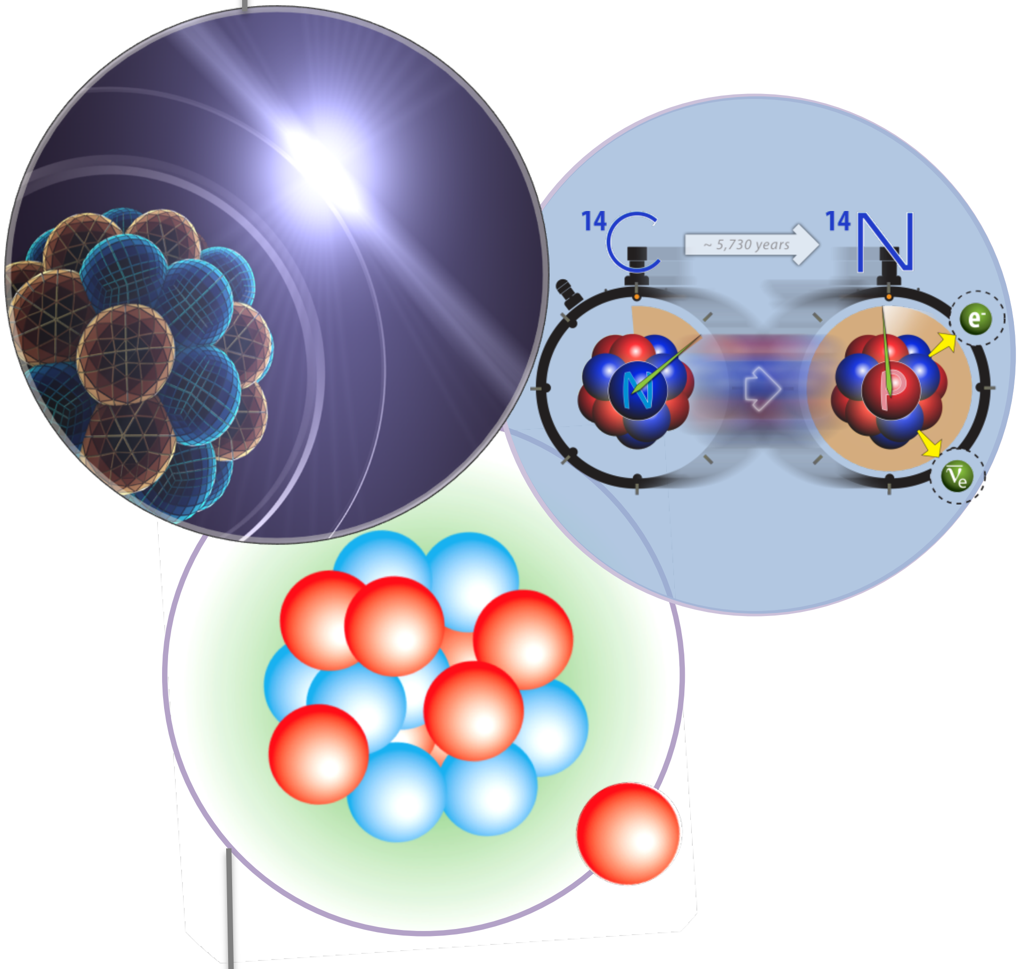
Coupled-cluster computations of atomic nuclei



Gaute Hagen

Oak Ridge National Laboratory

Frontiers in Nuclear Physics
KITP, October 4th, 2016

U.S. DEPARTMENT OF ENERGY
NUCLEI
Nuclear Computational Low-Energy Initiative
BSF
United States – Israel
Binational Science Foundation
OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Collaborators

@ ORNL / UTK: **S. Binder**, G. R. Jansen, **T. Morris**, T. Papenbrock, **M. Schuster**

@ MSU: W. Nazarewicz

@ Chalmers: **B. Carlsson**, A. Ekström, C. Forssén

@ Hebrew U: N. Barnea, D. Gazit

@ MSU/ U Oslo: M. Hjorth-Jensen

@ Trento: G. Orlandini

@ TRIUMF: S. Bacca, **M. Miorelli**, P. Navratil

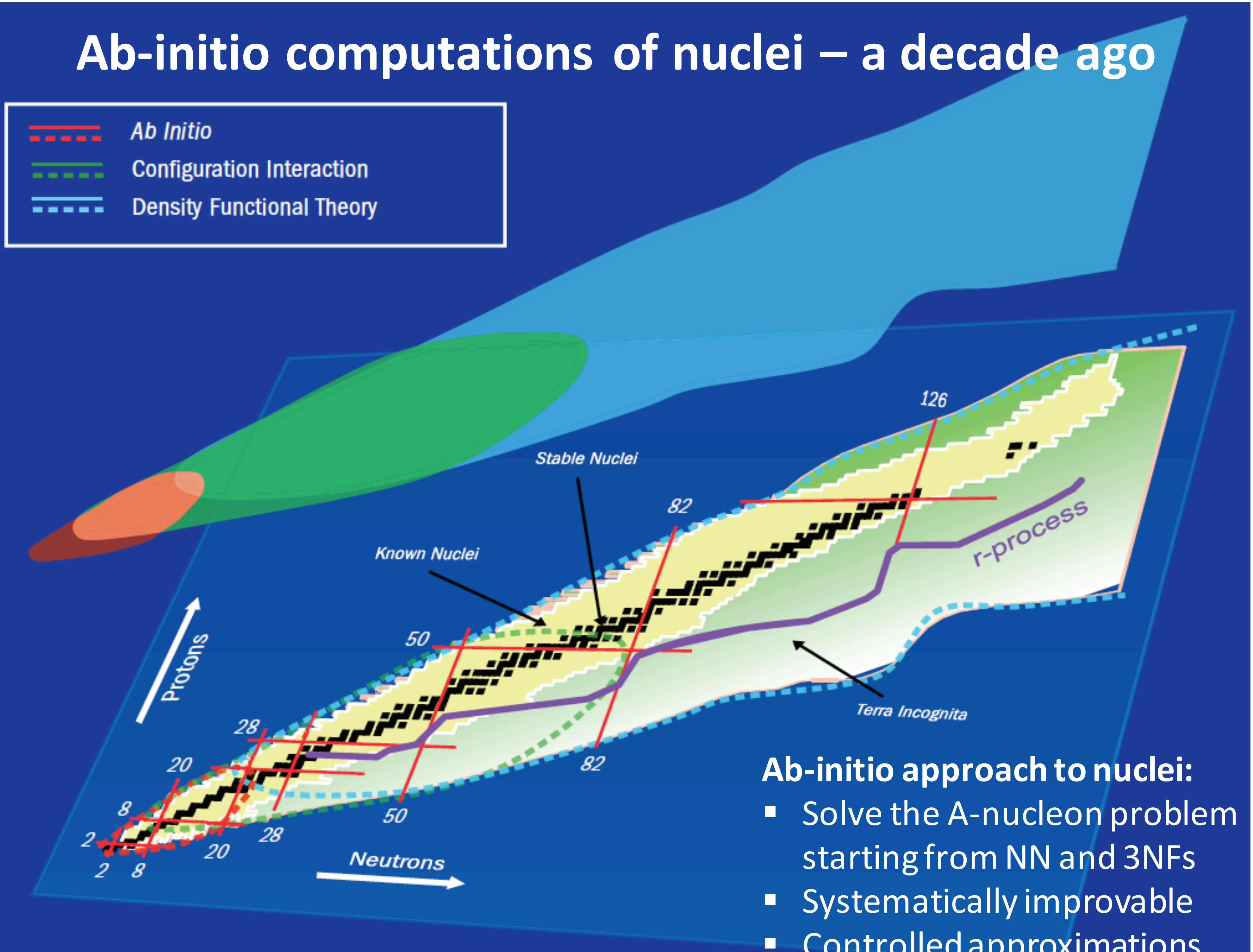
@ TU Darmstadt: **C. Drischler**, H.-W. Hammer, K. Hebeler, A. Schwenk, **J. Simonis, K. Wendt**

@ CERN/ISOLDE: **R. Garcia Ruiz** (COLLAPS collaboration)

Outline

- Status of ab-initio computations of nuclei
- Accurate binding energies and radii from a chiral interaction
- The neutron skin and dipole polarizability of ^{48}Ca
- Charge radii of neutron-rich calcium isotopes
- Structure of ^{78}Ni
- Structure and decay of ^{100}Sn

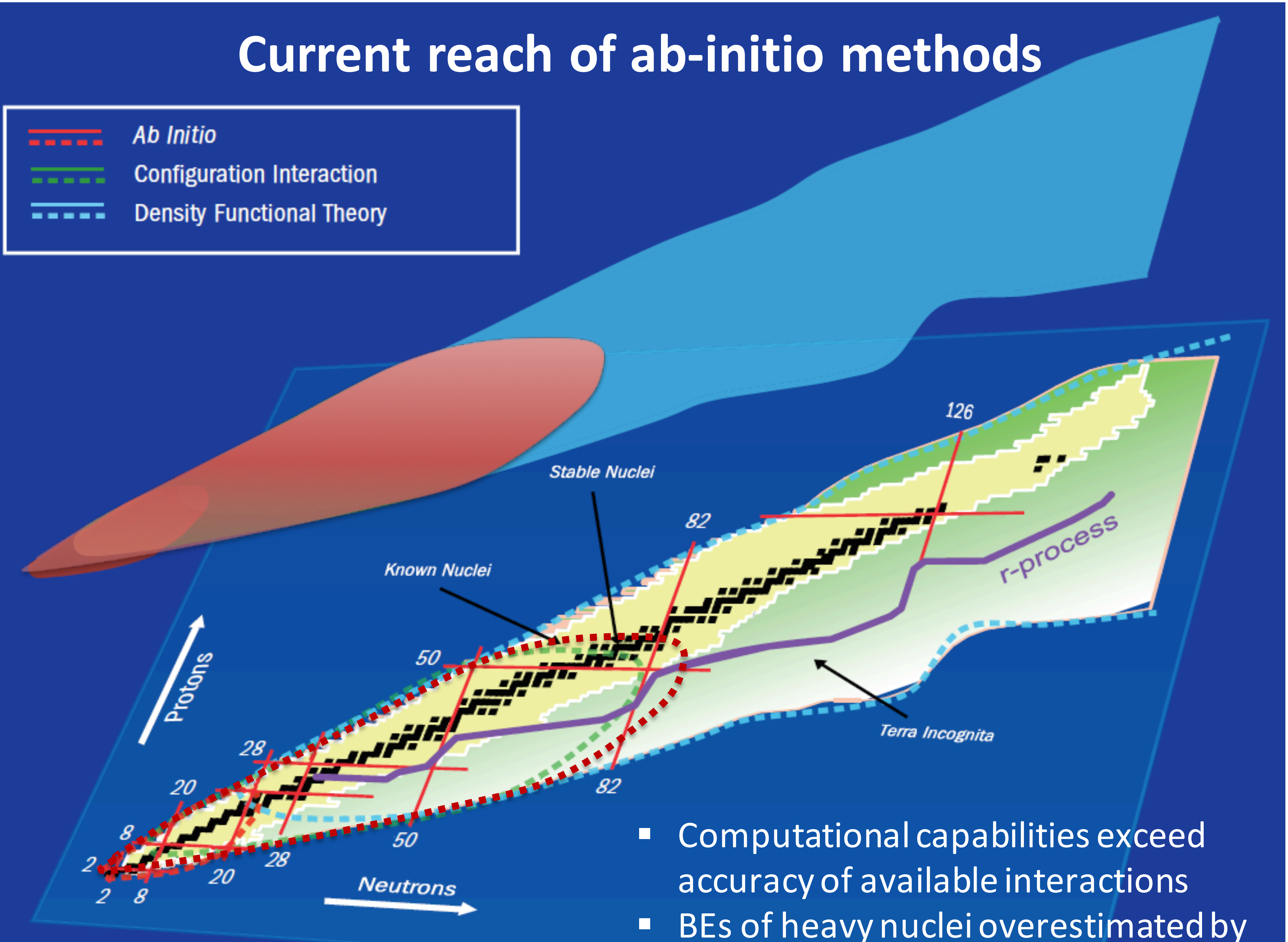
Ab-initio computations of nuclei – a decade ago



Ab-initio approach to nuclei:

- Solve the A-nucleon problem starting from NN and 3NFs
- Systematically improvable
- Controlled approximations

Current reach of ab-initio methods

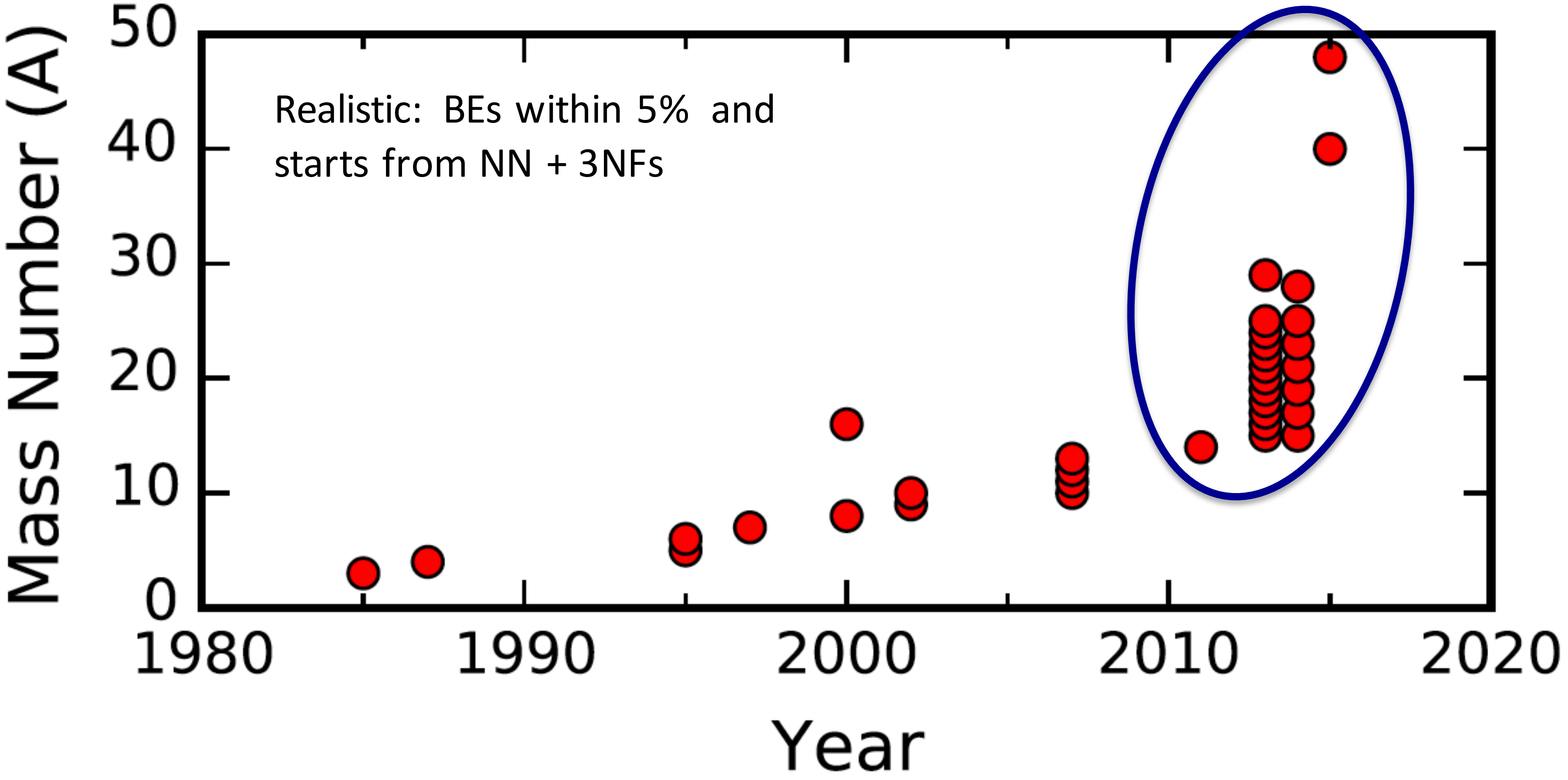


- Computational capabilities exceed accuracy of available interactions
- BEs of heavy nuclei overestimated by 1-2MeVs/A, [Binder *et al*, PLB (2014)]

Trend in realistic ab-initio calculations

Explosion of many-body methods (Coupled clusters, Green's function Monte Carlo, In-Medium SRG, Lattice EFT, MCSM, No-Core Shell Model, Self-Consistent Green's Function, UMOA, …)

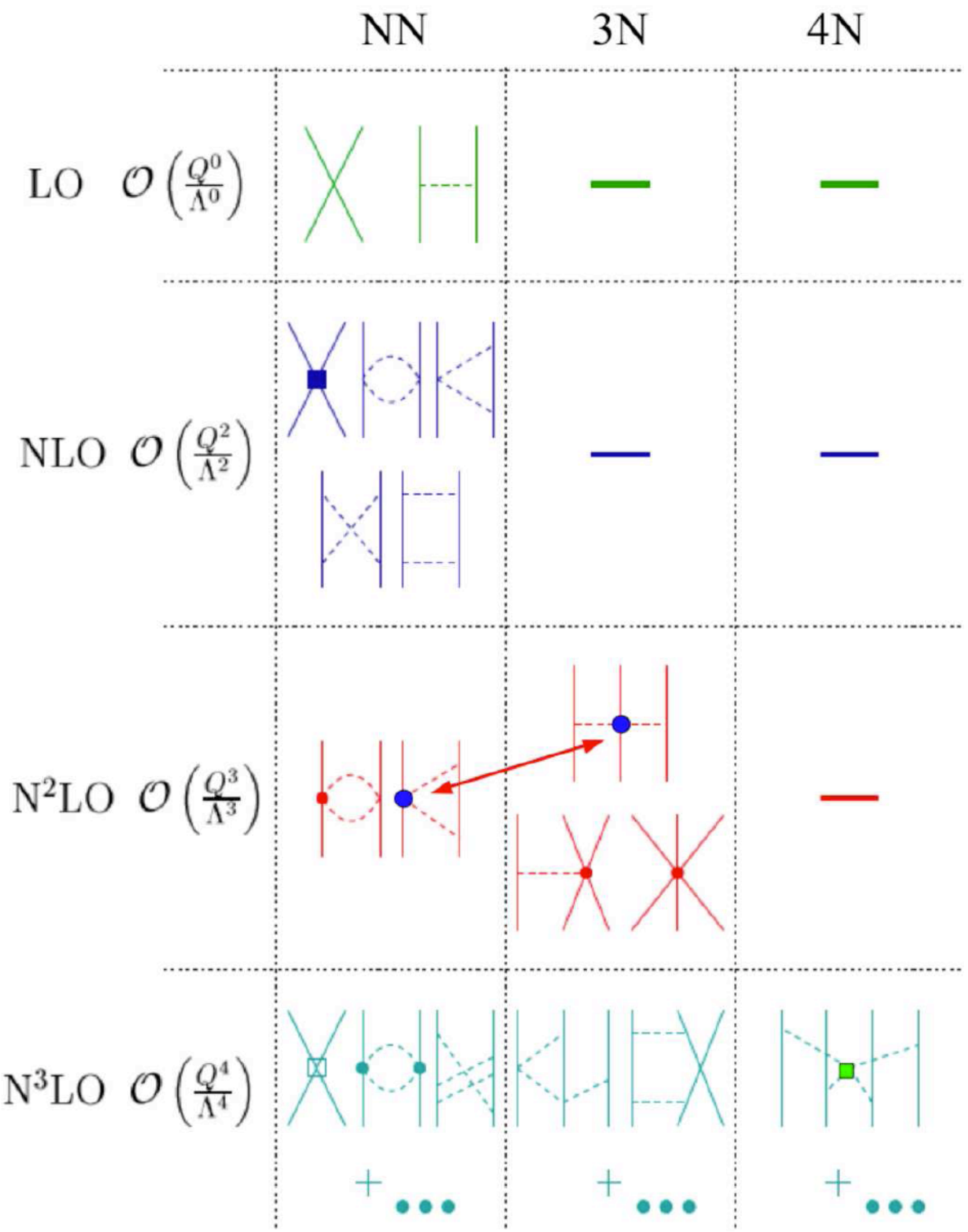
Application of ideas from EFT and renormalization group (V_{low-k}, Similarity Renormalization Group, …)



Realistic: BEs within 5% and starts from NN + 3NFs

Nuclear forces from chiral effective field theory

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



- Developing higher orders and higher rank (3NF, 4NF) [Epelbaum 2006; Bernard et al 2007; Krebs et al 2012; Hebeler et al 2015; …]
- Propagation of uncertainties on the horizon [Navarro Perez 2014, Carlsson et al 2015]
- Different optimization protocols [Ekström et al 2013, Carlsson et al 2016]
- Improved understanding/handling via SRG [Bogner et al 2003; Bogner et al 2007]
- local / semi-local / non-local formulations [Epelbaum et al 2015, Gezerlis et al 2013/2014]
- RG invariant? Different power counting schemes being explored

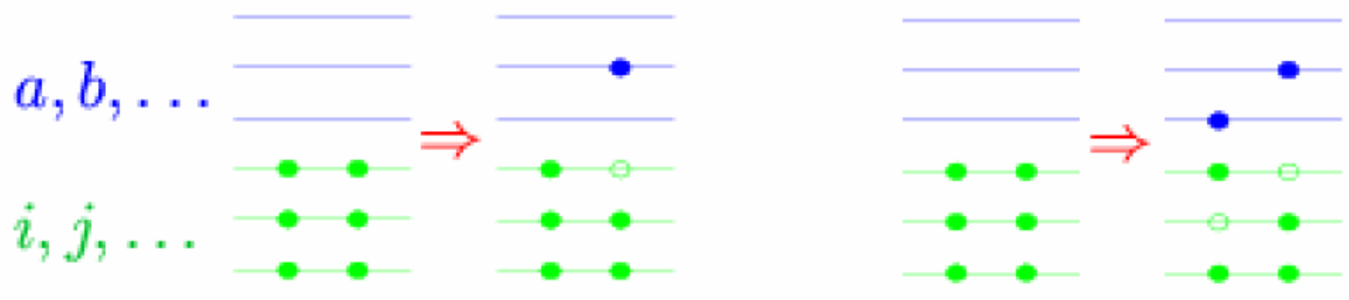
Coupled-cluster method (CCSD approximation)

Ansatz:

$$
\begin{aligned}
|\Psi\rangle &= e^{T}|\Phi\rangle \\
T &= T_1 + T_2 + \ldots \\
T_1 &= \sum_{ia} t_i^a a_a^\dagger a_i \\
T_2 &= \sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i
\end{aligned}
$$

- ☺ Scales gently (polynomial) with increasing problem size o^2u^4 .
- ☺ Truncation is the only approximation.
- ☺ Size extensive (error scales with A)
- ☹ Most efficient for closed (sub-)shell nuclei

Correlations are *exponentiated* 1p-1h and 2p-2h excitations. Part of np-nh excitations included!

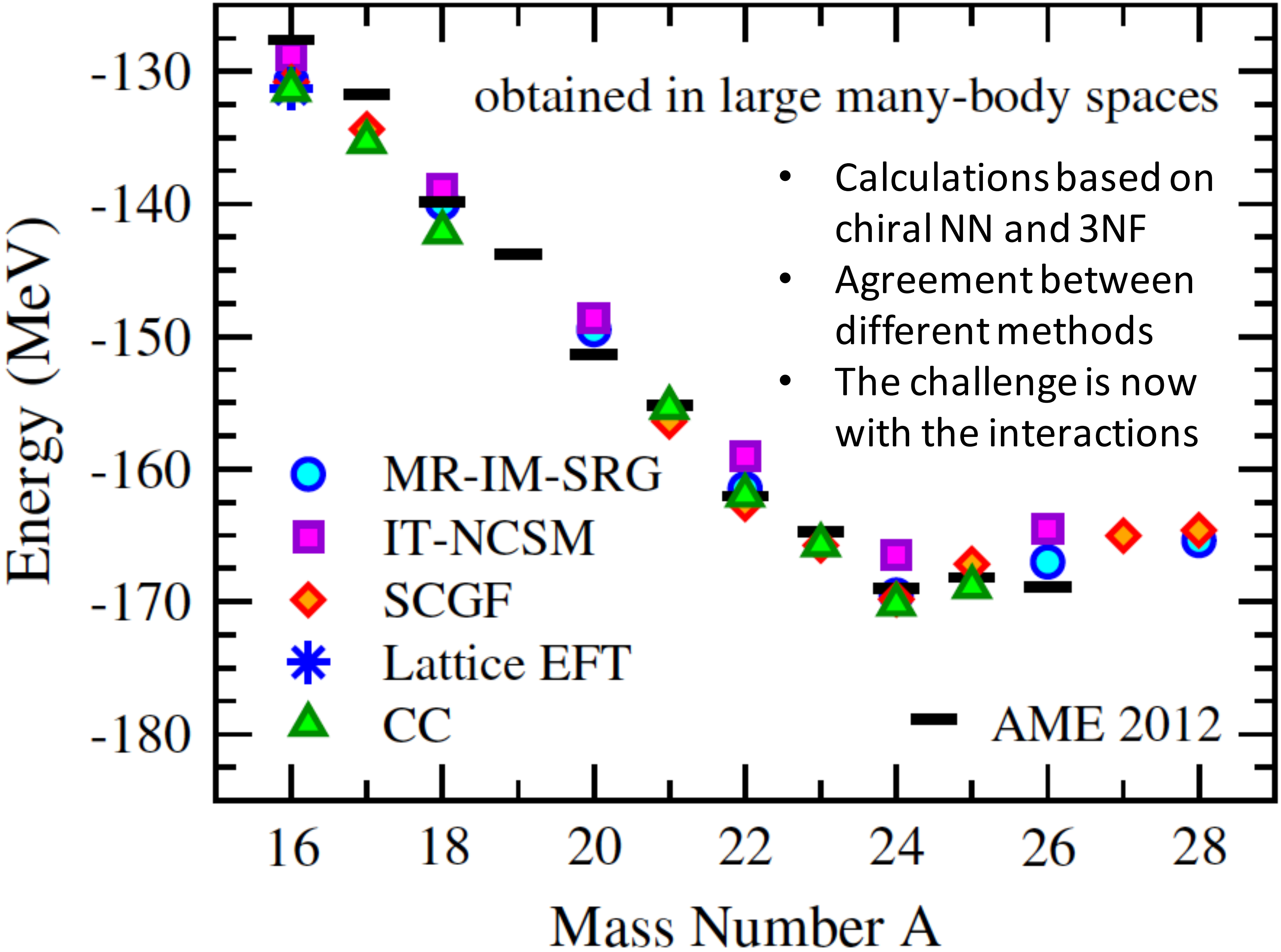


Coupled cluster equations

$$
\begin{aligned}
E &= \langle\Phi|\overline{H}|\Phi\rangle \\
0 &= \langle\Phi_i^a|\overline{H}|\Phi\rangle \\
0 &= \langle\Phi_{ij}^{ab}|\overline{H}|\Phi\rangle \\
\overline{H} &\equiv e^{-T}He^{T} = \left(He^{T}\right)_c = \left(H + HT_1 + HT_2 + \frac{1}{2}HT_1^2 + \ldots\right)_c
\end{aligned}
$$

Alternative view: CCSD generates similarity transformed Hamiltonian with no 1p-1h and no 2p-2h excitations.

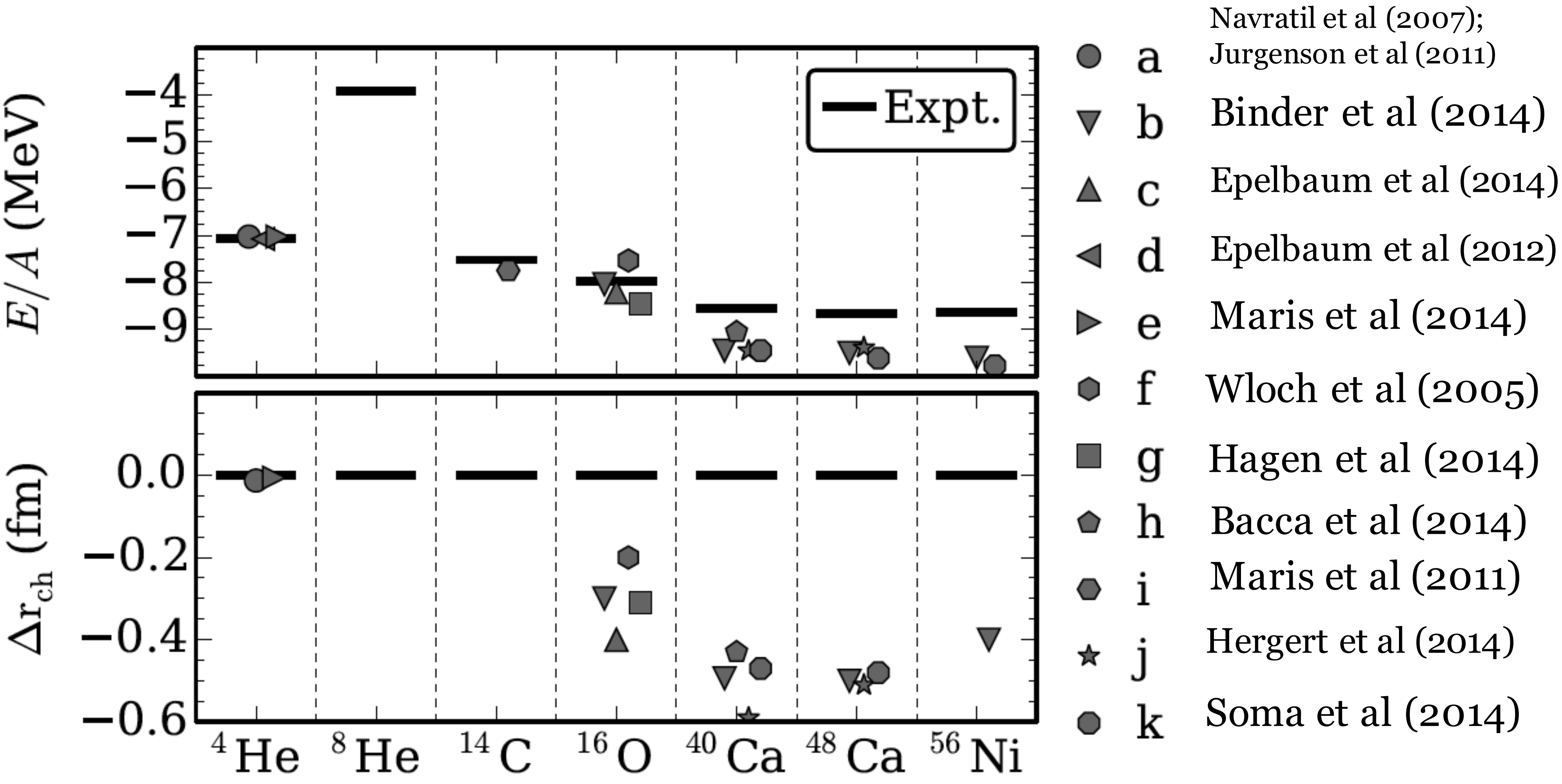
Oxgyen chain with interactions from chiral EFT



- Calculations based on chiral NN and 3NF
- Agreement between different methods
- The challenge is now with the interactions

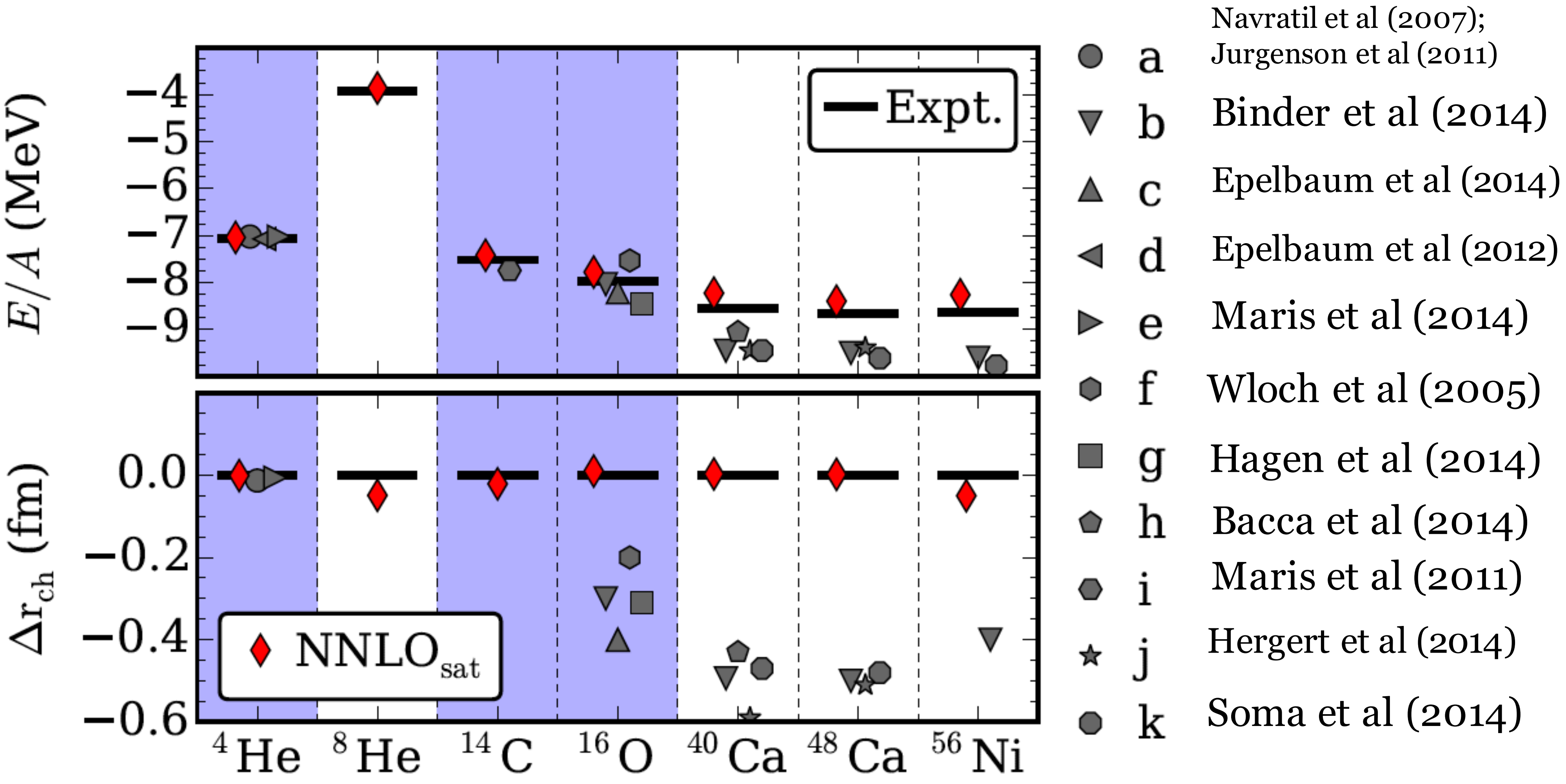
Hebeler, Holt, Menendez, Schwenk, Annu. Rev. Nucl. Part. Sci. 65, 457 (2015)

Accurate nuclear binding energies and radii from a chiral interaction



- Chiral interactions have failed at describing both binding energies and radii of nuclei
- Predictive power does not go together with large extrapolations
- Nuclear saturation may be viewed as an emergent property

Accurate nuclear binding energies and radii from a chiral interaction



Solution: Simultaneous optimization of NN and 3NFs

Include charge radii and binding energies of ^{3}H, ^{3,4}He, ^{14}C, ^{16}O in the optimization (NNLO$_{\text{sat}}$)

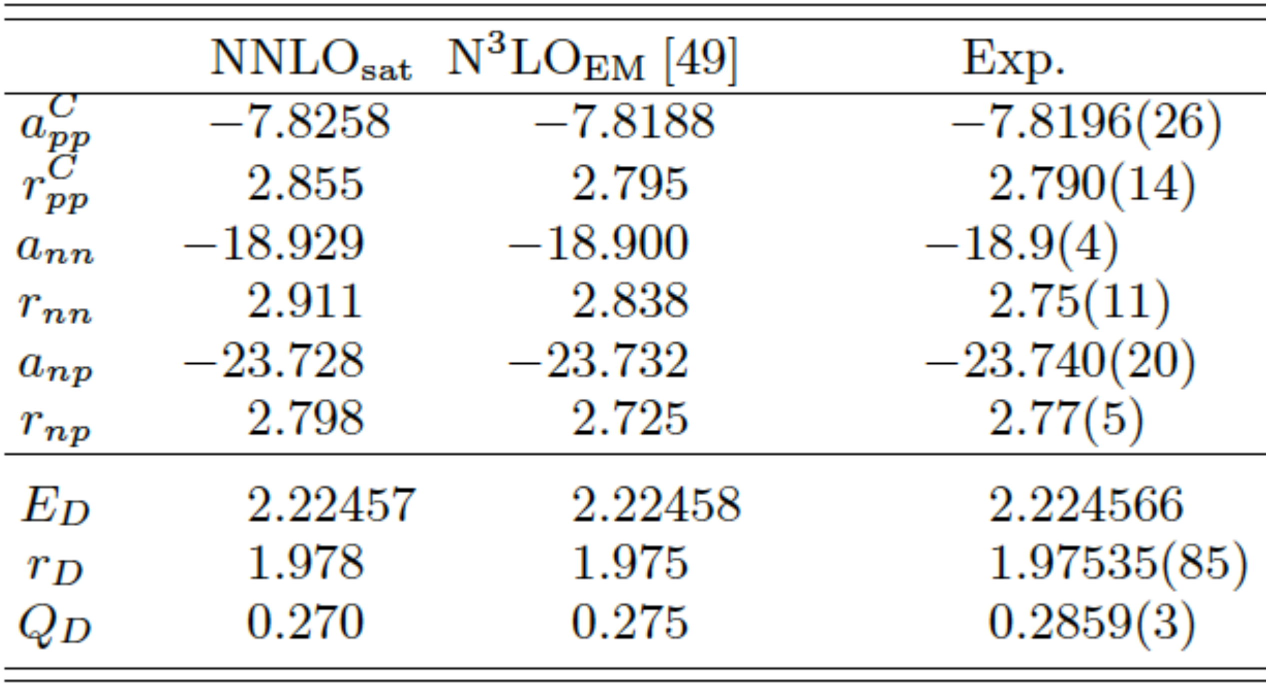
A. Ekström *et al*, Phys. Rev. C **91**, 051301(R) (2015).

G. Hagen et al, Phys. Scr. 91, 063006 (2016).

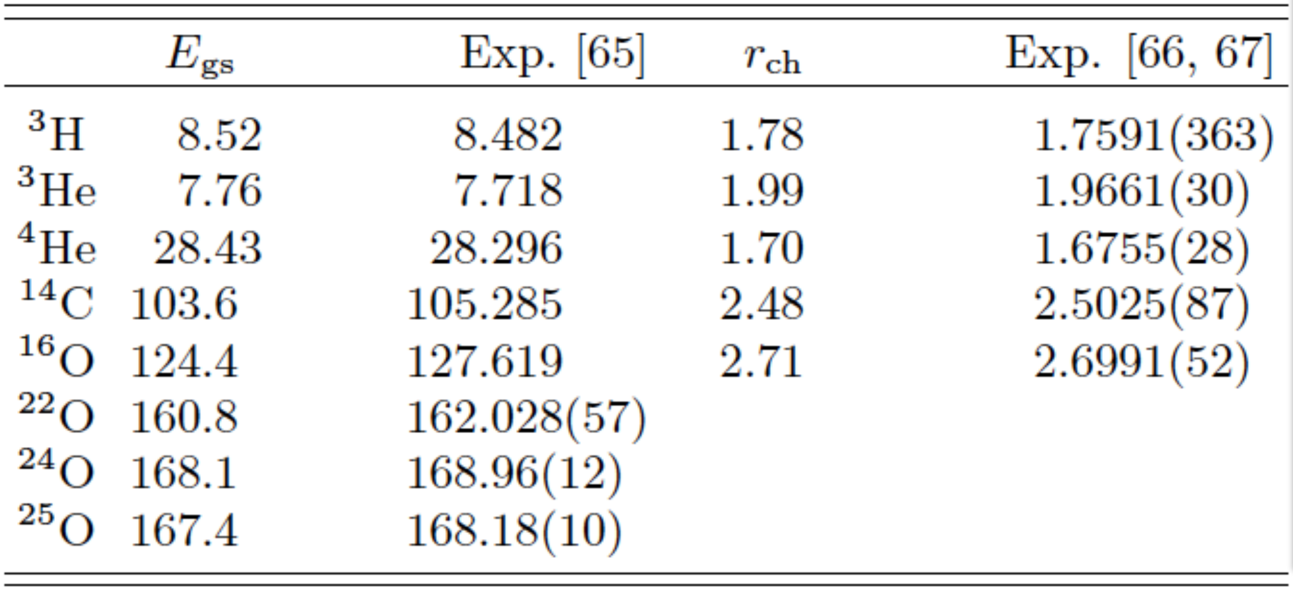
Not new: GFMC with AV18 and Illinois-7 are fit to 23 levels in nuclei with A <10

Optimizing NNLO$_{sat}$

A. Ekström, G. Jansen, K. Wendt et al, PRC 91, 051301 (2015)



	NNLO$_{sat}$	N^{3}LO$_{EM}$ [49]	Exp.
a_{pp}^C	-7.8258	-7.8188	$-7.8196(26)$
r_{pp}^C	2.855	2.795	2.790(14)
a_{nn}	-18.929	-18.900	$-18.9(4)$
r_{nn}	2.911	2.838	2.75(11)
a_{np}	-23.728	-23.732	$-23.740(20)$
r_{np}	2.798	2.725	2.77(5)
E_D	2.22457	2.22458	2.224566
r_D	1.978	1.975	1.97535(85)
Q_D	0.270	0.275	0.2859(3)



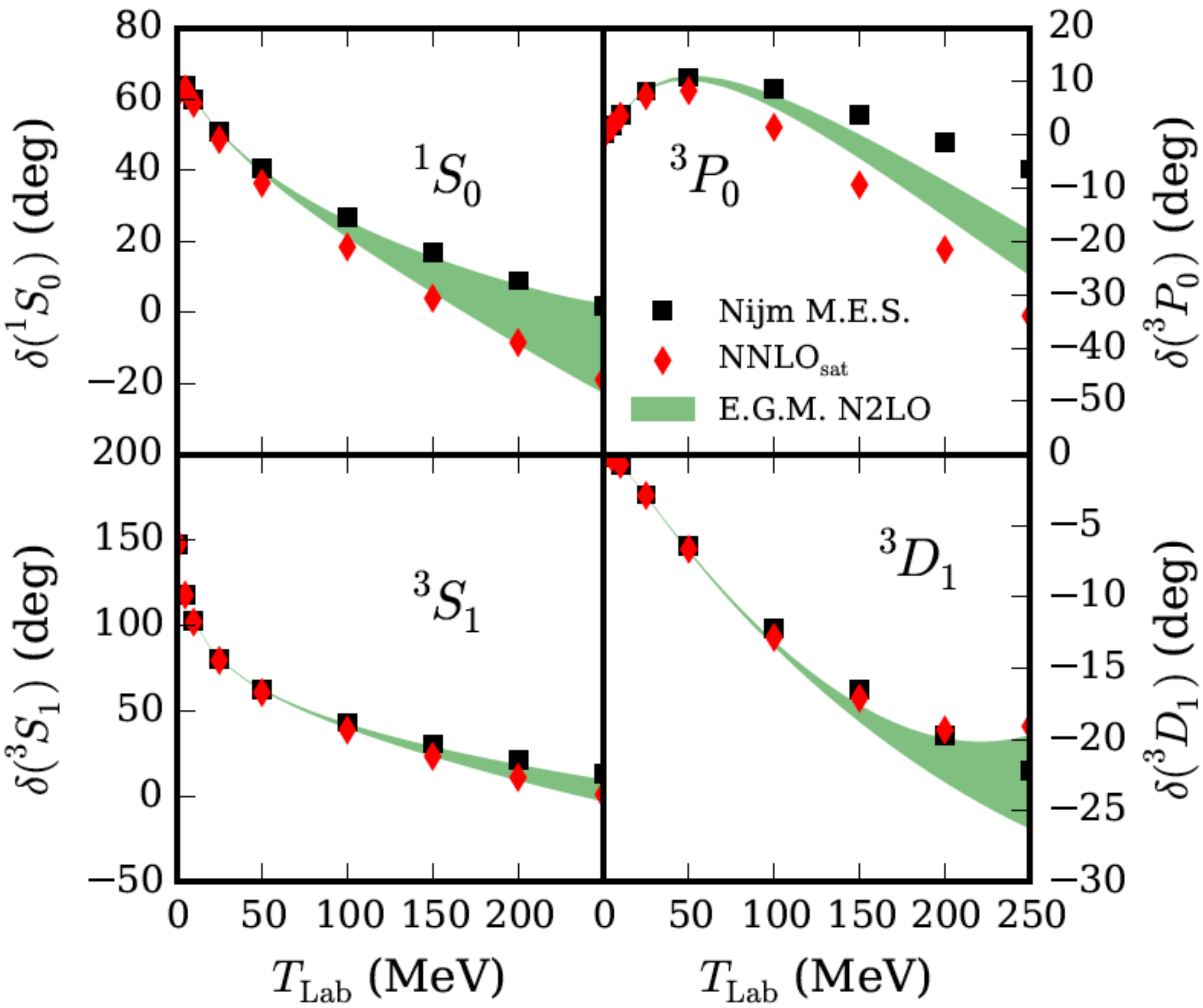
	E_{gs}	Exp. [65]	r_{ch}	Exp. [66, 67]
^{3}H	8.52	8.482	1.78	1.7591(363)
^{3}He	7.76	7.718	1.99	1.9661(30)
^{4}He	28.43	28.296	1.70	1.6755(28)
^{14}C	103.6	105.285	2.48	2.5025(87)
^{16}O	124.4	127.619	2.71	2.6991(52)
^{22}O	160.8	162.028(57)		
^{24}O	168.1	168.96(12)		
^{25}O	167.4	168.18(10)		

Objective function:

- Chi square optimization using POUNDerS
- Include BEs and radii in light nuclei and selected carbon and oxygen isotopes
- NN scattering data is included up to scattering energies of 35MeV
- Phase shifts are at the limit of expectations one can have at NNLO

Optimizing NNLO$_{\text{sat}}$

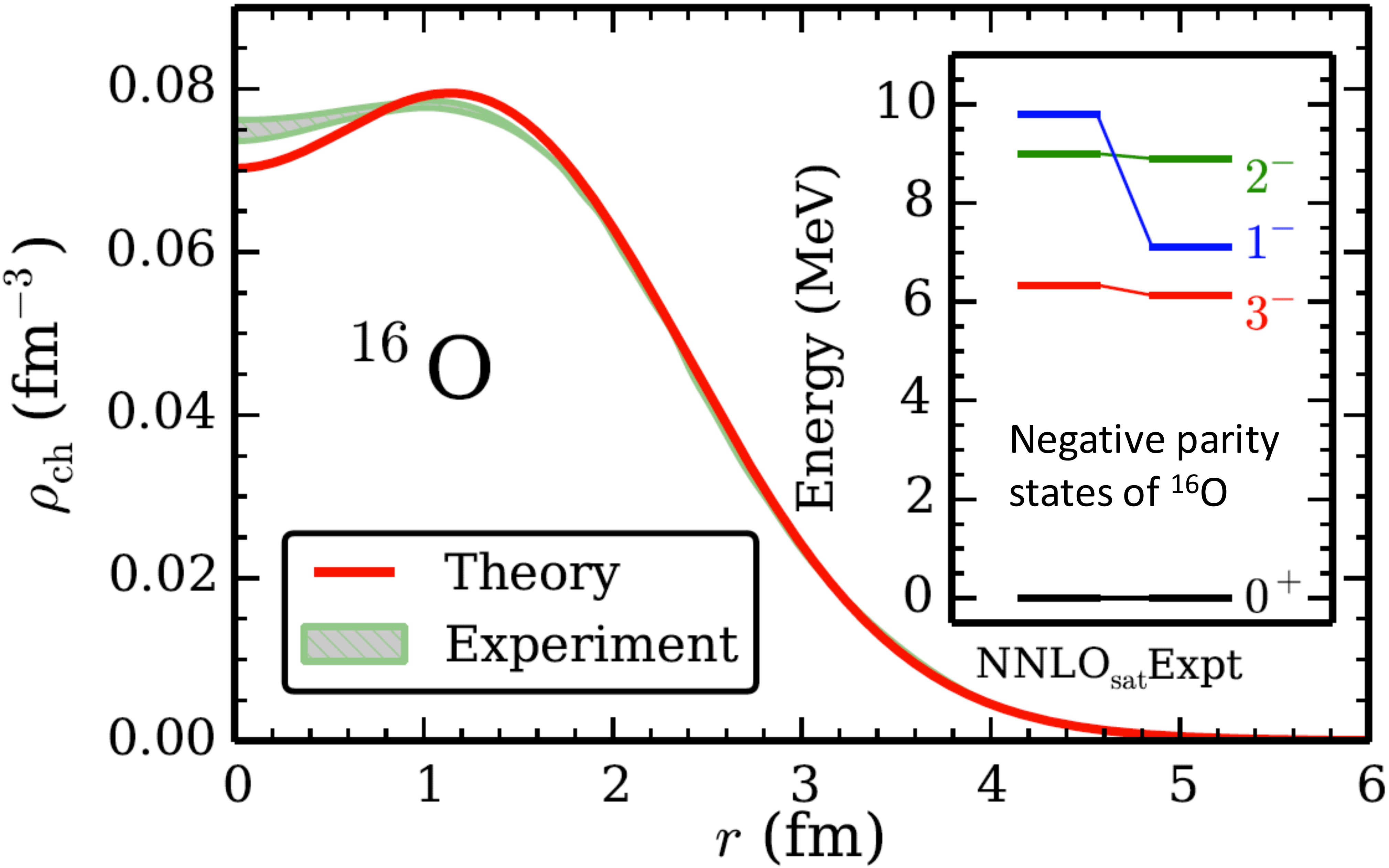
A. Ekström, G. Jansen, K. Wendt et al, PRC 91, 051301 (2015)



Objective function:

- Chi square optimization using POUNDerS
- Include BEs and radii in light nuclei and selected carbon and oxygen isotopes
- NN scattering data is included up to scattering energies of 35MeV
- Phase shifts are at the limit of expectations one can have at NNLO

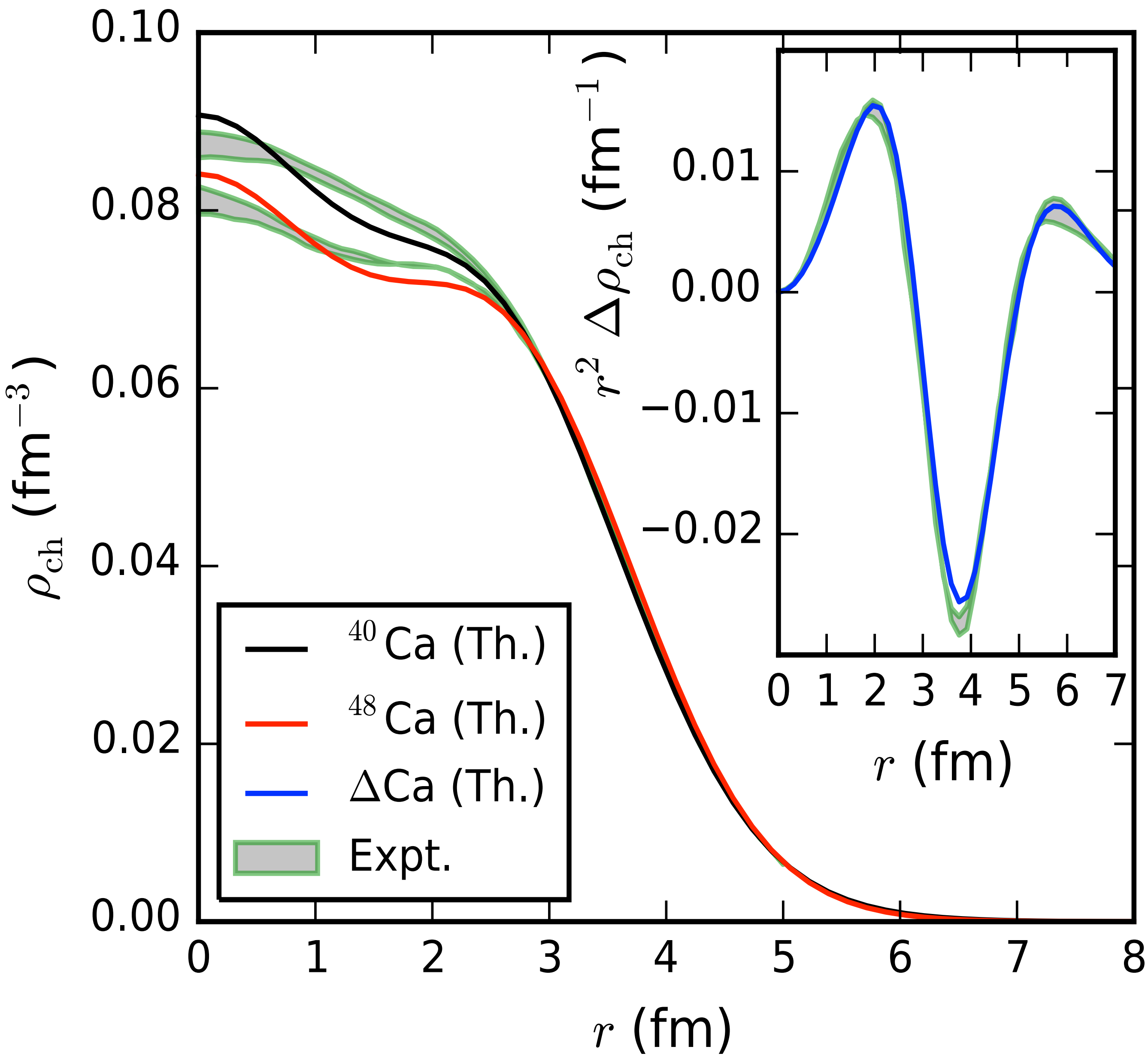
Charge density of ^{16}O



A. Ekström, G. Jansen, K. Wendt et al, PRC 91, 051301 2015

Charge densities of ^{40,48}Ca from NNLO$_{\text{sat}}$

G. Hagen *et al*, Nature Physics **12**, 186–190 (2016)



Electric charge distributions have been a long-standing problem for *ab initio* theory

^{40}Ca

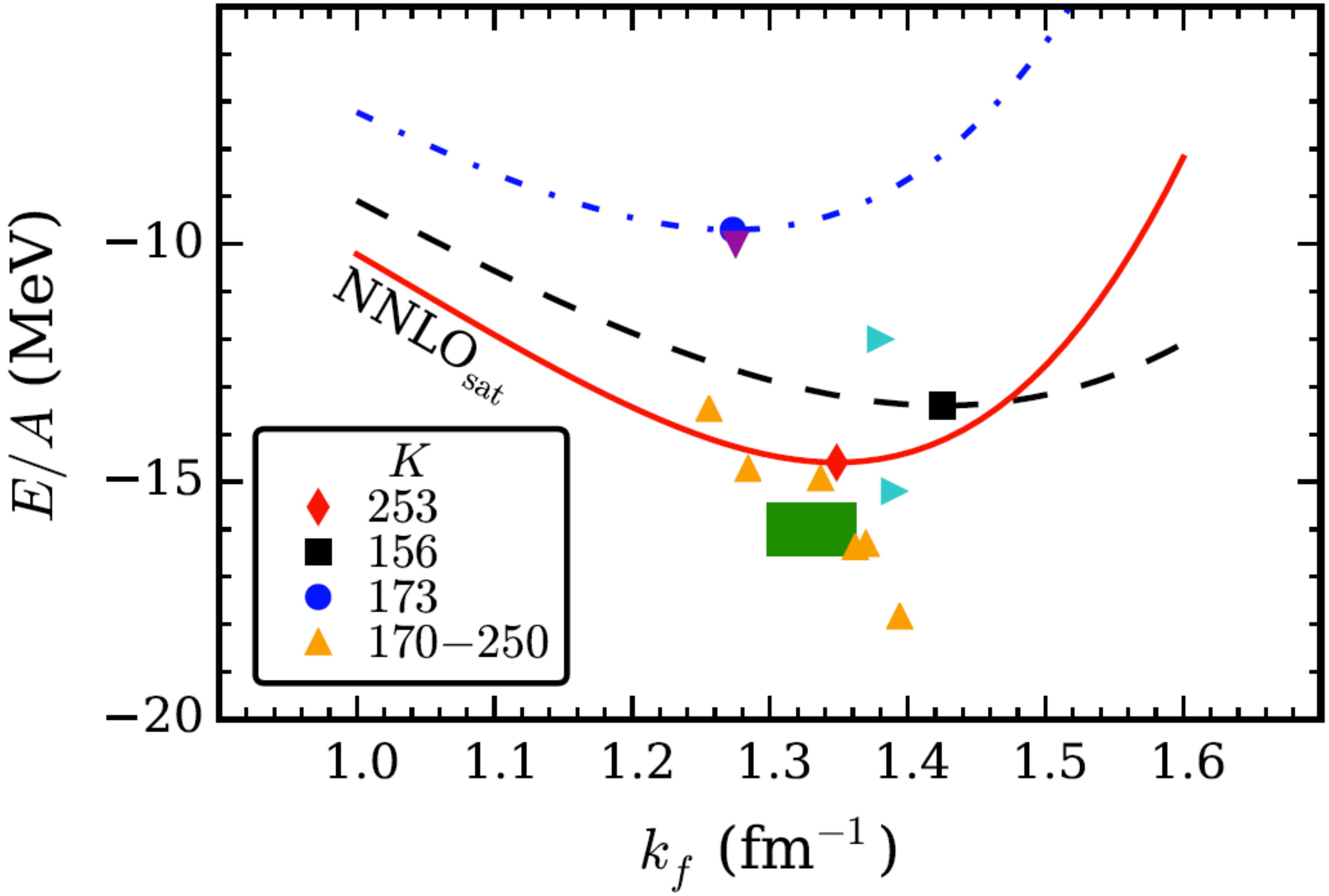
BE(Th)	*BE*(Exp)
326(3) MeV	342 MeV
R_{Ch} (Th)	$R_{Ch.}$(Exp)
3.49(2) fm	3.4776 fm

^{48}Ca

BE(Th)	*BE*(Exp)
404(3) MeV	416 MeV
R_{Ch} (Th)	$R_{Ch.}$(Exp)
3.48(3) fm	3.4771 fm

Nuclear matter from NNLO$_{sat}$

A. Ekström, G. Jansen, K. Wendt et al, PRC 91, 051301 (2015)



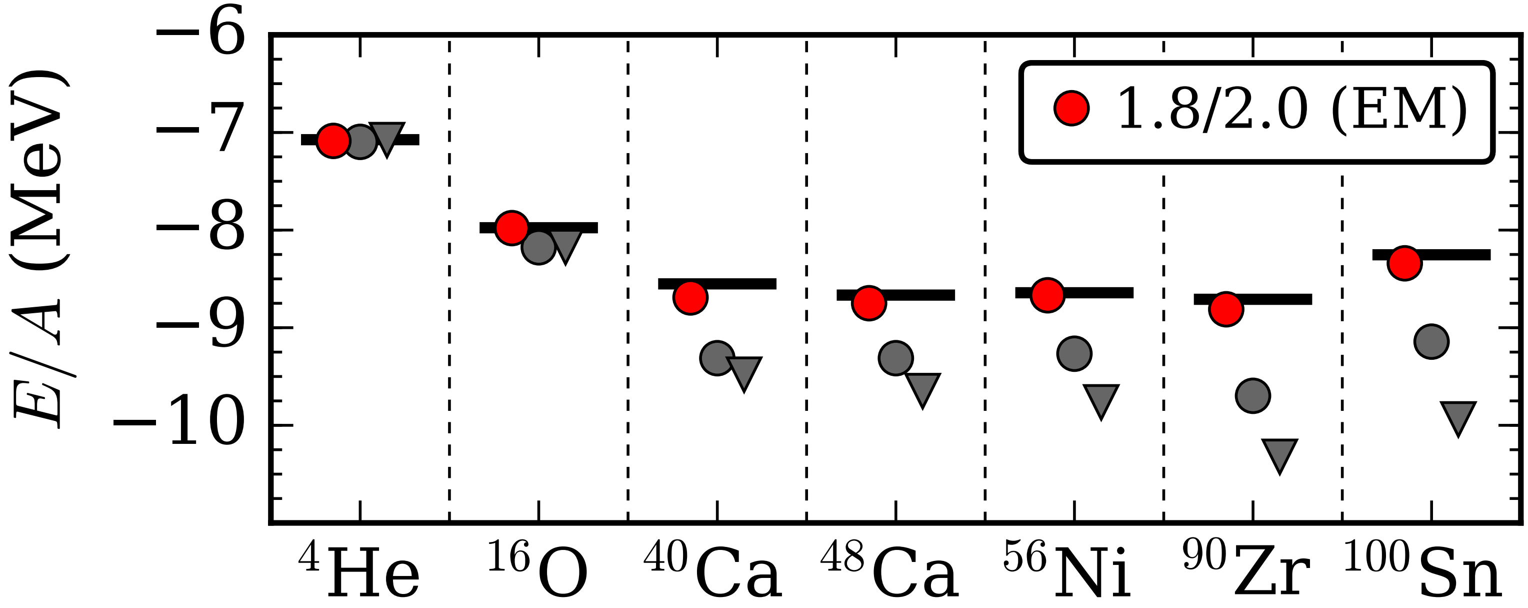
Nuclear matter saturation curves for NNLO$_{sat}$ and other interactions.

Hagen et al (2014); Carbone et al (2013); Coraggio et al 2014;

▲ **Hebeler *et al* PRC 2011.**

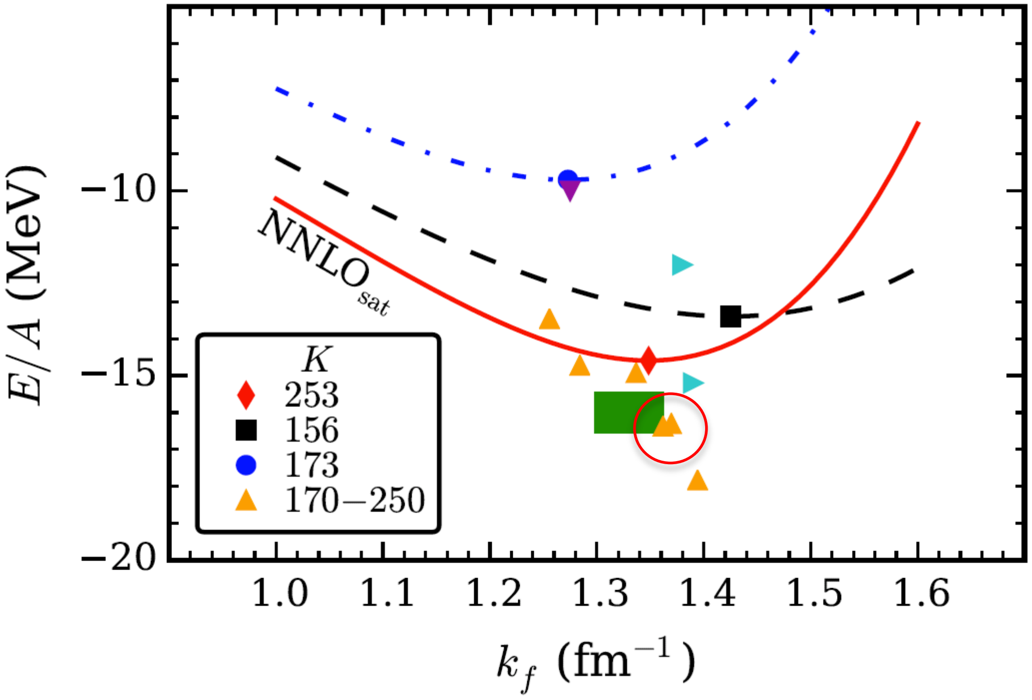
- Interactions from Hebeler *et al* not constrained by heavier nuclei.
- They reproduce binding energy and radii of few-body systems
- Non-local regulators in the 3NF important for saturation

Accurate BEs from light → heavy → infinite matter from a chiral interaction



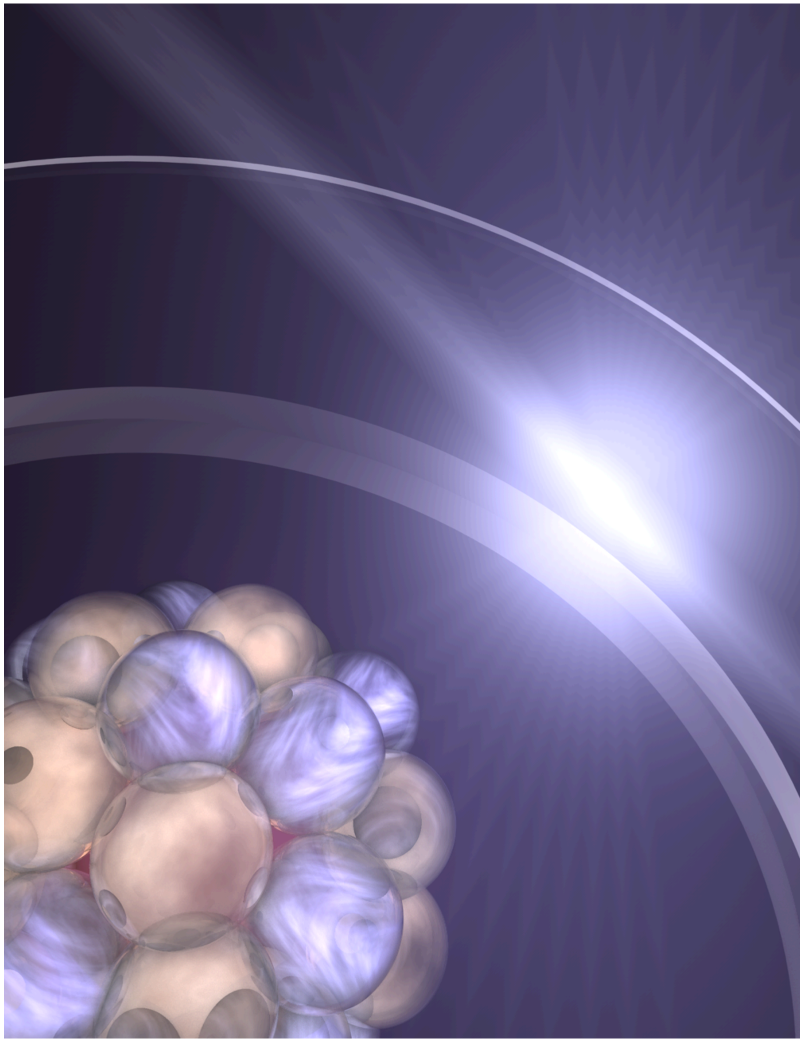
1.8/2.0 (EM) from K. Hebeler *et al* PRC (2011)

The other chiral NN + 3NFs are from Binder et al, PLB (2014)



- Accurate binding energies up to mass 100 from a chiral NN + 3NF
- Fit to nucleon-nucleon scattering and BEs and radii of A=3,4 nuclei
- Reproduces saturation point in nuclear matter within uncertainties
- Deficiencies: Radii are less accurate

What is the neutron skin of ^{48}Ca



Neutron skin = Difference between radii of neutron and proton distributions

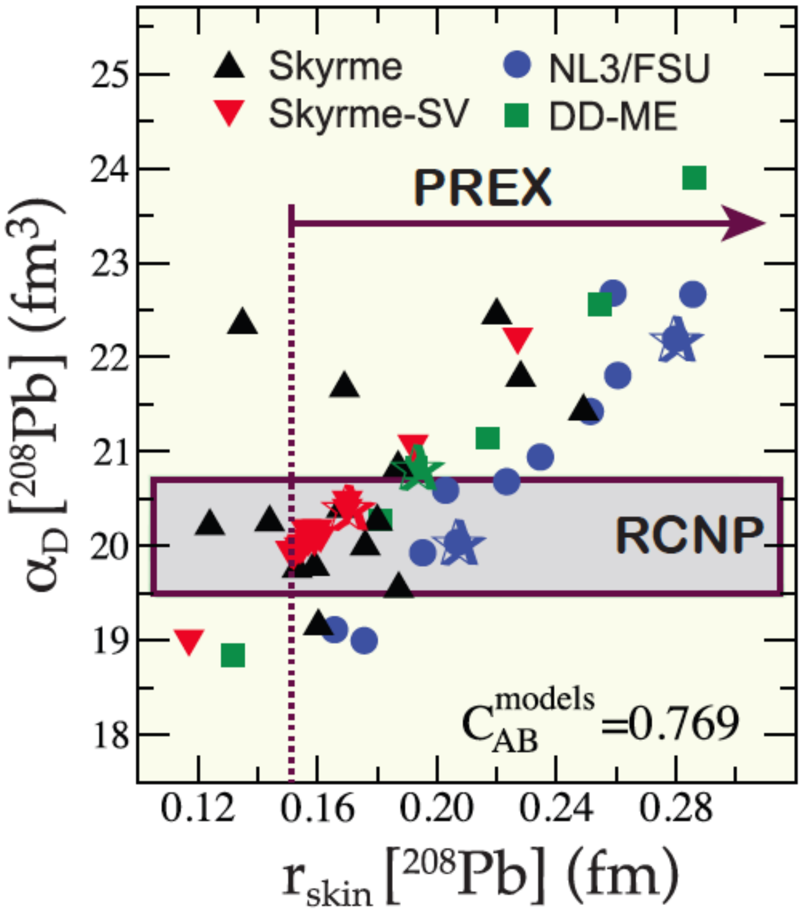
Relates atomic nuclei to neutron stars via neutron EOS

Correlated quantity: dipole polarizability

Model-independent measurement possible via parity-violating electron scattering (P-REX/C-REX at JLab)

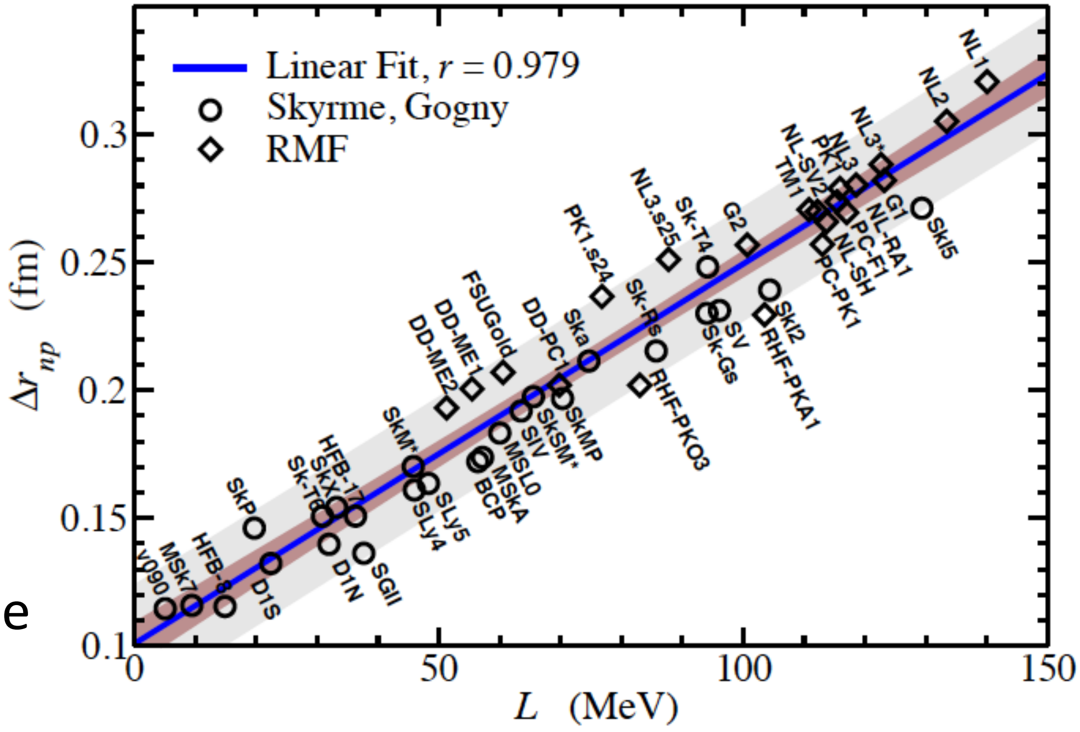
Neutron skin and dipole polarizability of ^{48}Ca

J. Piekarewicz e al, PRC 85, 041302(R) (2012)



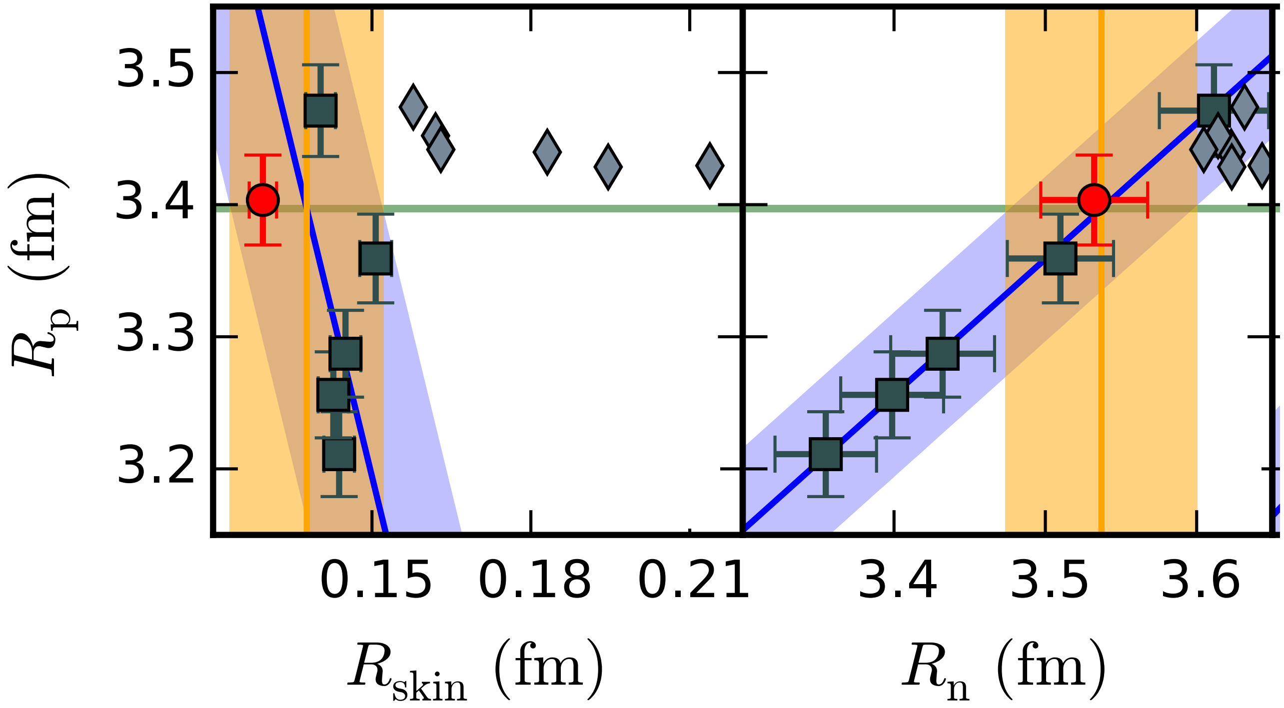
- Impacts limits of stability and physics of neutron stars
- C-REX will measure the weak charge form
- Darmstadt-Osaka collaboration has measured α_D

X. Viñas et al, Eur. Phys. J. A 50, 27 (2014)



- Our knowledge about neutron skins is so far mainly based on DFT models.
- What does ab-initio theory add to our knowledge of the neutron skin and size of nuclei?

Neutron radius and skin of ^{48}Ca

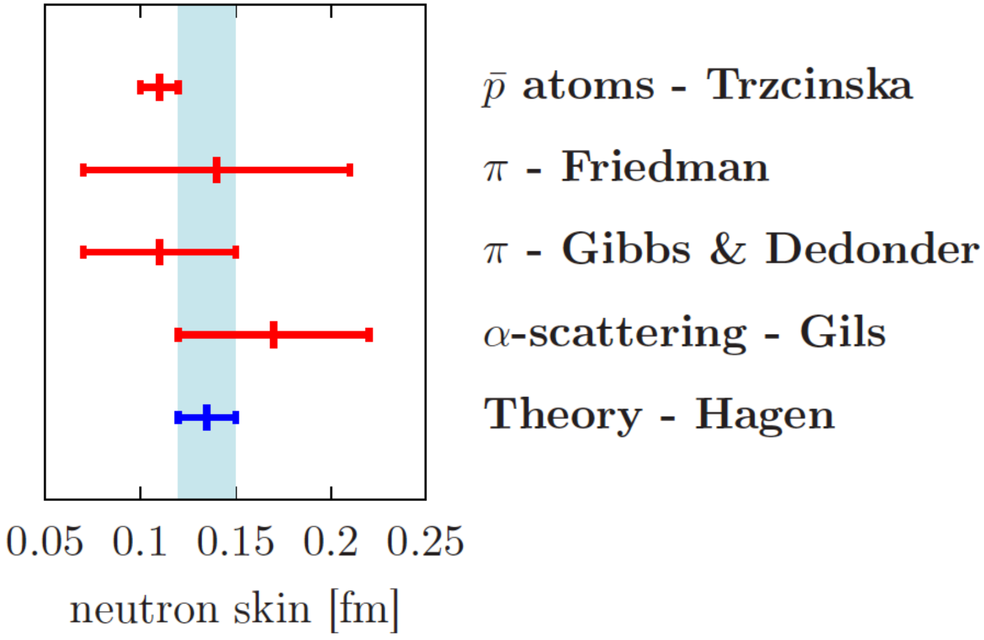


G. Hagen *et al*, Nature Physics **12**, 186–190 (2016)

Uncertainty estimates from family of chiral interactions: K. Hebeler *et al* PRC (2011)

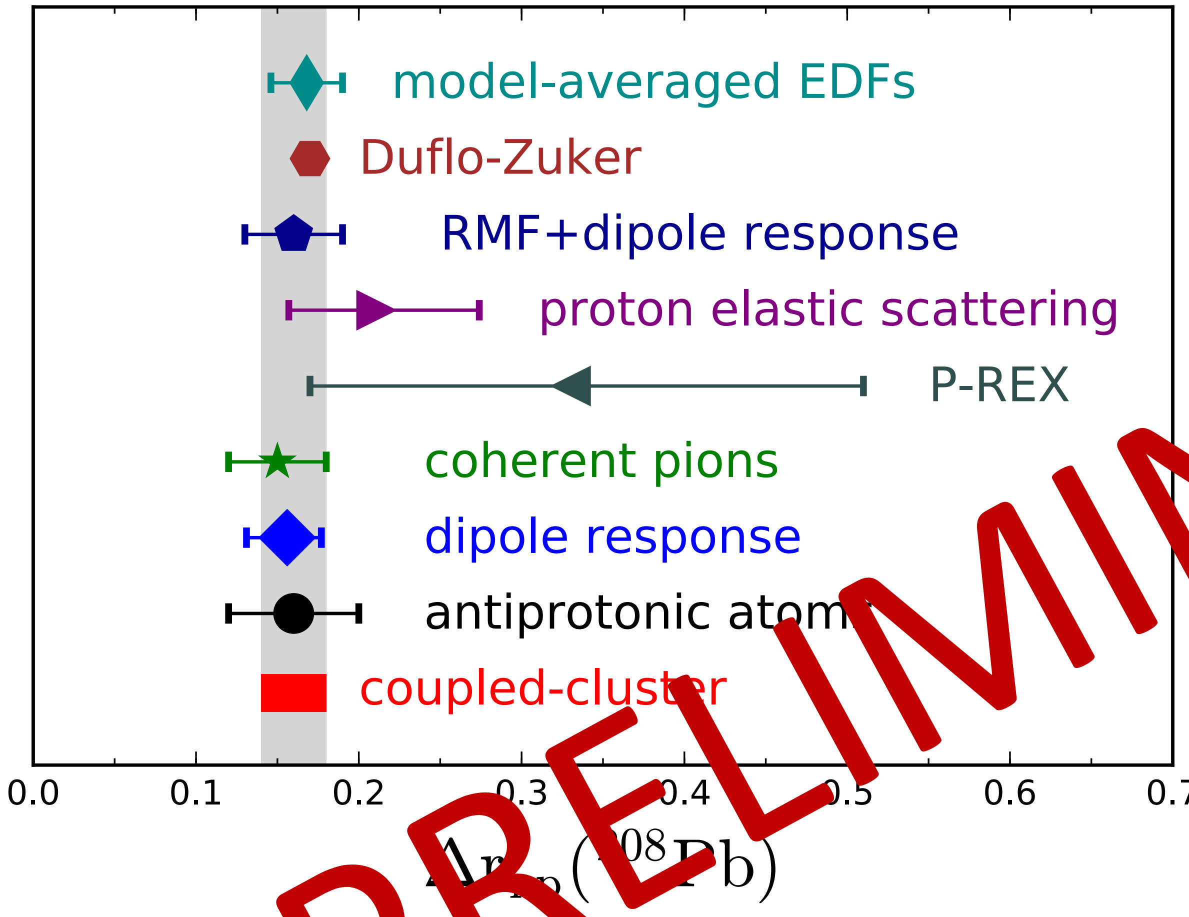
DFT:
SkM*, SkP, Sly4, SV-min, UNEDF0, and UNEDF1

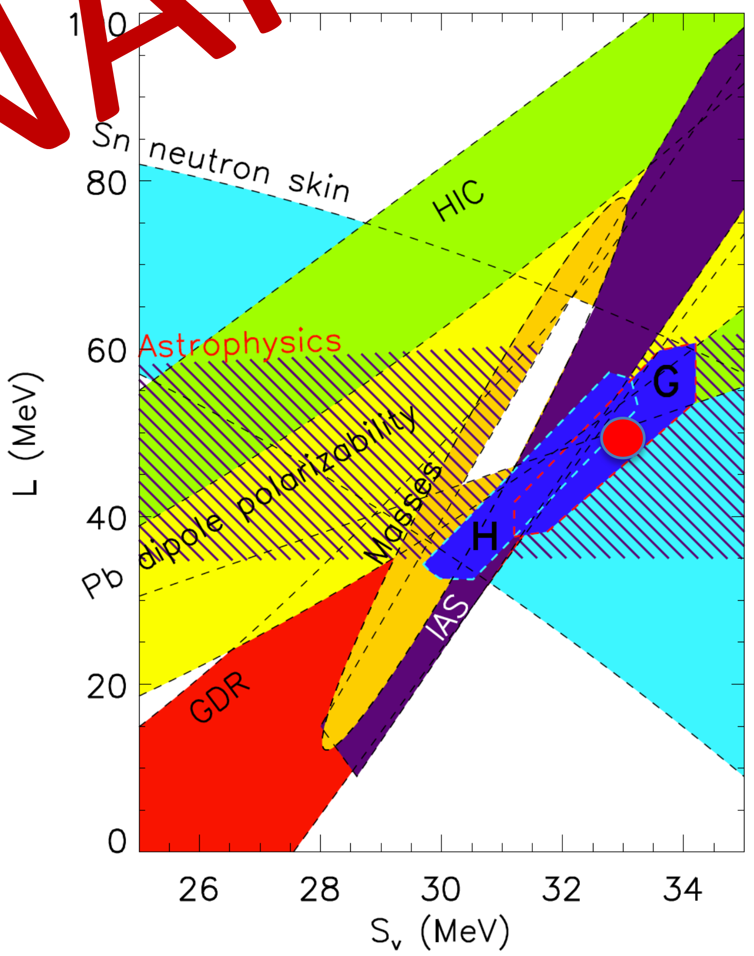
- Neutron skin significantly smaller than in DFT
- Neutron skin almost independent of the employed Hamiltonian
- Our predictions for ^{48}Ca are consistent with existing data



Neutron skin of ^{208}Pb

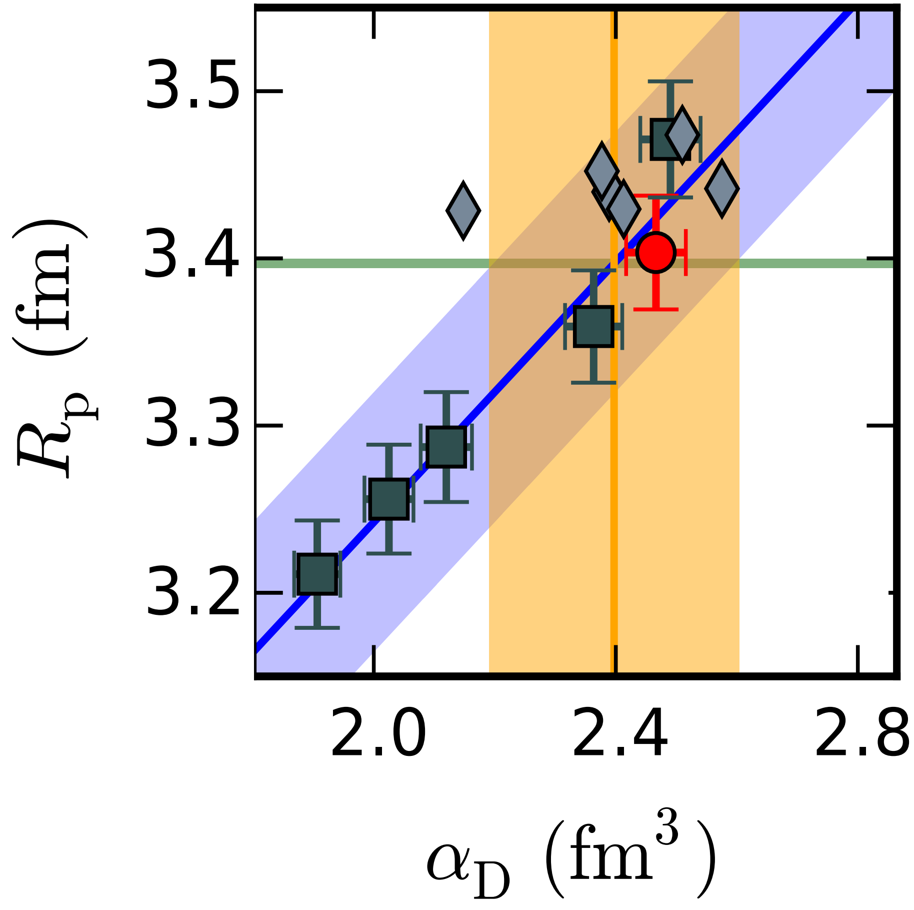
- Differences in radii converges more rapidly
- BE/A = 7.6(3)MeV in good agreement with data 7.87MeV





- Neutron skin consistent with experiments
- Symmetry energy (S) and its slope (L) consistent with existing data and theory

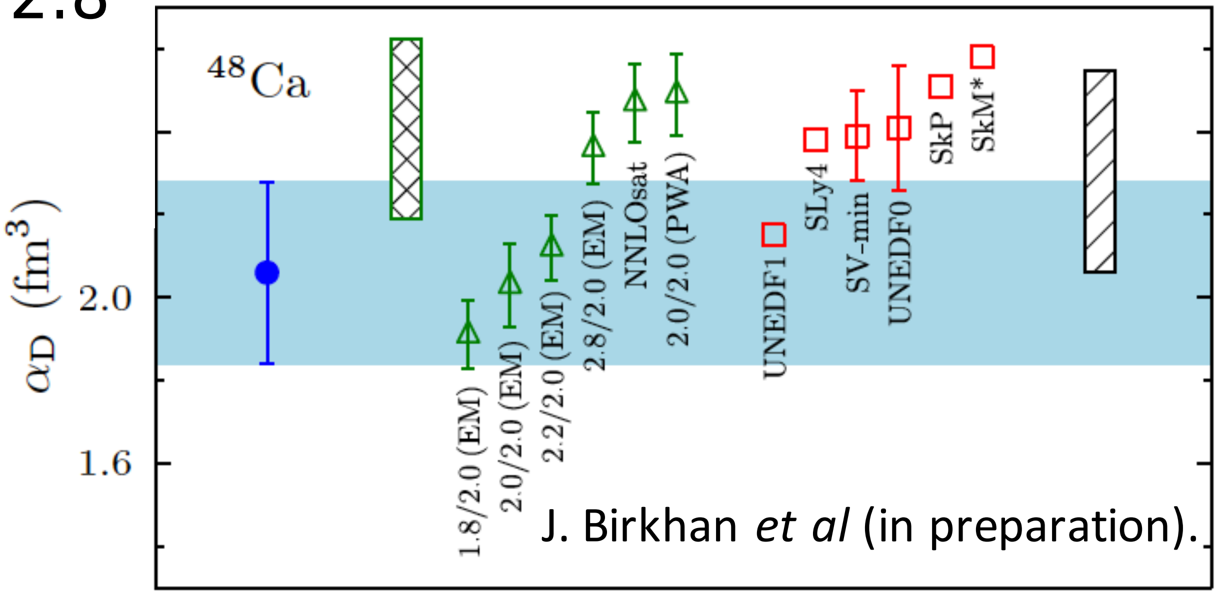
Dipole polarizability of ^{48}Ca



- DFT results are consistent and within band of ab-initio results
- Data has been analyzed by Osaka-Darmstadt collaboration
- Ab-initio prediction overlaps with experimental uncertainty

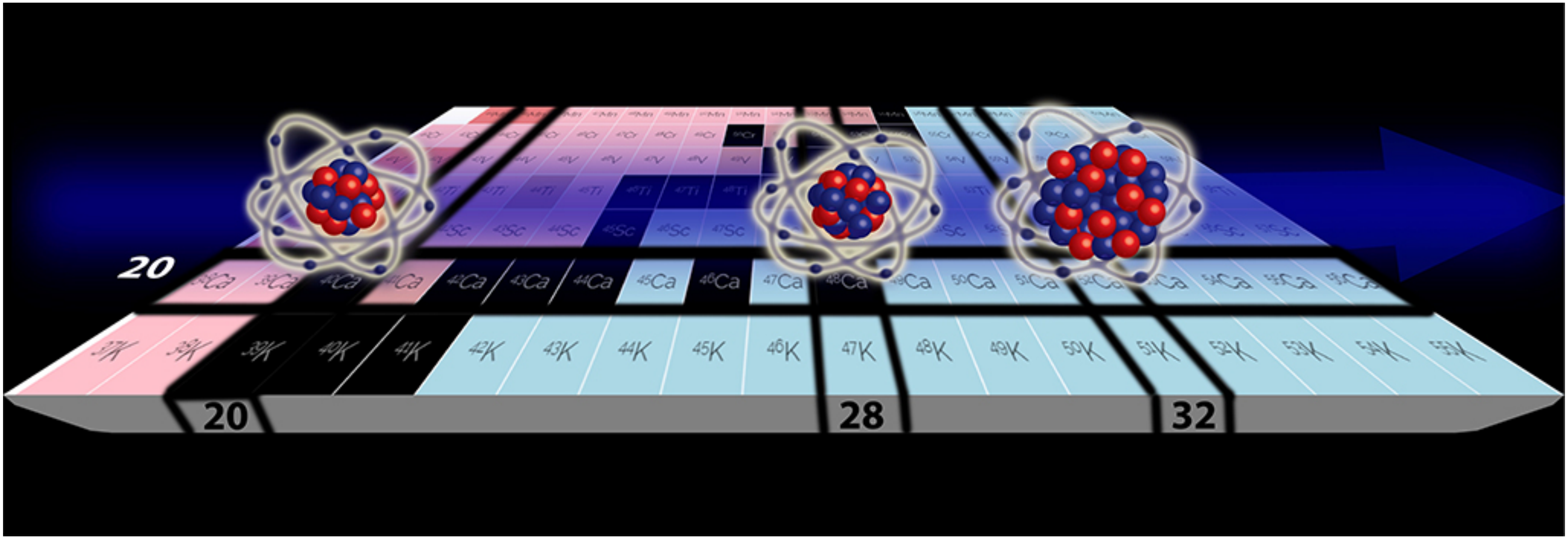
G. Hagen *et al*, Nature Physics **12**, 186–190 (2016)

Ab-initio prediction from correlation with R_p:
$2.19 \lesssim \alpha_\mathrm{D} \lesssim 2.60$ fm^3



J. Birkhan *et al* (in preparation).

Magicity of neutron-rich calcium isotopes

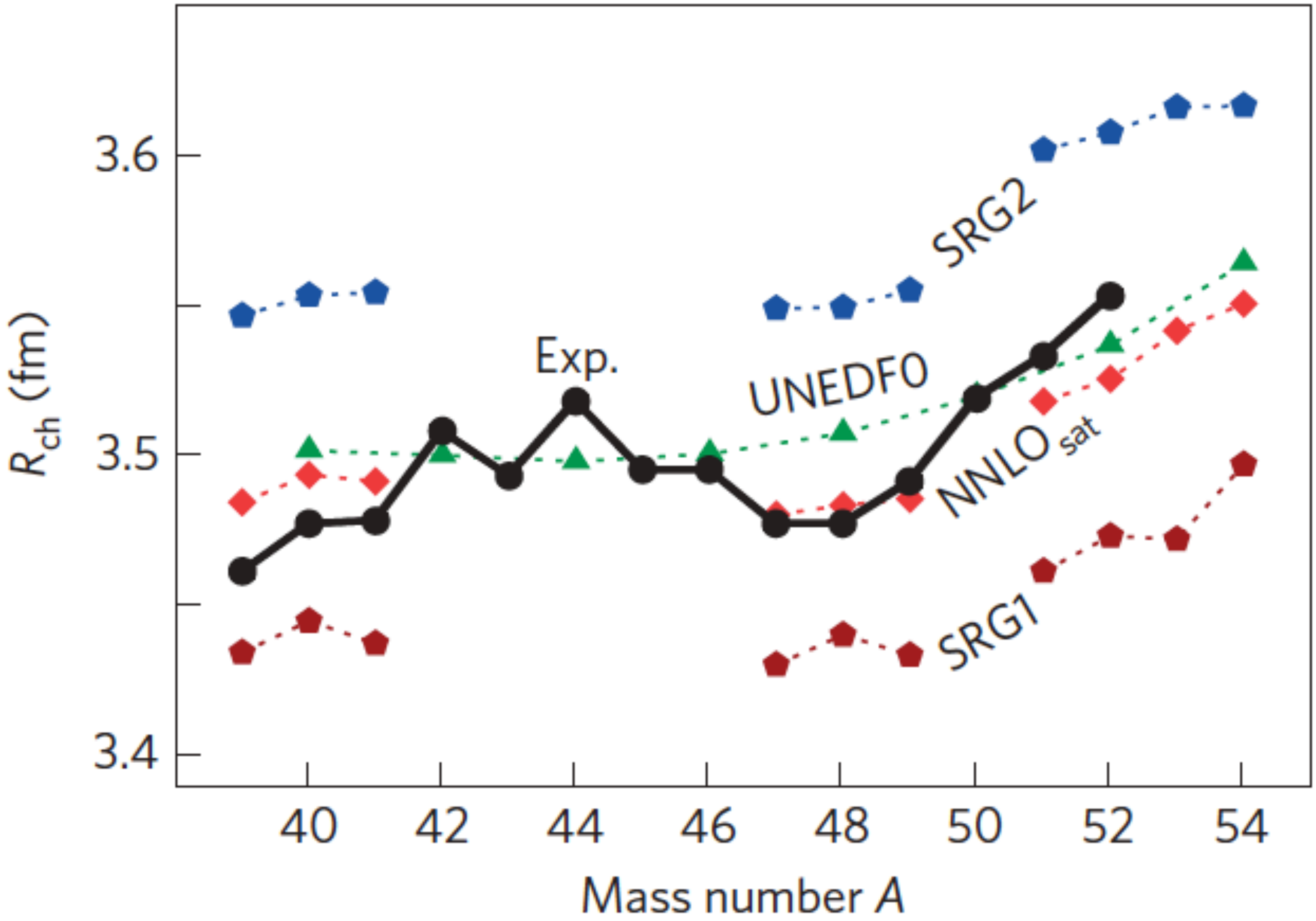


Magicity manifests itself through many observables:

- Separation energies
- Energy of 2^+ excited state
- Charge radii
- …

Figure: R. Garcia Ruiz and COLLAPS collaboration

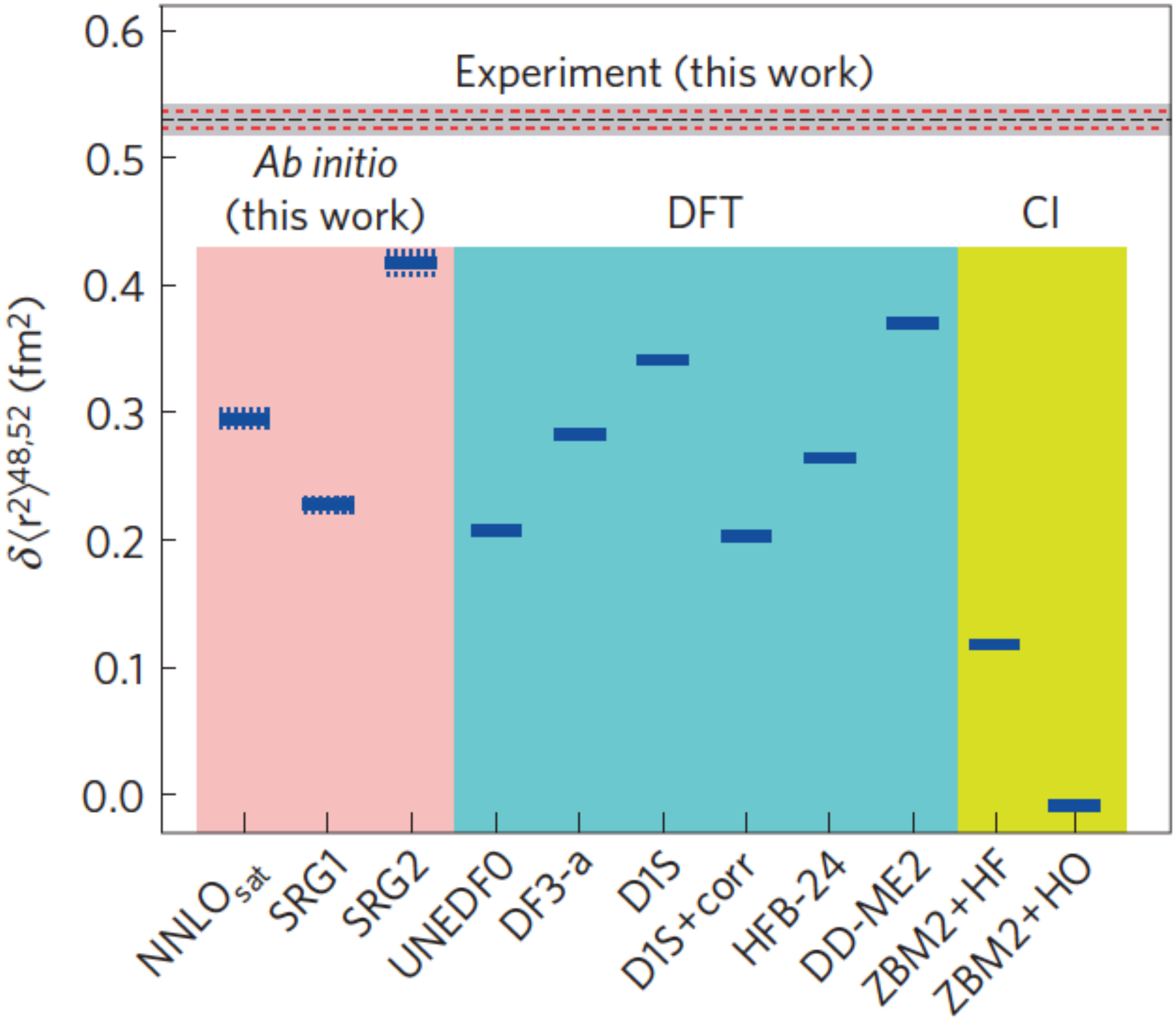
Charge radii of neutron-rich calcium isotopes



… question the magicity at N=32.

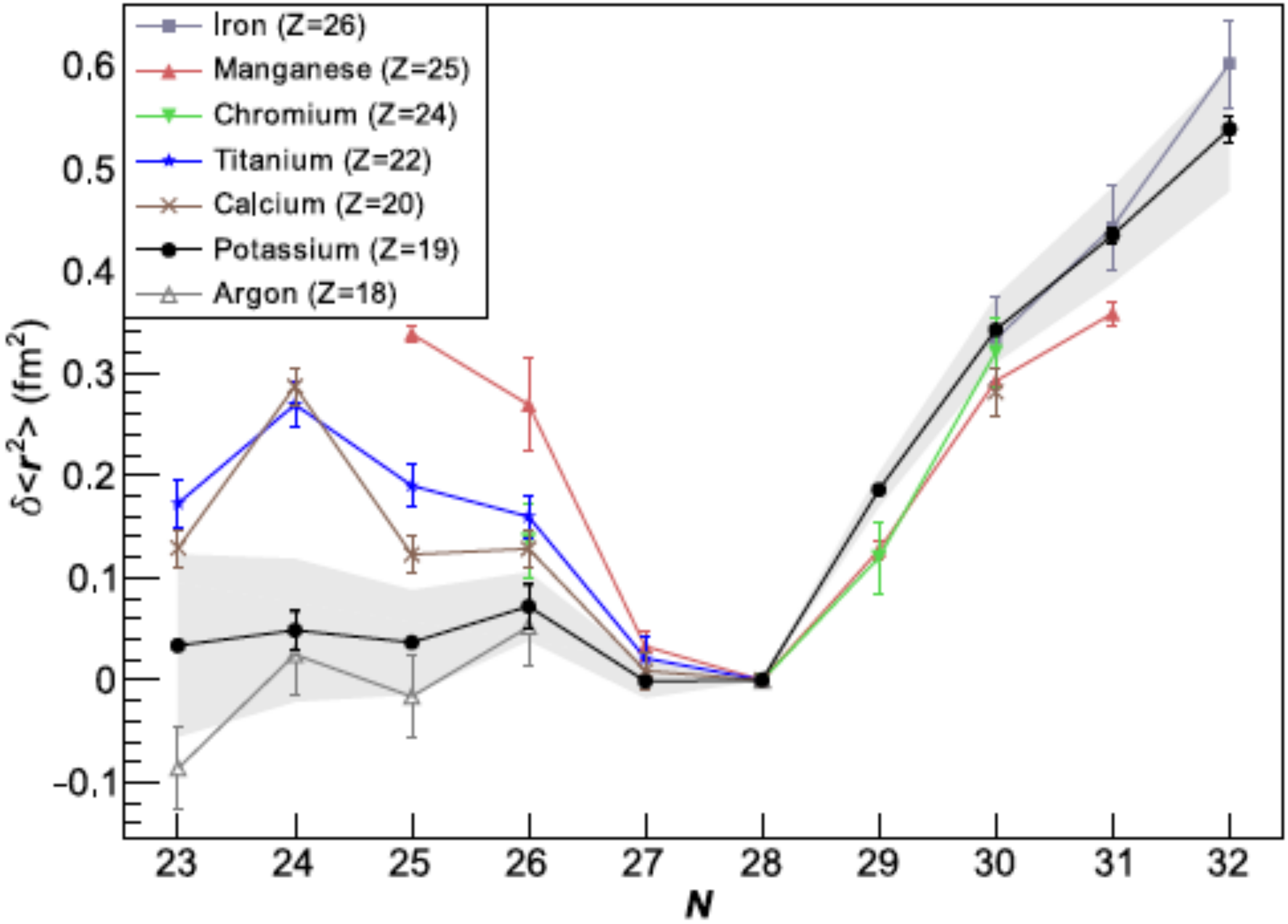
R. F. Garcia Ruiz *et al*, Nature Physics (2016) **12**, 594–598 (2016)

Theory challenge: Charge radius of ^{52}Ca



R. F. Garcia Ruiz *et al*, Nature Physics (2016) **12**, 594–598 (2016)

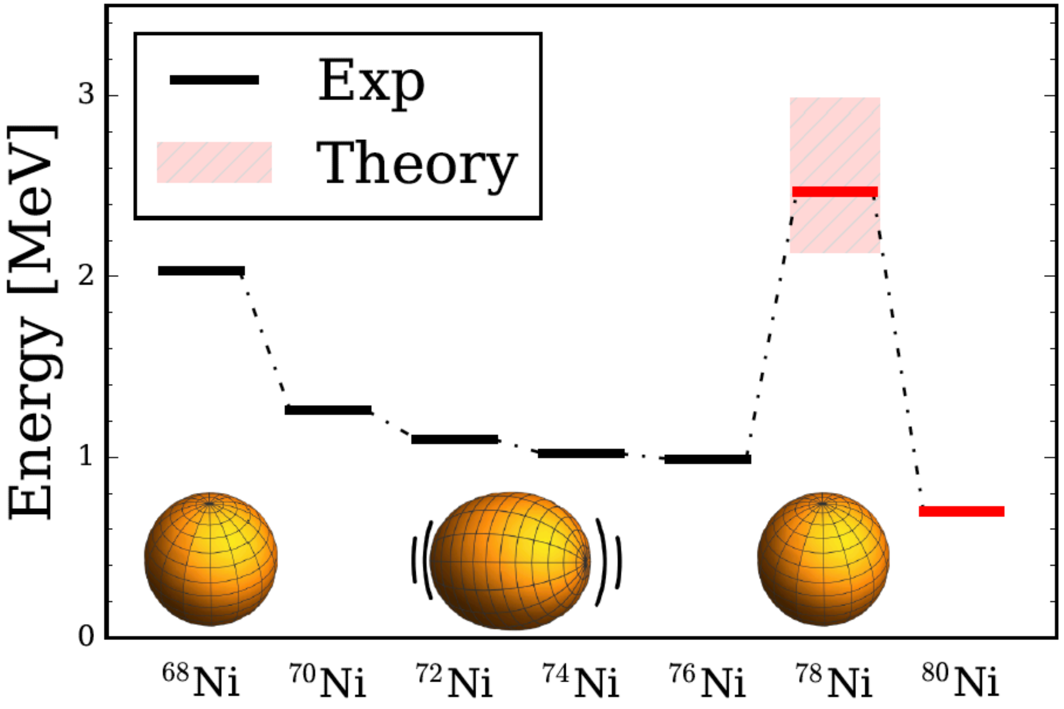
Isotope shifts around N=28



Ca isotopes similar to K isotopes
Beyond N=28

Kreim *et al.*, Phys. Lett. B (2014)

Structure of ^{78}Ni from first principles

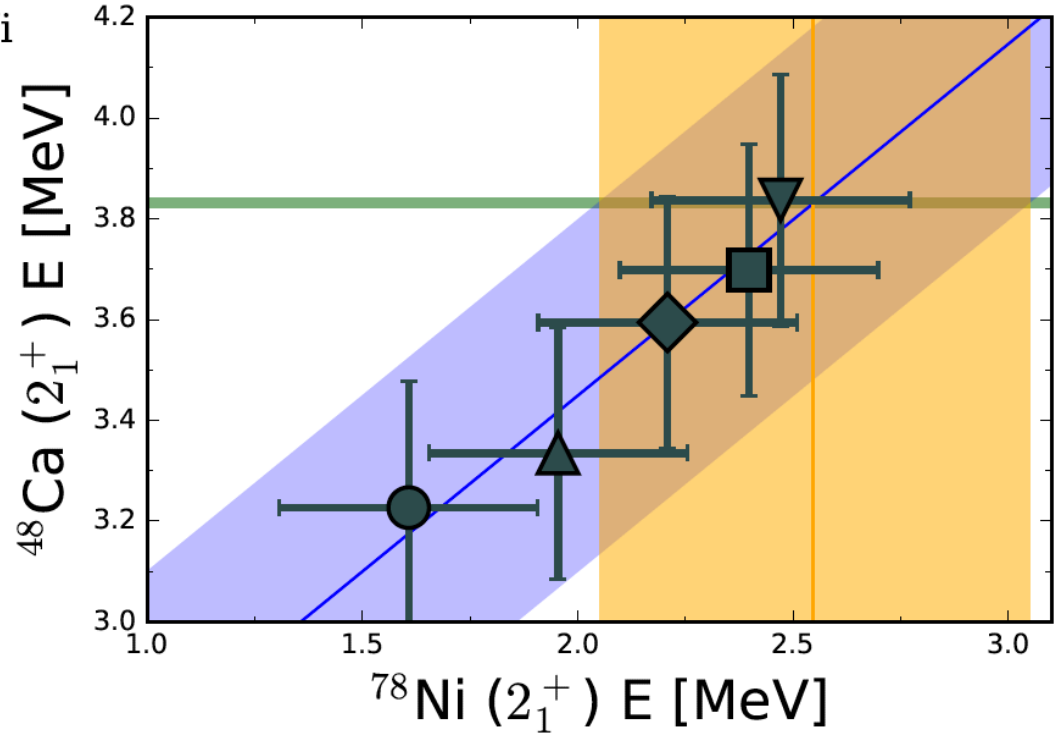


A high 2$^+$ energy in ^{78}Ni indicates that this nucleus is doubly magic

A measurement of this state has been made at RIBF, RIKEN
R. Taniuchi *et al.*, in preparation

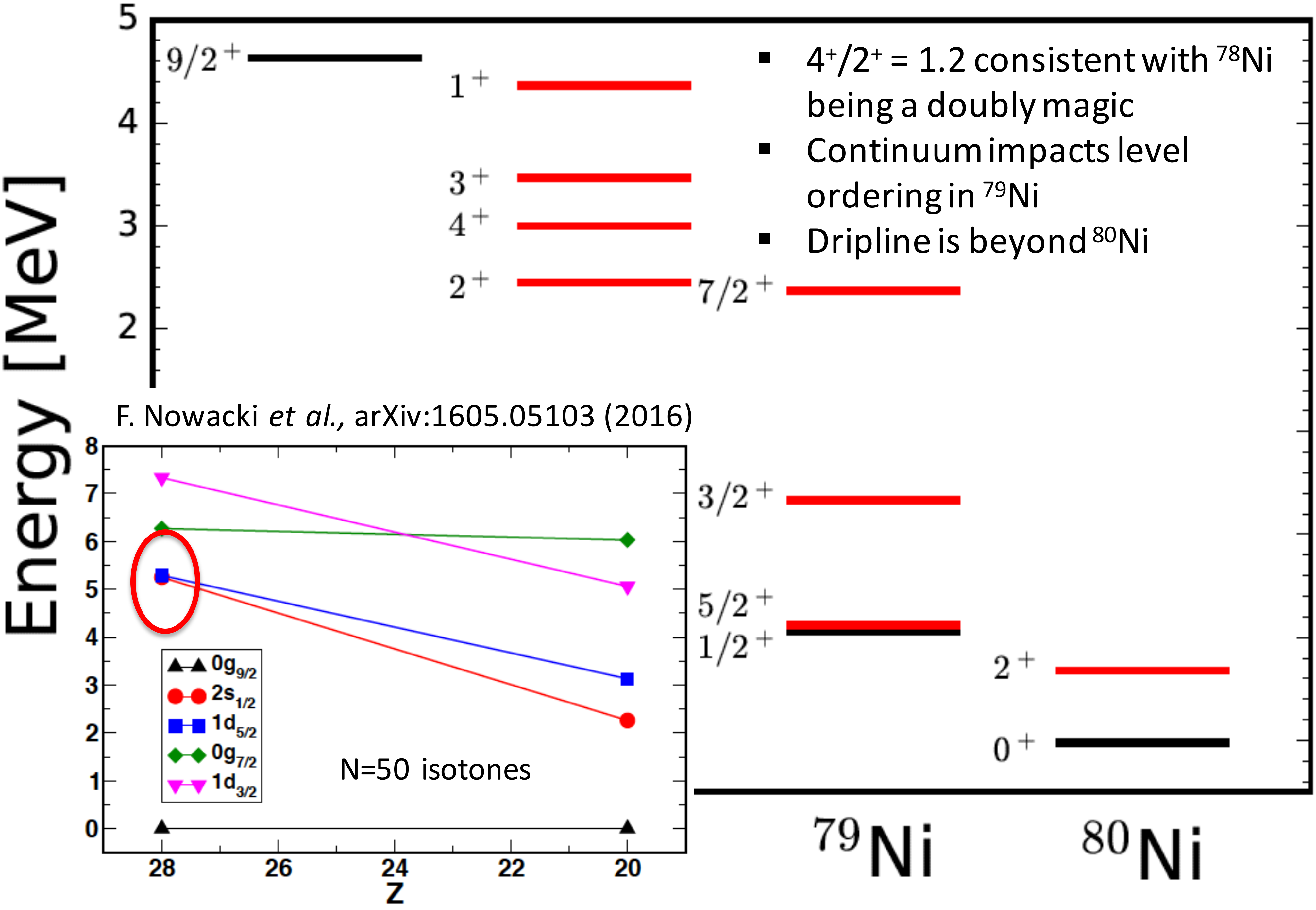
Consistent with recent shell-model studies
F. Nowacki *et al.*, arXiv:1605.05103 (2016)

- From an observed correlation we predict the 2$^+$ excited state in ^{78}Ni using the experimental data for the 2$^+$ state in ^{48}Ca
- Similar correlations have been observed in other nuclei, e.g. Tjon line in light nuclei



G. Hagen, G. R. Jansen, and T. Papenbrock
accepted for publication in PRL (2016)

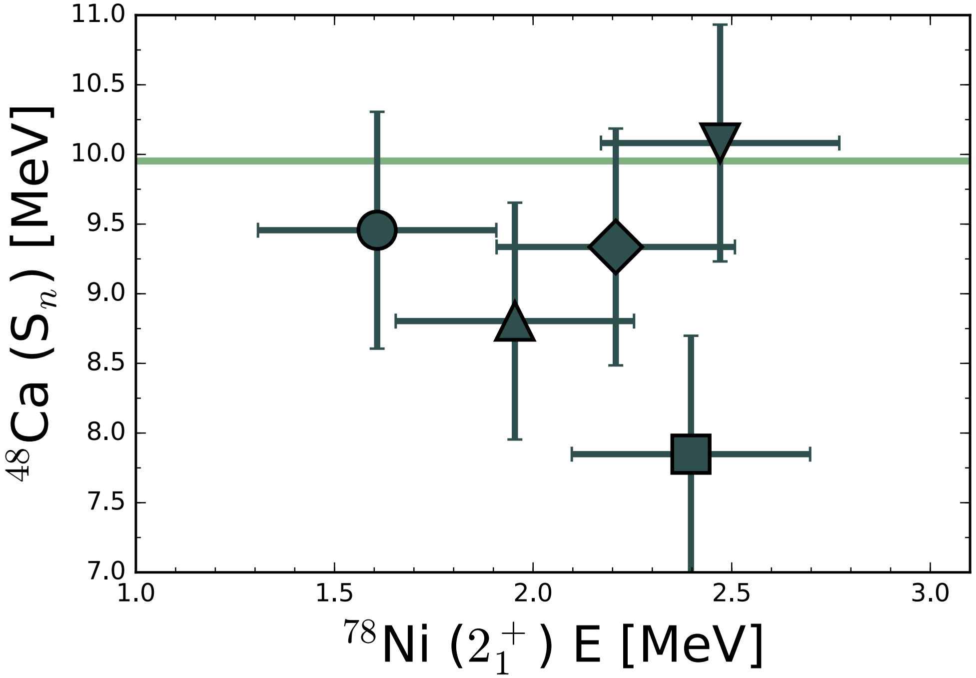
Excited states in ^{78}Ni and its neighbors



- $4^+/2^+ = 1.2$ consistent with ^{78}Ni being a doubly magic
- Continuum impacts level ordering in ^{79}Ni
- Dripline is beyond ^{80}Ni

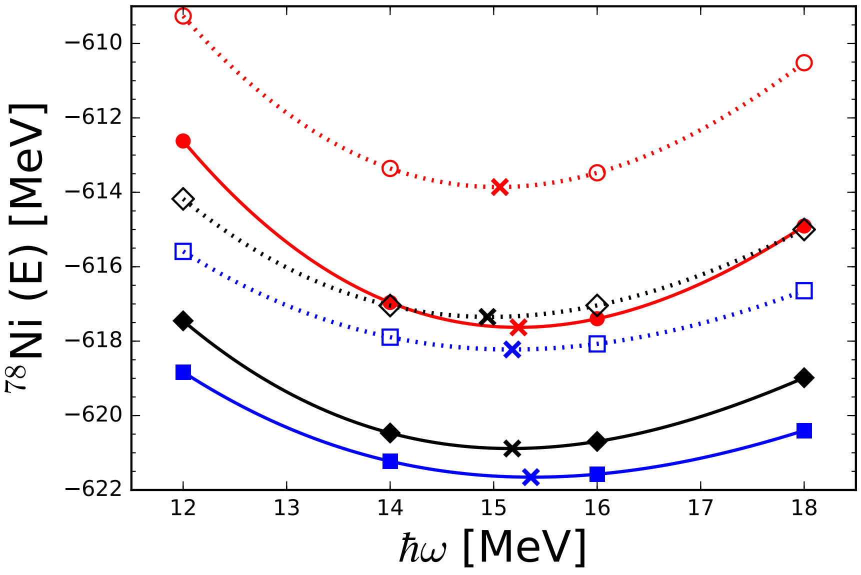
F. Nowacki *et al.*, arXiv:1605.05103 (2016)

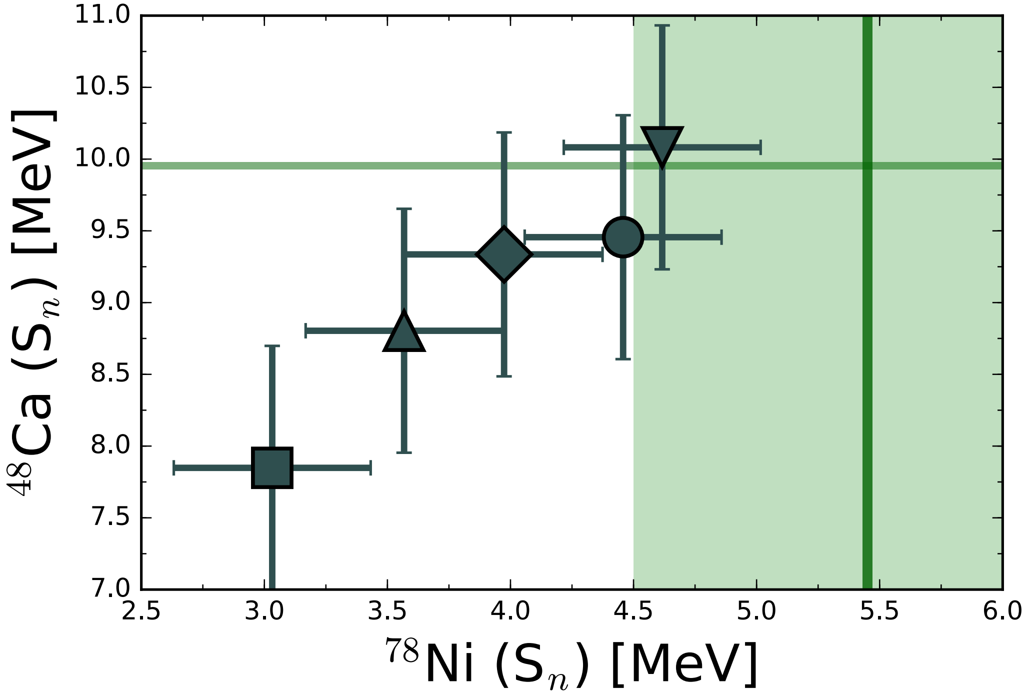
Other correlations in ^{48}Ca and ^{78}Ni



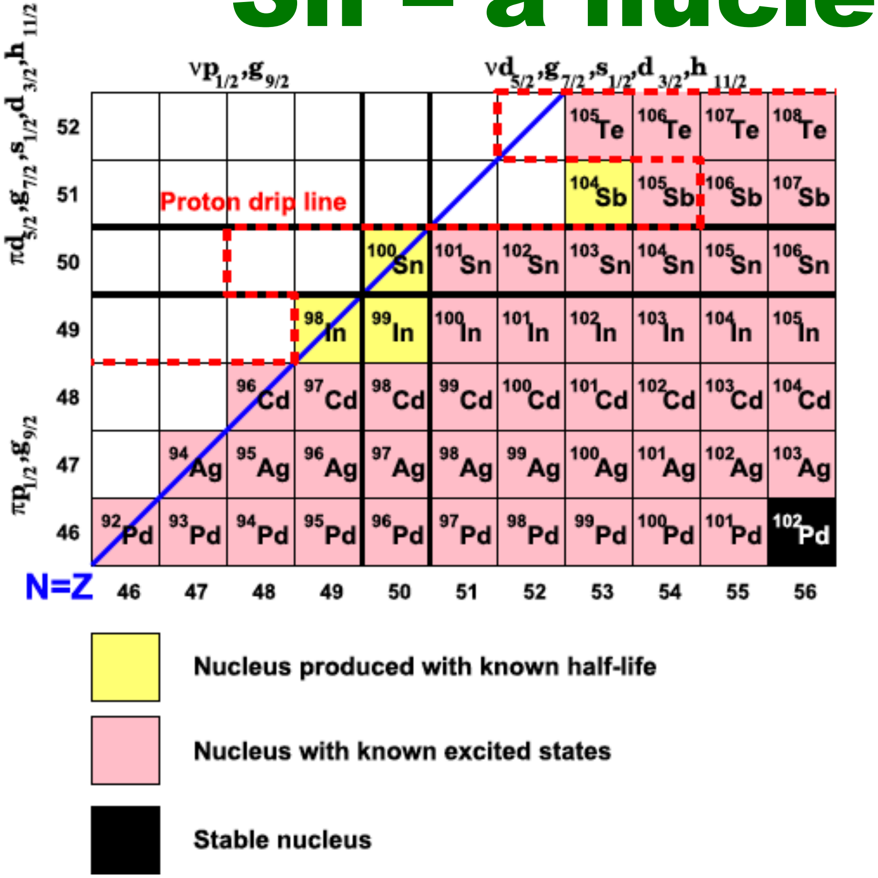
- Separation energy of ^{48}Ca and 2^+ energy of ^{78}Ni does not correlate
- Separation energies of ^{48}Ca and ^{78}Ni do correlate
- Non-trivial correlation between the 2^+ energy of ^{78}Ni and ^{48}Ca

Convergence of g.s. and 2^+

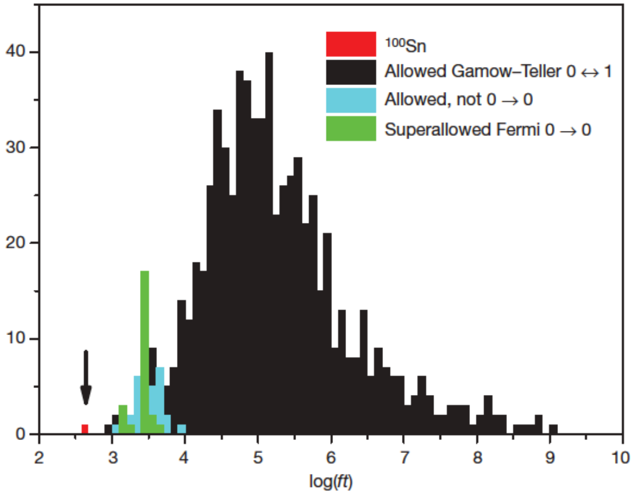




^{100}Sn – a nucleus of superlatives



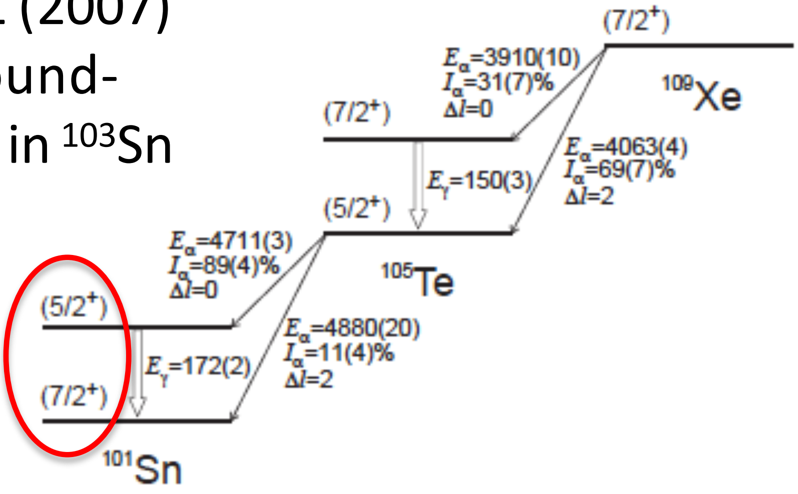
- Heaviest self-conjugate doubly magic nucleus
- Largest known strength in allowed nuclear β-decay
- In the closest proximity to the proton dripline
- At the endpoint of the rapid proton capture process (Sn-Sb-Te cycle)
- Unresolved controversy regarding s.p. structure of ^{101}Sn



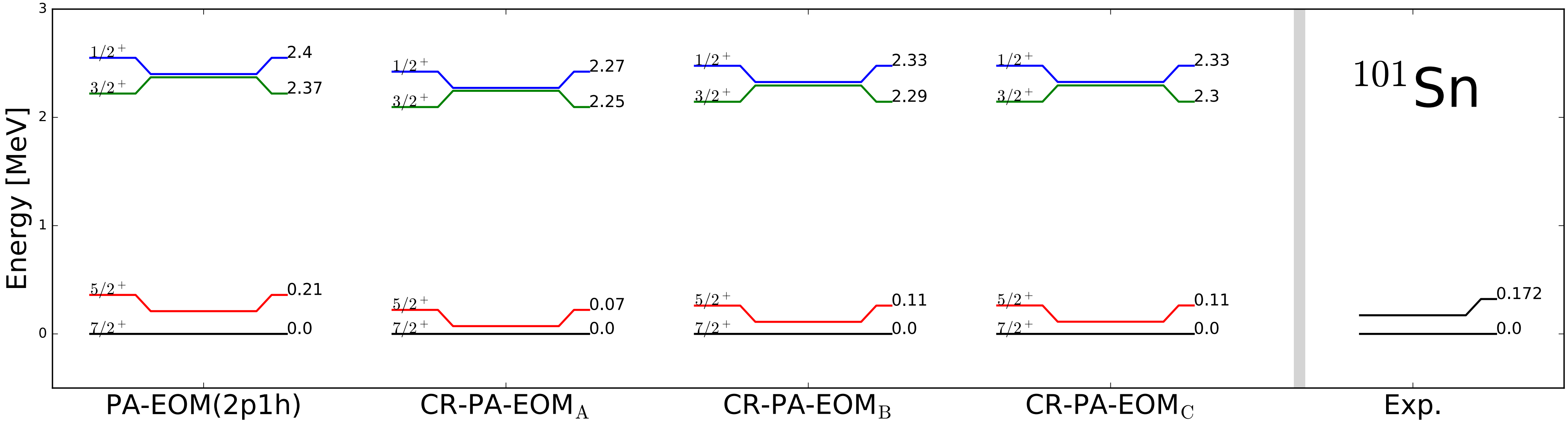
Hinke et al, Nature (2012)

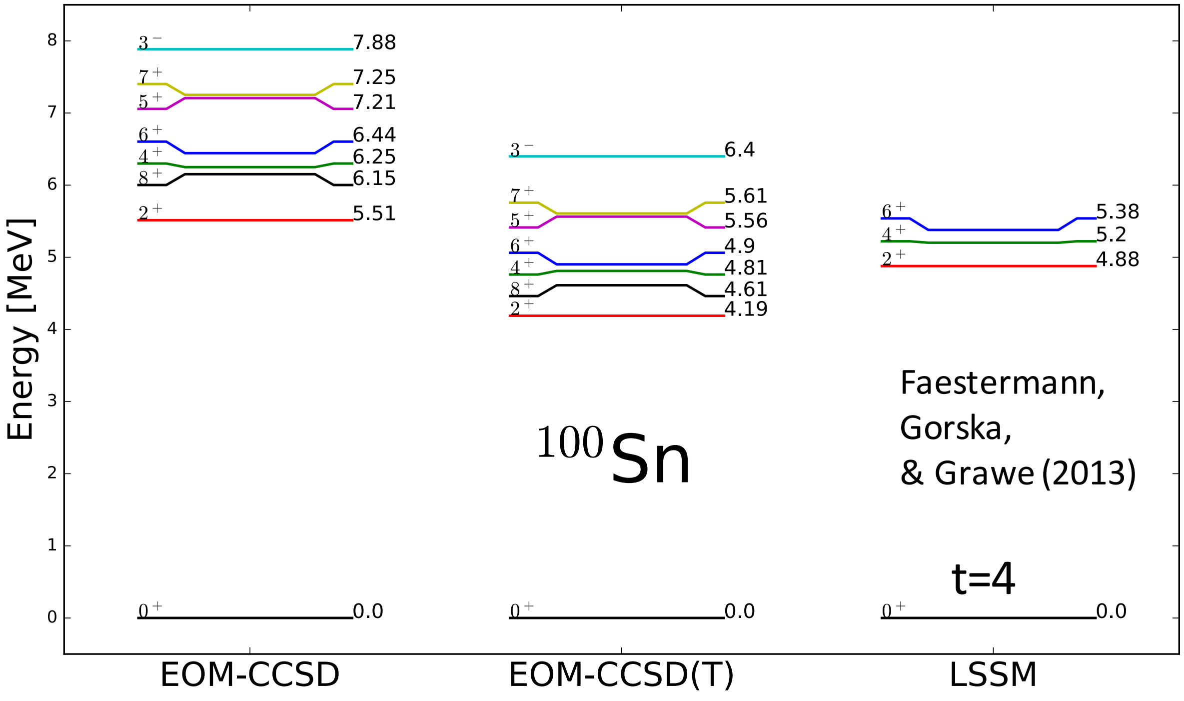
Sewernyiak et al PRL (2007) predicted a 5/2+ ground-state as presumably in ^{103}Sn

Darby et al, PRL (2010)



Structure of the ligthest tin isotopes

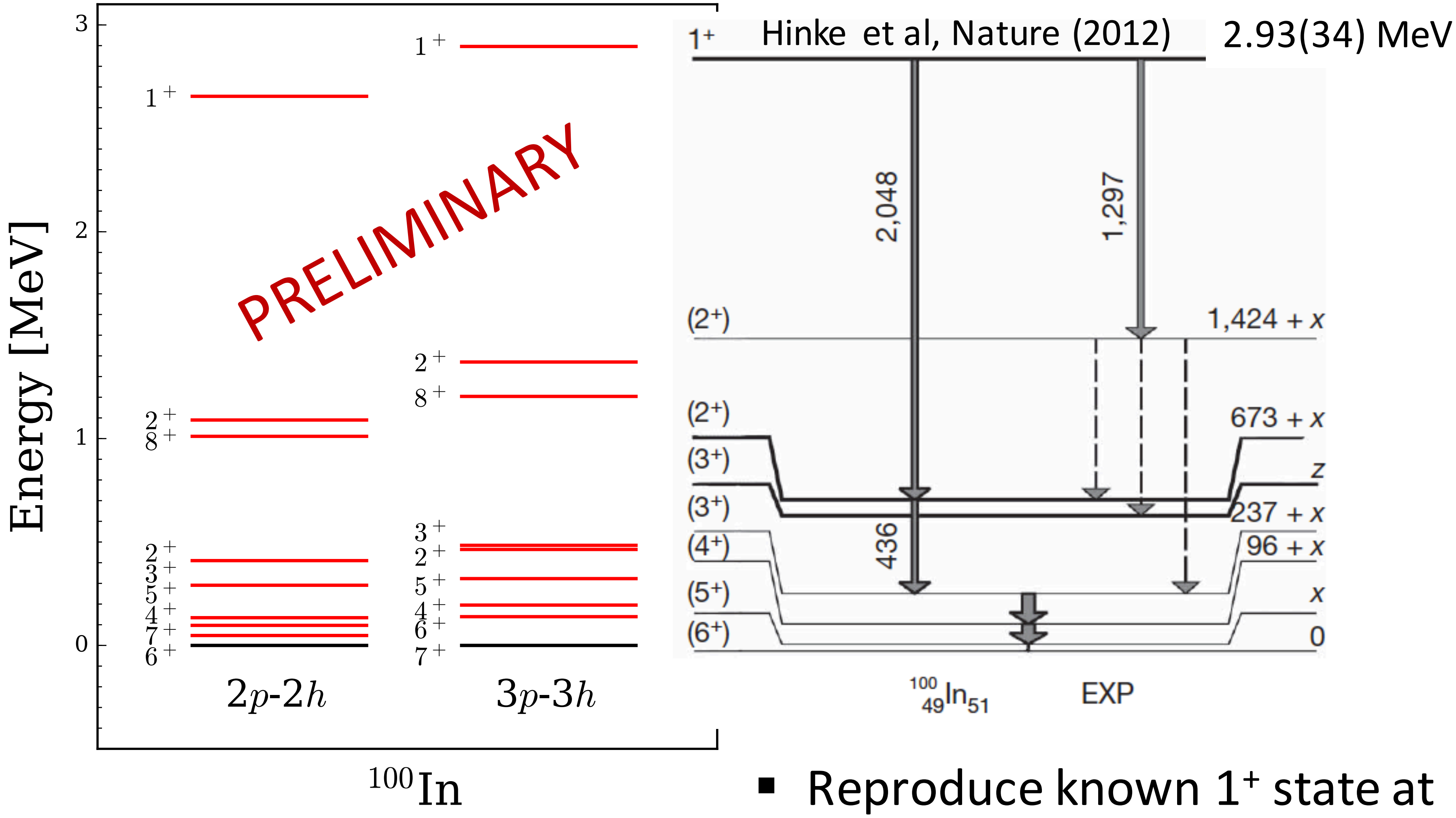




- High 2^+ energy in ^{100}Sn indicates it is doubly magic
- Theory predict the ground-state of ^{101}Sn to be $7/2^+$
- Experimental splitting between $7/2^+$ and $5/2^+$ reproduced

PRELIMINARY

^{100}In from a novel charge exchange coupled-cluster equation-of-motion method



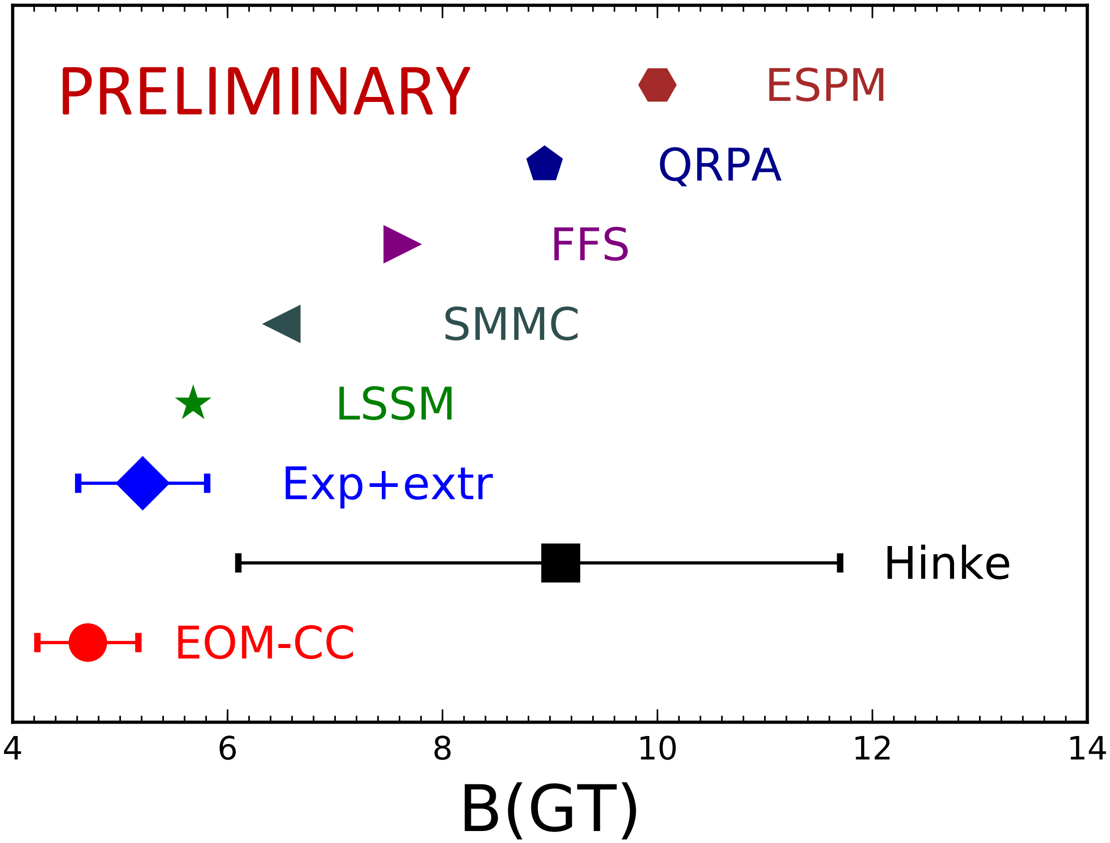
New method: 3p-3h charge-exchange EOM

$$\overline{H}_N R_\mu |\Phi_0\rangle = E_\mu R_\mu |\Phi_0\rangle$$

- Reproduce known 1^+ state at 2.93(34) MeV
- Predict a 7^+ ground-state for ^{100}In
- Spectra could be more complex than observed so far

Superallowed Gamow-Teller transition

- Prediction for the Gamow-Teller transition consistent with data
- Towards understanding the quenching of g_A
- Important implications for computations of $0\nu\beta\beta$ decay

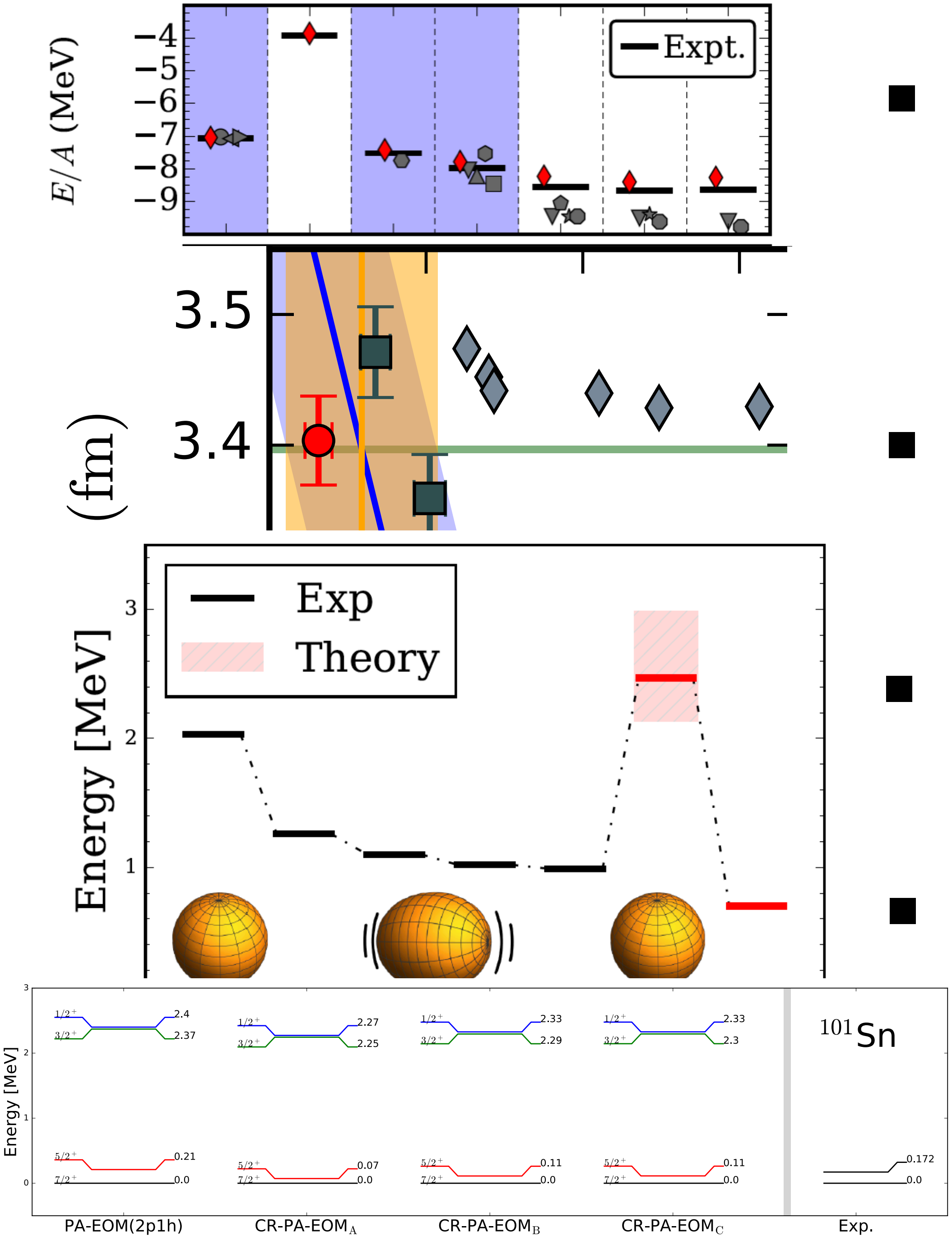


Hinke et al, Nature (2012)

Model	Ref	unquenched	quenched
ESPM	[30]	17.78	10.00
MCSM	[8]	10.3	6.5
QRPA	[9]	8.95	
FFS	[9]	7.63	
extrapol.	[10]	9.8	5.2
SM+corr.	[7]	14.2	
LSSM	this work	~ 13.90	~ 7.82
LSSM (only 1^+_1)	this work	10.10	5.68

- First principles coupled-cluster computations predict a B(GT) of **4.7(5)**
- B(GT) is currently targeted by upcoming precision measurements

Summary



- Chiral interaction with accurate saturation properties
- Predictions for the neutron skin of ^{48}Ca
- ^{78}Ni is predicted to be doubly magic
- Resolution to controversy of ground-state spin of ^{101}Sn