

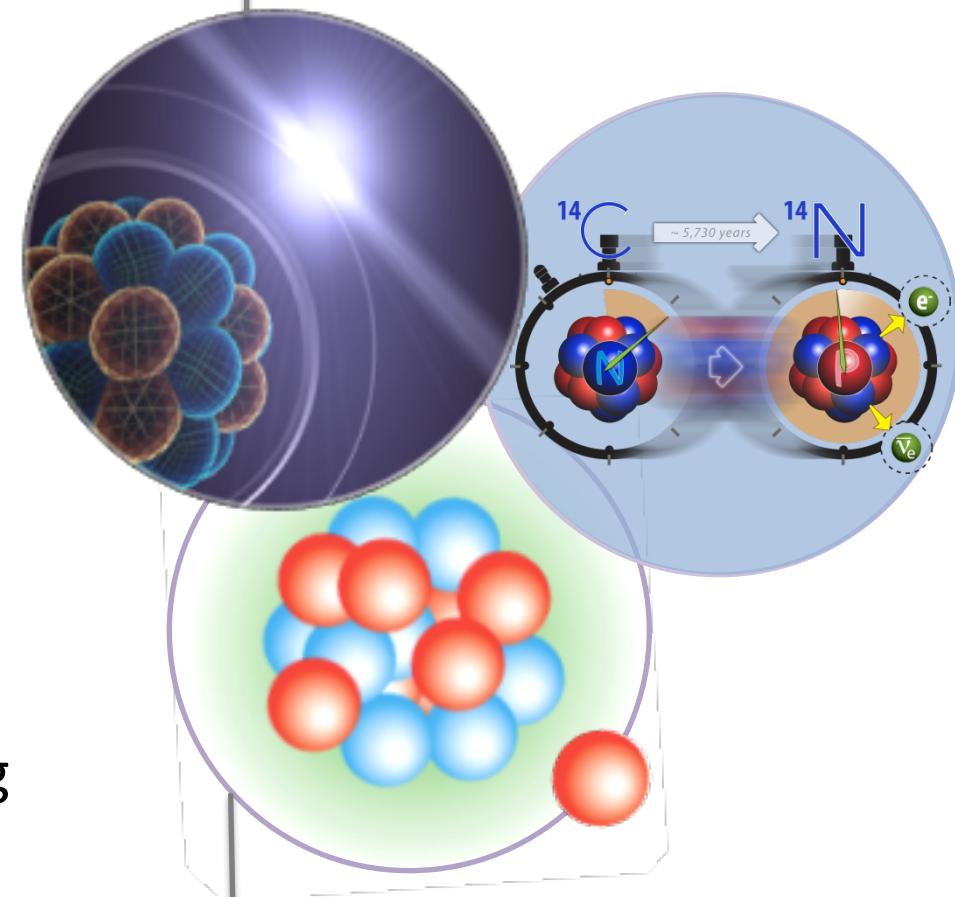
# Current topics in nuclear structure theory:

## Coupled-cluster computations of nuclei

Gaute Hagen  
Oak Ridge National Laboratory

54th International Winter Meeting  
on Nuclear Physics

Bormio, Italy, January 27<sup>th</sup>, 2016



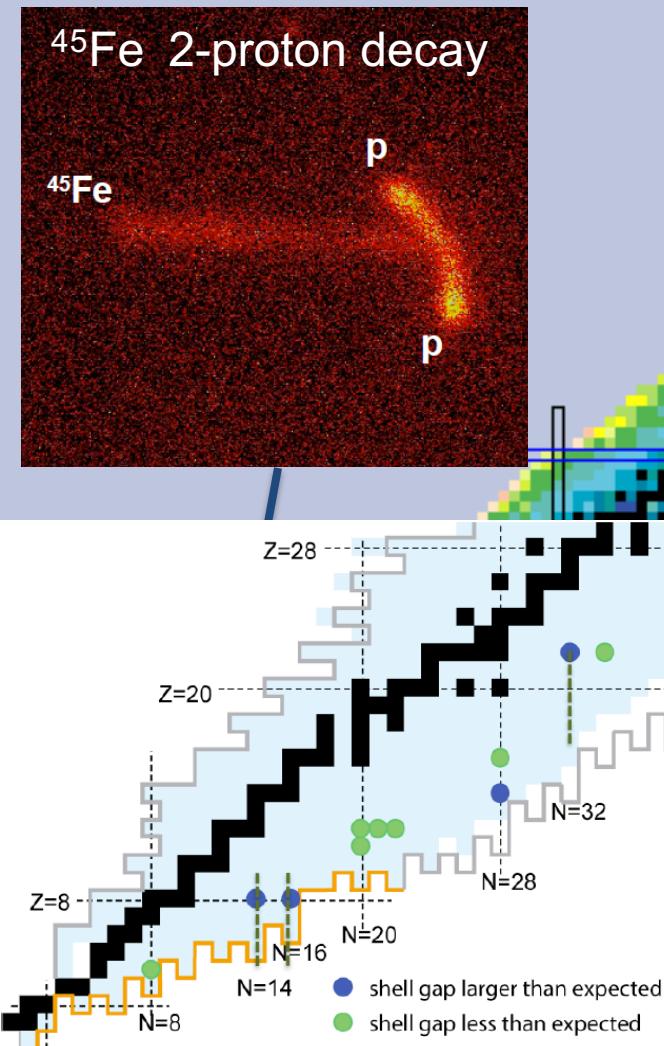
# Outline

- Status of ab-initio computations of nuclei
- Accurate radii and binding energies from a chiral interaction
- The neutron radius and dipole polarizability of  $^{48}\text{Ca}$
- Coupled-cluster effective interactions with application to *sd*-shell nuclei
- Role of two-body currents and three-nucleon forces on quenching of Gamow-Teller strengths  $^{14}\text{C}$ ,  $^{22,24}\text{O}$

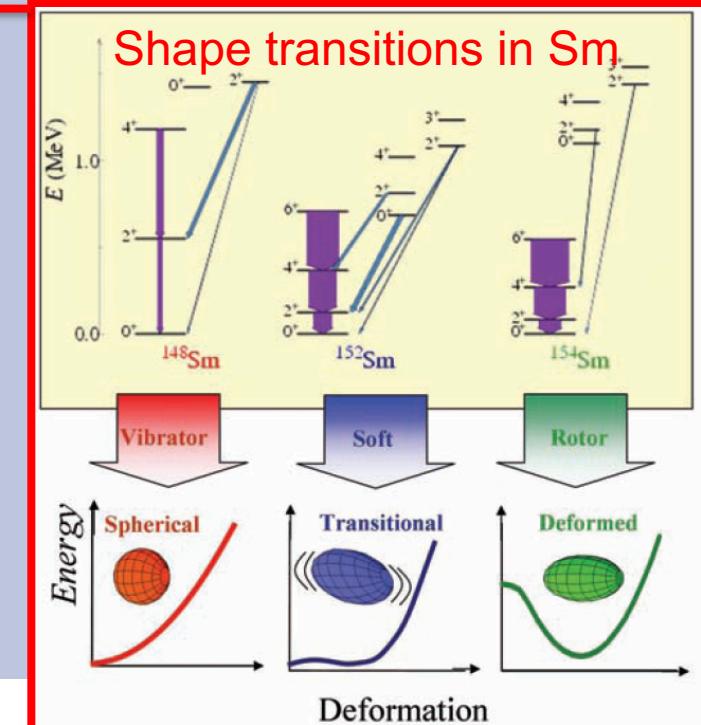
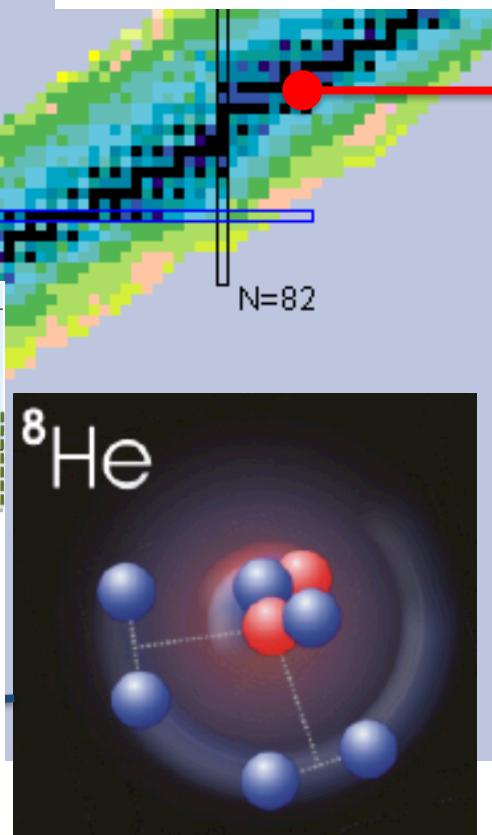
# Nuclei across the chart

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
- Challenge for ab-initio theory



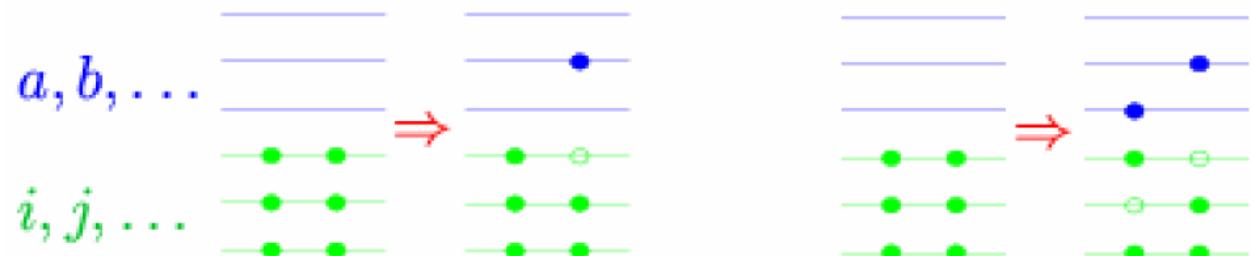
# Coupled-cluster method (CCSD approximation)

Ansatz:

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

- ☺ Scales gently (polynomial) with increasing problem size  $\mathcal{O}^2 u^4$ .
- ☺ 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!



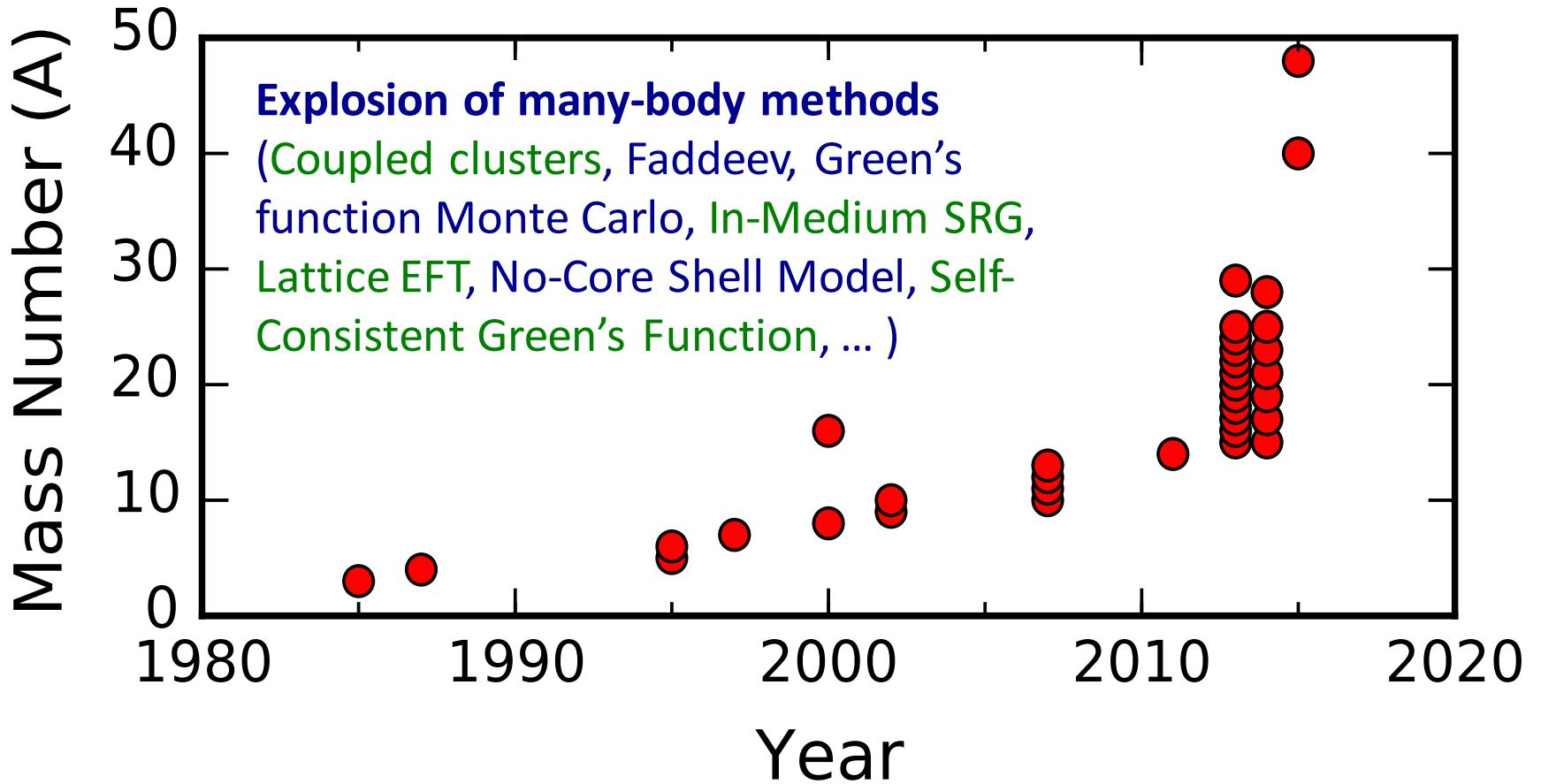
Coupled cluster equations

$$\begin{aligned} E &= \langle \Phi | \bar{H} | \Phi \rangle \\ 0 &= \langle \Phi_i^a | \bar{H} | \Phi \rangle \\ 0 &= \langle \Phi_{ij}^{ab} | \bar{H} | \Phi \rangle \end{aligned}$$

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

$$\bar{H} \equiv e^{-T} H e^T = (H e^T)_c = \left( H + H T_1 + H T_2 + \frac{1}{2} H T_1^2 + \dots \right)_c$$

# Ab-initio calculations of nuclei

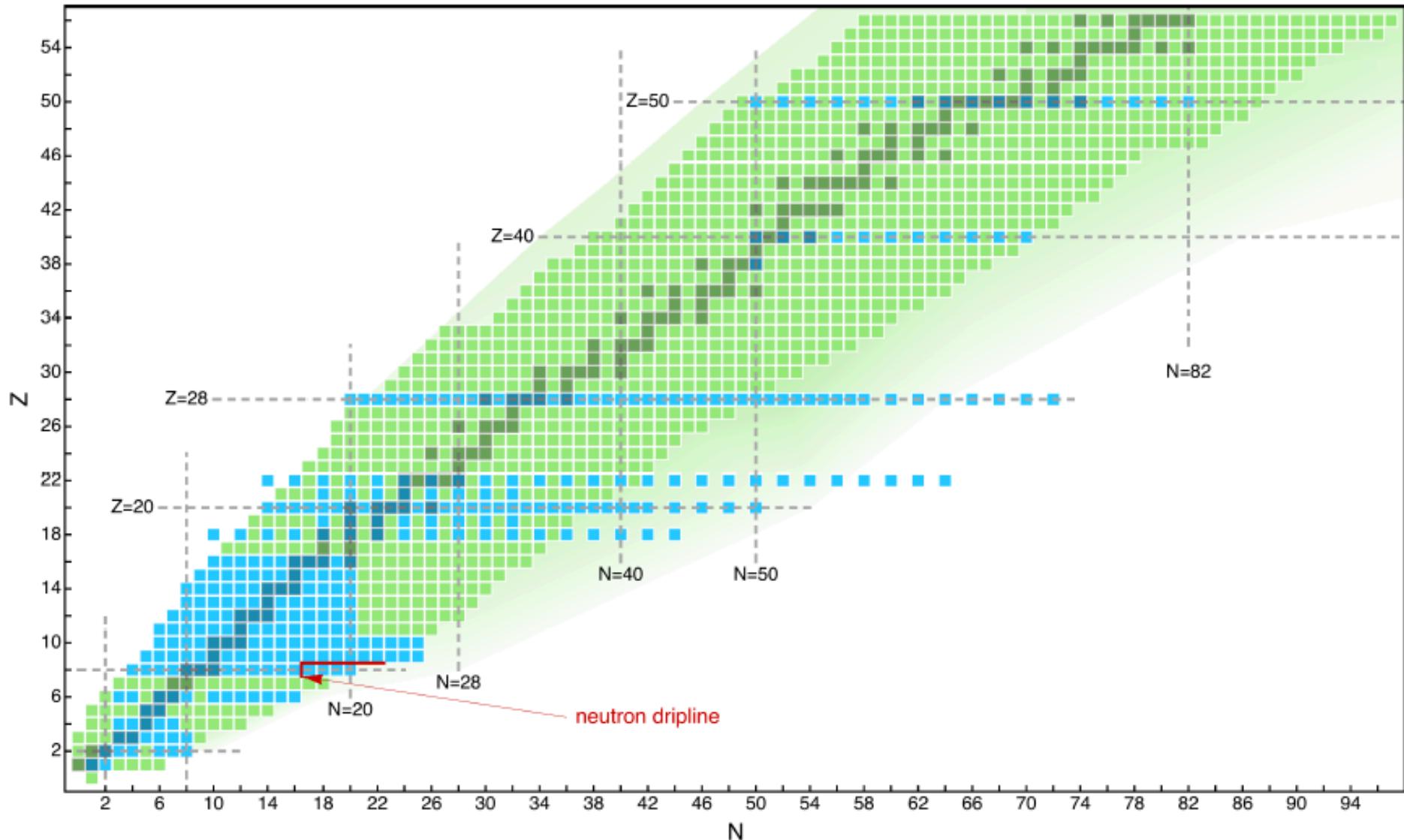


Algorithms with  
Exponential scaling in  $A$

Computing power increases  
exponentially (Moore's law)

Algorithms with  
polynomial scaling in  $A$

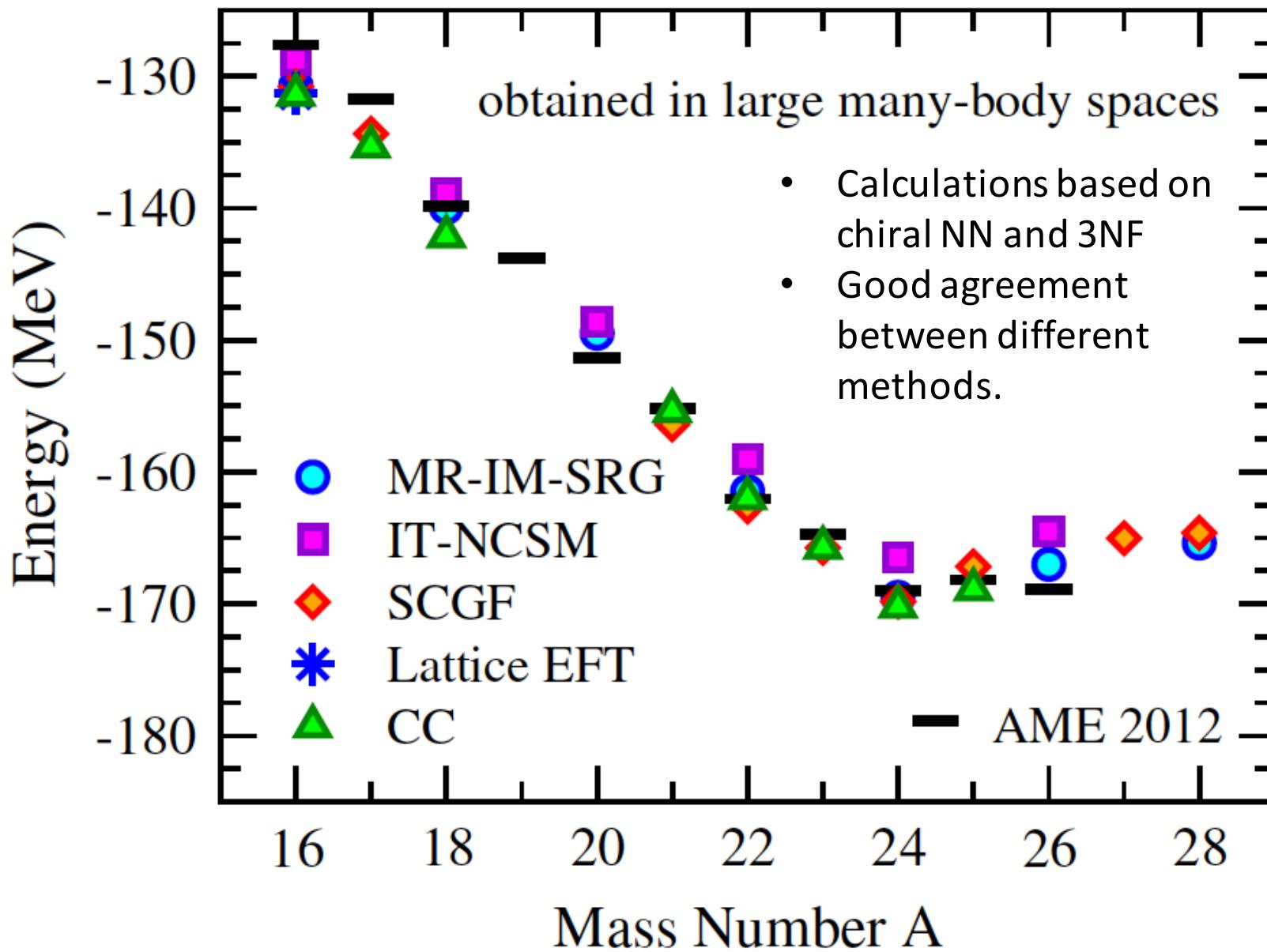
# Reach of ab-initio calculations of nuclei



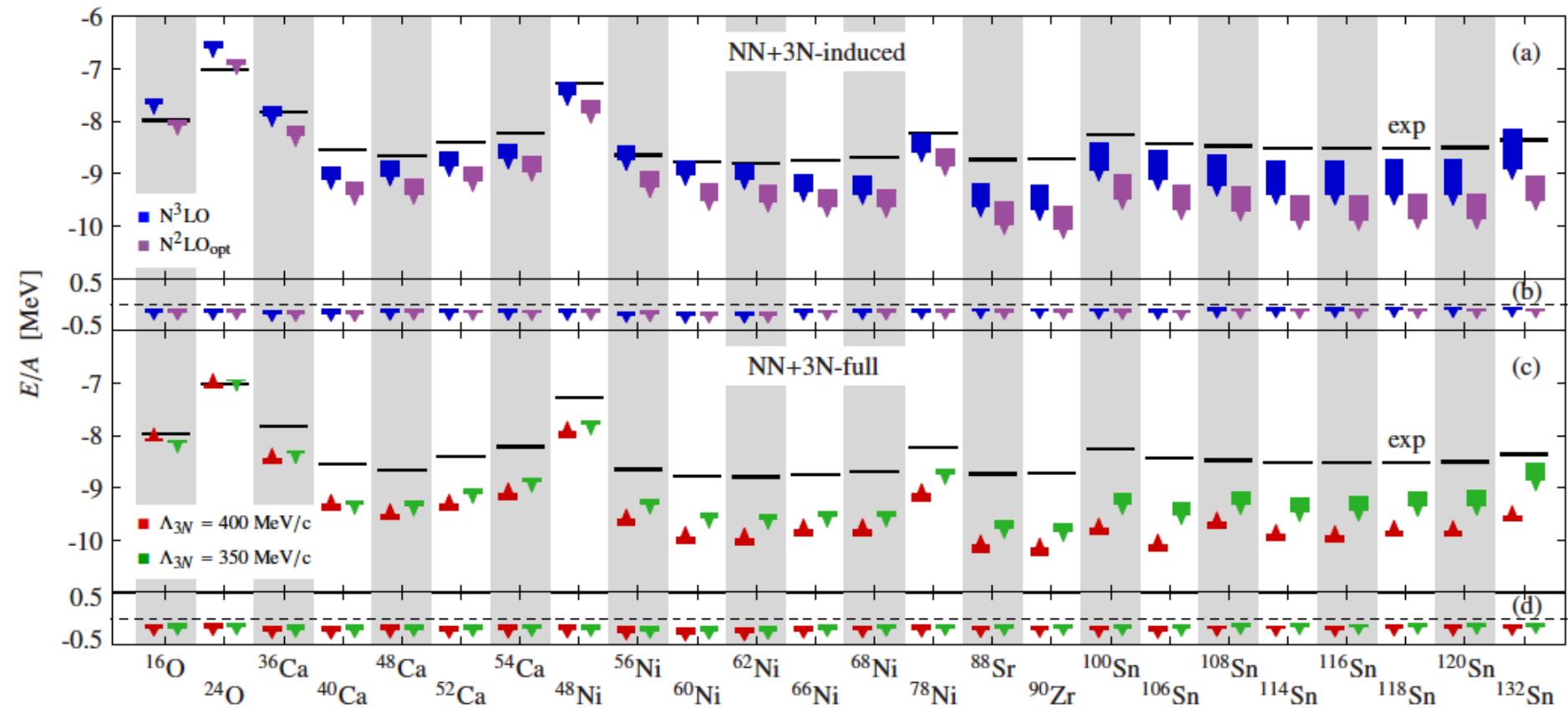
Nuclei for which ab-initio computations have been attempted.

H. Hergert *et al*, arXiv:1512.06956 (2015)

# Oxygen chain with interactions from chiral EFT



# Ab-initio computations towards heavy nuclei



S. Binder et al, Physics Letters B 736 119, (2014)

- Overbinding of 1-2 MeV/A for increasing mass  $A$
- The challenge is now with the interactions

# Effective theories for nuclei

Physics of Hadrons

Degrees of Freedom



quarks, gluons

Energy (MeV)



constituent quarks

940  
neutron mass

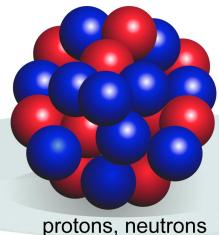
140  
pion mass

ab initio



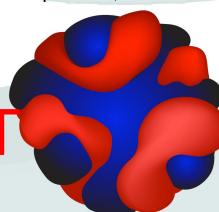
baryons, mesons

CI



protons, neutrons

DFT



nucleonic densities  
and currents

collective  
models

collective coordinates

Energy or Resolution



Effective theories provide us with model independent approaches to atomic nuclei

Key: Separation of scales

Ab-initio low-energy nuclear physics deals with nucleons and pions as dynamical degrees of freedom

# Nuclear forces from chiral effective field theory

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

	NN	3N	4N
LO $\mathcal{O}\left(\frac{Q^0}{\Lambda^0}\right)$			—
NLO $\mathcal{O}\left(\frac{Q^2}{\Lambda^2}\right)$		—	—
N <sup>2</sup> LO $\mathcal{O}\left(\frac{Q^3}{\Lambda^3}\right)$		—	—
N <sup>3</sup> LO $\mathcal{O}\left(\frac{Q^4}{\Lambda^4}\right)$		+ ...	+ ...

- developing higher orders and higher rank (3NF, 4NF) [Epelbaum 2006; Bernard et al 2007; Krebs et al 2012; Hebeler et al 2015; ...]

- implemented in continuum and on lattice [Borasoy et al 2007]

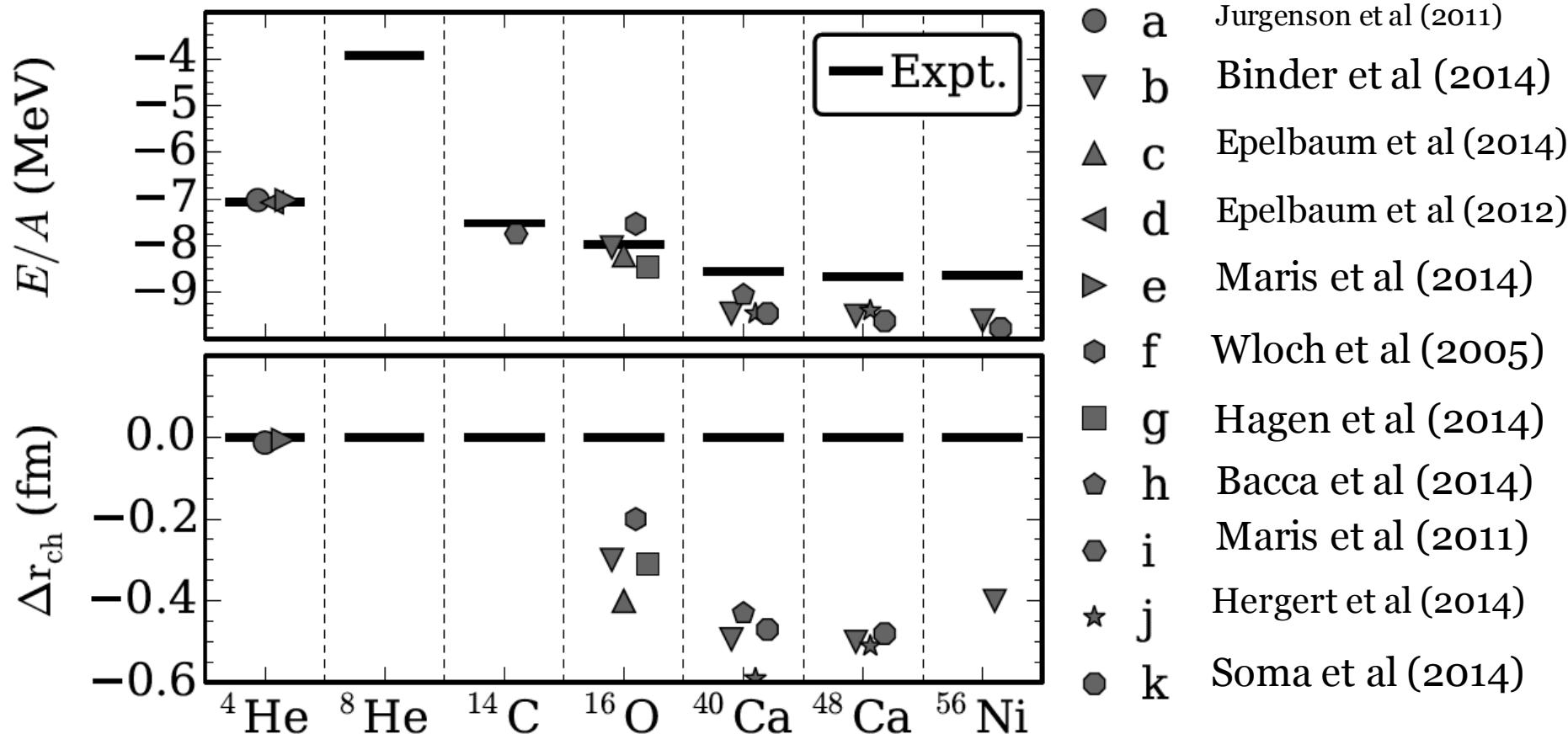
- local / non-local formulations [Gezerlis et al 2013/2014]

- propagation of uncertainties on horizon [Navarro Perez 2014, Carlsson et al 2015]

- different optimization protocols [Ekström et al 2015]

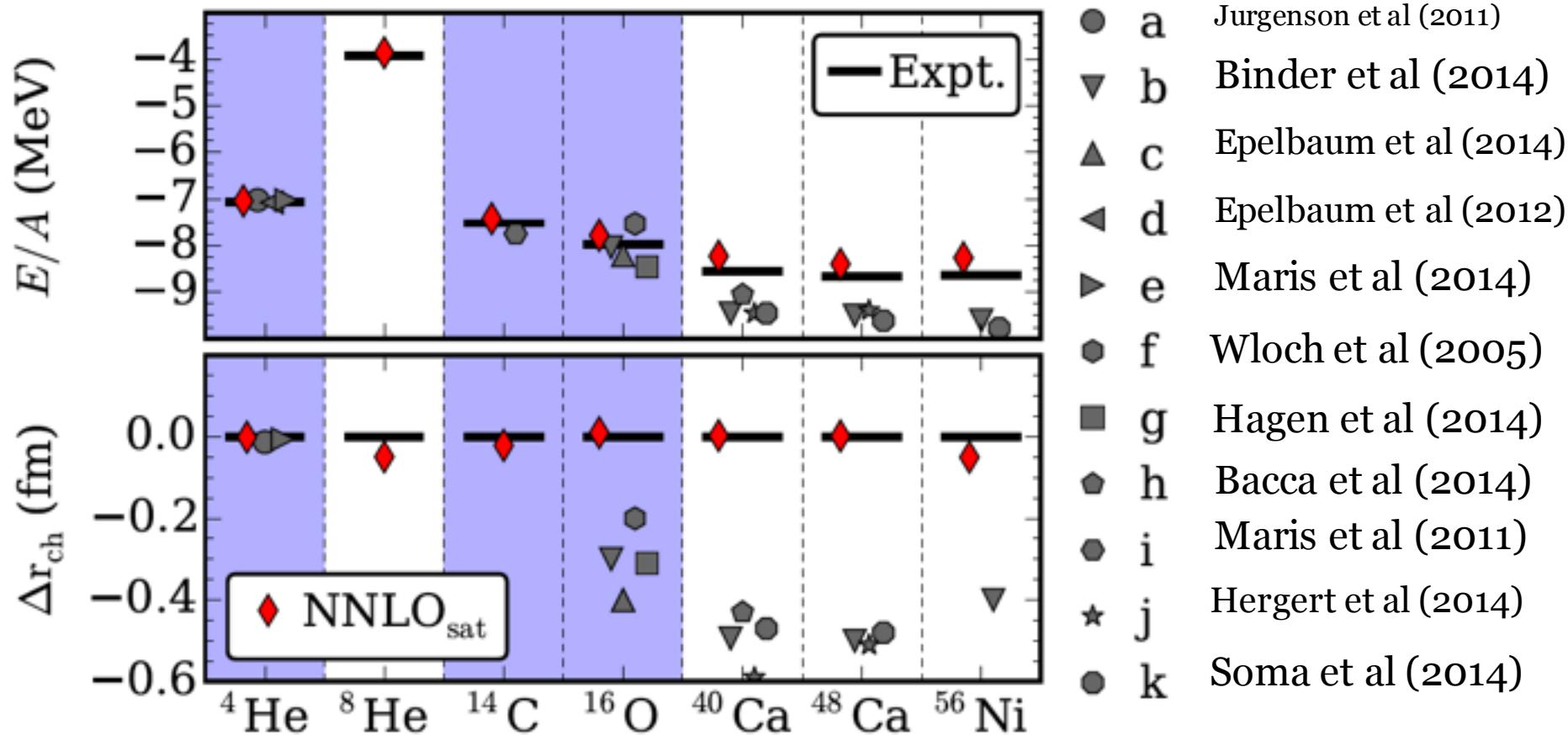
Much improved understanding and handling via renormalization group transformations [Bogner et al 2003; Bogner et al 2007]

# 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



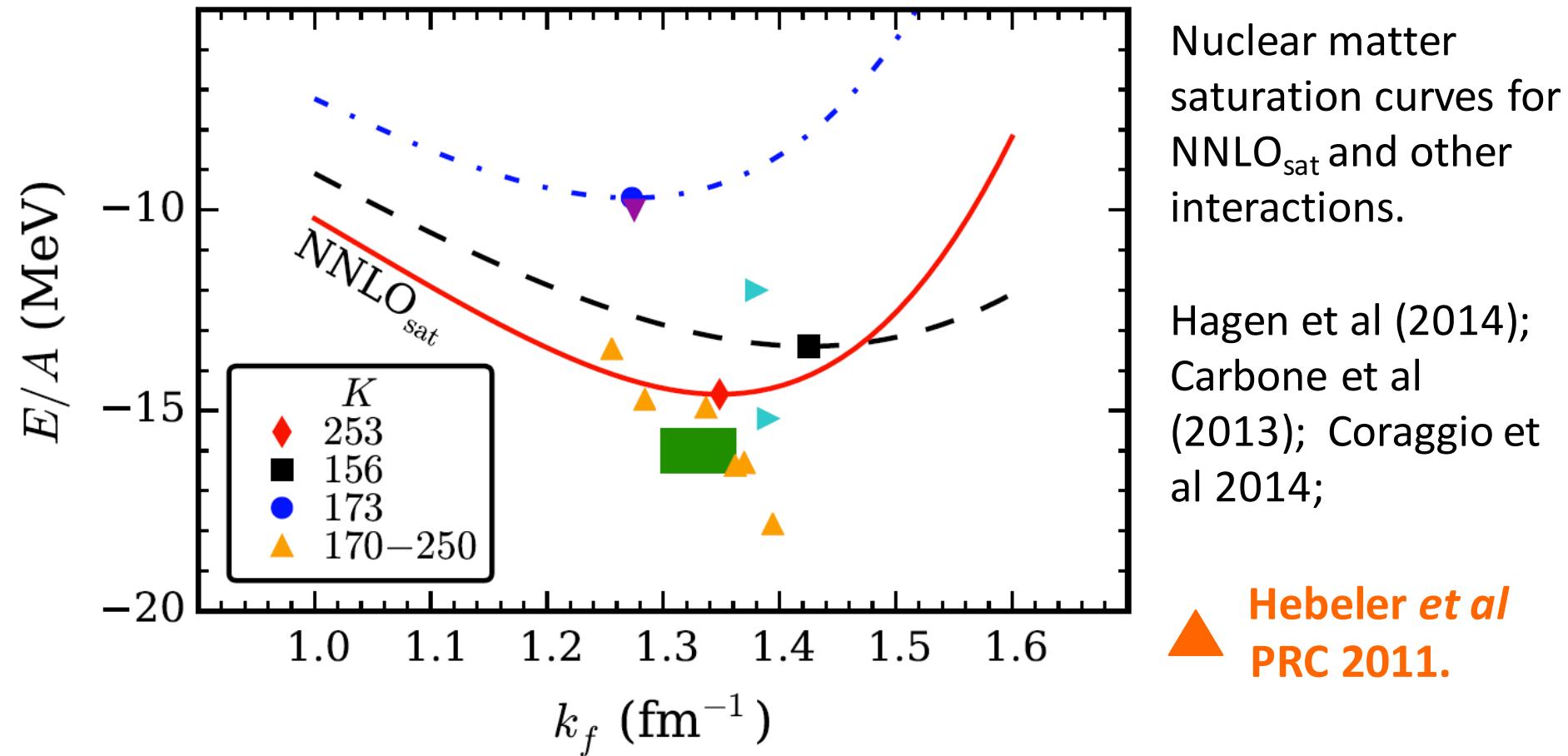
**Solution:** Simultaneous optimization of NN and 3NFs  
Include charge radii and binding energies of  
 $^3\text{H}$ ,  $^{3,4}\text{He}$ ,  $^{14}\text{C}$ ,  $^{16}\text{O}$  in the optimization (NNLO<sub>sat</sub>)  
A. Ekström *et al*, Phys. Rev. C **91**, 051301(R) (2015).

- a Navratil et al (2007);  
Jurgenson et al (2011)
- ▼ b Binder et al (2014)
- ▲ c Epelbaum et al (2014)
- d Epelbaum et al (2012)
- e Maris et al (2014)
- f Wloch et al (2005)
- g Hagen et al (2014)
- h Bacca et al (2014)
- i Maris et al (2011)
- ★ j Hergert et al (2014)
- k Soma et al (2014)

**Critical ingredient:**  
Three-nucleon forces  
with non-local  
regulators

# Nuclear matter from NNLO<sub>sat</sub>

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



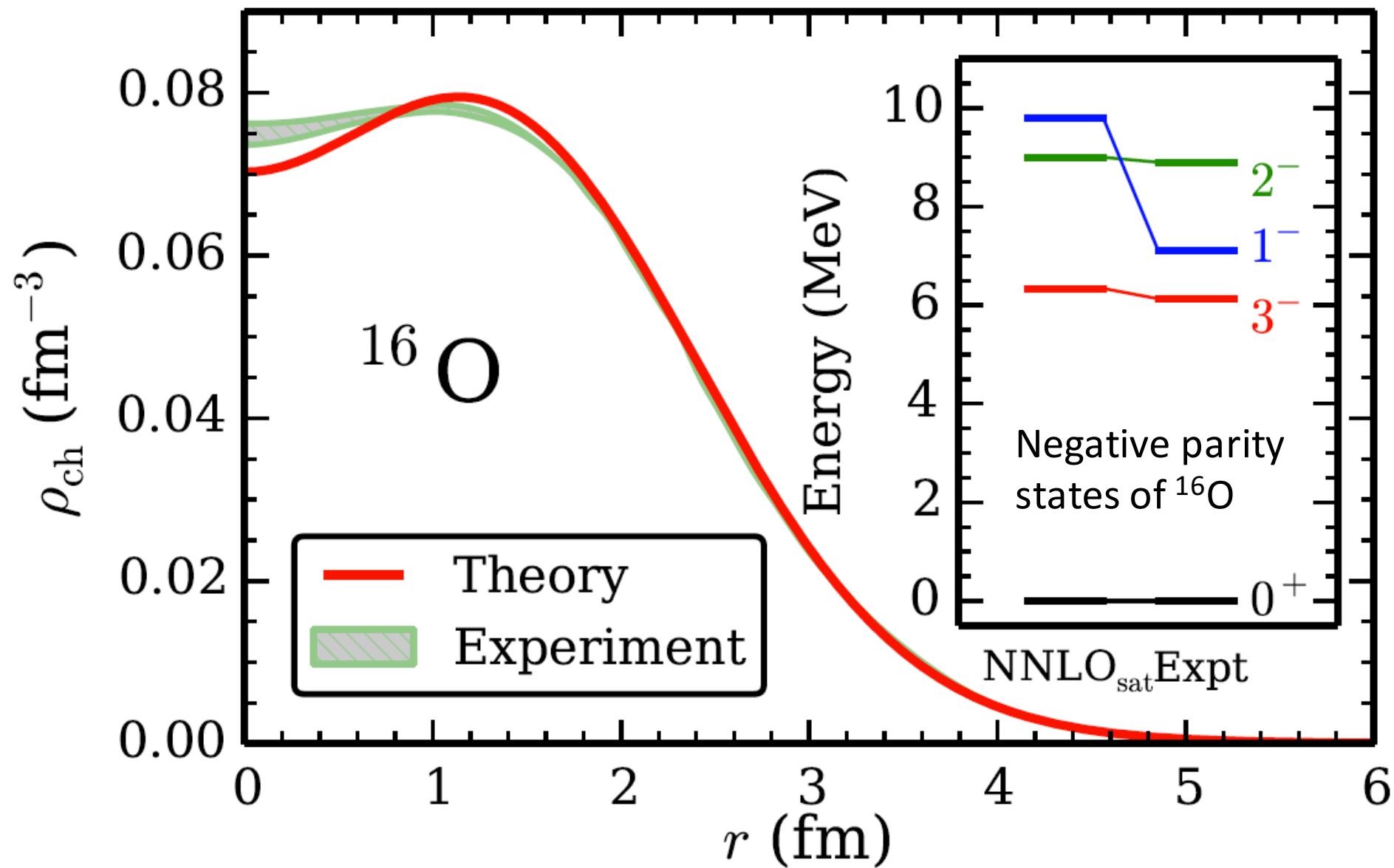
Nuclear matter saturation curves for NNLO<sub>sat</sub> and other interactions.

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

Hebeler *et al*  
PRC 2011.

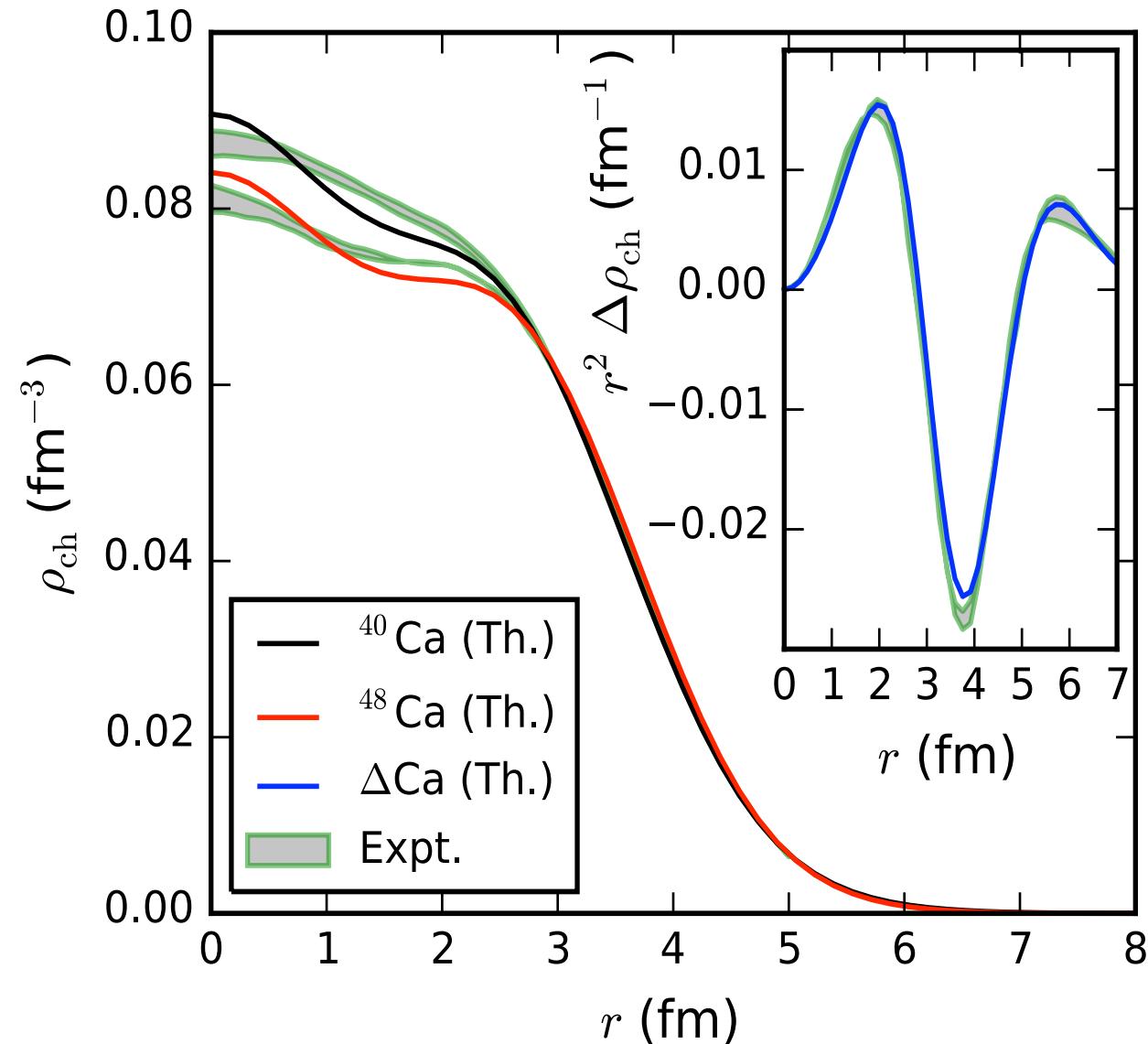
- Interactions from Hebeler *et al* not constrained by heavier nuclei.
- They reproduce binding energy and radii of few-body systems
- Non-local regulators in the 3NF important for saturation

# Charge density of $^{16}\text{O}$ from NNLO<sub>sat</sub>



# Charge densities of $^{40,48}\text{Ca}$ from NNLO<sub>sat</sub>

G. Hagen *et al*, Nature Physics (2015) doi:10.1038/nphys3529



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

$$BE(\text{Th}) = 404(3) \text{ MeV}$$

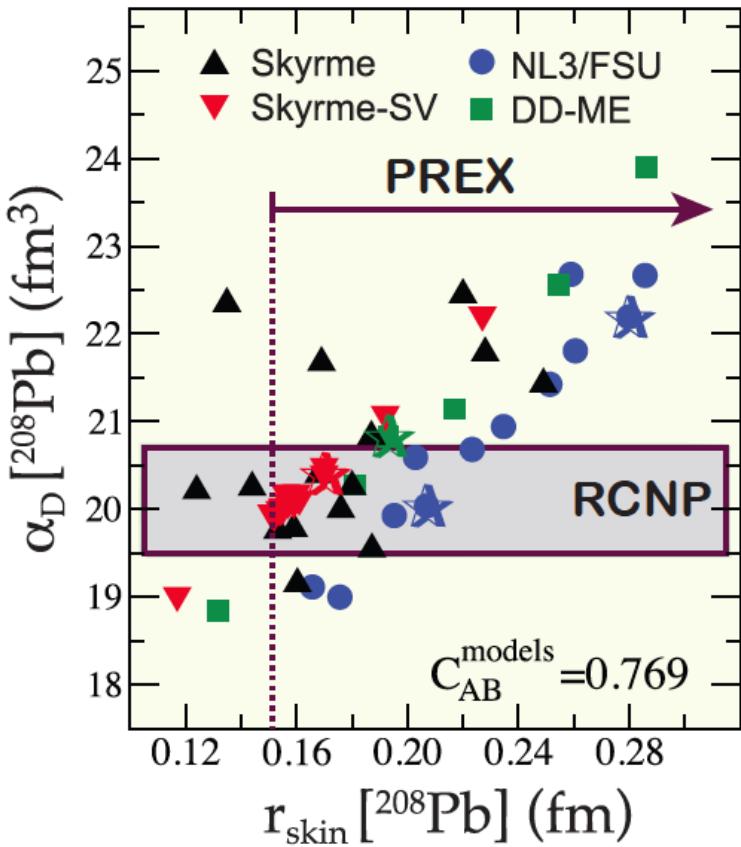
$$BE(\text{Exp}) = 416 \text{ MeV}$$

$$R_{Ch}(\text{Th}) = 3.48(3) \text{ fm}$$

$$R_{Ch.}(\text{Exp}) = 3.477(2) \text{ fm}$$

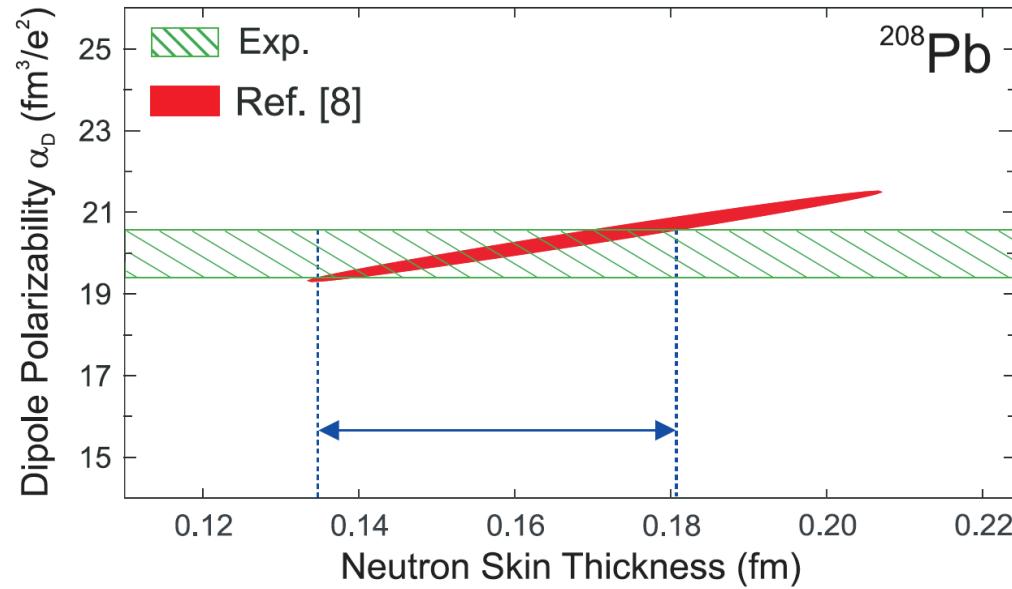
# Neutron radii and dipole polarizability

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



$\alpha_D$ : <sup>208</sup>Pb by Tamii et al, PRL 2011; <sup>68</sup>Ni by Rossi et al, PRL 2013; <sup>120</sup>Sn by Hashimoto et al. (2015); <sup>48</sup>Ca coming soon (Darmstadt/Osaka collaboration)

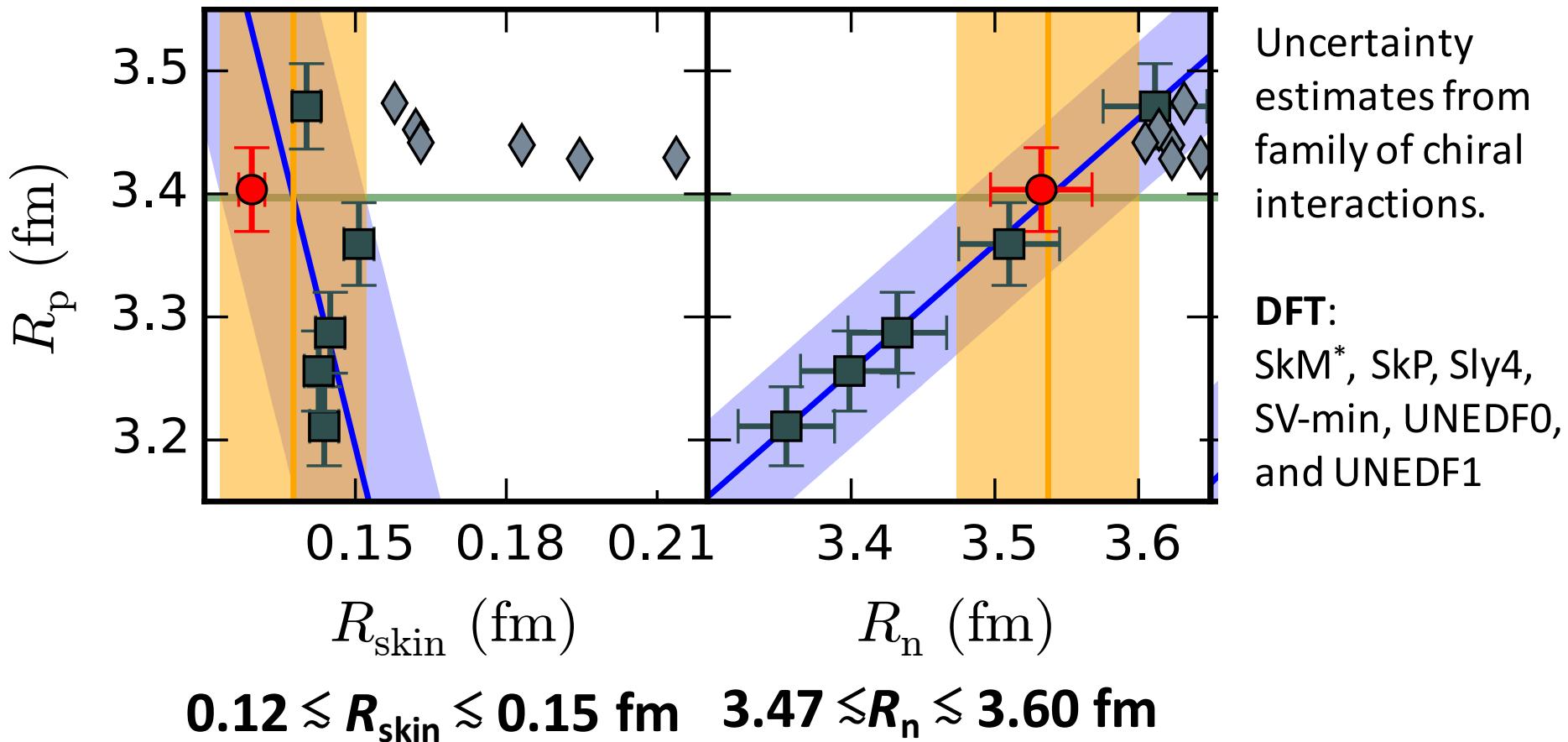
$R_n$ : <sup>208</sup>Pb by Abrahamyan et al, PRL 2012; <sup>48</sup>Ca → CREX



- 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 $^{48}\text{Ca}$

G. Hagen *et al*, Nature Physics (2015) doi:10.1038/nphys3529



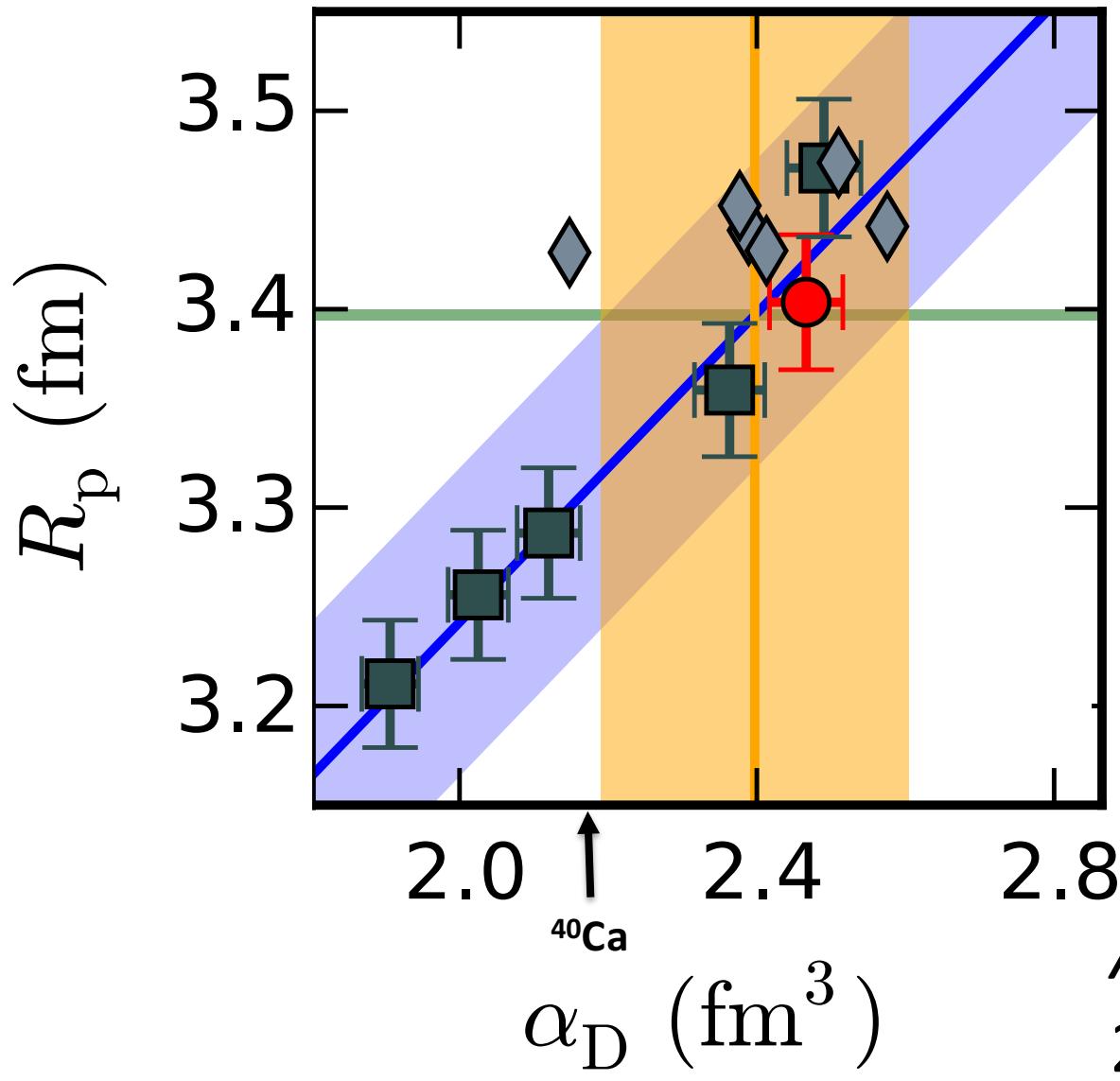
Uncertainty estimates from family of chiral interactions.

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

- Neutron skin significantly smaller than in DFT
- Neutron skin almost independent of the employed Hamiltonian
- Proton radii about 1% too large in DFT
- Ab-initio reproduce  $N=28$  shell gap/DFT underestimates shell gaps

# Dipole polarizability of $^{48}\text{Ca}$

G. Hagen *et al*, Nature Physics (2015) doi:10.1038/nphys3529



DFT results are consistent and within band of ab-initio results

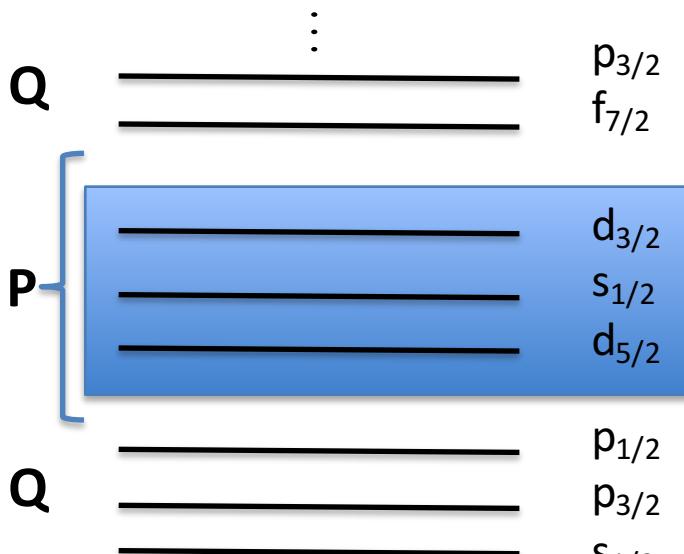
Data being analyzed by Osaka-Darmstadt collaboration

*Ab-initio* prediction:  
 $2.19 \lesssim \alpha_D \lesssim 2.60$  fm $^3$

# Coupled-cluster effective interactions (CCEI)

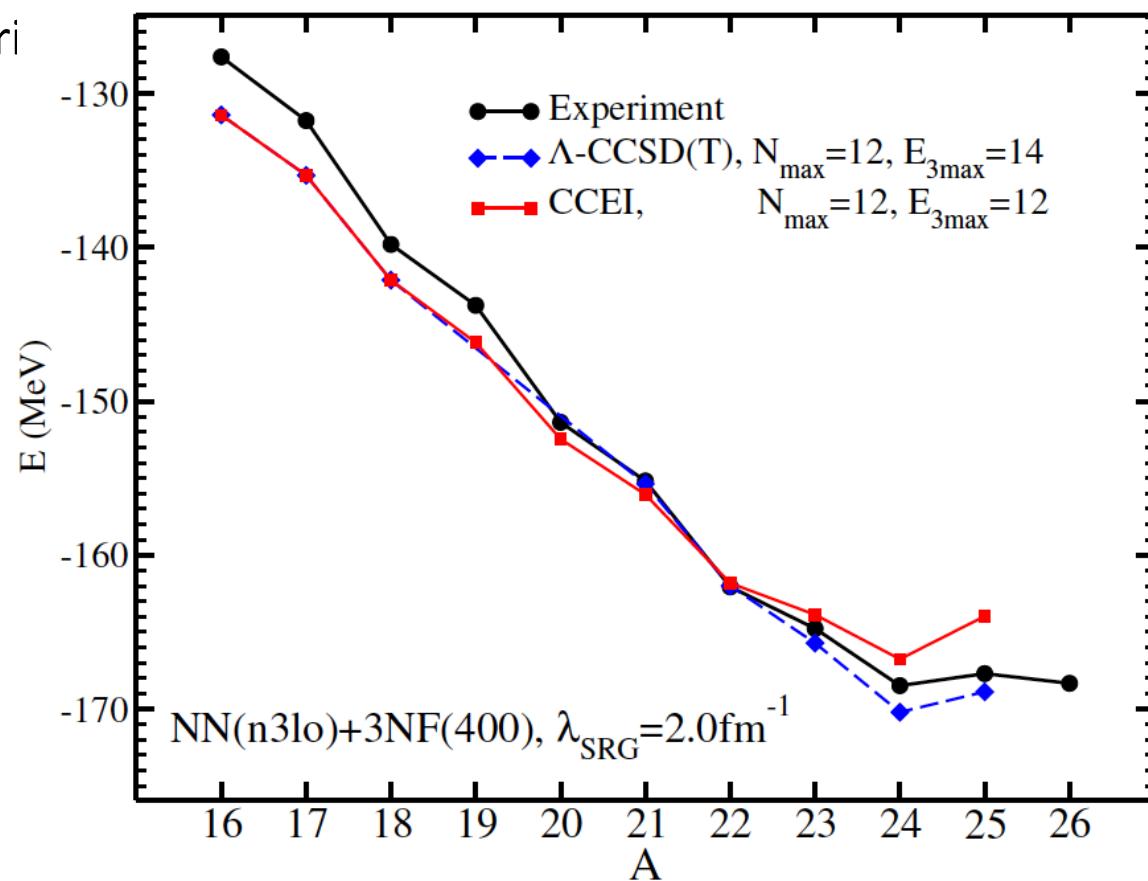
G. R. Jansen, J. Engel, GH, P. Navratil, A. Signoracci, Phys. Rev. Lett. **113**, 142502 (2014).

- Start from chiral NN+3NFs
- Solve for A, A+1 and A+2 using CC.
- Project A+1 and A+2 CC wave functions onto the *s-d* model space using Lee-Suzuki similarity transformation.

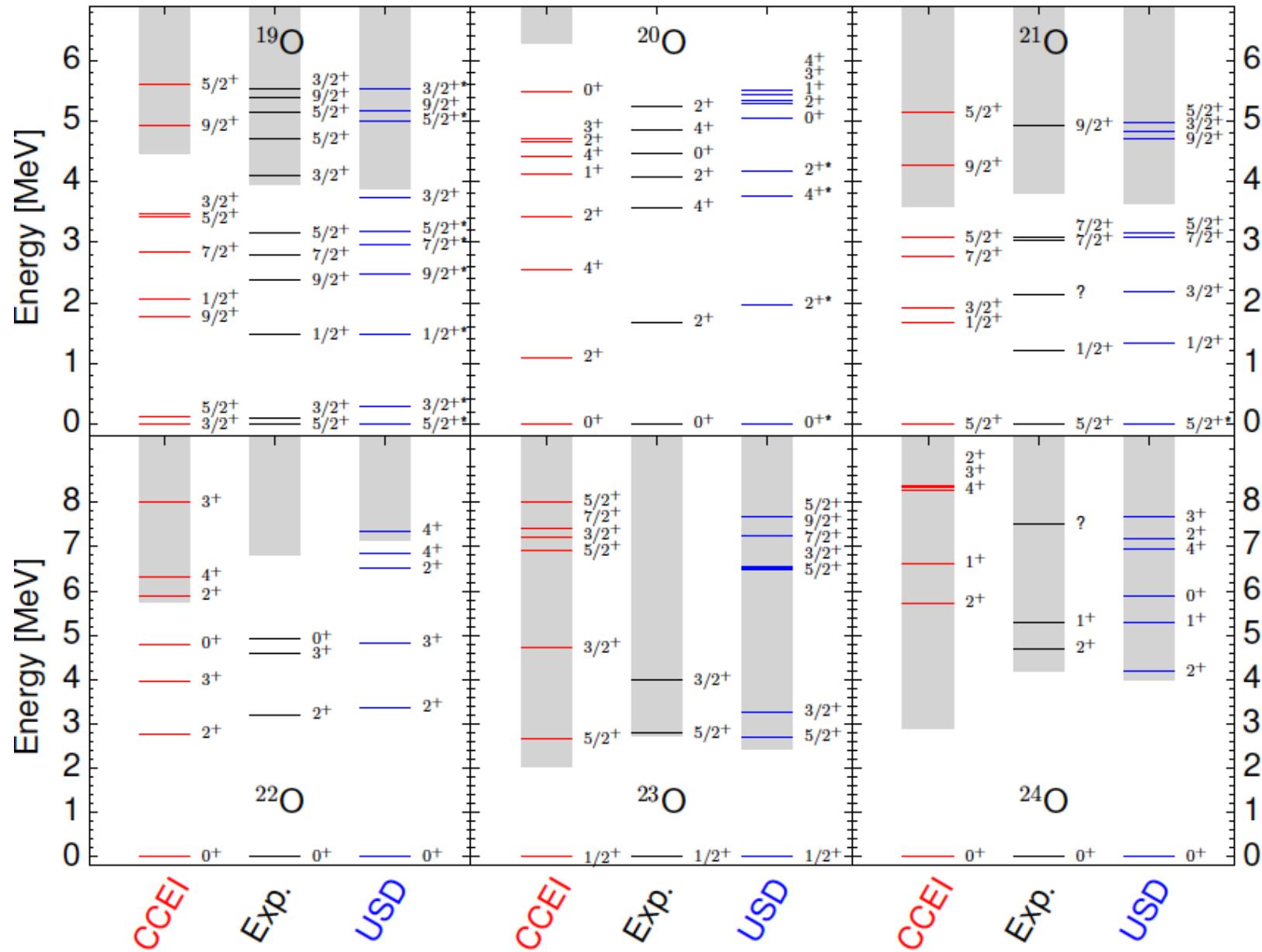


- Diagonalize the effective hamiltonian in the valence space.

Comparison between coupled-cluster effective interaction (CCEI) and “exact” coupled-cluster calculation with inclusion of perturbative triples ( $\Lambda$ -CCSD(T))

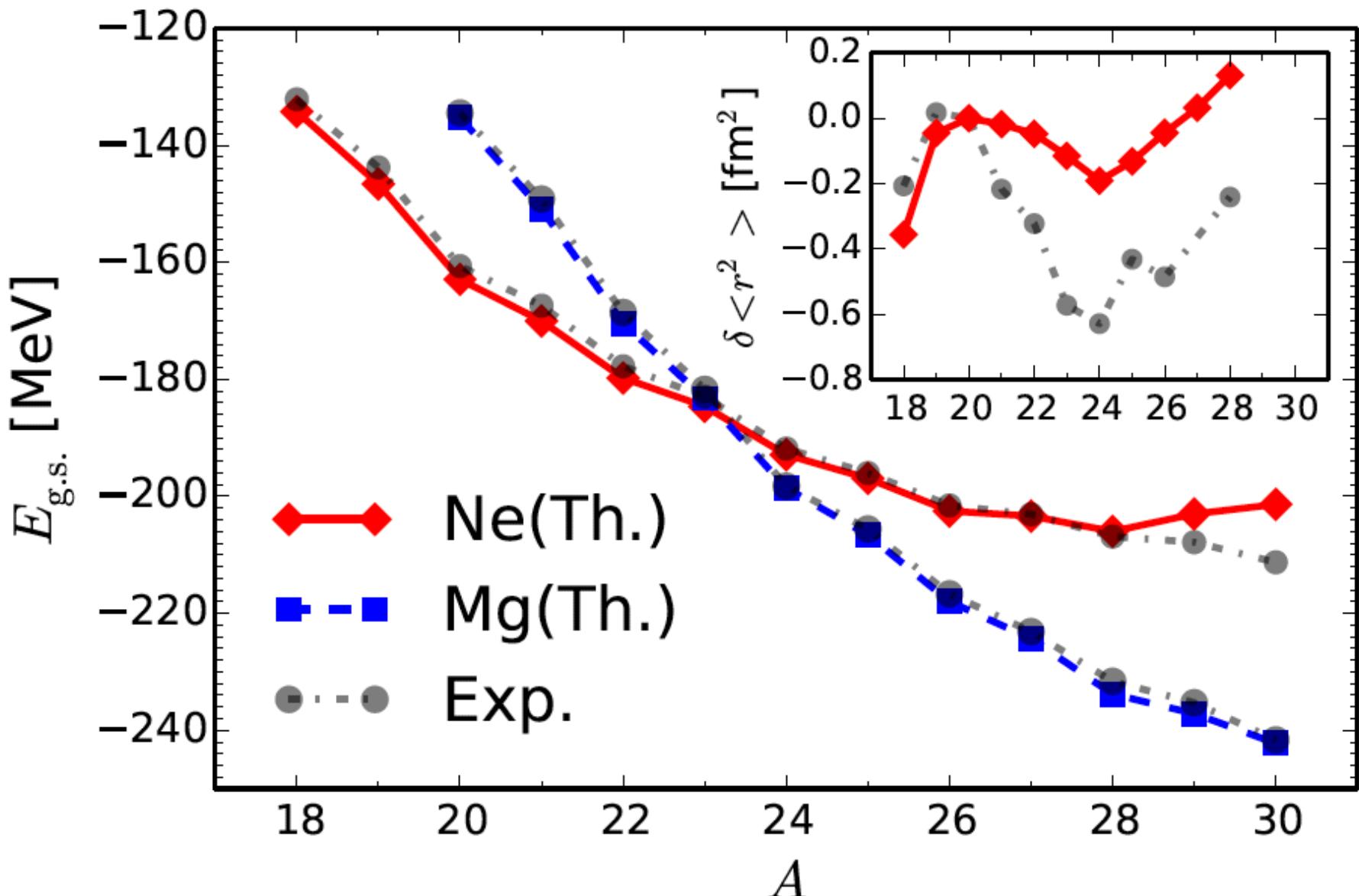


# Coupled-cluster effective interactions for the shell model: Oxygen isotopes



# Deformed sd-shell nuclei from first principles

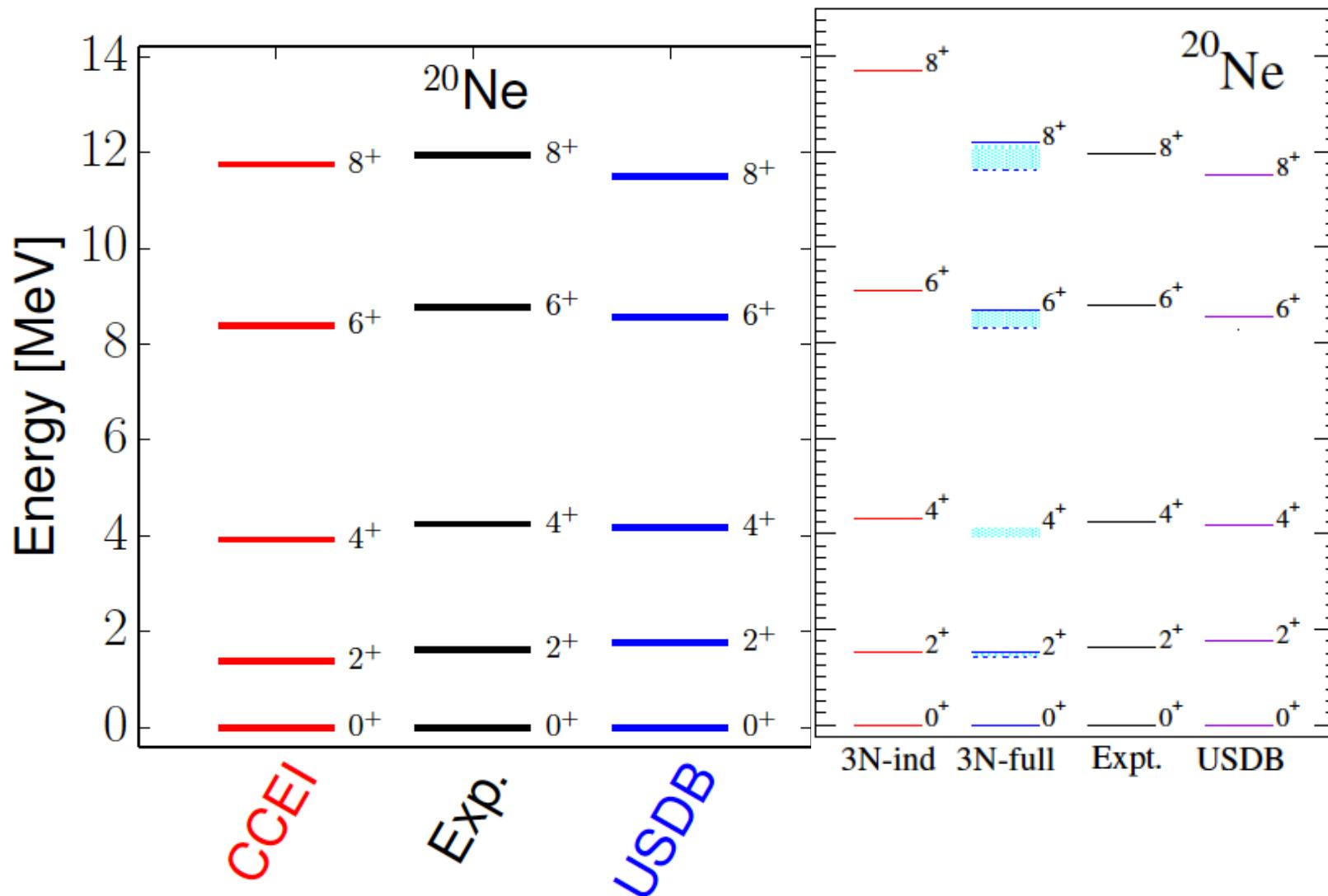
G. R. Jansen, A. Signoracci, GH, P. Navratil arXiv:1511.00757 (2015).



# Deformed sd-shell nuclei from first principles

G. R. Jansen, A. Signoracci, GH, P. Navratil arXiv:1511.00757 (2015).

S. R. Stroberg et al,  
arXiv:1511.02802 (2015).

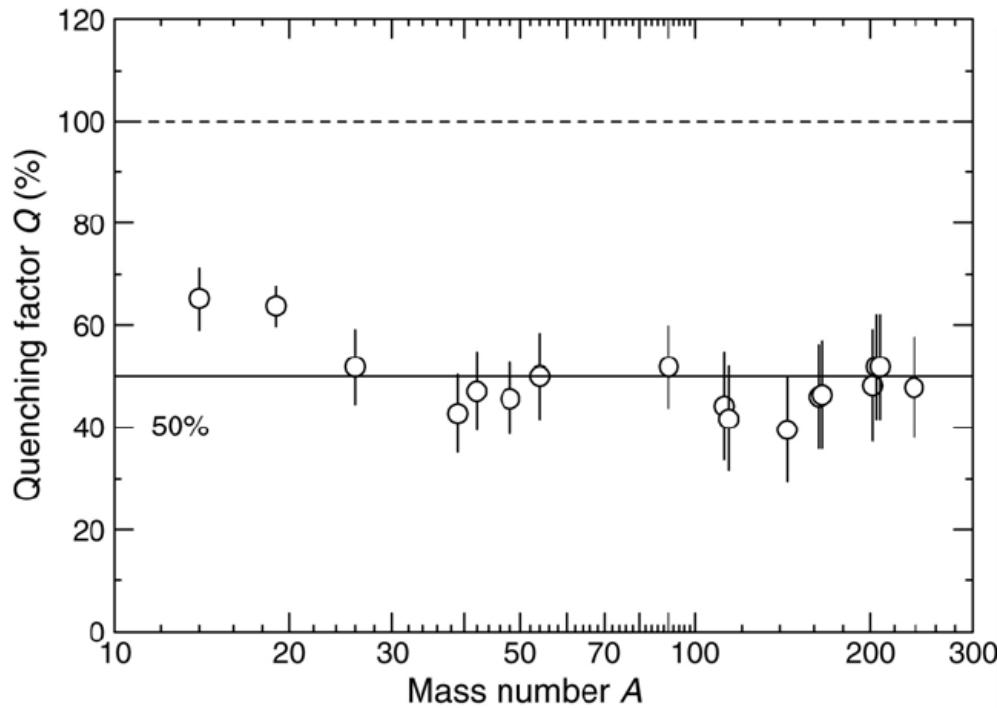


# Quenching of Gamow-Teller strength in nuclei

The Ikeda sum-rule  $S^N(\text{GT}) = S^N(\text{GT}^-) - S^N(\text{GT}^+) = 3(N - Z)$

**Long-standing problem:** Experimental beta-decay strengths quenched compared to theoretical results.

$$Q = \frac{S_{\text{GT}}^-(\omega_{\text{top}}^-) - S_{\text{GT}}^+(\omega_{\text{top}}^+)}{3(N - Z)}$$



Surprisingly large quenching  $Q$  (50%) obtained from  $(p,n)$  experiments. The excitation energies were just above the giant Gamow-Teller resonance  $\sim 10\text{-}15\text{MeV}$  (Gaarde 1983).

- Measurement of GT strengths to high energies (Sasano et al 2009, Yako et al 2005), suggests a much smaller quenching  $Q = 0.88\text{-}0.92$



- Renormalizations of the Gamow-Teller operator?
- Missing correlations in nuclear wave functions?
- Model-space truncations?

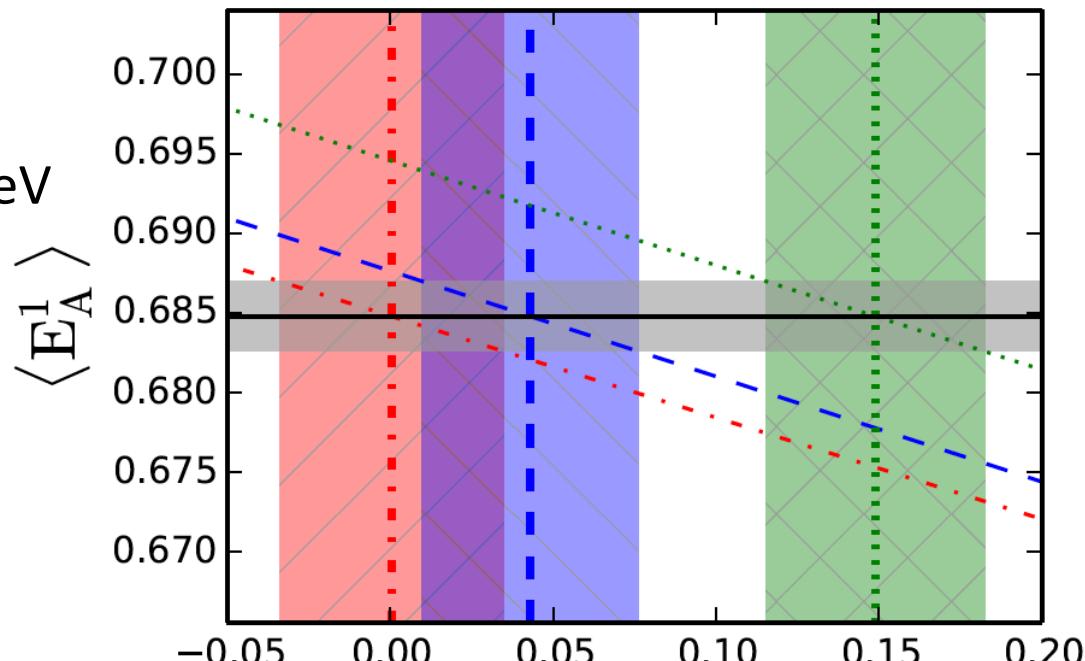
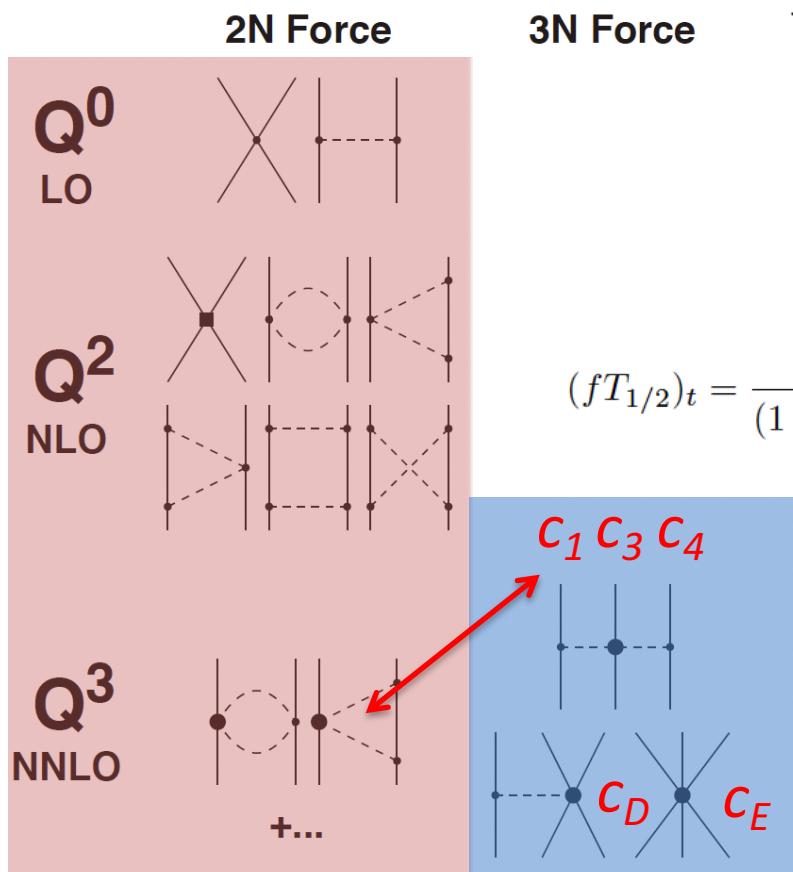


- **What does two-body currents and three-nucleon forces add to this long-standing problem?**

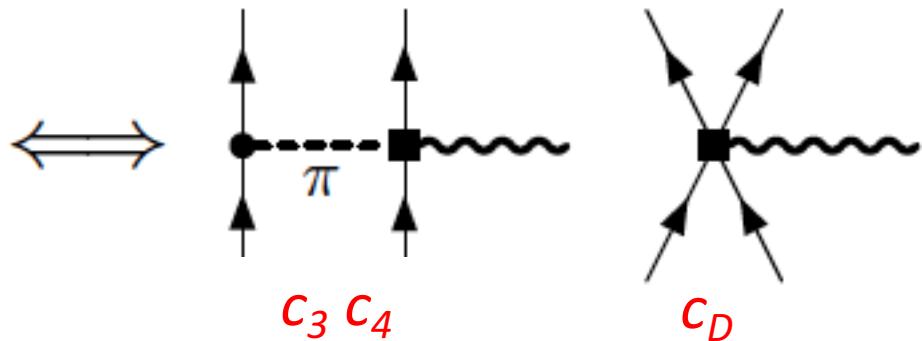
# Weak decays from first principles

A. Ekström, G. Jansen, K. Wendt et al, PRL 113 262504 (2014)

$c_D - c_E$  fit of A=3 binding energies  
and the  $^3\text{H}$  half life at NNLO for  
chiral cutoffs  $\Lambda = 450, 500, 550$  MeV  
 $[c_D, c_E] = [0.043, -0.501]$



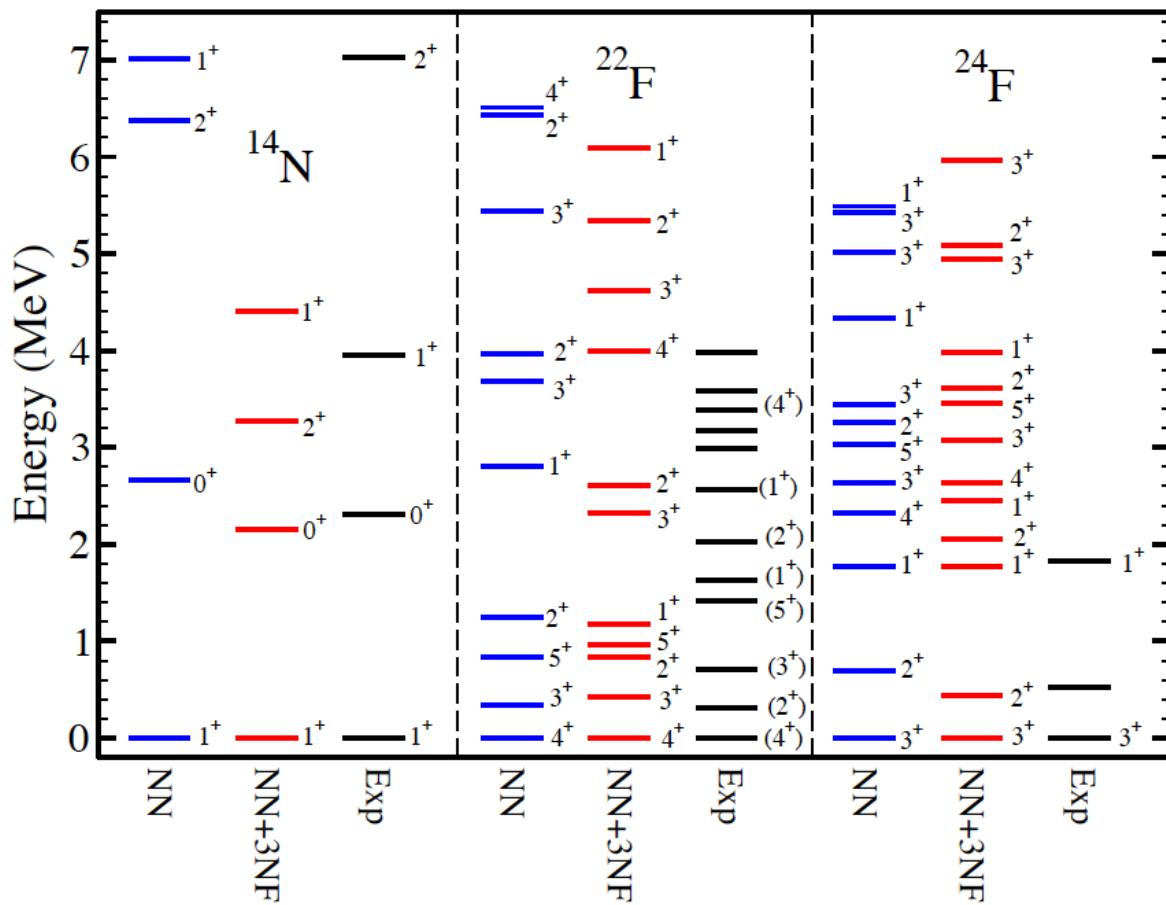
$$(fT_{1/2})_t = \frac{K/G_V^2}{(1 - \delta_c) + 3\pi \frac{f_A}{f_V} \langle E_1^A \rangle^2} c_D$$



# Charge-exchange coupled cluster method for odd-odd nuclei

Diagonalize  $\overline{H} = e^{-T} H_N e^T$  via charge-exchange equation-of-motion technique:

$$R \equiv \sum_{ia} r_i^a p_a^\dagger n_i + \frac{1}{4} \sum_{ijab} r_{ij}^{ab} p_a^\dagger N_b^\dagger N_j n_i$$



- Compute spectra of daughter nuclei as beta decays of mother nuclei
- Level densities in daughter nuclei increase slightly with 3NF
- Predict several states in neutron rich Fluorine

# Quenching of Gamow-Teller strength in nuclei

A. Ekström, G. Jansen, K. Wendt et al, PRL 113 262504 (2014)

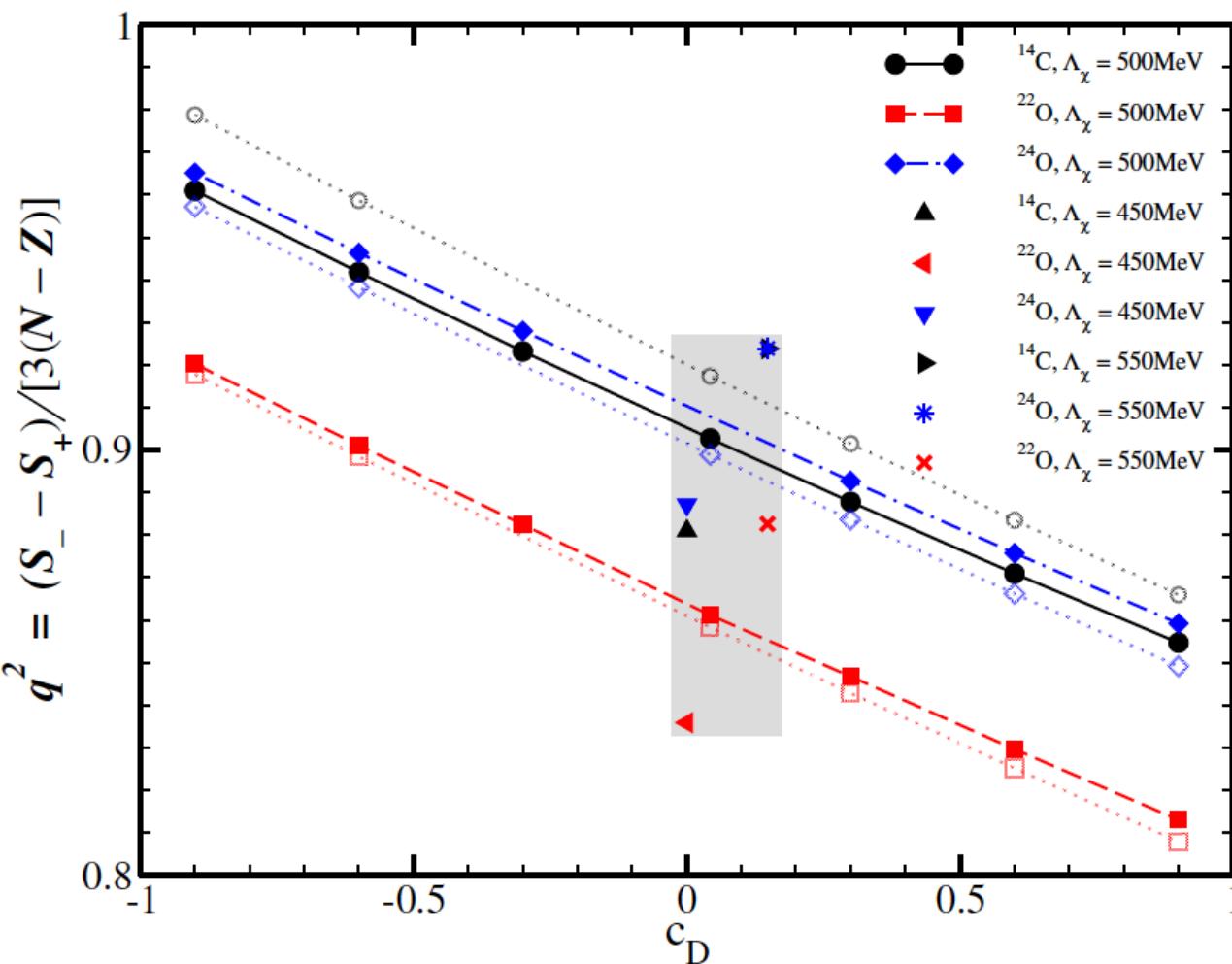
Gamow-Teller matrix element:

$$\hat{O}_{\text{GT}} \equiv \hat{O}_{\text{GT}}^{(1)} + \hat{O}_{\text{GT}}^{(2)} \equiv g_A^{-1} \sqrt{3\pi} E_1^A$$

Total GT strength functions:

$$S_- = \langle \Lambda | \overline{\hat{O}_{\text{GT}}^\dagger} \cdot \overline{\hat{O}_{\text{GT}}} | \text{HF} \rangle$$

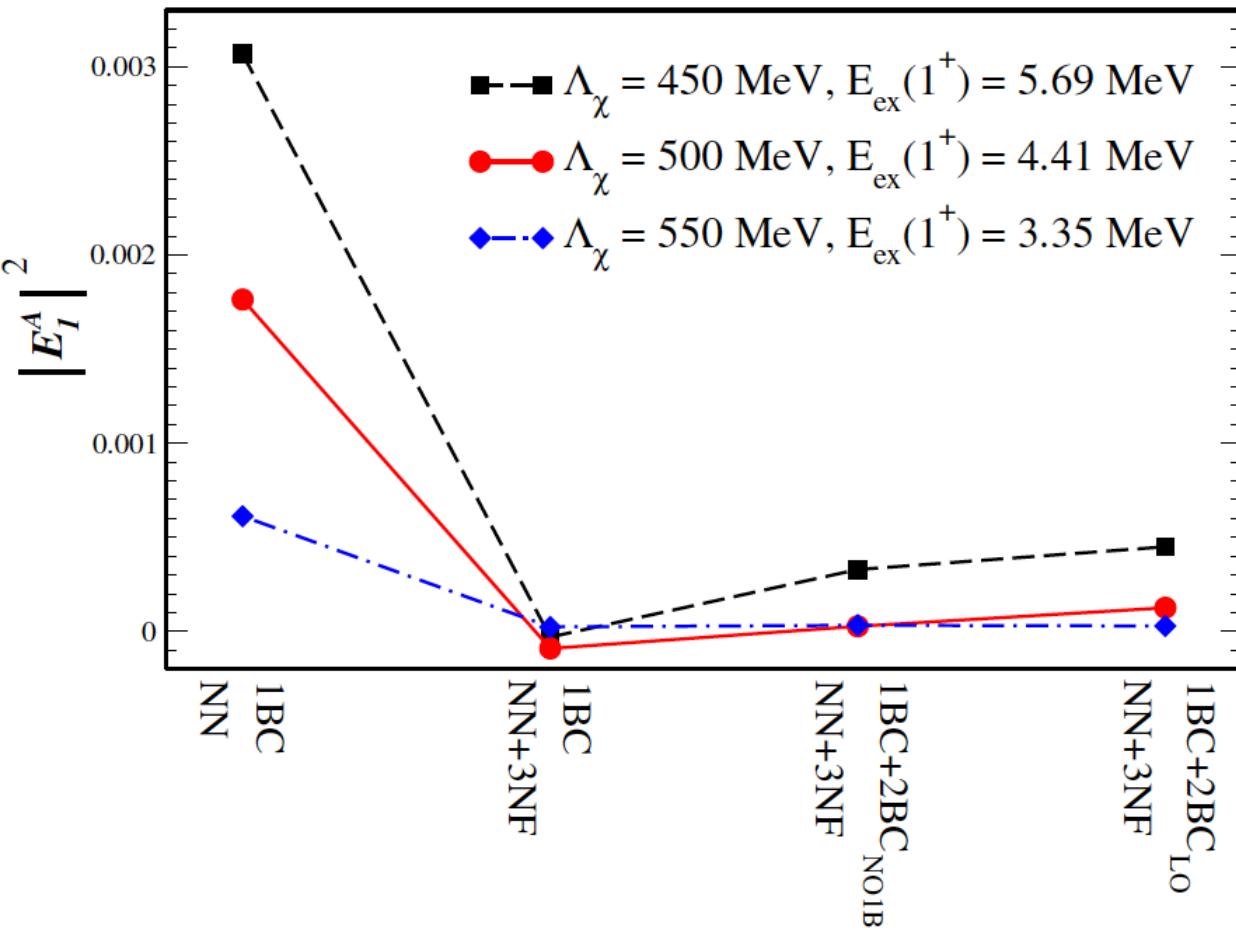
$$S_+ = \langle \Lambda | \overline{\hat{O}_{\text{GT}}} \cdot \overline{\hat{O}_{\text{GT}}^\dagger} | \text{HF} \rangle$$



- Quenching of the Ikeda sum rule in  $^{14}\text{C}$  and  $^{22,24}\text{O}$  for different cutoffs.
- Grey area is region which reproduce triton half-life
- The quenching  $q^2$  is about 8-16% and consistent with estimates in  $^{90}\text{Zr}$

# Anomalous life-time of $^{14}\text{C}$ revisited

A. Ekström, G. Jansen, K. Wendt et al, PRL 113 262504 (2014)



$E_A^A$  varies between  $5 \times 10^{-3}$  to  $2 \times 10^{-2}$  which is more than one order of magnitude larger than the empirical value  $\sim 6 \times 10^{-4}$  extracted from the 5700 a half life of  $^{14}\text{C}$

- 3NFs decrease the transition matrix element significantly
- 2BC counter the effect of 3NFs to some degree.
- The matrix element depends on the first excited  $1^+$  state in  $^{14}\text{N}$ .



# Summary

- Accurate radii and binding energies from a chiral interactions at NNLO
- Predictions for weak charge form-factor and distribution and dipole polarizability of  $^{48}\text{Ca}$
- Developed non-perturbative shell-model interactions for the shell-model with application to deformed nuclei
- Quenching of Gamow-Teller strength in selected nuclei due to two-body currents

# Collaborators

@ ORNL / UTK: **A. Ekström**, T. Papenbrock, G. R. Jansen, L. Platter

@ MSU: W. Nazarewicz

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

@ Hebrew U: N. Barnea, D. Gazit

@ MSU/ U Oslo: M. Hjorth-Jensen

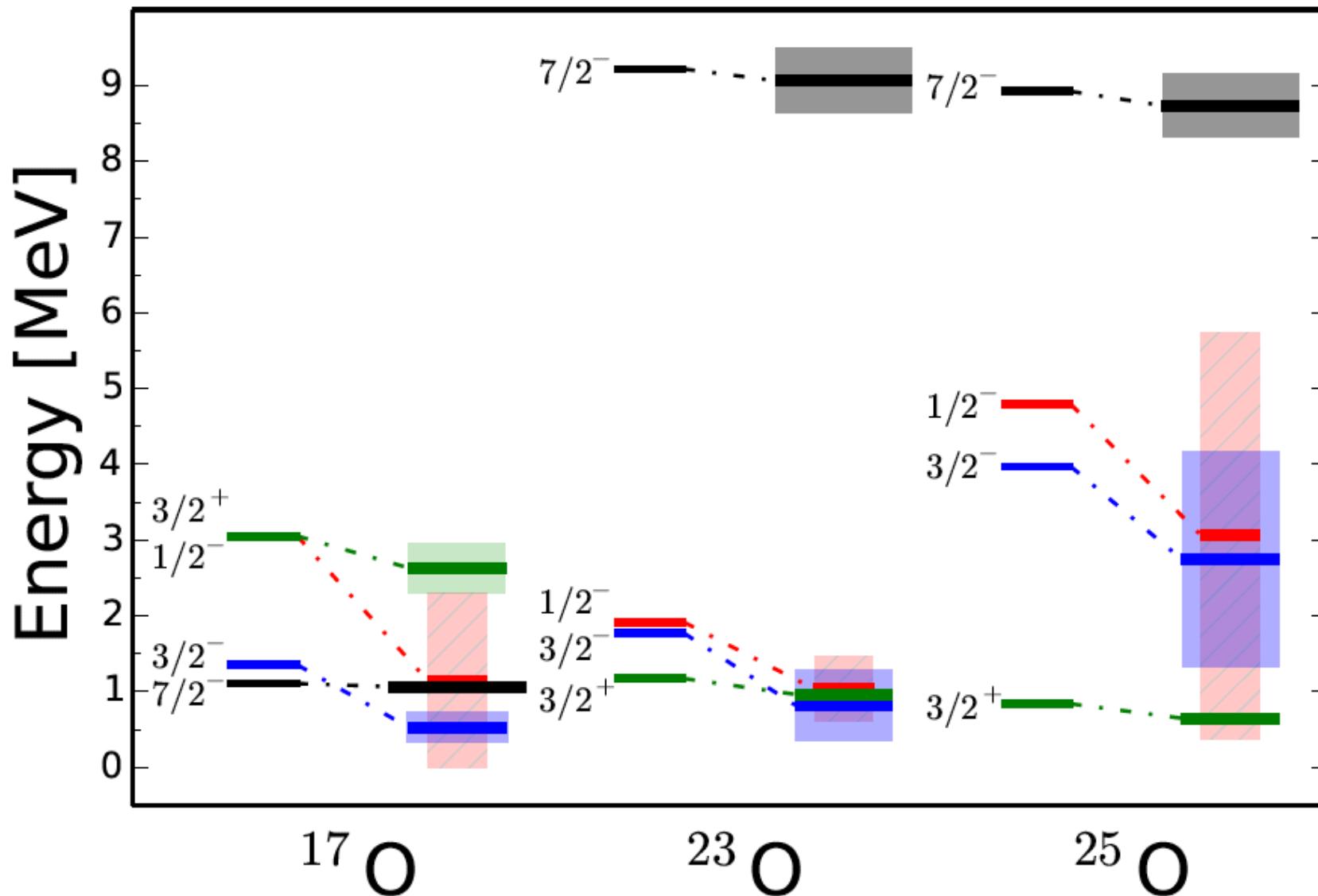
@ U. Idaho: R. Machleidt

@ Trento: G. Orlandini

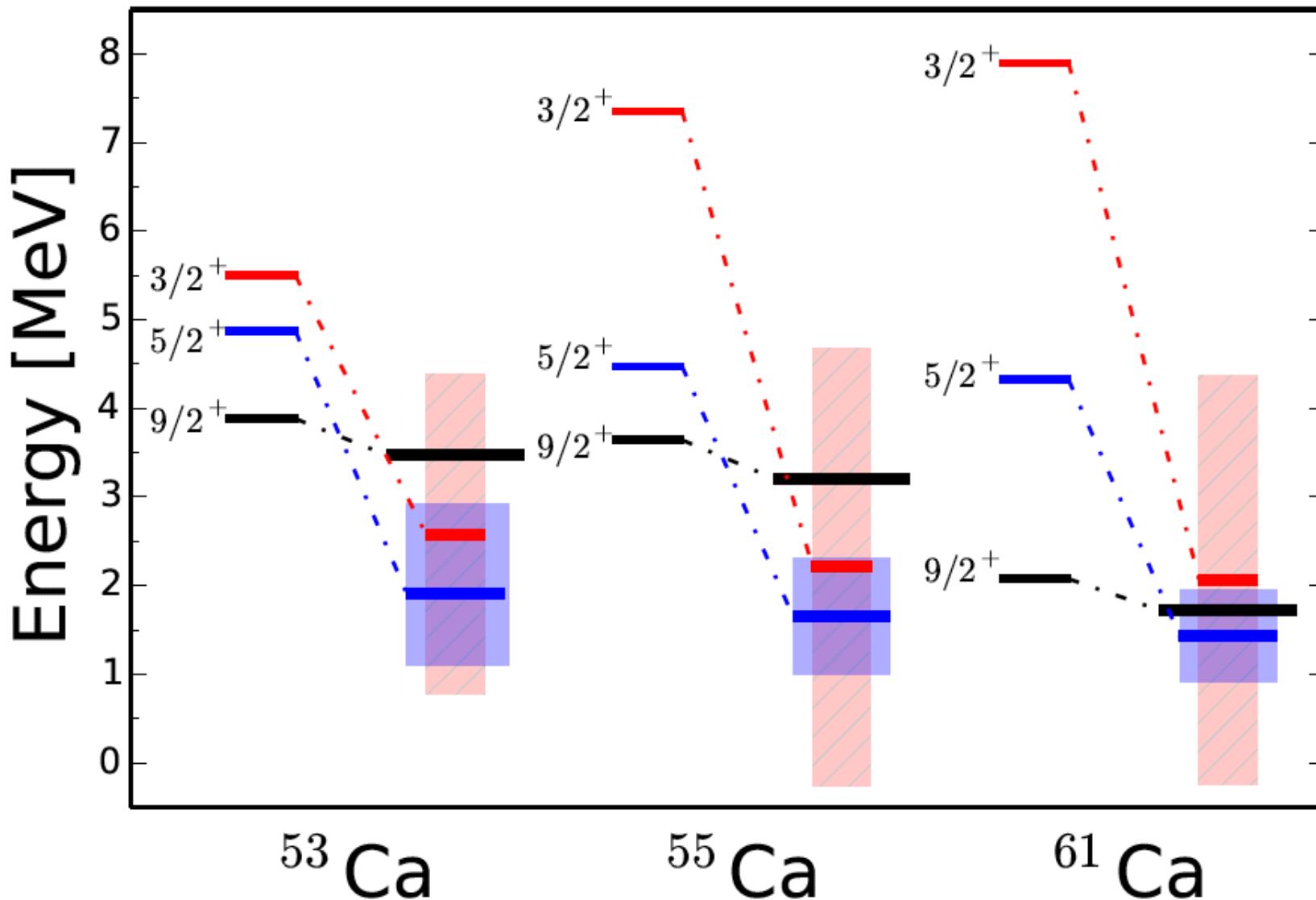
@ TRIUMF: S. Bacca, **M. Miorelli**, P. Navratil

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

# Role of continuum on unbound states in oxygen isotopes



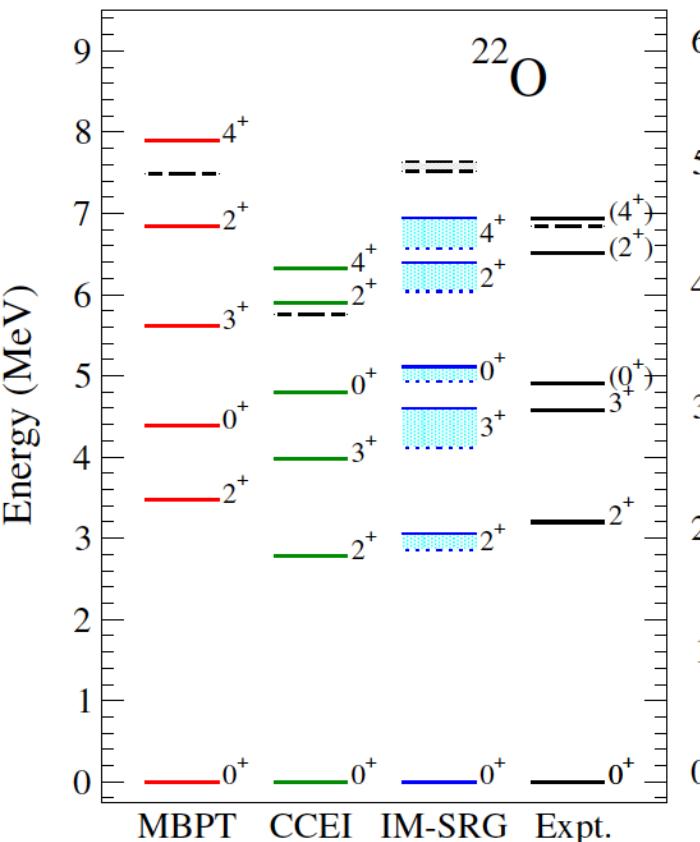
# Role of continuum on unbound states in neutron rich calcium



# Benchmarking different methods: Spectra in $^{22,23,24}\text{O}$

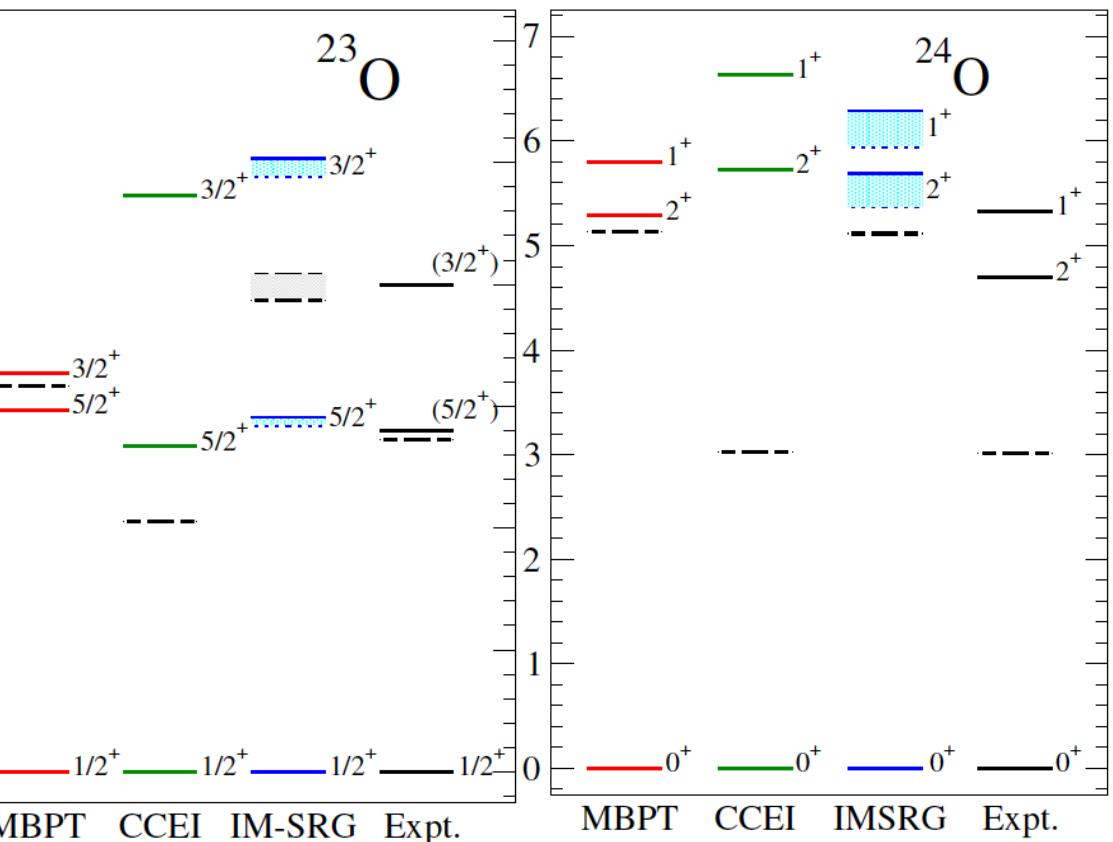
## In-medium SRG

S. Bogner et al, Phys. Rev. Lett. 113,  
142501 (2014)  
Hebeler, Holt, Menendez, Schwenk, Ann.  
Rev. Nucl. Part. Sci. in press (2015)

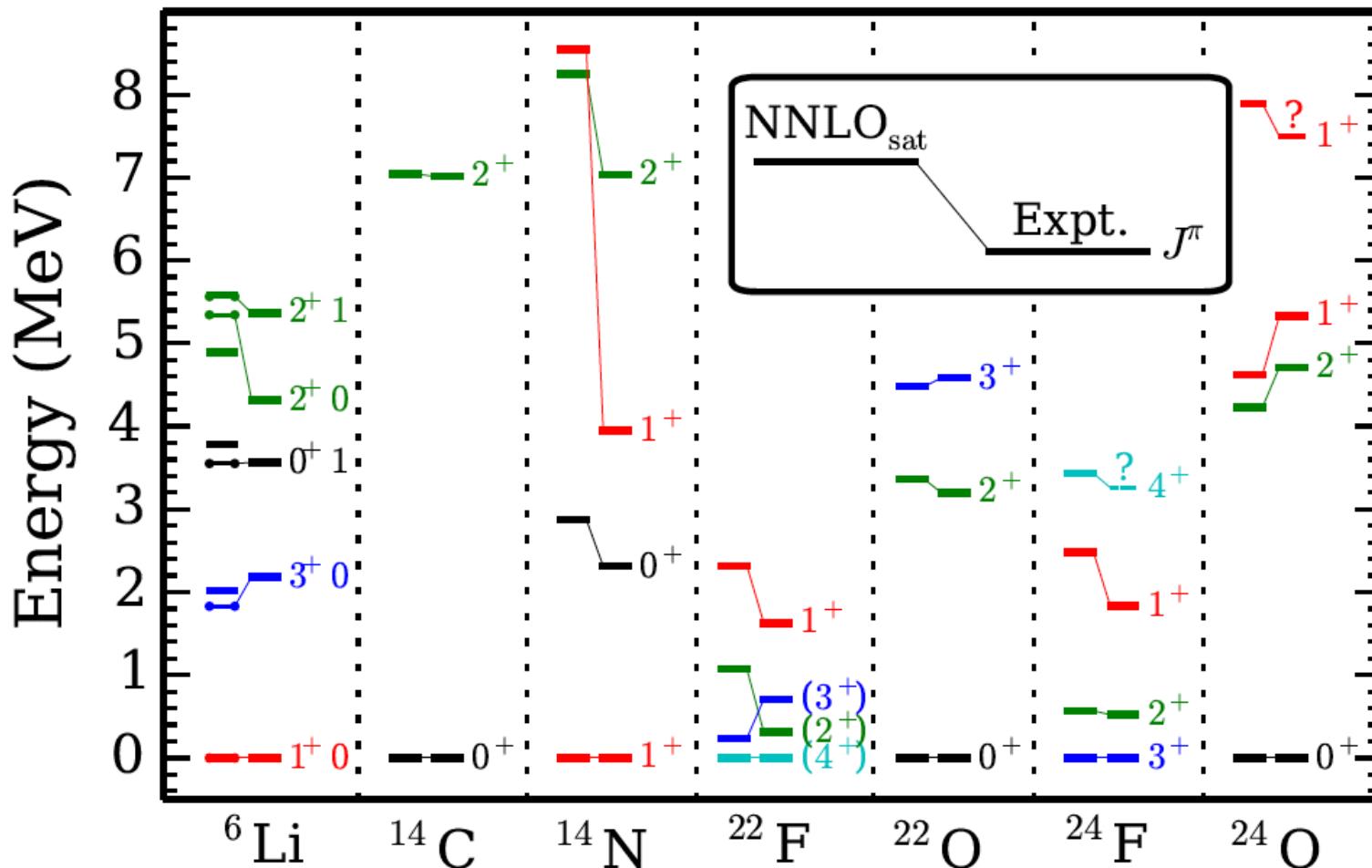


## Coupled-Cluster Effective Interactions

G. R. Jansen et al,  
Phys. Rev. Lett. 113, 142502 (2014)



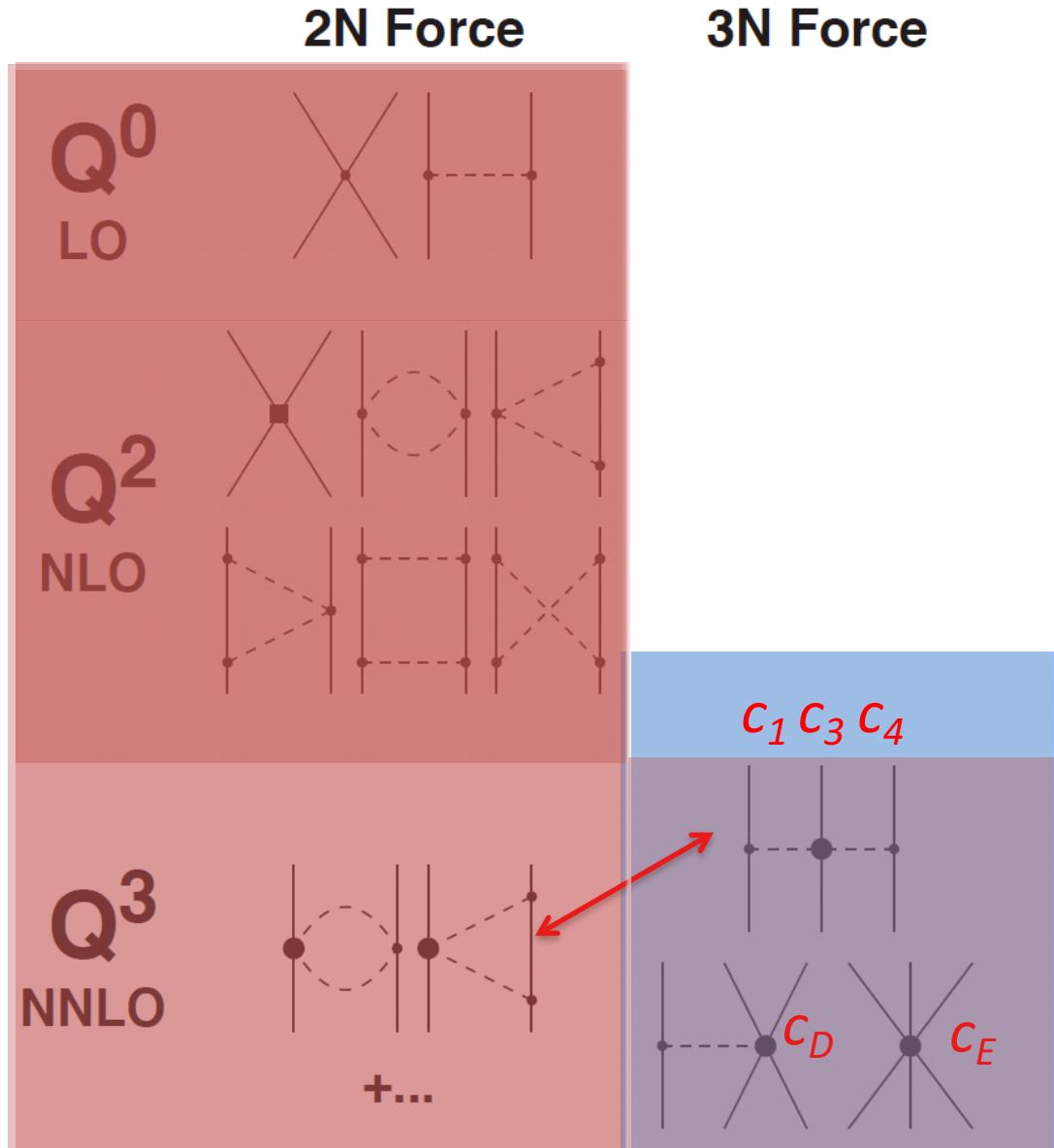
# Spectra with NNLO<sub>sat</sub>



Other deficiencies:  ${}^{17,18}\text{O}$  ( $1/2^+$  too high,  $2^+$  too low)

Overall NNLO<sub>sat</sub> spectra comparable to other chiral interactions

# Simultaneous optimization of NN and 3NFs



## Traditional approach:

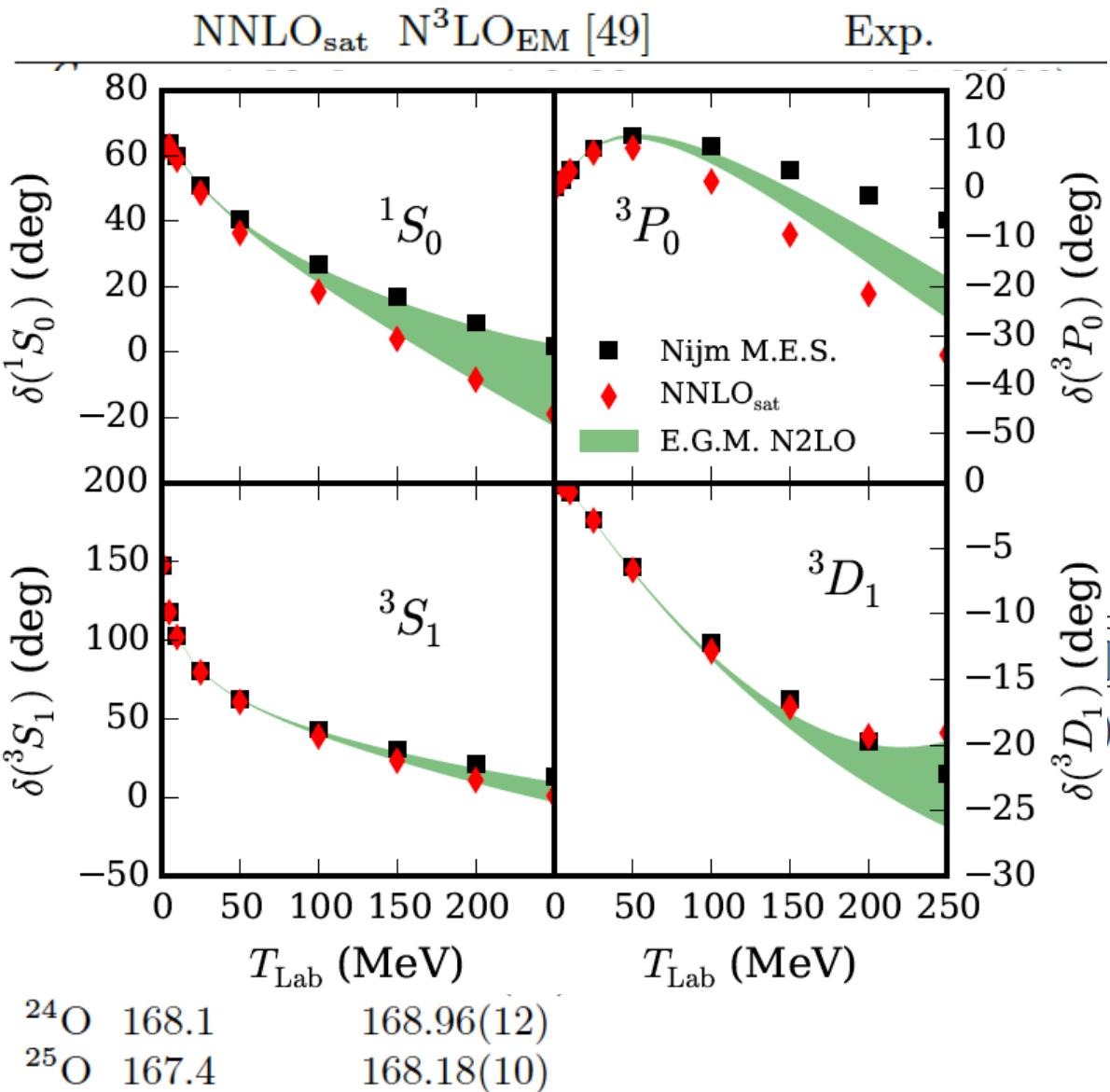
- Fit interactions nucleon by nucleon
- Fit to NN scattering data up to  $\sim 350\text{MeV}$
- cE and cD fit to  $A=3,4$

## New approach:

- Simultaneous optimization of NN and 3NFs
- Fit to few-body data and BEs/radii in nuclei with  $A \sim 25$

# Optimizing NNLO<sub>sat</sub>

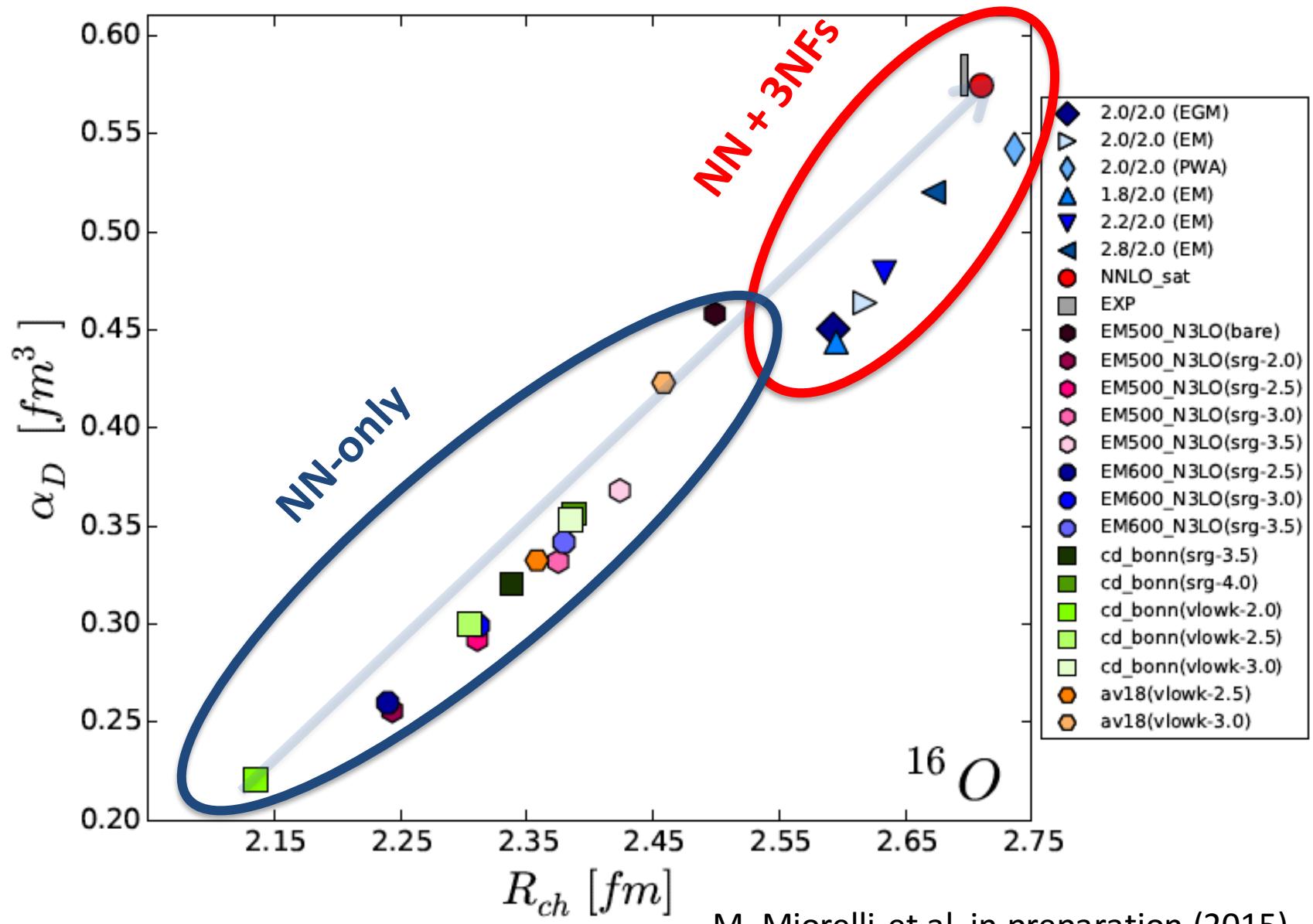
A. Ekström, G. Jansen, K. Wendt et al, PRC 91, 051301 (2015)



## 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 35 MeV
- Phase shifts are at the limit of expectations one can have at NNLO

# Dipole polarizability of $^{16}\text{O}$ : The role of three-nucleon forces



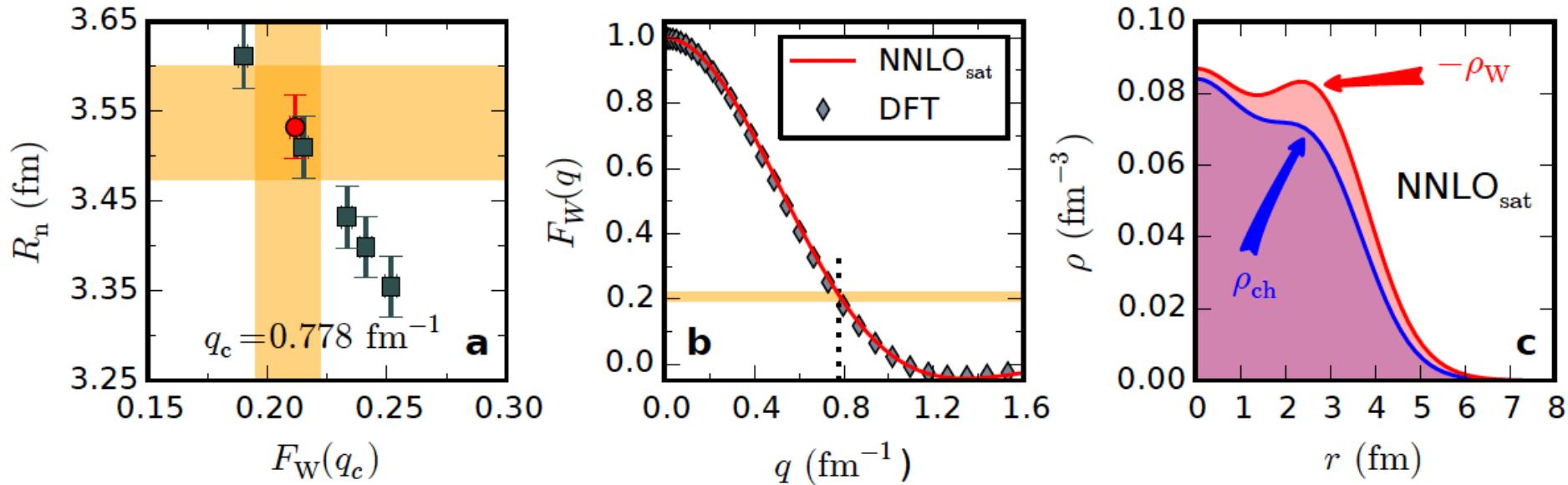
# Family of chiral interactions

G. Hagen et al, in preparation (2015)

Interaction	$BE$	$S_n$	$\Delta$	$R_{ch}$	$R_w$	$S_v$	$L$
NNLO <sub>sat</sub>	404(3)	9.5	2.69	3.48	3.65	26.9	40.8
1.8/2.0 (EM)	420(1)	10.1	2.69	3.30	3.47	33.3	48.6
2.0/2.0 (EM)	396(2)	9.3	2.66	3.34	3.52	31.4	46.7
2.2/2.0 (EM)	379(2)	8.8	2.61	3.37	3.55	30.2	45.5
2.8/2.0 (EM)	351(3)	8.0	2.41	3.44	3.62	28.5	43.8
2.0/2.0 (PWA)	346(4)	7.8	2.82	3.55	3.72	27.4	44.0
Experiment	415.99	9.995	2.399	3.477			

# Weak charge form-factor of $^{48}\text{Ca}$

G. Hagen *et al*, Nature Physics (2015) doi:10.1038/nphys3529



***Ab-initio* predictions:**

$$0.195 \lesssim F_W(q_c) \lesssim 0.222, \quad 3.59 \lesssim R_W \lesssim 3.71 \text{ fm}, \quad 0.12 \lesssim R_{\text{skin}} \lesssim 0.15 \text{ fm}$$

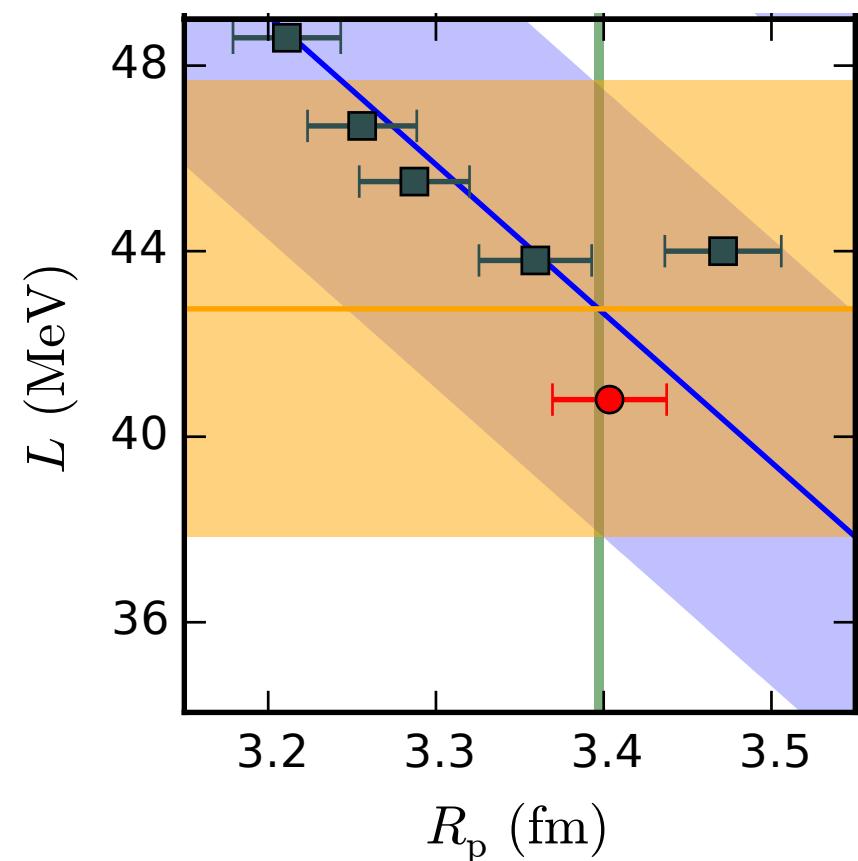
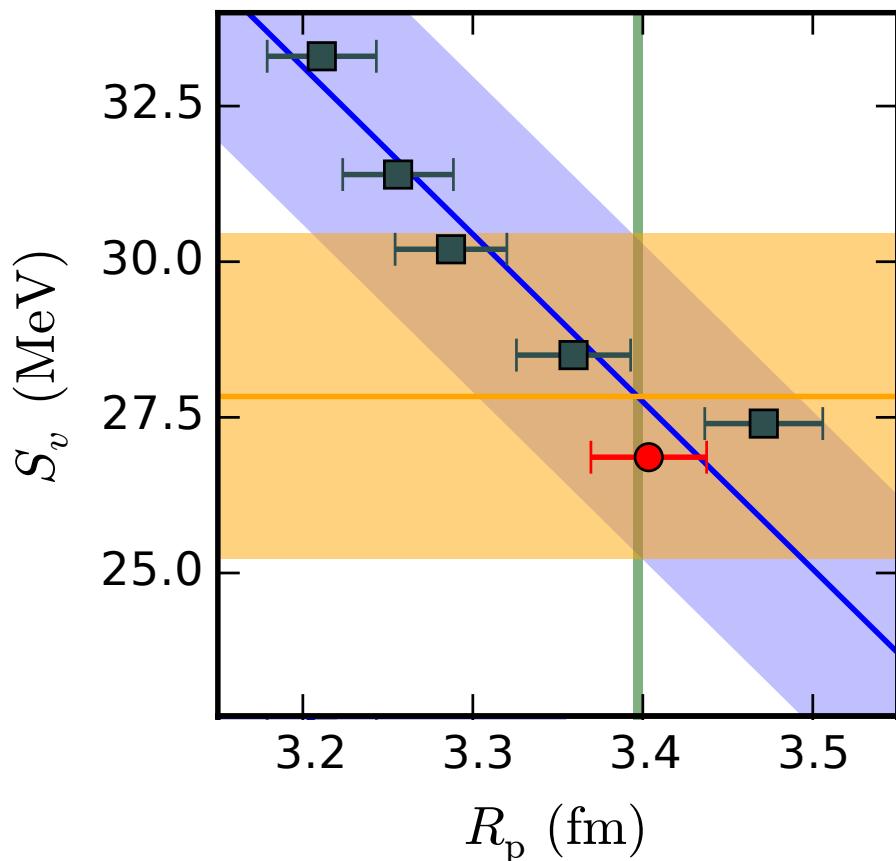
**DFT predictions:**

$$\text{SV-min: } F_W(q_C) = 0.1986 \quad R_{\text{skin}} = 0.1830 \text{ fm}$$

$$\text{FSUBJ: } F_W(q_C) = 0.205 \quad R_{\text{skin}} = 0.1925 \text{ fm}$$

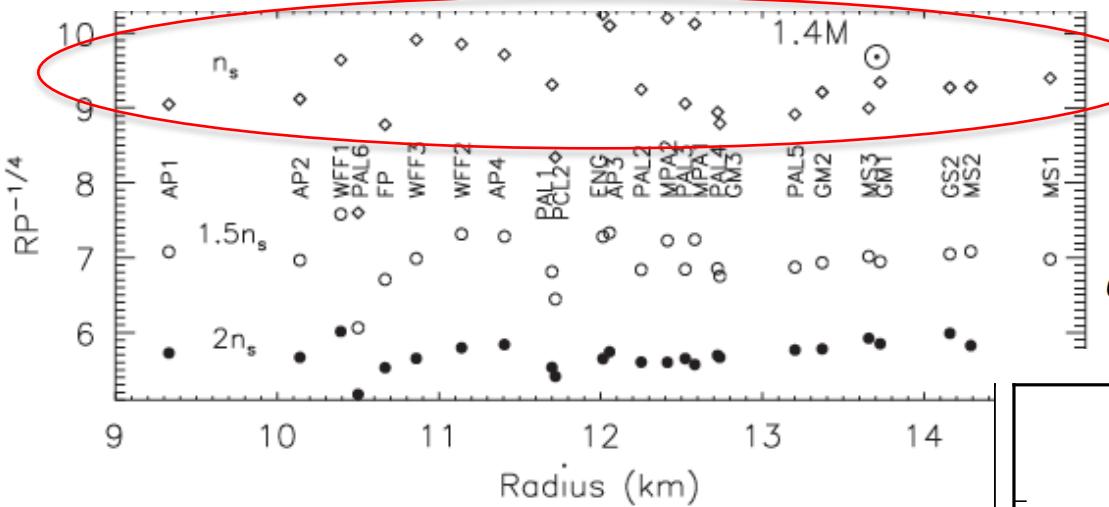
Can we reliably extract the neutron skin from a single measurement?

# Symmetry energy and L from chiral EFT



- $S_v$  and  $L$  correlates with dipole polarizability and proton radius
- Ab-initio prediction for  $S_v$  and  $L$  from chiral EFT:  
 $25.2 \lesssim S_v \lesssim 30.4$  MeV,  $37.8 \lesssim L \lesssim 47.7$  MeV
- Consistent with Lattimer and Lim:  
 $29 \lesssim S_v \lesssim 32.7$  MeV and  $40.5 \lesssim L \lesssim 61.9$  MeV

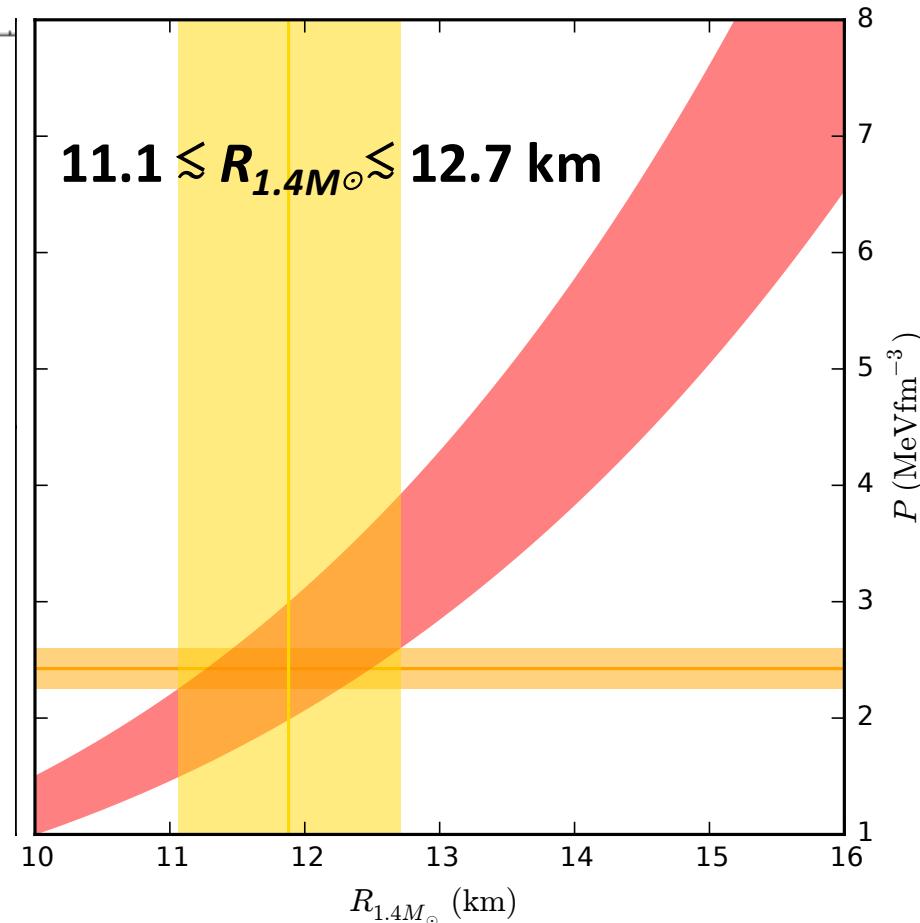
# The radius of a $1.4M_{\odot}$ neutron star



Lattimer and Prakash, Phys. Rep. 442, 109 (2007)

$$R(M) = C(\rho, M)(P(\rho)/\text{MeV fm}^{-3})^{1/4}$$

$$C(\rho = 0.16 \text{ fm}^{-3}, M = 1.4 M_{\odot}) = 9.52 \pm 0.49 \text{ km}$$

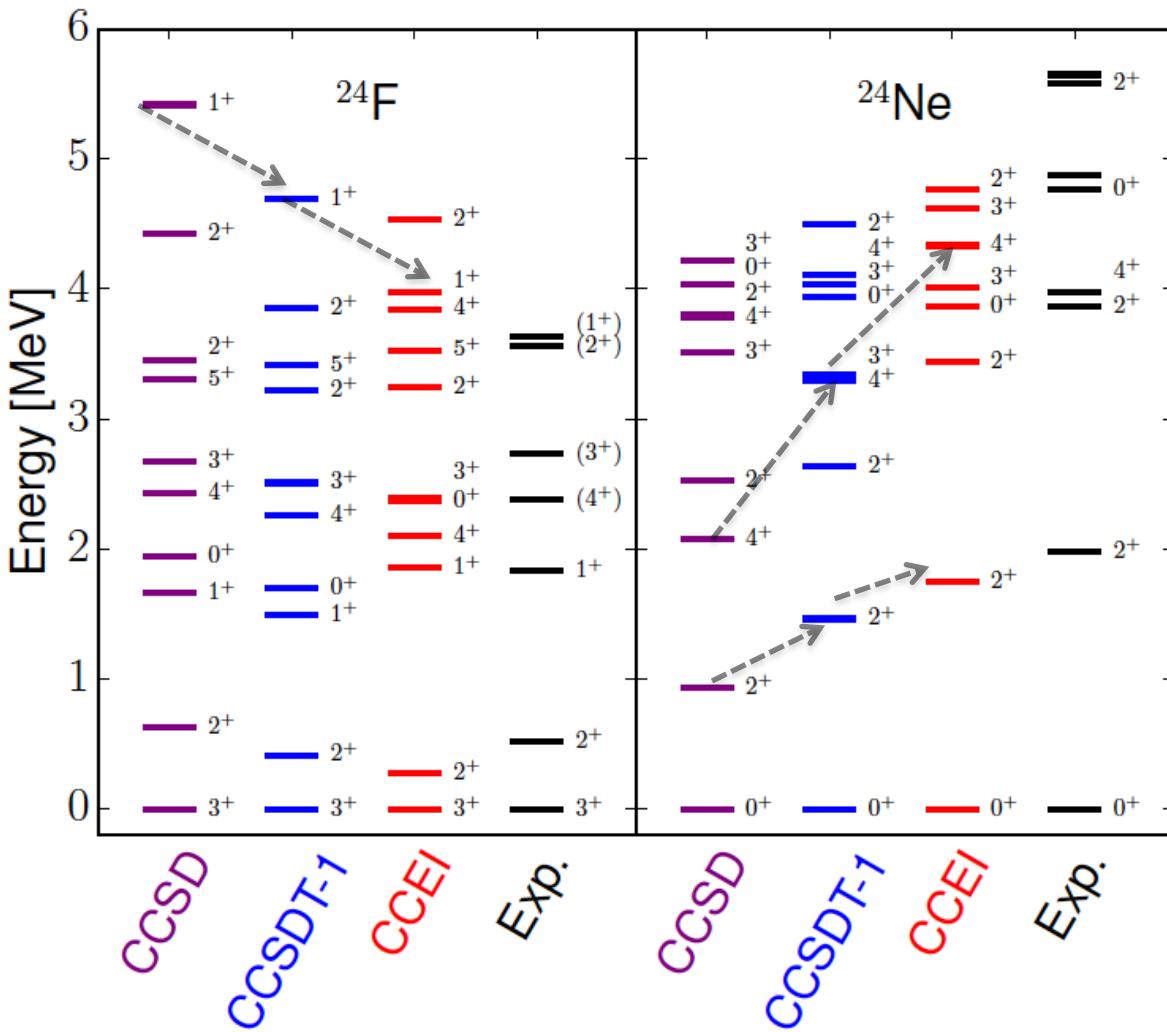


- Use empirical power law that relates neutron-star radii to the pressure  $P$  at nuclear saturation density.
- $P$  is strongly connected to  $S_v$  and  $L$
- We correlate  $P$  with the charge radius of  $^{48}\text{Ca}$  and get at an estimate:  
 $2.3 \lesssim P \lesssim 2.6 \text{ MeV fm}^{-3}$
- Ab-initio prediction consistent with Lattimer and Lim  $10.7 \lesssim R_{1.4M_{\odot}} \lesssim 13.1$

# Deformed sd-shell nuclei from first principles

G. R. Jansen, A. Signoracci, GH, P. Navratil arXiv:1511.00757 (2015).

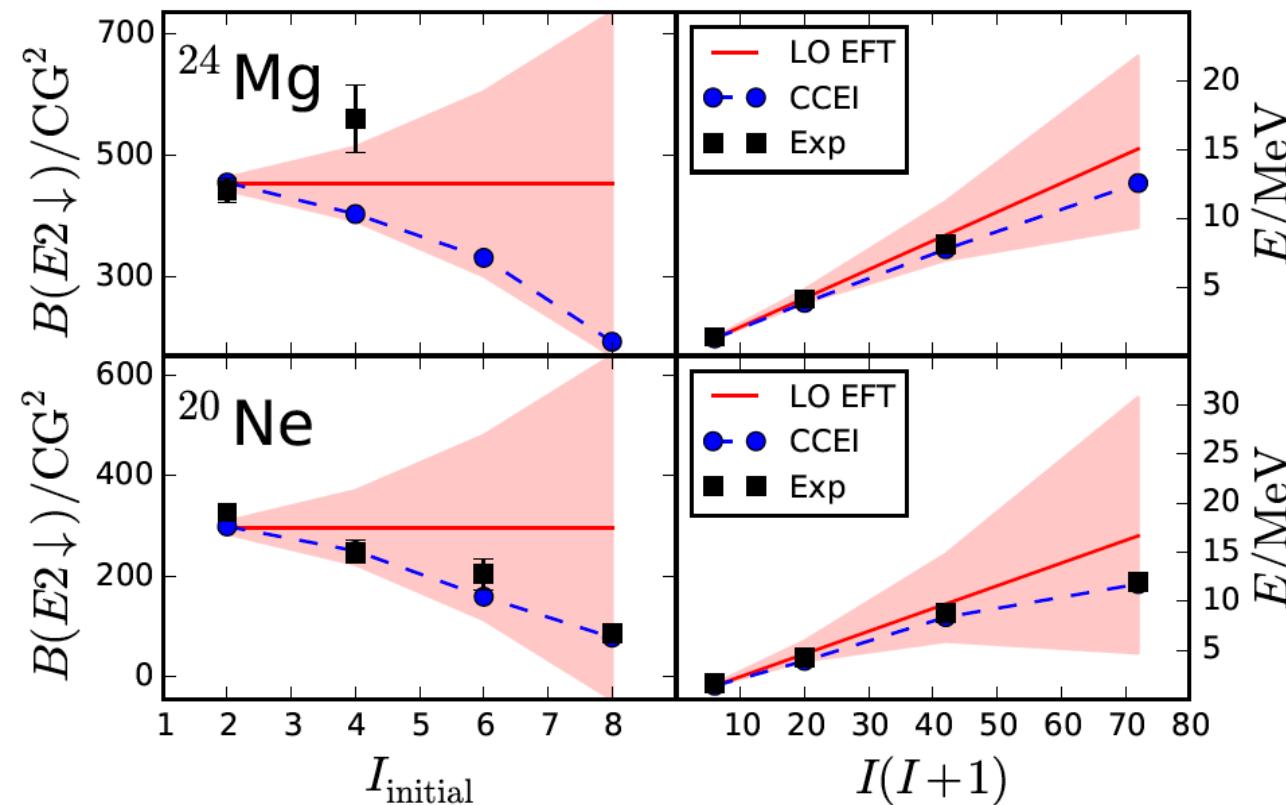
Single and double charge exchange equation-of-motion coupled cluster way to compute ground- and excited states of open-shell nuclei



- Good agreement between EOM-CCSD, EOM-CCSDT-1 and CCEI for excited states in  $^{24}\text{F}$
- Role of 3p-3h excitations small except for second 1<sup>+</sup> state
- For  $^{24}\text{Ne}$  we find overall satisfactory agreement between EOM-CCSDT-1 and CCEI.
- Larger role of 3p-3h excitations and they overall improve the agreement with CCEI.

# Deformed sd-shell nuclei from first principles

G. R. Jansen, A. Signoracci, GH, P. Navratil arXiv:1511.00757 (2015).



Rotational bands emerge from *ab-initio* calculations. CCEI results are within the uncertainties of EFT at LO.

Effective theory for deformed nuclei: E. A. Coello Perez and T. Papenbrock PRC 92, 014323 (2015)

LO EFT is straight line (rigid rotor). Error band from fit to first two excited states.

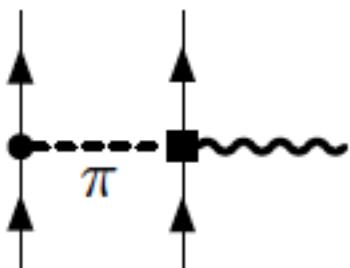
Within EFT, the  $B(E2)$  are that of a non-rigid rotor, and the deviation from the rigid rotor is as expected from the spectrum.

$$E(I) = \frac{I(I+1)}{2C_0} - \frac{C_2}{4C_0^4} (I(I+1))^2$$

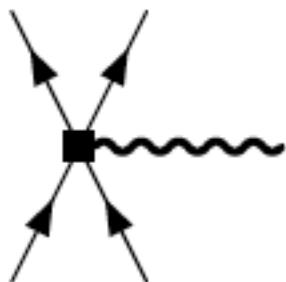
$$B(E2, i \rightarrow f) = \frac{(aqR)^2}{60} \left( C_{I_i 020}^{I_f 0} \right)^2 \left[ 1 + \frac{b}{a} I_i (I_i - 1) \right]$$

# Normal ordered one- and two-body current

Gamow-Teller matrix element:



$$\hat{O}_{\text{GT}} \equiv \hat{O}_{\text{GT}}^{(1)} + \hat{O}_{\text{GT}}^{(2)} \equiv g_A^{-1} \sqrt{3\pi} E_1^A$$



Normal ordered operator:

$$\hat{O}_{\text{GT}} = O_N^0 + O_N^1 + O_N^2$$

$$O_N^0 = \sum_{i \leq E_f} \langle i | O^{(1)} | i \rangle + \frac{1}{2} \sum_{i,j \leq E_f} \langle ij | O^{(2)} | ij \rangle$$

$$O_N^1 = \sum_{pq} \langle p | O^{(1)} | q \rangle \{ p^\dagger q \} + \sum_{pq} \sum_{i \leq E_f} \langle pi | O^{(2)} | qi \rangle \{ p^\dagger q \}$$

$$O_N^2 = \frac{1}{4} \sum_{pqrs} \langle pq | O^{(2)} | rs \rangle \{ p^\dagger q^\dagger sr \}$$

# One- and two-body currents and normal ordering in Coupled-Cluster

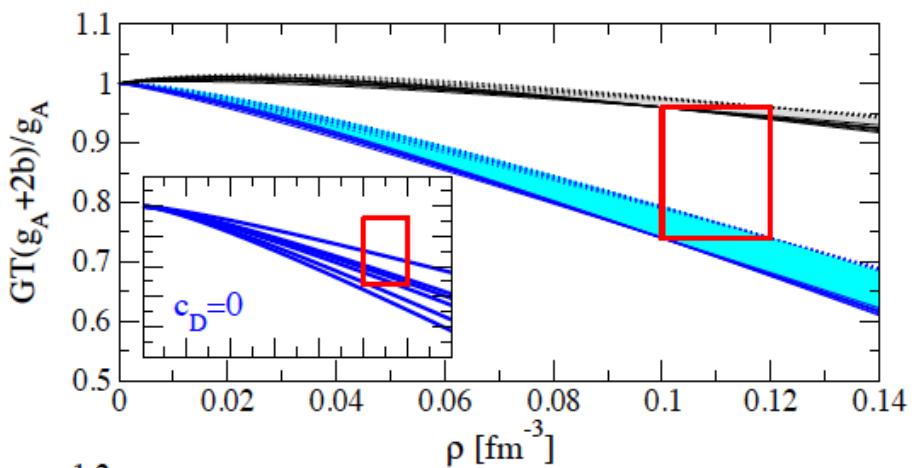
CCSD similarity transformed normal-ordered current operator:

$$\overline{O_{\text{GT}}} = e^{-T} O_N e^T = e^{-T} O_N^1 e^T + e^{-T} \cancel{O_N^2} e^T$$

3-body terms                            6-body terms

Normal ordered 1-body contribution

$$e^{-T} O_N^2 e^T \approx O_N^2 = \frac{1}{4} \sum_{pqrs} \langle pq | O^{(2)} | rs \rangle \{ p^\dagger q^\dagger s r \}$$

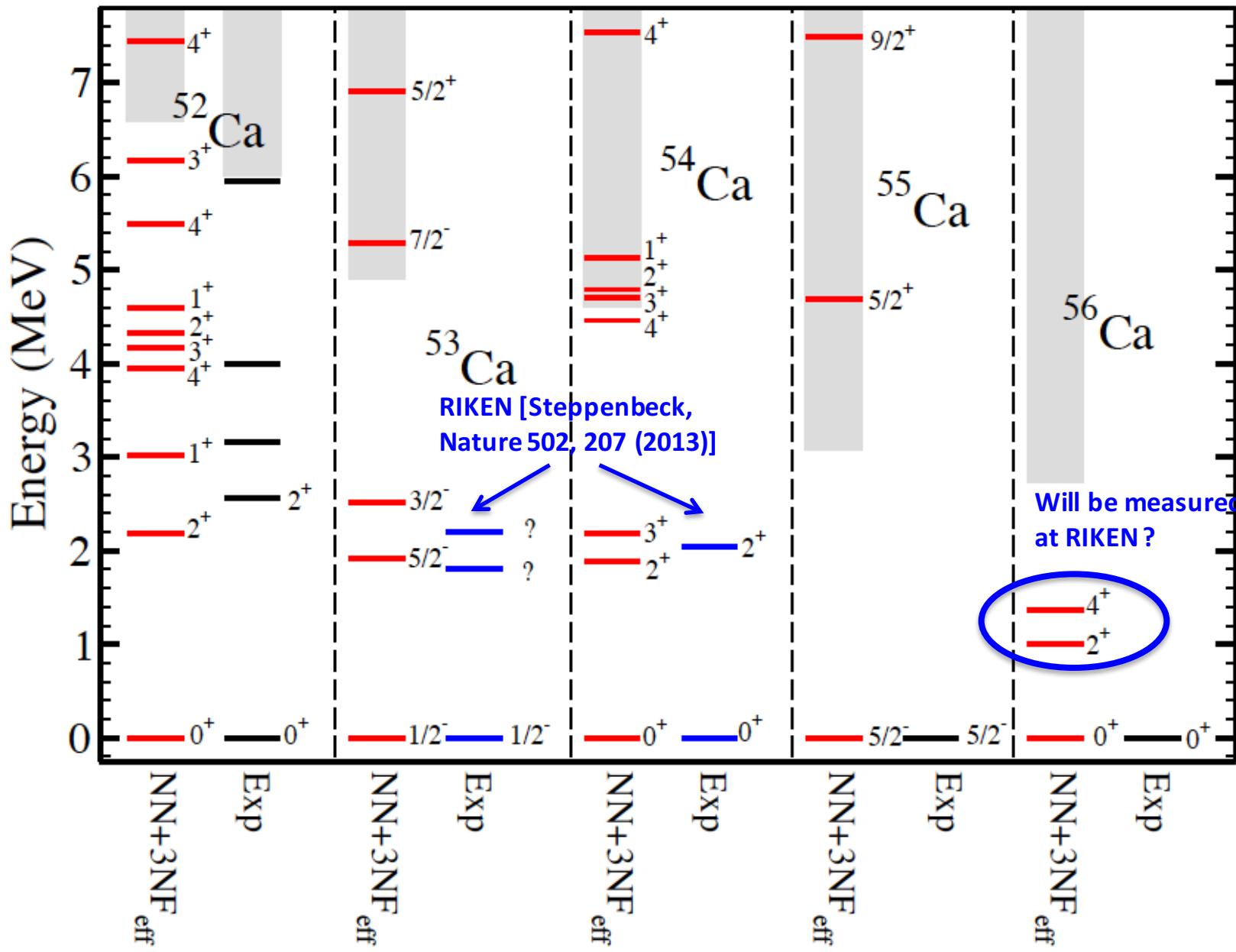


J. Menéndez, D. Gazit, A. Schwenk  
PRL 107, 062501 (2011)

Normal order with respect to free Fermi gas.  
One-body normal ordered approximation gives  
quenching of  $g_A$  by a factor  $q = 0.74...0.96$  for  
different set of coupling constants

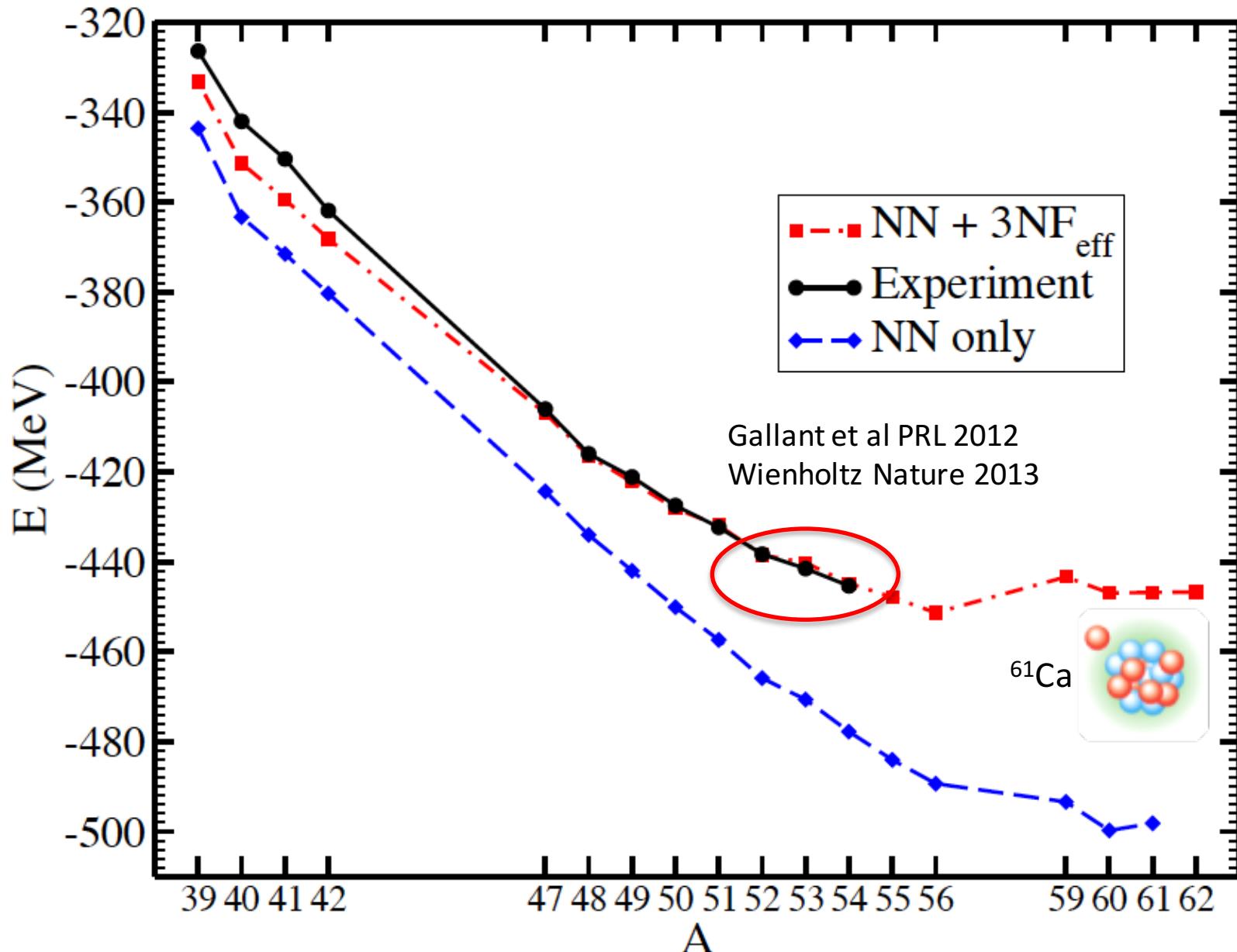
# Spectra and shell evolution in Calcium isotopes

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

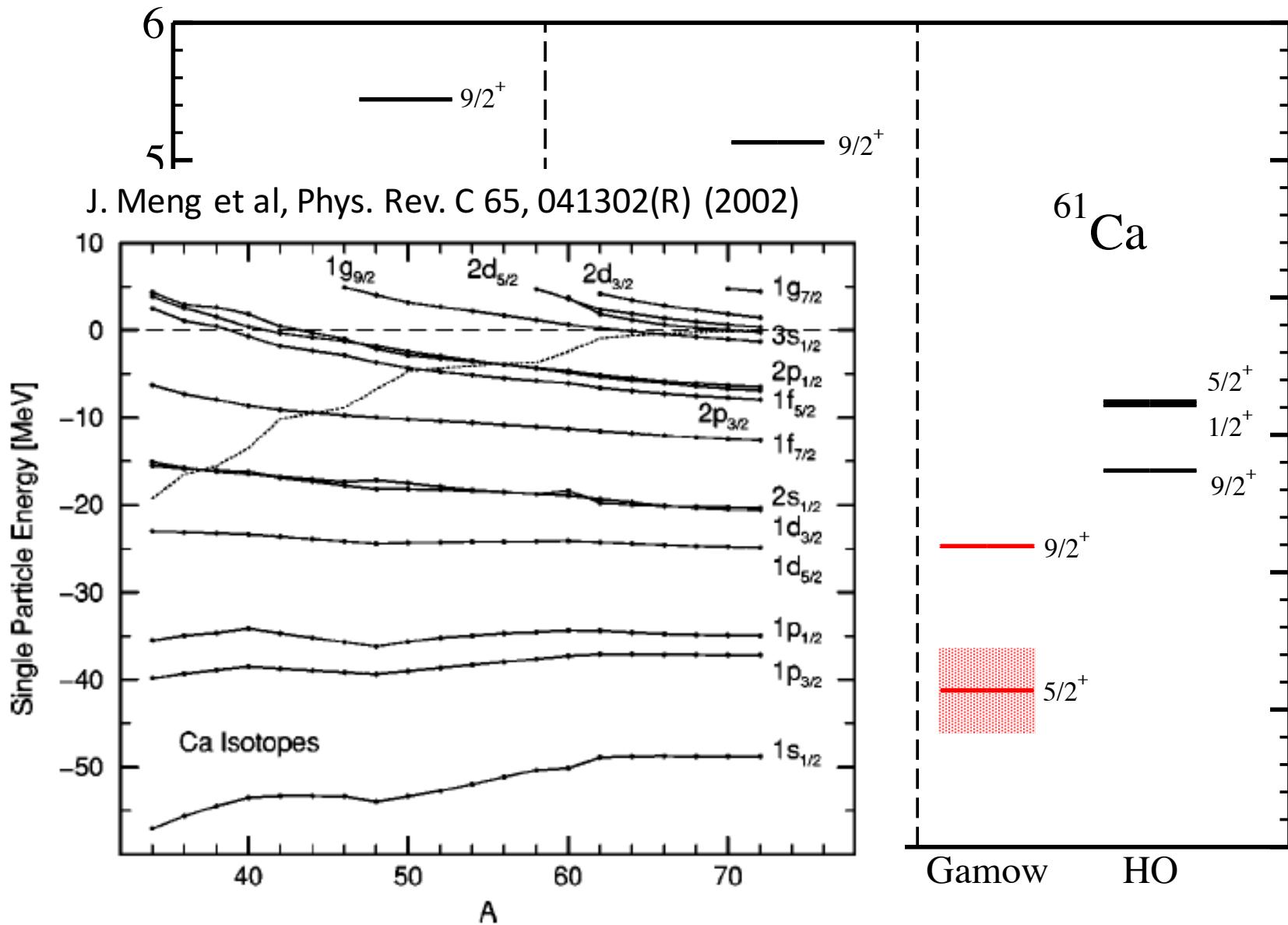


# Calcium isotopes from chiral interactions

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

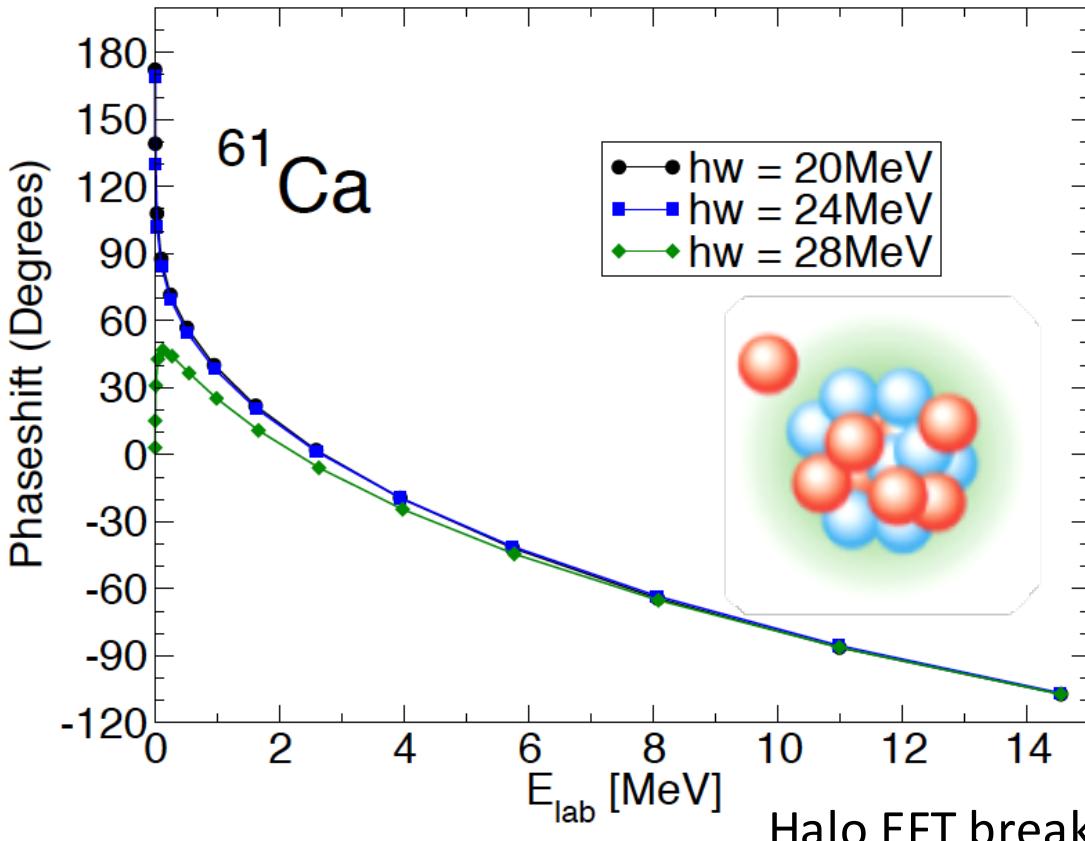


# Effect of continuum on excited states in odd neutron rich Calcium isotopes



# Efimov physics around neutron rich $^{60}\text{Ca}$

G. Hagen, P. Hagen, H.-W. Hammer, and L. Platter, PRL 111, 132501 (2013)

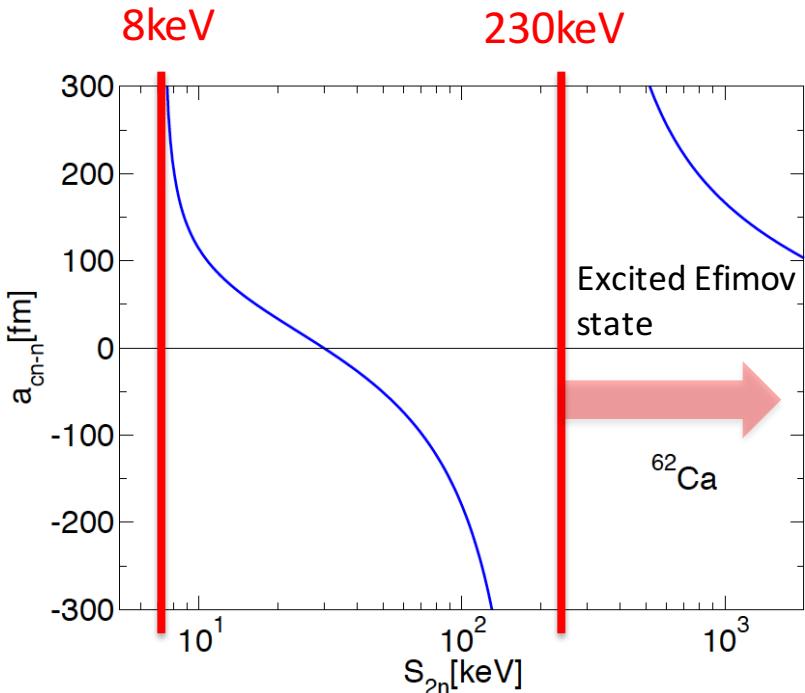


- Large S-wave scattering length in  $^{61}\text{Ca}$  implies Halo phenomena
- Core- $n$ - $n$  are effective degrees of freedom
- New Approach: Merge halo-EFT and input from CC to study properties of  $^{62}\text{Ca}$

$\hbar\omega$ [MeV]	$a_{cn}$ [fm]	$r_{cn}$ [fm]	$S_n$ [keV]	$S_{\text{deep}}$ [keV]
20	55.0	8.8	8.4	544
24	53.2	9.1	5.3	509
28	-26.1	10.8	-	361

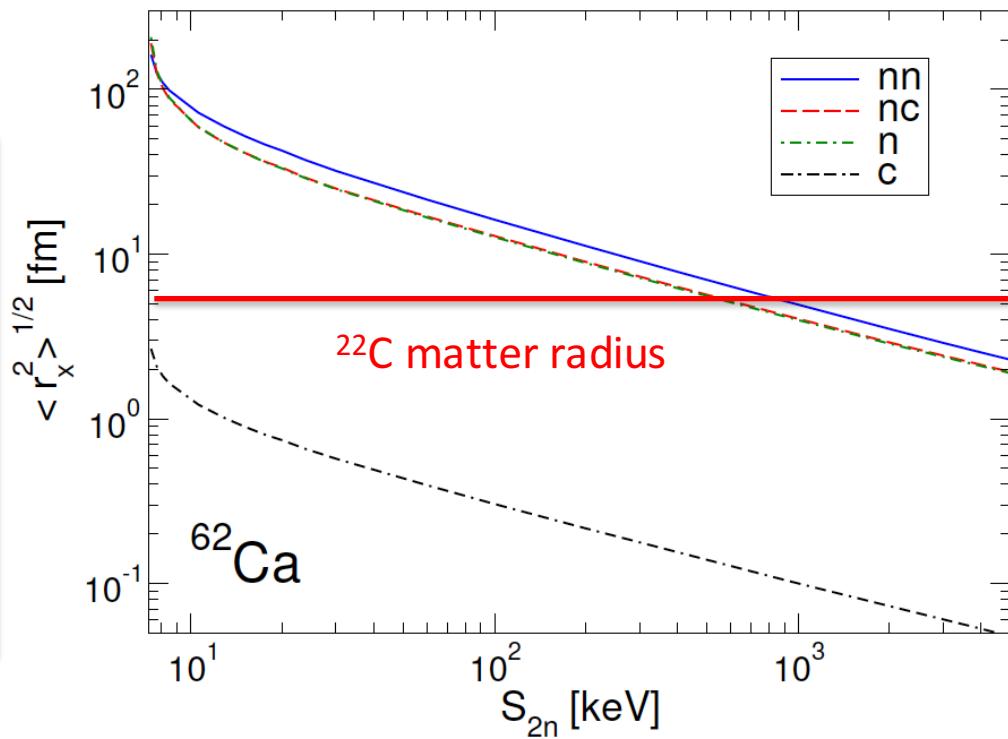
$J^\pi$	$^{53}\text{Ca}$		$^{55}\text{Ca}$		$^{61}\text{Ca}$	
	$\text{Re}[E]$	$\Gamma$	$\text{Re}[E]$	$\Gamma$	$\text{Re}[E]$	$\Gamma$
$5/2^+$	1.99	1.97	1.63	1.33	1.14	0.62
$9/2^+$	4.75	0.28	4.43	0.23	2.19	0.02

# Efimov physics around neutron rich $^{60}\text{Ca}$

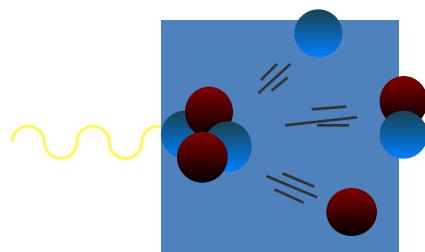


- $^{22}\text{C}$  is the largest known two-neutron halo  $R_{\text{rms}} \sim 5.4\text{fm}$  (Tanaka PRL 2010)
- Computed matter radii for  $^{62}\text{Ca}$  indicates that it can be the largest and heaviest halo in the chart of nuclei so far.

- For  $S_{2n}$  larger than  $\sim 230\text{keV}$  another state appears in the spectrum
- $^{62}\text{Ca}$  is likely to have an Efimov state (large halo)
- It is conceivable that  $^{62}\text{Ca}$  displays an excited Efimov state



# Break-up observables for medium-mass nuclei



Cross section is related to the Response Function in the continuum

$$S(\omega) = \sum_f \left| \langle \psi_f | \hat{O} | \psi_0 \rangle \right|^2 \delta(E_f - E_0 - \omega)$$



Cannot be calculated beyond 3-body break-up even for A=4

**Solution:** Lorentz Integral Transform method

(Efros, Leidemann, Orlandini, Barnea, Bacca)

Efros *et al.*, J. Phys. G: Nucl. Part. Phys. 34 (2007)

$$\mathcal{L}(\sigma, \Gamma) = \int d\omega \frac{S(\omega)}{(\omega - \sigma)^2 + \Gamma^2} = \langle \tilde{\Psi} | \tilde{\Psi} \rangle$$

$$(H - E_0 - \sigma + i\Gamma) |\tilde{\Psi}\rangle = O|\Psi_0\rangle$$

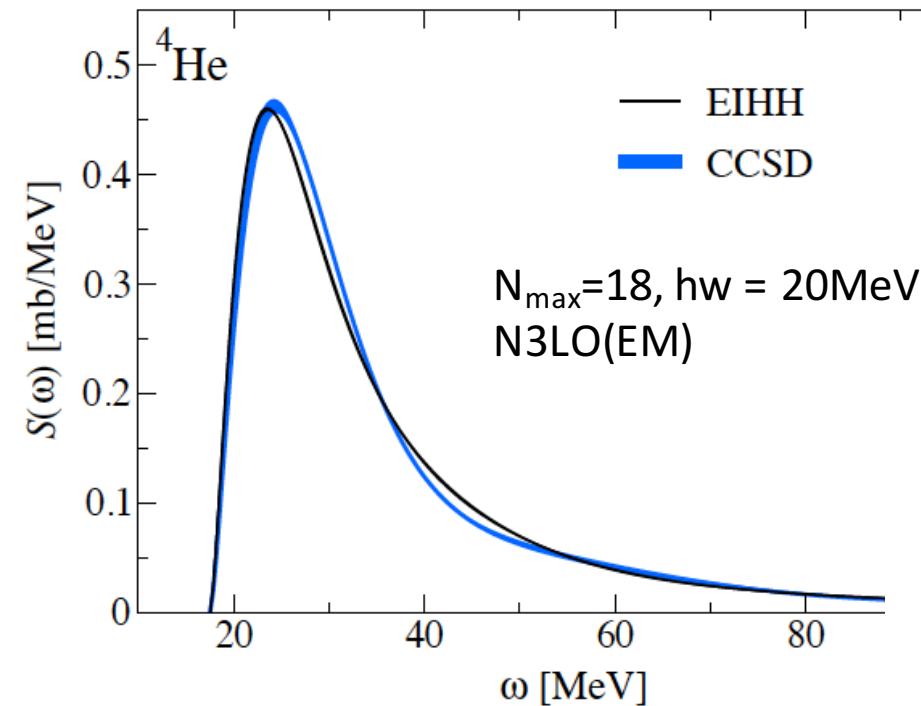


Bound-state-like object. Need bound state technique to calculate it

# Dipole response in ${}^4\text{He}$ from coupled-cluster

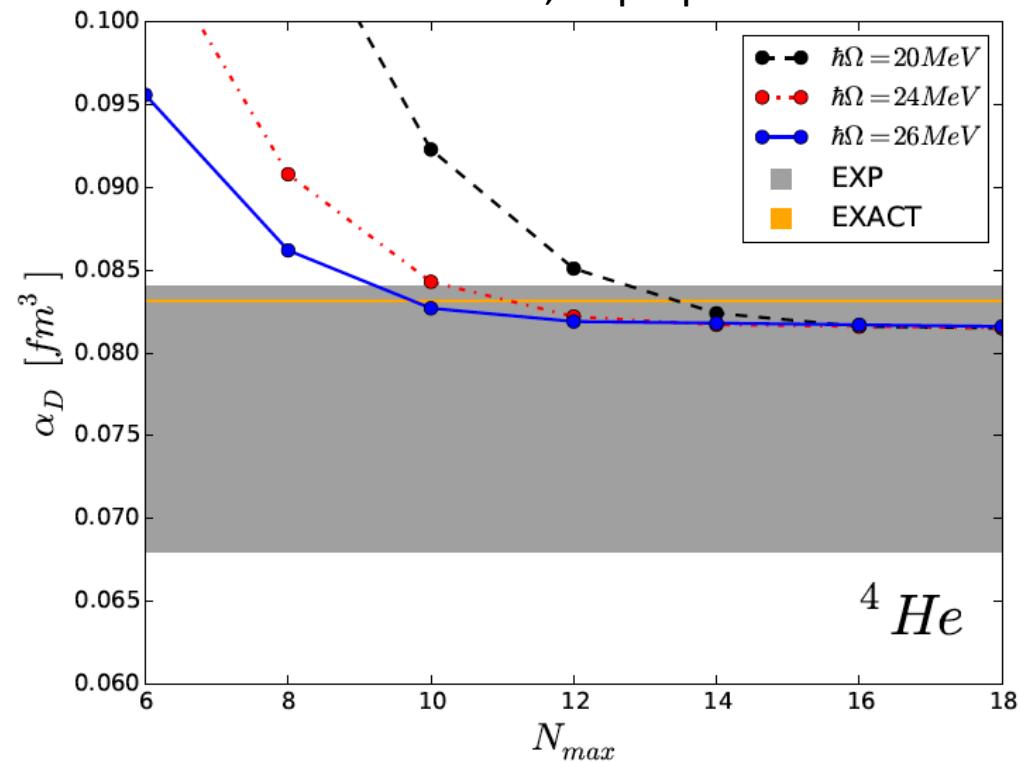
S. Bacca, N. Barnea, G. Hagen, G. Orlandini, T. Papenbrock, PRL 111, 143402 (2013).

S. Bacca, N. Barnea, G. Hagen, M. Miorelli, G. Orlandini, T. Papenbrock, PRC 90, 064610 (2014)



Lorentz Integral transform from coupled-cluster benchmarked with “exact” hyper-spherical harmonics for  ${}^4\text{He}$

M. Miorelli *et al*, in preparation



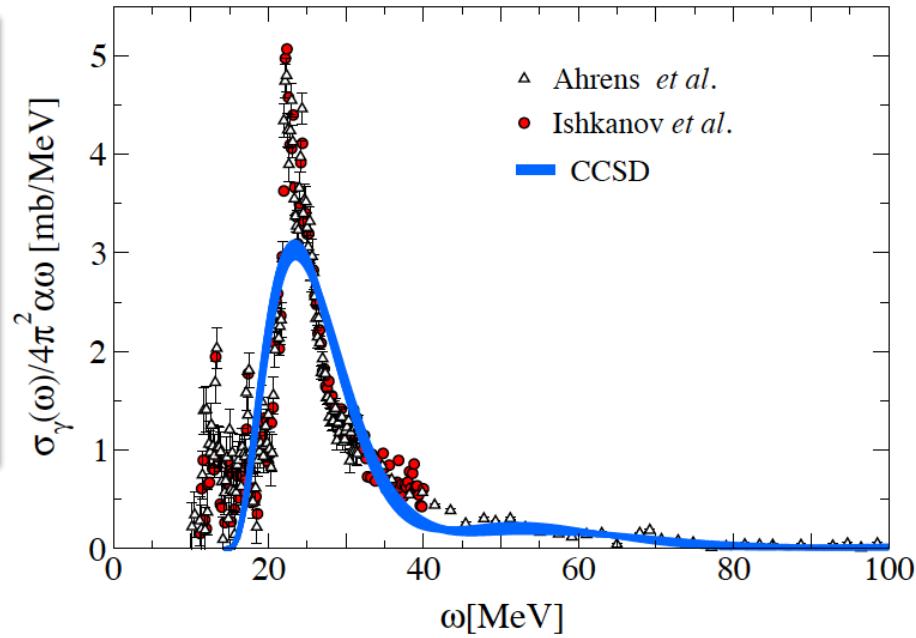
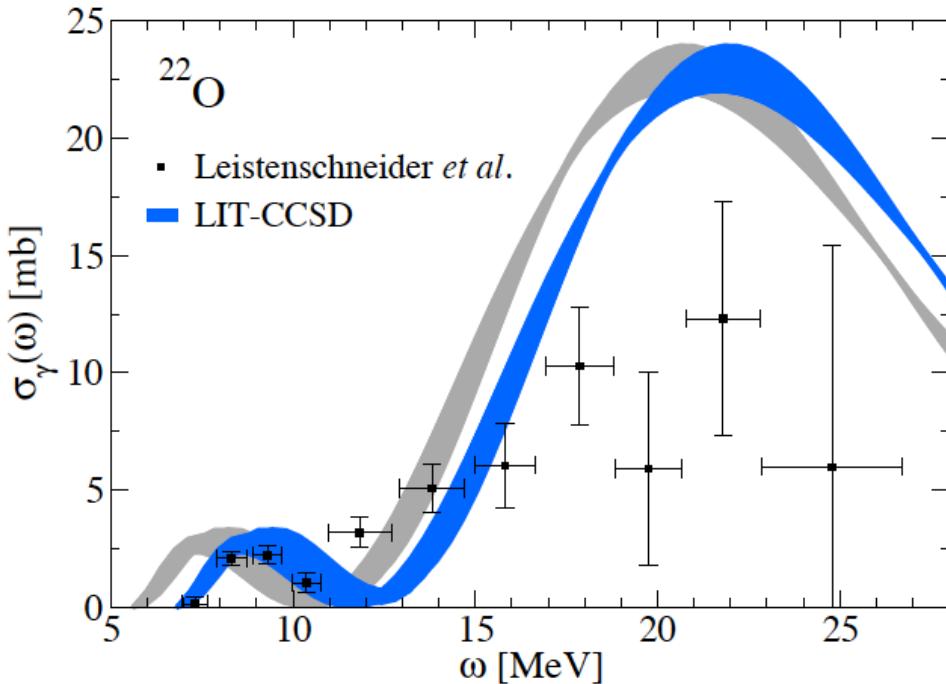
Dipole polarizability in  ${}^4\text{He}$  from CCSD within 1% of exact Hyper-spherical harmonics

$$\alpha_D = 2\alpha \int_{\omega_{\text{th}}}^{\infty} d\omega \frac{S(\omega)}{\omega}$$

# Dipole response in $^{16,22}\text{O}$

We find low-lying dipole strength consistent with experiment

Total dipole strength is enhanced in  $^{22}\text{O}$  as compared to  $^{16}\text{O}$  which can be explained by the excess of neutrons in  $^{22}\text{O}$

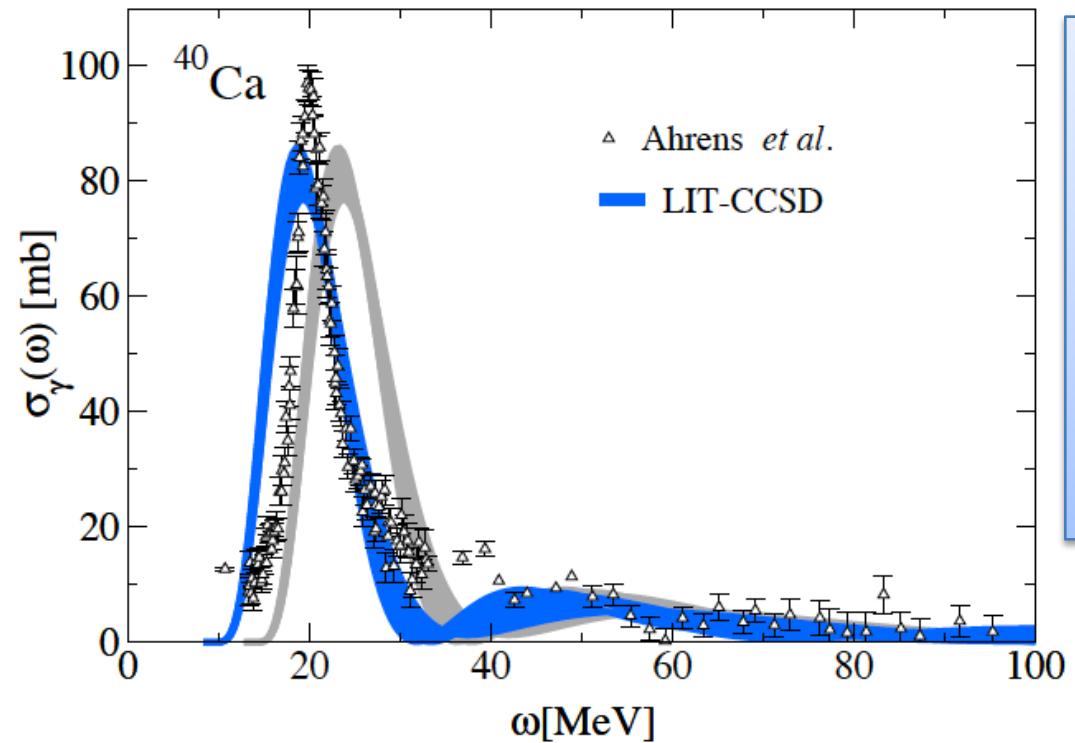


S. Bacca, N. Barnea, G. Hagen, G. Orlandini, T. Papenbrock, PRL 111, 143402 (2013).

S. Bacca, N. Barnea, G. Hagen, M. Miorelli, G. Orlandini, T. Papenbrock, PRC 90, 064610 (2014)

# Dipole response and polarizability in $^{40}\text{Ca}$

## $\text{N}^3\text{LO}$ Entem & Machleidt (NN only)



$$R_{\text{ch}}(\text{Th}) = 3.05 \text{ fm}$$

$$R_{\text{ch}}(\text{Exp}) = 3.48 \text{ fm}$$

$$E(\text{Th}) = 362 \text{ MeV}$$

$$E(\text{Exp}) = 342 \text{ MeV}$$

- Dipole response in  $^{40}\text{Ca}$  compared to data.
- Dipole resonance at too high energy, implies too small electric dipole polarizability.

$$\alpha_D(\text{Th}) = 1.47 \text{ fm}^3$$

$$\alpha_D(\text{Exp}) = 2.23(3) \text{ fm}^3$$

Current chiral interactions do not have good saturation properties. Radii and binding energies are off the experimental target values

**How to solve the problem of saturation?**

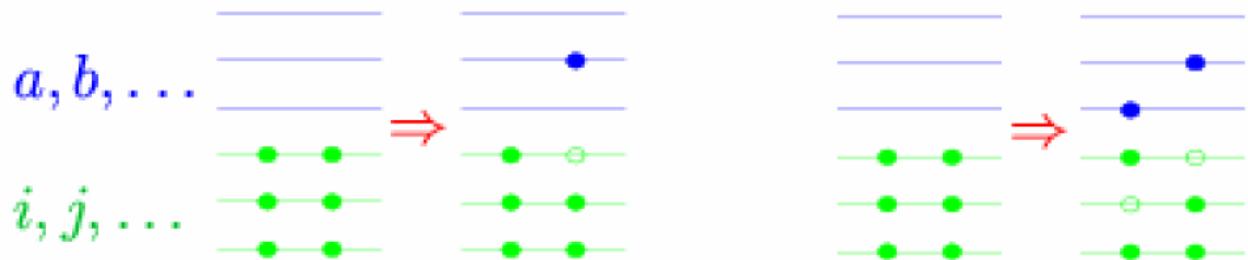
# Coupled-cluster method (in CCSD approximation)

Ansatz:

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

- ☺ Scales gently (polynomial) with increasing problem size  $\mathcal{O}^2 u^4$ .
- ☺ 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!



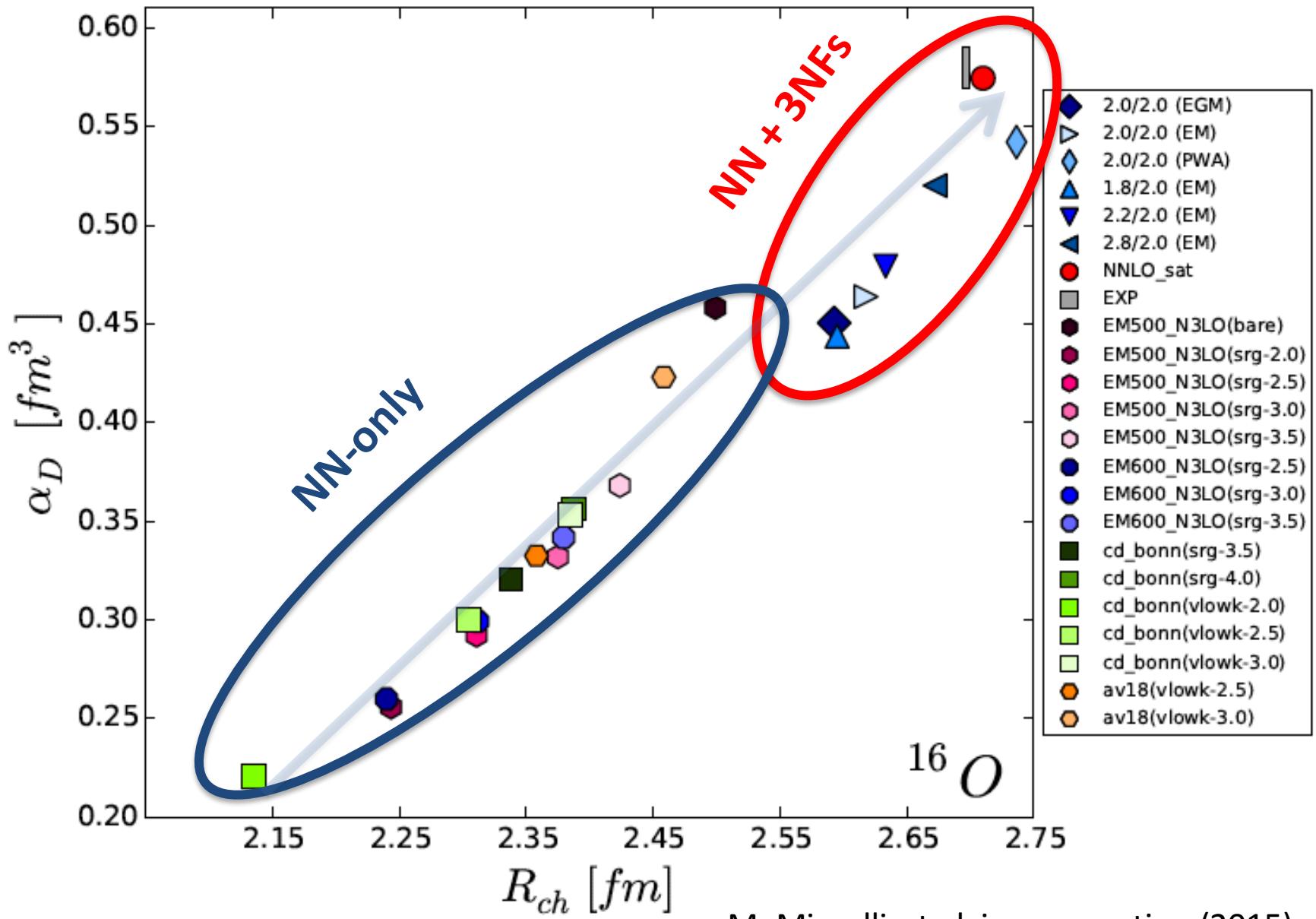
Coupled cluster equations

$$\begin{aligned} E &= \langle \Phi | \bar{H} | \Phi \rangle \\ 0 &= \langle \Phi_i^a | \bar{H} | \Phi \rangle \\ 0 &= \langle \Phi_{ij}^{ab} | \bar{H} | \Phi \rangle \end{aligned}$$

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

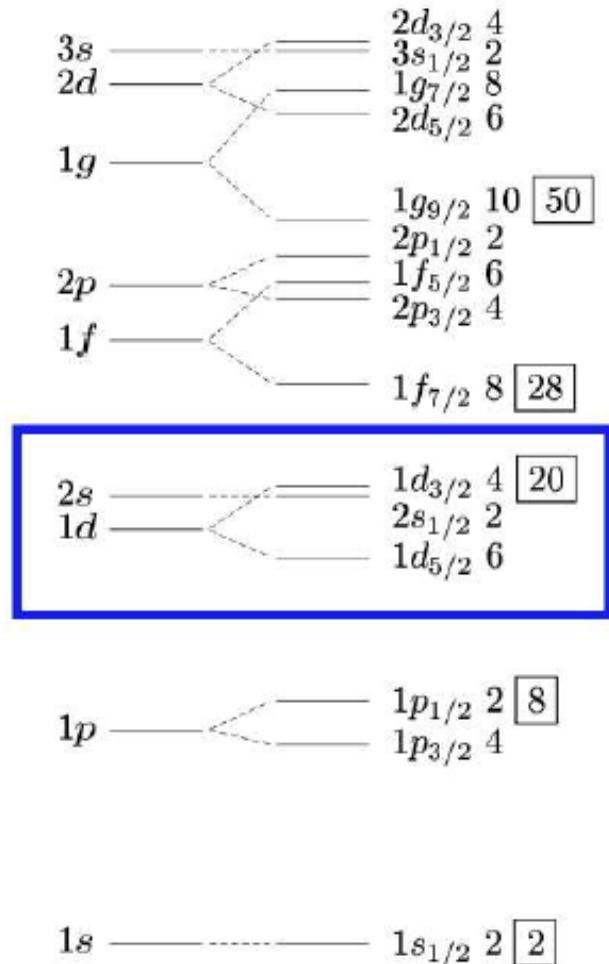
$$\bar{H} \equiv e^{-T} H e^T = (H e^T)_c = \left( H + H T_1 + H T_2 + \frac{1}{2} H T_1^2 + \dots \right)_c$$

# Dipole polarizability of $^{16}\text{O}$

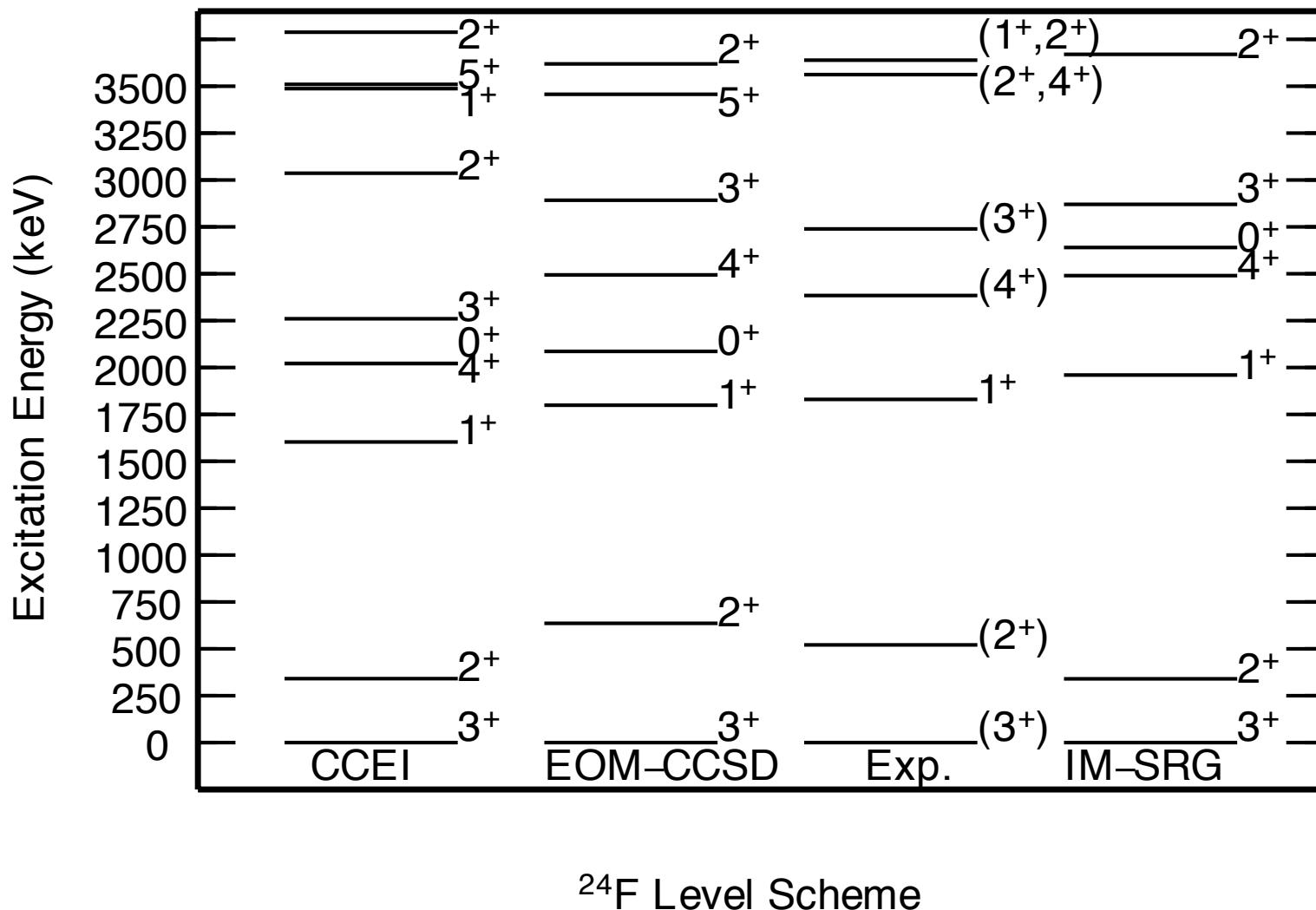


# Coupled-cluster effective interaction in practice

- Obtain excited states of  $A_c+1$  and  $A_c+2$  from **PA-EOMCCSD(2p1h)** and **2PA-EOMCCSD(3p1h)**
- The  $A_c+1$  Hamiltonian is diagonal and given by the  $A_c+1$  lowest eigenvalues
- Are results sensitive to the choice of left/right eigenvector projections for  $A+2$ ?
- How do we choose the  $d$  “exact”  $A+2$  wavefunctions?
  - Largest overlap with model space
  - Lowest energies



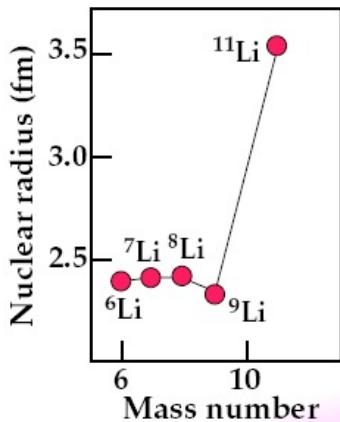
# Benchmarking different methods in $^{24}\text{F}$



$^{24}\text{F}$  Level Scheme

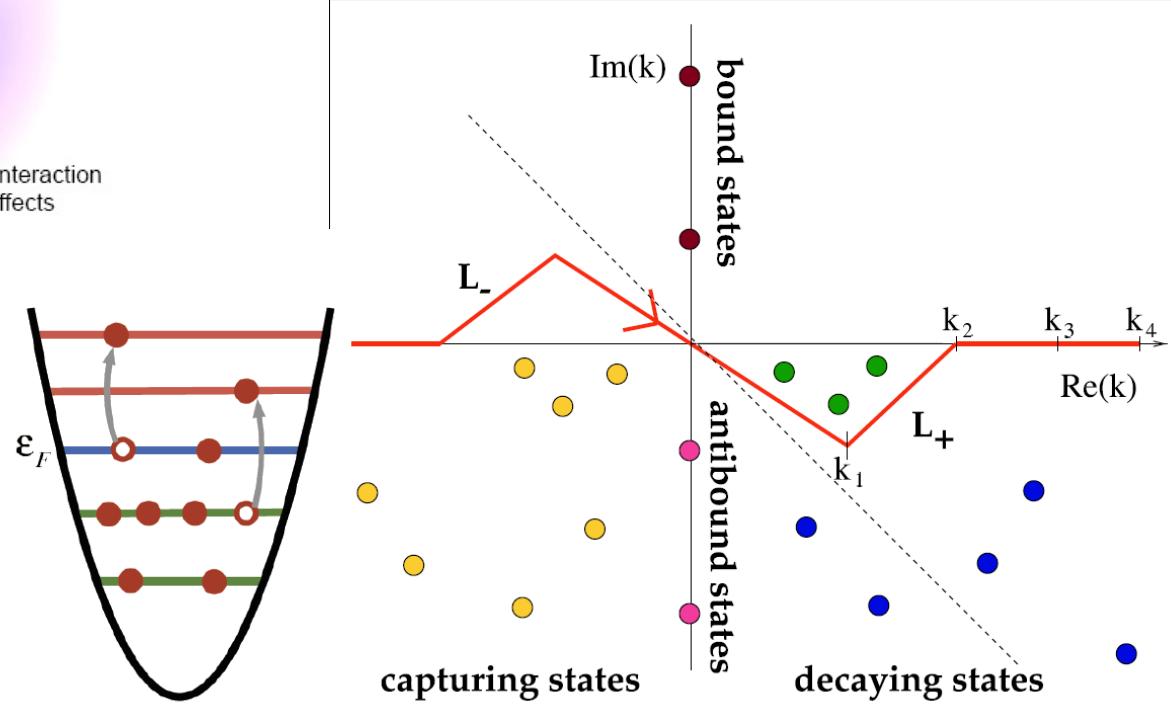
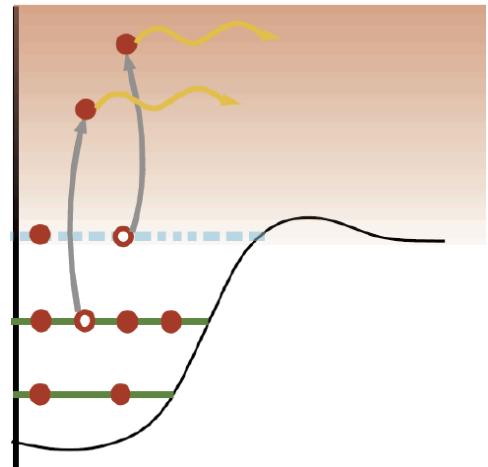
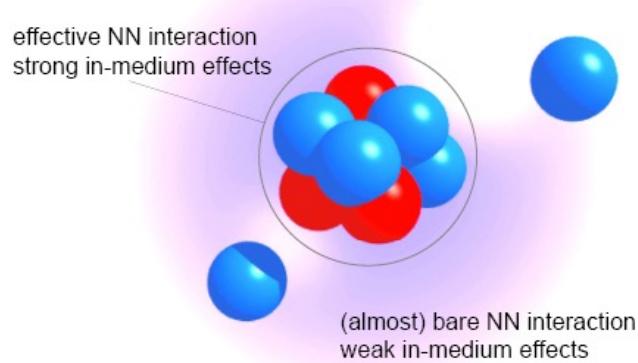
IM-SRG: L. Caceres et al arXiv:1501.01166 (2015)

# 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)



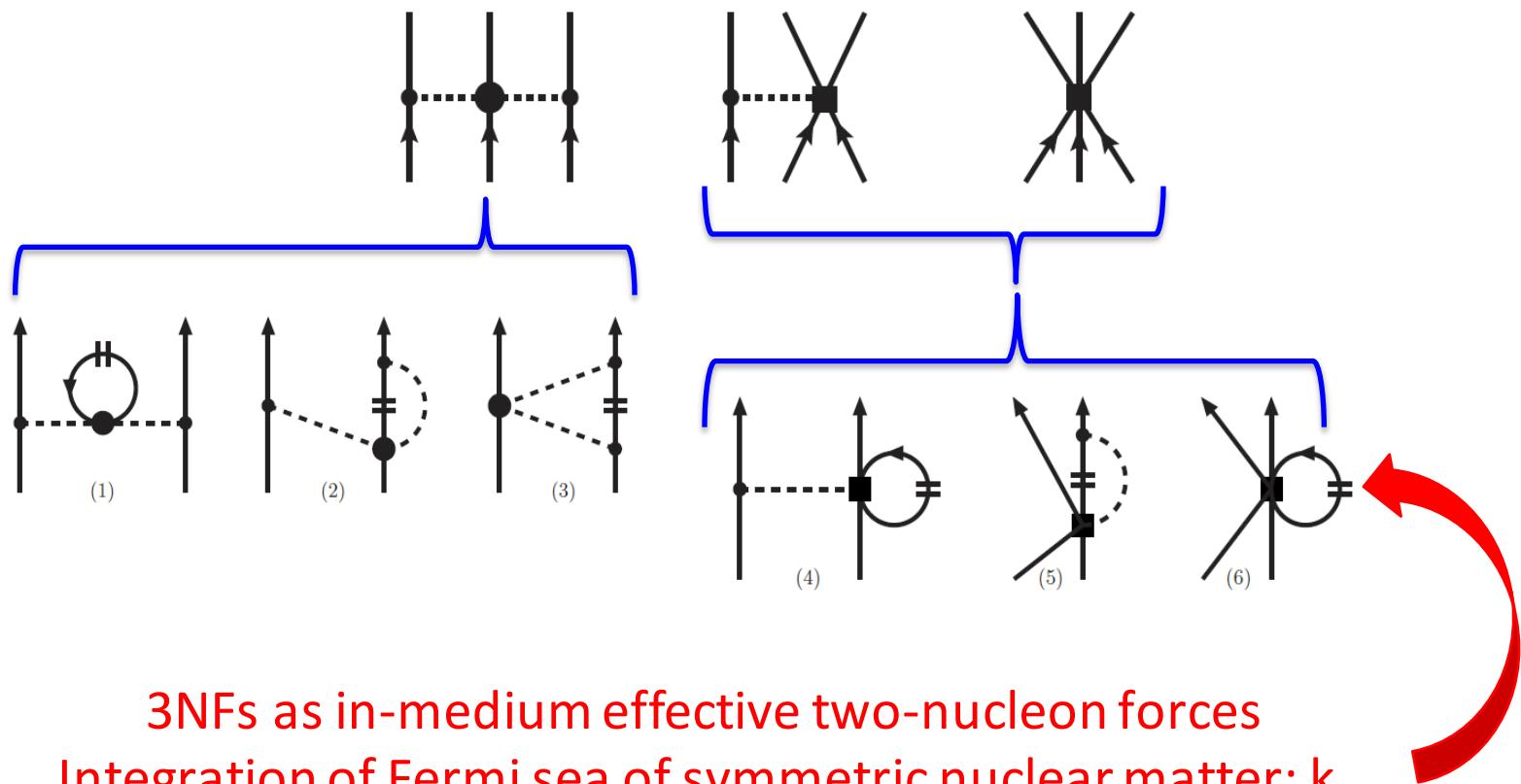
The Berggren completeness treats bound, resonant and scattering states on equal footing.

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).

# Including the effects of 3NFs (approximation!)

[J.W. Holt, Kaiser, Weise, PRC 79, 054331 (2009); Hebeler & Schwenk, PRC 82, 014314 (2010)]

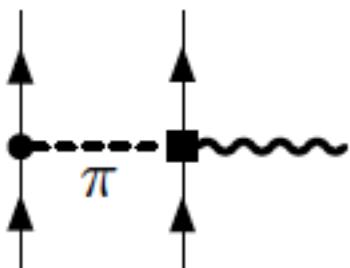


3NFs as in-medium effective two-nucleon forces  
Integration of Fermi sea of symmetric nuclear matter:  $k_F$

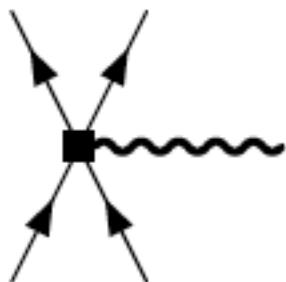
**Parameters:** For Calcium we use  $k_F = 0.95 \text{ fm}^{-1}$ ,  $c_E = 0.735$ ,  $c_D = -0.2$  from binding energy of  $^{40}\text{Ca}$  and  $^{48}\text{Ca}$  (The parameters  $c_D$ ,  $c_E$  differ from values proposed for light nuclei)

# Normal ordered one- and two-body current

Gamow-Teller matrix element:



$$\hat{O}_{\text{GT}} \equiv \hat{O}_{\text{GT}}^{(1)} + \hat{O}_{\text{GT}}^{(2)} \equiv g_A^{-1} \sqrt{3\pi} E_1^A$$



Normal ordered operator:

$$\hat{O}_{\text{GT}} = O_N^0 + O_N^1 + O_N^2$$

$$O_N^0 = \sum_{i \leq E_f} \langle i | O^{(1)} | i \rangle + \frac{1}{2} \sum_{i,j \leq E_f} \langle ij | O^{(2)} | ij \rangle$$

$$O_N^1 = \sum_{pq} \langle p | O^{(1)} | q \rangle \{ p^\dagger q \} + \sum_{pq} \sum_{i \leq E_f} \langle pi | O^{(2)} | qi \rangle \{ p^\dagger q \}$$

$$O_N^2 = \frac{1}{4} \sum_{pqrs} \langle pq | O^{(2)} | rs \rangle \{ p^\dagger q^\dagger sr \}$$

# One- and two-body currents and normal ordering in Coupled-Cluster

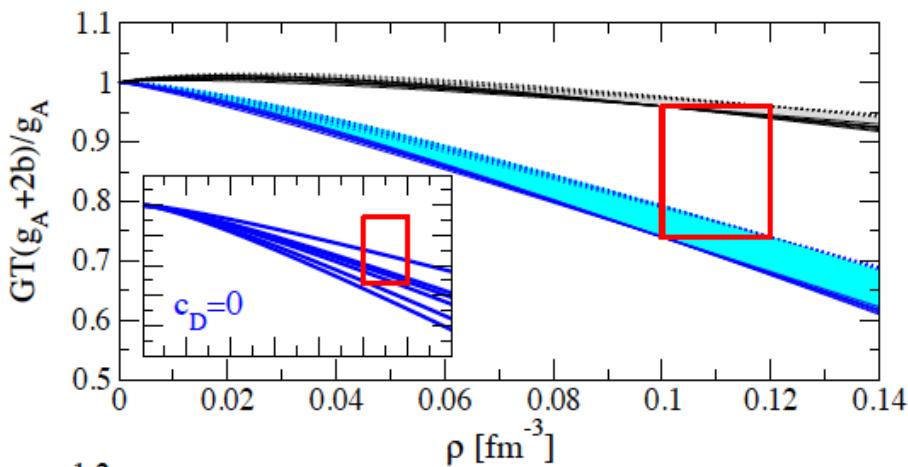
CCSD similarity transformed normal-ordered current operator:

$$\overline{O_{\text{GT}}} = e^{-T} O_N e^T = e^{-T} O_N^1 e^T + e^{-T} \cancel{O_N^2} e^T$$

3-body terms                            6-body terms

Normal ordered 1-body contribution

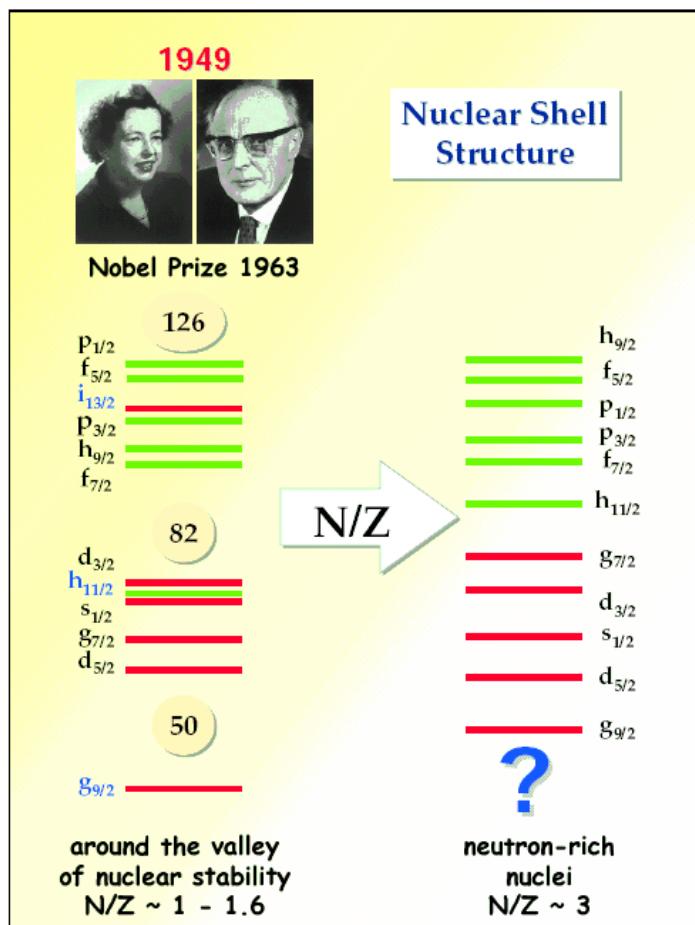
$$e^{-T} O_N^2 e^T \approx O_N^2 = \frac{1}{4} \sum_{pqrs} \langle pq | O^{(2)} | rs \rangle \{ p^\dagger q^\dagger s r \}$$



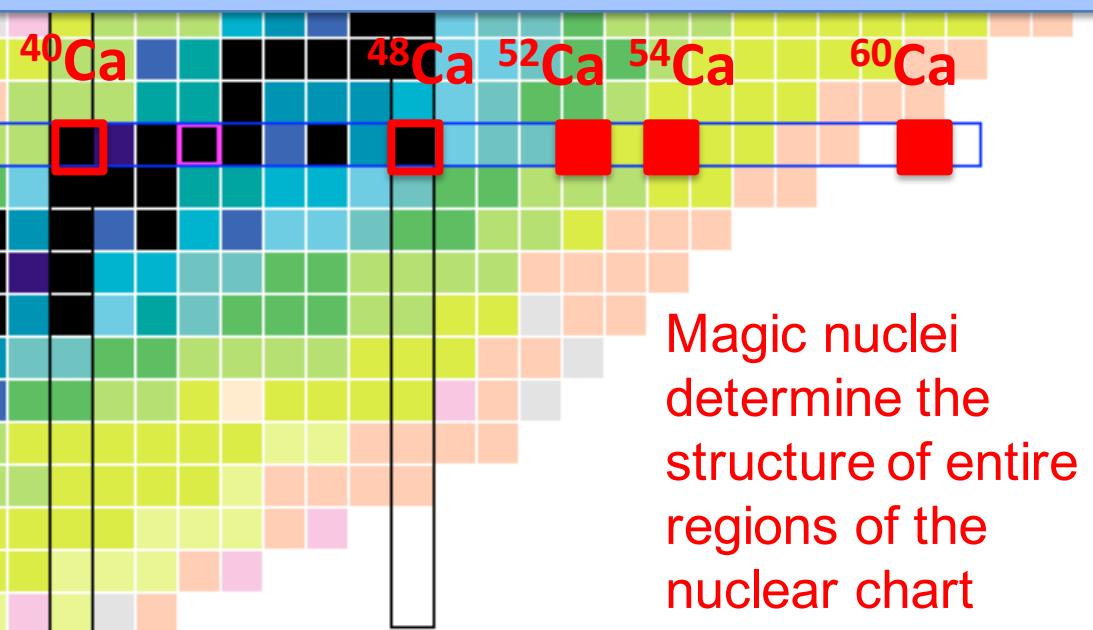
J. Menéndez, D. Gazit, A. Schwenk  
PRL 107, 062501 (2011)

Normal order with respect to free Fermi gas.  
One-body normal ordered approximation gives  
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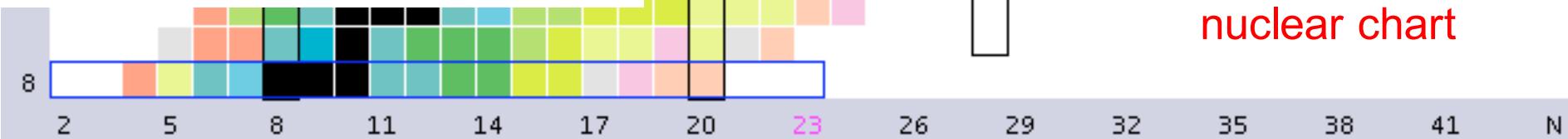
# Evolution of shell structure in neutron rich Calcium



- 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 for new shell structure?



Magic nuclei determine the structure of entire regions of the nuclear chart



# Evolution of shell structure in neutron rich Calcium

- Effects of three-nucleon forces and continuum is essential to describe shell structure
- We predict an inversion of the gds shell-model orbitals
- Our prediction for excited states in  $^{53}\text{Ca}$  and weak sub-shell closure in  $^{54}\text{Ca}$  was verified by experiment at RIKEN (Nature 2013, D. Steppenbeck et al)

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

