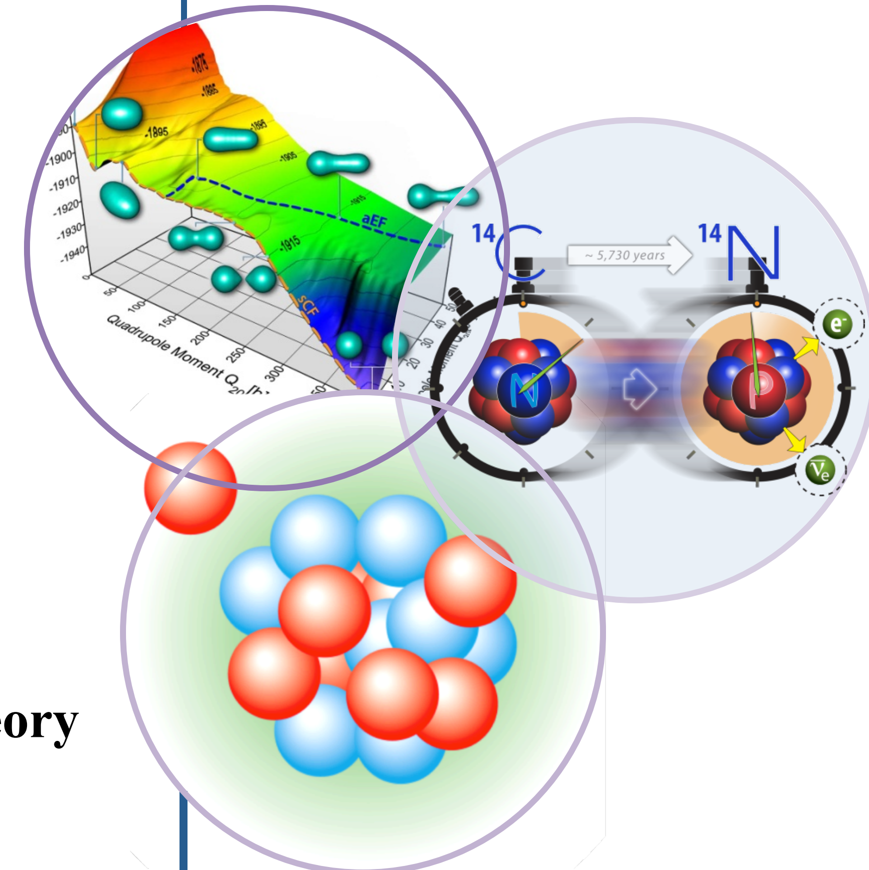
Ab initio Nuclear Structure – From Light to Medium Weight Nuclei

Gaute Hagen



International Conference on Nuclear Theory in the Supercomputing Era - 2013

May 13, Ames, Iowa.

U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY
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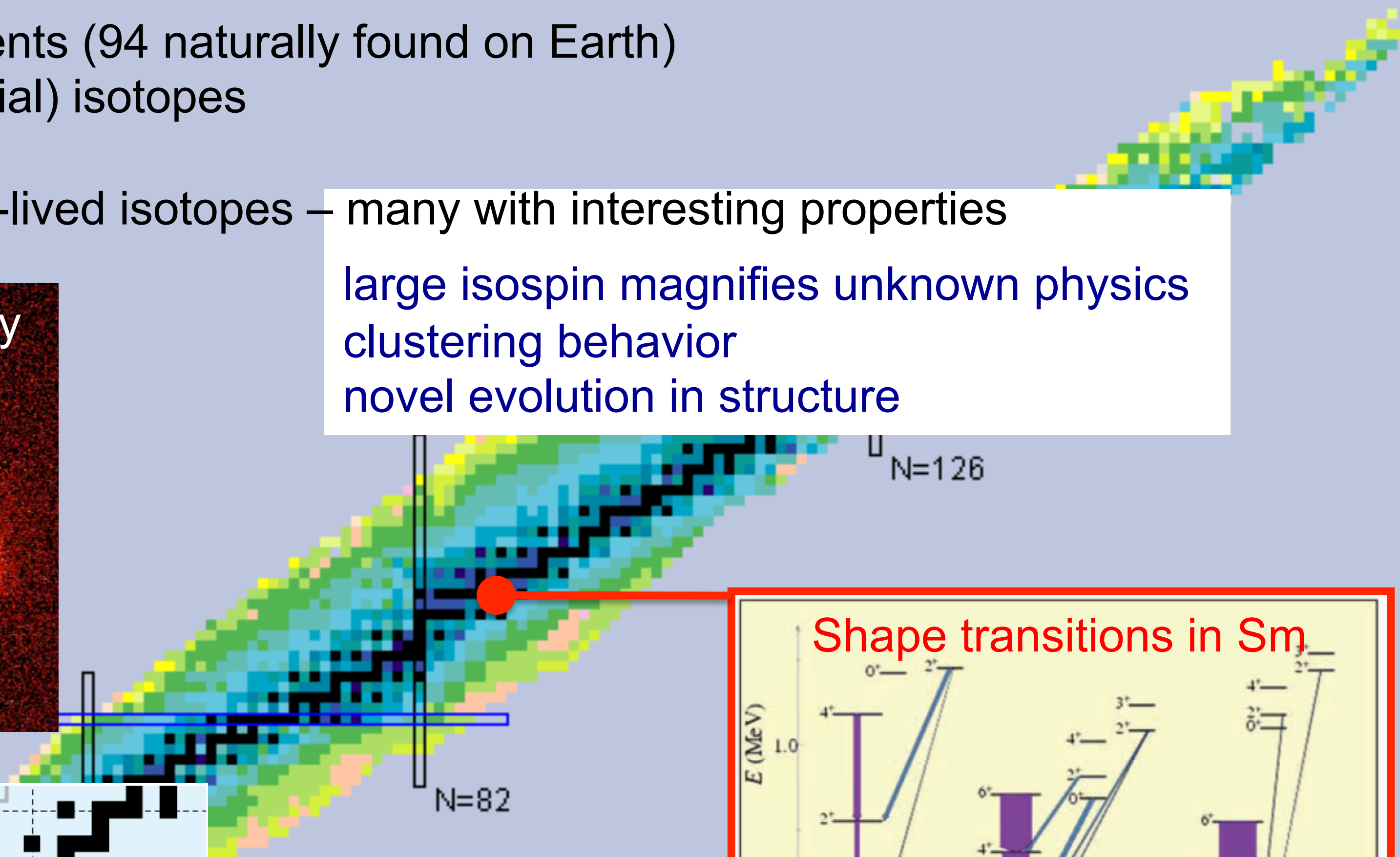
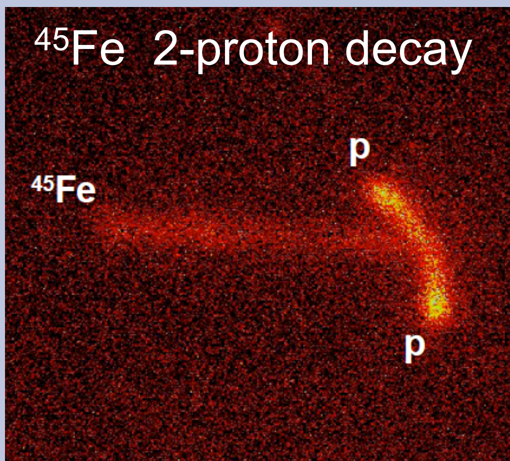
Nuclei across the chart

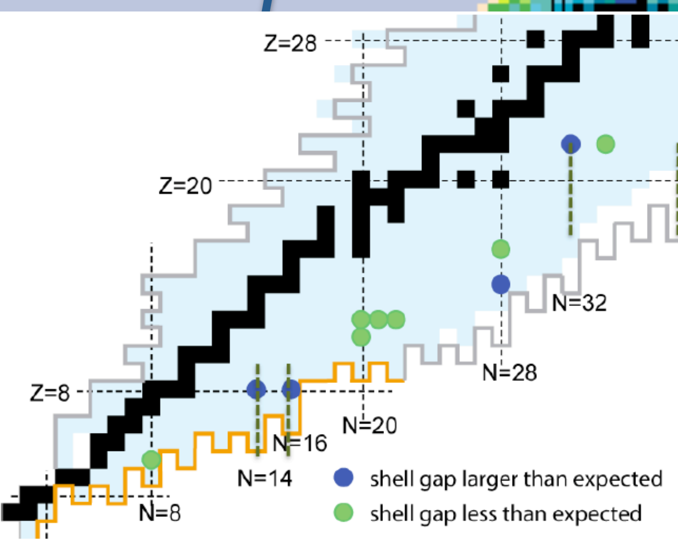
118 chemical elements (94 naturally found on Earth)
288 stable (primordial) isotopes

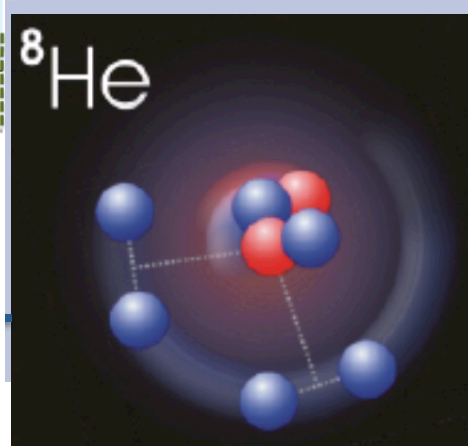
Thousands of short-lived isotopes – many with interesting properties

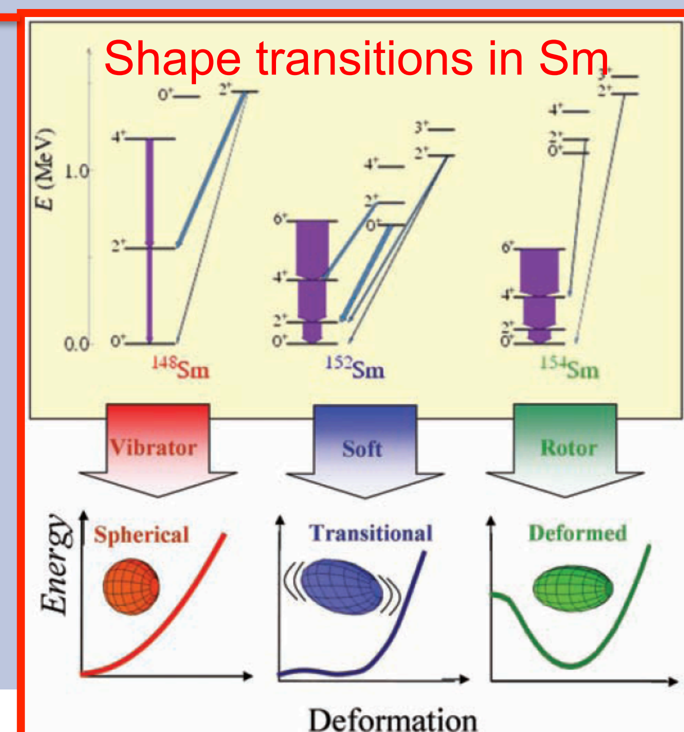
- large isospin magnifies unknown physics
- clustering behavior
- novel evolution in structure

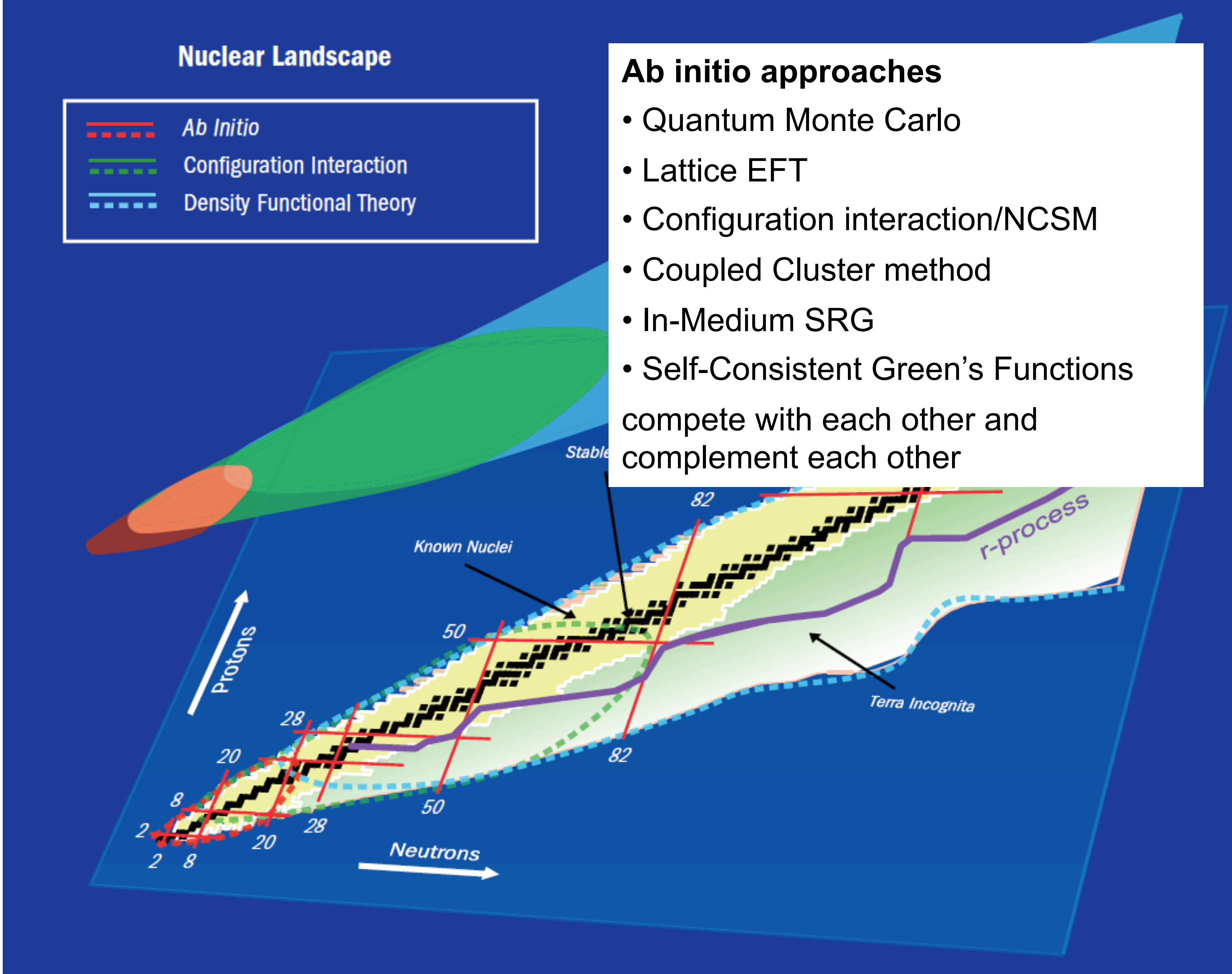










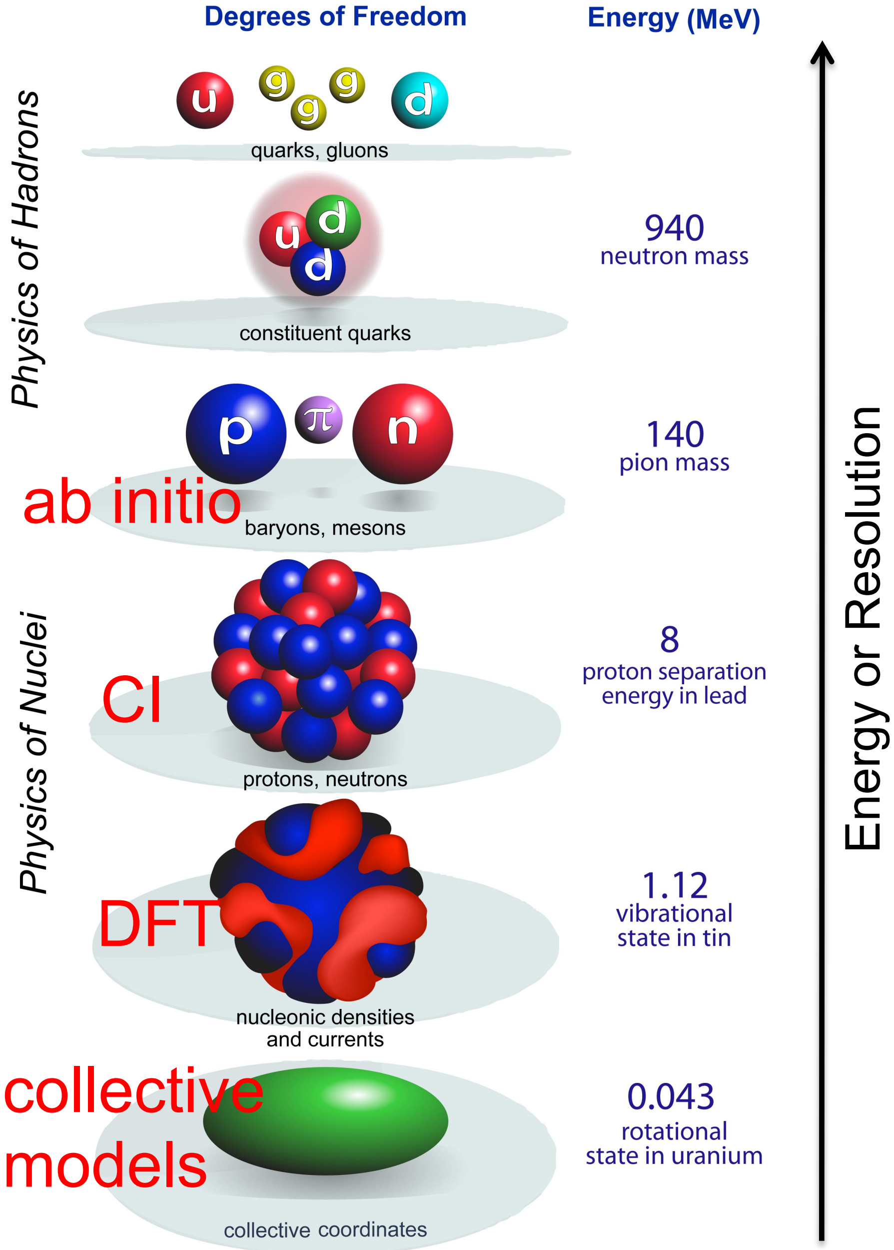


Ab initio approaches

- Quantum Monte Carlo
- Lattice EFT
- Configuration interaction/NCSM
- Coupled Cluster method
- In-Medium SRG
- Self-Consistent Green's Functions

compete with each other and complement each other

Energy scales and relevant degrees of freedom



Chiral symmetry is broken

Pion is Nambu-Goldstone boson

Tool: Chiral effective field theory

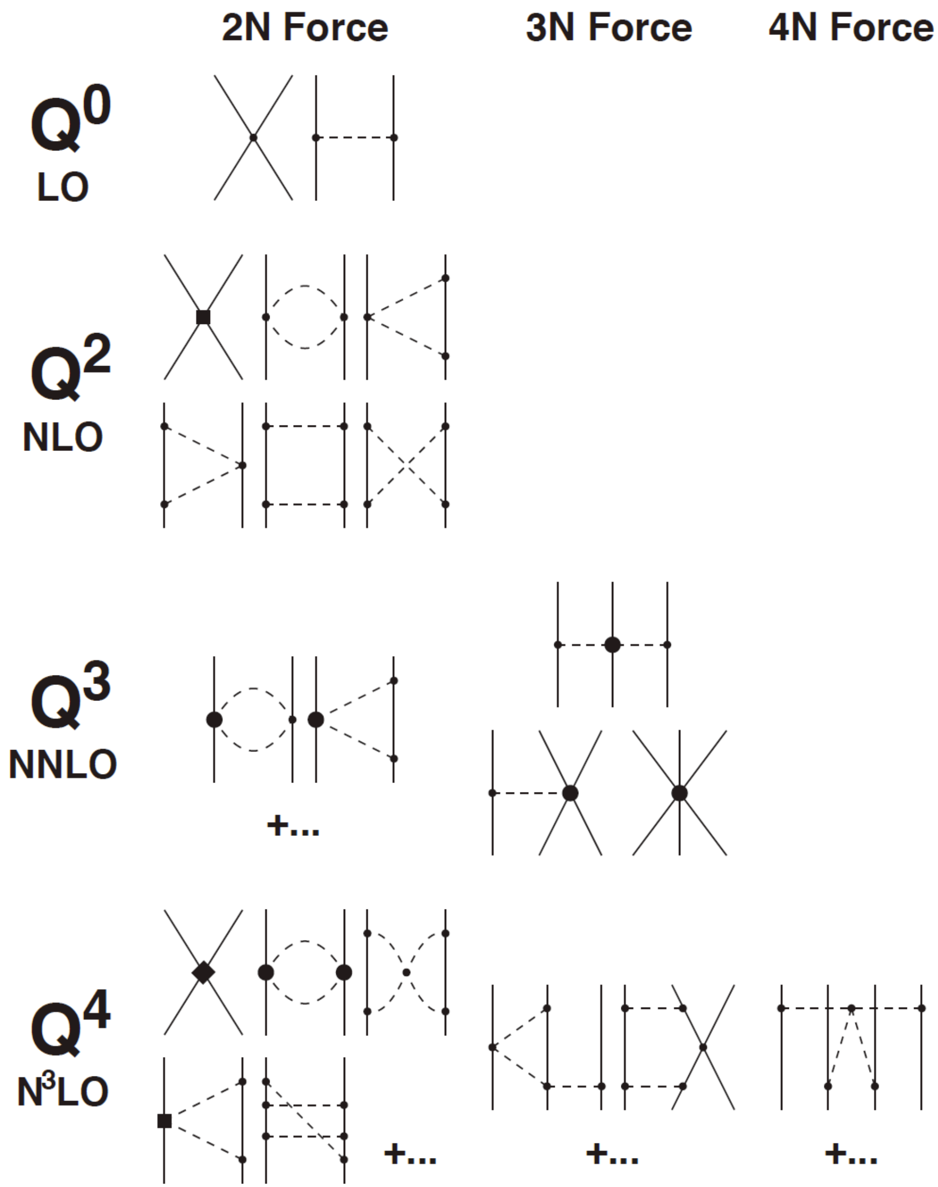
Effective theories provide us with model independent approaches to atomic nuclei

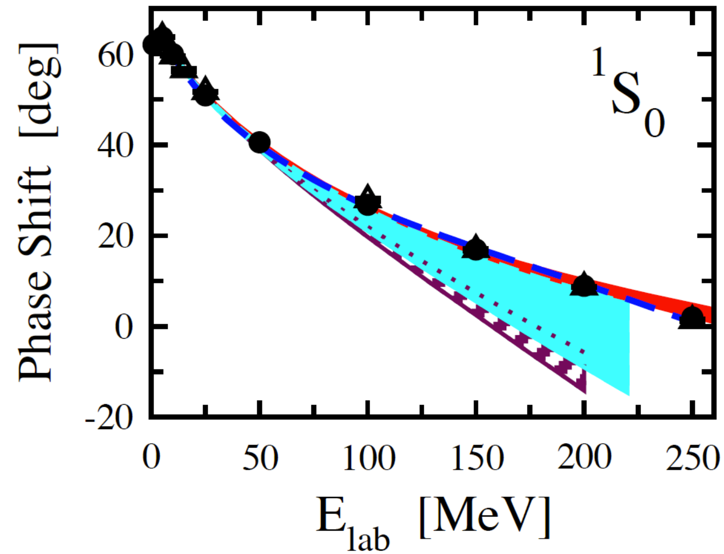
Key: Separation of scales

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

Nuclear forces from chiral effective field theory

[Weinberg; van Kolck; Epelbaum *et al*.; Entem & Machleidt; …]





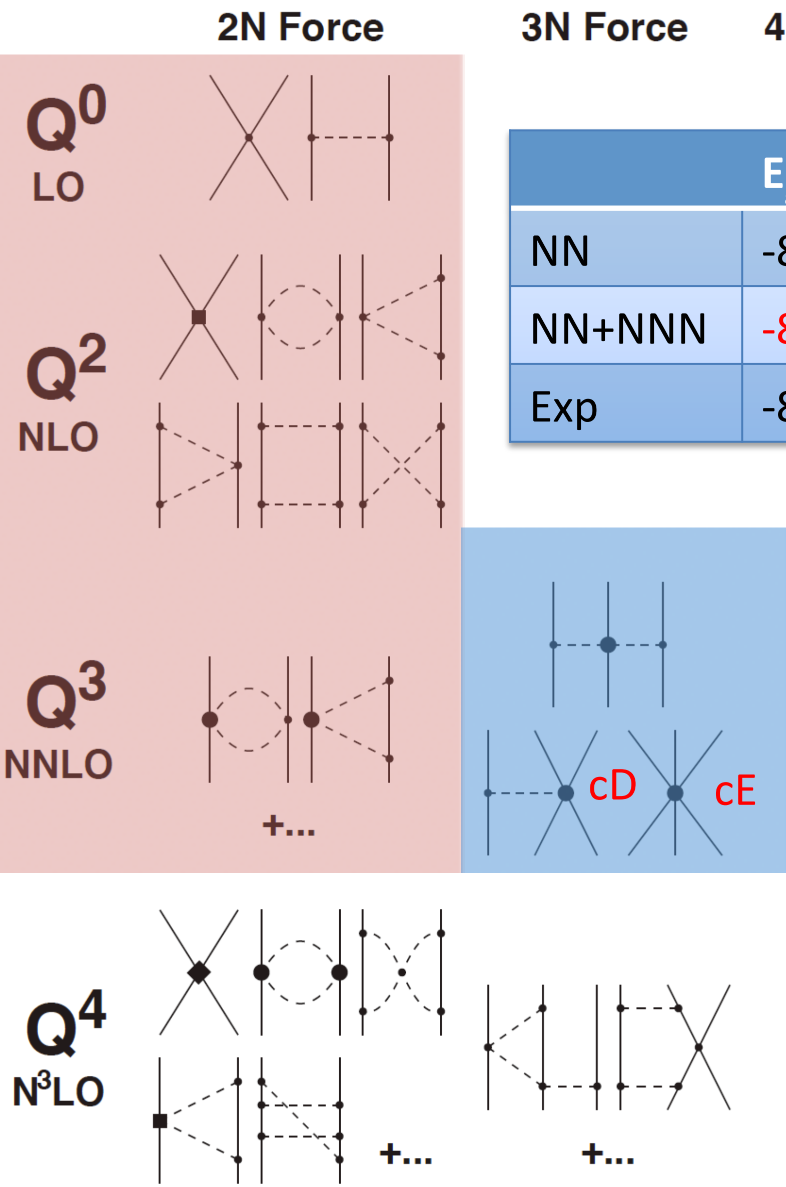
[Epelbaum, Hammer, Meissner RMP 81, 1773 (2009)]

Low energy constants from fit of NN data, A=3,4 nuclei, or light nuclei.

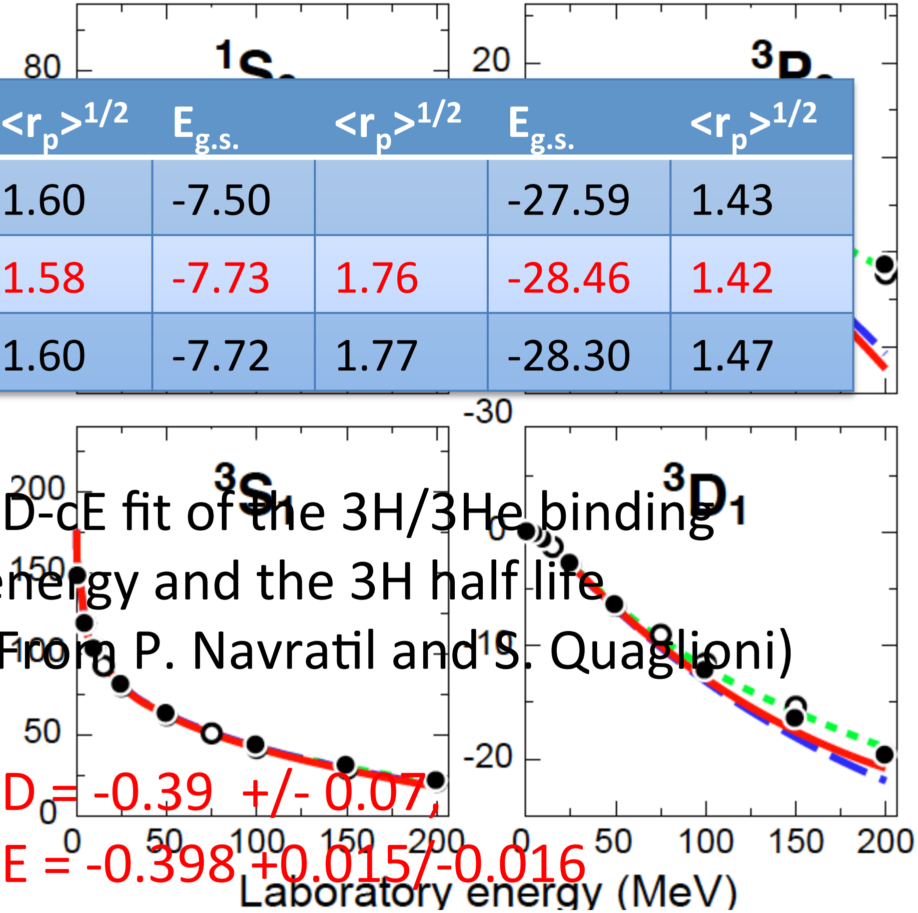
- Model inadequacy: optimization of the parameters order-by-order
- Parameter uncertainties: Covariance and sensitivity analysis of parameters in few- AND many-body systems

Optimization of Chiral interactions at NNLO

A. Ekström et al, Phys. Rev. Lett. 110, 192502 (2013)



	$E_{g.s.}$	$\langle r_p\rangle^{1/2}$	$E_{g.s.}$	$\langle r_p\rangle^{1/2}$	$E_{g.s.}$	$\langle r_p\rangle^{1/2}$
NN	-8.25	1.60	-7.50		-27.59	1.43
NN+NNN	-8.48	1.58	-7.73	1.76	-28.46	1.42
Exp	-8.48	1.60	-7.72	1.77	-28.30	1.47



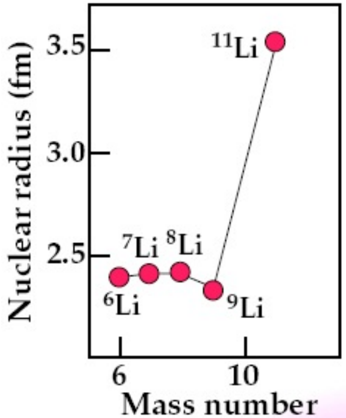
cD-cE fit of the 3H/3He binding energy and the 3H half life (From P. Navratil and S. Quaglioni)

cD = -0.39 +/- 0.07,

cE = -0.398 +0.015/-0.016

T_{lab} (MeV)	0–35	35–125	125–183	183–290	0–290
$pp\ \chi^2$/datum	1.11	1.56	23.95 4.35^a	29.26	17.10 14.03^a
$np\ \chi^2$/datum	0.85	1.17	1.87	6.09	2.95

Physics of nuclei at the edges of stability



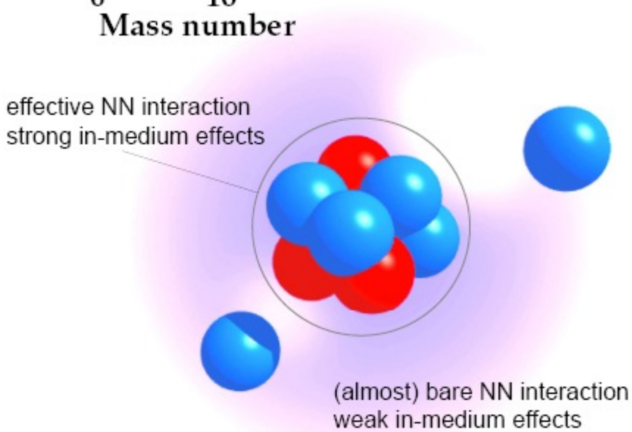
I. Tanihata et al.
Phys. Rev. Lett. 55, 2676 (1985)

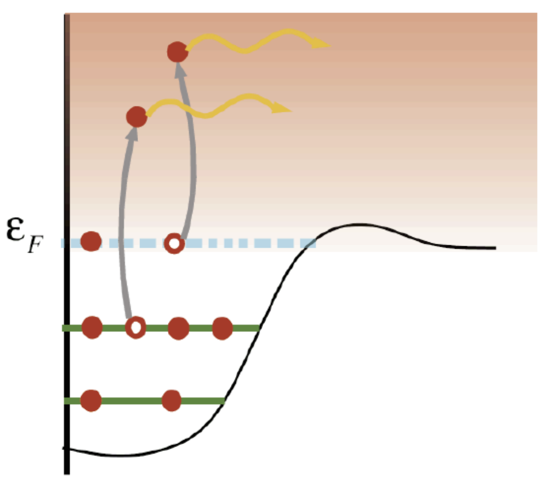
Interaction cross section measurements at Bevalac (790 MeV/u)

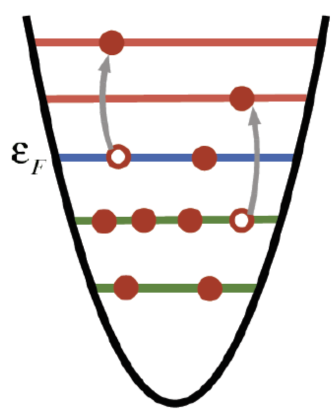
The Berggren completeness treats bound, resonant and scattering states on equal footing.

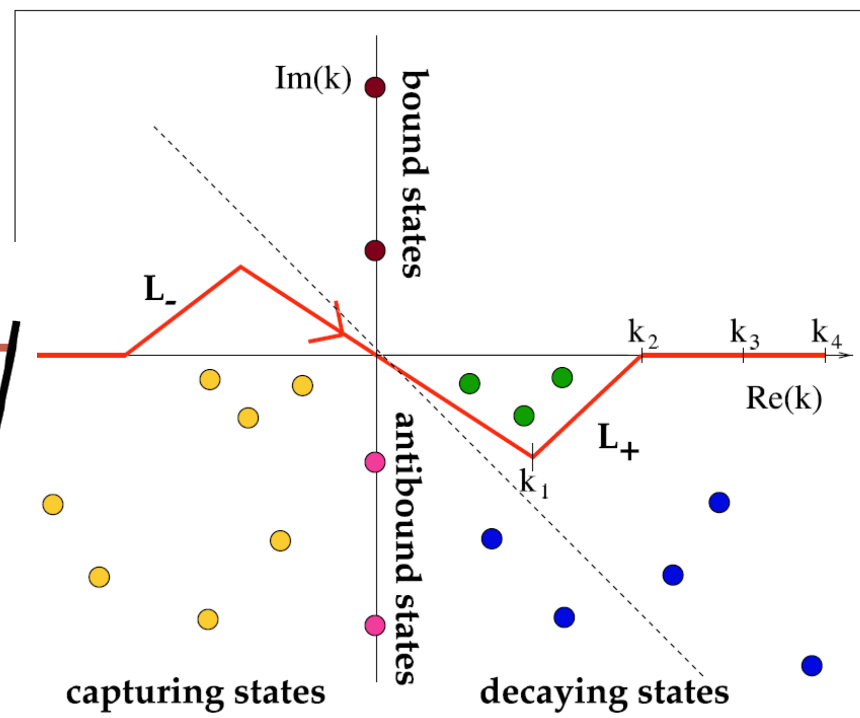
Has been successfully applied in the shell model in the complex energy plane to light nuclei. For a review see

N. Michel et al J. Phys. G 36, 013101 (2009).



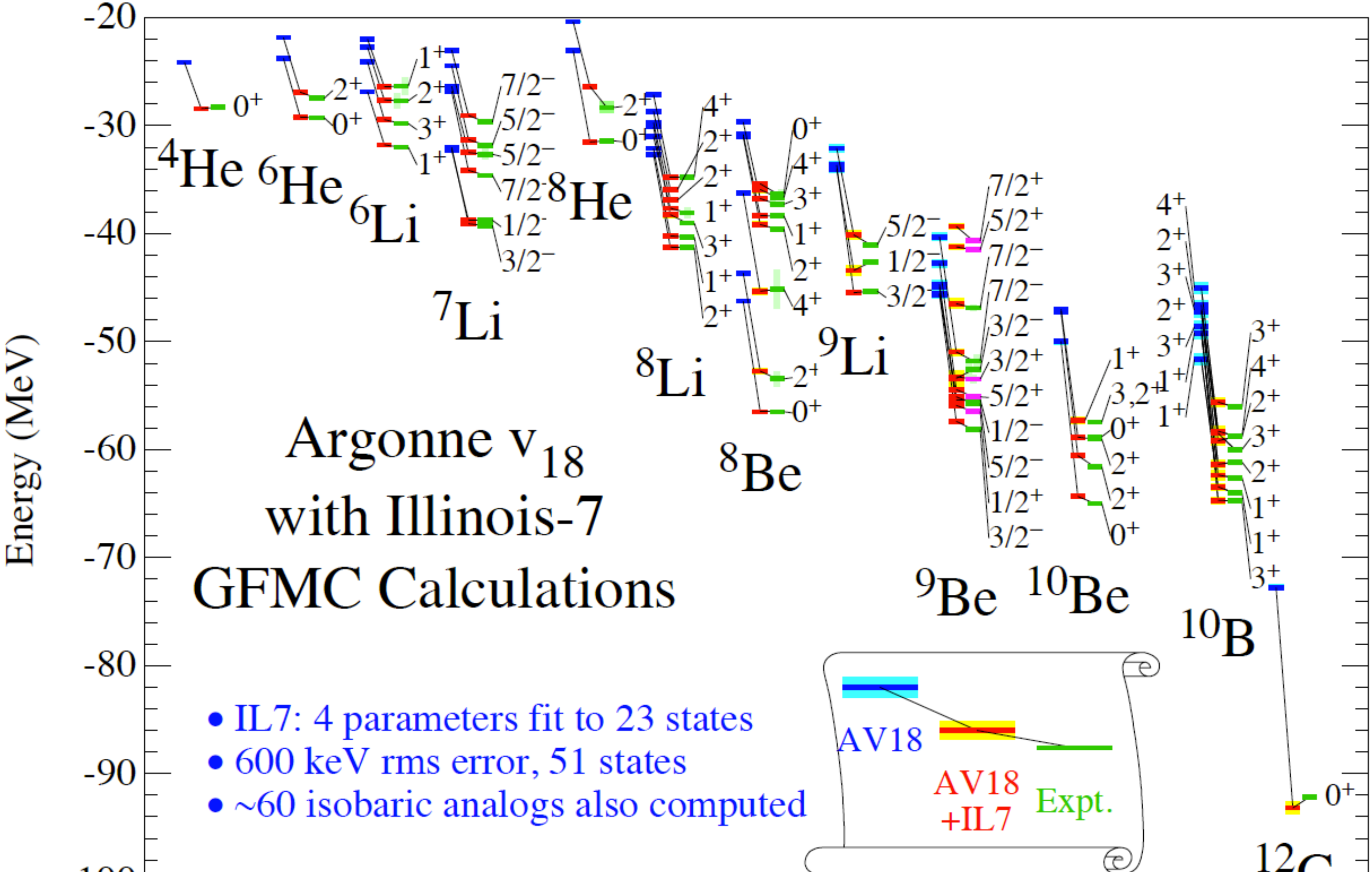






Green's function Monte Carlo computations

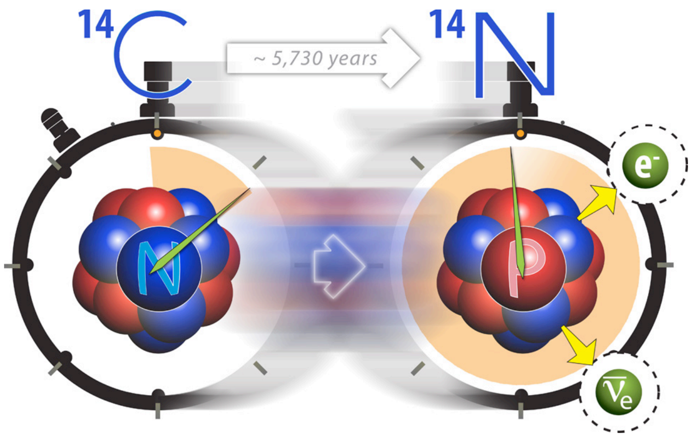
Demonstration that light nuclei can be build from scratch



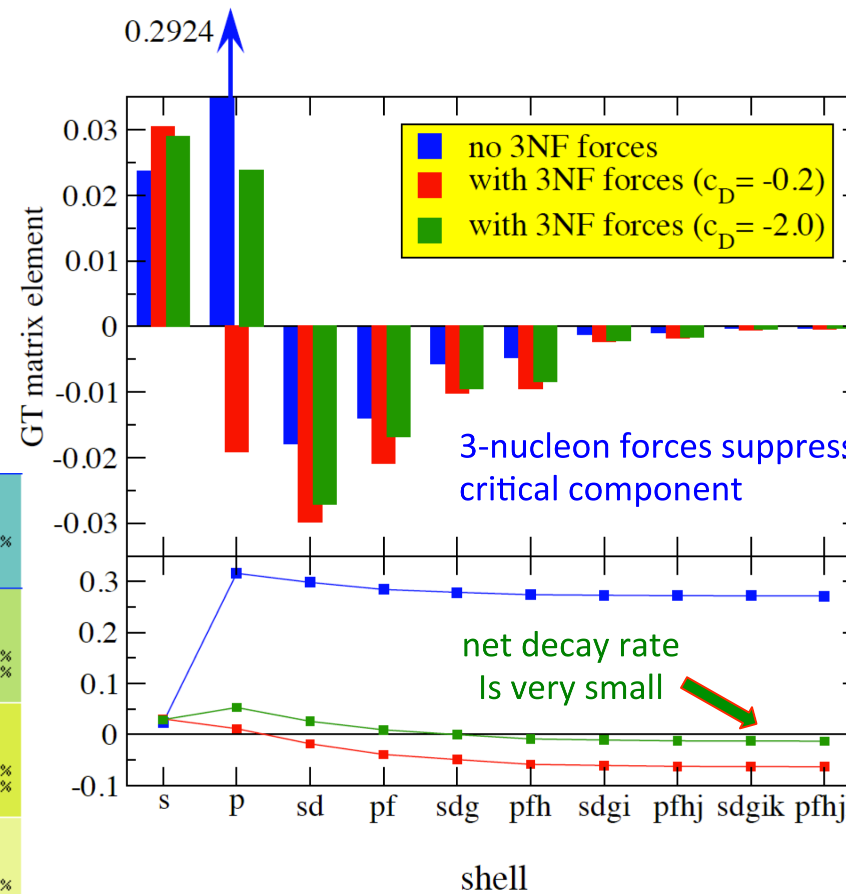
Pieper & Wiringa, Ann. Rev. Nucl. Part. Sci. 51, 53 (2001)

Anomalous Long Lifetime of Carbon-14

Anomalous long lifetime of Carbon-14 (used in carbon dating) explained by ab-initio CI calculations using NN and NNN forces. Three-nucleon forces yield suppression of transition matrix element.



Z \ N	4	5	6	7	8	9	10	11	N
Z	12O 0.40 MeV P	13O 8.58 MS εp: 100.00% ε: 100.00%	14O 70.620 S ε: 100.00%	15O 122.24 S ε: 100.00%	16O STABLE 99.757%	17O STABLE 0.038%	18O STABLE 0.205%	19O 26.88 S β-: 100.00%	20O 13.51 S β-: 100.00%
7	11N 0.83 MeV P: 100.00%	12N 11.000 MS ε: 100.00%	13N 9.965 M ε: 100.00%	14N STABLE 99.636%	15N STABLE 0.364%	16N 7.13 S β-: 100.00% β-α: 1.2E-3%	17N 4.173 S β-: 100.00% β-n: 95.1%	18N 620 MS β-: 100.00% β-α: 12.20%	19N 336 MS β-: 100.00% β-n: 41.80%
6	10C 19.308 S ε: 100.00%	11C 20.334 M ε: 100.00%	12C STABLE 98.93%	13C STABLE 1.07%	14C 5700 Y β-: 100.00%	15C 2.449 S β-: 100.00%	16C 0.747 S β-: 100.00% β-n: 99.00%	17C 193 MS β-: 100.00% β-n: 32.00%	18C 92 MS β-: 100.00% β-n: 31.50%
5	9B 0.54 KeV 2α: 100.00% P: 100.00%	10B STABLE 19.9%	11B STABLE 80.1%	12B 20.20 MS β-: 100.00% B3A: 1.58%	13B 17.33 MS β-: 100.00%	14B 12.5 MS β-: 100.00%	15B 9.93 MS β-: 100.00% β-n: 93.60%	16B <190 PS N	17B 5.08 MS β-: 100.00% β-n: 63.00%
4	8Be 5.57 eV α: 100.00%	9Be STABLE 100.%	10Be 1.387E+6 Y β-: 100.00%	11Be 13.81 S β-: 100.00% β-α: 3.1%	12Be 21.49 MS β-: 100.00% β-n≤ 1.00%	13Be 2.7E-21 S N	14Be 4.35 MS β-: 100.00% β-n: 81.00%	15Be <200 NS N	16Be <200 NS 2N

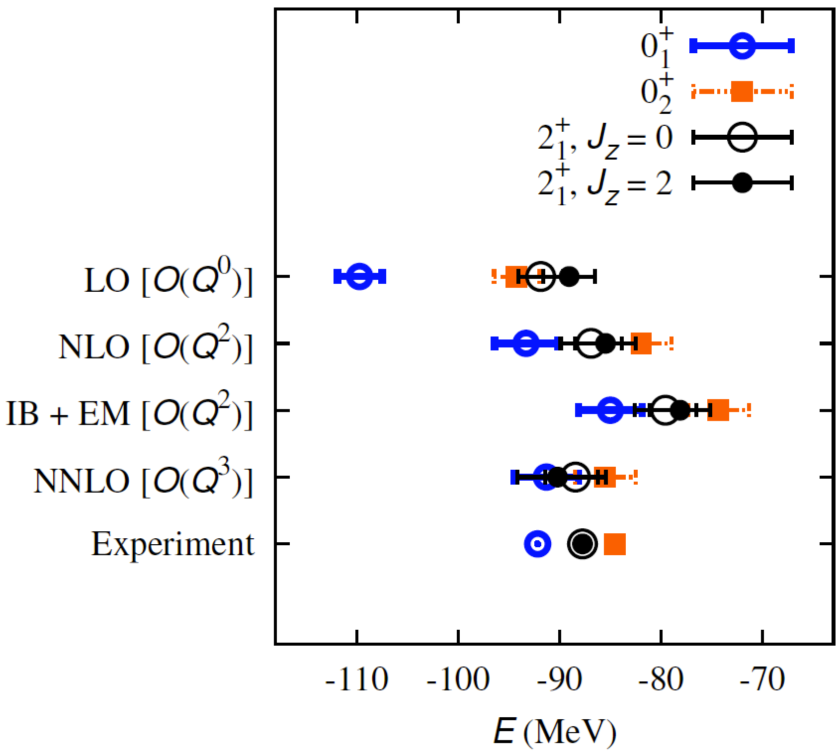


Maris, Vary, Navrátil, Ormand, Nam, Dean, Phys. Rev. Lett. 106, 202502 (2011)

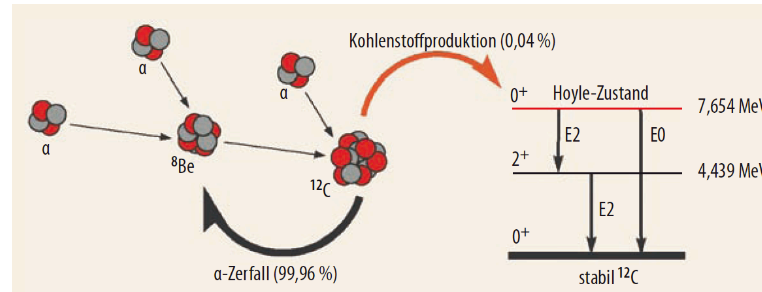
Computation of the Hoyle state

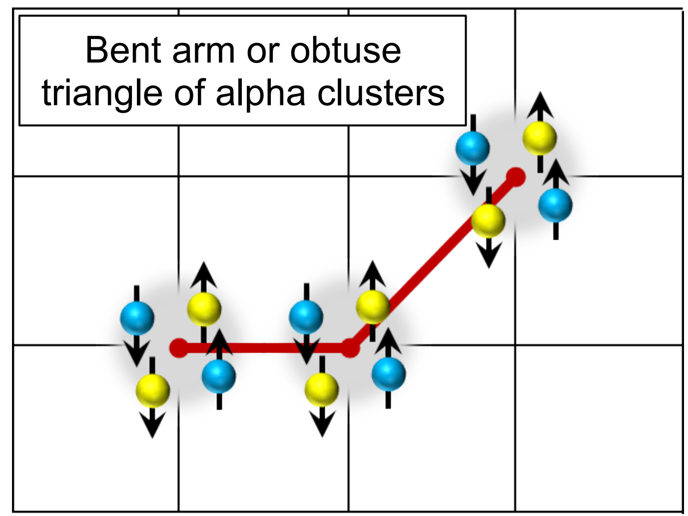
The Hoyle state (postulated in 1954) explains the abundance of ^{12}C in stars.

Nuclear Lattice Effective Field Theory Collaboration



Epelbaum, Krebs, Lee, Meißner,
Phys. Rev. Lett. 106, 192501 (2011)

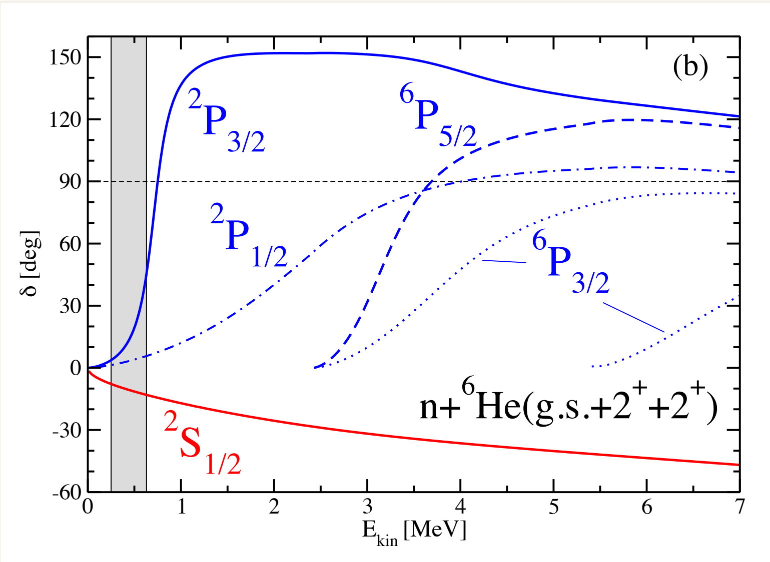




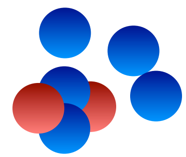
Epelbaum, Krebs, Lähde, Lee, Meißner,
Phys. Rev. Lett. 109, 252501 (2012)

NCSM with continuum: ^{7}He ↔ ^{6}He + *n*

S. Baroni, P. Navrátil, and S. Quaglioni, Phys. Rev. Lett. **110**, 022505 (2013)



^{7}He



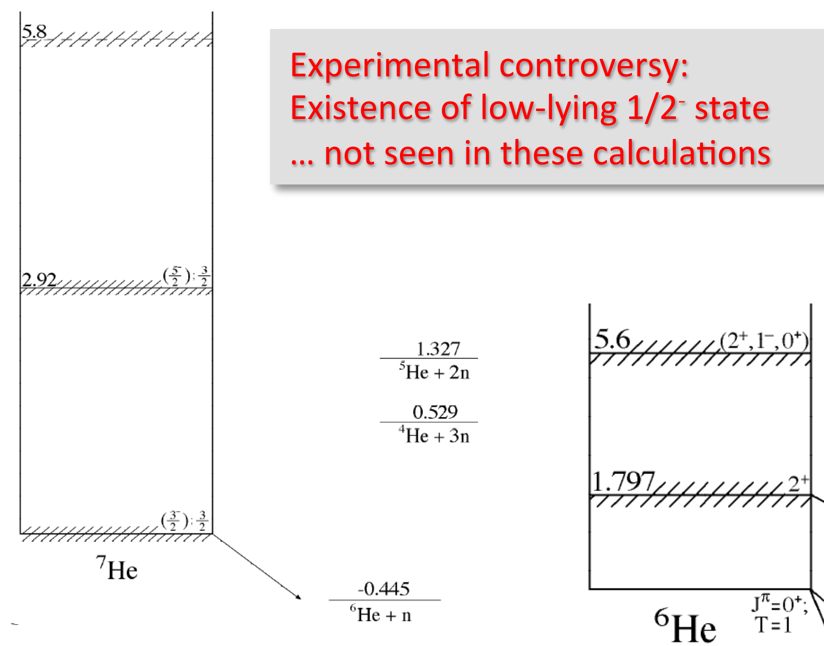
unbound

J^π	experiment			NCSMC	
	E_R	Γ	Ref.	E_R	Γ
$3/2^-$	0.430(3)	0.182(5)	[2]	0.71	0.30
$5/2^-$	3.35(10)	1.99(17)	[40]	3.13	1.07
$1/2^-$	3.03(10)	2	[11]	2.39	2.89
	3.53	10	[15]		
	1.0(1)	0.75(8)	[5]		

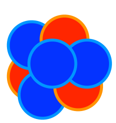
[11] A. H. Wuosmaa *et al.*, Phys. Rev. C **72**, 061301 (2005).

NCSMC
with three ^{6}He states
and ten ^{7}He eigenstates
More **7-nucleon correlations**
Fewer ^{6}He-core states needed

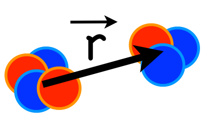
Experimental controversy:
Existence of low-lying $1/2^-$ state
… not seen in these calculations



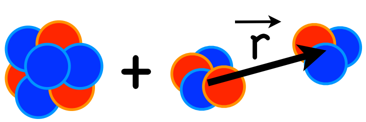
NCSM



NCSM/RGM

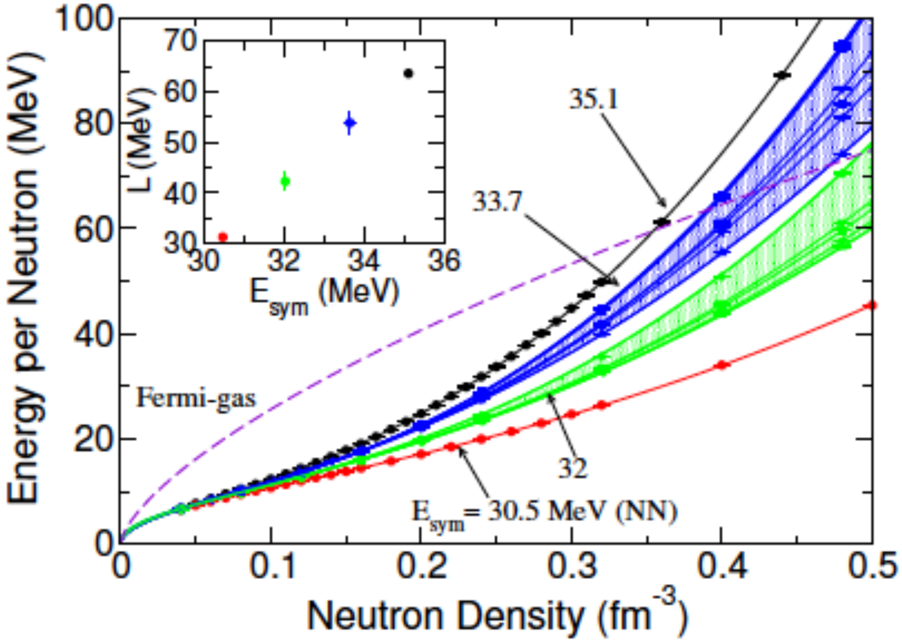


NCSMC

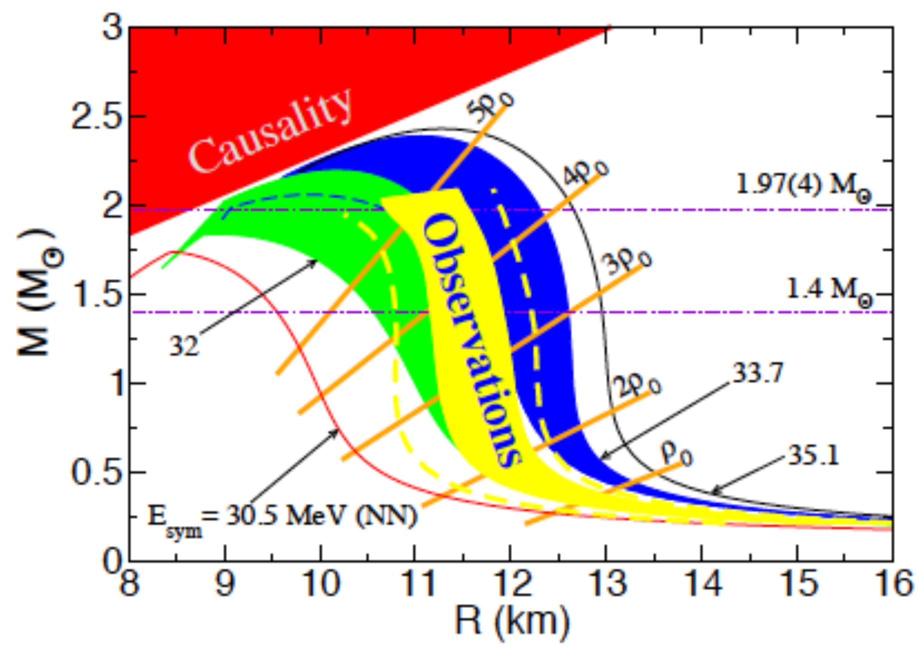


Effect of three-body force in neutron matter and neutron star structure

Auxiliary Field Diffusion Quantum Monte Carlo calculations of neutron matter and equation of state with Argonne and Urbana/Illinois NN + NNN forces.
Constraining the maximum mass and radius of neutron stars and the nuclear symmetry energy



Gandolfi, Carlson, Reddy, PRC 85, 032801 (2012)

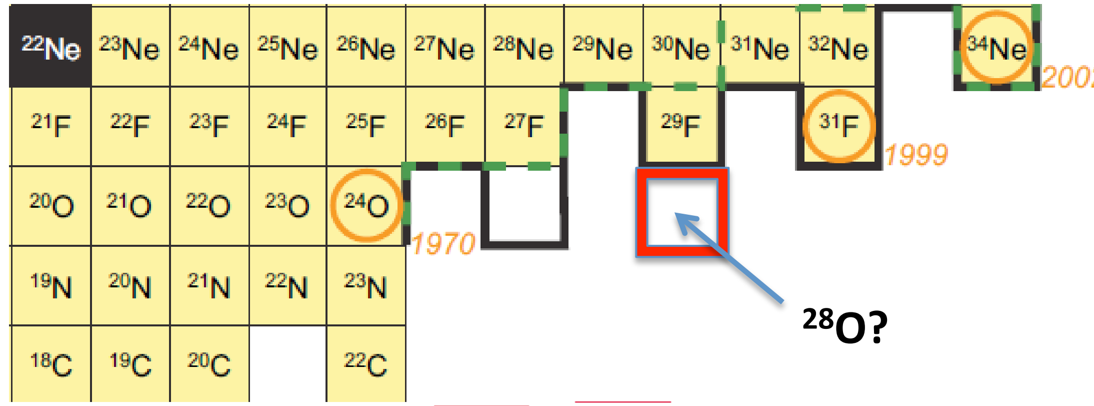


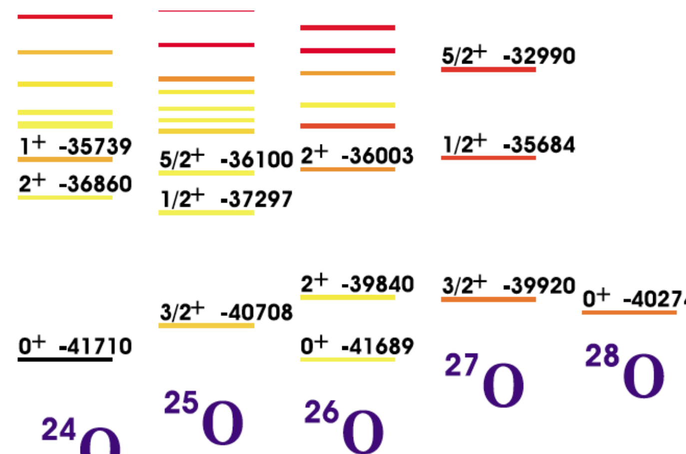
adapted from
Steiner, Gandolfi, PRL 108, 081102 (2012)

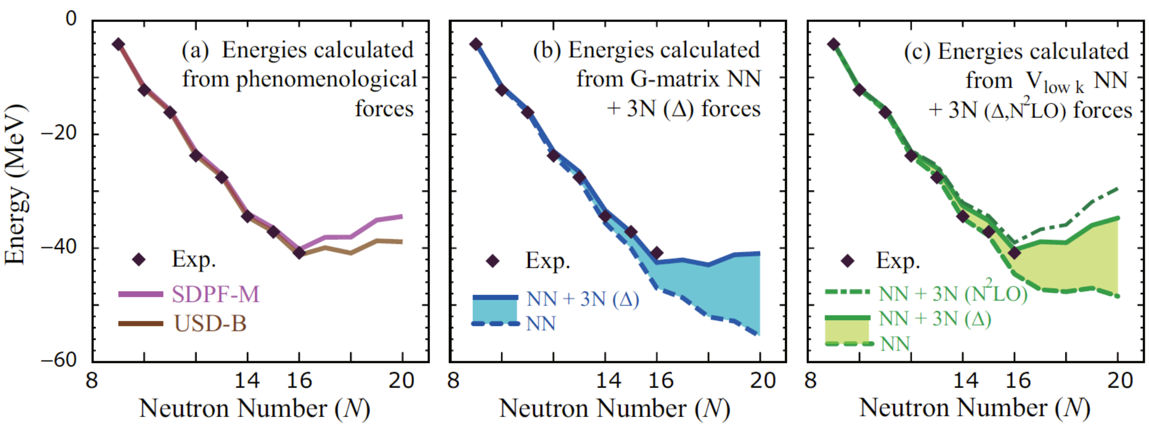
Is ^{28}O a bound nucleus?

Experimental situation

- "Last" stable oxygen isotope ^{24}O
- ^{25,26}O unstable (Hoffman et al 2008, Lunderberg et al 2012)
- ^{28}O not seen in experiments
- ^{31}F exists (adding on proton shifts drip line by 6 neutrons!?)





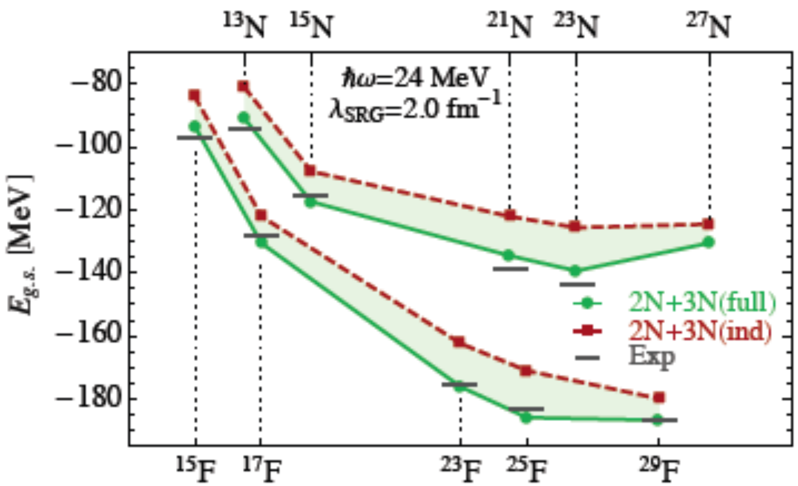


Continuum shell model with HBUSD interaction predict ^{28}O unbound. A. Volya and V. Zelevinsky PRL (2005)

Shell model (sd shell) with monopole corrections based on three-nucleon force predicts 2nd O as last stable isotope of oxygen. [Otsuka, Suzuki, Holt, Schwenk, Akaishi, PRL (2010), arXiv:0908.2607]

Ab-initio Gorkov-Green's function theory with 3NFs

A. Cipollone, CB, P.Navrátil, arXiv:1303.4900 [nucl-th], V. Somà, C.B., and T. Duguet, Phys. Rev. C87, 011303 (2013).



-> 3NF inlcuded as density dep. NN forces (**beyond normal ordering and <u>all</u> symmetry factors correct**)

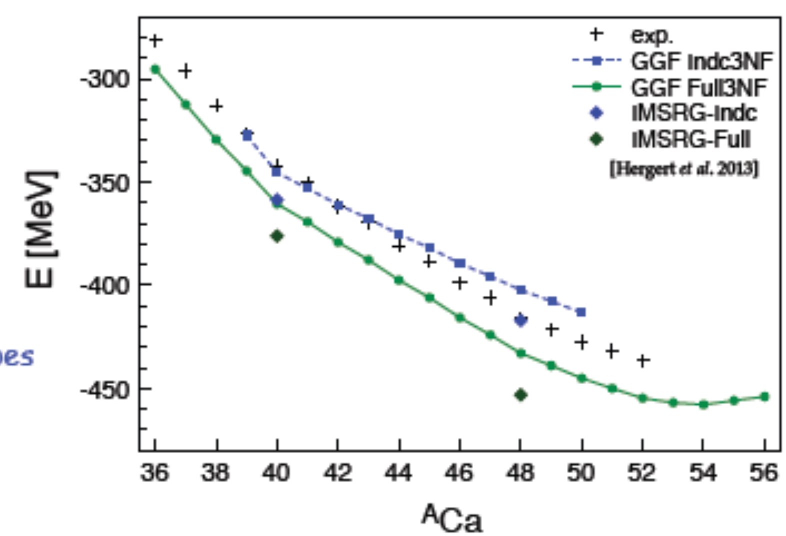
-> Near-dripline Fluorine and Nitrogen isotopes significantly affected by 2-π/Fujita-Miyazawa terms

-> Leading 3NF consistently bring results F and N close to experiment

-> ***Ab-initio*** studies of **open-shell semi-magic** isotopes have become reachable by breaking particle number symmetry.

-> *Good agreement with IM-SRG (quantitative when 3rd order included)*

-> *Original leading 3NFs correct the curvature in Calcium isotopes*

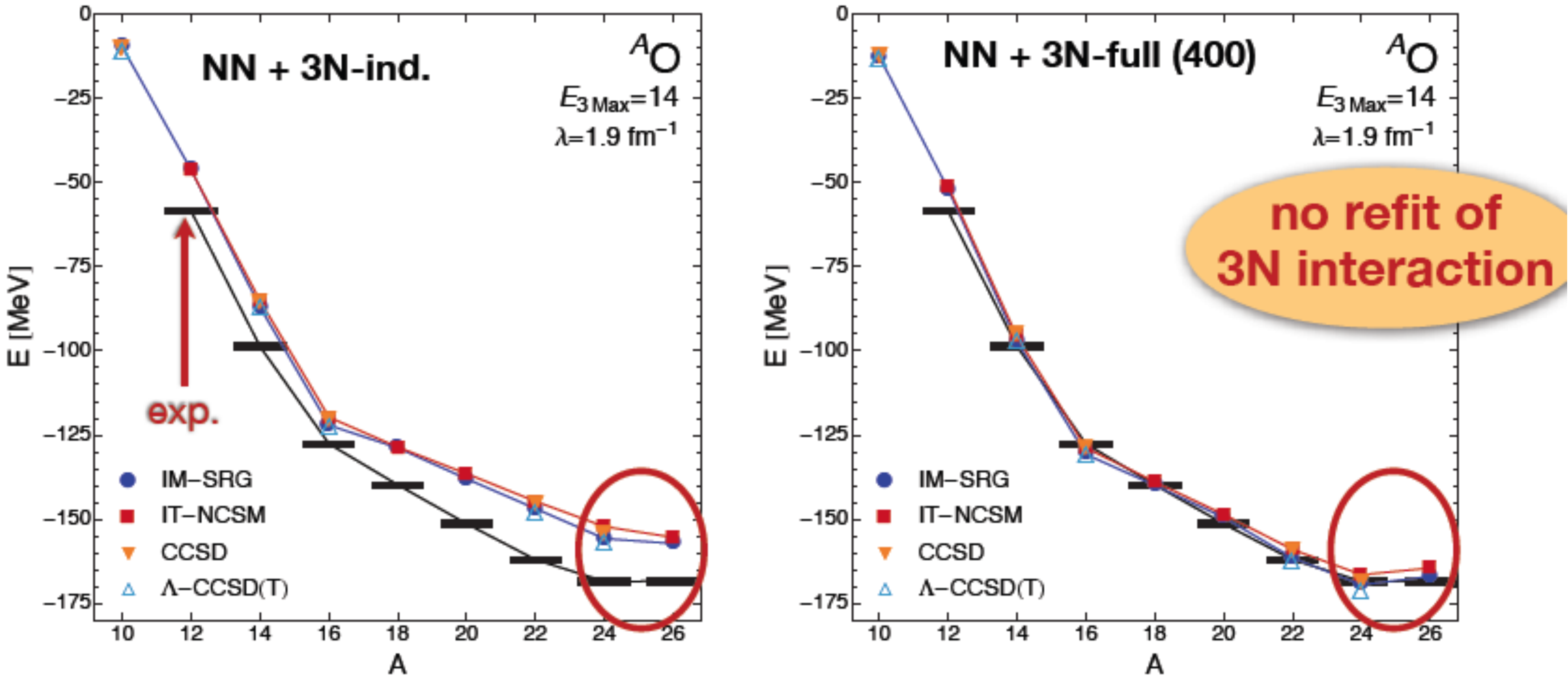


INDUCED Hamiltonian: N3LO (Λ = 500Mev/c) chiral <u>NN</u> interaction evolved to 2N + 3N forces (2.0fm^{-1})

FULL Hamiltonian: N2LO (Λ = 400Mev/c) chiral <u>3N</u> interaction evolved (2.0fm^{-1})

[from R. Roth et al., PRL (2012)]

Ab-initio computation of all even oxygen isotopes from multi-reference IM-SRG

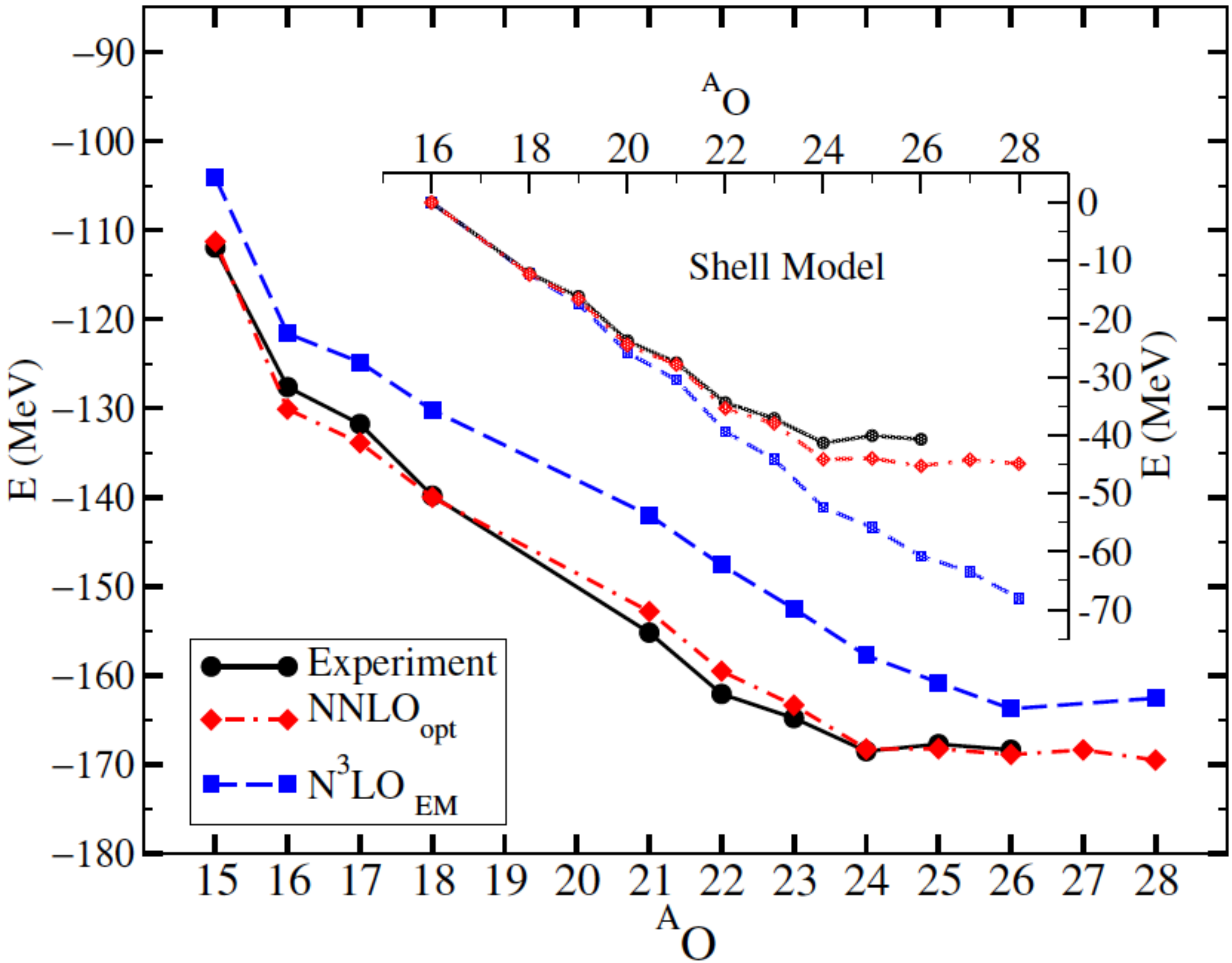


H. Hergert, S. Binder, A. Calci, J. Langhammer, R. Roth, arXiv: 1302.7294 [nucl-th]

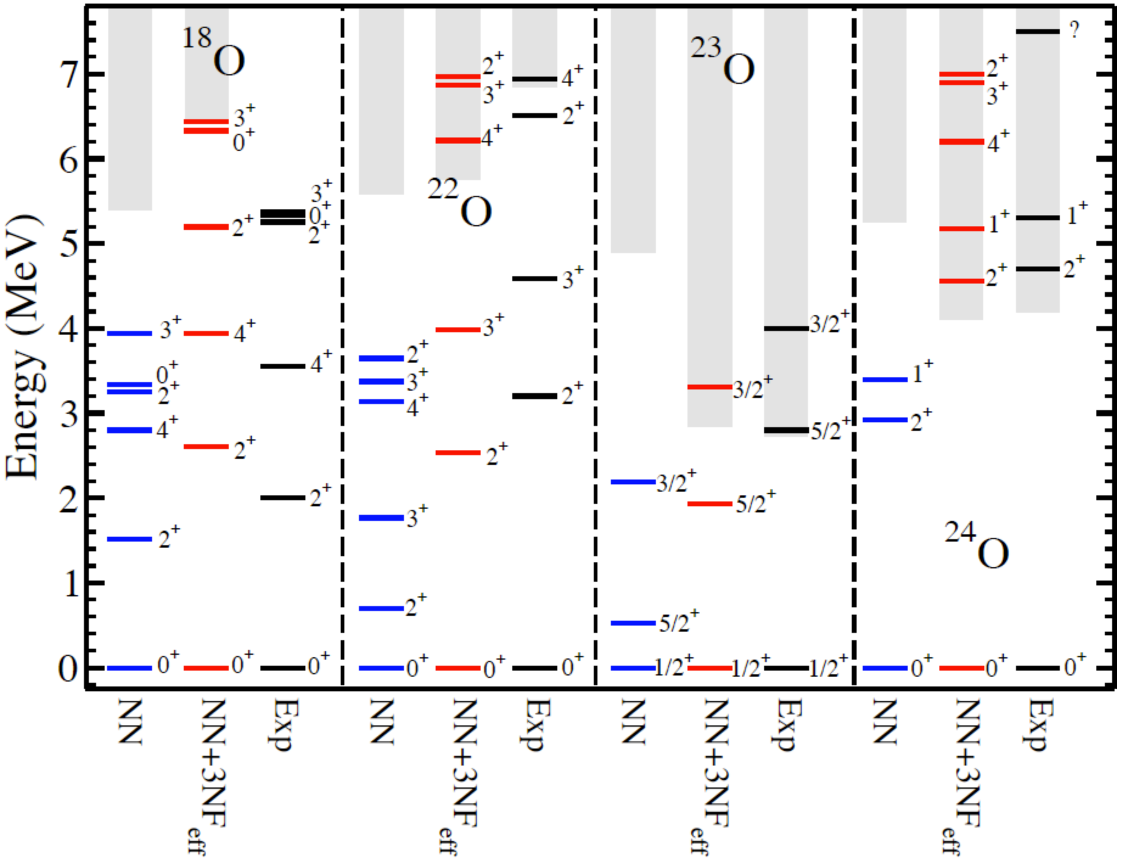
- IM-SRG: decouple ground state from excitations via flow equations
- multi-reference formulation for open-shell nuclei
- agreement between different methods

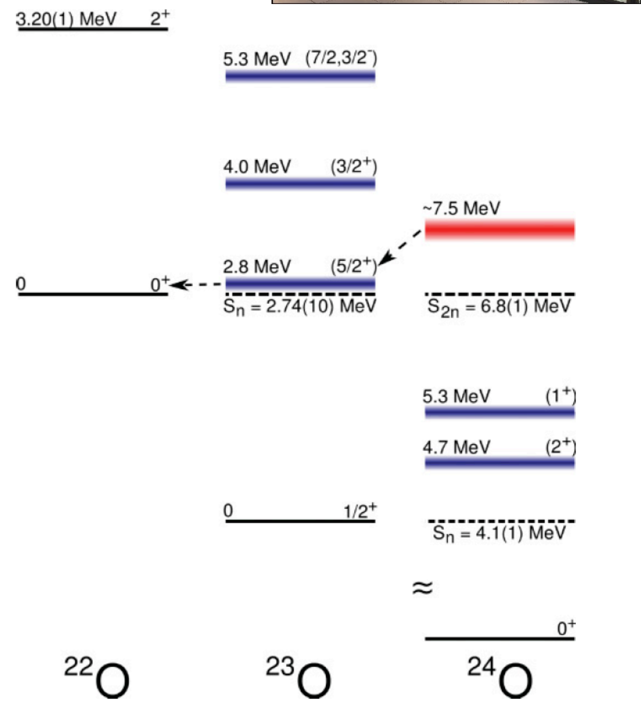
Oxygen isotopes from NNLO(POUNDerS)

A. Ekström et al, Phys. Rev. Lett. 110, 192502 (2013)



Excited states in neutron rich oxygen isotopes





Inclusion of schematic 3NFs:
k_F=1.05 fm^{-1}, c_E=0.71, c_D=-0.2

Hagen, Hjorth-Jensen, Jansen, Machleidt, Papenbrock, Phys. Rev. Lett. 108 242501 (2012)

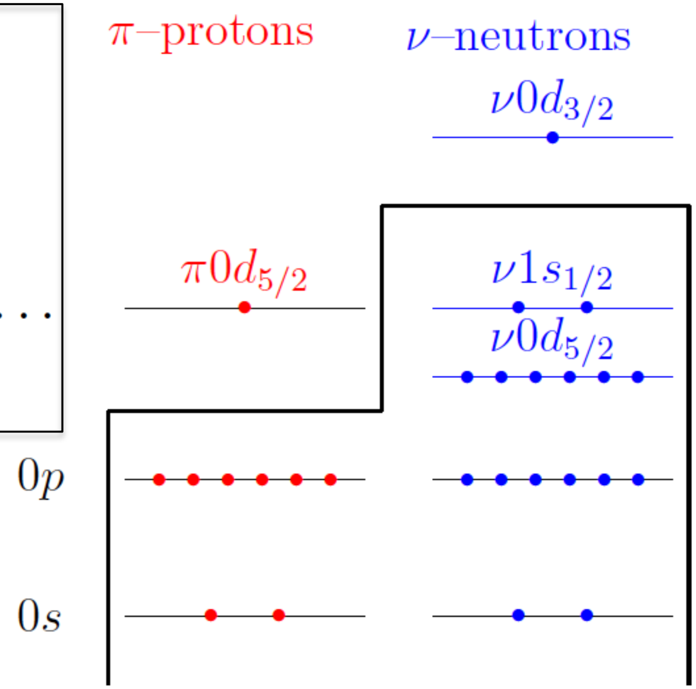
Experment

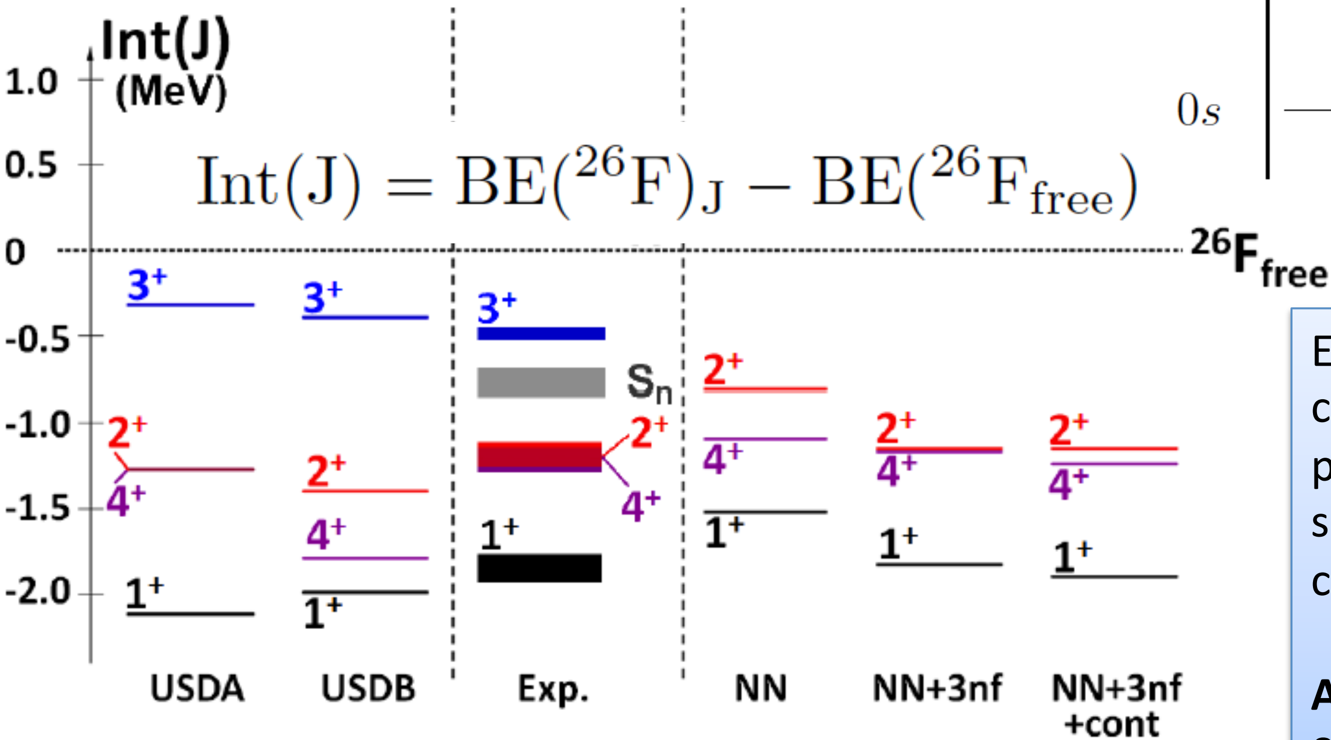
[Hoffman et al., PRC 83, 031303 (2011)] Unbound states in ^{24}O populated by knockout from ^{26}F. Observation of ^{22}O and two-neutron cascade. Speculation: single resonance or superposition of states with J^π= 1$^+$ to 4$^+$.

Computing open-shell Fluorine-26

$$(\bar{H}\hat{R}_\mu^{(A\pm2)})_C|\Phi_0\rangle = \omega_\mu \hat{R}_\mu^{(A\pm2)}|\Phi_0\rangle$$

$$\hat{R}^{(A+2)} = \frac{1}{2}\sum_{ba} r^{ab} a_a^\dagger a_b^\dagger + \frac{1}{6}\sum_{iabc} r_i^{abc} a_a^\dagger a_b^\dagger a_c^\dagger a_i + \ldots$$

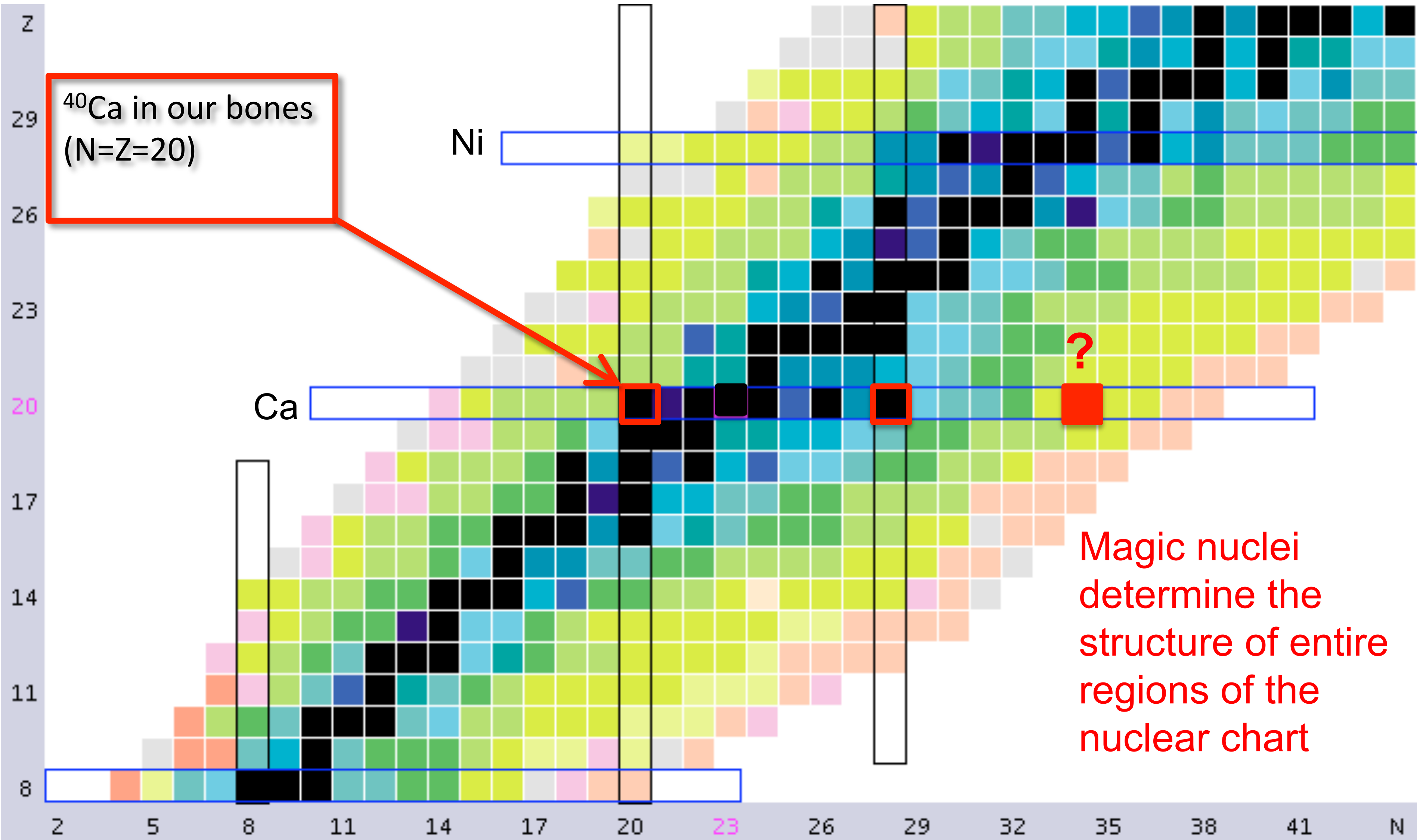




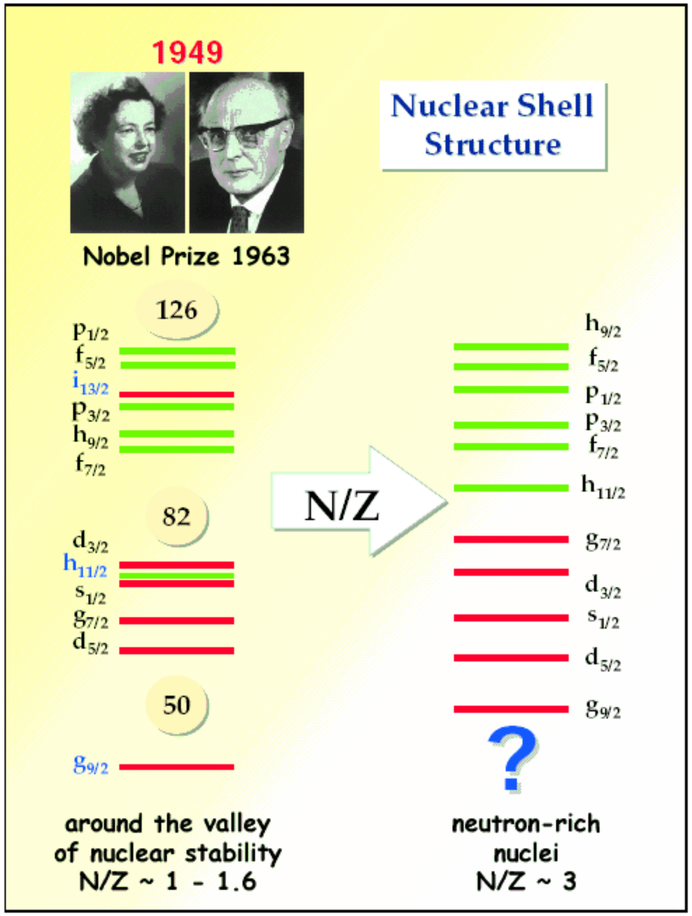
Experimental spectra in ^{26}F compared with phenomenological USD shell-model calculations and coupled-cluster calculations

A. Lepailleur et al, PRL 110 082502 (2013)

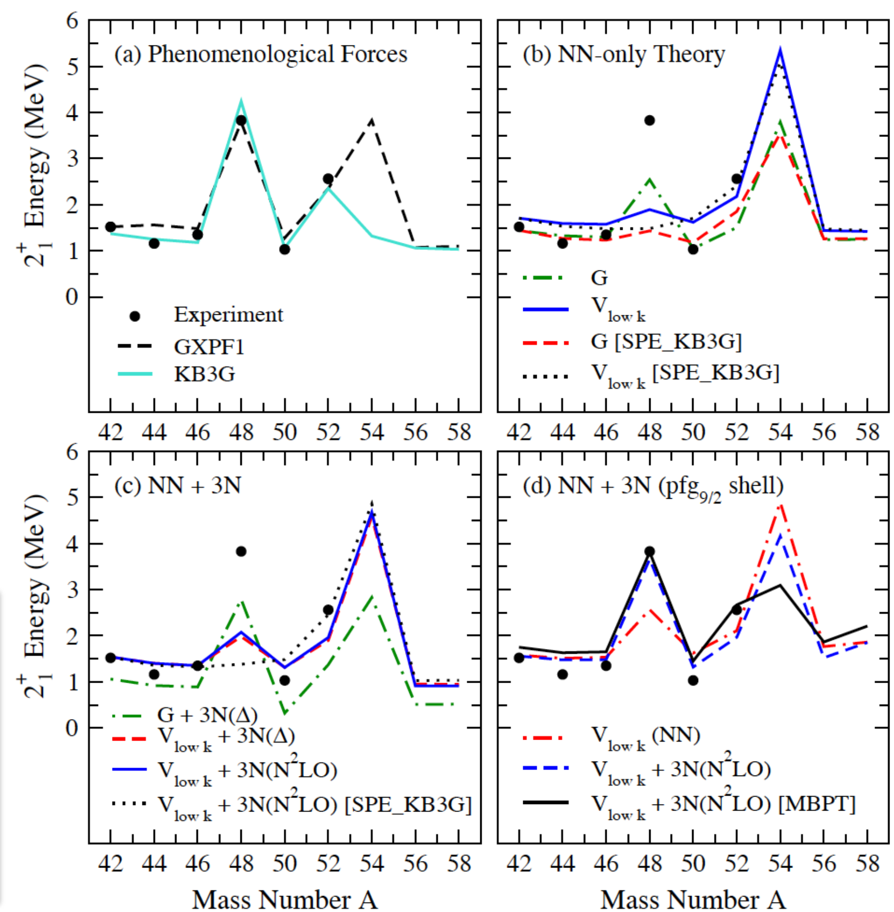
Is ^{54}Ca a magic nucleus?



Evolution of shell structure in neutron rich Calcium



- How do shell closures and magic numbers evolve towards the dripline?
- Is the naïve shell model picture valid at the neutron dripline?



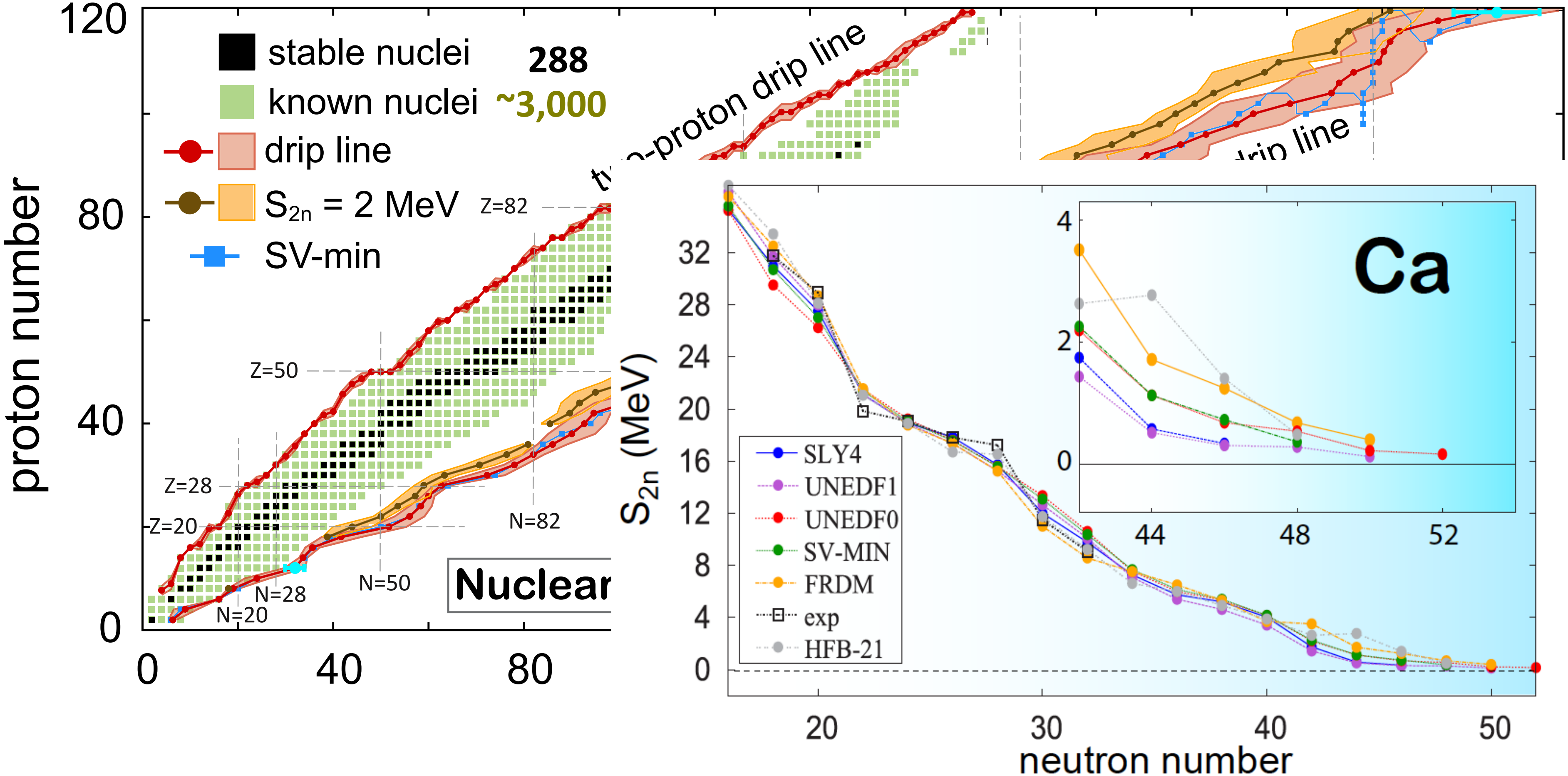
- What are the mechanisms responsible for shell closure in ^{48}Ca?
- Different models give conflicting result for shell closure in ^{54}Ca.

J. D. Holt et al, J. Phys. G **39**, 085111 (2012)

How many protons and neutrons can be bound in a nucleus?

Literature: 5,000-12,000

Skyrme-DFT: $6{,}900 \pm 500_{syst}$

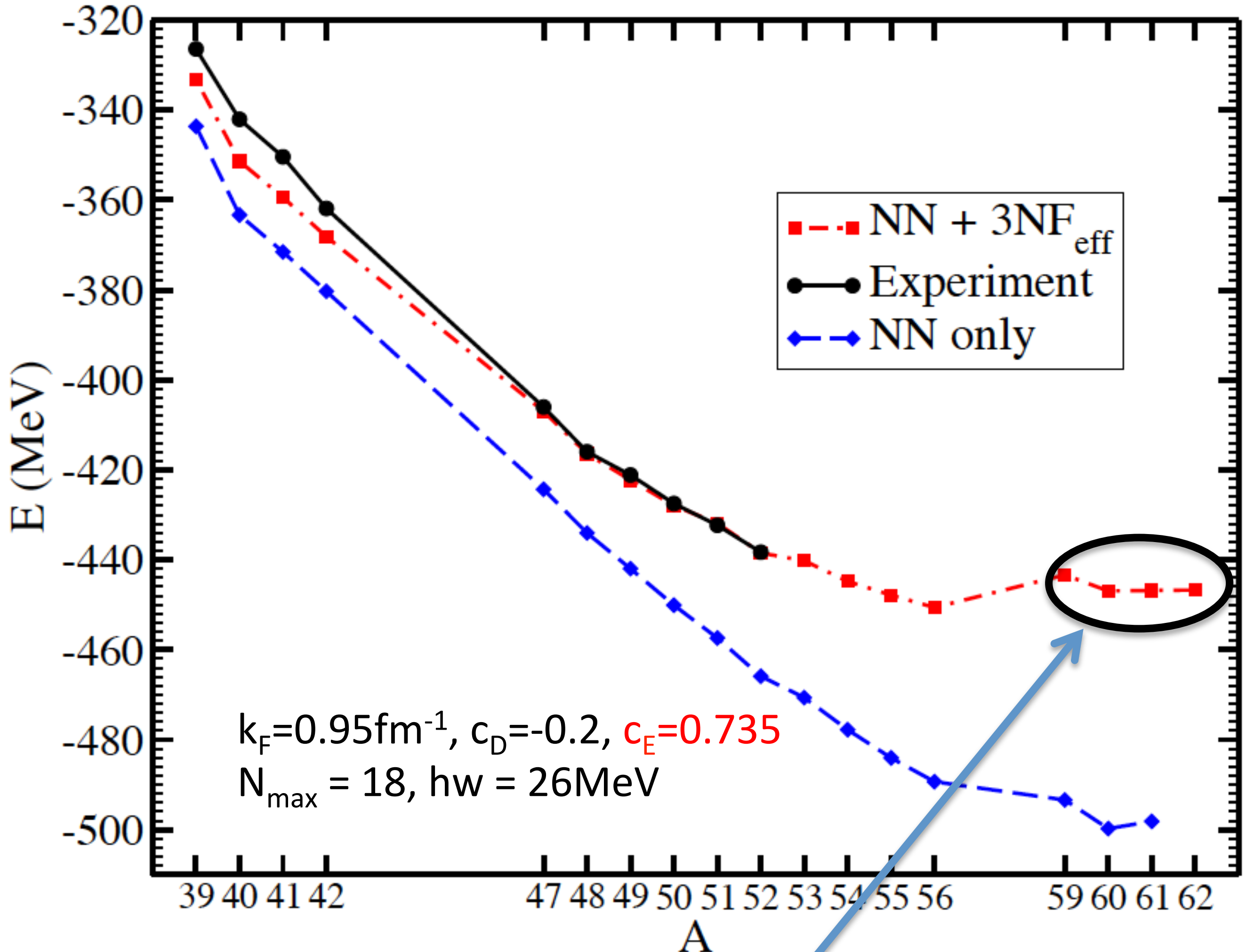


Description of observables and model-based extrapolation

- Systematic errors (due to incorrect assumptions/poor modeling)
- Statistical errors (optimization and numerical errors)

Erler et al., Nature 486, 509 (2012)

Calcium isotopes from chiral interactions



NN forces from chiral EFT and in-medium effective 3NF: k_F=0.95 fm^{-1}, c_E=0.735, c_D=-0.2

Main Features:

1. Energies agree well with experimental masses.
2. ^{60}Ca is not magic
3. $^{61\text{-}62}$Ca are located right at threshold.

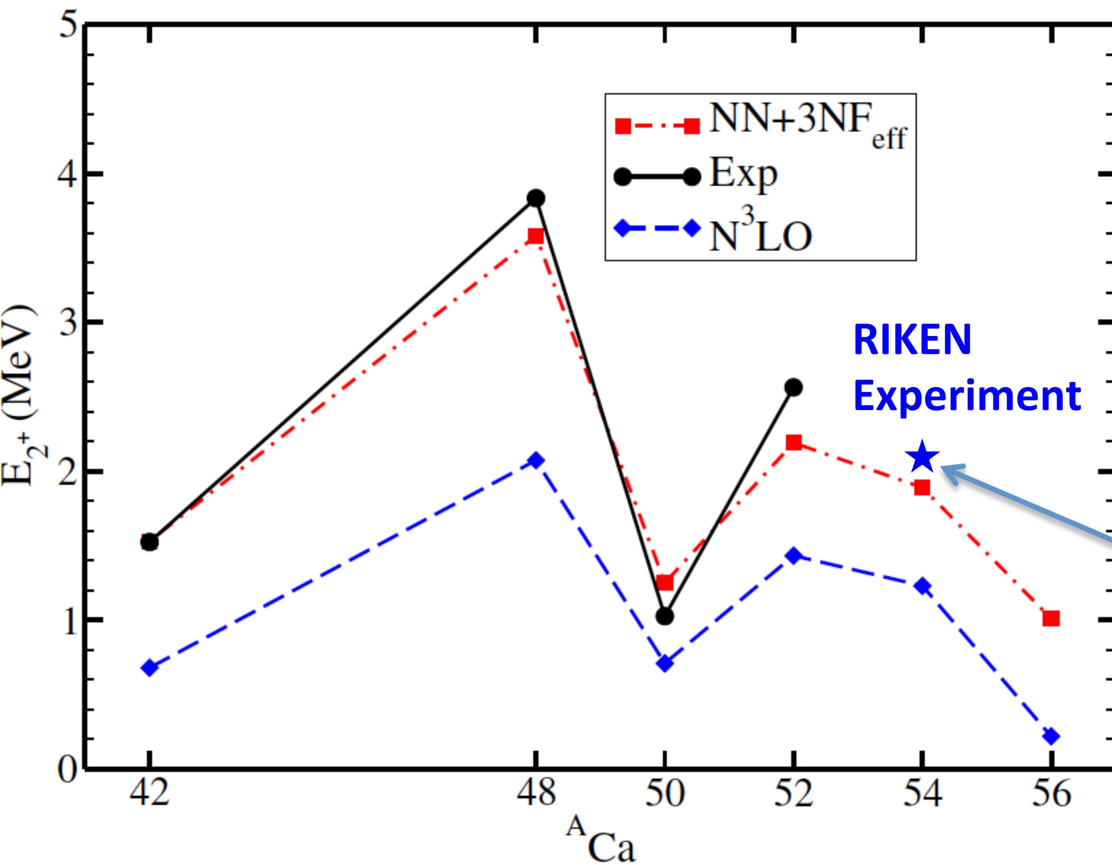
See also:

Meng et al PRC 65, 041302 (2002), Lenzi et al PRC 82, 054301 (2010) and Erler et al, Nature 486, 509 (2012)

G. Hagen, M. Hjorth-Jensen, G. R. Jansen, R. Machleidt, T. Papenbrock, Phys. Rev. Lett. 109, 032502 (2012).

A peninsula of weak stability?

Is ^{54}Ca a magic nucleus? (Is N=34 a magic number?)



Main Features:

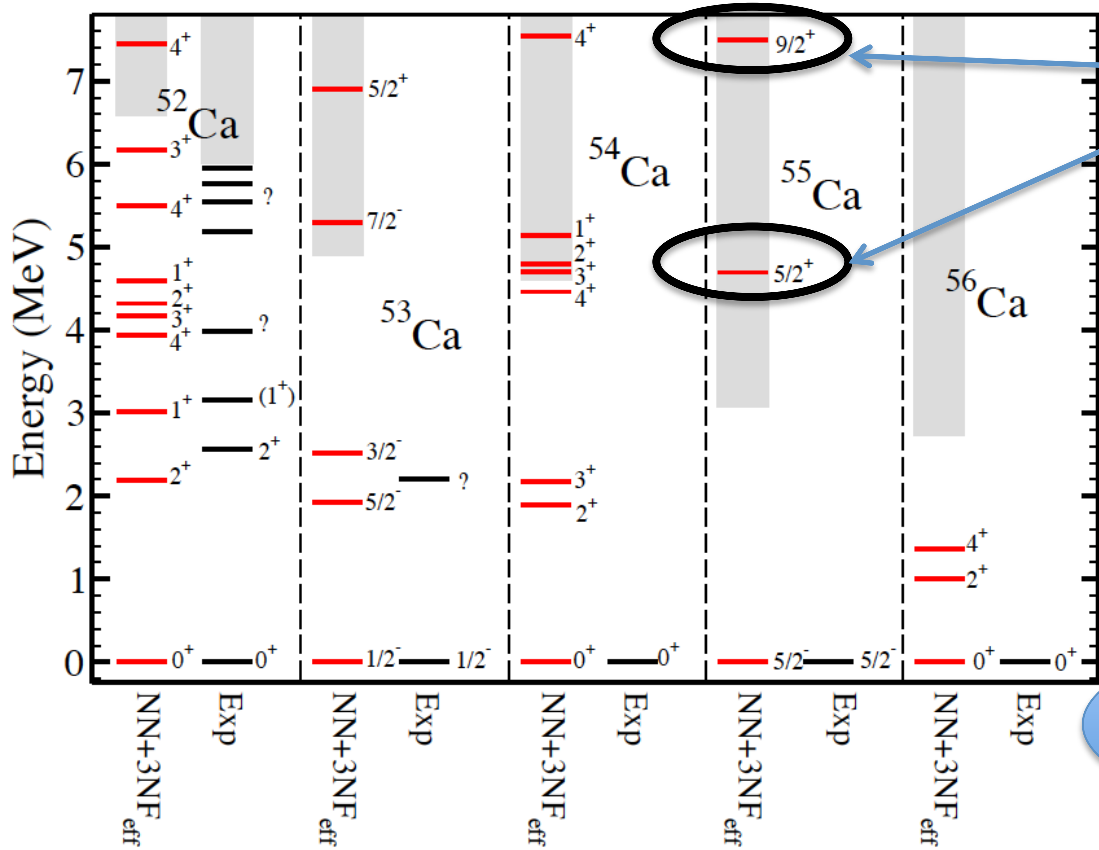
1. Good agreement between theory and experiment.
2. Shell closure in ^{48}Ca due to effects of 3NFs
3. Predict weak (sub-)shell closure in ^{54}Ca.

Measurement at RIKEN (Japan) agrees with theoretical prediction.

G. Hagen, M. Hjorth-Jensen, G. R. Jansen, R. Machleidt, T. Papenbrock, Phys. Rev. Lett. 109, 032502 (2012).

	^{48}Ca			^{52}Ca			^{54}Ca		
	2^+	4^+	$4^+/2^+$	2^+	4^+	$4^+/2^+$	2^+	4^+	$4^+/2^+$
CC	3.58	4.20	1.17	2.19	3.95	1.80	1.89	4.46	2.36
Exp	3.83	4.50	1.17	2.56	?	?	?	?	?

Spectra and shell evolution in Calcium isotopes



1. Inversion of the 9/2+ and 5/2+ resonant states in $^{53,55,61}Ca$
2. We find the ground state of ^{61}Ca to be ½+ located right at threshold.
3. A harmonic oscillator basis gives the naïve shell model ordering of states.

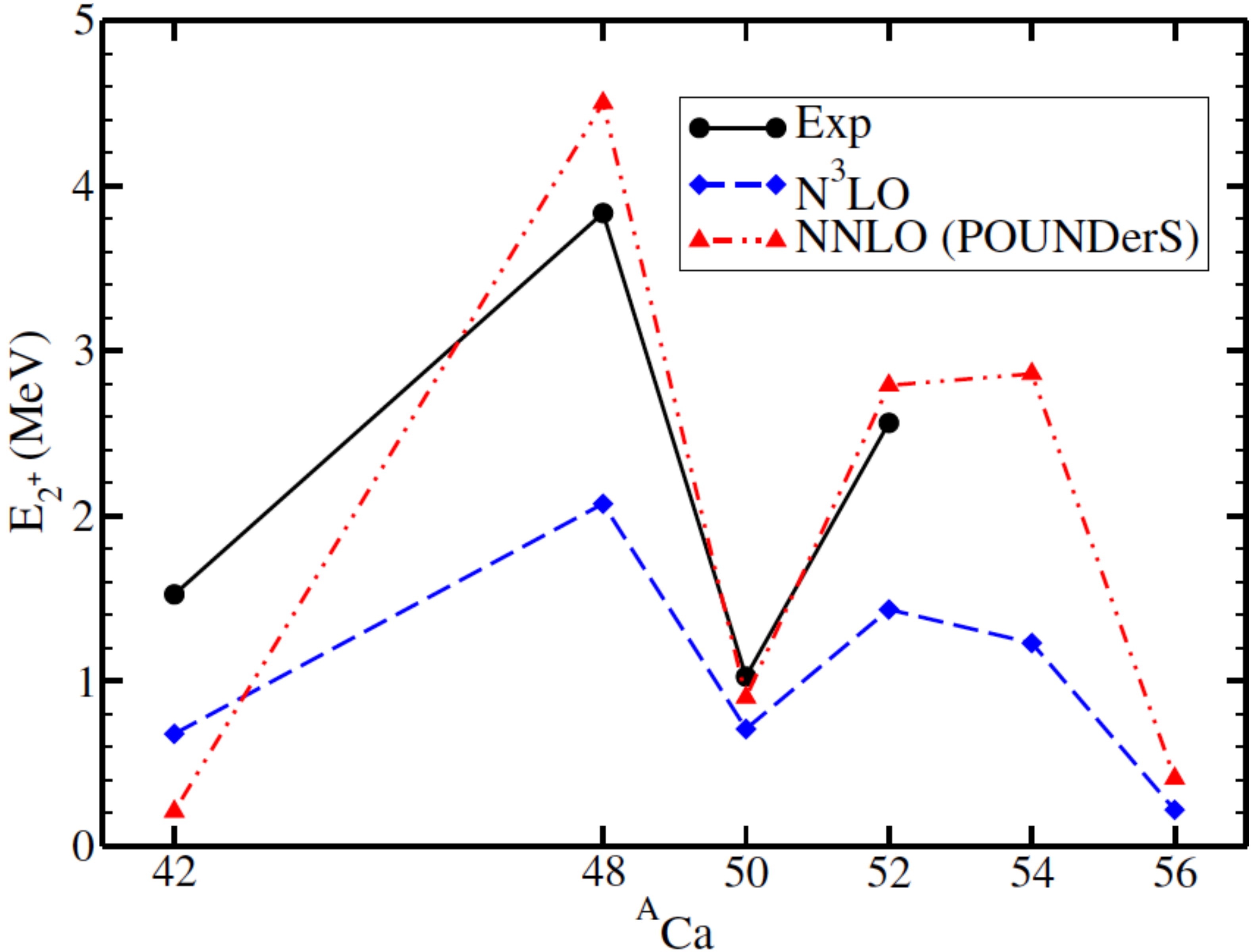
Continuum coupling is crucial!

	^{48}Ca	^{52}Ca	^{54}Ca
E_{2^+}(CC)	3.58	2.19	1.89
E_{2^+}(Exp)	3.83	2.56	n.a.
E_{4^+}/E_{2^+}(CC)	1.17	1.80	2.36
E_{4^+}/E_{2^+}(Exp)	1.17	n.a.	n.a.
S_n(CC)	9.45	6.59	4.59
S_n(Exp)	9.95	6.0*	4.0†

New penning trap measurement of masses of $^{51,52}Ca$
A. T. Gallant et al Phys. Rev. Lett. **109**, 032506 (2012)

	^{53}Ca		^{55}Ca		^{61}Ca	
J^π	Re[E]	Γ	Re[E]	Γ	Re[E]	Γ
$5/2^+$	1.99	1.97	1.63	1.33	1.14	0.62
$9/2^+$	4.75	0.28	4.43	0.23	2.19	0.02

Shell evolution in Calcium isotopes from NNLO(POUNDerS)



Comput

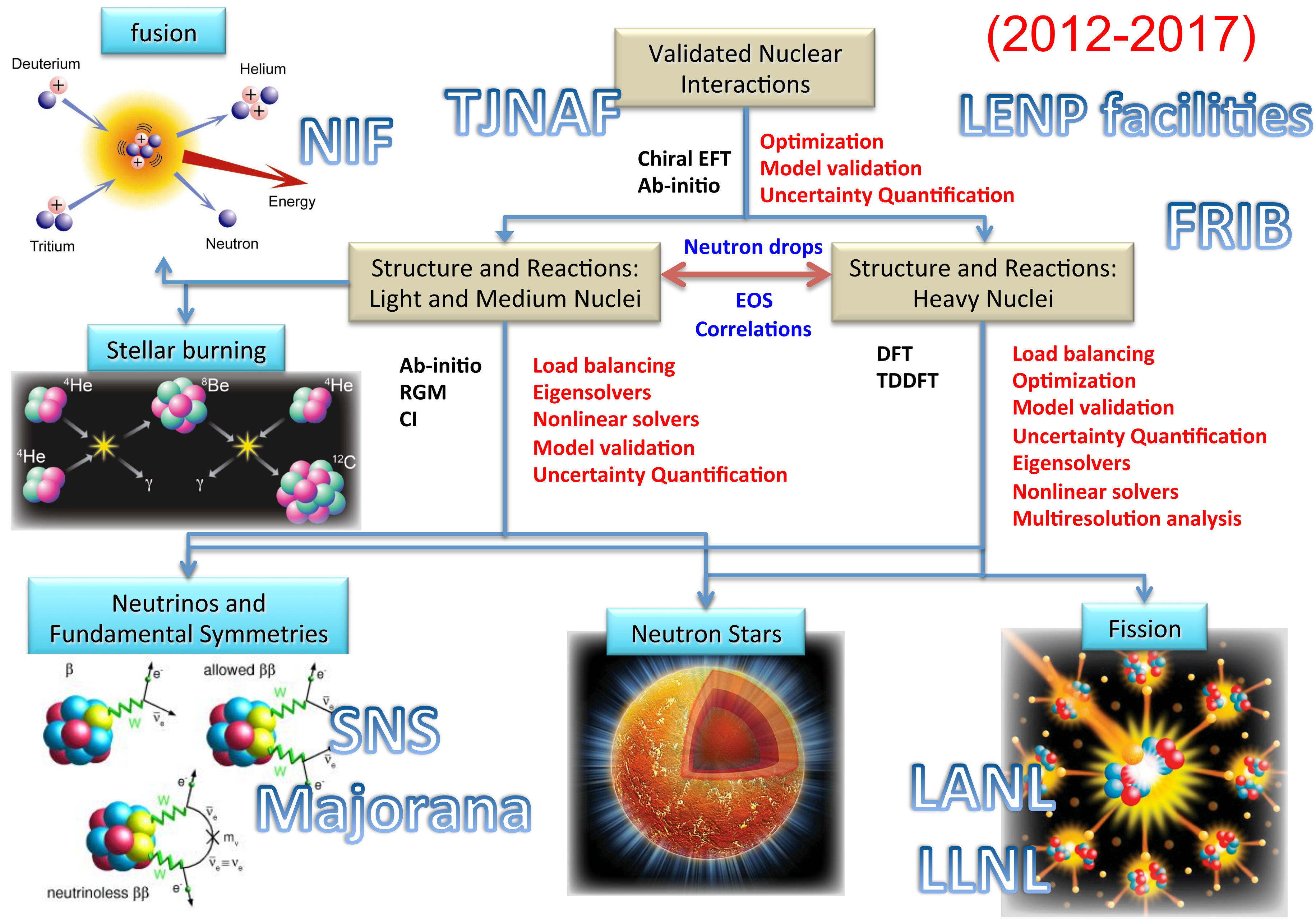
High Performance Computing provides answer … *her*
experiment nor analytic theory c
hence, it becomes the third leg supporting th … *cs*

National Academy Report
(2012)

SciDAC-2 UNEDF
SciDAC-3 NUCLEI

From M. Savage

NUclear Computational Low-Energy Initiative



Summary

- Super computing is an essential part of nuclear theory
- Purpose: Understanding of complex processes, guidance of experiment, and predictions into *terra incognita*
- Suite of *ab initio* methods: complementary and competing
- Aim: anchor low-energy nuclear theory into theory of strong interactions, with reliable predictions
- Quantification of theoretical uncertainties on the horizon
- Collaboration between nuclear theorists, and computer scientists and applied mathematicians crucial and most beneficial

HaPpY BiRtHdAy!

Excited states in oxygen isotopes from NNLO(POUNDerS)