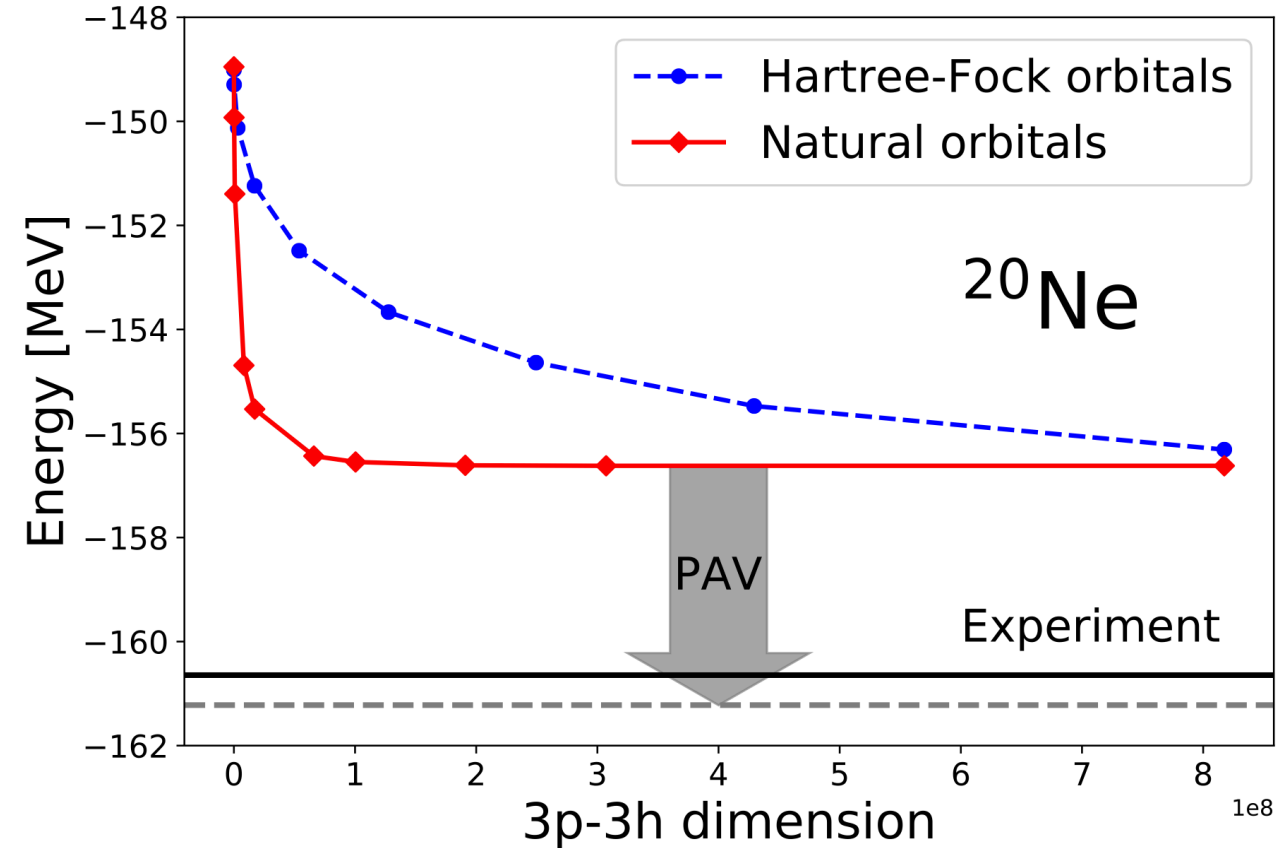
$$T = T_1 + T_2 + \dots$$

- Include long-range correlations via symmetry projections

- Small contribution to total energy
- Relevant for rotational bands and transition matrix elements

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

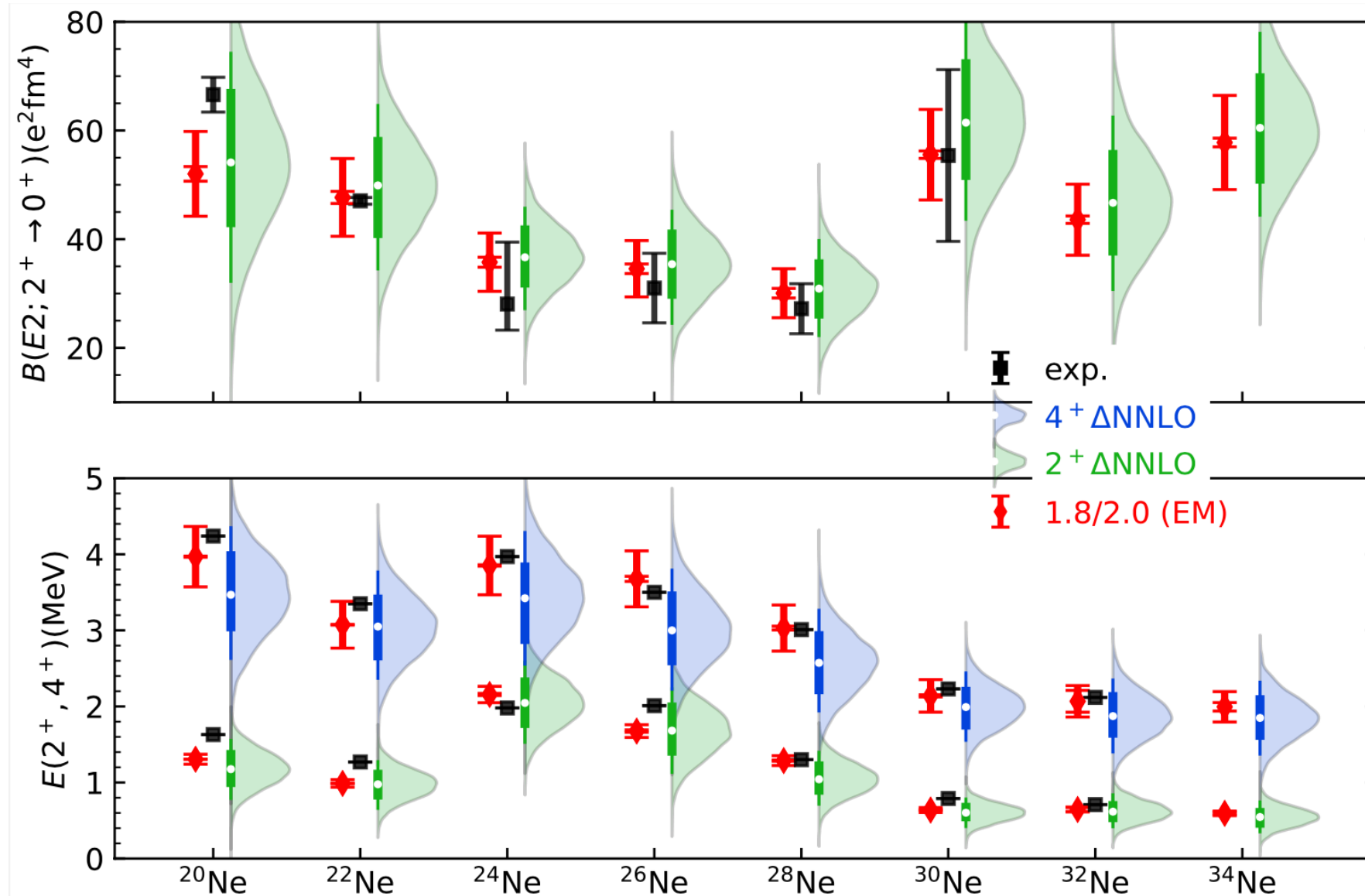
S. J. Novario, et al PRC 102, 051303 (2020)



Total energy:

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

Collectivity in neon isotopes

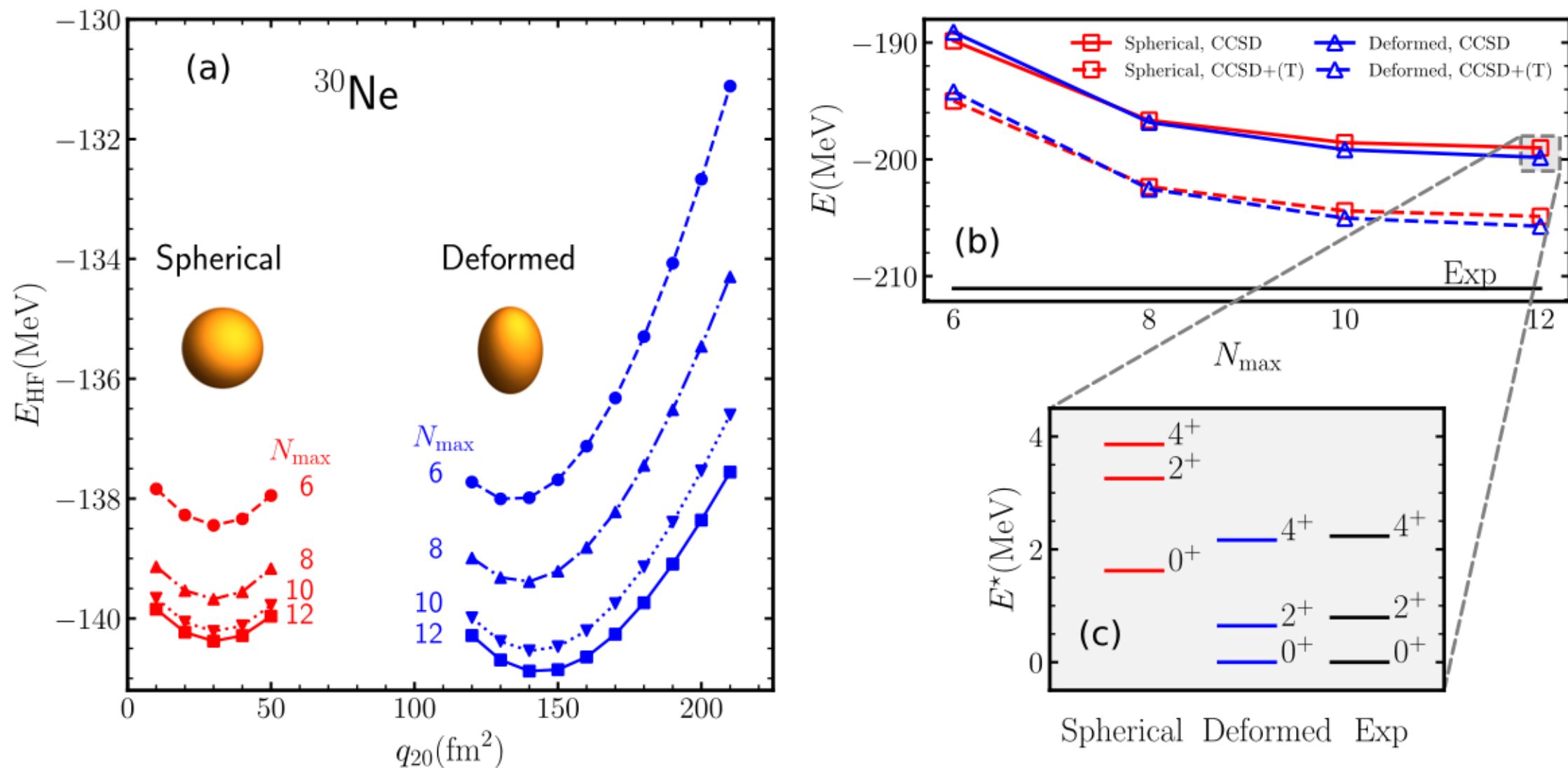


- Small energies reflect a large moment of inertia and a strong deformation
- Radii are underpredicted and leads to smaller moment of inertia
- Could it be that pairing effects are lacking?

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

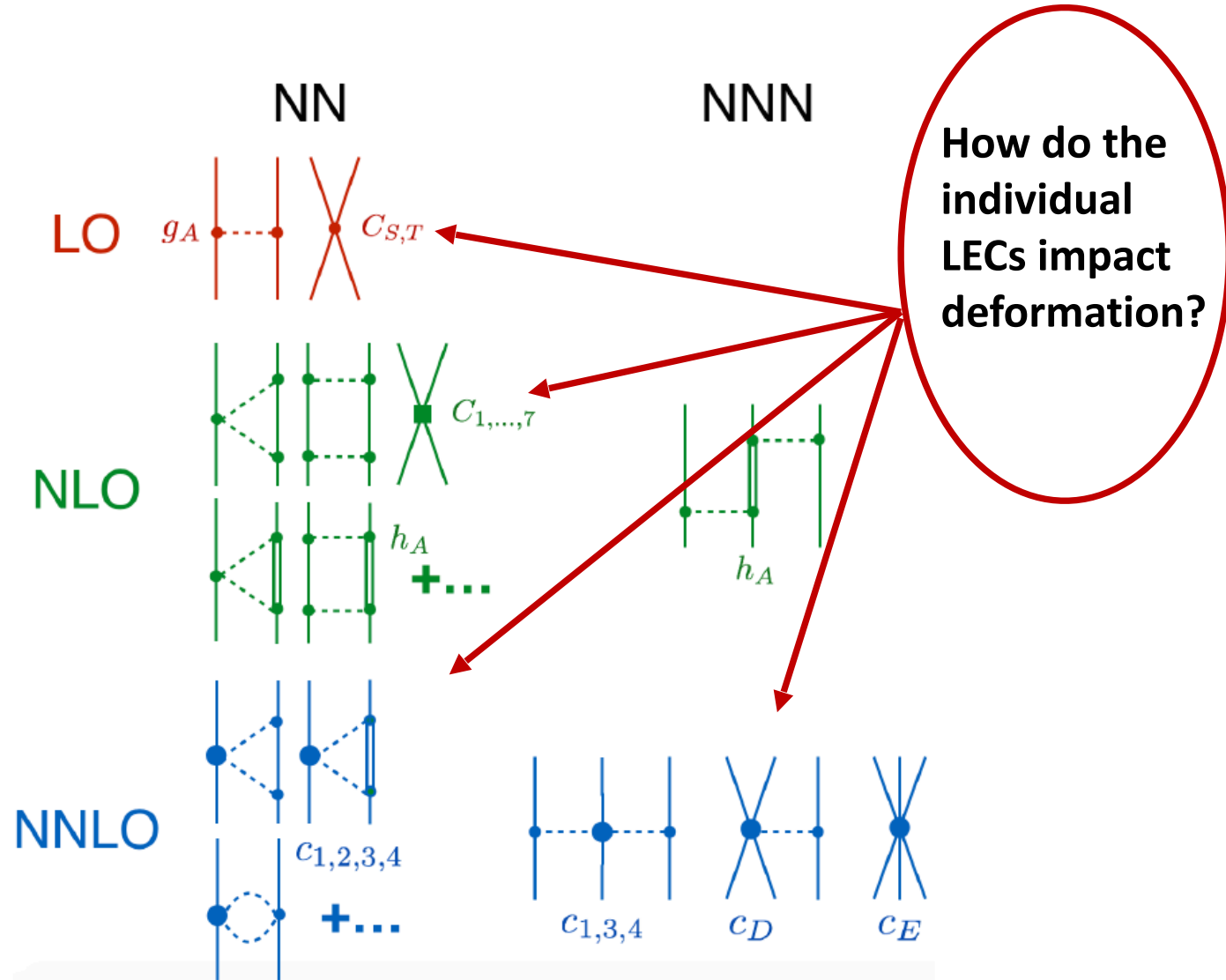
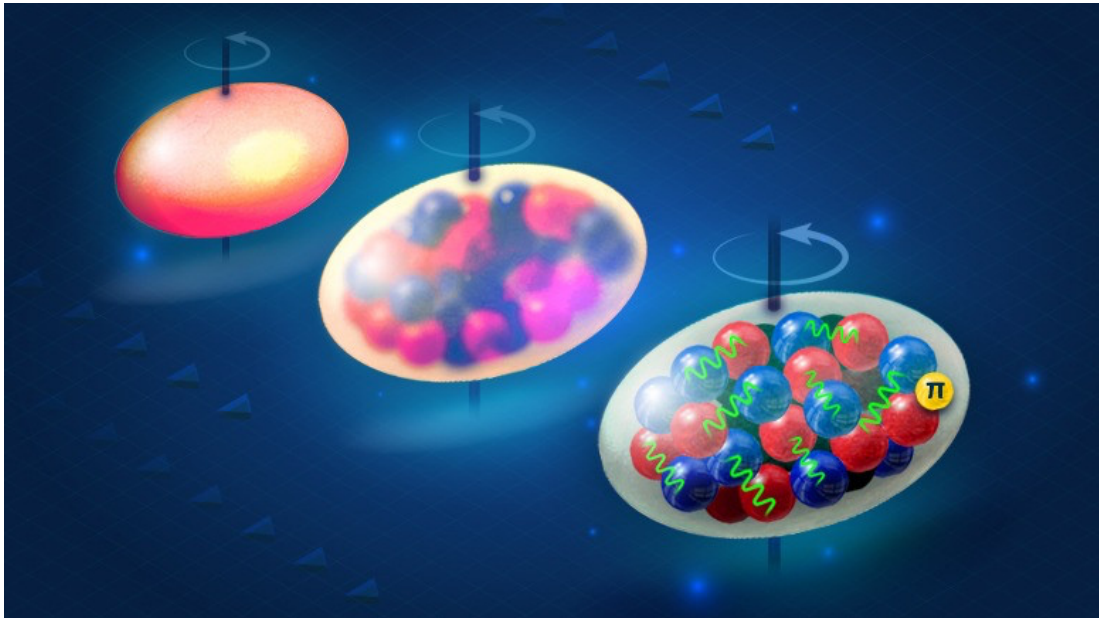
Y. Kondo et al.,
Nature **620**, 965–970 (2023)

Shape co-existence in ^{30}Ne



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

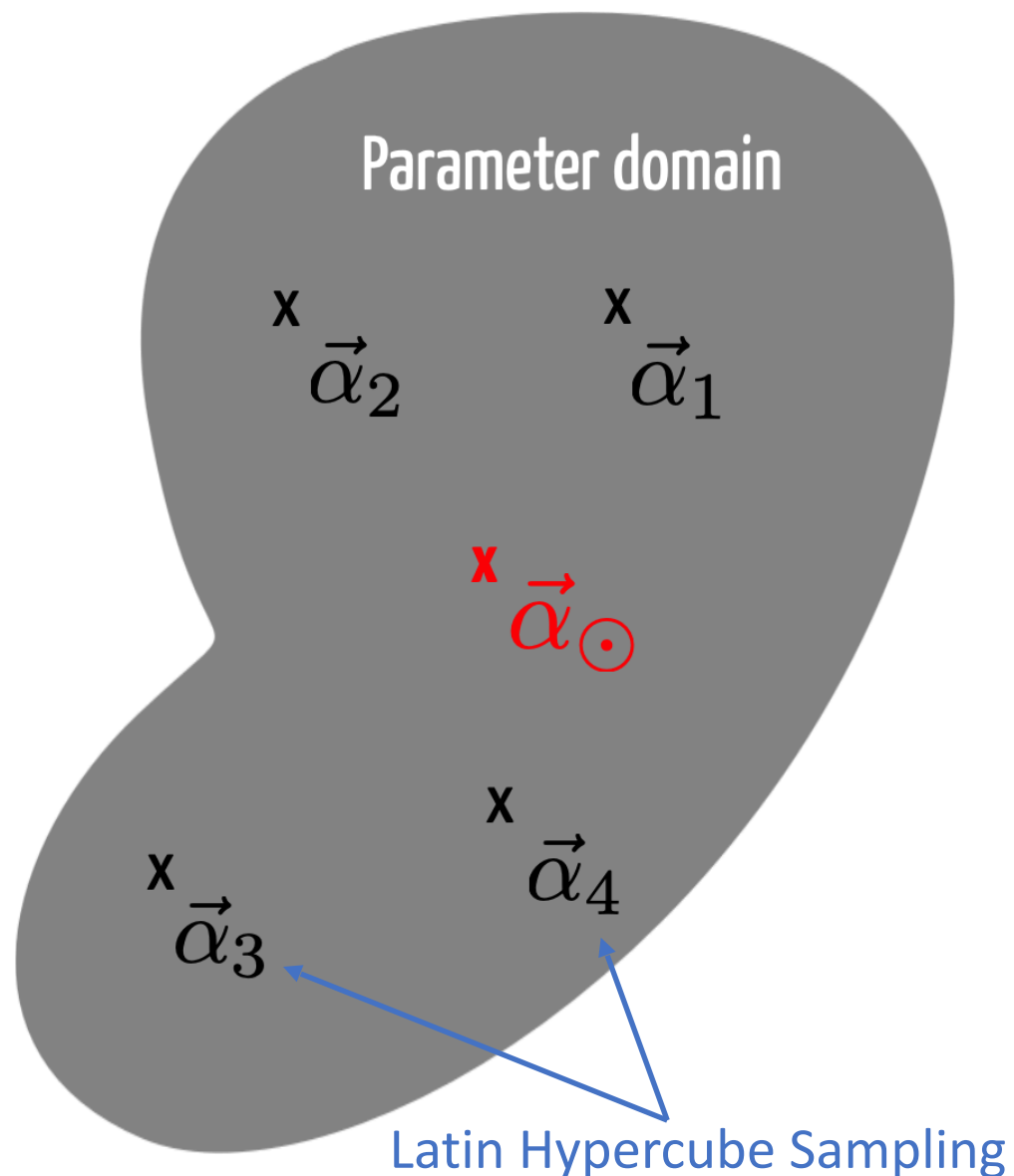
Sensitivity analysis of the radius and binding energy of ^{16}O

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



Reduced order model for deformed states

Zhonghao Sun, A. Ekstrom, C. Forssen, G. Hagen. G. R. Jansen, T. Papenbrock arXiv:2404.00058 (2024)



- 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

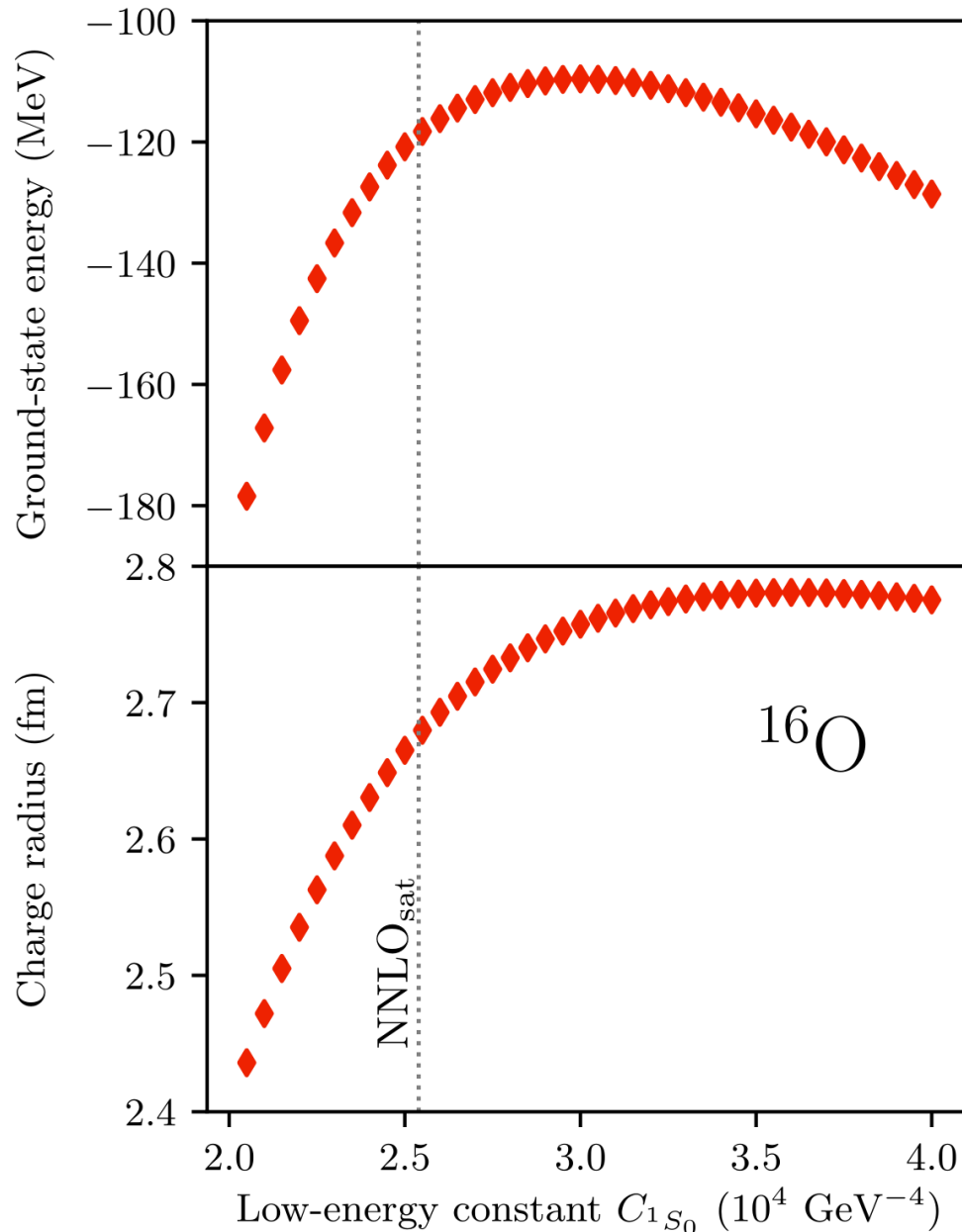
$$H(\vec{\alpha}) = h_0 + \sum_{i=1}^{N_{\text{LECs}}=17} \alpha_i h_i$$

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

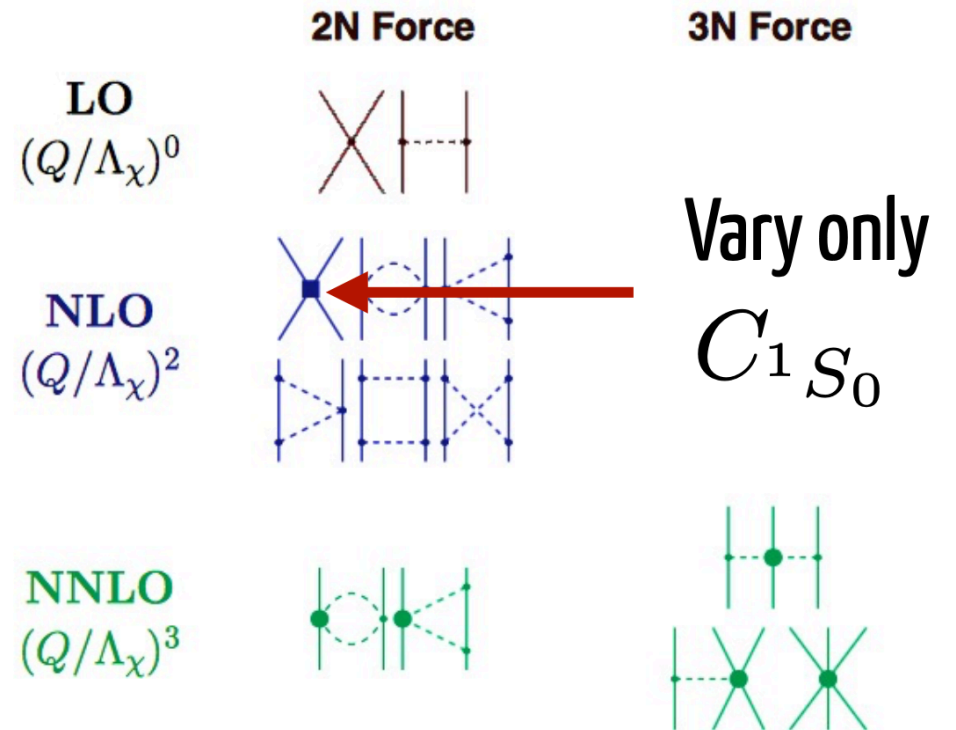
$$\mathbf{H}(\vec{\alpha}_{\odot}) \vec{c} = E(\vec{\alpha}_{\odot}) \mathbf{N} \vec{c},$$

Emulating ab-initio coupled-cluster calculations

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

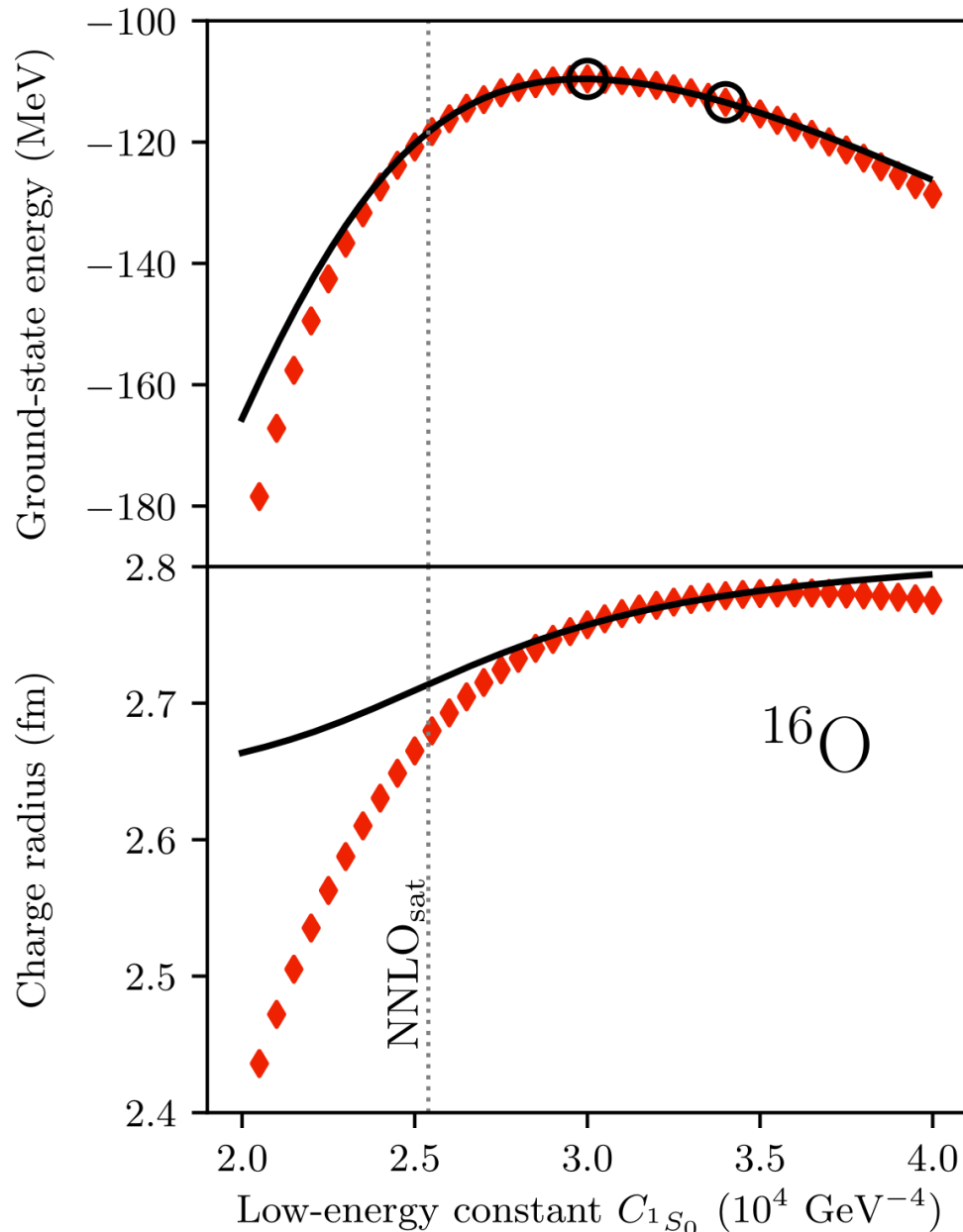


Exact coupled cluster calculations at the singles and doubles level

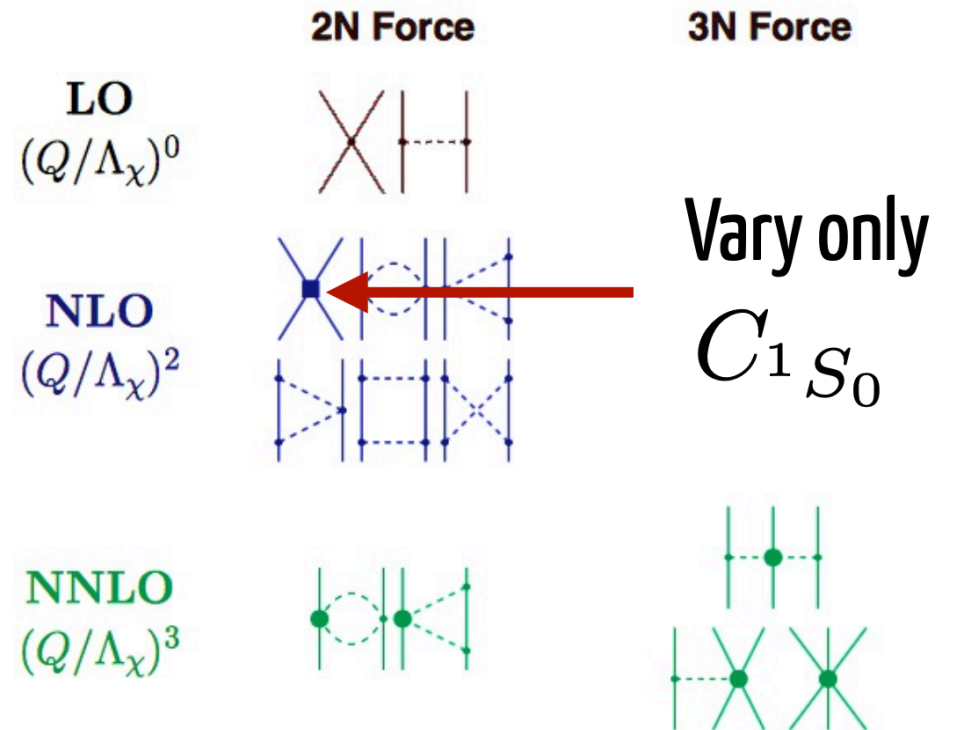


Emulating ab-initio coupled-cluster calculations

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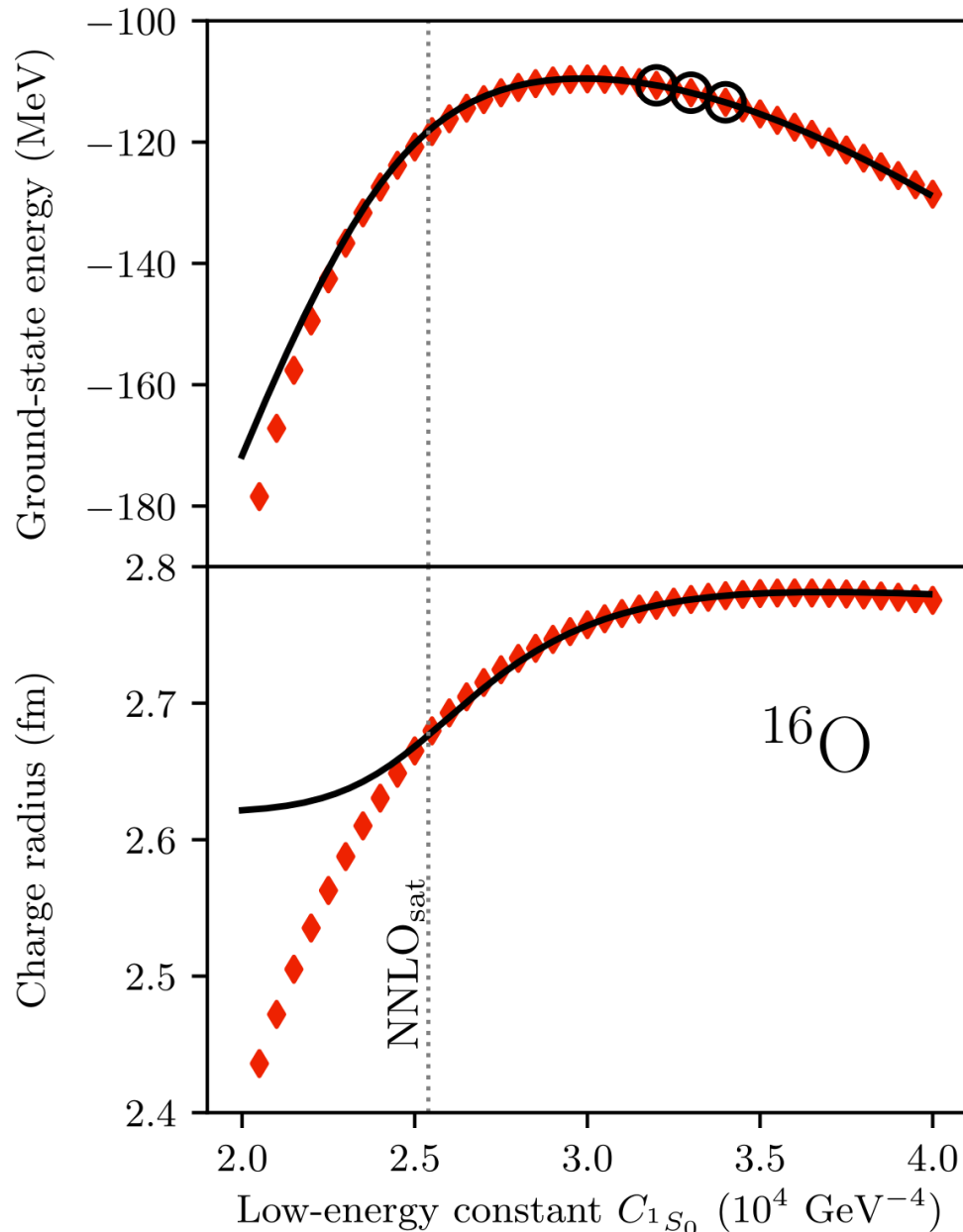


Exact coupled cluster calculations at the singles and doubles level

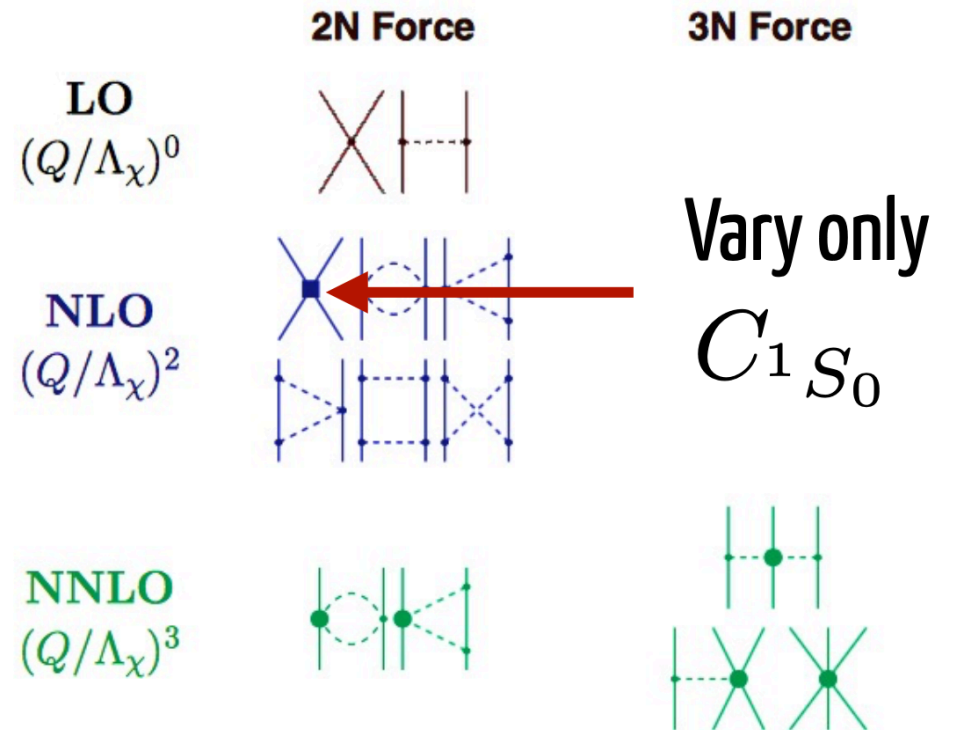


Emulating ab-initio coupled-cluster calculations

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

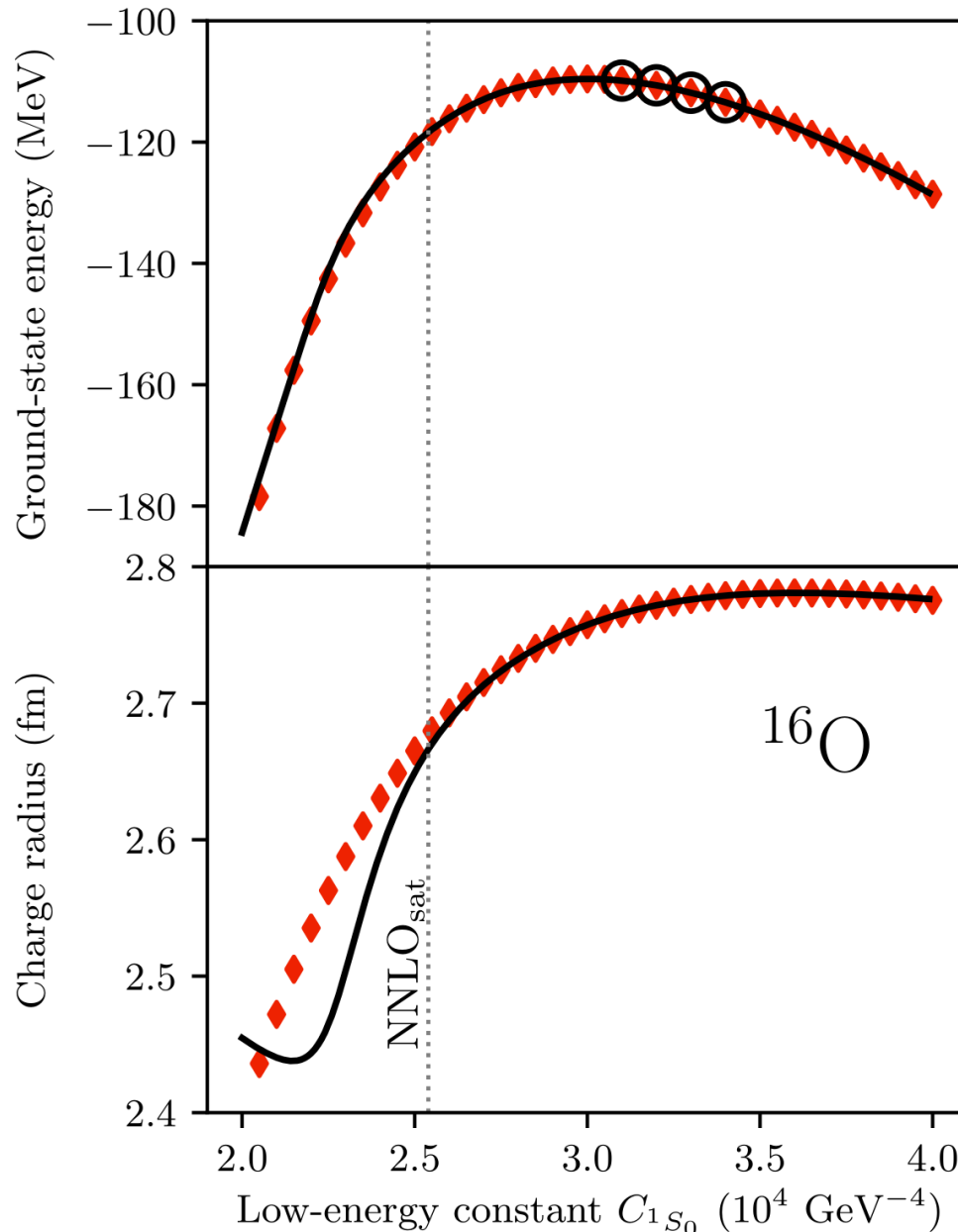


Exact coupled cluster calculations at the singles and doubles level

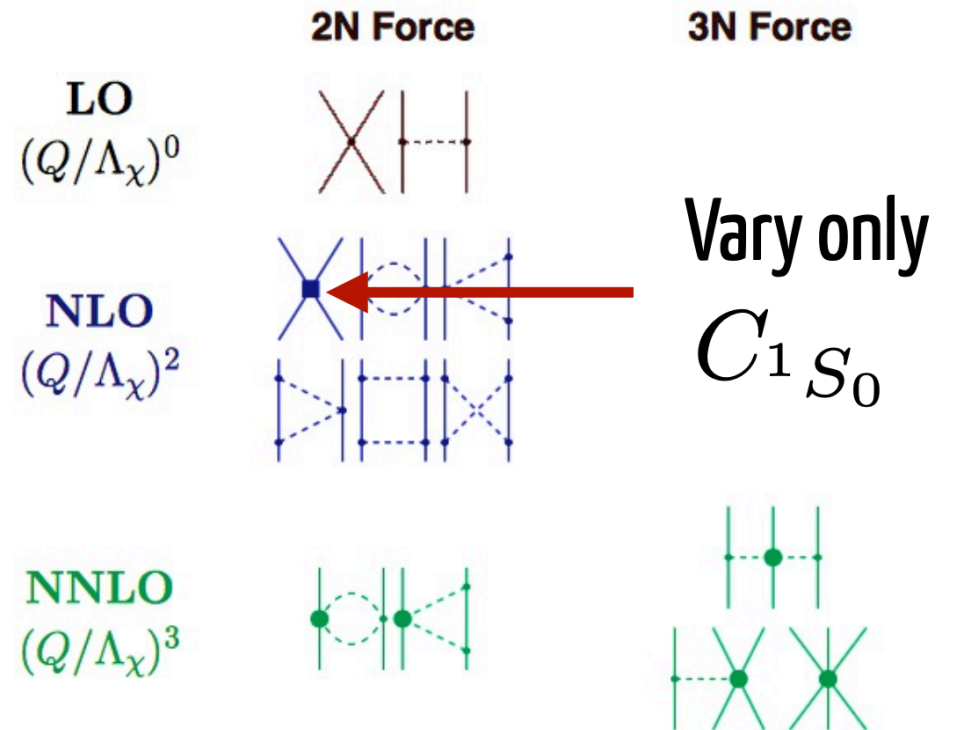


Emulating ab-initio coupled-cluster calculations

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

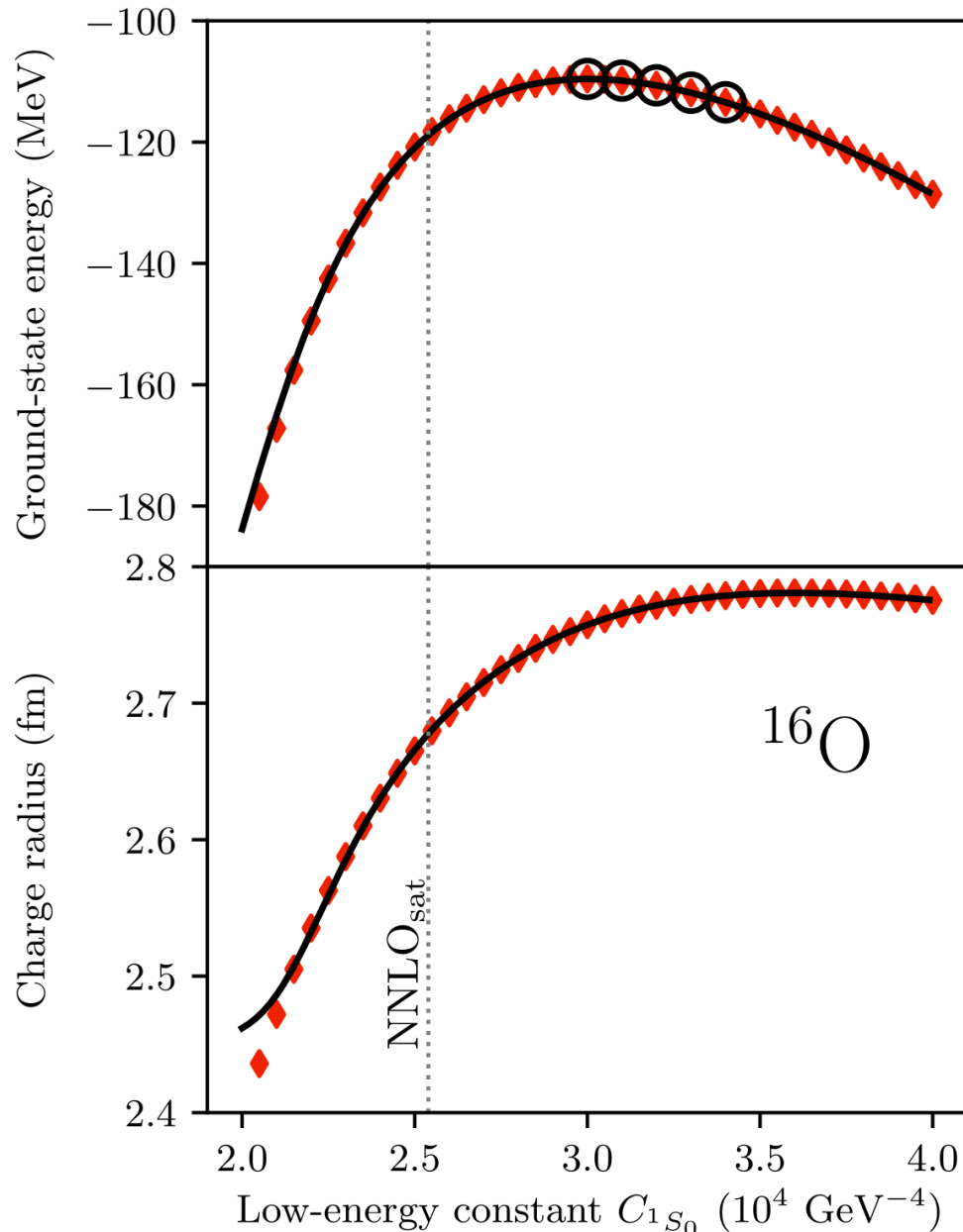


Exact coupled cluster calculations at the singles and doubles level

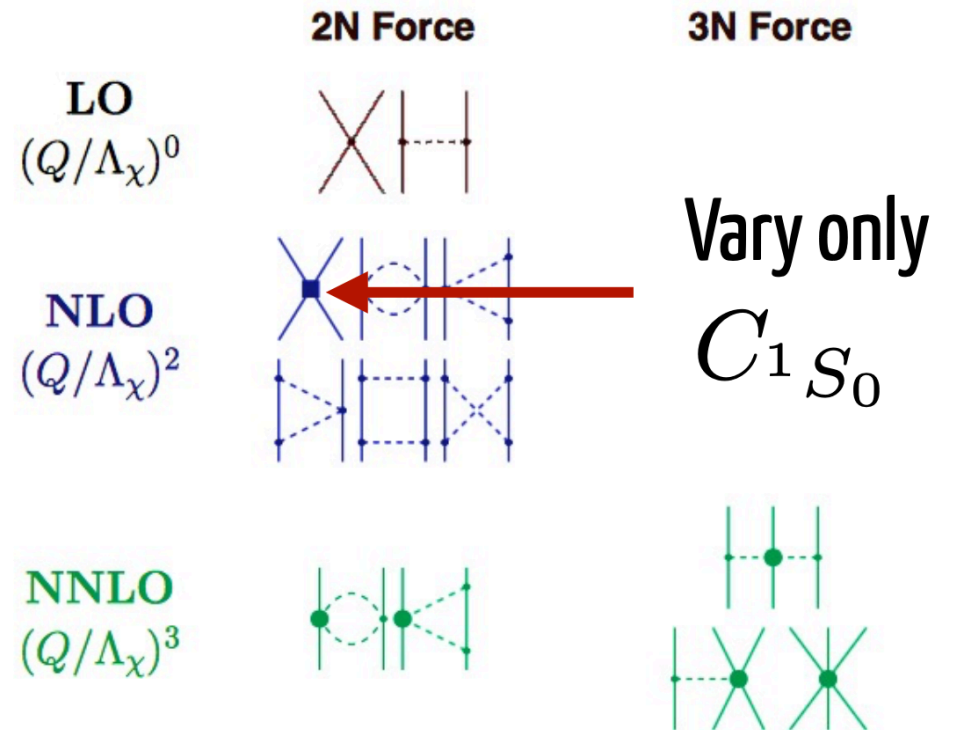


Emulating ab-initio coupled-cluster calculations

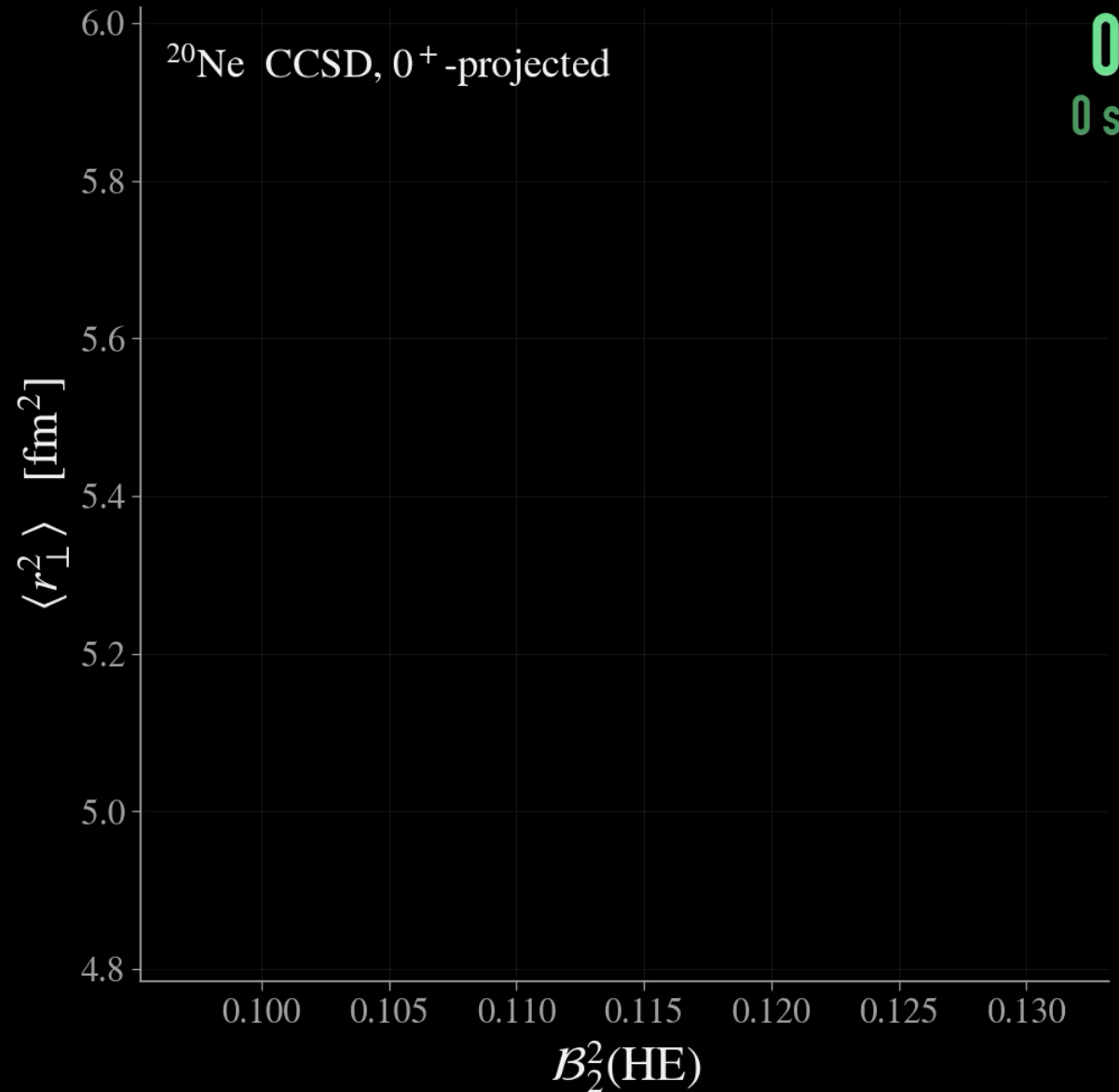
Andreas Ekström, Gaute Hagen PRL **123**, 252501 (2019)



Exact coupled cluster calculations at the singles and doubles level



Computing nuclei at lightning speed



(~1 min: ~**10⁵** 0⁺ projected calculations of ²⁰Ne)

Realtime speed of emulated transverse radius and shape parameter for different values of interaction parameters in ²⁰Ne

$$H(\vec{\alpha}) = \sum_{i=0}^{N_{\text{LECs}}=16} \alpha_i h_i$$

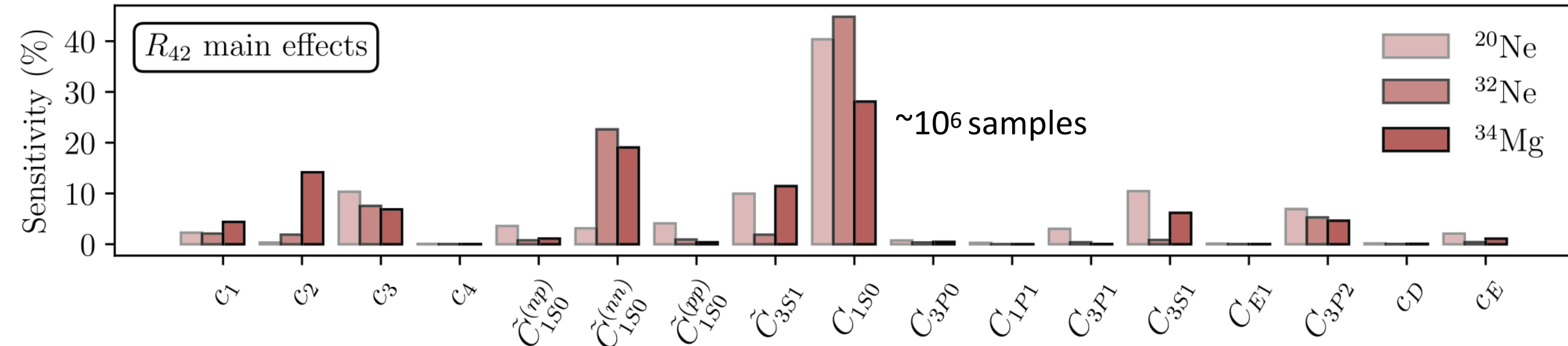
Accuracy: 1%

Speedup: 20 years of single node computations can be replaced by a one hour run on a laptop

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

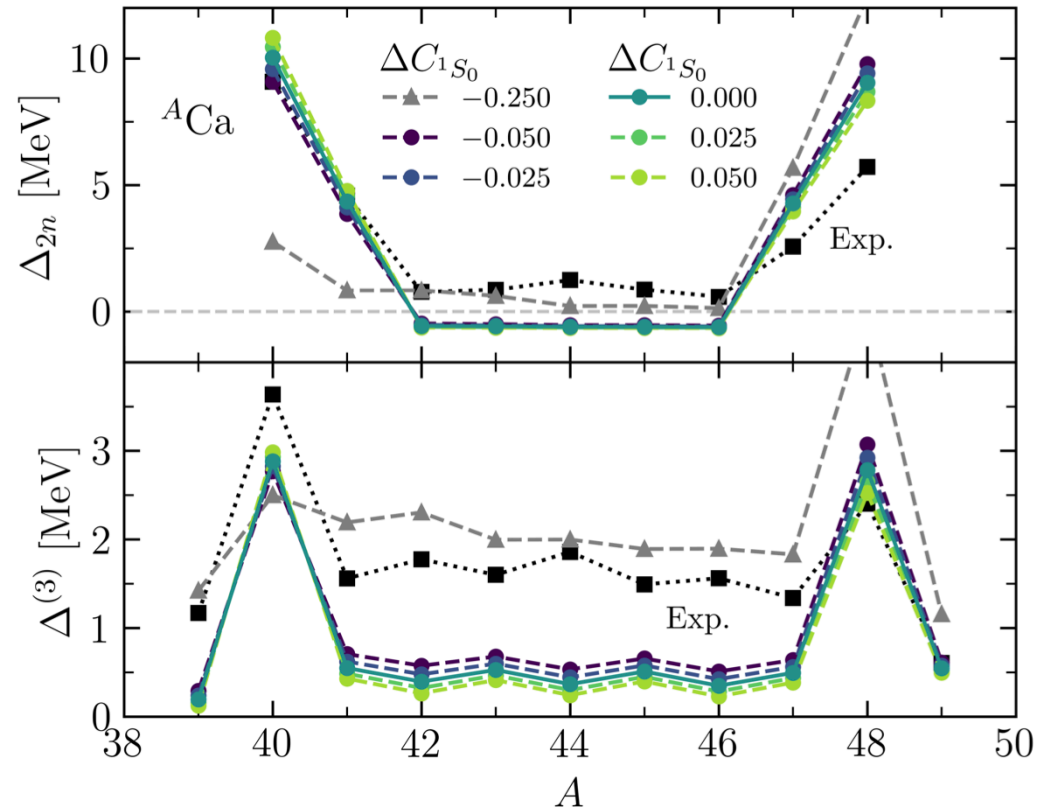
Linking deformation to nuclear forces

- 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

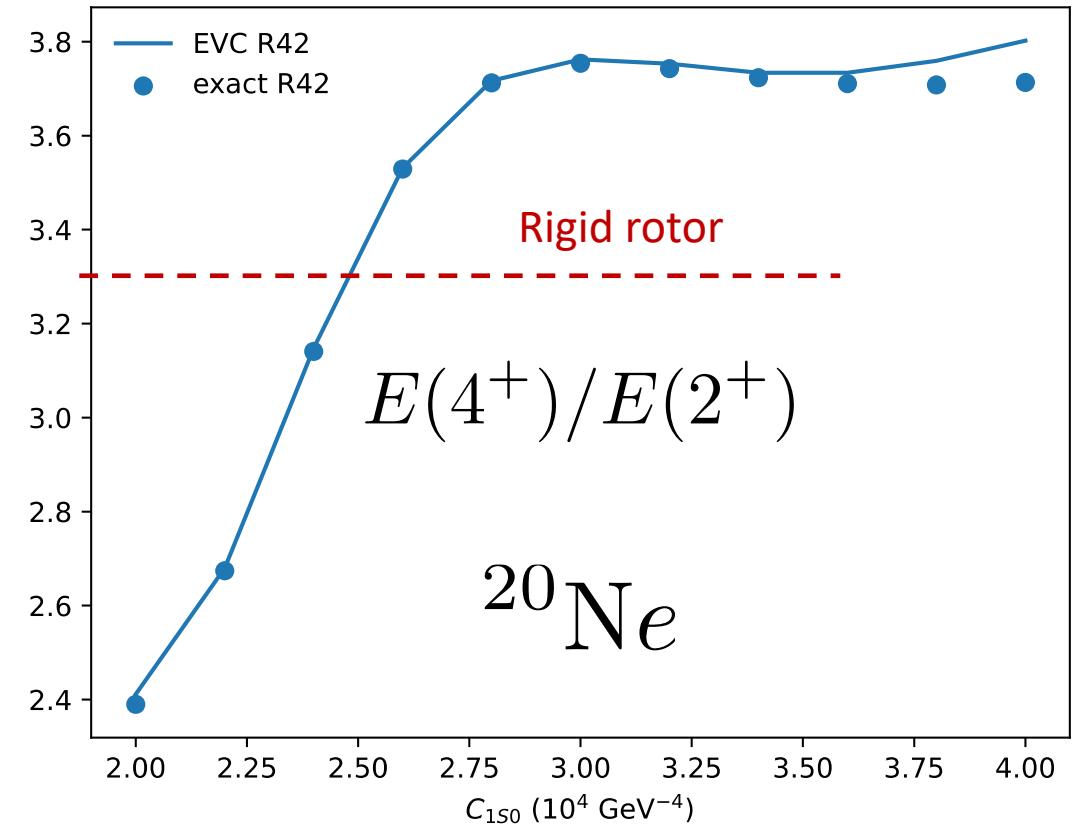


Linking deformation to nuclear forces

Varying only one parameter $C_1 S_0$



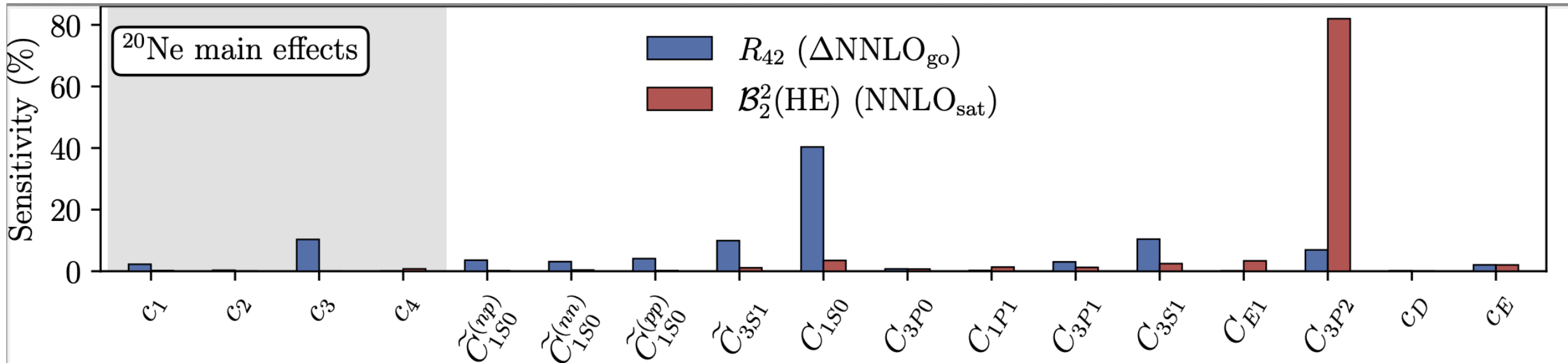
Two neutron shell gap and three point mass difference in calcium isotopes



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

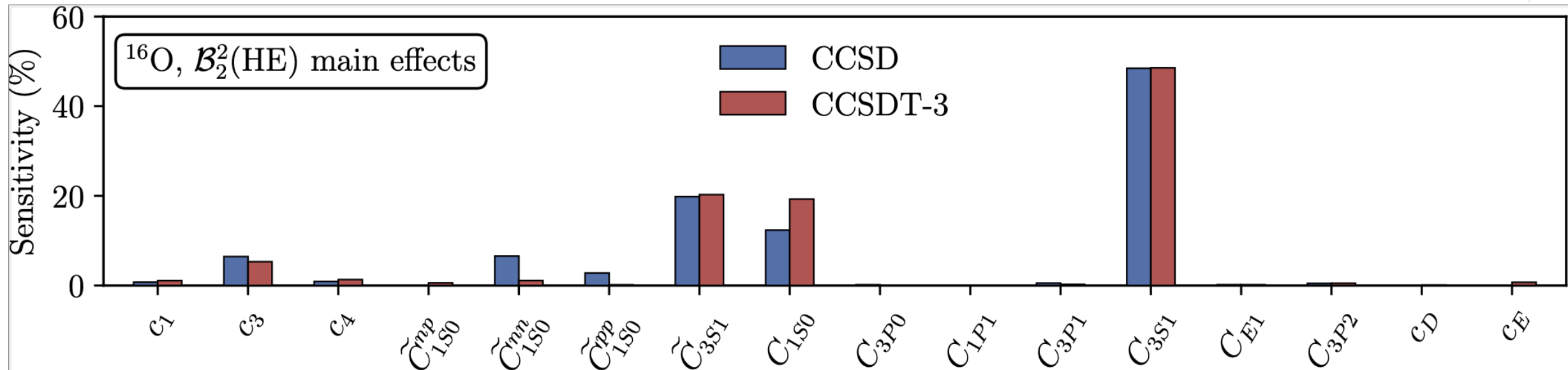
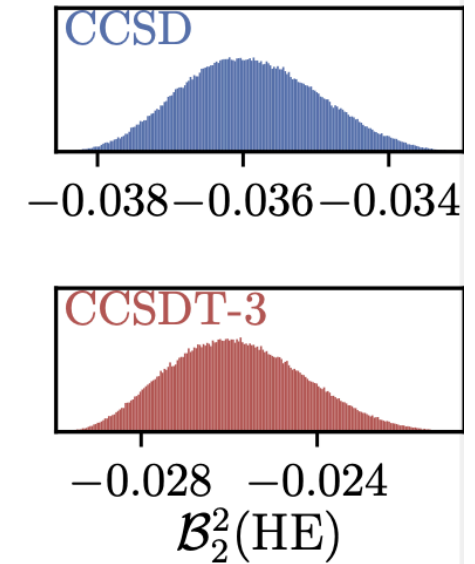
Linking deformation to nuclear forces

- $\mathcal{B}_2^2(\text{HE})$ is the deformation the collision sees: $\langle \delta \varepsilon_2^2 \rangle \approx 1/A + (3/4\pi) \cdot \mathcal{B}_2^2(\text{HE})$, and $\mathcal{B}_2^2(\text{HE}) = \beta_{20}^2$ for a rigid rotor.
- R_{42} and $\mathcal{B}_2^2$ respond to different LECs: C_{1S0} carries 40% of R_{42} but 4% of $\mathcal{B}_2^2$; C_{3P2} carries 7% of R_{42} but 82% of $\mathcal{B}_2^2$
- The P-wave contacts carry the two-body spin-orbit force, ${}^3P_2$ strongest. Spin-orbit sets the sd-shell ordering and so the quadrupole strength; pairing (${}^1S_0$) sets the level spacings that R_{42} measures



Linking deformation to nuclear forces

- In contrast to ^{20}Ne the sensitivity of $\mathcal{B}_2^2(\text{HE})$ in ^{16}O is dominated by the 3S1 partial wave
- The sensitivity analysis is robust with respect to many-body truncations in the coupled-cluster wave-function



Summary

Breaking and restoring symmetries

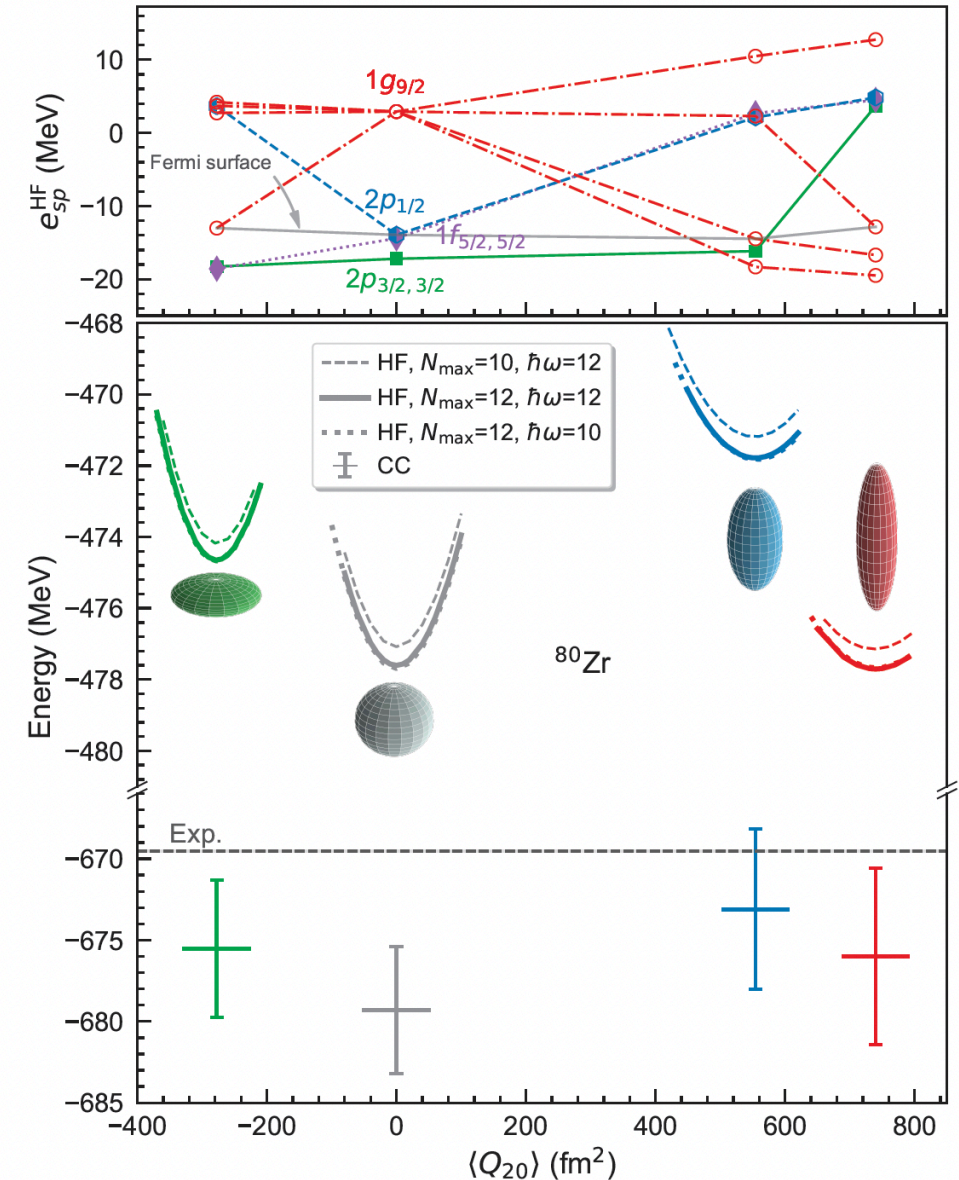
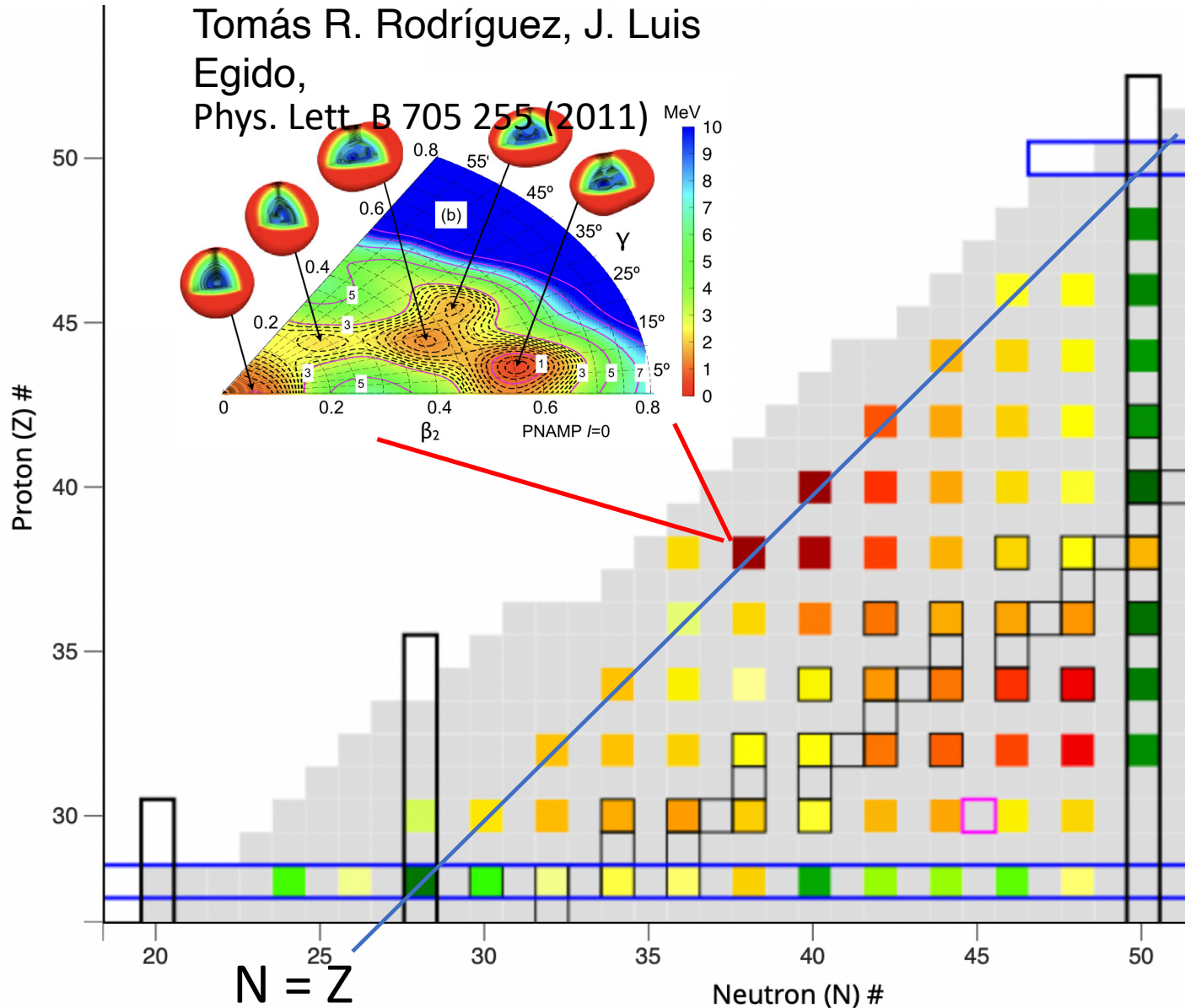
Exploits separation of scale between collective and specific UV physics

Conceptually simple & computationally affordable

- Shape coexistence in ^{30}Ne and ^{32}Mg
- Much improved $B(E2)$ values with no effective charges in ^{3x}Ne , ^{3x}Mg
- Connected deformation to microscopic forces
- Shape parameter in ^{20}Ne probe $^3P_2$ — complementary to R_{42}
- Challenges: many-body UQ, beyond quadrupole shape parameters, deformed heavy mass nuclei...

Strongly deformed nuclei around ^{80}Zr

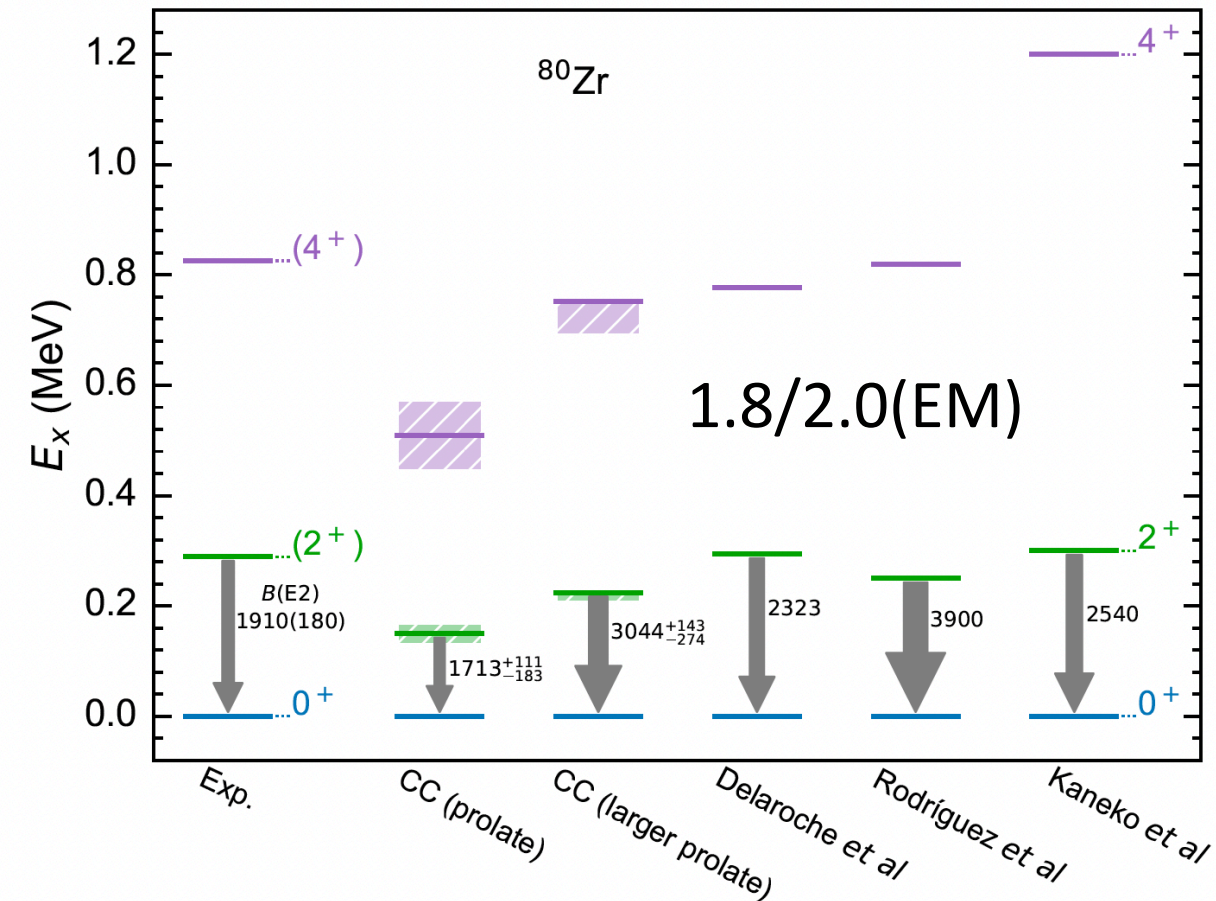
Tomás R. Rodríguez, J. Luis Egido,
Phys. Lett. B 705 255 (2011)



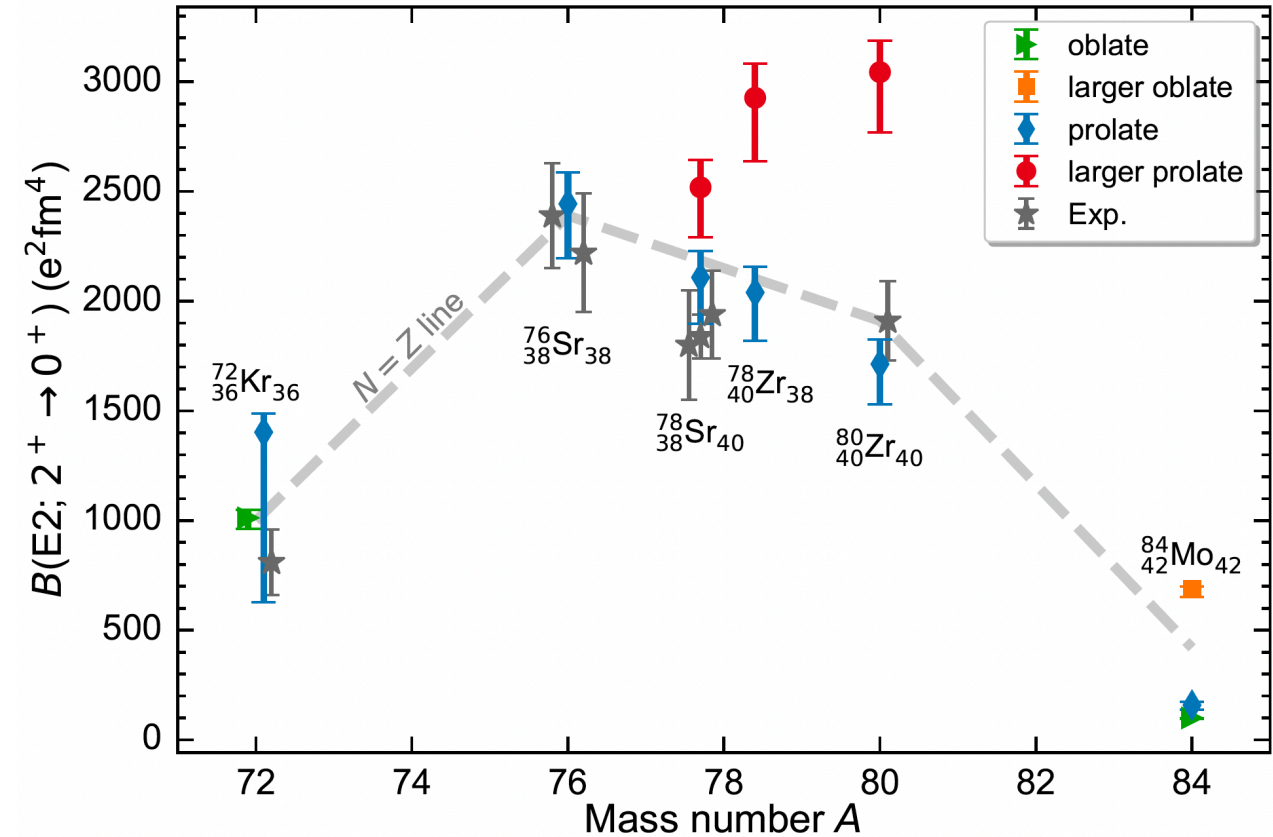
Baishan Hu, Zhonghao Sun, G. Hagen, T. Papenbrock.
Phys. Rev. C **110**, L011302 (2024)

Strongly deformed nuclei around ^{80}Zr

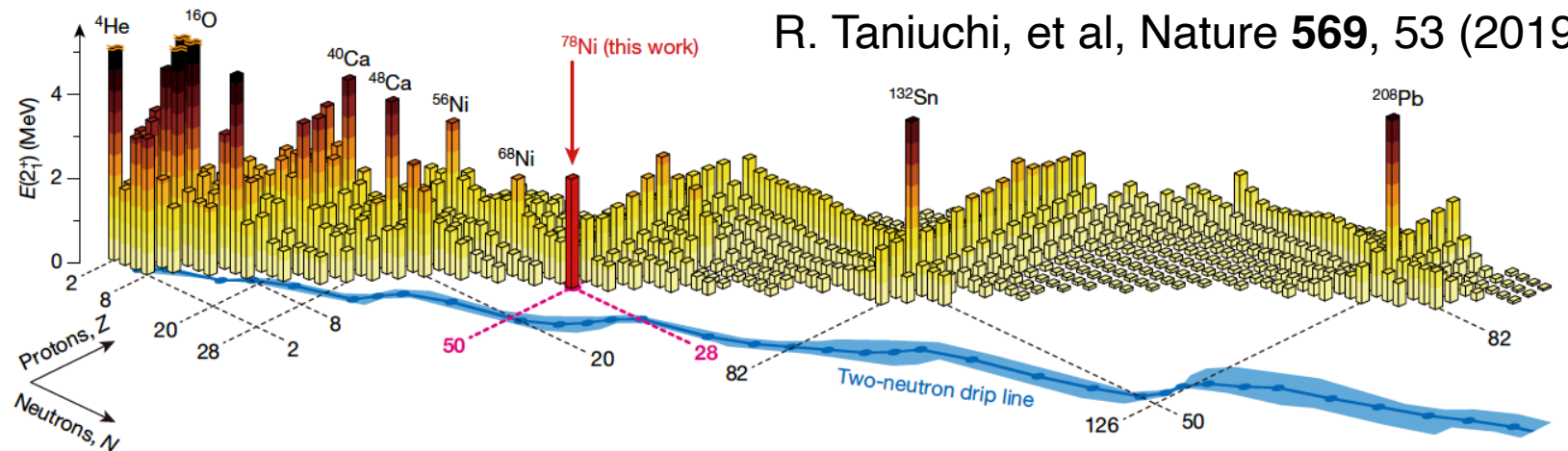
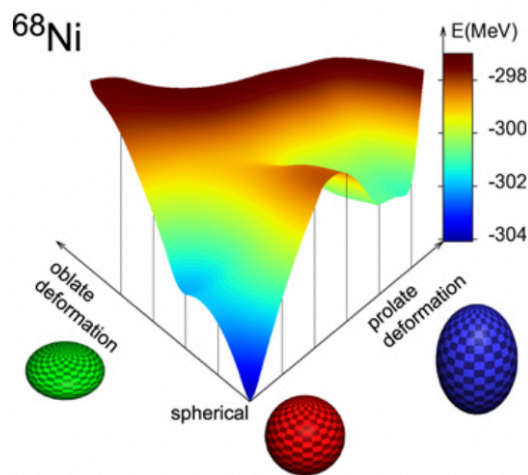
Spectrum prefers larger prolate shape



$B(E2)$ prefers prolate band

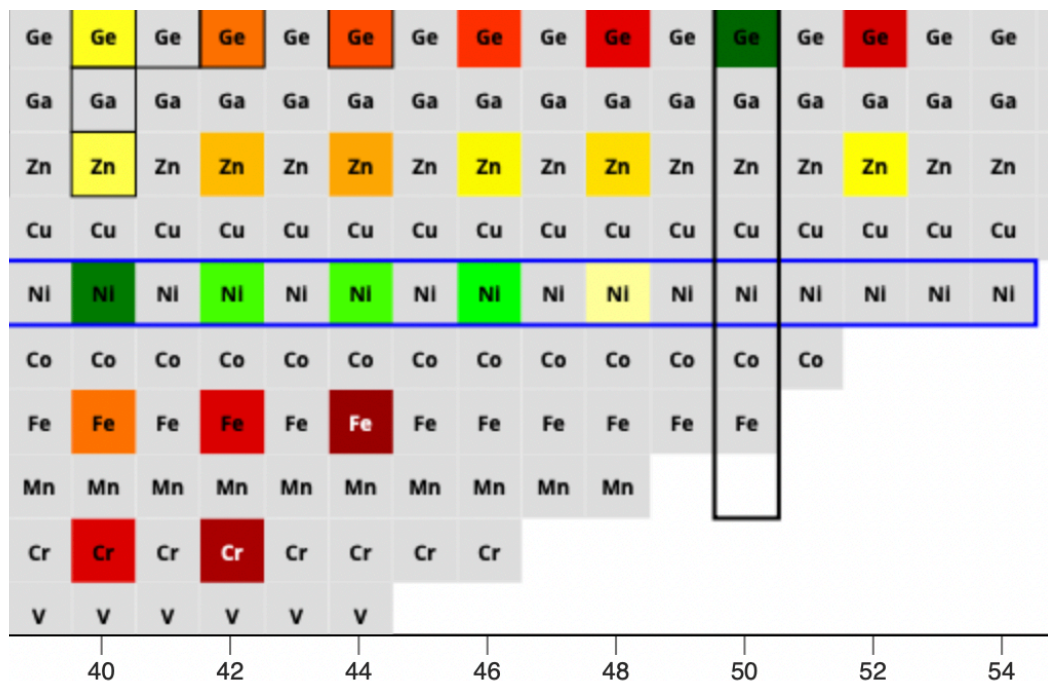


Shape co-existence in ^{78}Ni ?

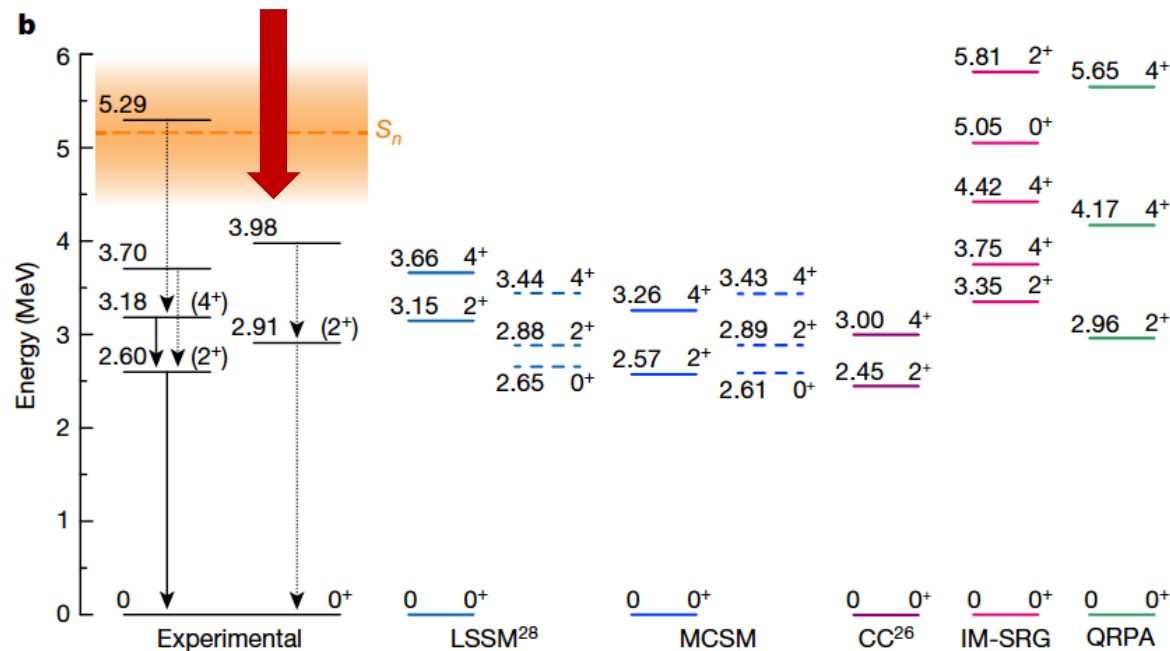


R. Taniuchi, et al, Nature **569**, 53 (2019)

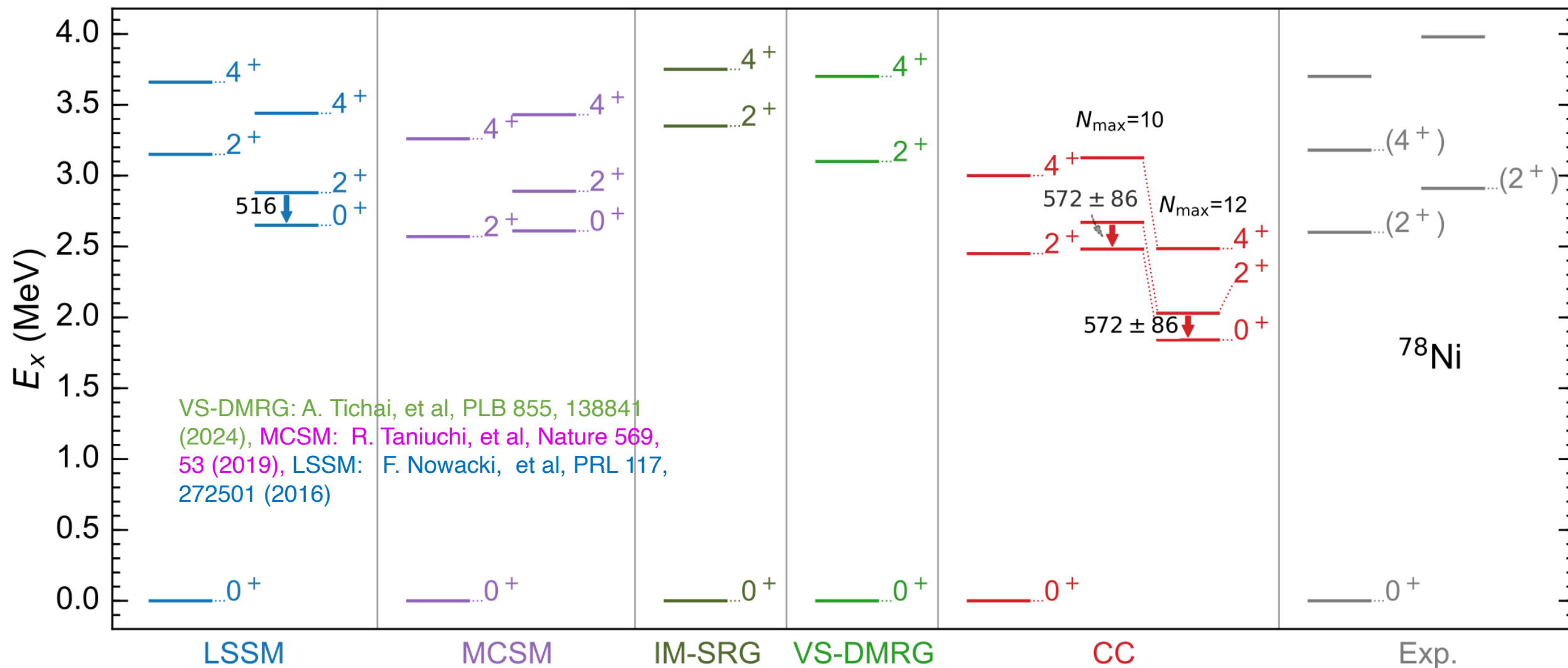
T Otsuka and Y Tsunoda *J. Phys. G* **43** 024009 (2016)



Deformed band?
Where is the band head?



Shape co-existence in ^{78}Ni ?



Convergence of coupled-cluster method

$$C_1 = T_1,$$

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

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

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

$\vdots,$

CCSD

CCSDT

Exact CI:

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

- 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!

