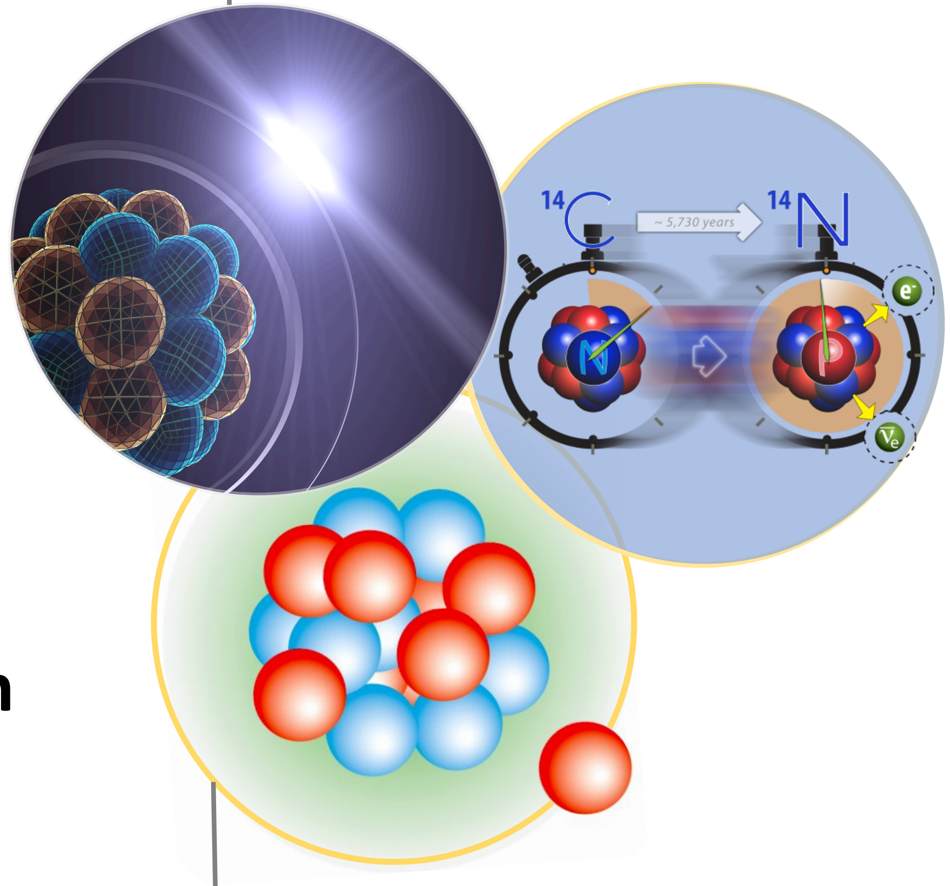
Calcium dripline from a new chiral interaction

Gaute Hagen
Oak Ridge National Laboratory

PAINT 2026 – Workshop on Progress in Ab Initio Nuclear Theory

TRIUMF, February 27th, 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
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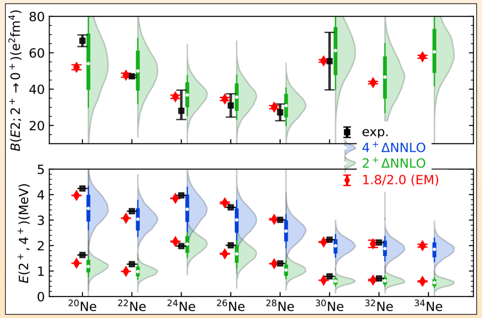
Thank you for making this another successful workshop!

Some interactions work "better" than others

"Magic" utilize regulator and SRG off-shell freedom

K. Hebeler, et al. (2011)

N³LO-NN (SRG evolved) N²LO-3N fit LECs

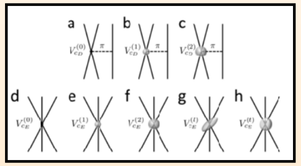


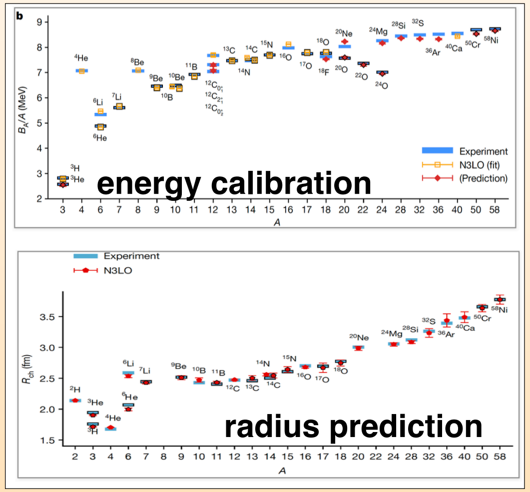
Accurate binding energies and spectra

Z. Sun, et al. (2025) and many more

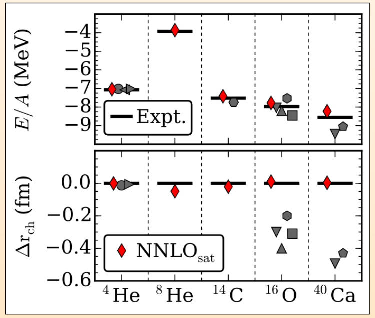
Nuclear lattice EFT with promoted 3N terms

S. Elhatisari et al. (2024)



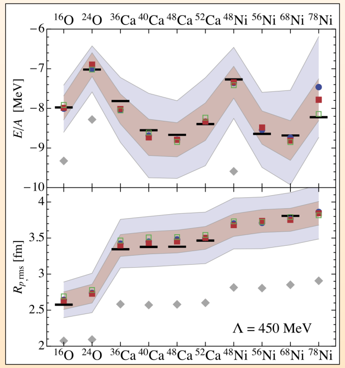


Optimization with ¹⁶O energy (and radius)



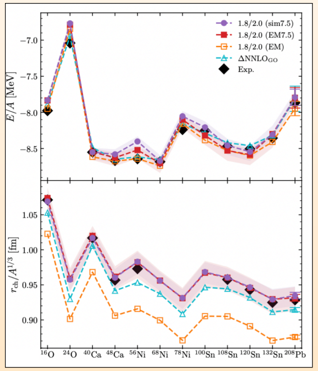
NNLOsat

A. Ekström et al. (2015)



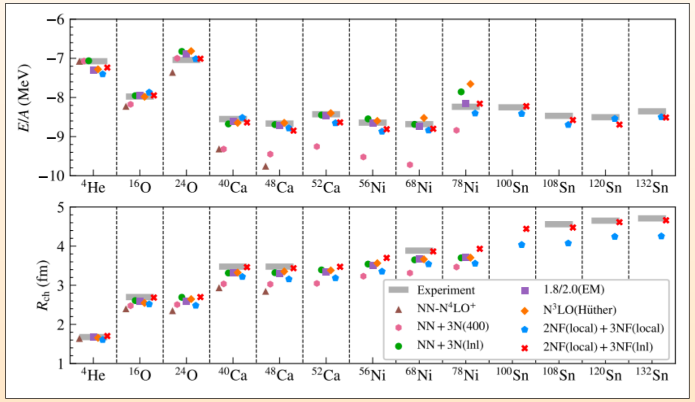
Order-by-order family

T. Hüther et al. (2020)



"Magic interaction" family

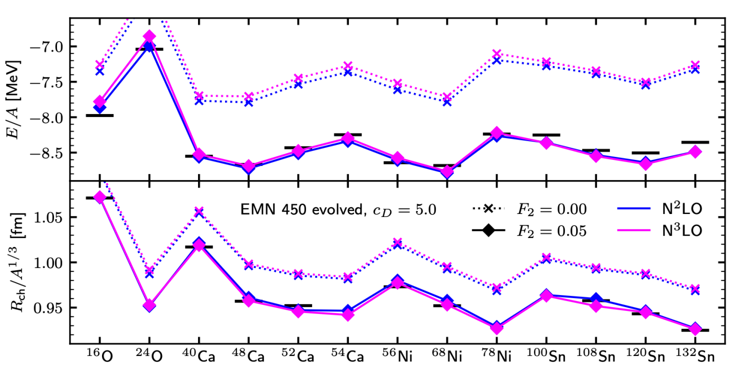
P. Arthuis, et al. (2024)



Local-non-local regulators

R.Z. Hu et al. (2026)

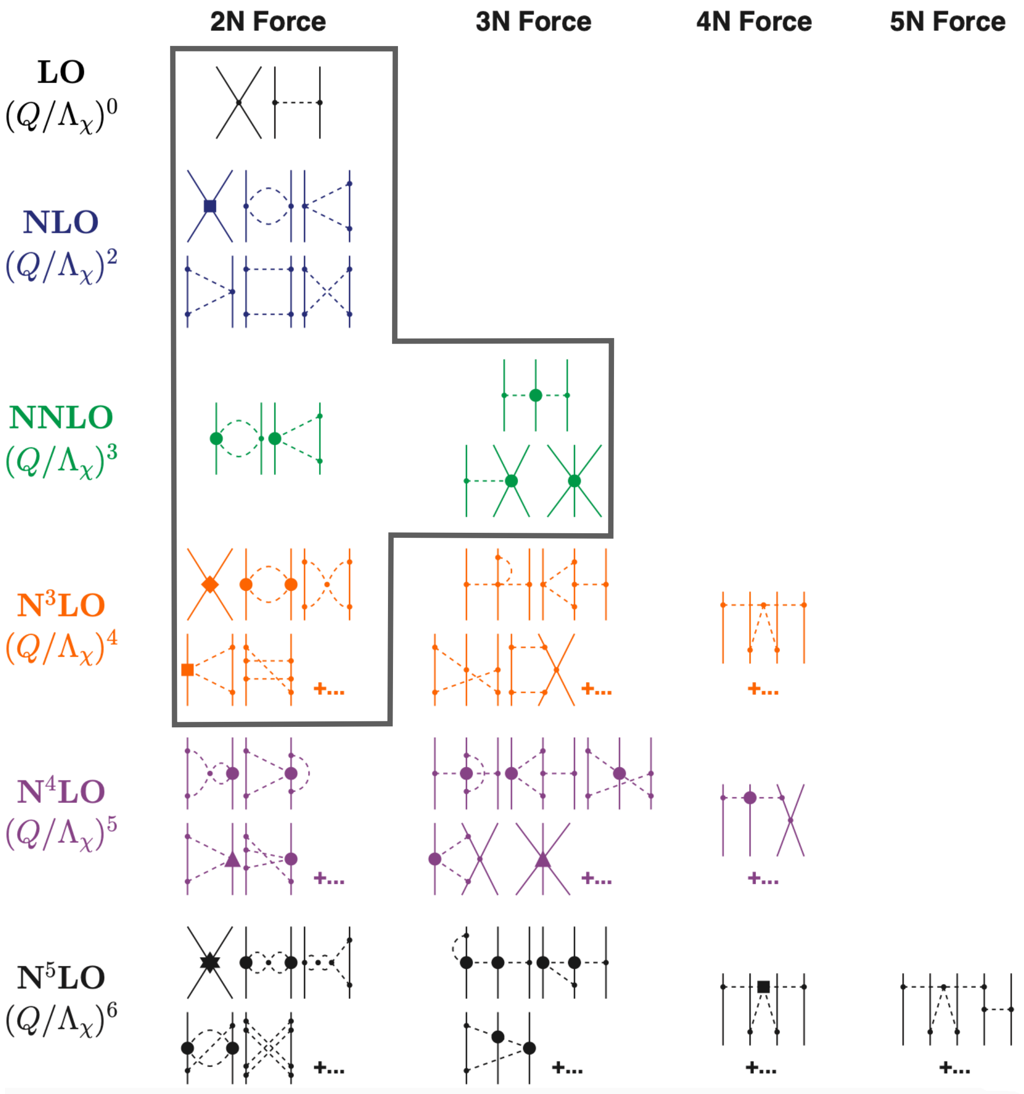
N³LO-NN (local, SRG) N²LO-3N fit LECs (lnl)

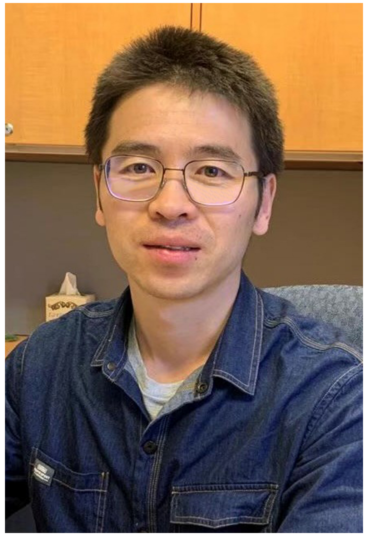


Quark mass dependent 3NFs

Urban Vernik, et al arXiv:2512.20454 (2025)

N3LO$_{\text{Texas}}$

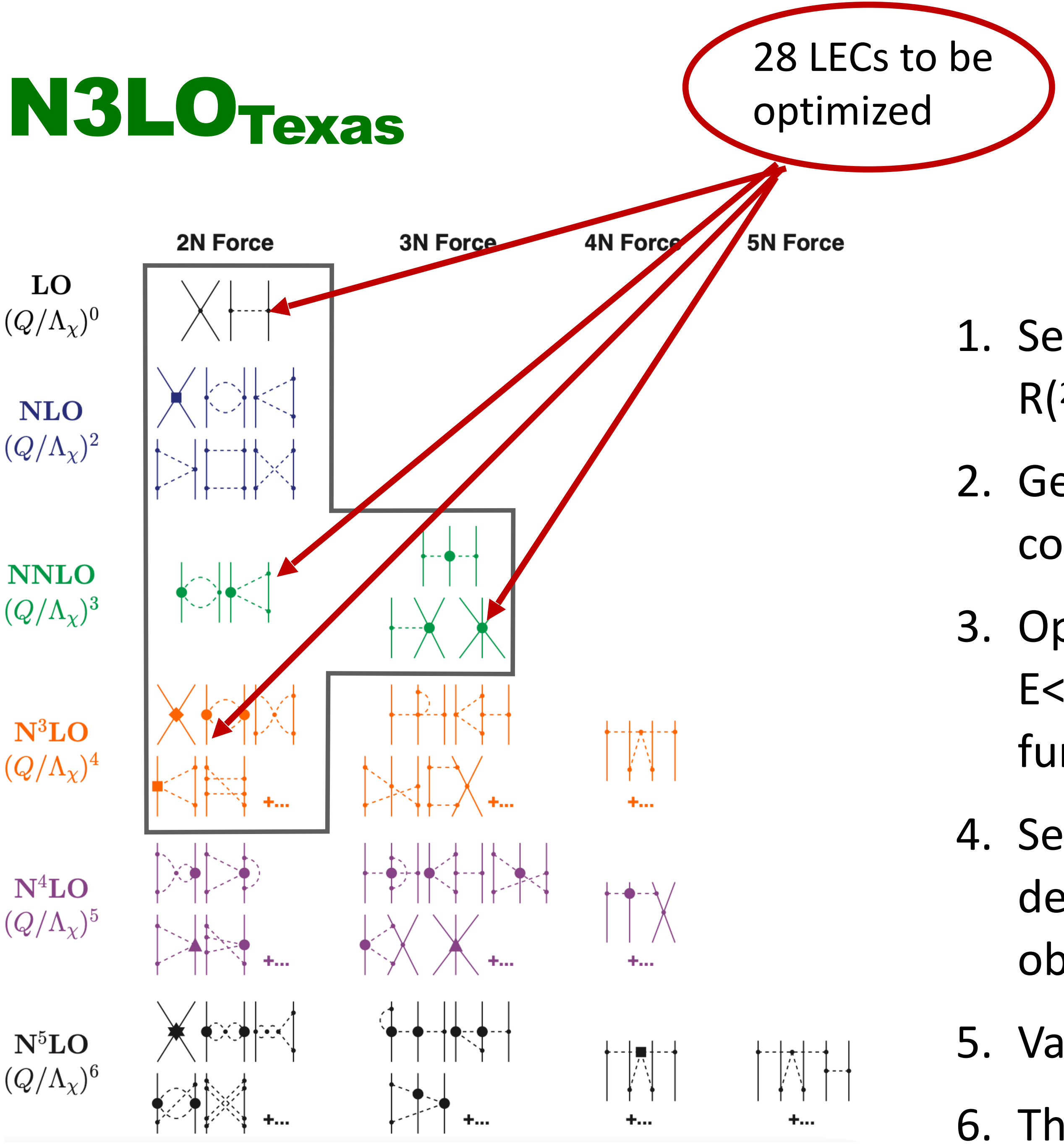




Baishan Hu
Texas A&M

Baishan Hu, A. Ekström, C. Forssén, G. Hagen, W. G. Jiang, T. Miyagi, T. Papenbrock
https://arxiv.org/abs/2512.11723

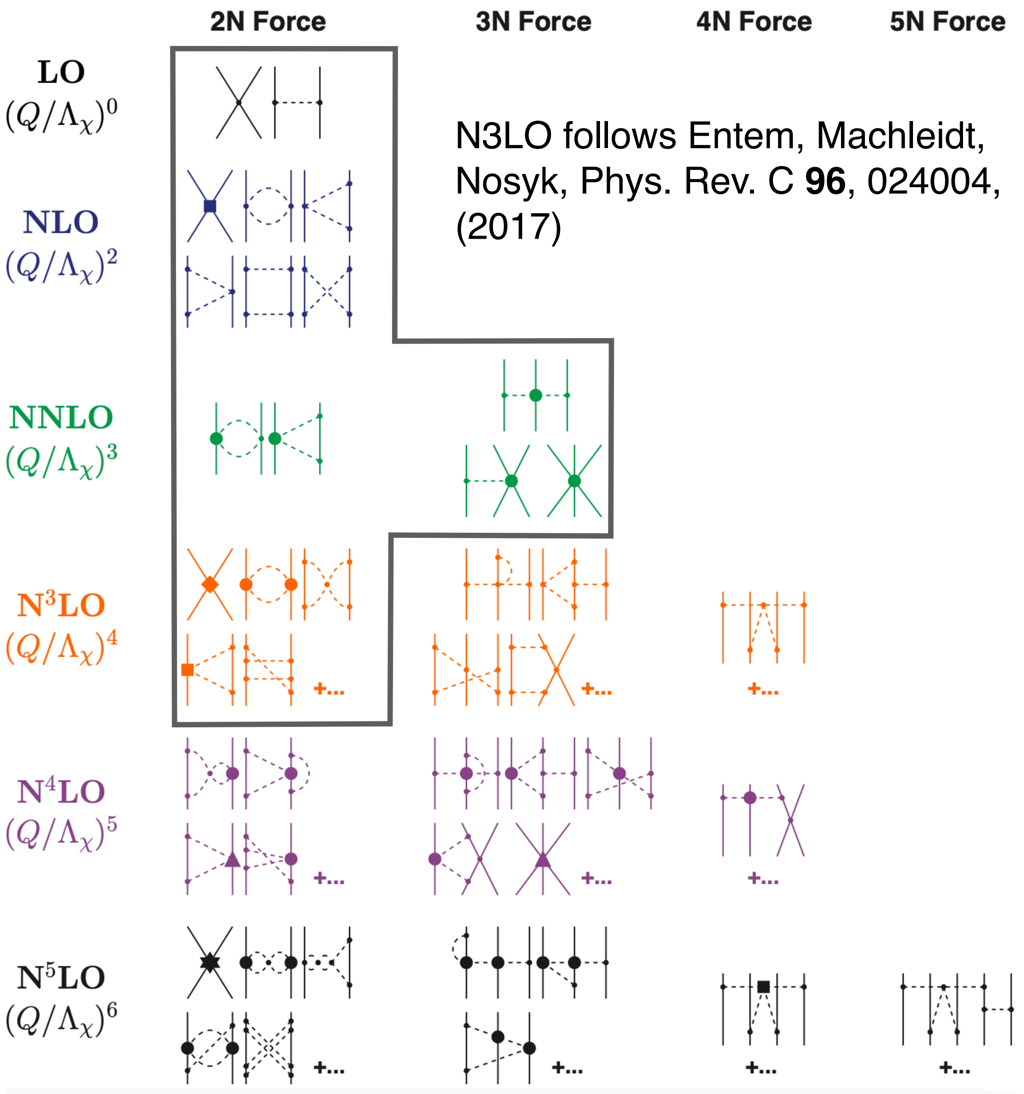
N3LO$_{\text{Texas}}$



Optimization strategy:

1. Setup emulators for np phase shifts, nn/pp, and E/R(^{2}H,^{4}He,^{16}O)
2. Generate 2000 random (LHS) points in space of 28 contact LECs (including cD and cE)
3. Optimize wrt L1 loss function (forgives outliers) for E<0 observables, heavy weight on R(^{16}O). L2 loss function (penalizes outliers) for phase shifts.
4. Select subset of 20 interactions that yield good description of phase shifts and A=2,4,16 observables.
5. Validate with gs energies of ^{22,24}O and ^{40,48}Ca.
6. The "greatest one" is N^{3}LO$_{\text{Texas}}$!

N3LOTexas



N3LO follows Entem, Machleidt, Nosyk, Phys. Rev. C **96**, 024004, (2017)

non-local momentum space regulators

$$\Lambda = 2\,\mathrm{fm}^{-1} = 394\,\mathrm{MeV}$$

$$f_\Lambda(p) = \exp\left[-\left(p^2/\Lambda^2\right)^{\{n=4\}}\right]$$

$$f_\Lambda(p,q) = \exp\left[-\left(\left(p^2 + 3/4q^2\right)/\Lambda^2\right)^{\{n=4\}}\right]$$

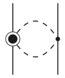
πN LECs according to Roy-Steiner analysis

$c_1\,[\mathrm{GeV}^{-1}]$	-1.07 ± 0.02	$\bar{d}_1 + \bar{d}_2\,[\mathrm{GeV}^{-2}]$	1.04 ± 0.06
$c_2\,[\mathrm{GeV}^{-1}]$	3.20 ± 0.03	$\bar{d}_3\,[\mathrm{GeV}^{-2}]$	-0.48 ± 0.02
$c_3\,[\mathrm{GeV}^{-1}]$	-5.32 ± 0.05	$\bar{d}_5\,[\mathrm{GeV}^{-2}]$	0.14 ± 0.05
$c_4\,[\mathrm{GeV}^{-1}]$	3.56 ± 0.03	$\bar{d}_{14} - \bar{d}_{15}\,[\mathrm{GeV}^{-2}]$	-1.90 ± 0.06

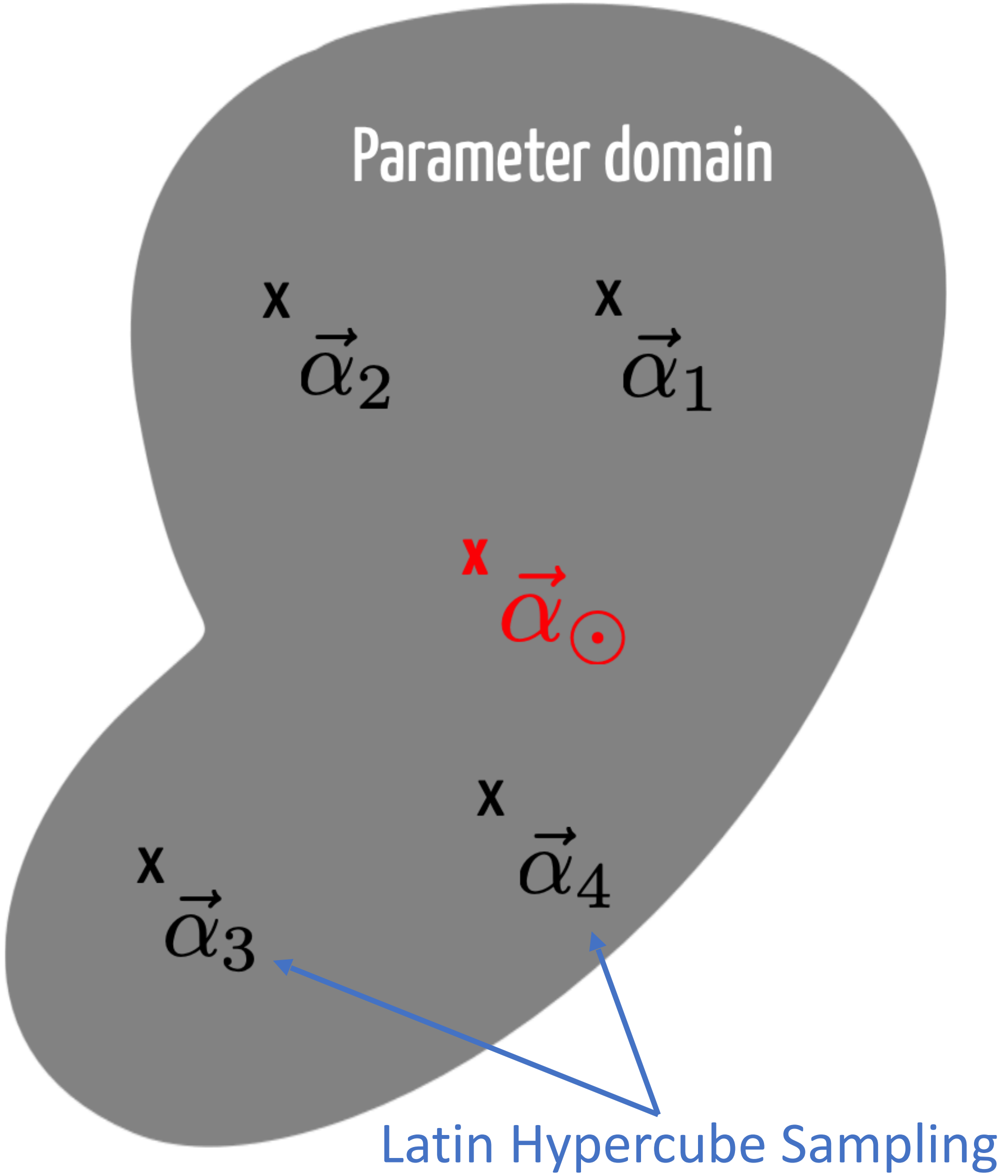
M. Hoferichter *et al.* Phys. Rev. Lett. **115**, 192301 (2015); Phys Rep. **625**, 1 (2016)

N3LO includes contacts $\widehat{D}_{^1S_0}, \widehat{D}_{^3S_1}, \widehat{D}_{^3S_1-^3D_1}$

N3LO 2π-exchange and “relativistic corrections”

$\frac{Q}{M_N} \sim \left(\frac{Q}{\Lambda_\chi}\right)^2$ We promote $V_{2\pi}^{(\mathrm{N4LO})} \propto \frac{c_i}{M_N}$  … to N3LO

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

$$H(\vec{\alpha}) = h_0 + \sum_{i=1}^{N_{\mathrm{LECs}=28}} \alpha_i h_i$$

- 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

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

Reduced order models for ab initio computations

Initial search domain

LEC	Min	Max	LEC	Min	Max
$\widetilde{C}^{pp}_{^1S_0}$	-0.30	-0.10	$\widetilde{C}^{np}_{^1S_0}$	-0.30	-0.10
$\widetilde{C}^{nn}_{^1S_0}$	-0.30	-0.10	$\widetilde{C}_{^3S_1}$	-0.30	-0.10
$C_{^1S_0}$	2.30	2.90	$C_{^3P_0}$	0.80	1.40
$C_{^1P_1}$	-1.00	1.00	$C_{^3P_1}$	-1.40	1.50
$C_{^3S_1}$	0.10	1.70	$C_{^3S_1-^3D_1}$	0.00	1.20
$C_{^3P_2}$	-2.10	2.40	$\widehat{D}_{^1S_0}$	-2.20	4.50
$D_{^1S_0}$	-28.00	-18.00	$D_{^3P_0}$	3.90	6.40
$D_{^1P_1}$	8.50	18.00	$D_{^3P_1}$	2.00	10.50
$\widehat{D}_{^3S_1}$	-9.70	9.30	$D_{^3S_1}$	-40.60	16.70
$D_{^3D_1}$	-8.20	4.50	$\widehat{D}_{^3S_1-^3D_1}$	-10.00	9.30
$D_{^3S_1-^3D_1}$	-7.40	10.00	$D_{^1D_2}$	-2.60	1.10
$D_{^3D_2}$	-8.00	-2.00	$D_{^3P_2}$	-3.00	15.30
$D_{^3P_2-^3F_2}$	-2.60	2.90	$D_{^3D_3}$	-3.00	1.00
c_D	-8.00	8.00	c_E	-8.00	8.00

Emulators reduces the computational cost of the optimization by several orders of magnitude and facilitates exploration across a broad LEC parameter domain

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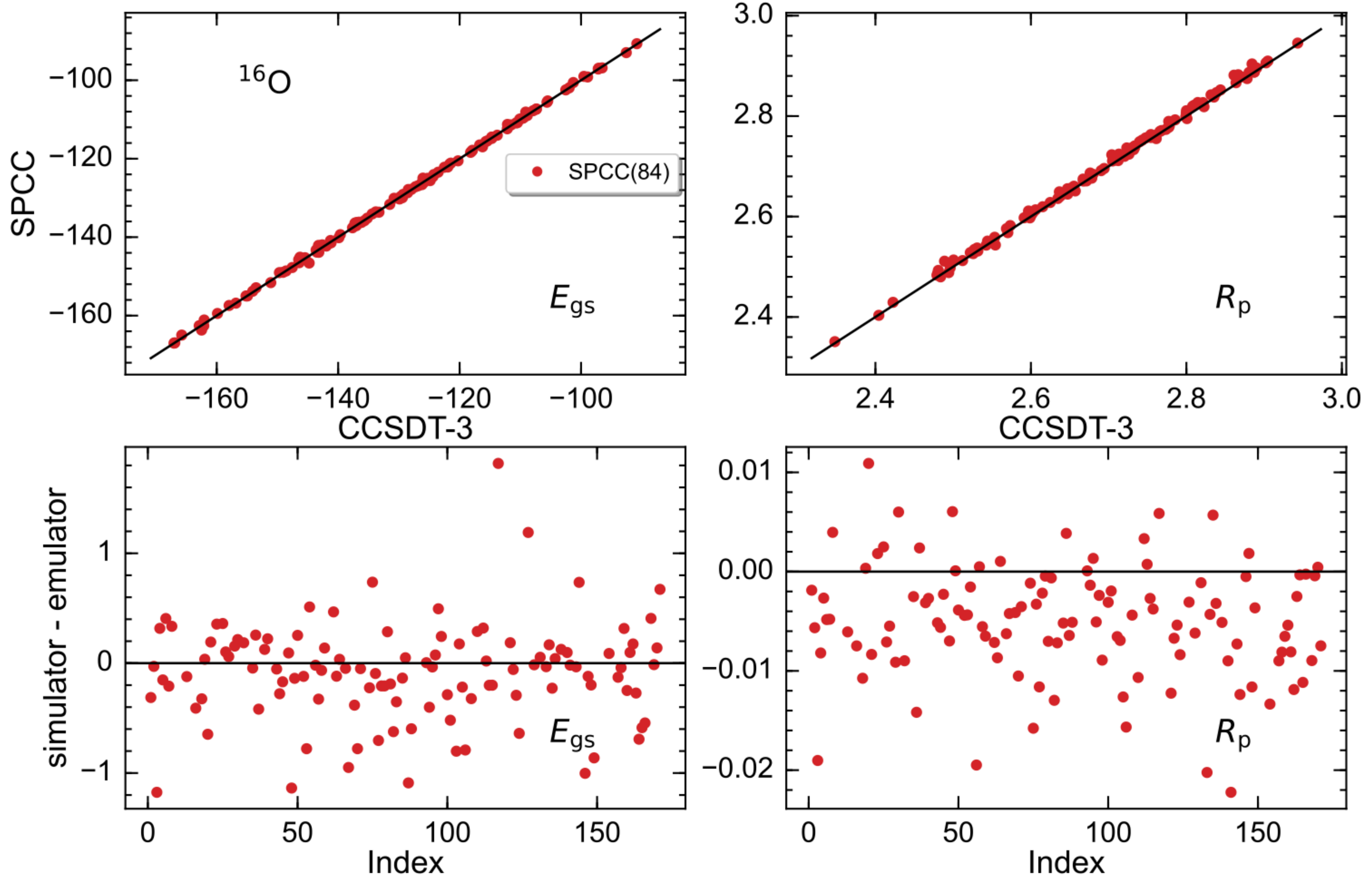
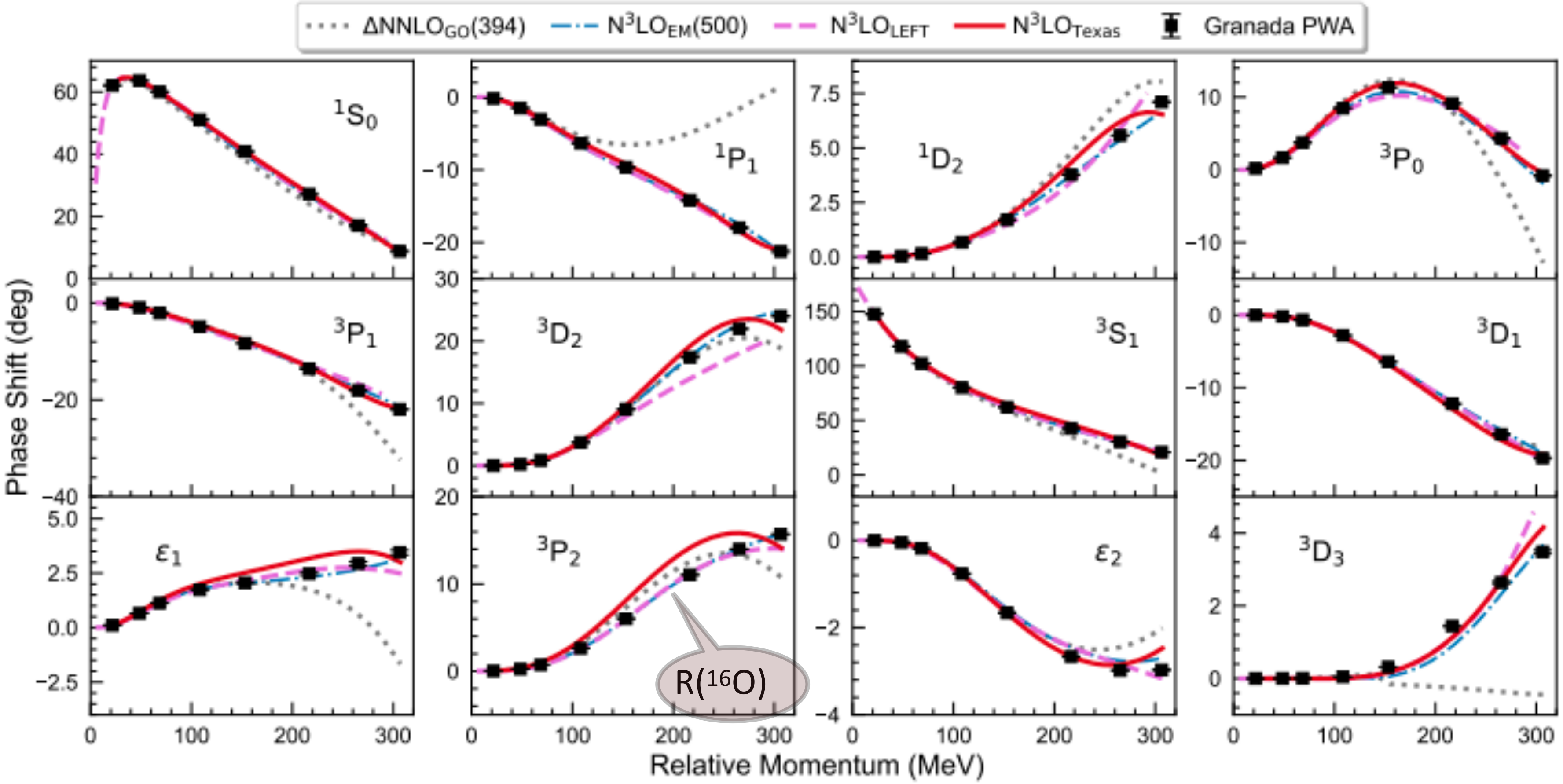
$$\mathbf{H}(\vec{\alpha}_{\odot})\,\vec{c} = E(\vec{\alpha}_{\odot})\,\mathbf{N}\,\vec{c},$$

Cross-validation of SPCC

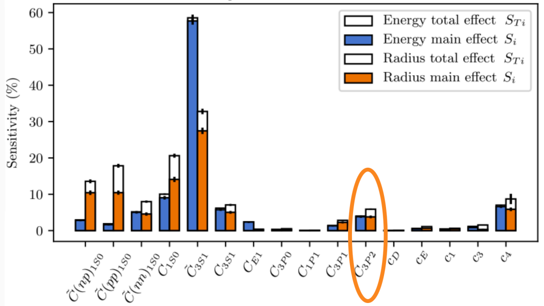


Baishan Hu et al, arXiv:2512.11723 (2025)

N^3LO_{Texas} accuracy: NN scattering



Ekström and Hagen (2019)



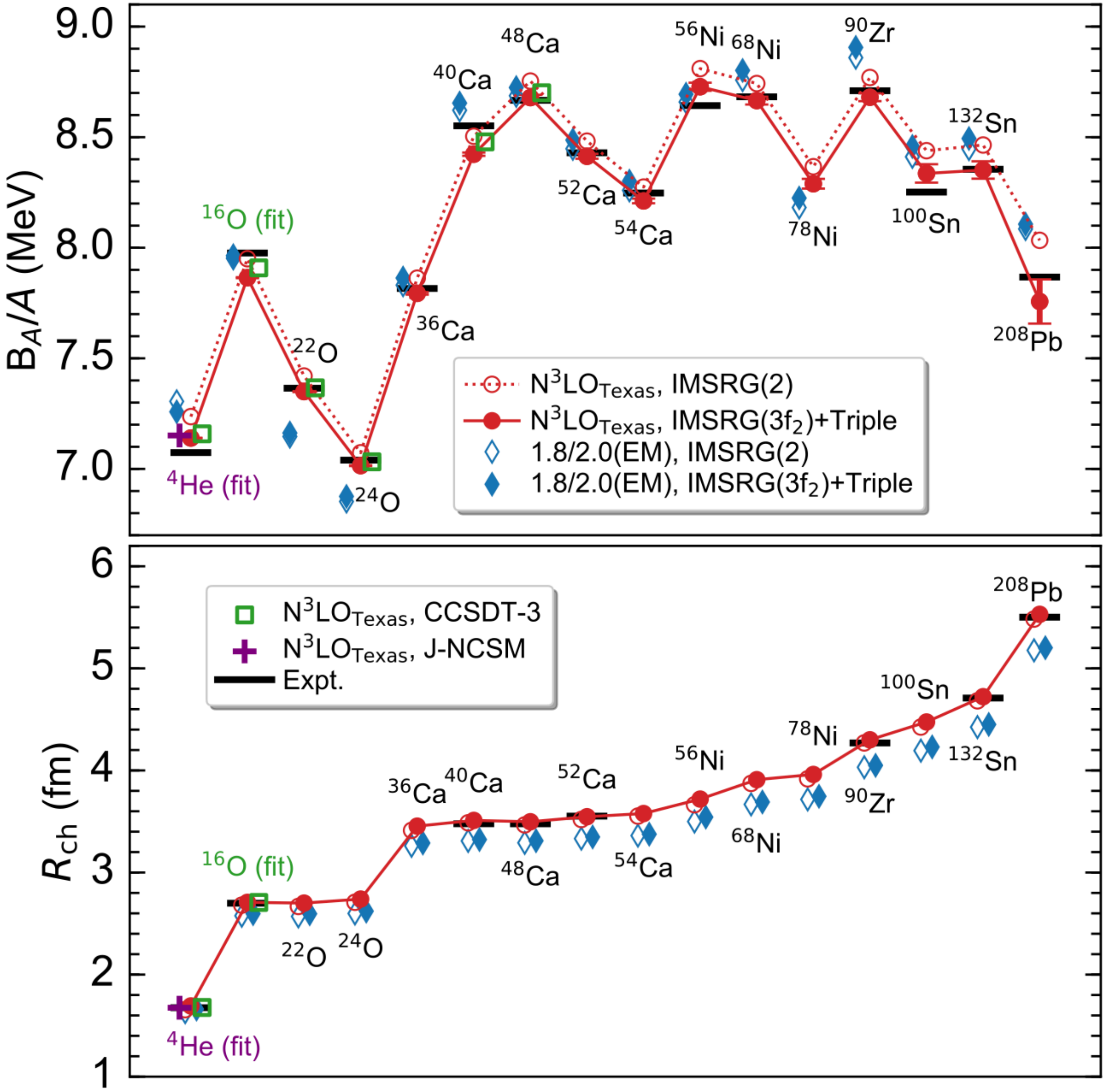
Some tension between the $^3P_2$ *NN* scattering phase shifts and radius of ^{16}O

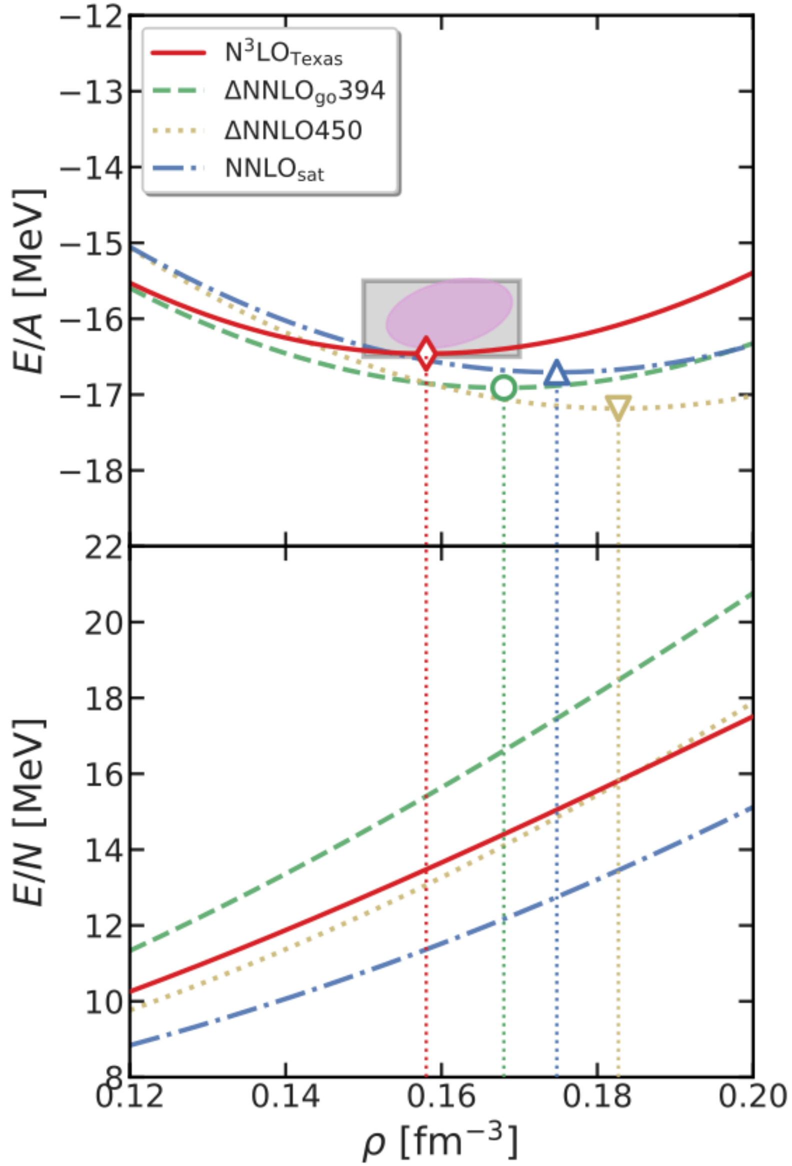
Optimization / Validation / Prediction

		N^3LO_{Texas}	Exp.
Optimization	a_{pp}^C	−7.820	−7.8196(26)[a]
	r_{pp}^C	2.757	2.790(14)[a]
	a_{nn}	−18.950	−18.95(40)
	r_{nn}	2.794	2.75(11)
	a_{np}	−23.741	−23.740(20)
	r_{np}	2.681	2.77(5)
	$E_{gs}(^2H)$	−2.225	−2.224575(9)
	$R_{ch}(^2H)$	2.131	2.1421(88)
	$Q(^2H)$	0.27	0.27[b]
	$P_D(^2H)$	2.68%	–
	$E_{gs}(^4He)$	−28.61	−28.2957
	$R_{ch}(^4He)$	1.675	1.6775(28)
	$E_{gs}(^{16}O)$	−126.54	−127.6193
	$R_{ch}(^{16}O)$	2.707	2.6991(52)
Validation	$E_{gs}(^{22}O)$	−162.06	−162.0272(572)
	$E_{gs}(^{24}O)$	−168.77	−168.9525(1680)
	$E_{gs}(^{40}Ca)$	−339.15	−342.0522
	$E_{gs}(^{48}Ca)$	−417.63	−416.0012

Prediction	$E_{gs}(^3H)$	−8.50	−8.4818
	$R_{ch}(^3H)$	1.769	1.7591(363)
	$E_{gs}(^3He)$	−7.76	−7.7180
	$R_{ch}(^3He)$	1.967	1.9661(30)
	$E_{2^+}(^{22}O)$	3.28(7)	3.199
	$E_{2^+}(^{24}O)$	4.05(11)	4.760
	$E_{gs}(^{78}Ni)$	−647(2)	−642.5640(3900)[c]
	$R_{ch}(^{78}Ni)$	3.961	–
	$E_{gs}(^{132}Sn)$	−1102(5)	−1102.8432(19)
	$R_{ch}(^{132}Sn)$	4.723	4.7093(76)
	$E_{gs}(^{208}Pb)$	−1613(21)	−1636.4302(12)
	$R_{ch}(^{208}Pb)$	5.530	5.5012(13)

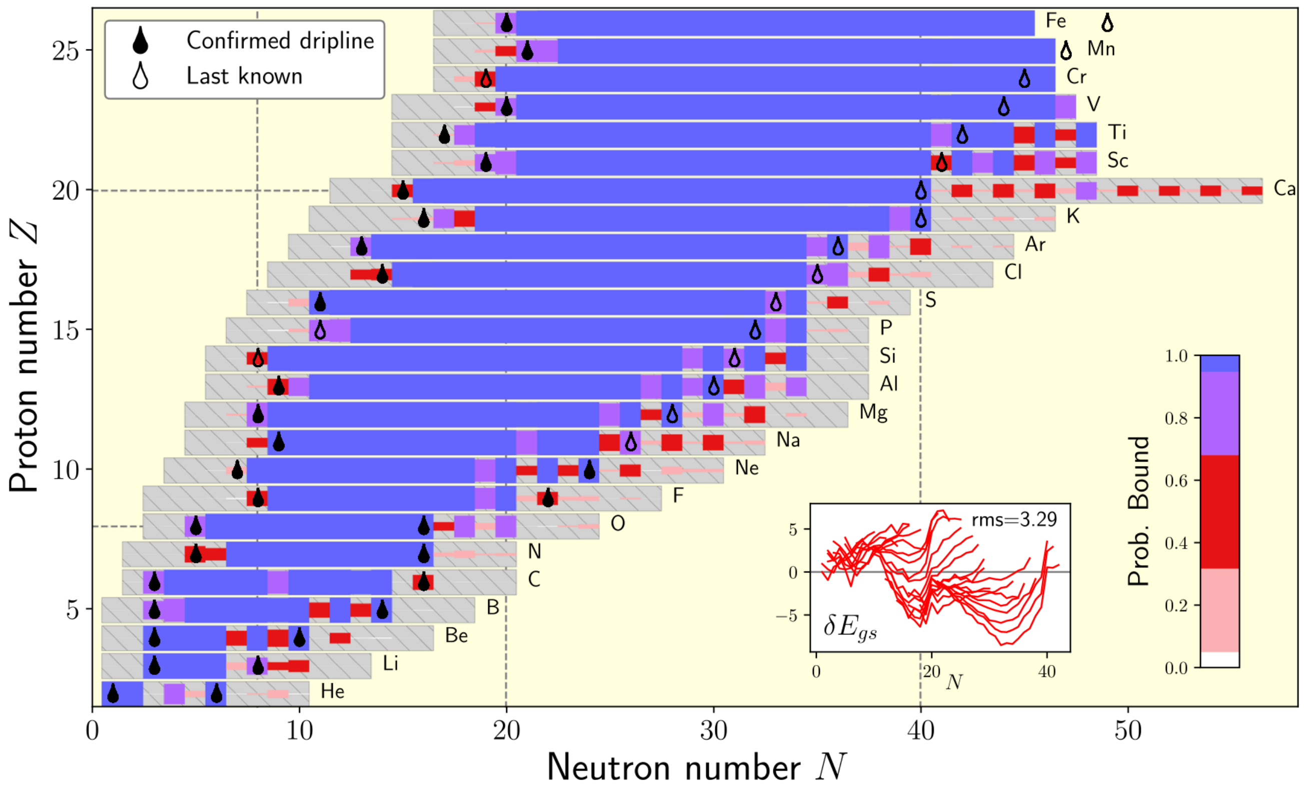
Saturation properties of nuclei and nuclear matter



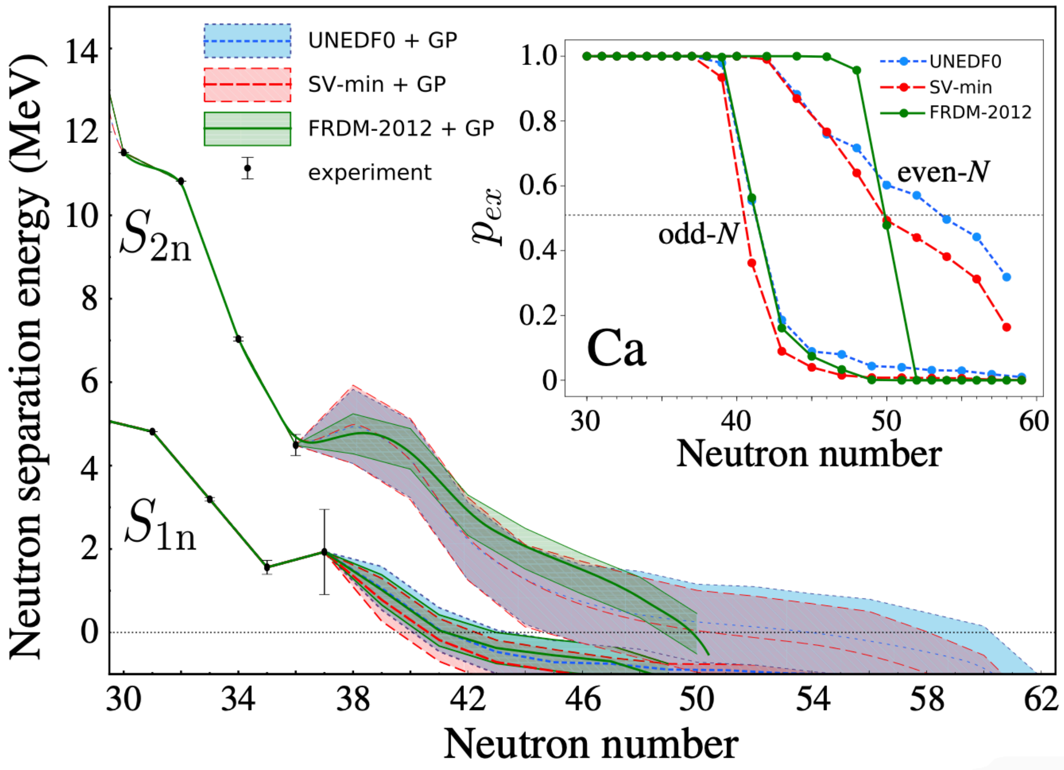


Baishan Hu et al, arXiv:2512.11723 (2025)

The dripline in calcium isotopes



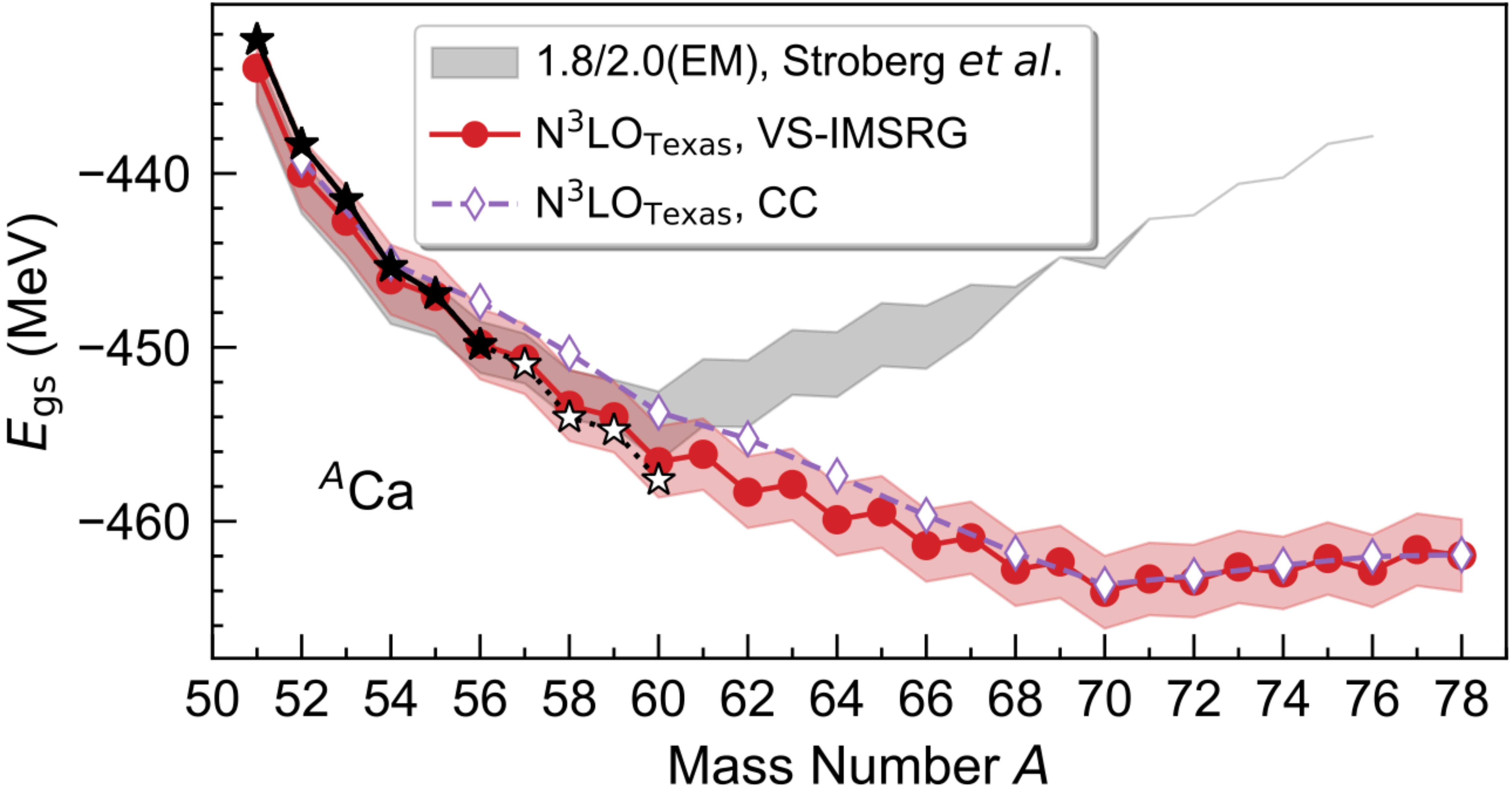
S. R. Stroberg et al, Phys. Rev. Lett. **126**, 022501 (2021)



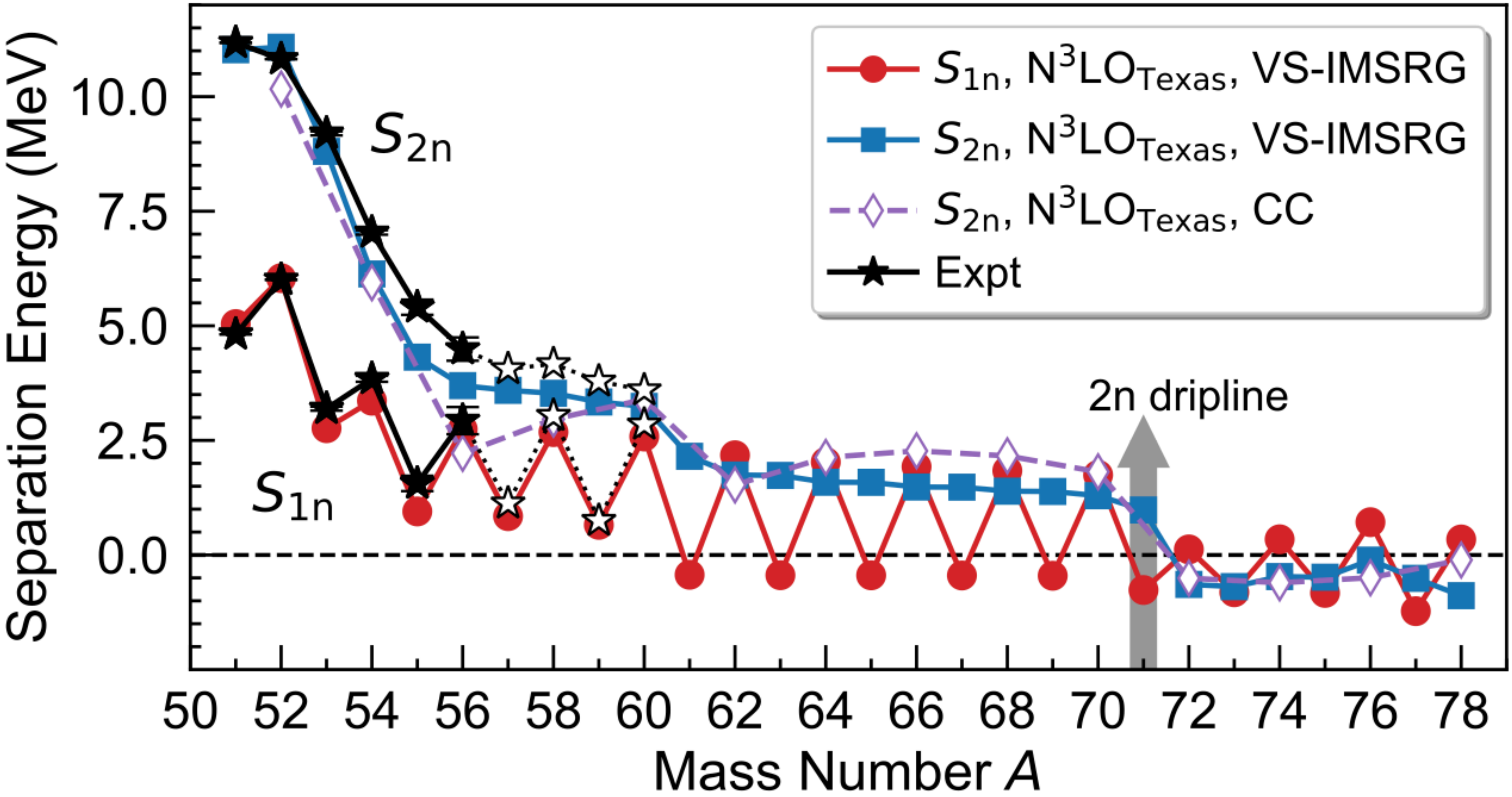
Leo Neufcourt, et al, PRL **122** 062502 (2019)

- 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

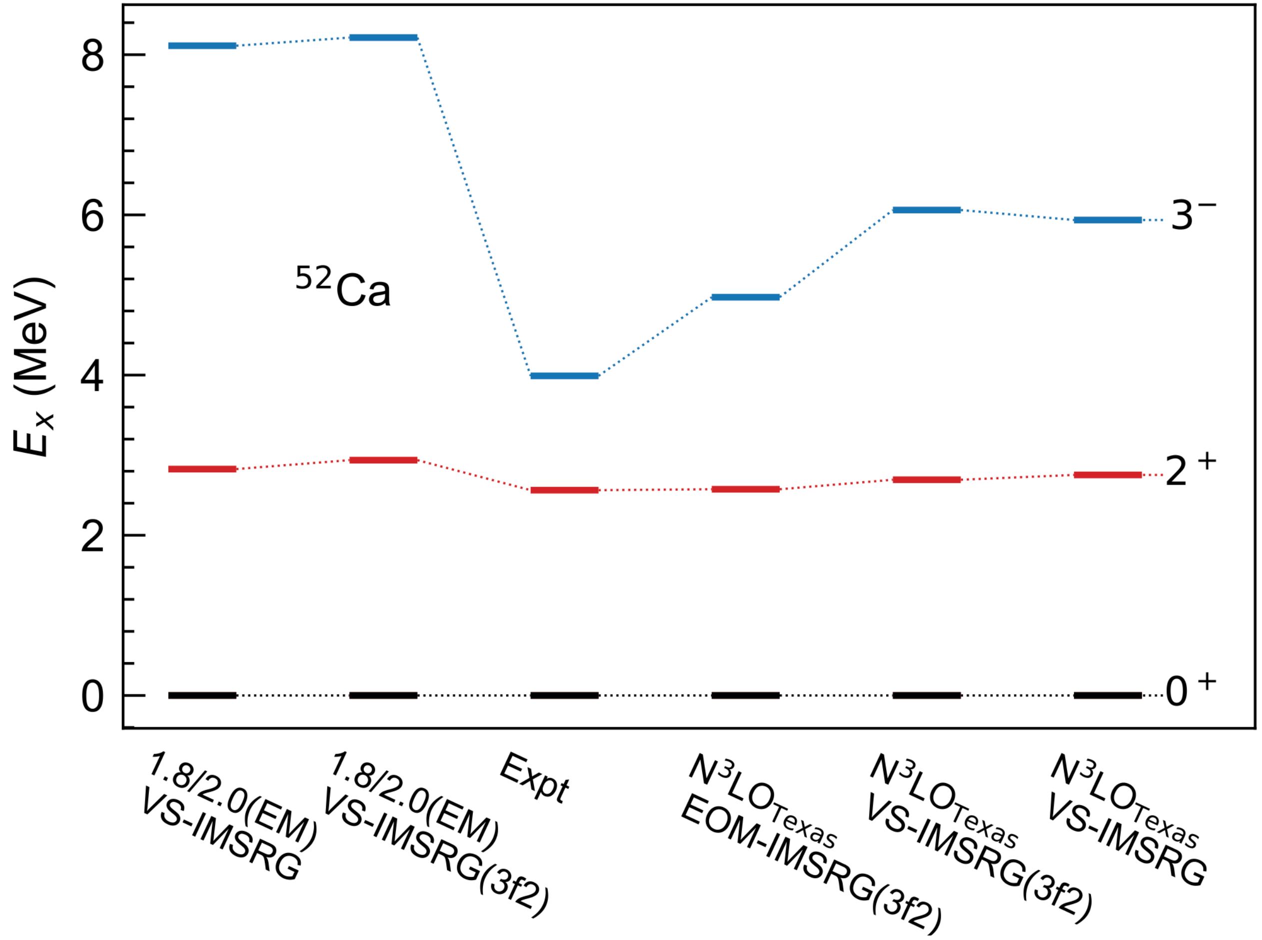
The dripline in calcium isotopes

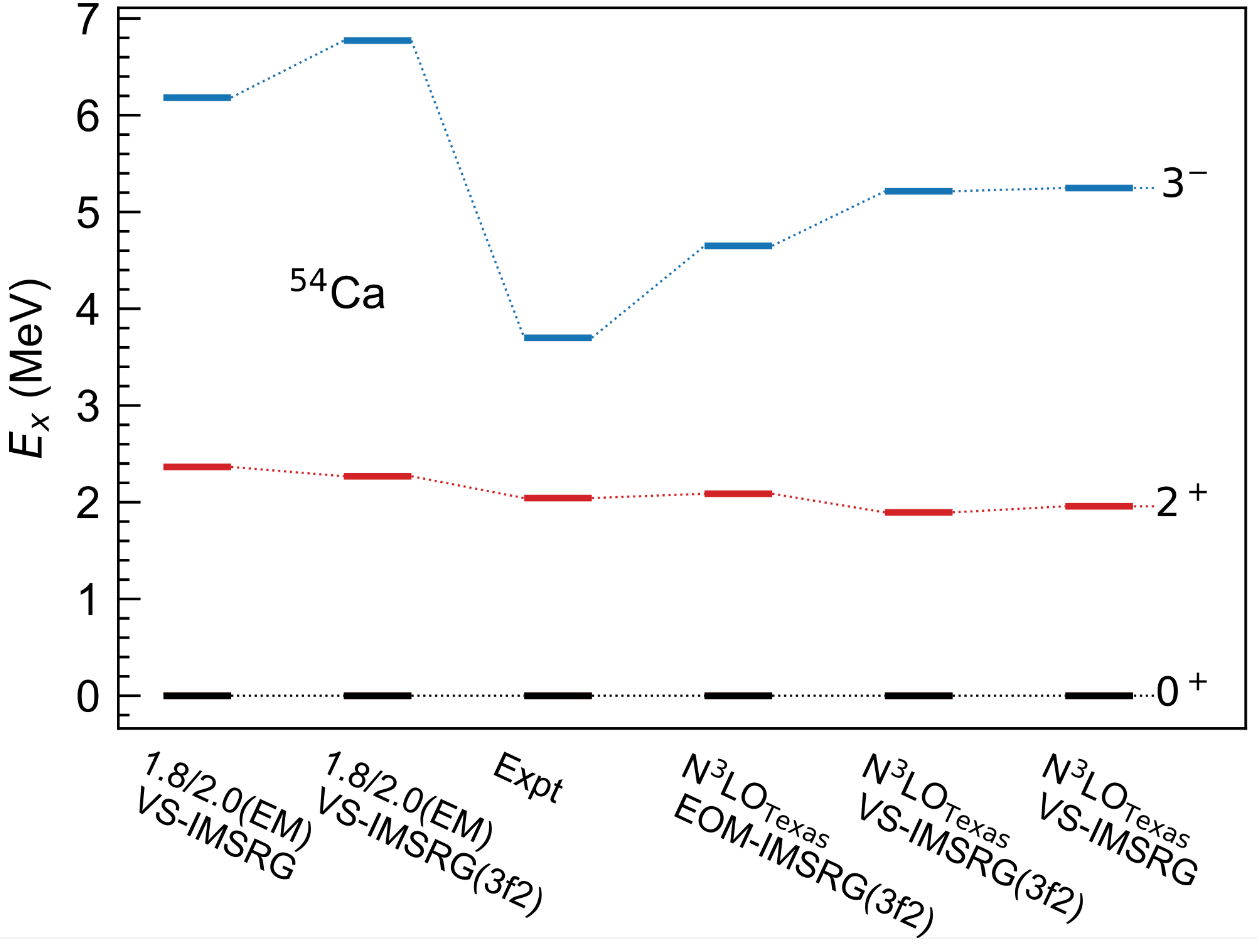


The dripline in calcium isotopes



Spectra of neutron-rich calcium

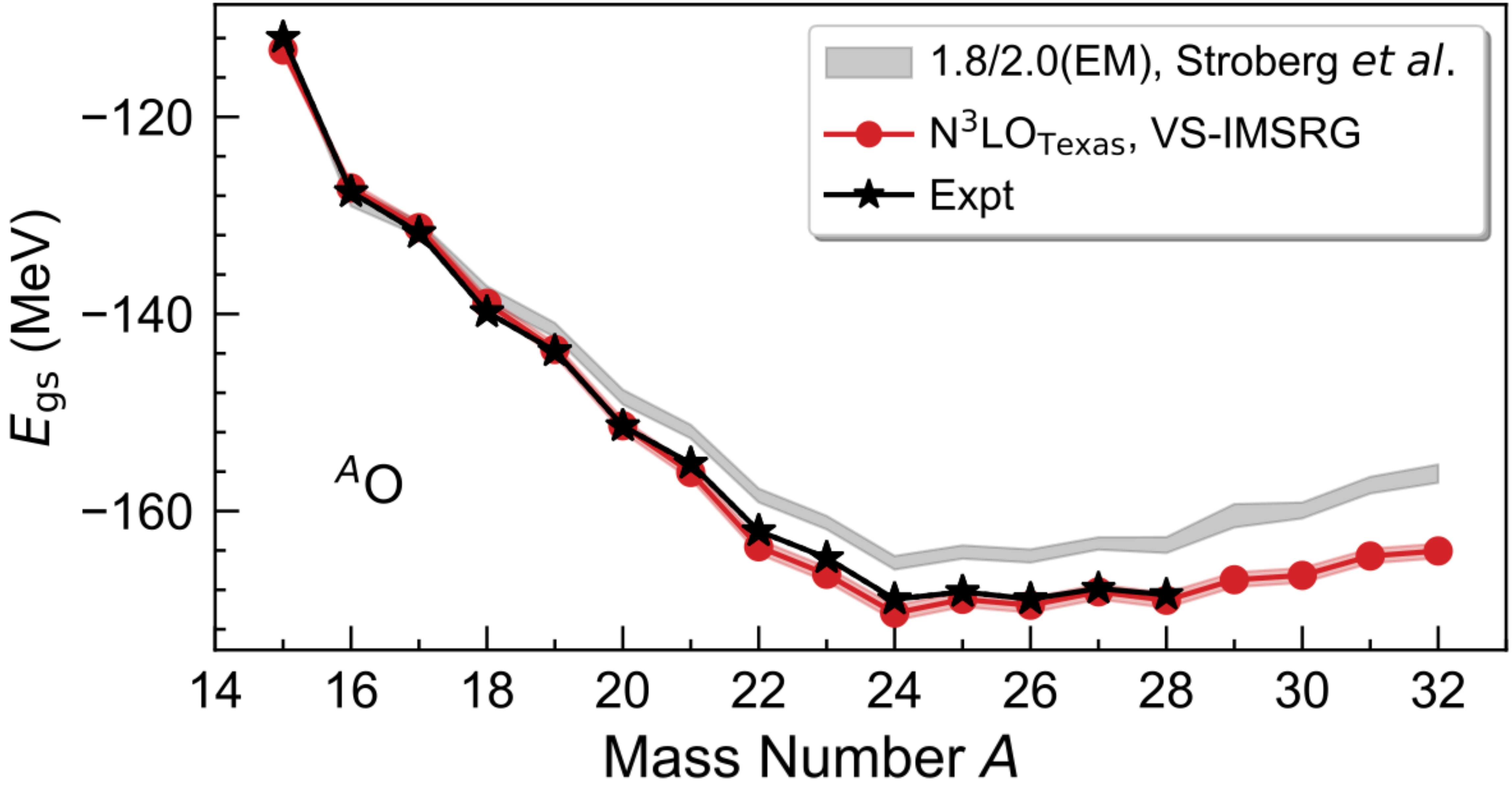




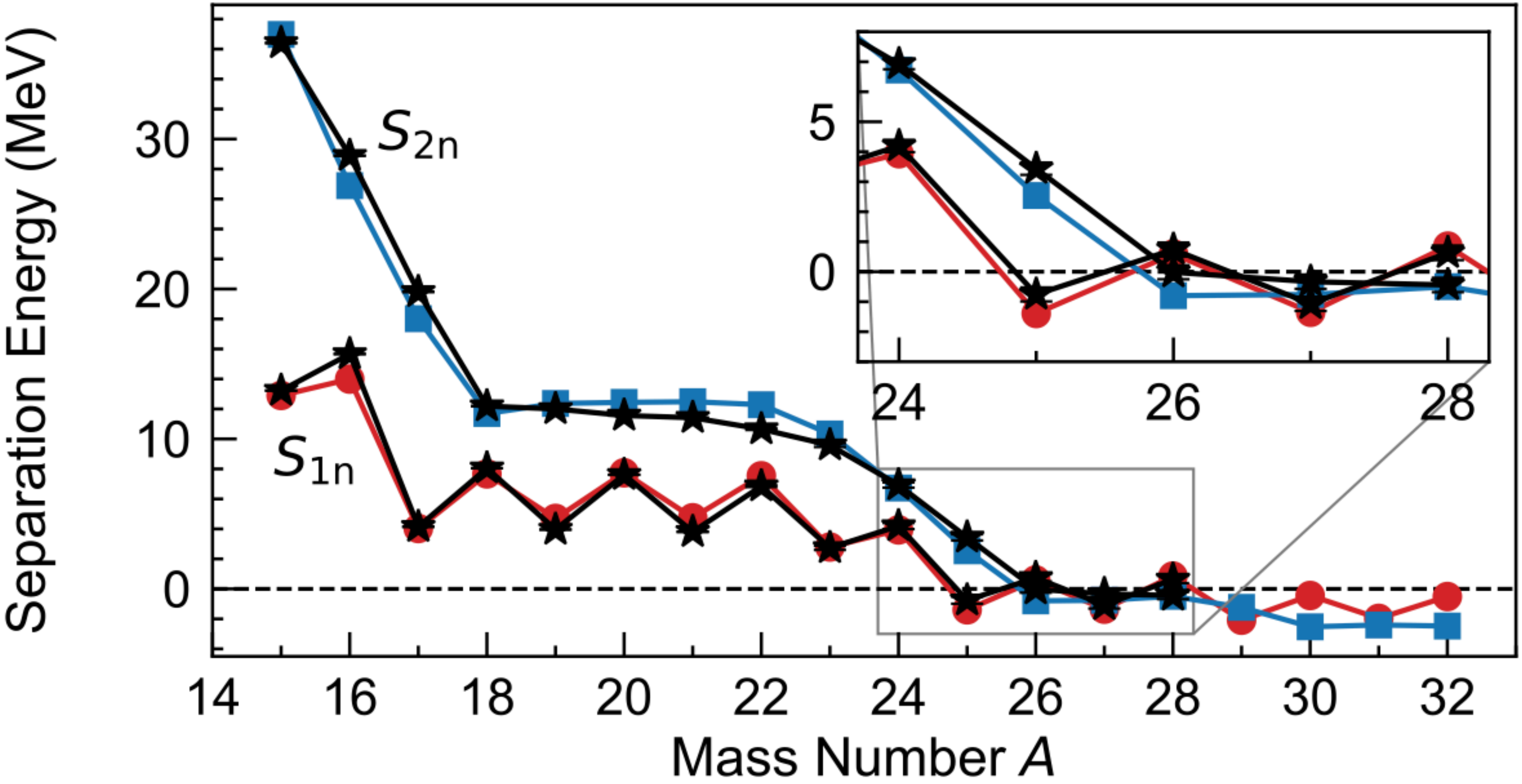
Negative parity states from N3LO$_{Texas}$ are significantly lower compared to 1.8/2.0(EM) indicating smaller N = 40 shell gap

VS-IMSRG: ^{48}Ca core and neutron 1p3/2, 1p1/2, 0f5/2, 0g9/2, 1d5/2, 2s1/2 valence space

The dripline in oxygen isotopes



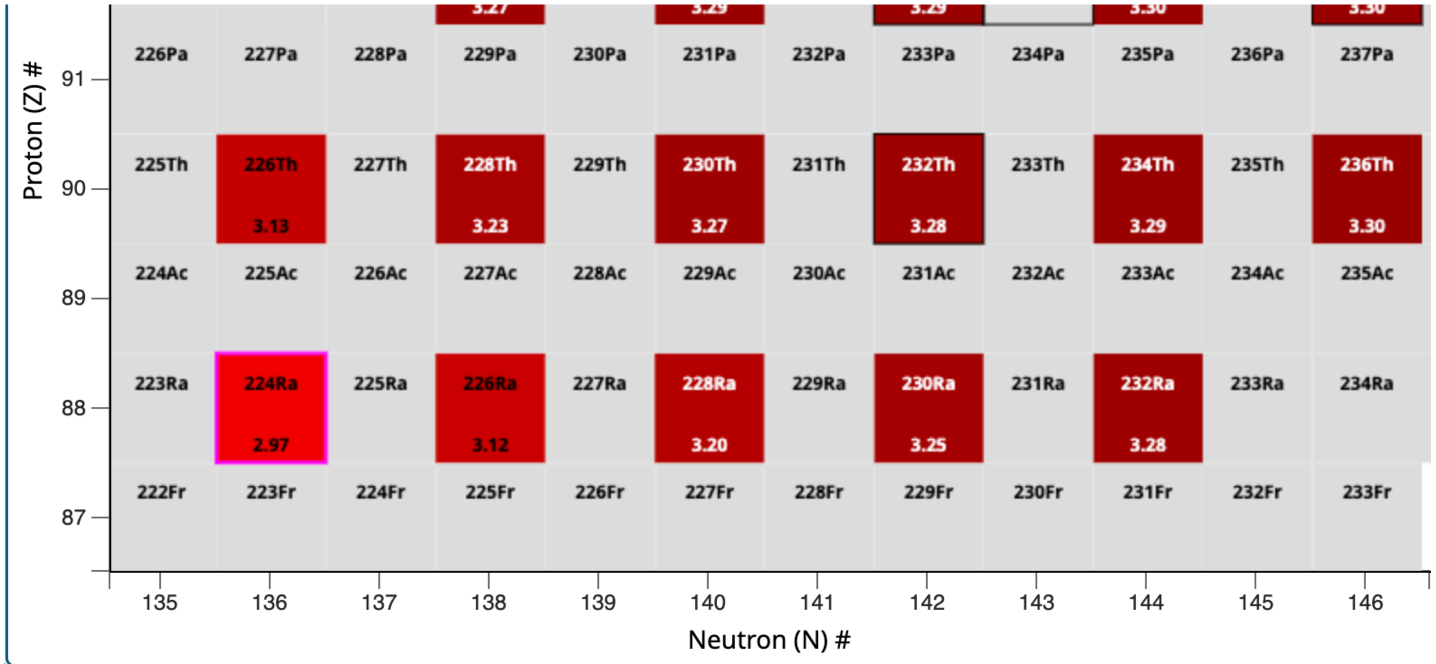
The dripline in oxygen isotopes



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

Coupled-cluster computations of deformed nuclei

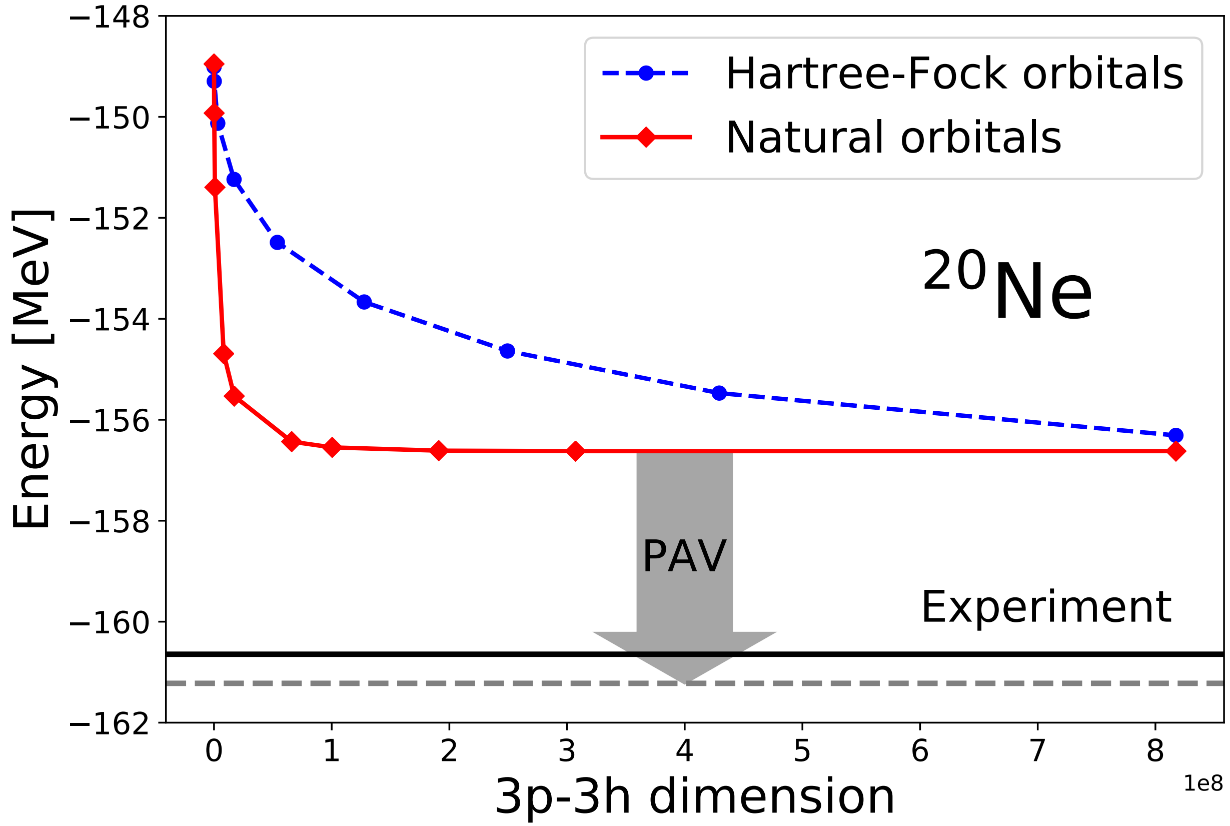
- Include short-range correlations via coupled-cluster theory
  - Large contribution to total energy
  - Cost increases polynomial with mass

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

- 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)



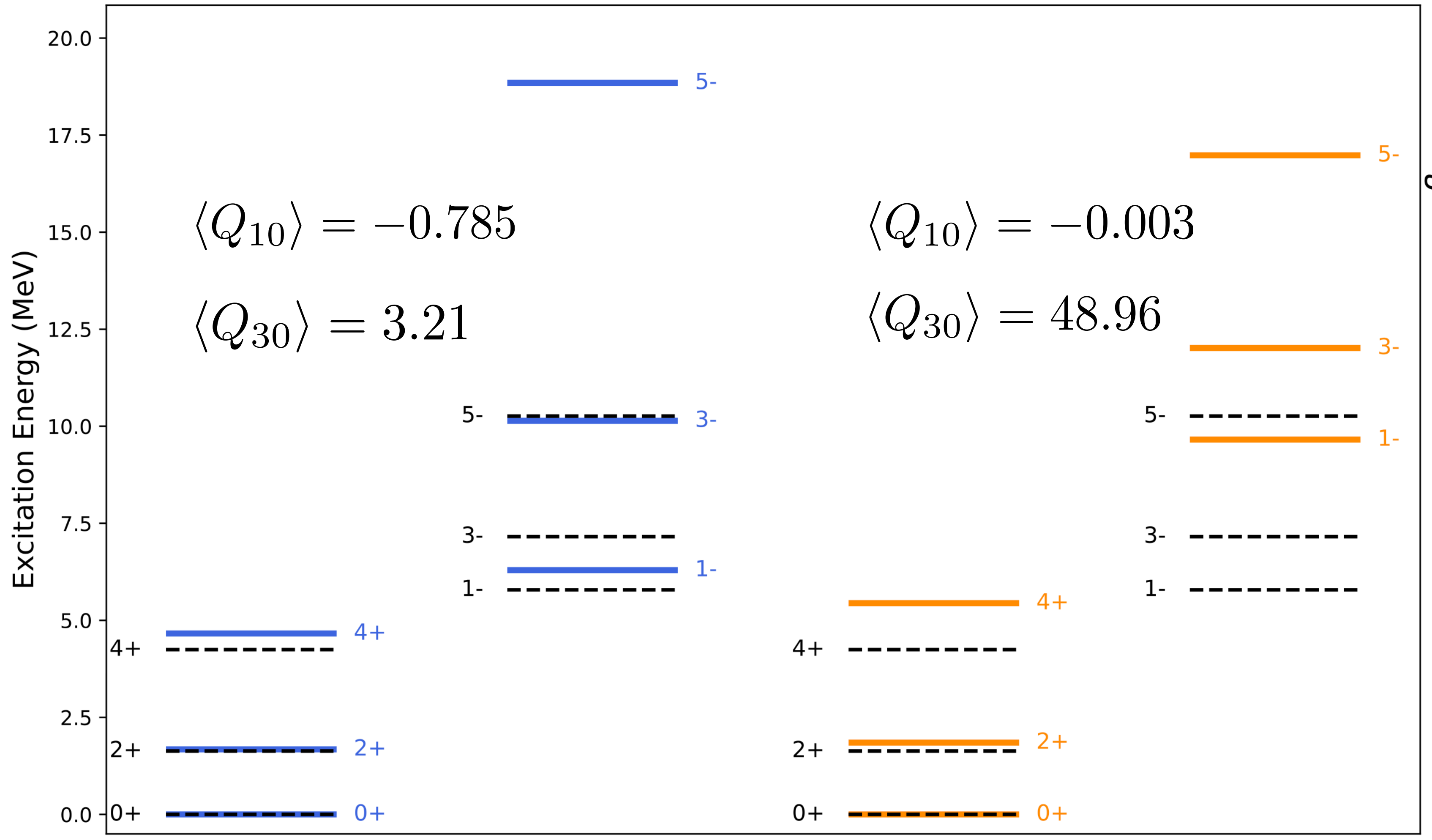
Total energy:

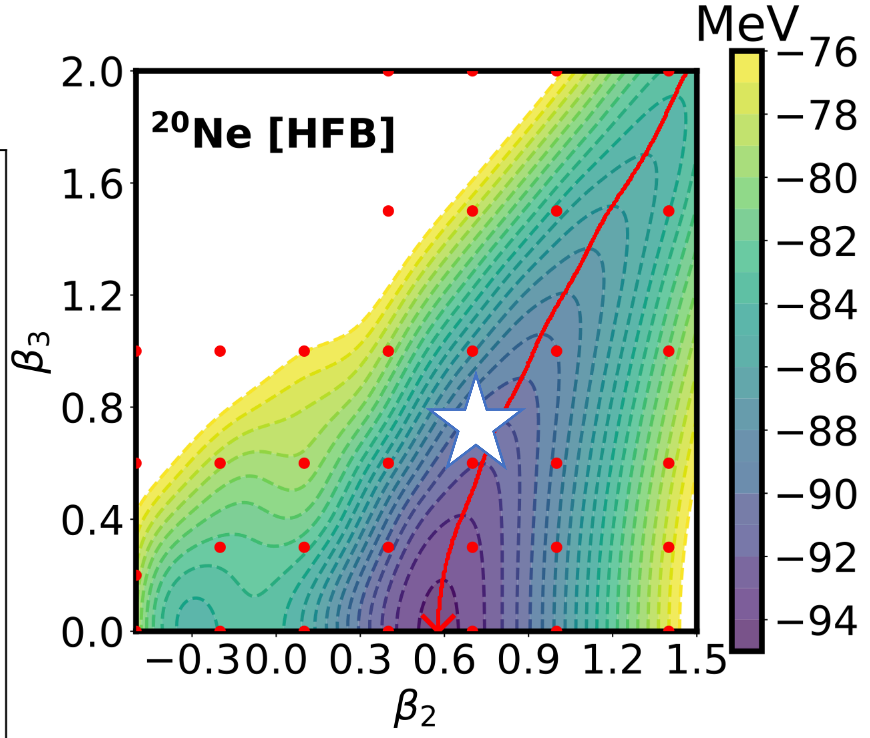
$$E = E_{\mathrm{ref}} + \Delta E_{\mathrm{CC}} + \delta E$$

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:

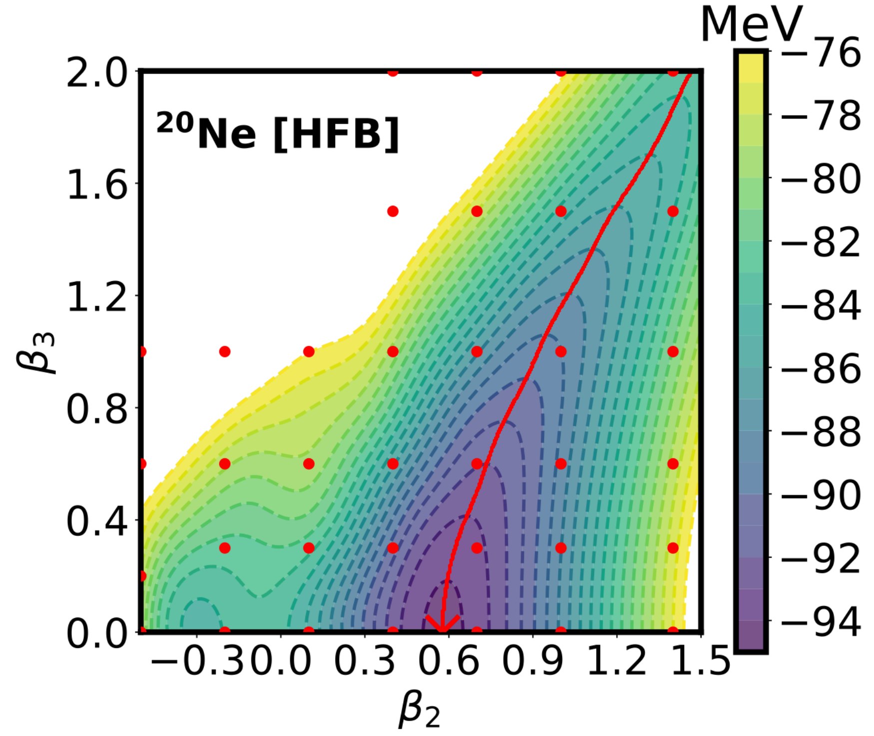
$$E'(T, \Lambda, \vec{\lambda}) = \langle \Phi_0 | (1+\Lambda) \overline{H'}(\vec{\lambda}) | \Phi_0 \rangle$$

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

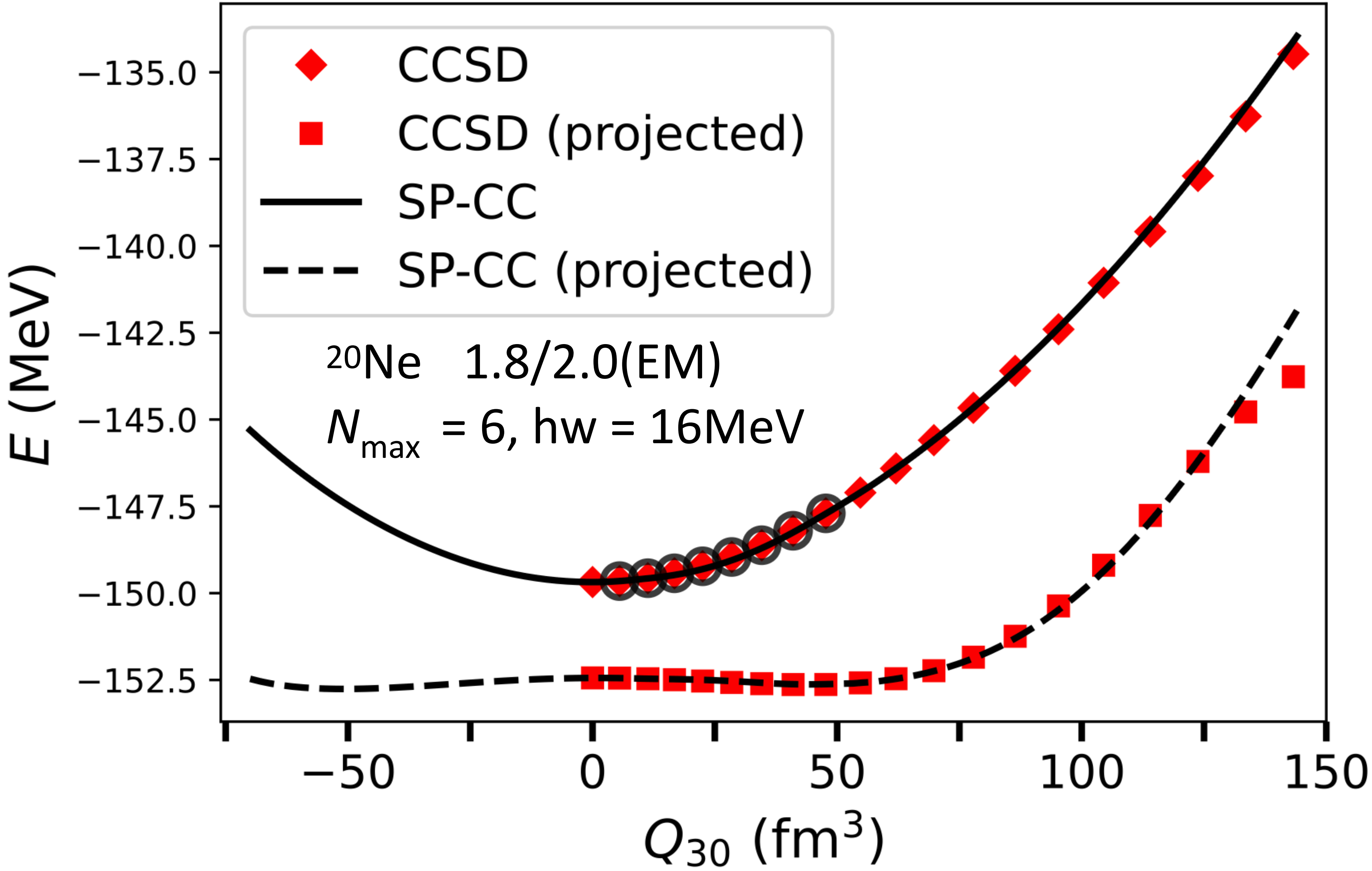
$$\left\{ \langle \Phi_0 | (1 + \Lambda_i) e^{-T_i}, \;\; e^{T_i} | \Phi_0 \rangle \right\}$$

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:

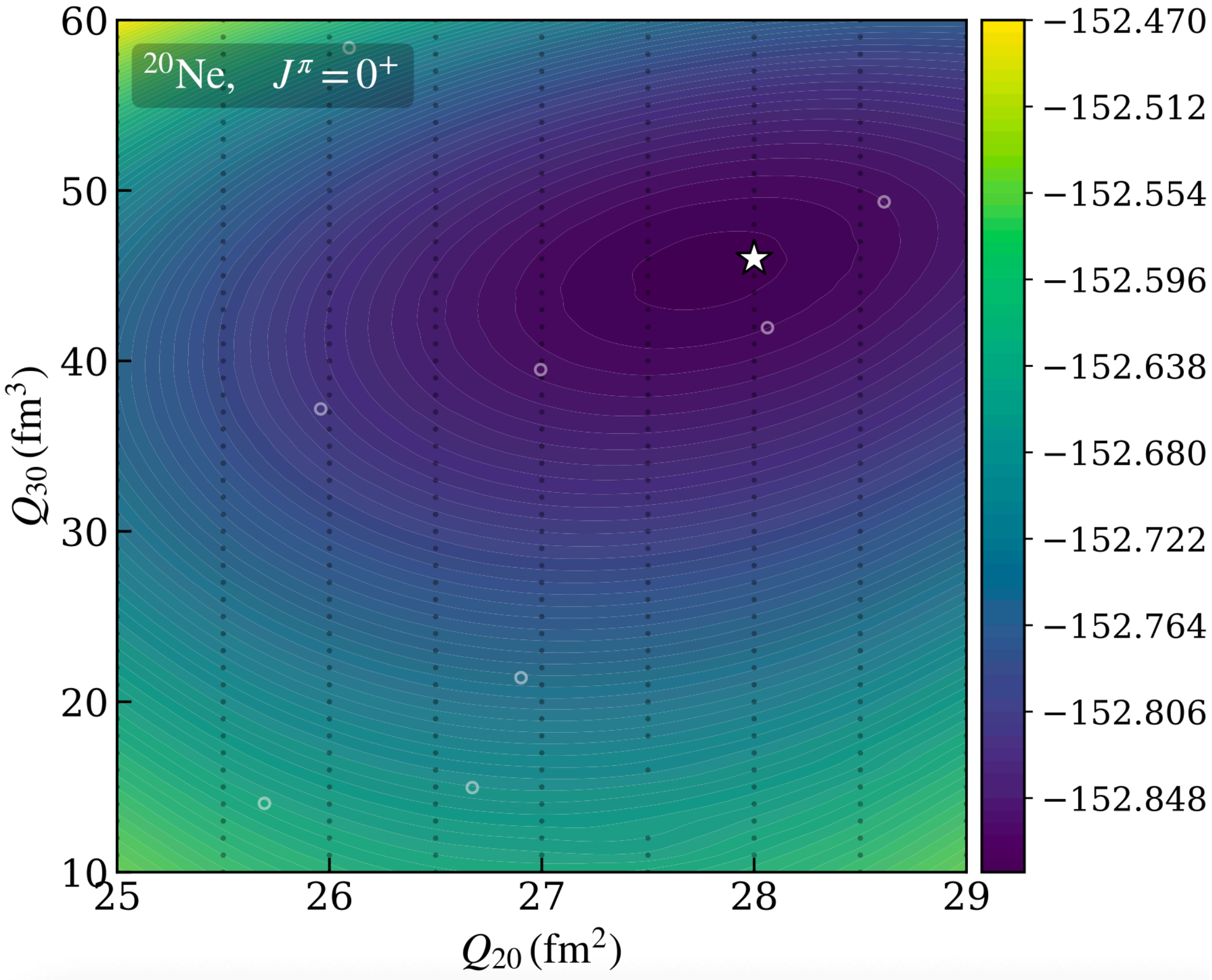
$$\min_{\vec{\lambda}} \left\{ \sum_{i=1}^{3} w_i (\langle Q_{i0}(\vec{\lambda}) \rangle - q_{i0})^2 \right\}.$$

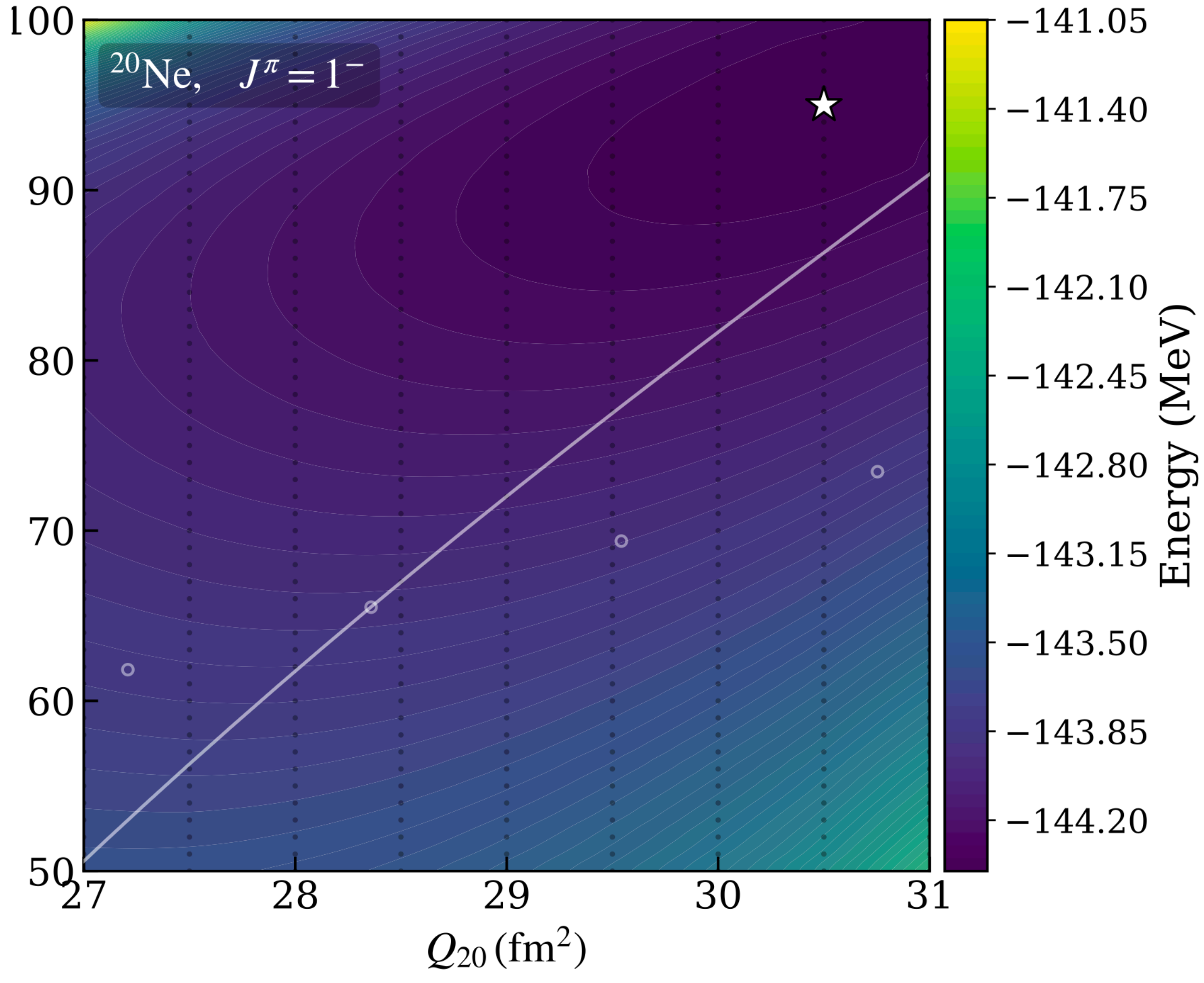
Constrained sub-space Coupled-Cluster



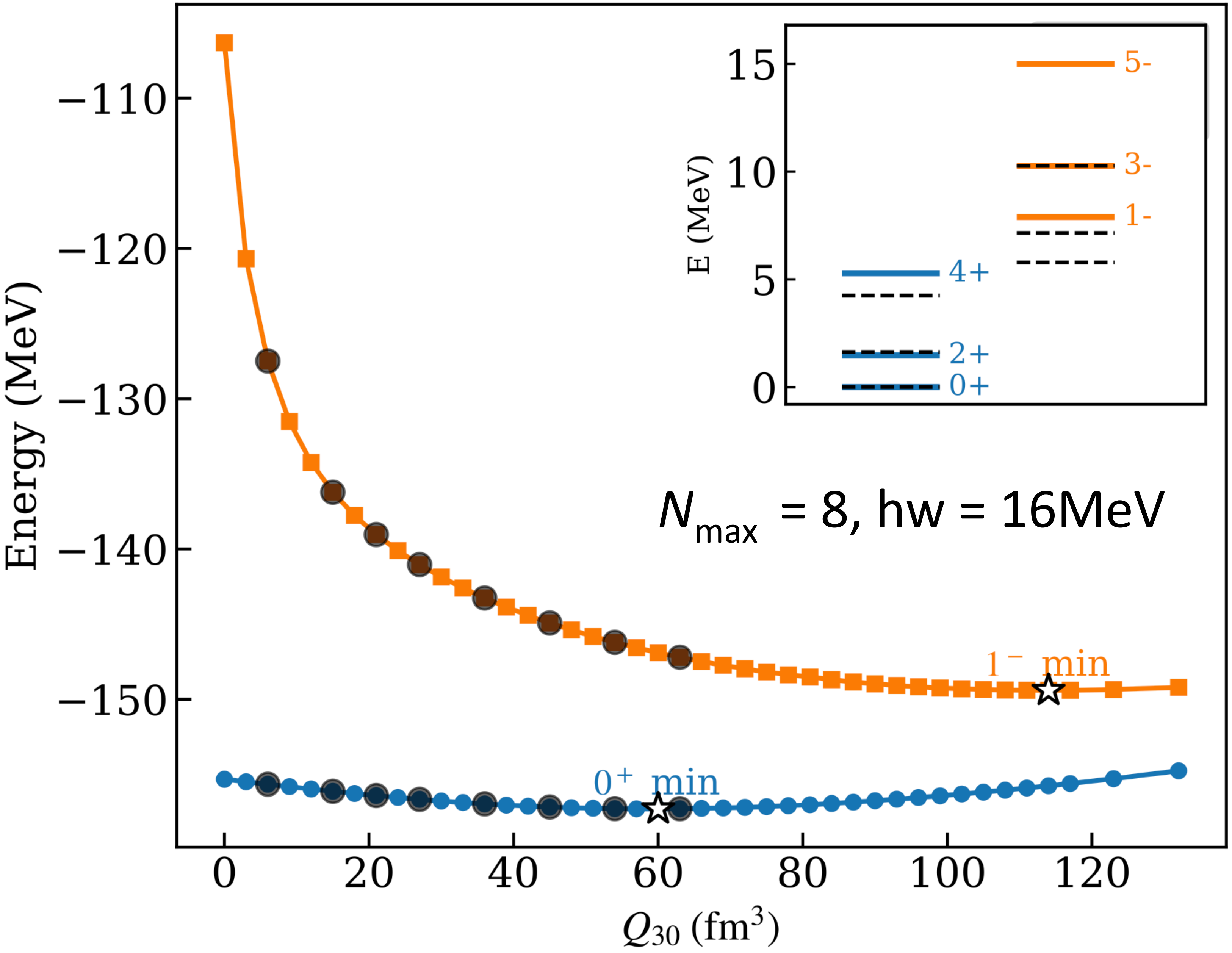
Constrained sub-space Coupled-Cluster

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



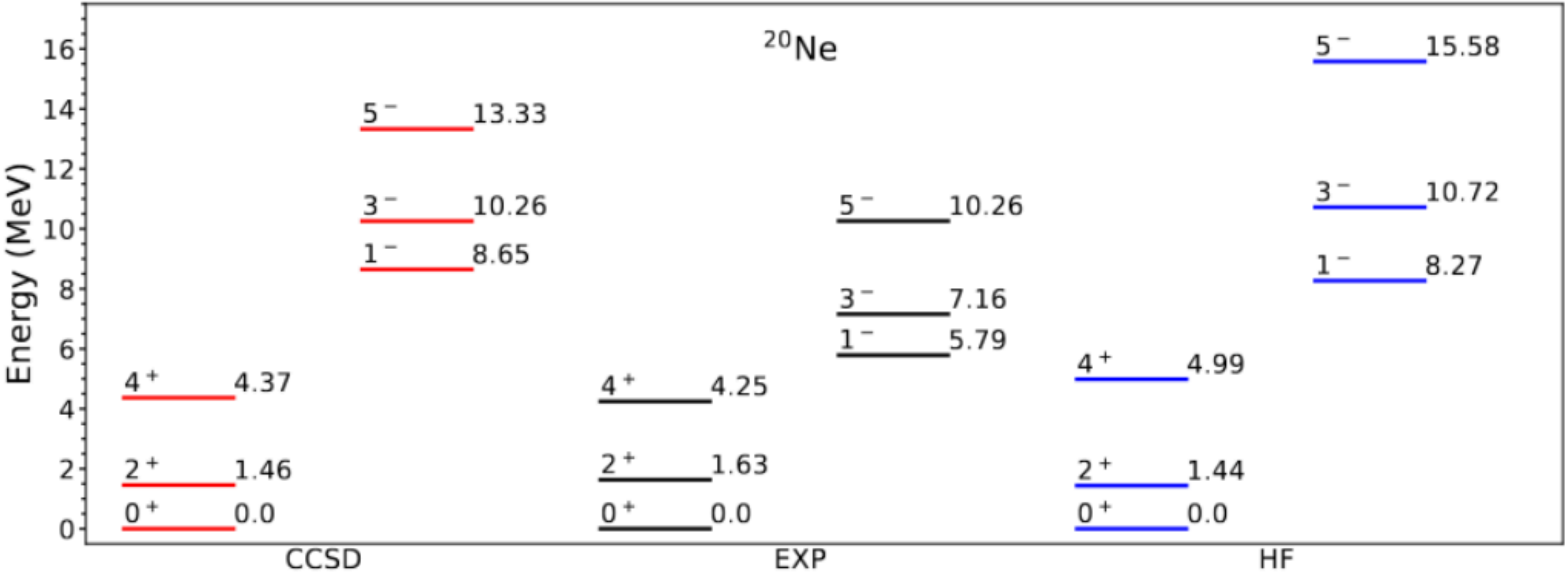


Constrained sub-space Coupled-Cluster



Constrained sub-space Coupled-Cluster

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



Summary

- Used emulators of scattering and properties of ^{16}O to optimize a new chiral interaction
- The resulting interaction is “soft” enough to converge medium mass and heavy nuclei
- N3LO$_{\text{Texas}}$ yields energy results that are comparable to 1.8/2.0(EM), while improving radii systematics and dripline physics.
- Two-neutron dripline extends to ^{70}Ca with N3LO$_{\text{Texas}}$
- Explicit symmetry breaking in deformed coupled-cluster promising tool to access negative parity states and nuclei that are soft towards octupole deformation

N3LO$_{\text{Texas}}$ interaction is available in NuHamil