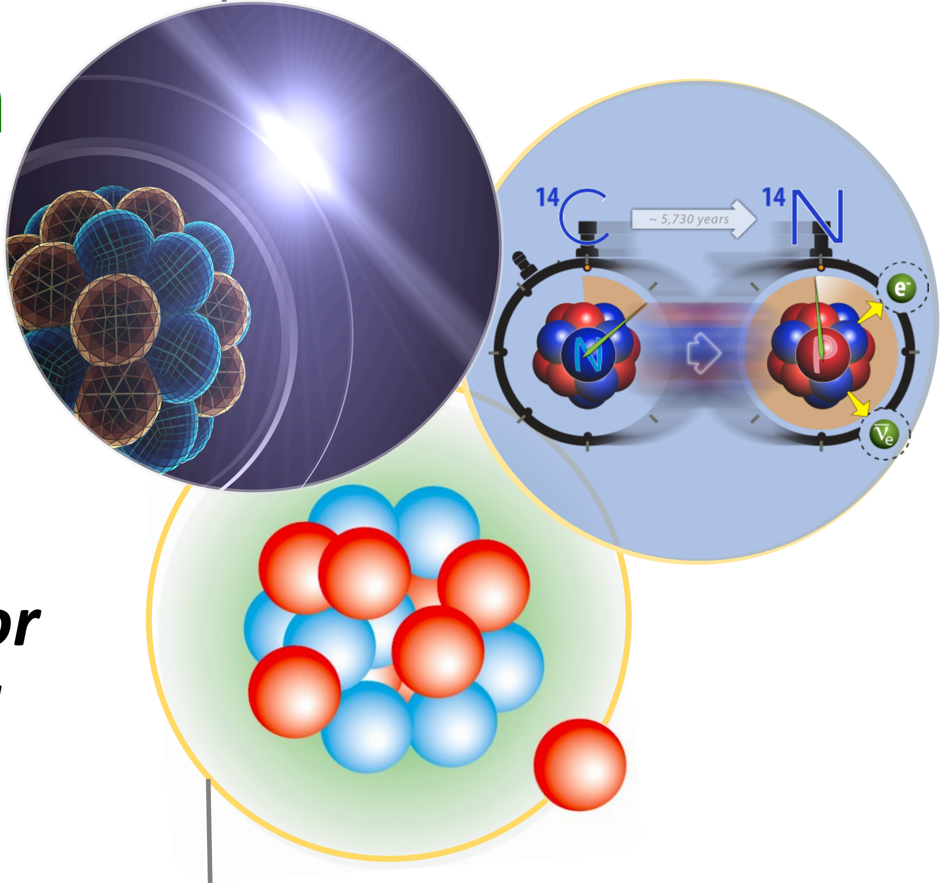
A Pragmatist Approach to a New Chiral Interaction: The Dripline in Calcium Isotopes

Gaute Hagen
Oak Ridge National Laboratory



INT workshop: *Nuclear Hamiltonians for Advancing Nuclear Physics and Beyond*

INT, May 6th, 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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Multiscale physics of nuclei from ab-initio methods

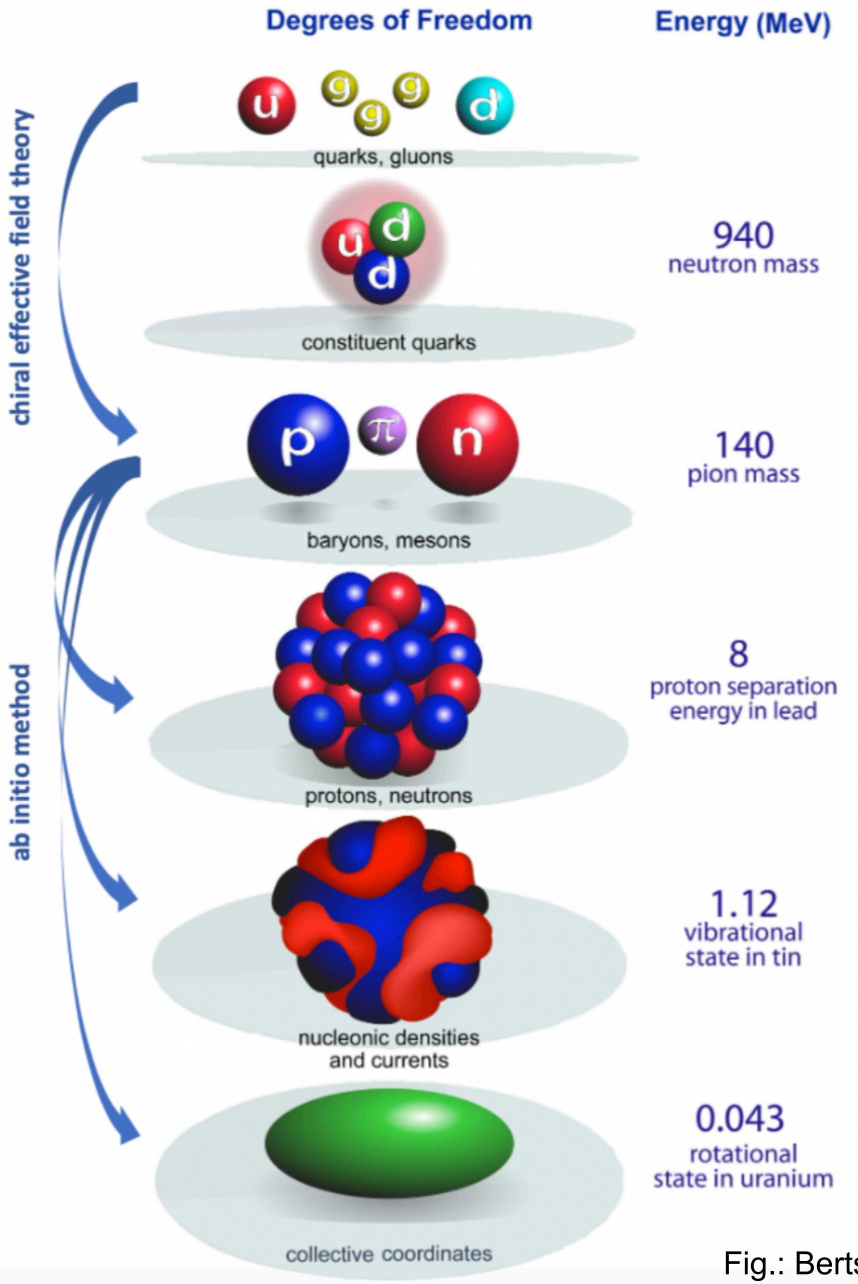


Fig.: Bertsch, Dean, Nazarewicz, SciDAC review (2007)

What is ab initio in nuclear theory?

A. Ekström et al, Frontiers (2023)

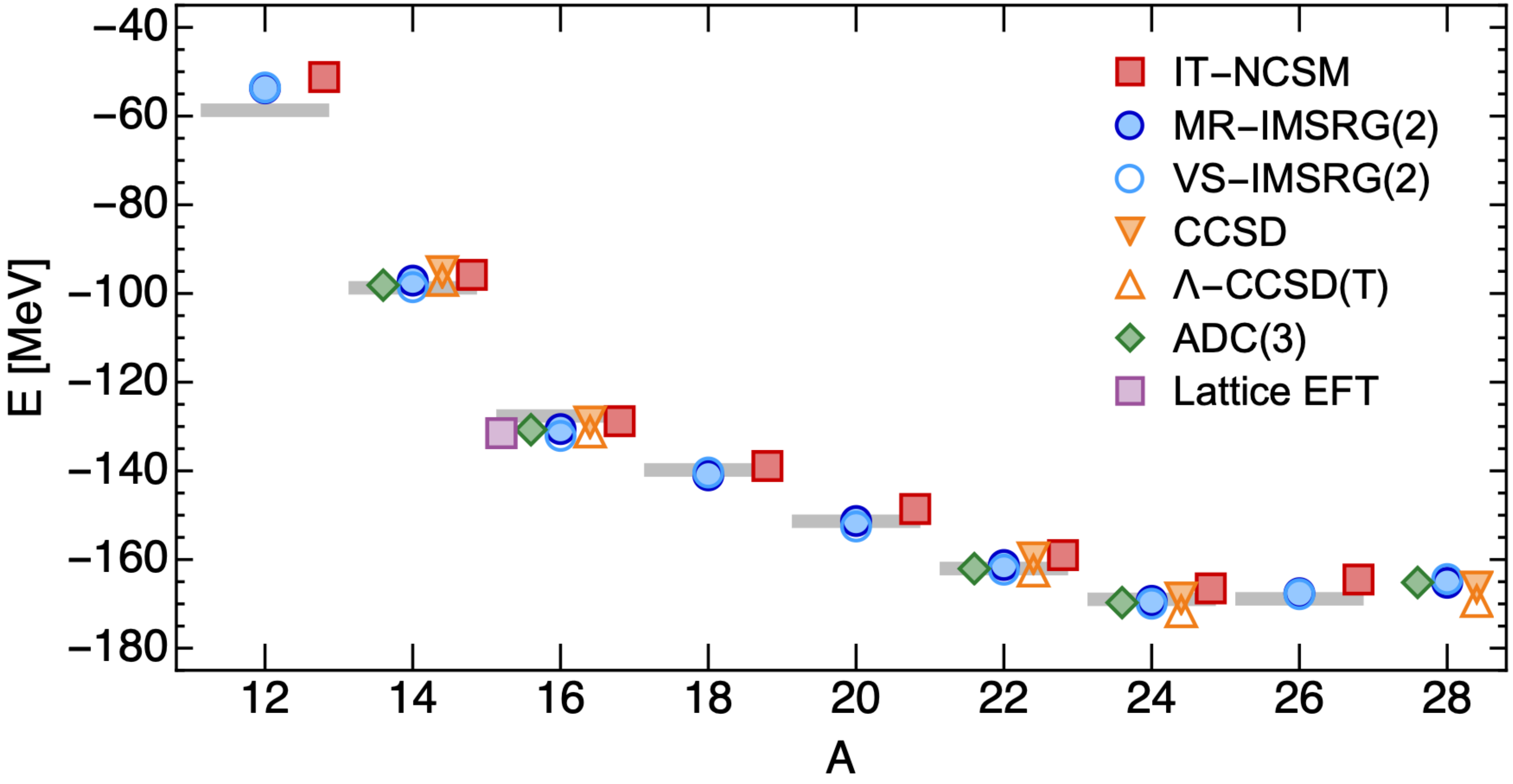
"we interpret the ab initio method to be a systematically improvable approach for quantitatively describing nuclei using the finest resolution scale possible while maximizing its predictive capabilities"

- 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

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

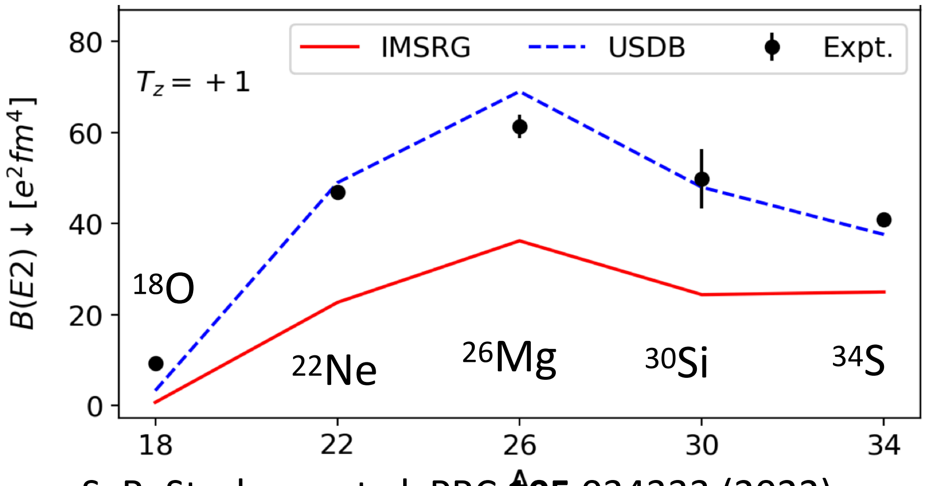
Different many-body approaches agree with each for binding energies and radii

(challenges exist for transitions, isotope shifts, and deformed shapes)

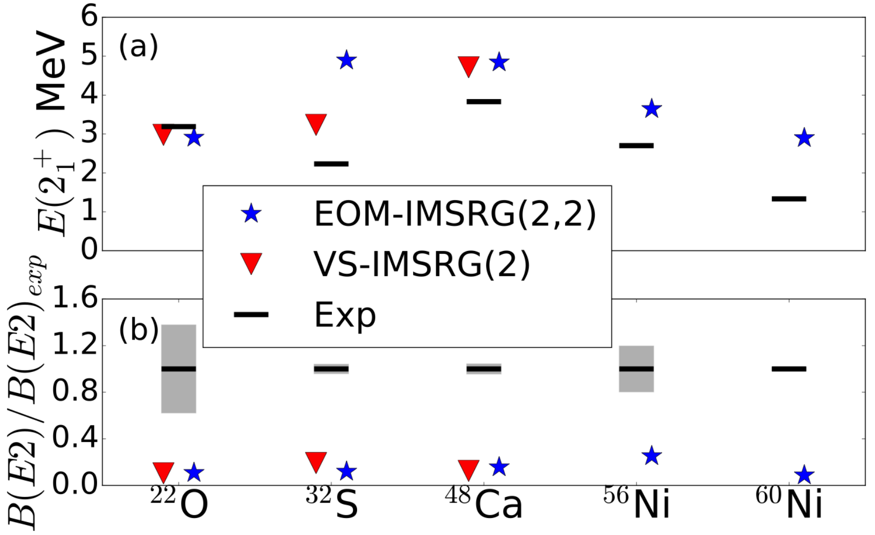


H. Hergert Front. Phys., (2020)

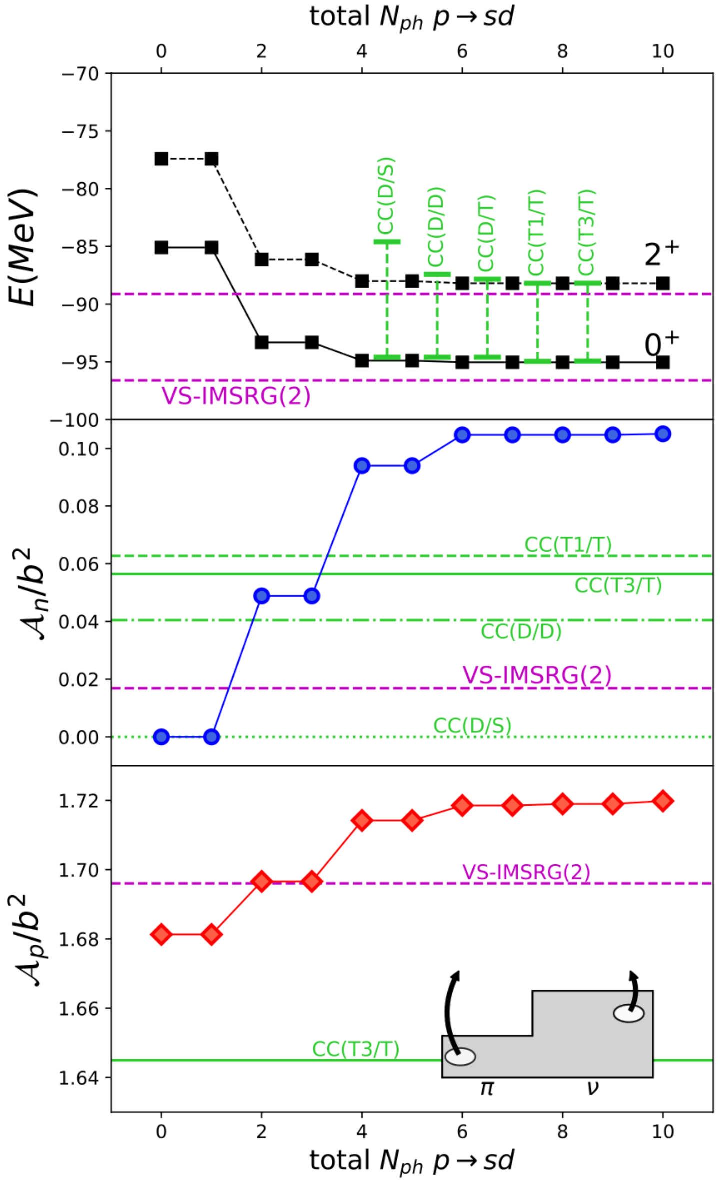
What precision/accuracy can we aim for in ab-initio modeling of nuclei?



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



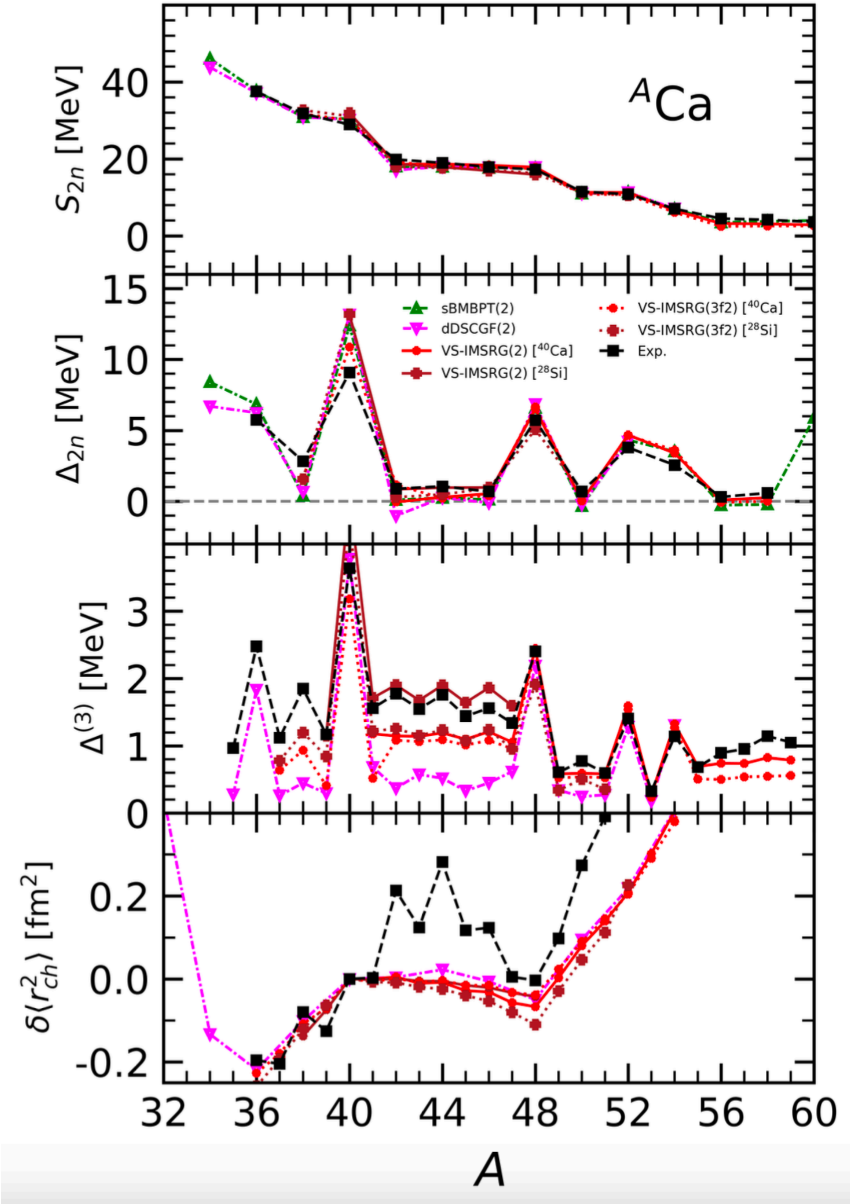
N. M. Parzuchowski, et al Phys. Rev. C 96, 034324 (2017)



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?

Where is the pairing gone?



A. Scalesi et al, unpublished

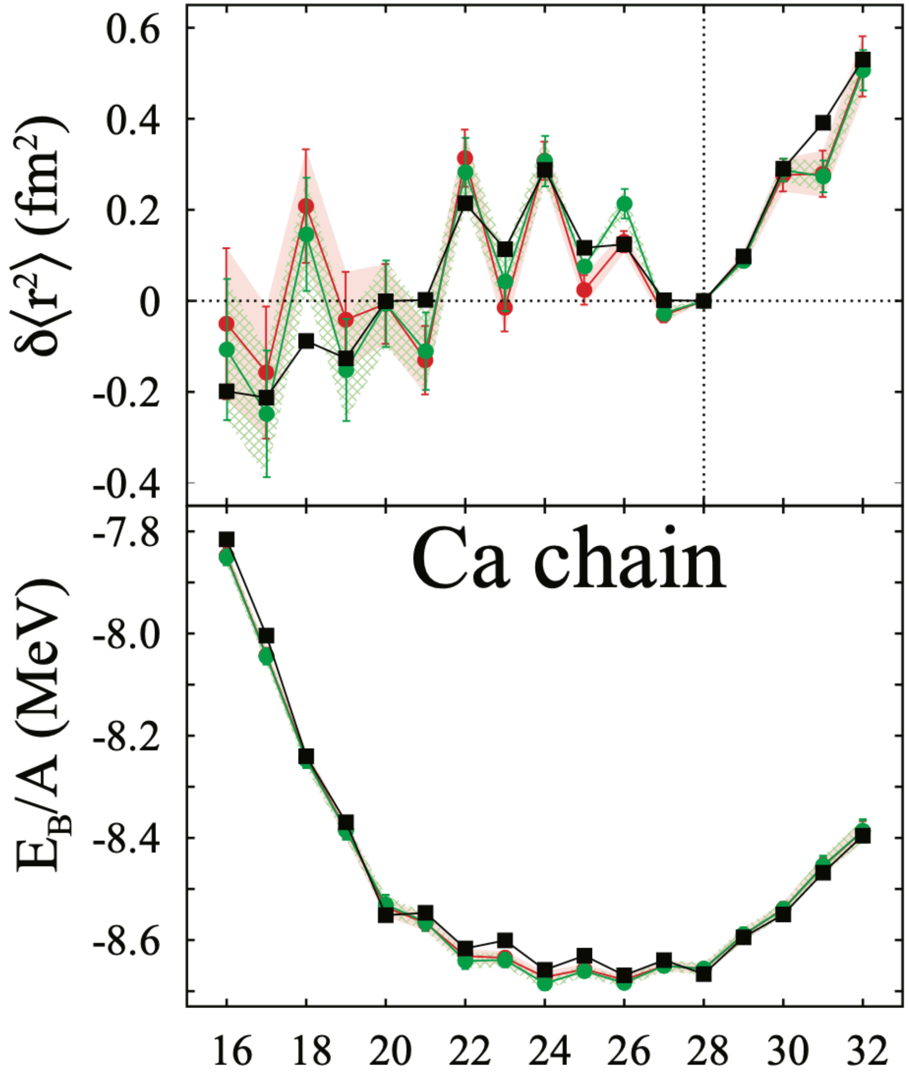
Fayans EDF
(density dependent
pairing functional)

Pairing

Ab initio computations based on chiral EFT interactions

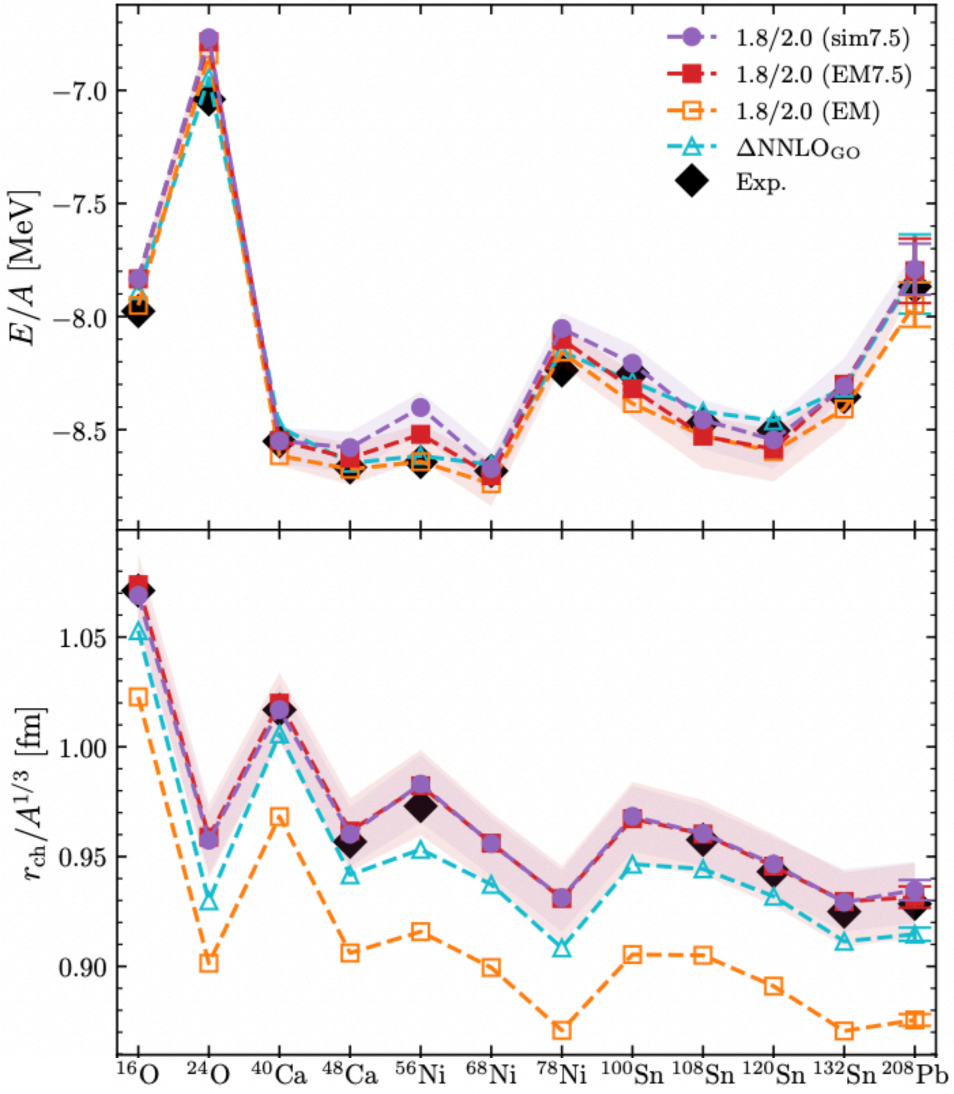
A. Scalesi, et al Eur. Phys. J. A **60**, 209 (2024).

No Pairing



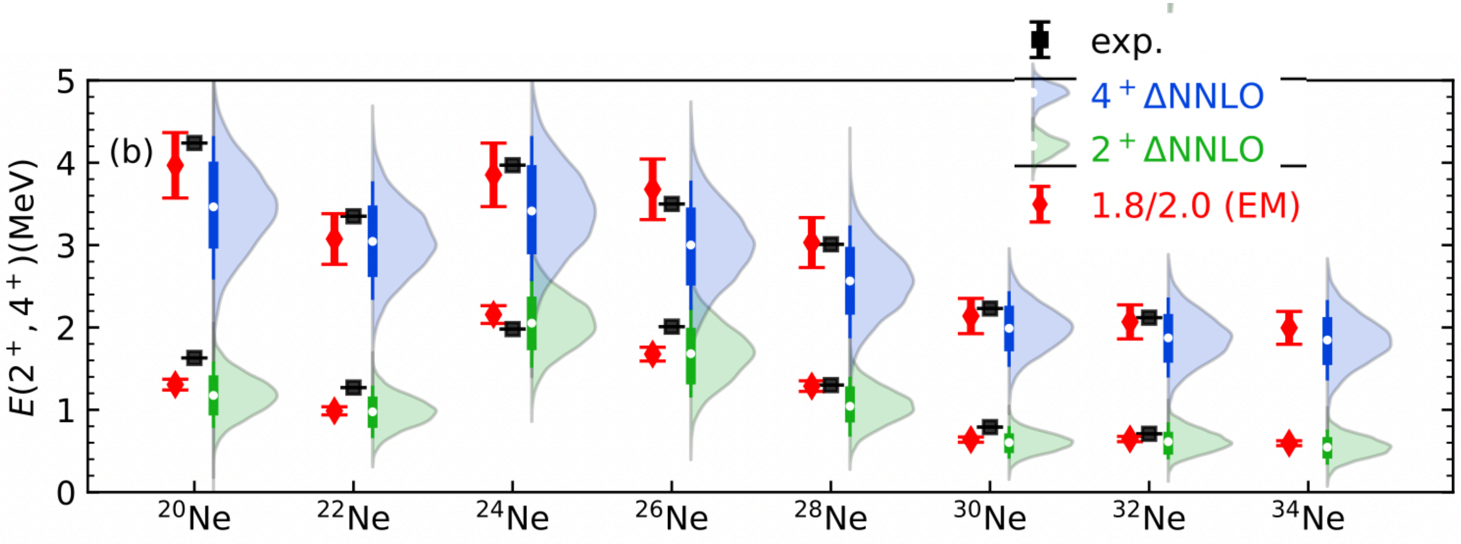
P-G Reinhard et al, J. Phys. G 51, 105101 (2024)

Some interactions work "better" than others



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

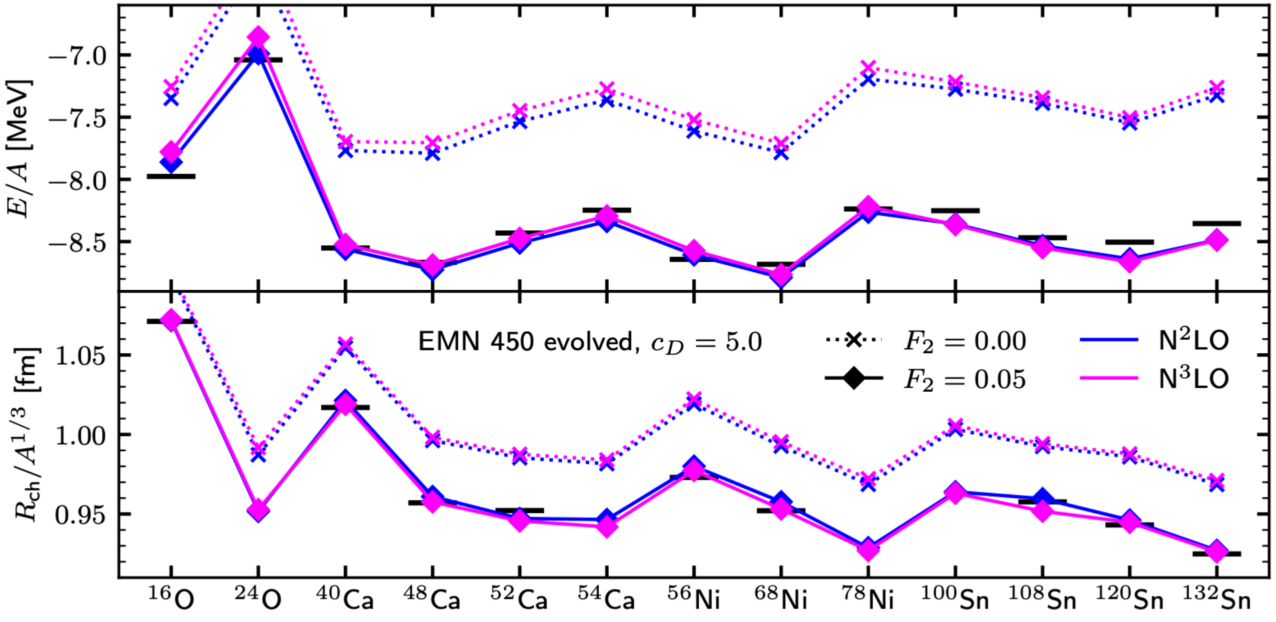


P. Arthuis, K. Hebeler, A. Schwenk, arXiv:2401.06675 (2024)

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

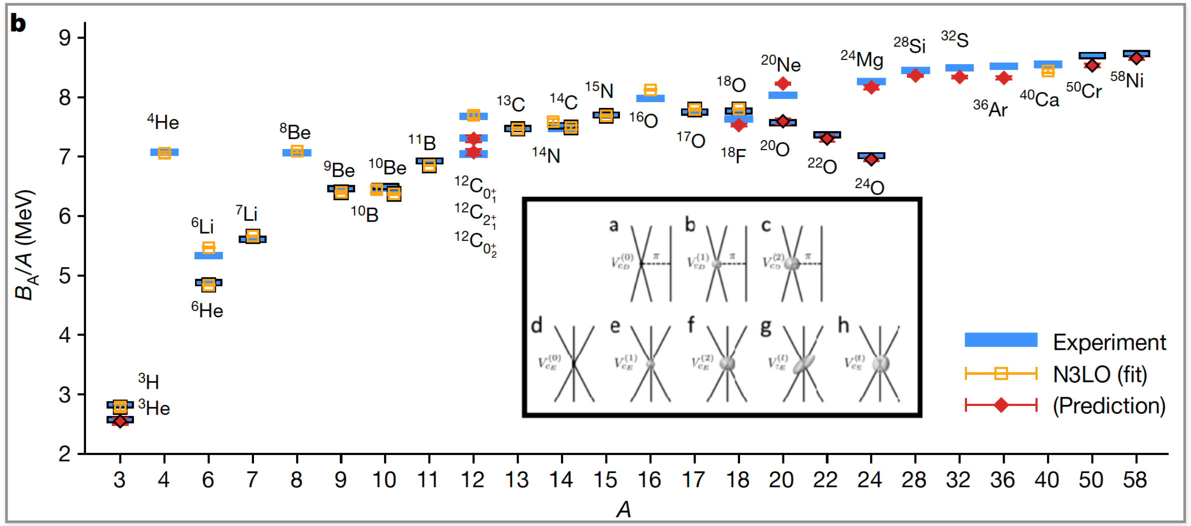
Some interactions work “better” than others

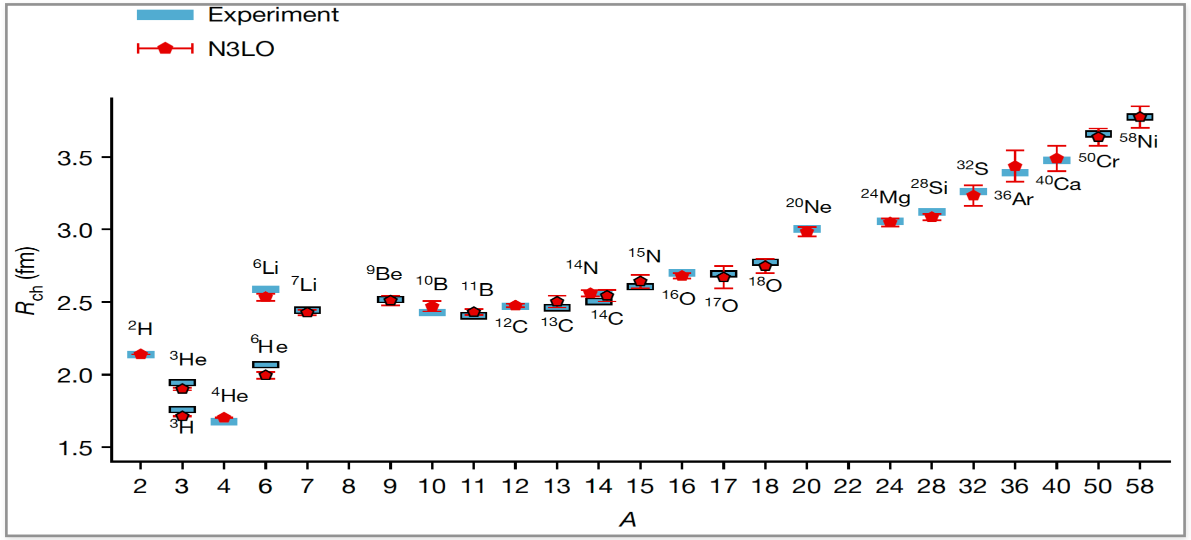
Quark mass dependent 3NFs



Urban Vernik, Kai Hebeler, Achim Schwenk, arXiv:2512.20454 (2025)

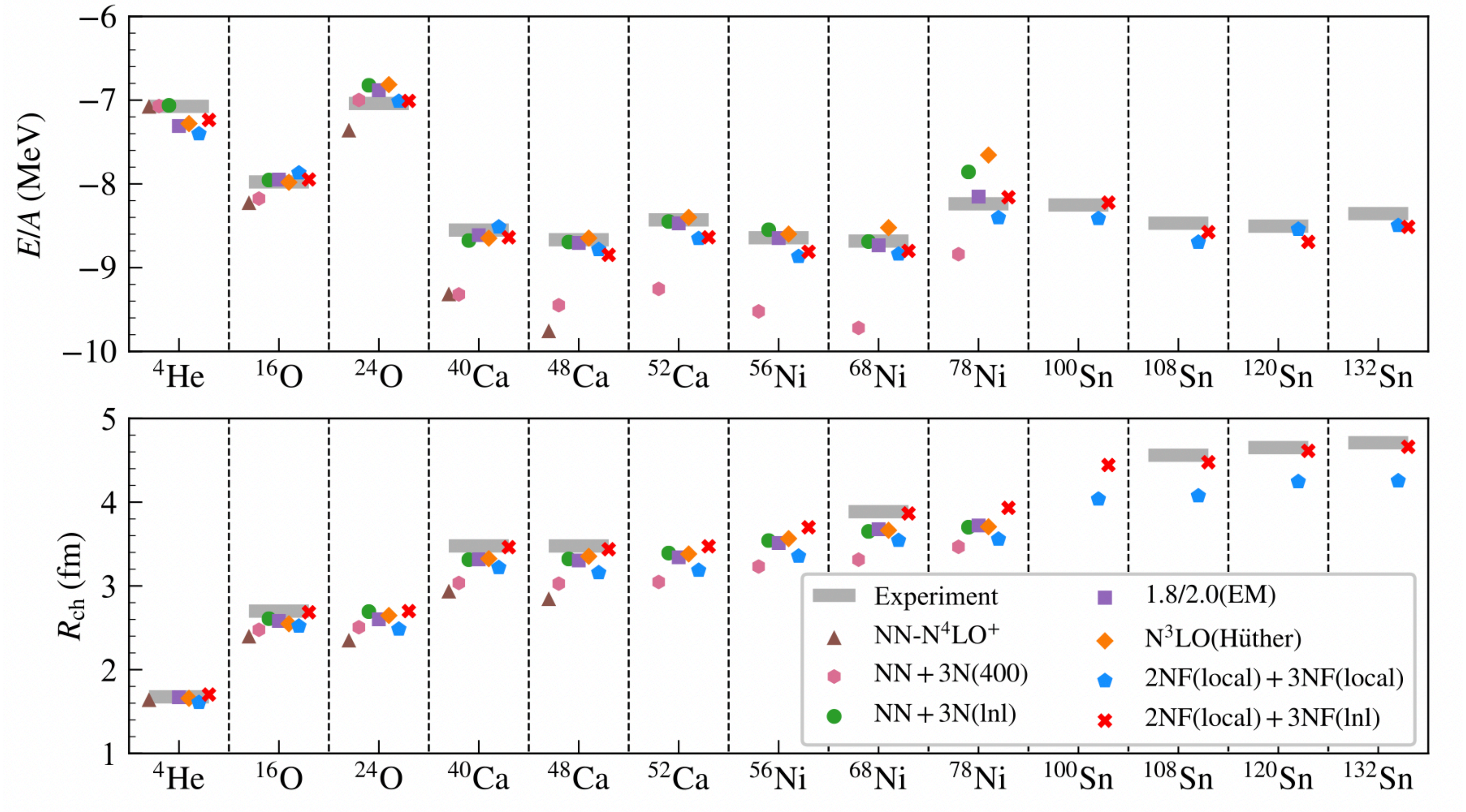
Lattice EFT with promoted 3NFs



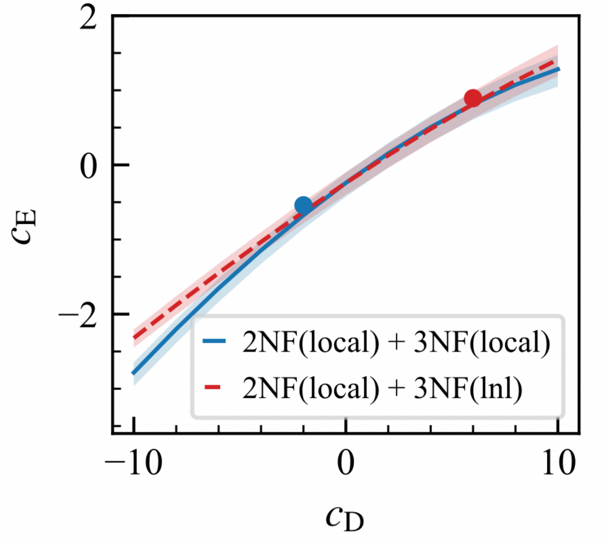


S Elhatisari, et al., Nature 630, 59 (2024)

Some interactions work "better" than others



Local and hybrid local-nonlocal chiral 3NFs fit to 3H and 16O

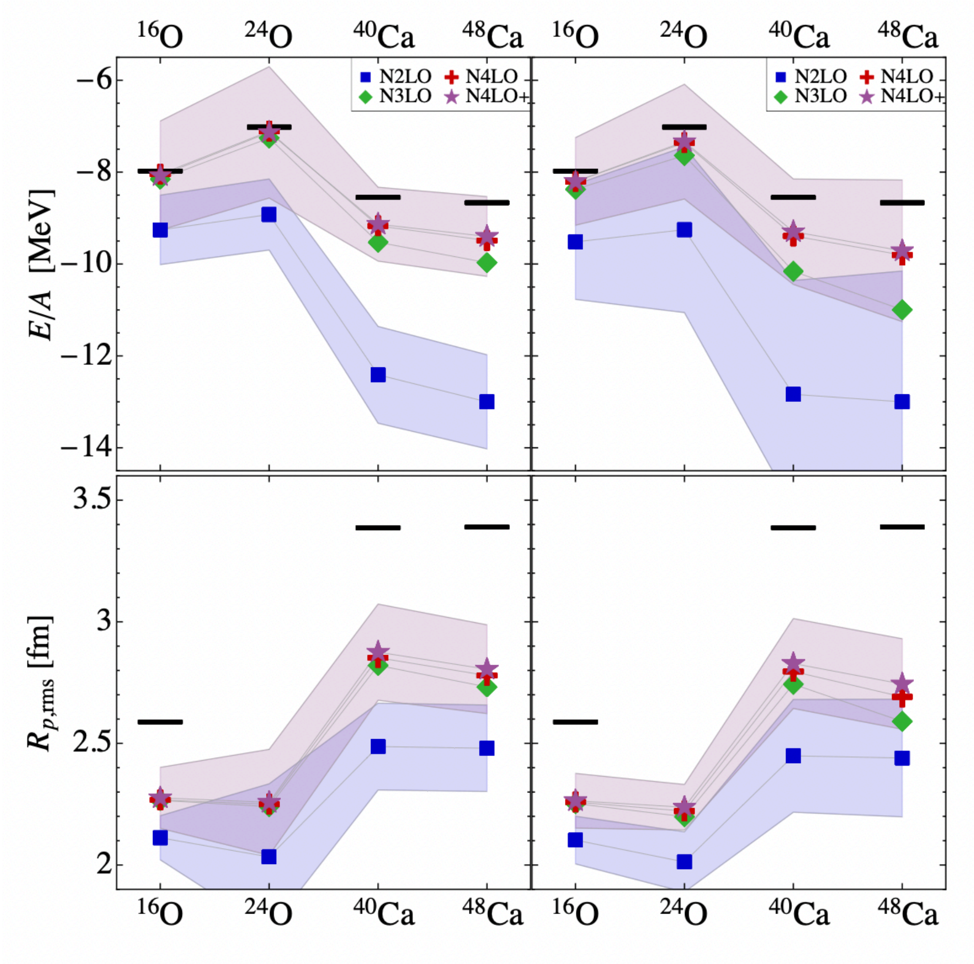


	c_D	c_E	$E(^3H)$	$E(^{16}O)$
3NF(local)	−2.0	−0.541	−8.78	−126.01
3NF(lnl)	6.0	0.894	−8.73	−127.15
Expt.			−8.482	−127.619

Rongzhe Hu, Jianguo Li, Siqin Fan, Furong Xu, arXiv:2601.08199 (2026)

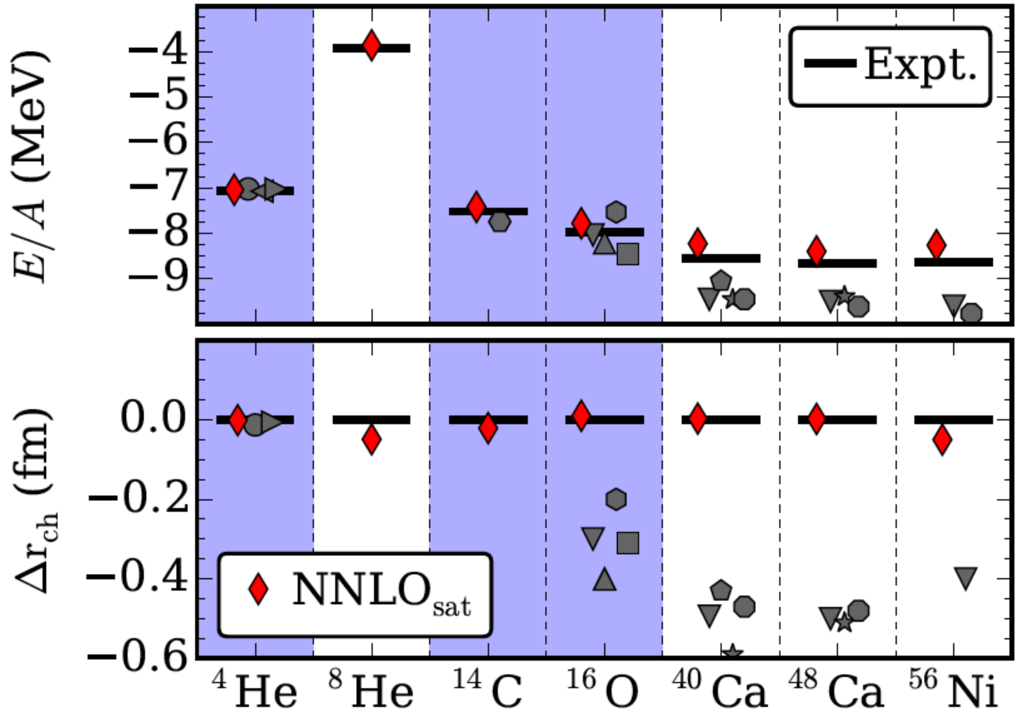
Different optimization strategies

Traditional approach fit to A <= 3 nuclei



P. Maris et al, (LENPIC collaboration)
Phys. Rev. C 106, 064002, 2022

Pragmatic approach fit to heavier nuclei

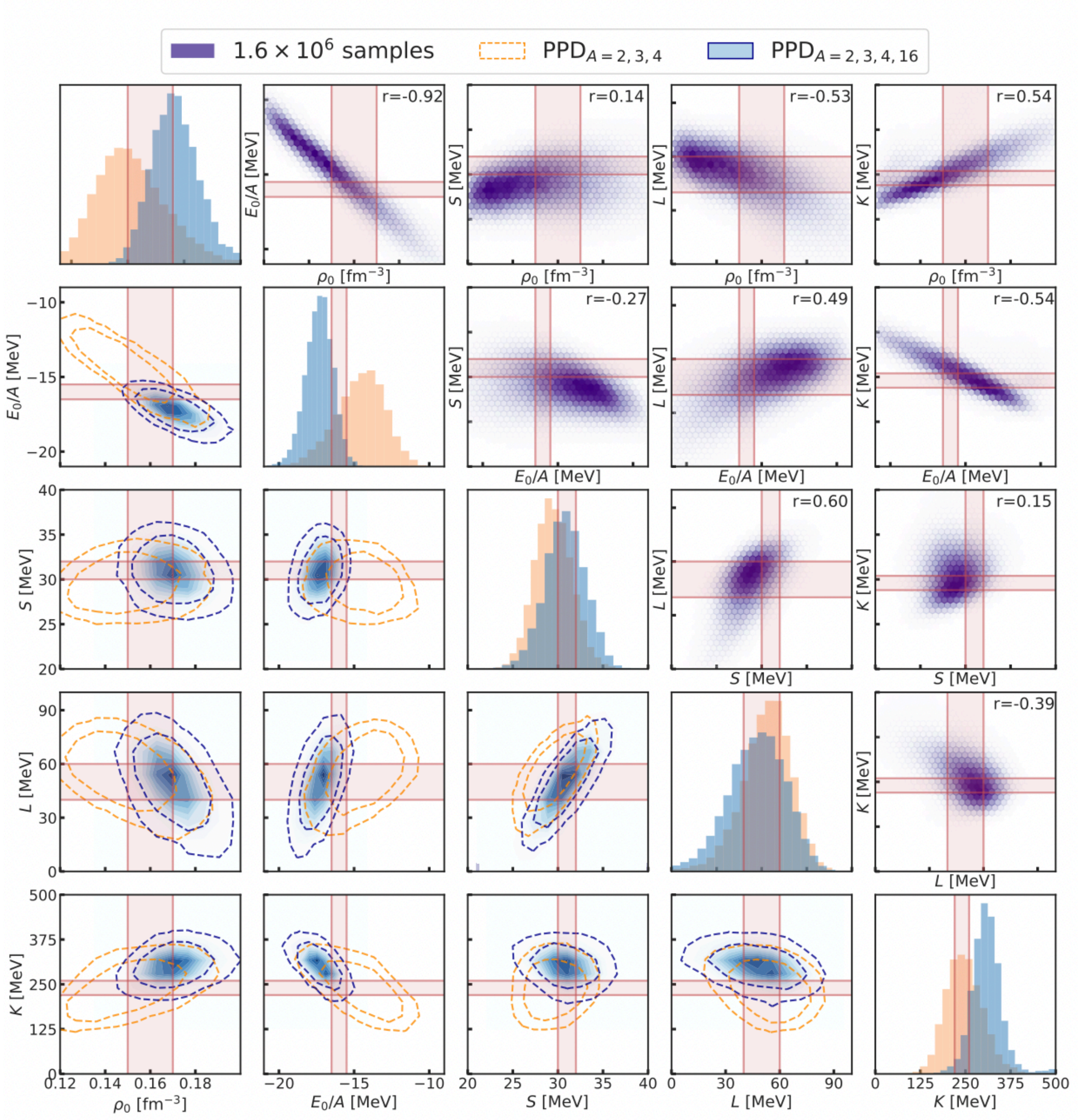


A. Ekström *et al*, Phys. Rev. C **91**, 051301(R) (2015).

Not new: GFMC with AV18 and Illinois-7 are fit to 23 levels in nuclei with A <10

What is ab initio in nuclear theory?
What are the "correct" observables to fit in chiral EFT?
Does predictive power go with large extrapolations?

Why include ^{16}O in the optimization?



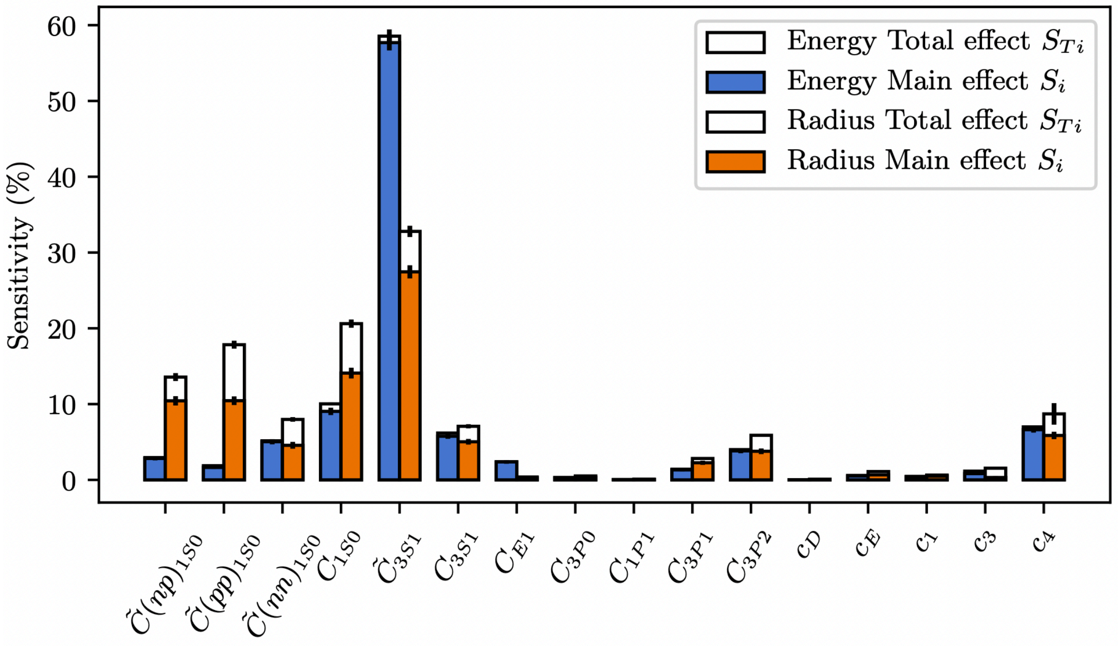
W. Jiang et al, Phys. Rev. C 109, L061302 (2024)

Constrains saturation physics directly:

^{16}O introduces the first meaningful density and many-body information, anchoring the interaction in a way few-body data cannot

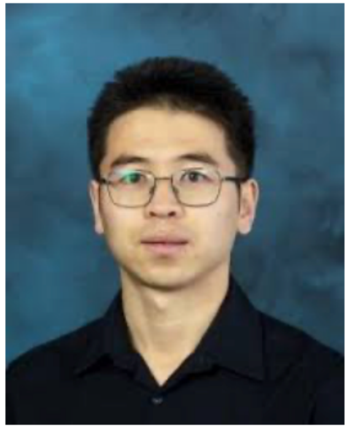
Reduces parameter degeneracy:

Including ^{16}O observables eliminates large regions of the LEC space, leading to significantly tighter and more reliable saturation predictions



A. Ekström, G. Hagen Phys. Rev. Lett. 123, 252501 (2019)

$N3LO_{Texas}$



Baishan Hu
Texas A&M

Disclaimer:
We will not address UQ in this talk

Initial search domain

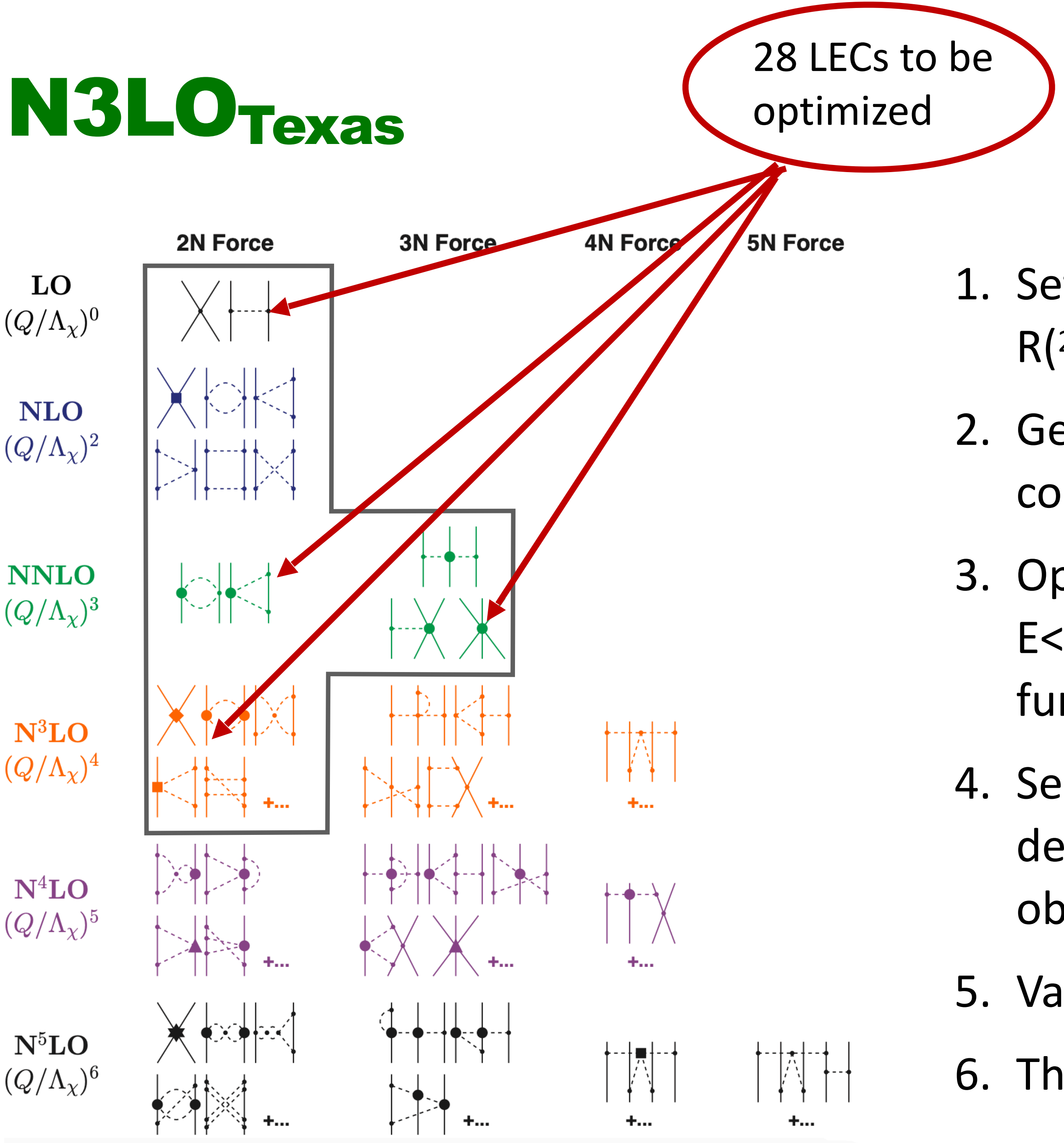
LEC	Min	Max
$\widetilde{C}^{pp}_{^1S_0}$	−0.30	−0.10
$\widetilde{C}^{nn}_{^1S_0}$	−0.30	−0.10
$C_{^1S_0}$	2.30	2.90
$C_{^1P_1}$	−1.00	1.00
$C_{^3S_1}$	0.10	1.70
$C_{^3P_2}$	−2.10	2.40
$D_{^1S_0}$	−28.00	−18.00
$D_{^1P_1}$	8.50	18.00
$\widehat{D}_{^3S_1}$	−9.70	9.30
$D_{^3D_1}$	−8.20	4.50
$D_{^3S_1-^3D_1}$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

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^3LO_{Texas}!

Baishan Hu, A. Ekström, C. Forssén, G. Hagen, W. G. Jiang, T. Miyagi, T. Papenbrock et al, arXiv:2512.11723 (2025)

N3LO_{Texas}



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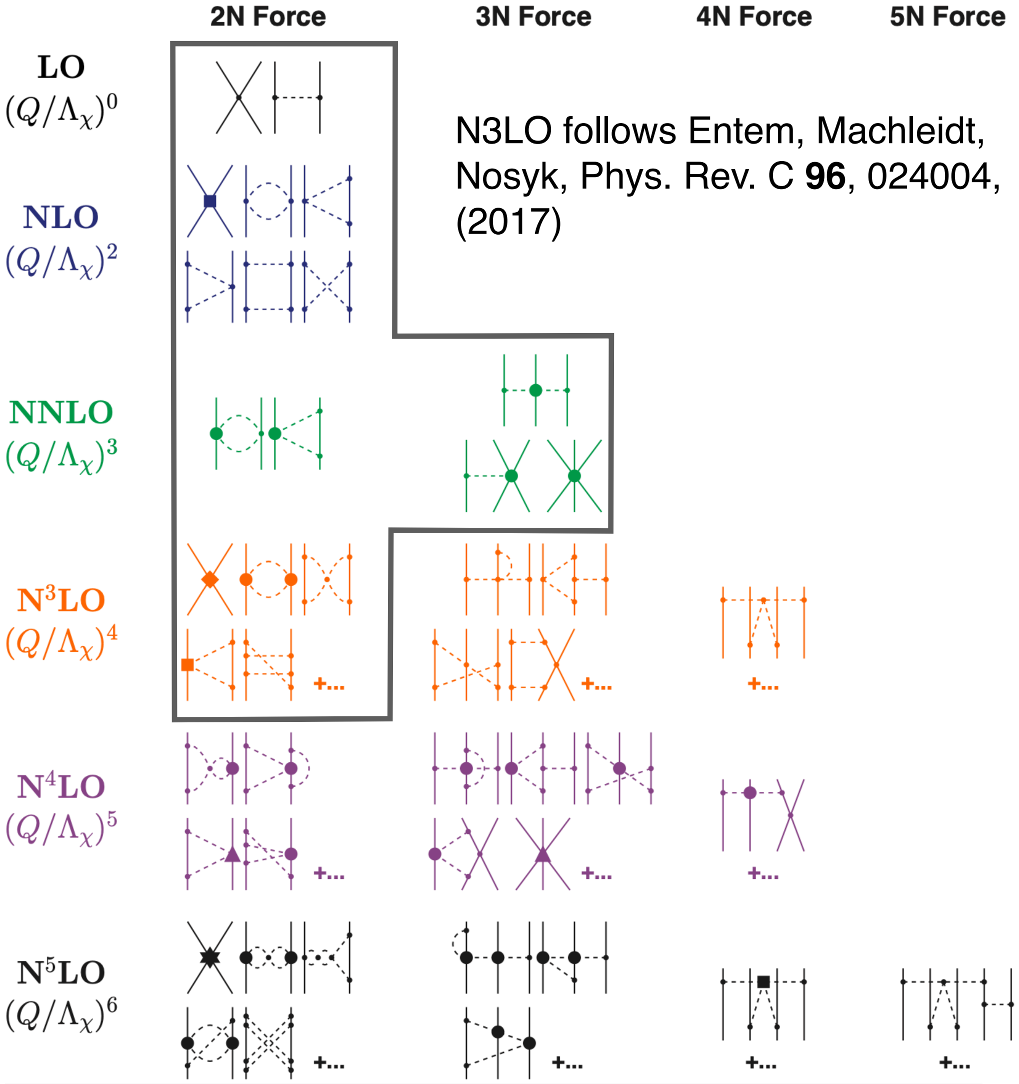
N3LO Texas



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

non-local momentum space regulators

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

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

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

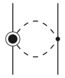
πN LECs according to Roy-Steiner analysis

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

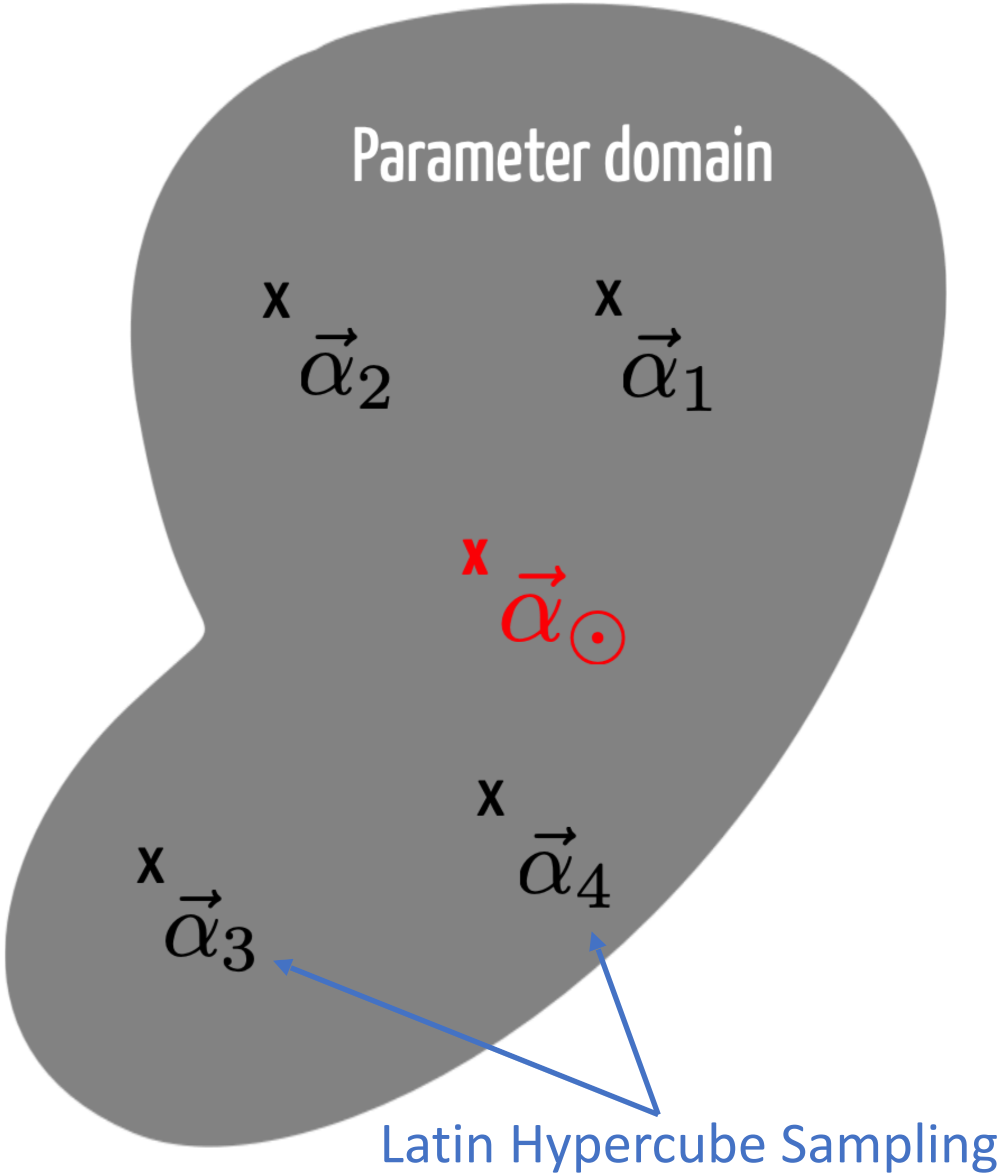
M. Hoferichter *et al.* Phys. Rev. Lett. **115**, 192301 (2015); Phys Rep. **625**, 1 (2016)

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



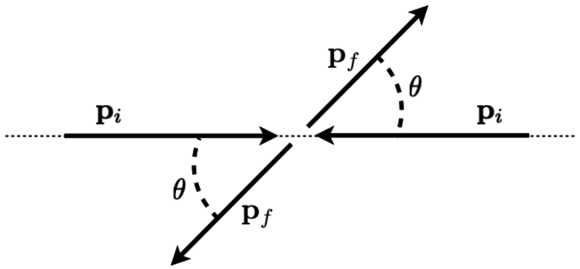
- Eigenvector continuation method [Frame D. et al., Phys. Rev. Lett. 121, 032501 (2018), A. Ekström, G. Hagen PRL 123, 252501 (2019), S. König et al Phys. Lett. B 810 (2020) 135814]
- Write the Hamiltonian in a linearized form

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

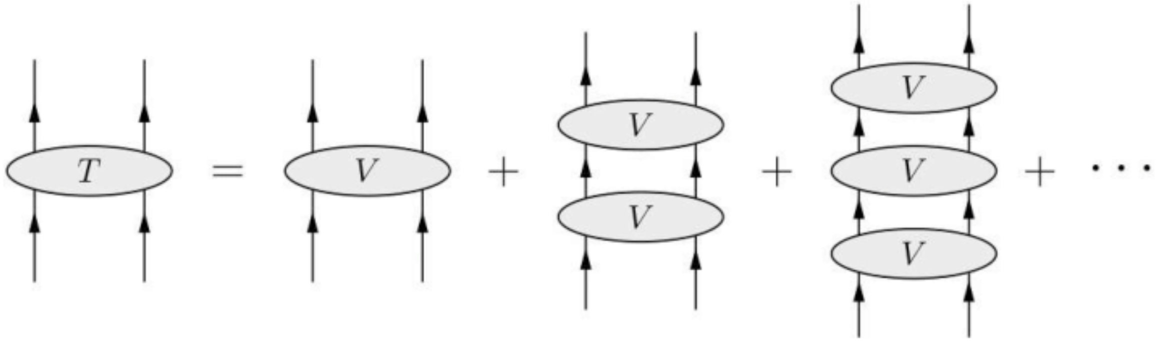
- Select "training points" (snap-shots) where we solve the exact problem
- Project a target Hamiltonian onto sub-space of training vectors and diagonalize the generalized eigenvalue problem

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

Emulating two-body scattering



$$T = V + VGT$$



Newton functional: $S[T] = V + VGT + TGV - TGT + TGVGT$

Assume a trial *T*-matrix $\tilde{T} = \sum_{i=1}^{N_t} \beta_i T_i$ ← **N_t $\alpha-$snapshots ("training points")**

The condition for stationarity $\frac{dS}{d\vec{\beta}} = 0$ yields the following equation for $\vec{\beta}_\star$: $\vec{m} + \mathbf{M}\vec{\beta}_\star = 0$

where $M_{ij} = (T_i[GVG - G]T_j + T_j[GVG - G]T_i)$ $m_i = (VGT_i + T_i GV)$

Inserting solution back into the functional, we approximate the *T*-matrix by

More than 300x improvement in CPU time $S[T_\star] = V - \frac{1}{2}\vec{m}^T \mathbf{M}^{-1} \vec{m}$

J. A. Melendez, et al Phys. Lett. B 821 136608 (2021)

Optimization → Validation → Prediction

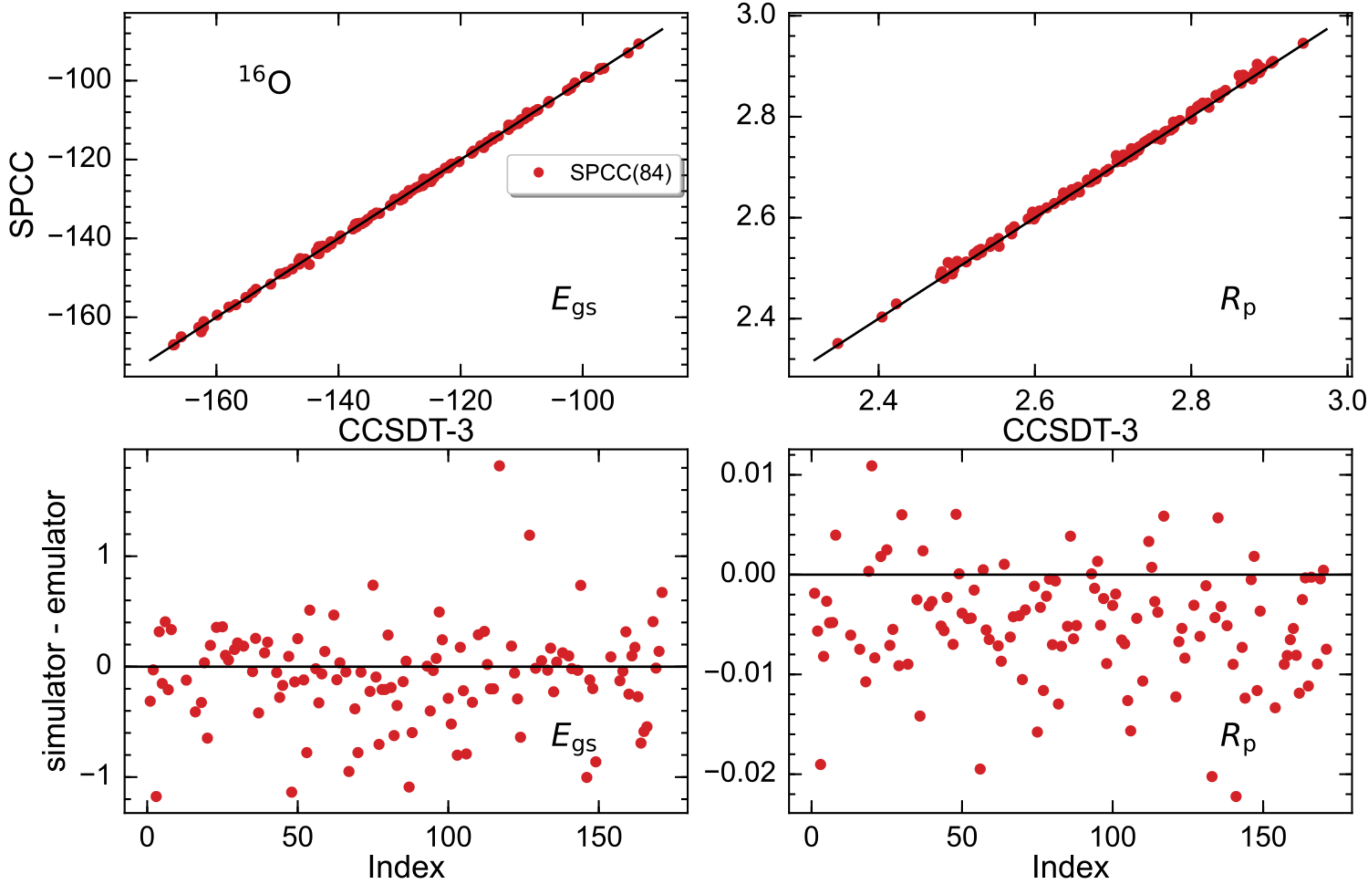
		N^3LO_{Texas}	Exp.
Optimization	a_{pp}^C	-7.820	$-7.8196(26)^a$
	r_{pp}^C	2.757	$2.790(14)^a$
	a_{nn}	-18.950	$-18.95(40)$
	r_{nn}	2.794	$2.75(11)$
	a_{np}	-23.741	$-23.740(20)$
	r_{np}	2.681	$2.77(5)$
	$E_{gs}(^2H)$	-2.225	$-2.224575(9)$
	$R_{ch}(^2H)$	2.131	$2.1421(88)$
	$Q(^2H)$	0.27	0.27^b
	$P_D(^2H)$	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	$5.5012(13)$

^{a}Including Coulomb (C) effects. Tuned separately after optimization.

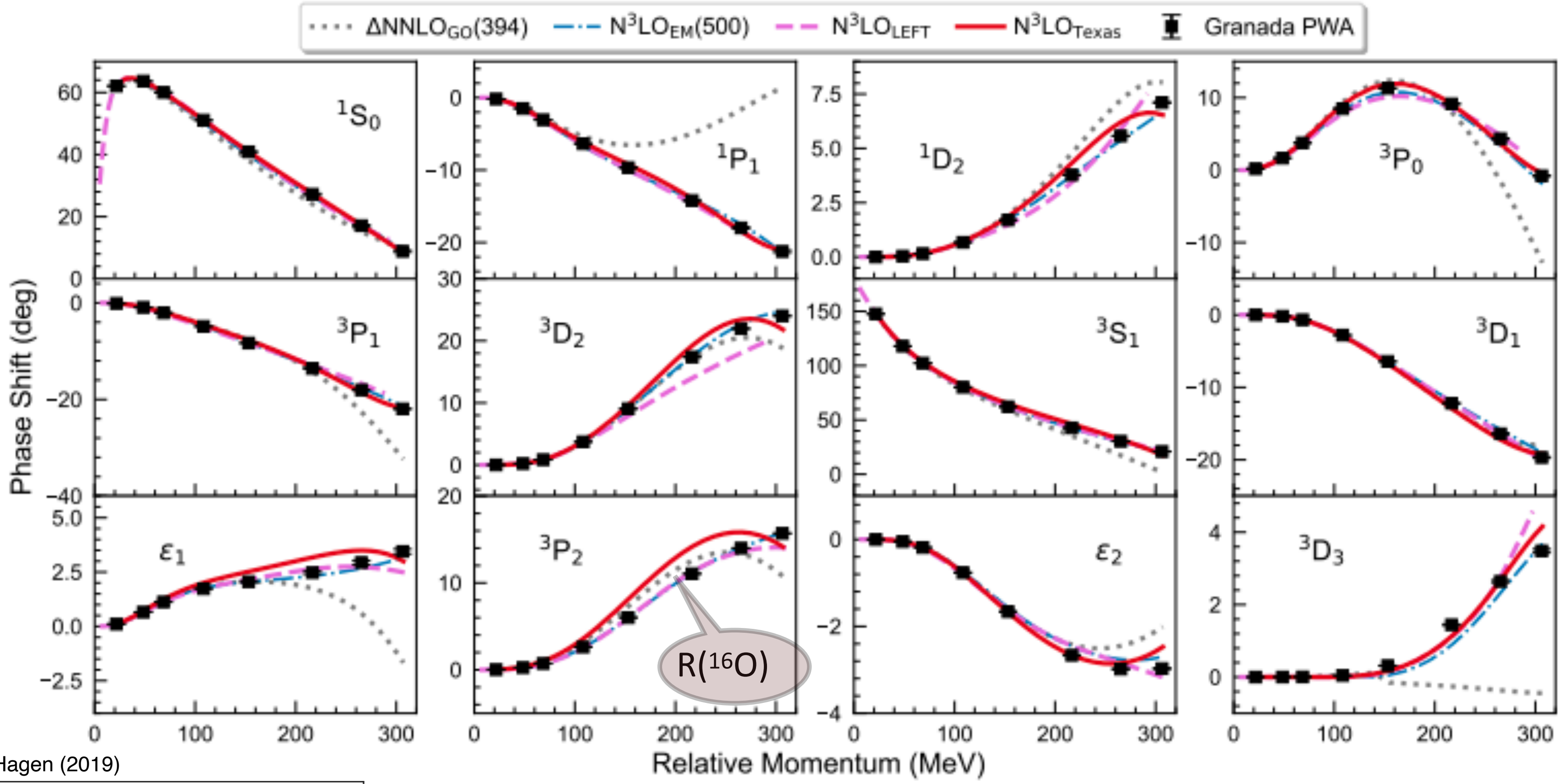
^{b}CD-Bonn value [103]

^{c}Trends from mass surface [13]

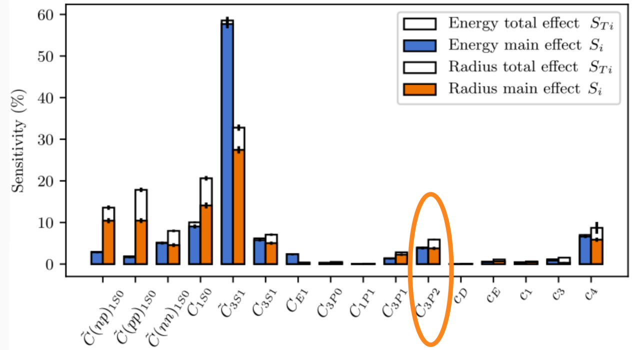
High-precision emulator of CCSDT-3



N^{3}LO$_{Texas}$ accuracy: NN scattering



Ekström and Hagen (2019)

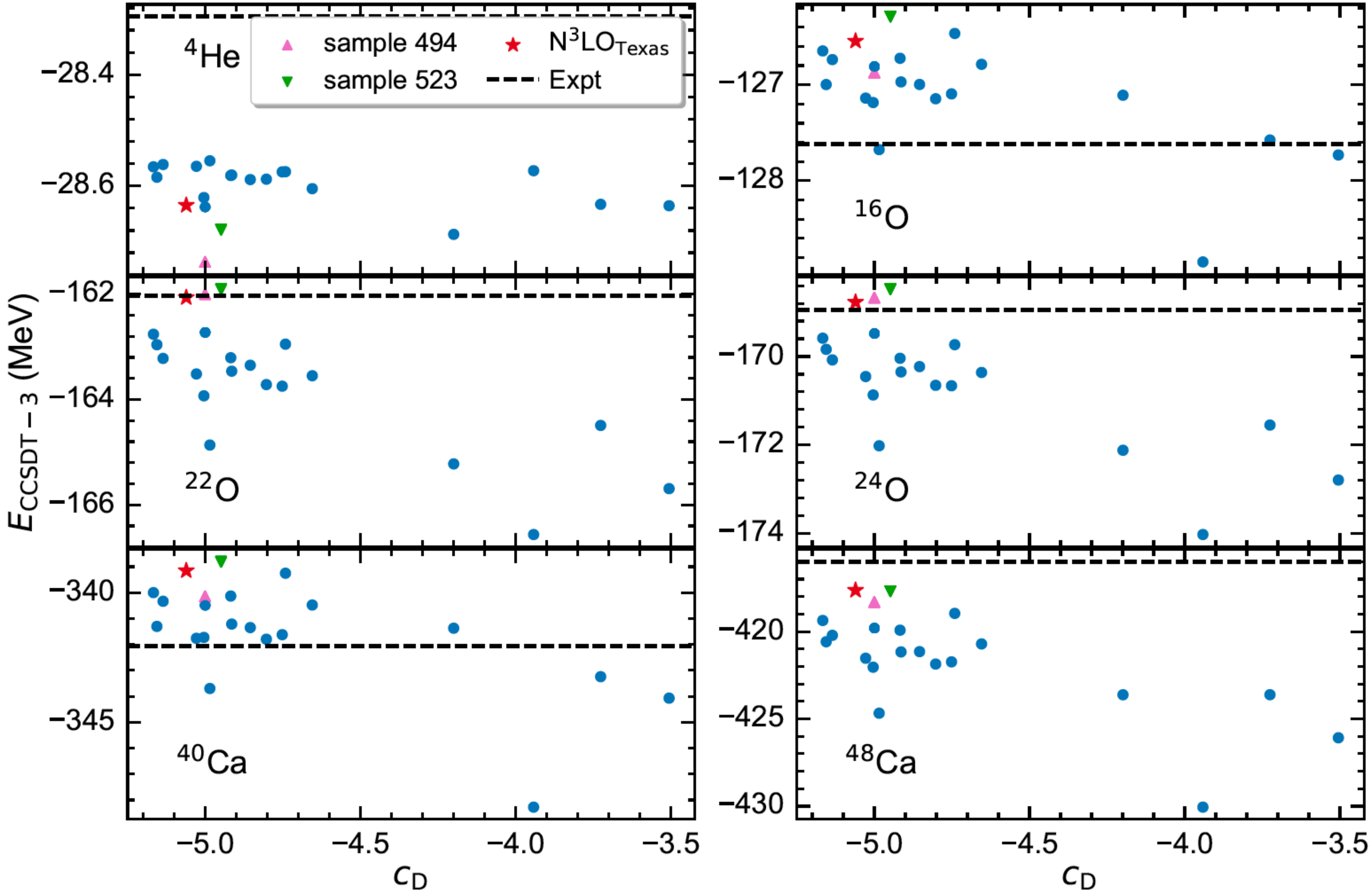


Some tension between the reproduction of the scattering phase shifts in the $^3P_2$ channel and the charge radius of ^{16}O

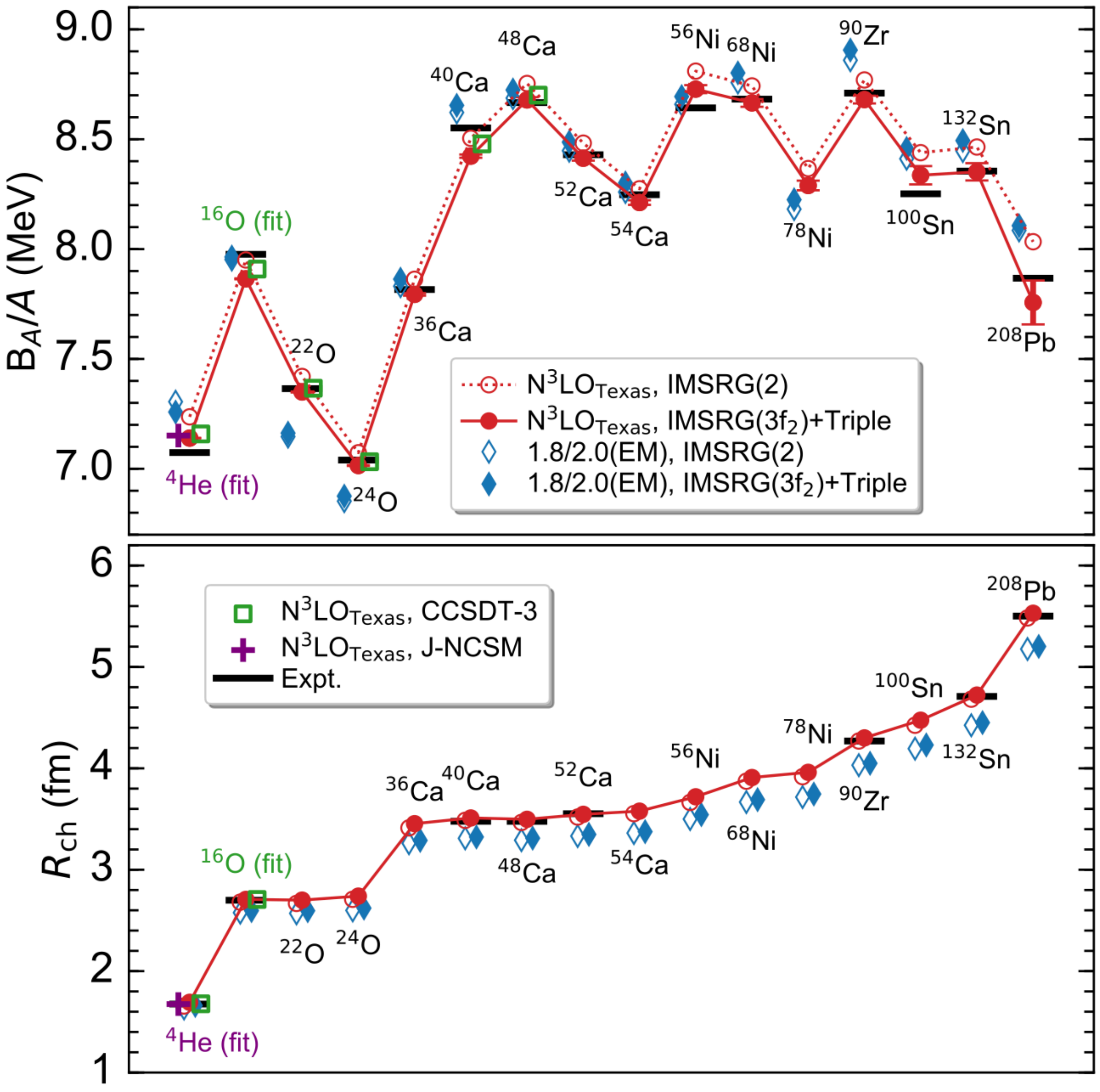
Consistent with the global sensitivity analysis

How much weight should one put on different observables in the fit?

The 20 "top" candidates



Saturation properties of nuclei and nuclear matter



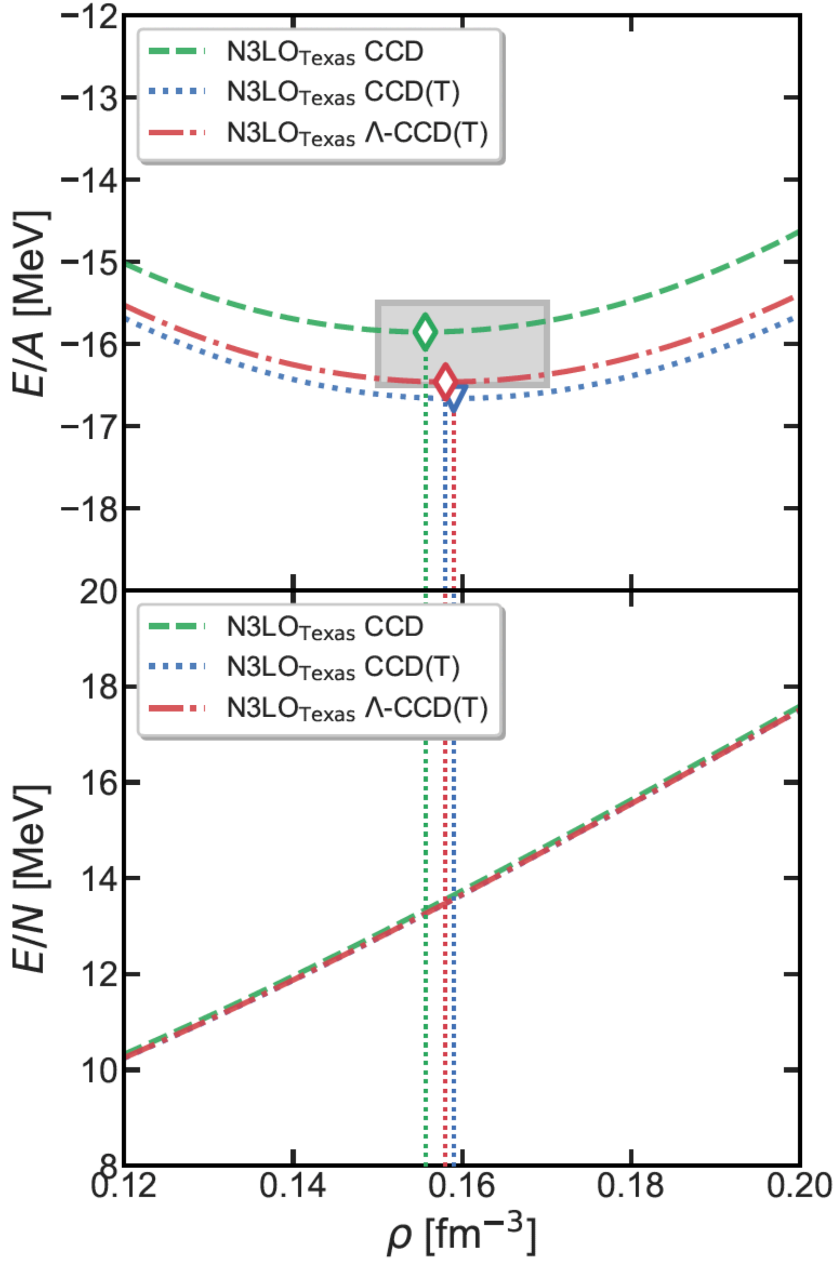
Binding energies and charge radii for closed shell nuclei in good agreement with data

Used different high precision many-body approaches: CCSDT-3 and VS-IMSRG(3f2)

Note that the N = Z doubly-magic nuclei ^{40}Ca, ^{56}Ni, and ^{100}Sn deviate a bit more from data →

^{16}O was optimized with CCSDT-3 while heavier nuclei were computed using IMSRG(3f2)

Properties of neutron/nuclear matter



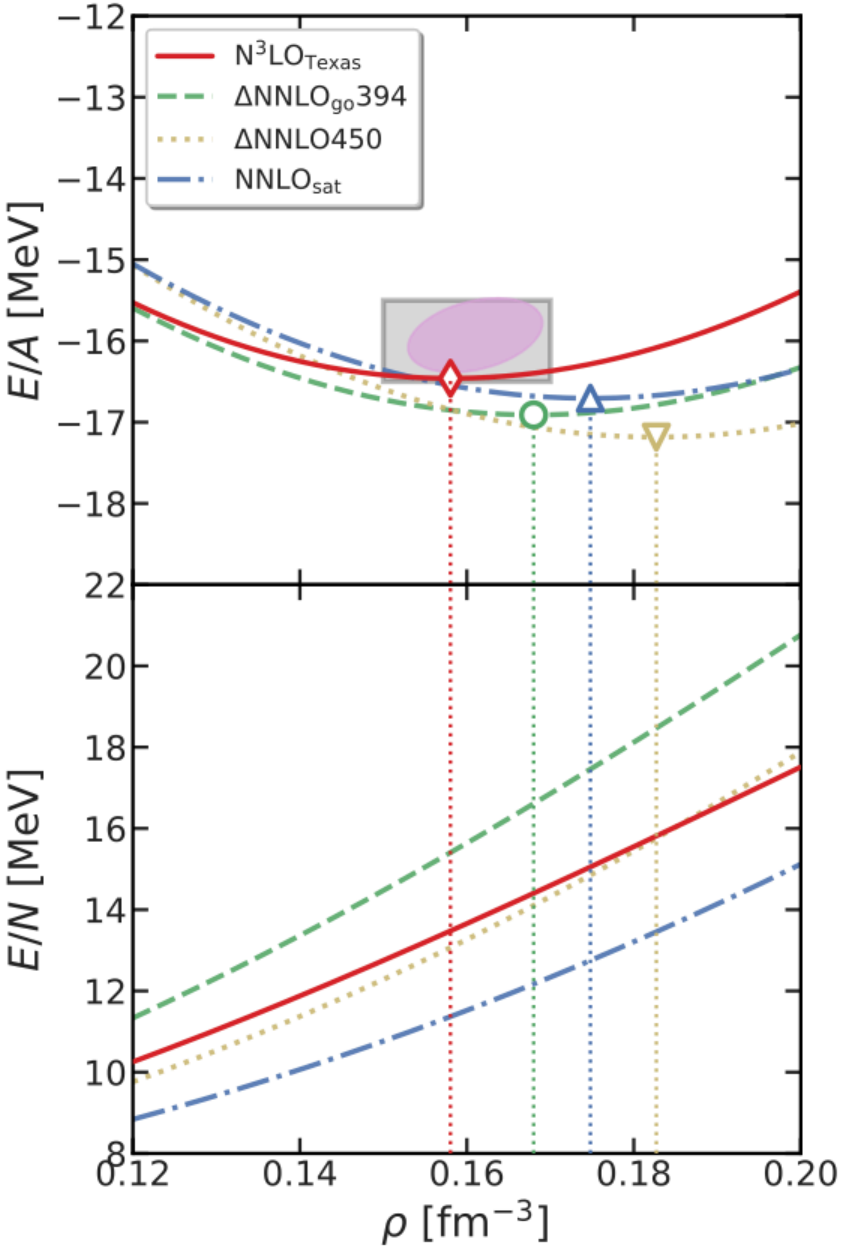
- Simulations used periodic boundary conditions

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

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

Λ-CCD(T) originally developed in quantum chemistry:
A. G. Taube and R. J. Bartlett, J. Chem. Phys. 128, 044110 (2008).

Properties of neutron/nuclear matter



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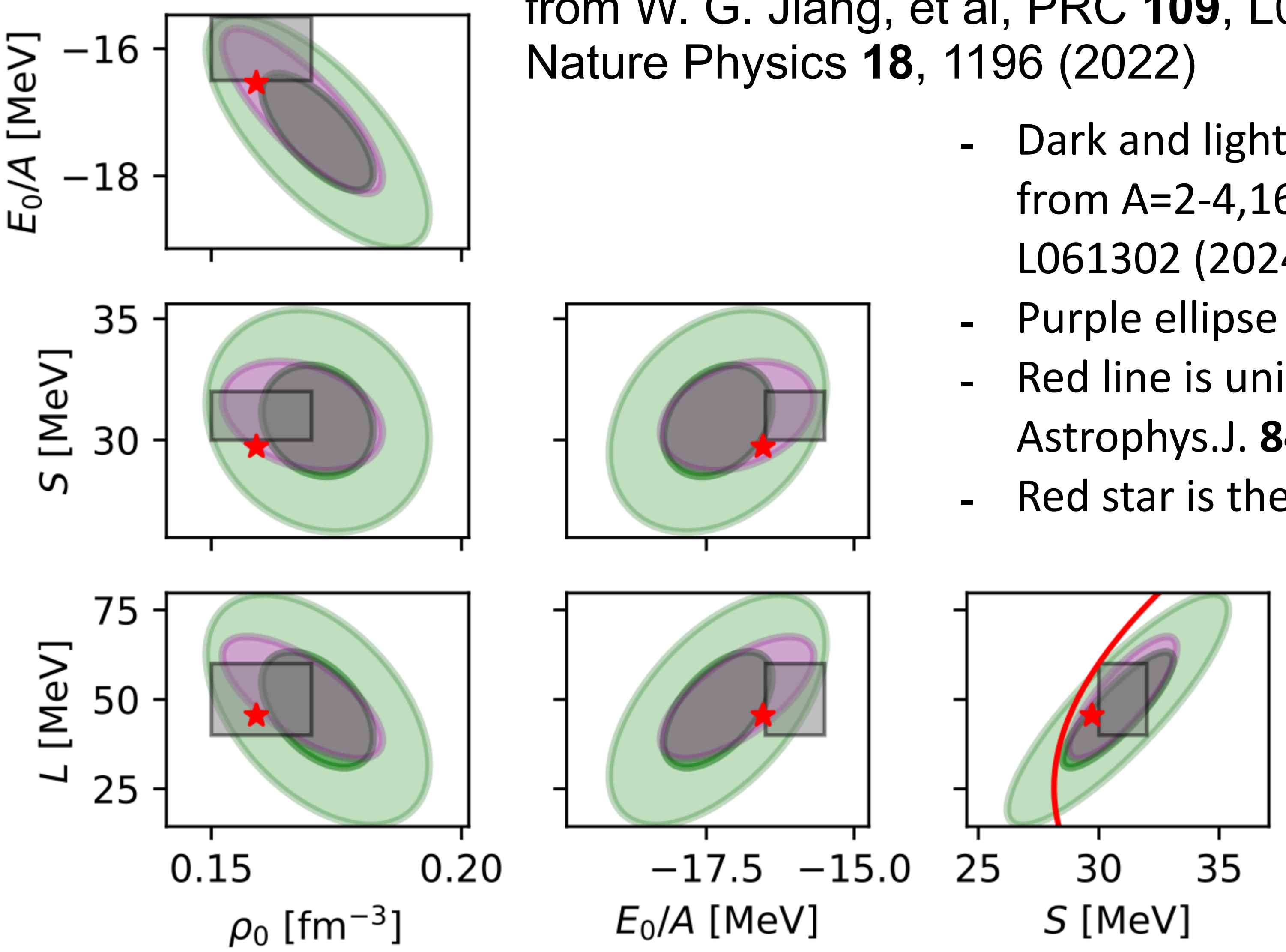
- New development: Λ-CCD(T) for infinite nuclear matter

N^3LO_{Texas} results are compared with coupled cluster computations using different interactions [**Francesco Marino, Weiguang Jiang, Samuel J. Novario, Phys. Rev. C 110, 054322 (2024)**]

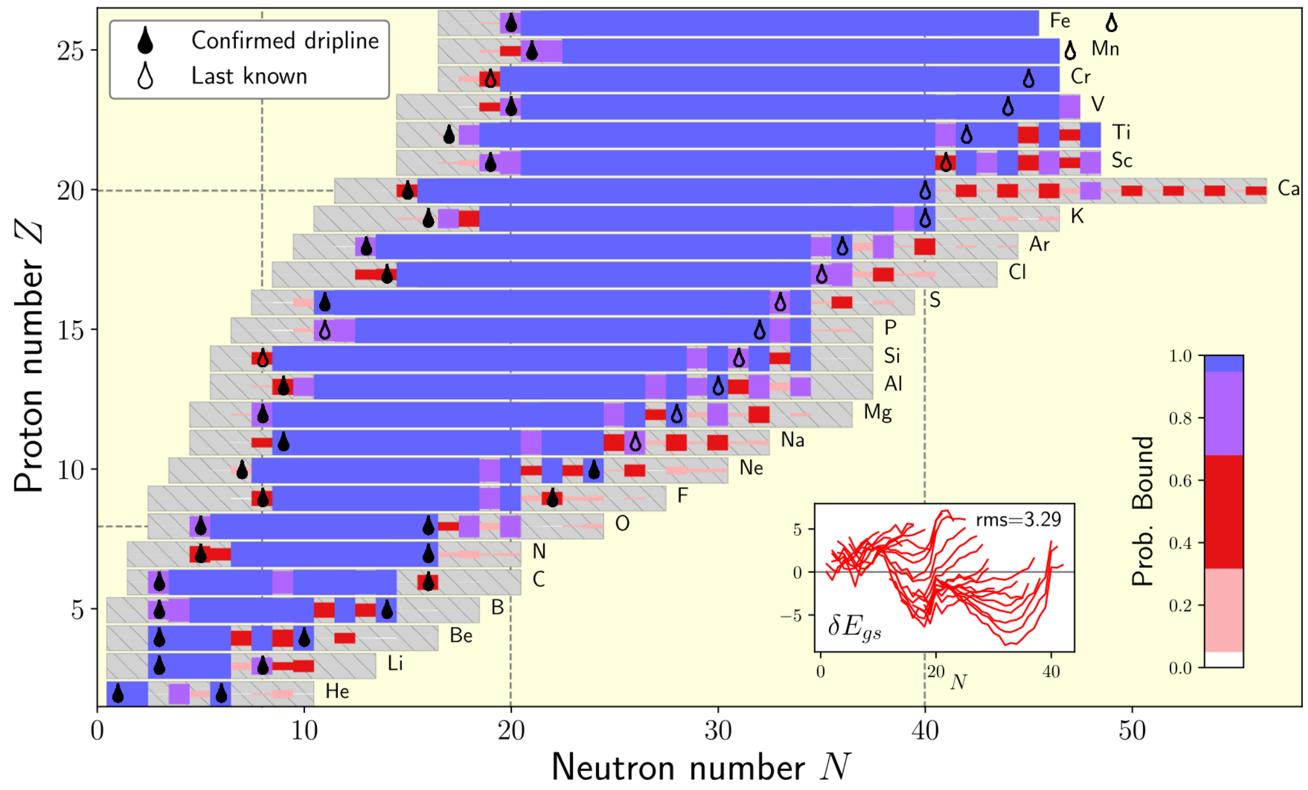
Properties of neutron/nuclear matter



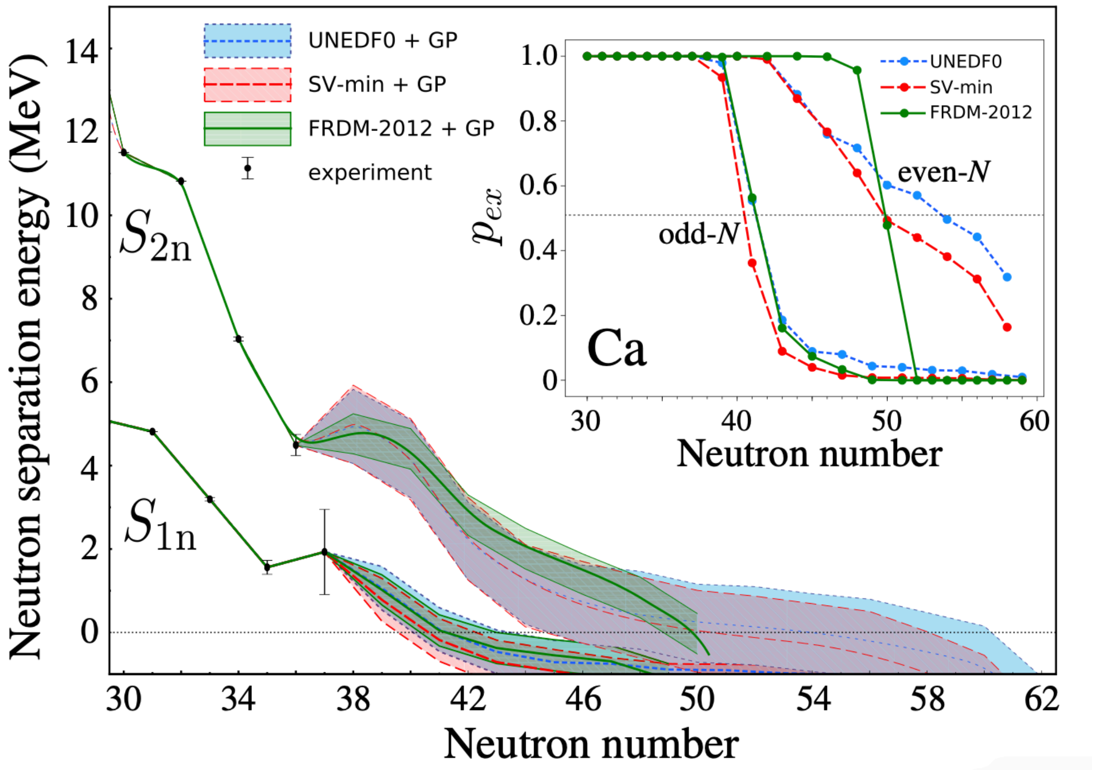
PPD (Gaussian approximation) ellipses for NM saturation properties from W. G. Jiang, et al, PRC **109**, L061302 (2024) and from B. Hu et al, Nature Physics **18**, 1196 (2022)

- 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$_{Texas}$ prediction

The dripline in calcium isotopes



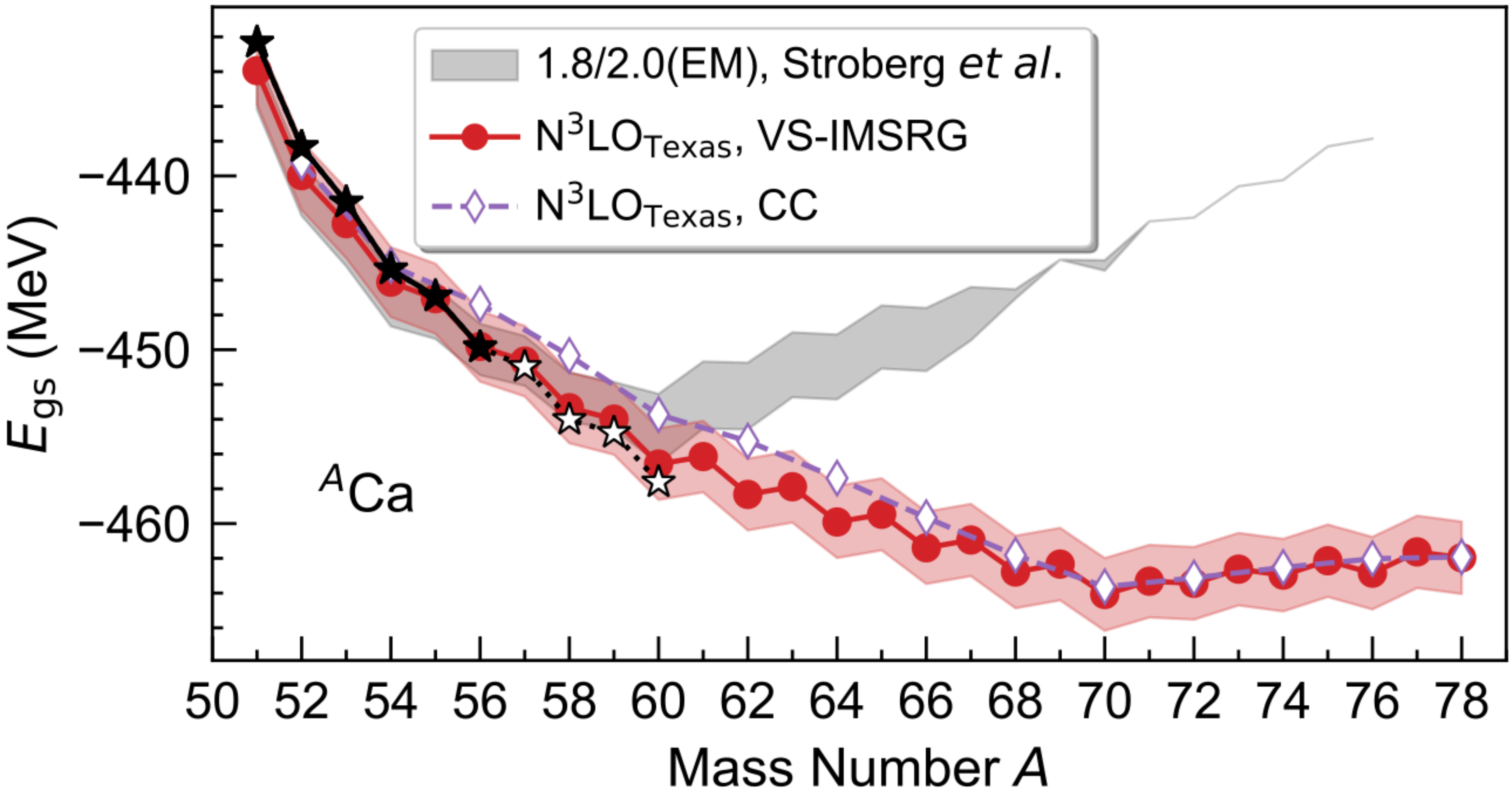
S. R. Stroberg et al, Phys. Rev. Lett. **126**, 022501 (2021)



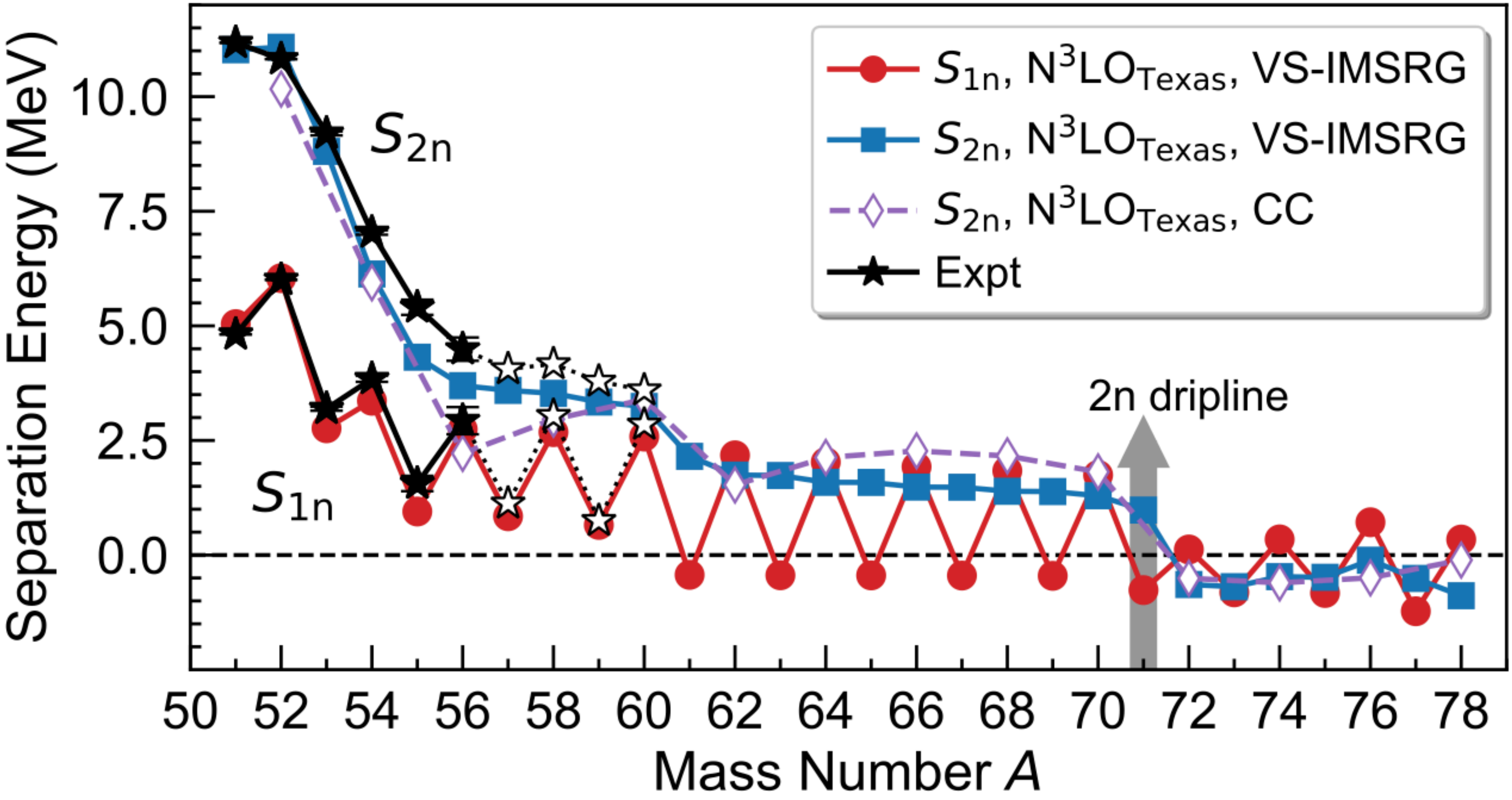
Leo Neufcourt, et al, PRL **122** 062502 (2019)

- 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

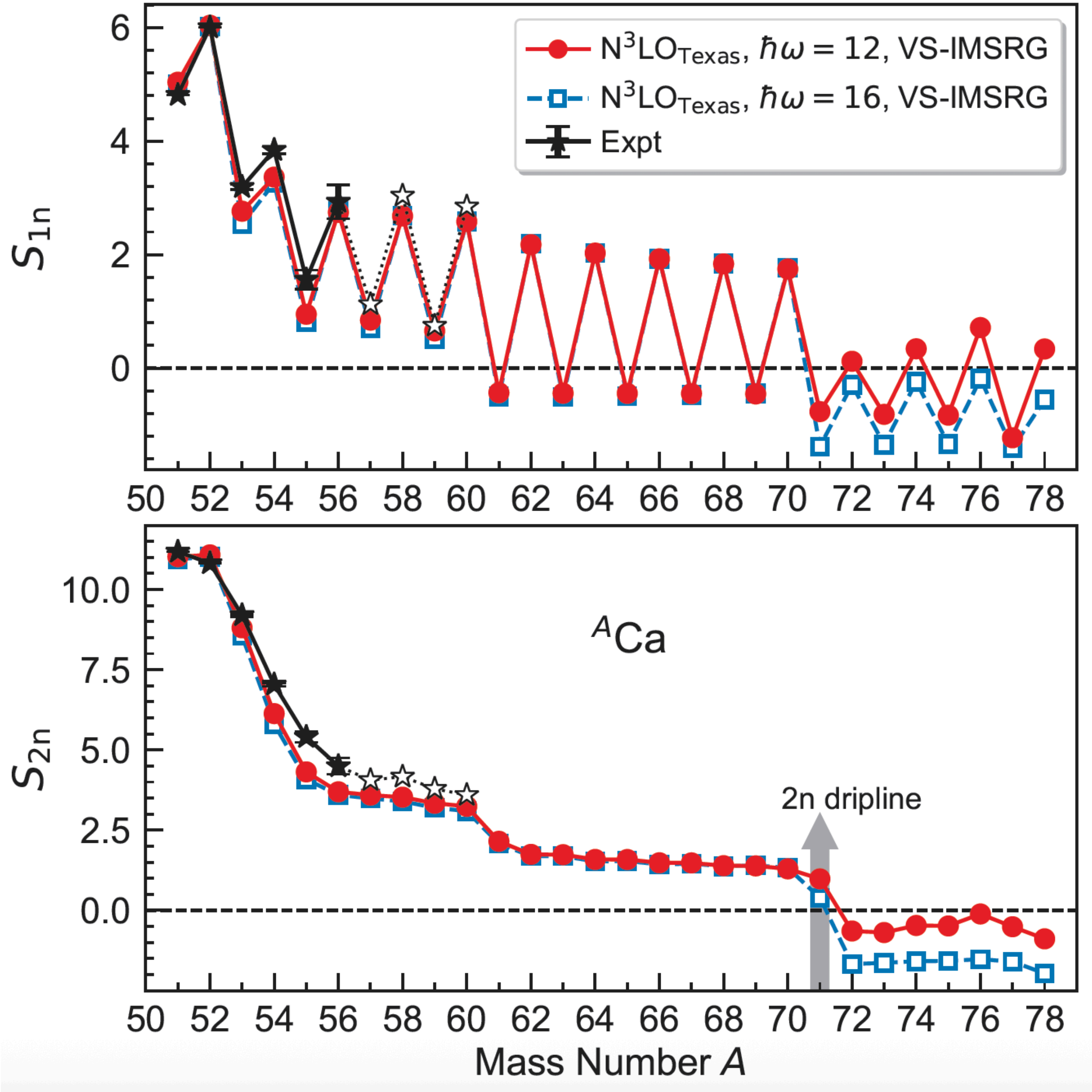
The dripline in calcium isotopes



The dripline in calcium isotopes

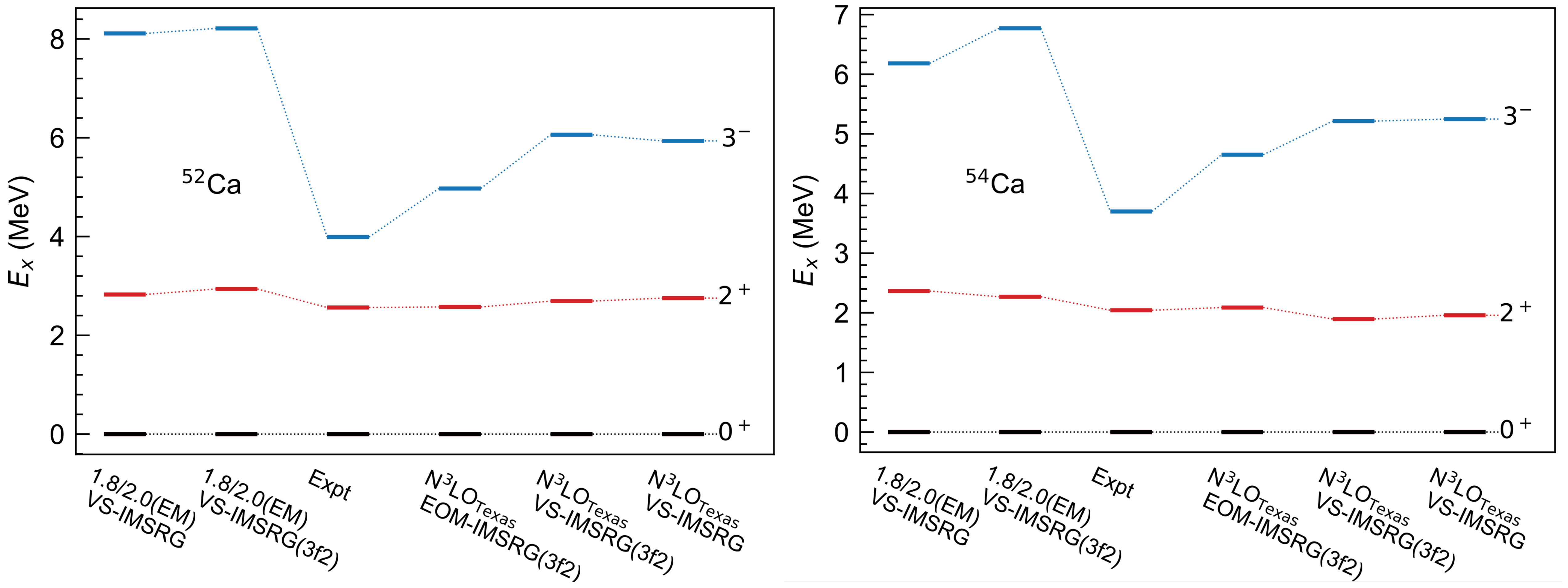


The dripline in calcium isotopes



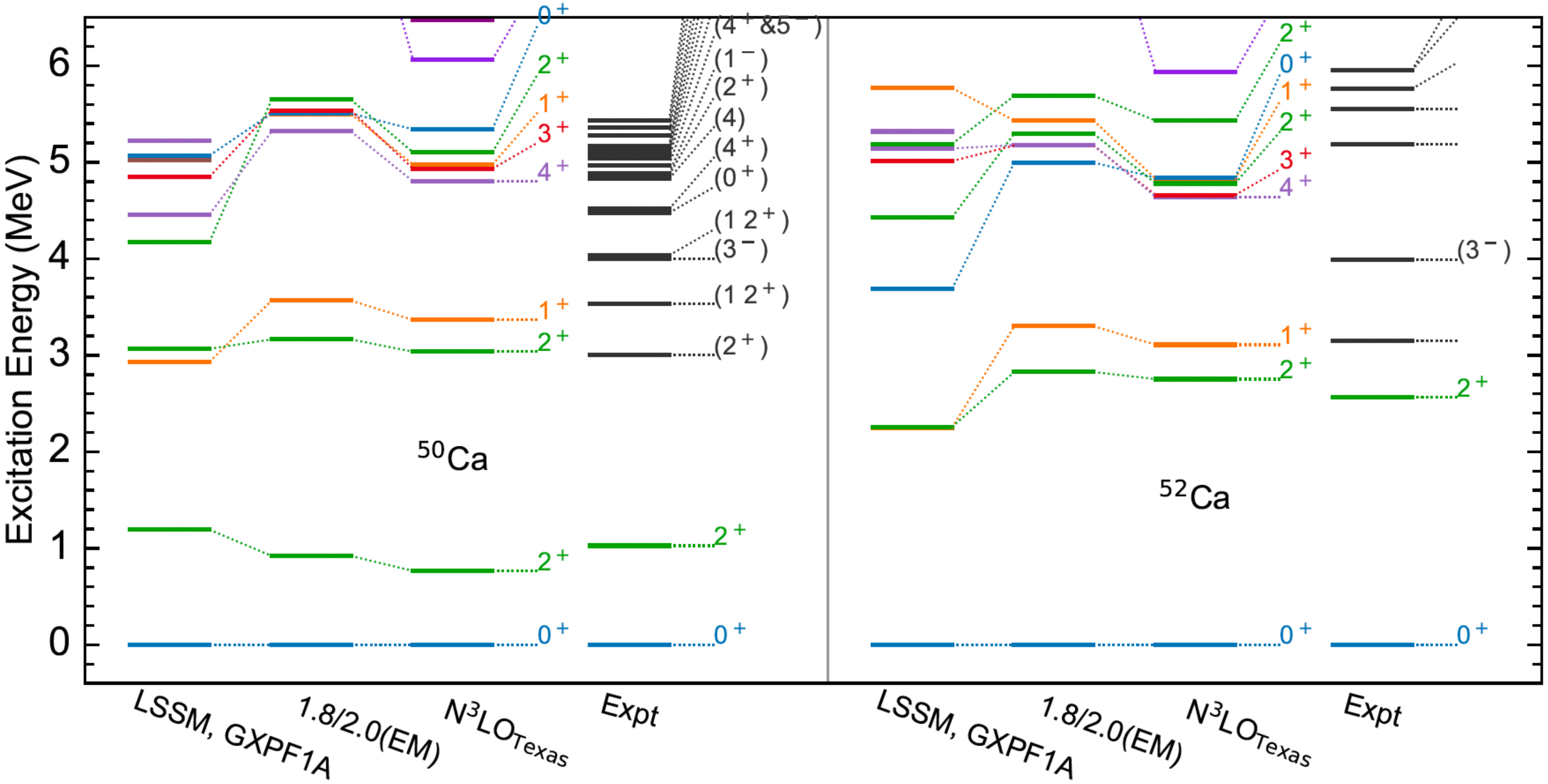
- We do not include coupling to the scattering continuum
- In order to better capture weak binding effects we choose a smaller hw = 12MeV
- We find the dripline at ^{70}Ca is robust with respect to different values of hw

The dripline in calcium isotopes

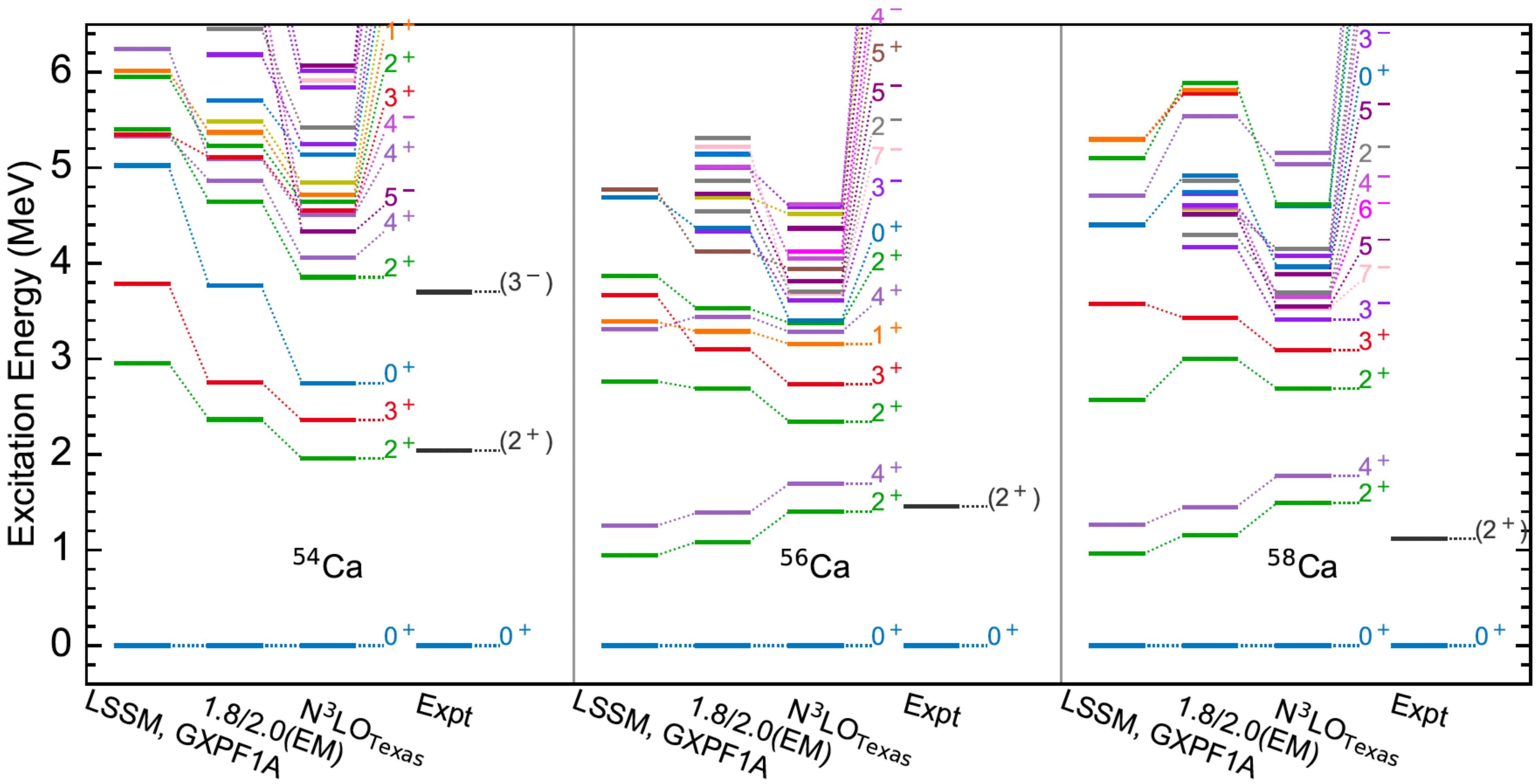


VS-IMSRG: ^{48}Ca core and neutron 1p3/2, 1p1/2, 0f5/2, 0g9/2, 1d5/2, 2s1/2 valence space

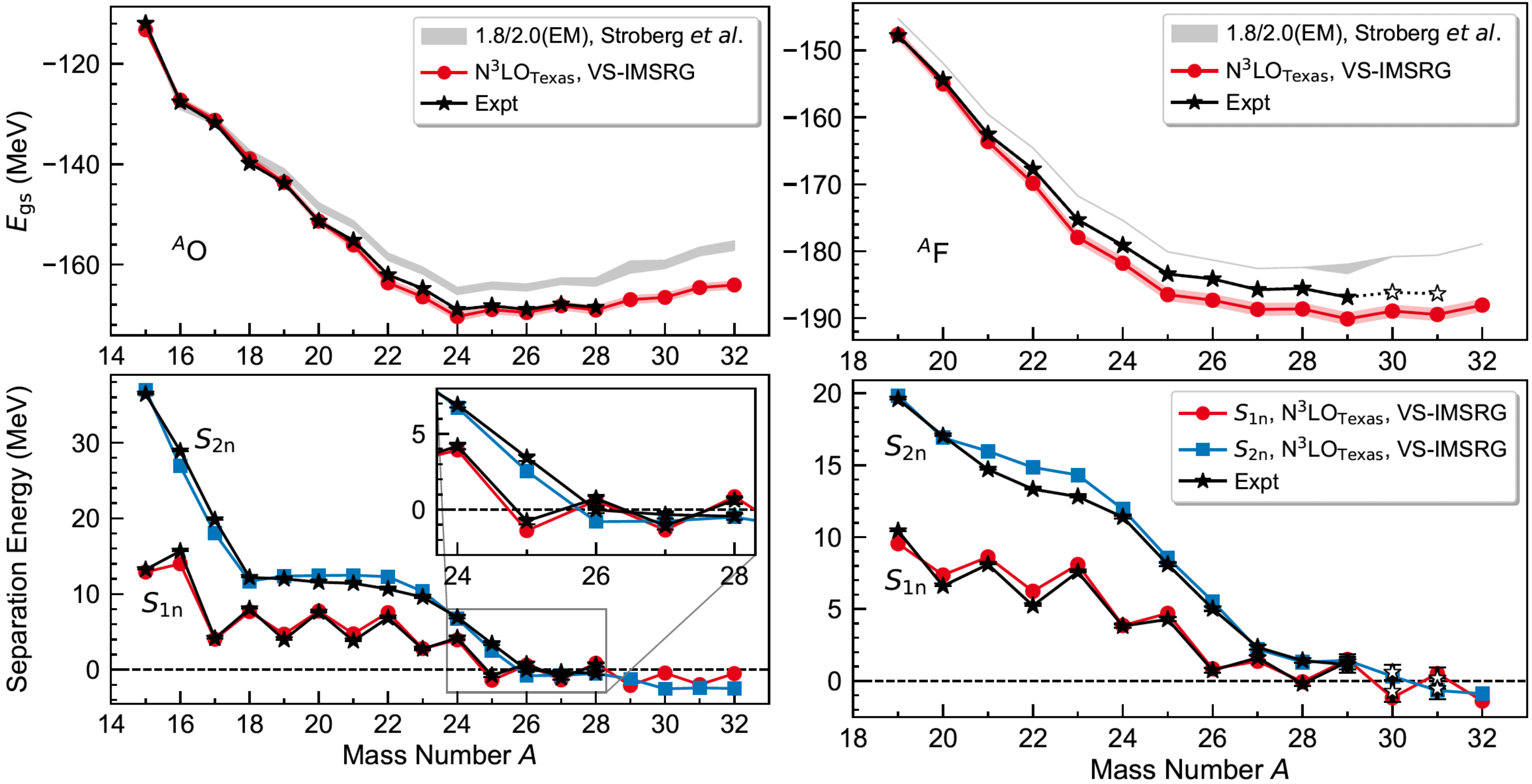
The dripline in calcium isotopes



The dripline in calcium isotopes



The dripline in oxygen and fluorine



Open problems/challenges

- What is ab initio in nuclear theory?
- Why do certain interaction models work better than others, but only for selected types of observables and in limited regions of the nuclear chart?
- In the pragmatic EFT approach by Weinberg what are the “correct” and most relevant observables to include in the optimization?
- How do we consistently quantify and understand our uncertainties: many-body versus interaction?
- Does predictive power go with large extrapolations?
- Can a pragmatic approach be too pragmatic?

Summary

- Utilizing high fidelity emulators we optimized a N3LO (NN) + N2LO (3NF)
- The objective function include scattering phase shifts, deuteron properties, and ^{4}He and ^{16}O properties
- Saturation properties are improved by including ^{16}O in the fit
- The resulting interaction is "soft" enough to converge medium mass and heavy nuclei and yields accurate results for the deuteron, scattering phase shifts, finite nuclei and infinite nuclear matter

Matrix elements available via NuHamil

Low-energy constants

TABLE S1. Low-energy constants (LECs) for the N^3LO_{Texas} interaction. The constants c_i, $\bar{d}_i$, $\widetilde{C}_i$, C_i, and D_i (also $\widehat{D}_i$) are in units of GeV^{-1}, GeV^{-2}, 10^4 GeV^{-2}, 10^4 GeV^{-4}, and 10^4 GeV^{-6}, respectively. The 3N LECs c_D and c_E are dimensionless.

LEC	Value	LEC	Value
	πN		
c_1	−1.07	c_2	3.20
c_3	−5.32	c_4	3.56
$\bar{d}_1 + \bar{d}_2$	1.04	$\bar{d}_3$	−0.48
$\bar{d}_5$	0.14	$\bar{d}_{14} - \bar{d}_{15}$	−1.90
	2N (LO)		
$\widetilde{C}^{pp}_{^1S_0}$	−0.154291	$\widetilde{C}^{np}_{^1S_0}$	−0.155631
$\widetilde{C}^{nn}_{^1S_0}$	−0.155010	$\widetilde{C}_{^3S_1}$	−0.202464
	2N (NLO)		
$C_{^1S_0}$	2.514273	$C_{^3P_0}$	1.025413
$C_{^1P_1}$	0.082796	$C_{^3P_1}$	−0.977112
$C_{^3S_1}$	1.075598	$C_{^3S_1-^3D_1}$	0.528490
$C_{^3P_2}$	−0.960907		
	2N (N^3LO)		
$\widehat{D}_{^1S_0}$	−1.643852	$D_{^1S_0}$	−19.286790
$D_{^3P_0}$	5.607692	$D_{^1P_1}$	10.529344
$D_{^3P_1}$	5.427348	$\widehat{D}_{^3S_1}$	5.715113
$D_{^3S_1}$	−40.129215	$D_{^3D_1}$	−4.622881
$\widehat{D}_{^3S_1-^3D_1}$	2.852185	$D_{^3S_1-^3D_1}$	0.505938
$D_{^1D_2}$	−2.369999	$D_{^3D_2}$	−4.984577
$D_{^3P_2}$	6.7635540	$D_{^3P_2-^3F_2}$	0.188085
$D_{^3D_3}$	−1.196276		
	3N (N^2LO)		
c_D	−5.060563	c_E	−1.034629