

Recent advances in coupled-cluster computations of nuclei

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Progress in Ab Initio Techniques in Nuclear Physics

TRIUMF, February 24th, 2016



U.S. DEPARTMENT OF
ENERGY

NUCLEI
Nuclear Computational Low-Energy Initiative

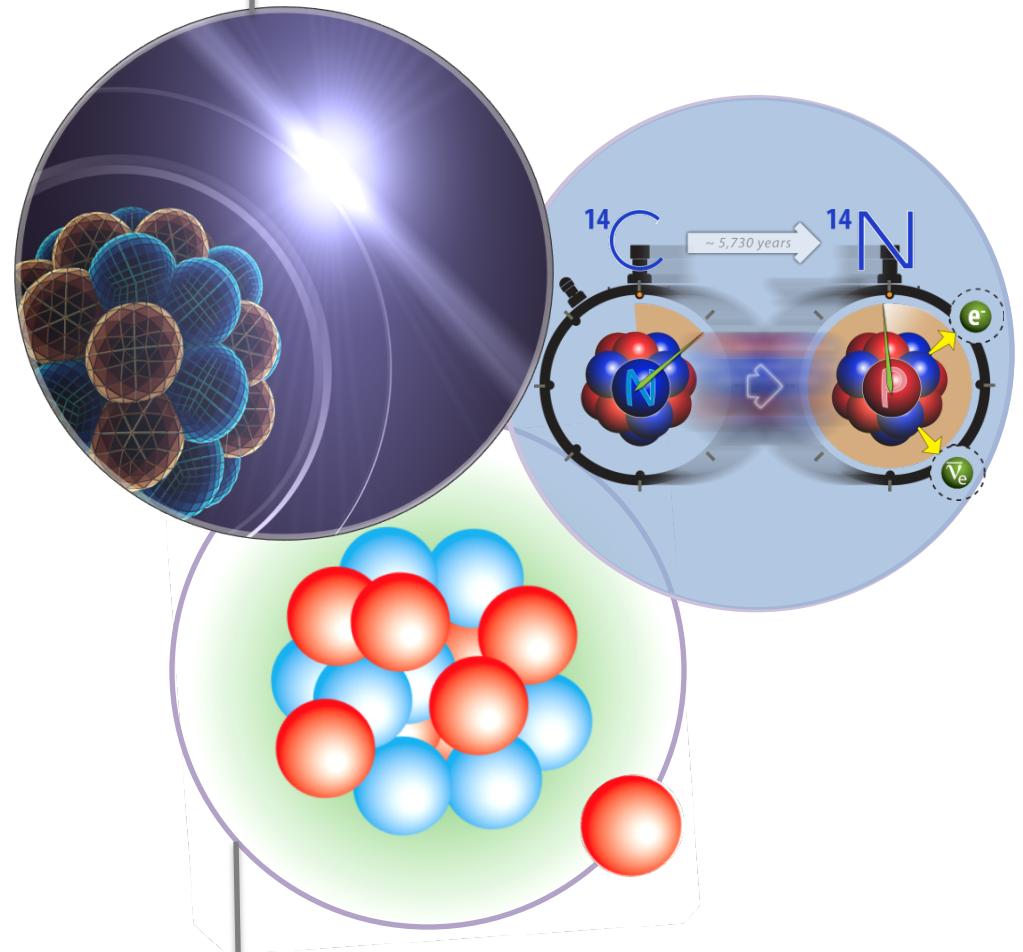


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OAK RIDGE NATIONAL LABORATORY

MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY



Collaborators

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

@ 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

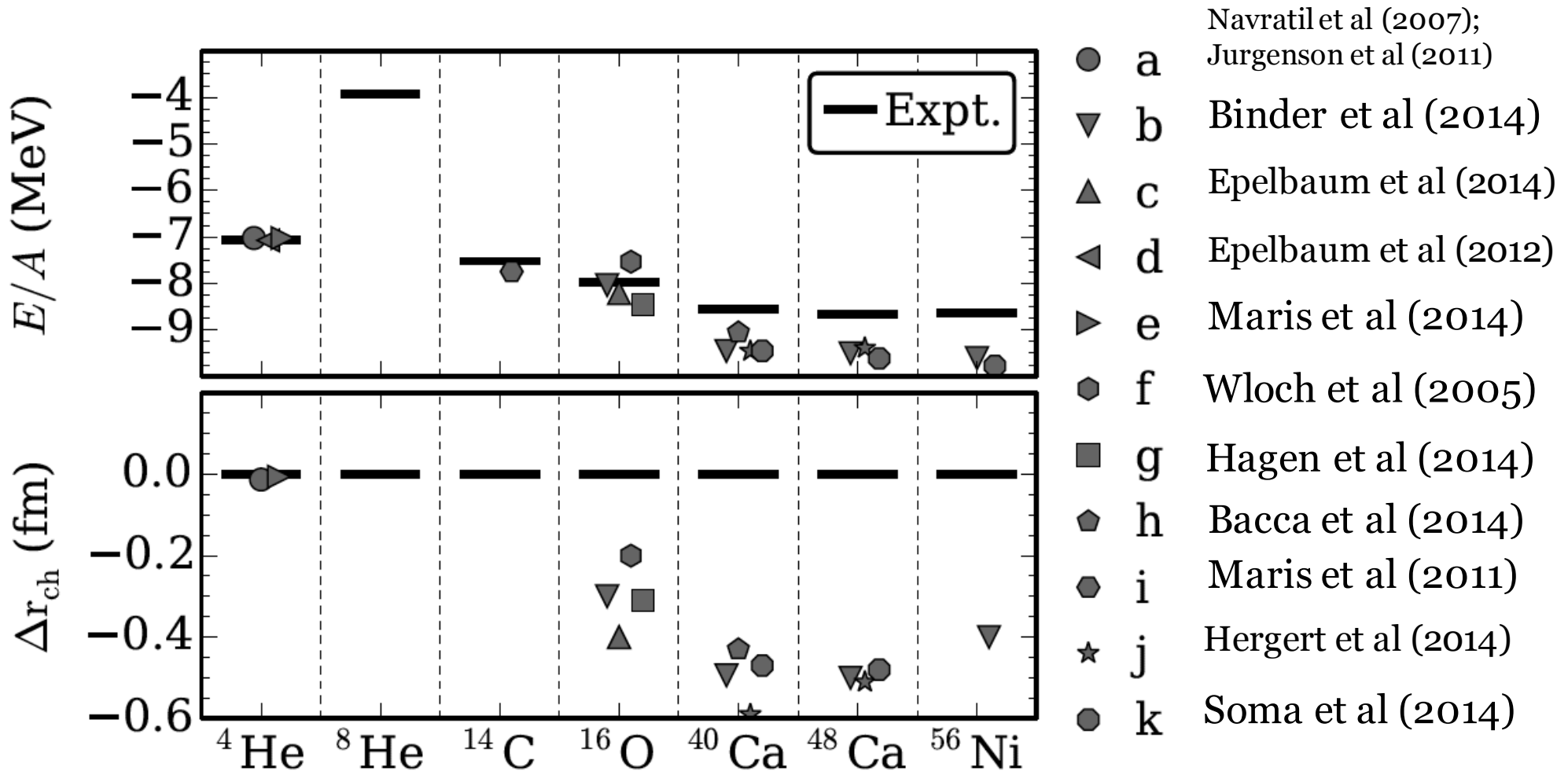
@ TRIUMF: S. Bacca, **M. Miorelli**, P. Navratil

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

Outline

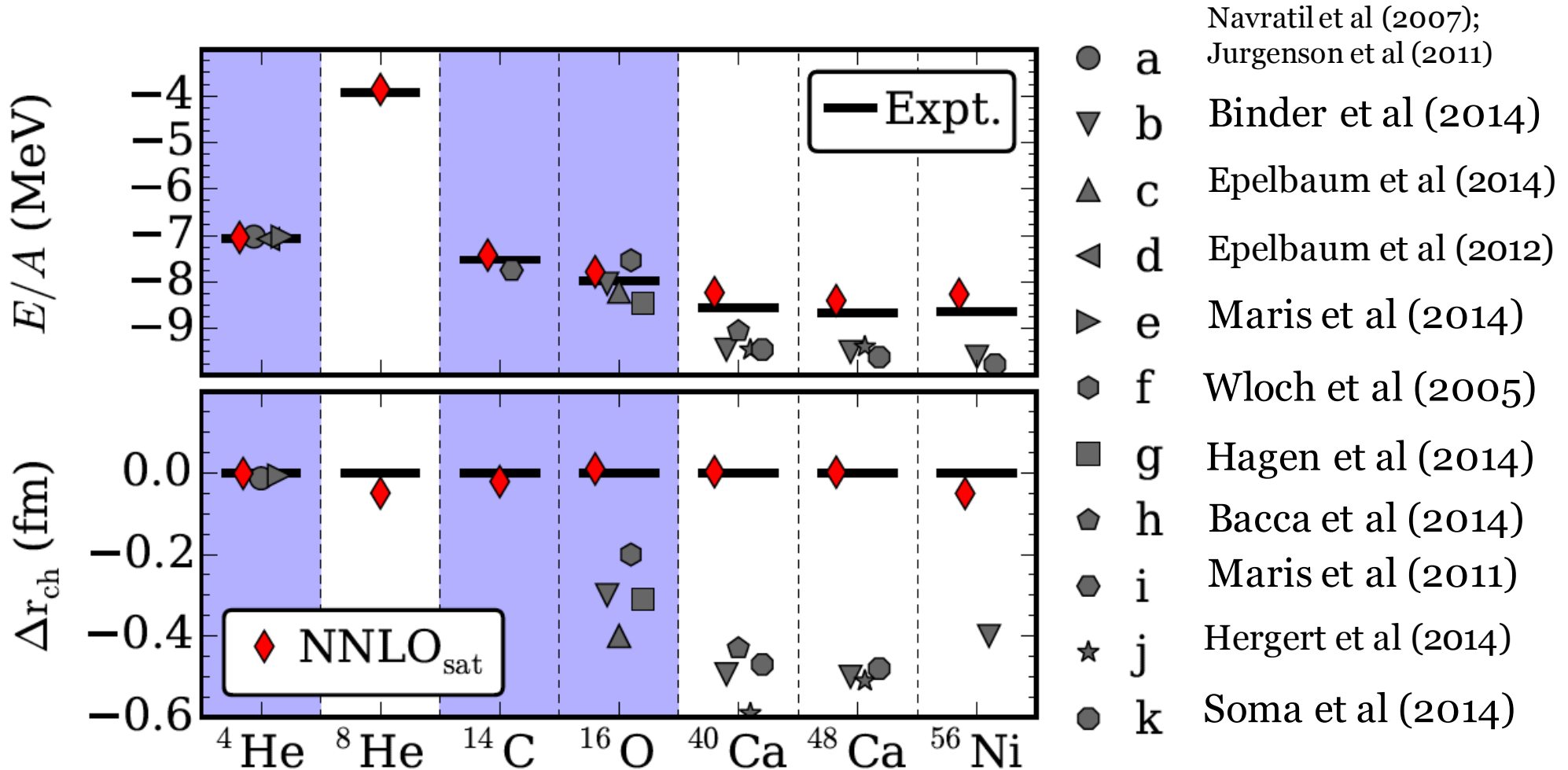
- Accurate radii and binding energies in light and medium mass nuclei
- The neutron radius and dipole polarizability of ^{48}Ca
- Unexpected large charge radii of ^{52}Ca questions its magicity
- Coupled-cluster effective interactions with application to *sd*-shell nuclei
- Giant “pygmy” resonance in ^8He
- Unbound states in neutron rich oxygen and calcium isotopes
- Towards heavy nuclei with HO-EFT

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



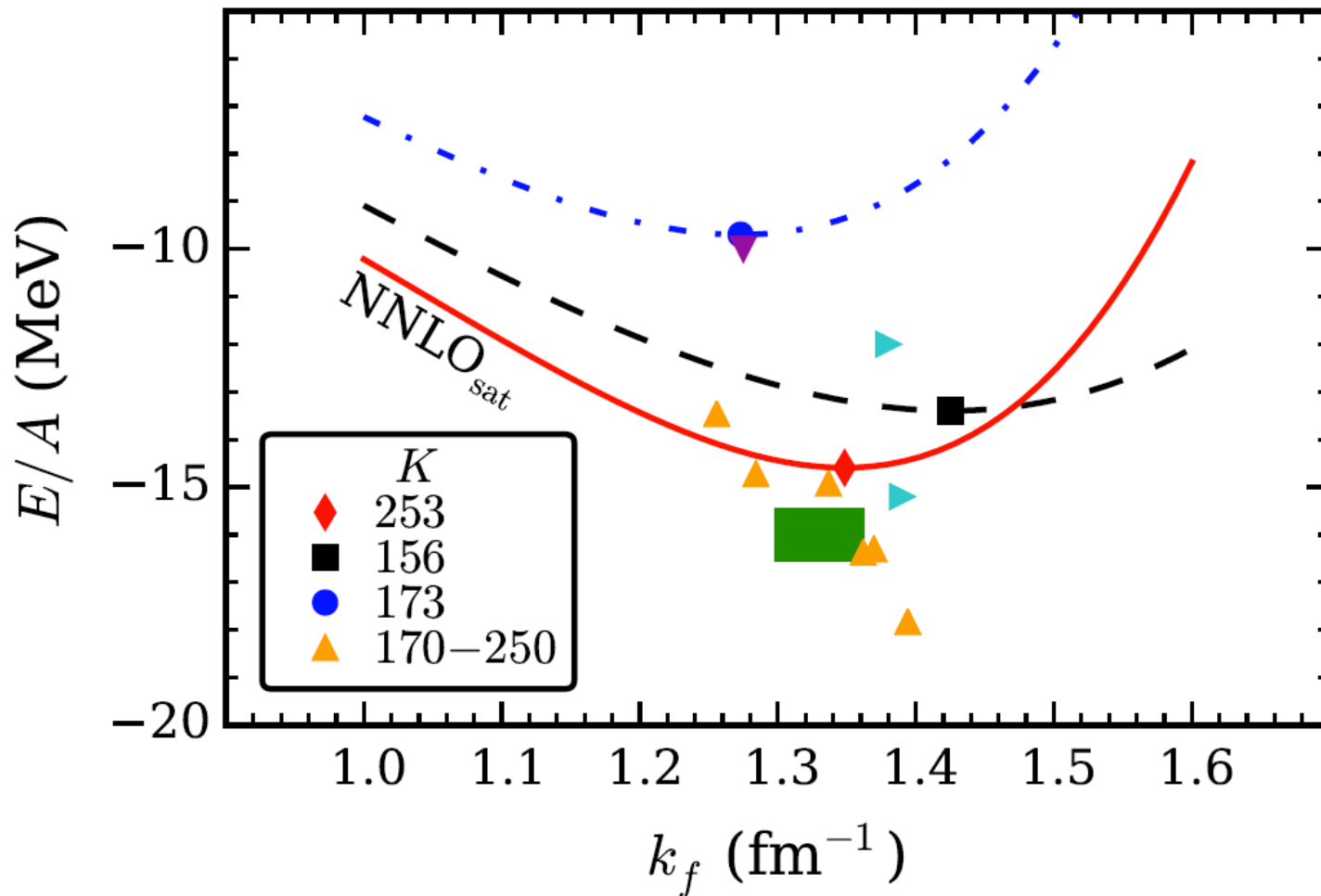
Solution: Simultaneous optimization of NN and 3NFs
 Include charge radii and binding energies of ${}^3\text{H}$, ${}^{3,4}\text{He}$, ${}^{14}\text{C}$, ${}^{16}\text{O}$ in the optimization (NNLO_{sat})

A. Ekström *et al*, Phys. Rev. C **91**, 051301(R) (2015).
 G. Hagen *et al*, arXiv:1601.08203 (2016).

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

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.

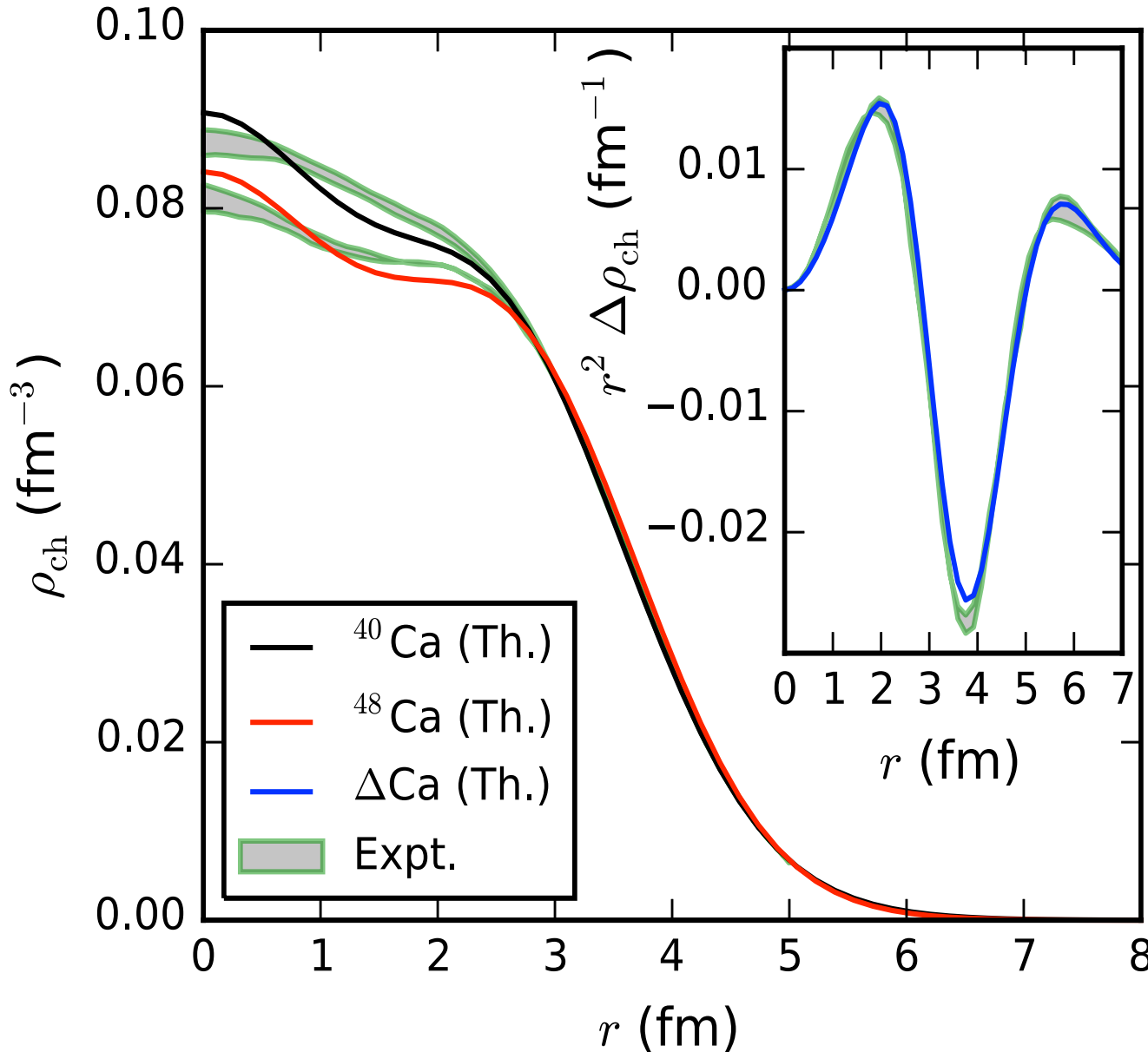
Hagen et al (2014);
Carbone et al (2013); Coraggio et al 2014;

K. Hebeler *et al*
▲ PRC 83, 031301
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 densities of $^{40,48}\text{Ca}$ from NNLO_{sat}

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



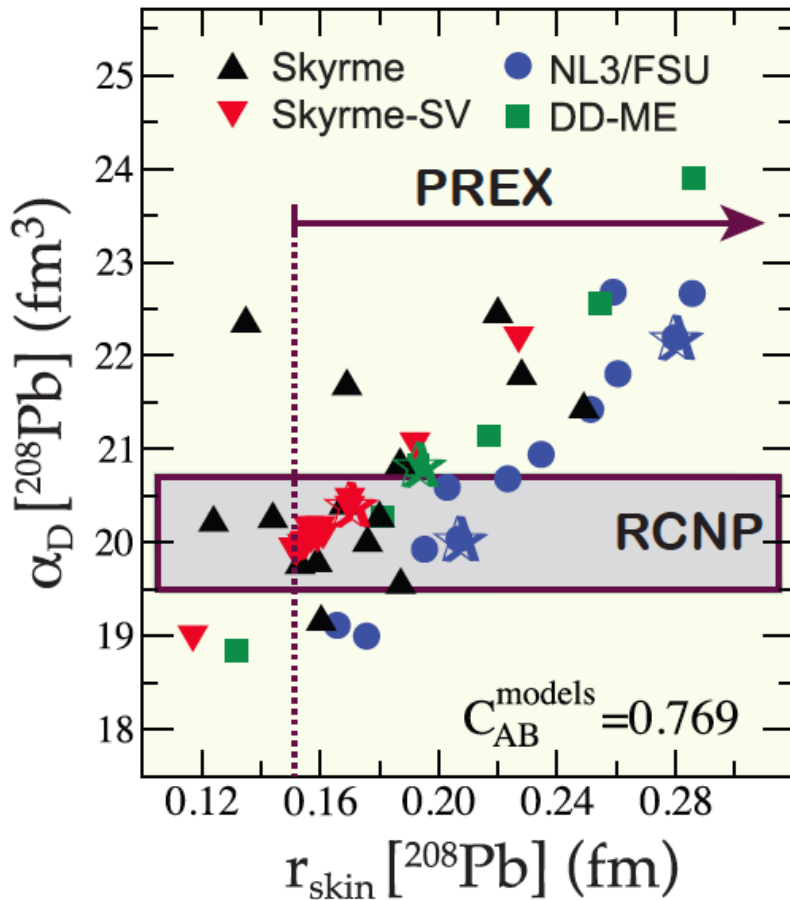
Electric charge distributions have been a long-standing problem for *ab initio* theory.

$$BE(\text{Th}) = 404(3) \text{ MeV}$$
$$BE(\text{Exp}) = 416 \text{ MeV}$$

$$R_{\text{Ch}}(\text{Th}) = 3.48(3) \text{ fm}$$
$$R_{\text{Ch.}}(\text{Exp}) = 3.477(2) \text{ fm}$$

Neutron radii and dipole polarizability

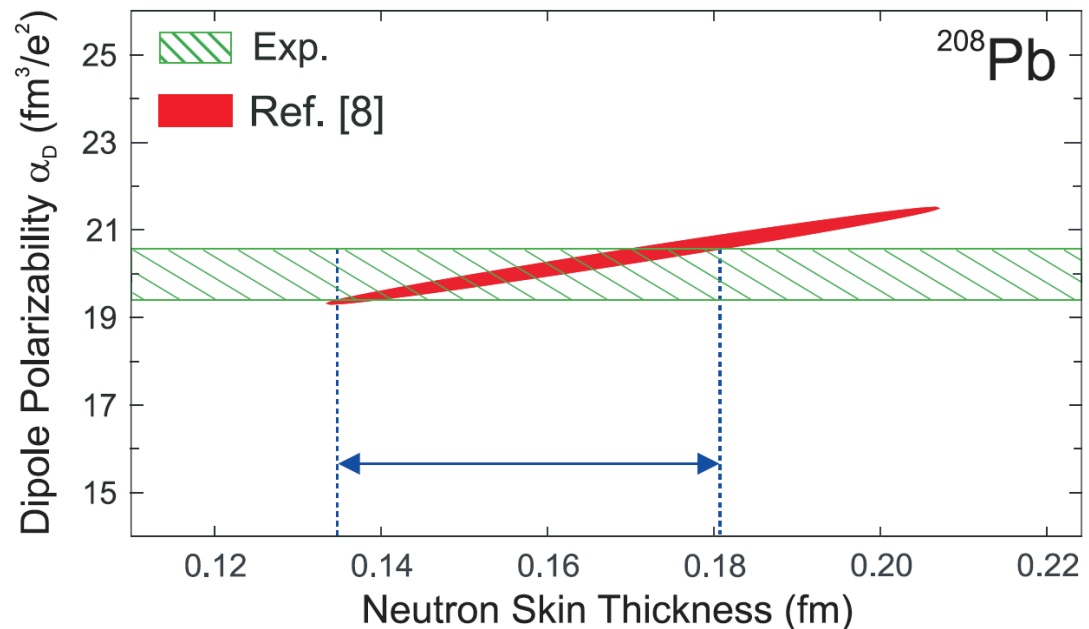
J. Piekarewicz et al, PRC 85, 041302(R) (2012)



- 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?

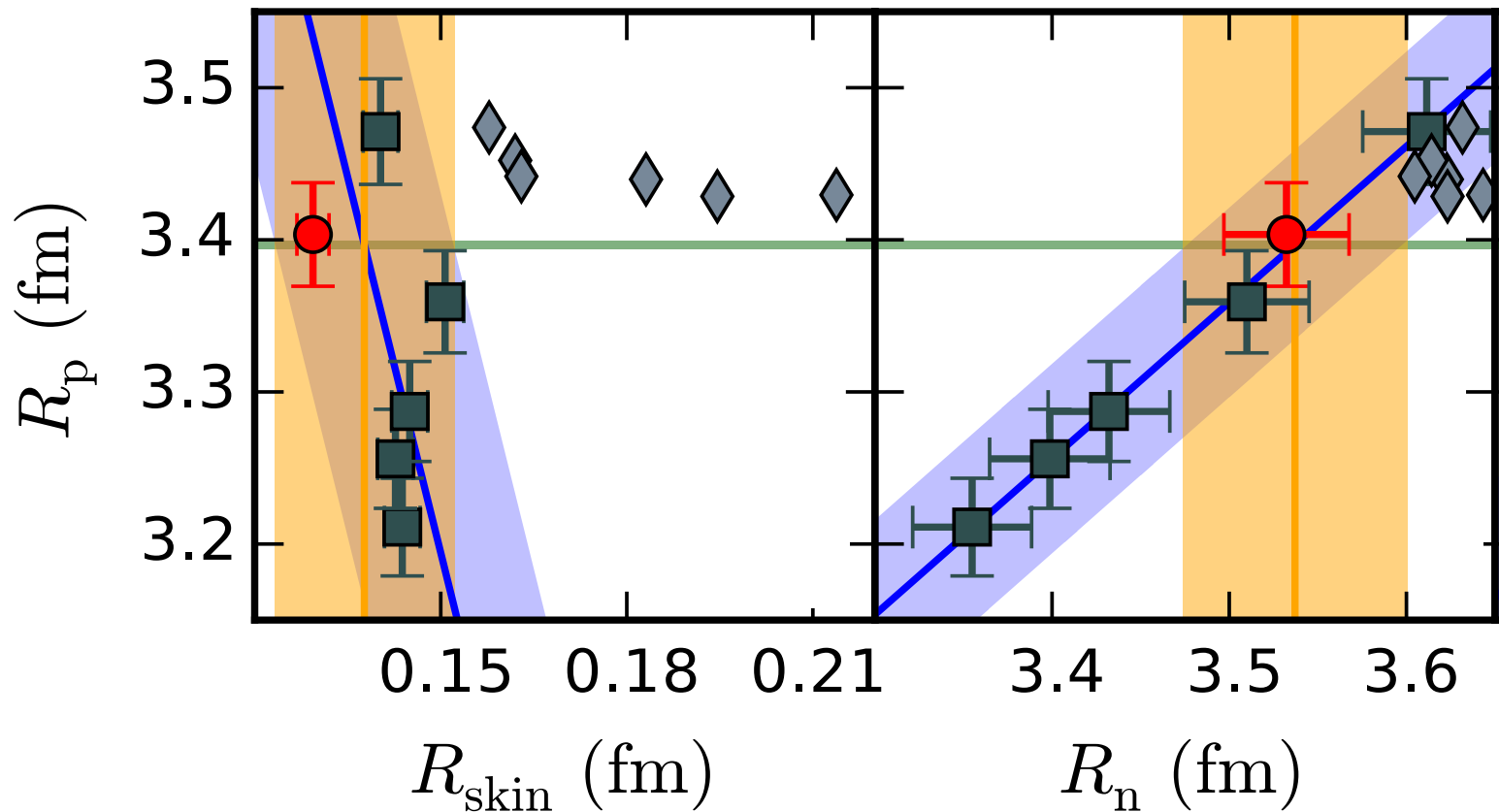
α_D : ^{208}Pb by Tamii et al, PRL 2011;
 ^{68}Ni by Rossi et al, PRL 2013; ^{120}Sn by Hashimoto et al. (2015); ^{48}Ca coming soon (Darmstadt/Osaka collaboration)

R_n : ^{208}Pb by Abrahamyan et al, PRL 2012; $^{48}\text{Ca} \rightarrow$ CREX



Neutron radius and skin of ^{48}Ca

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



Uncertainty estimates from family of chiral interactions.

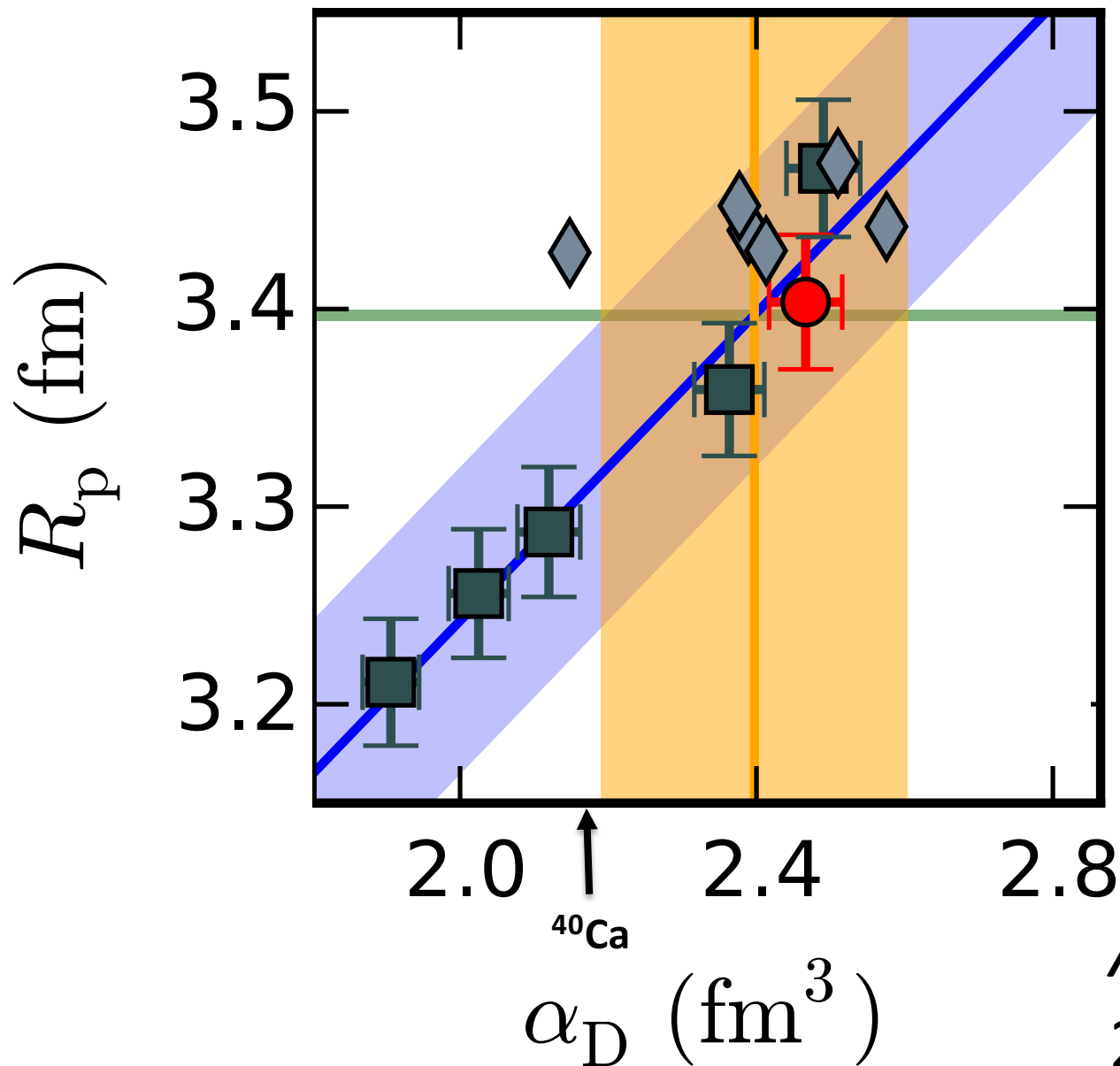
DFT:
SkM*, SkP, Sly4,
SV-min, UNEDF0,
and UNEDF1

$$0.12 \lesssim R_{\text{skin}} \lesssim 0.15 \text{ fm} \quad 3.47 \lesssim R_n \lesssim 3.60 \text{ fm}$$

- 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}Ca

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

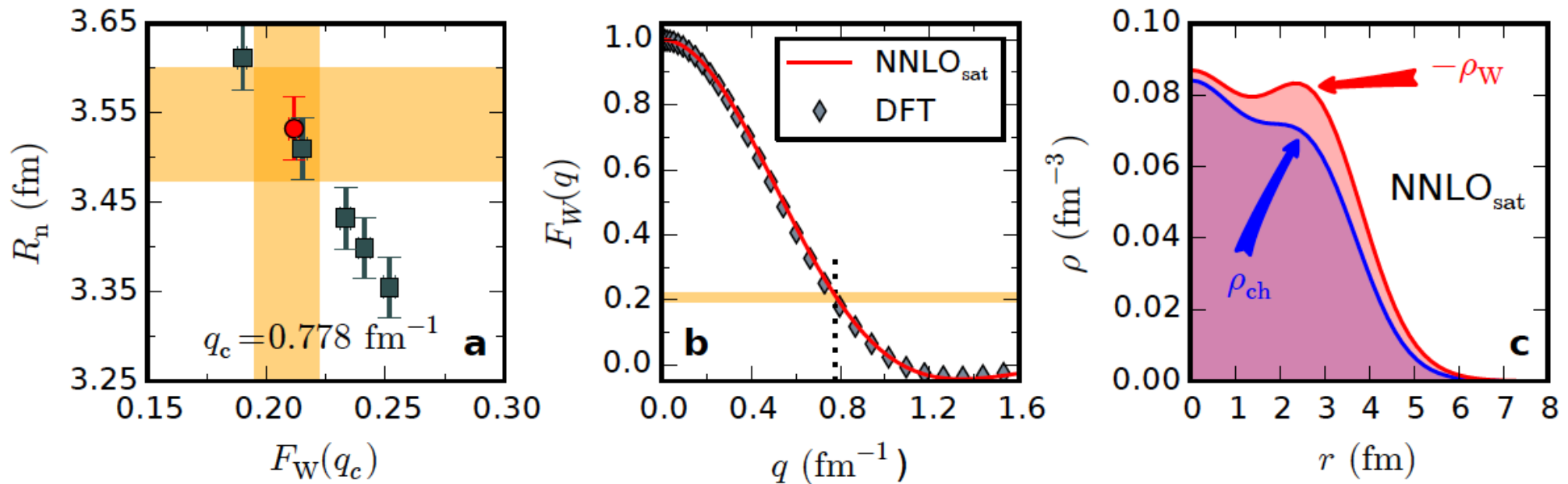


DFT results are consistent and within band of ab-initio results

Data being analyzed by Osaka-Darmstadt collaboration

Ab-initio prediction:
 $2.19 \lesssim \alpha_D \lesssim 2.60 \text{ fm}^3$

Weak charge form-factor of ^{48}Ca



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?

Unexpectedly large charge radii of ^{52}Ca

R. F. Garcia Ruiz *et al*, Nature Physics (2016)
doi:10.1038/nphys3645

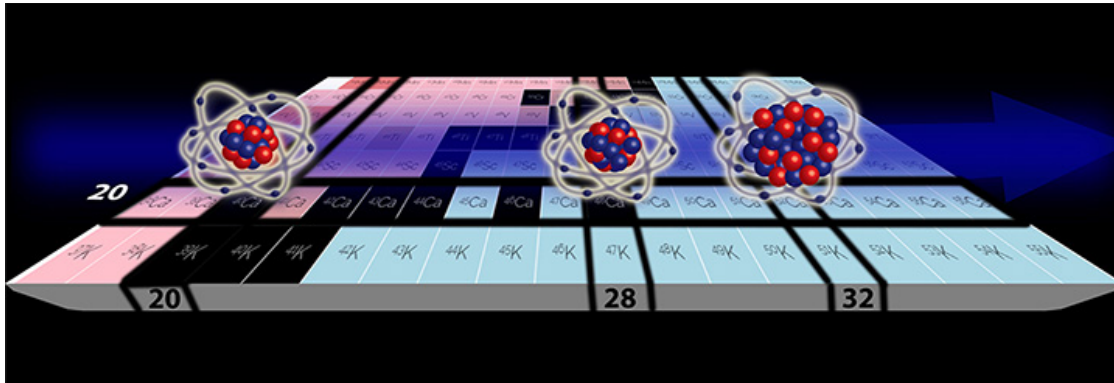
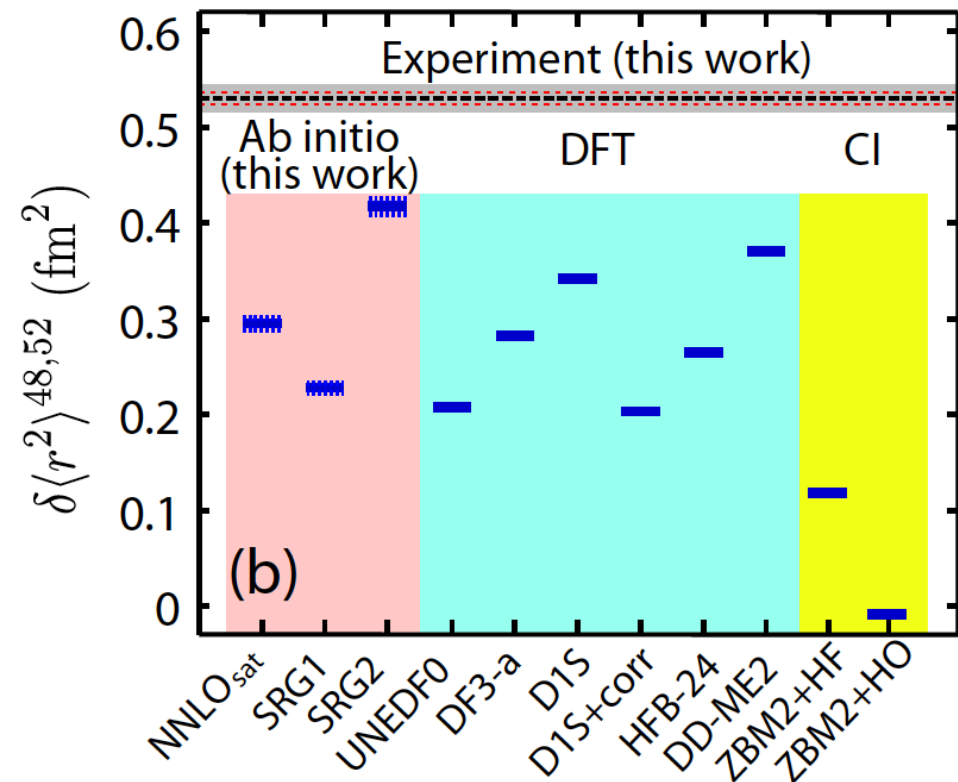
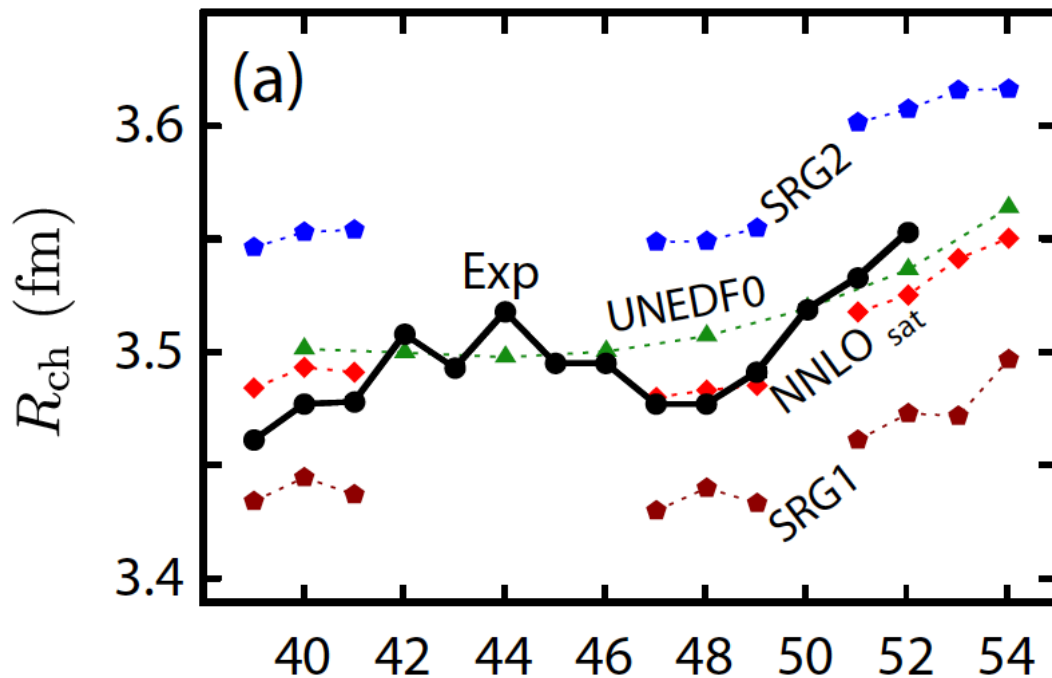
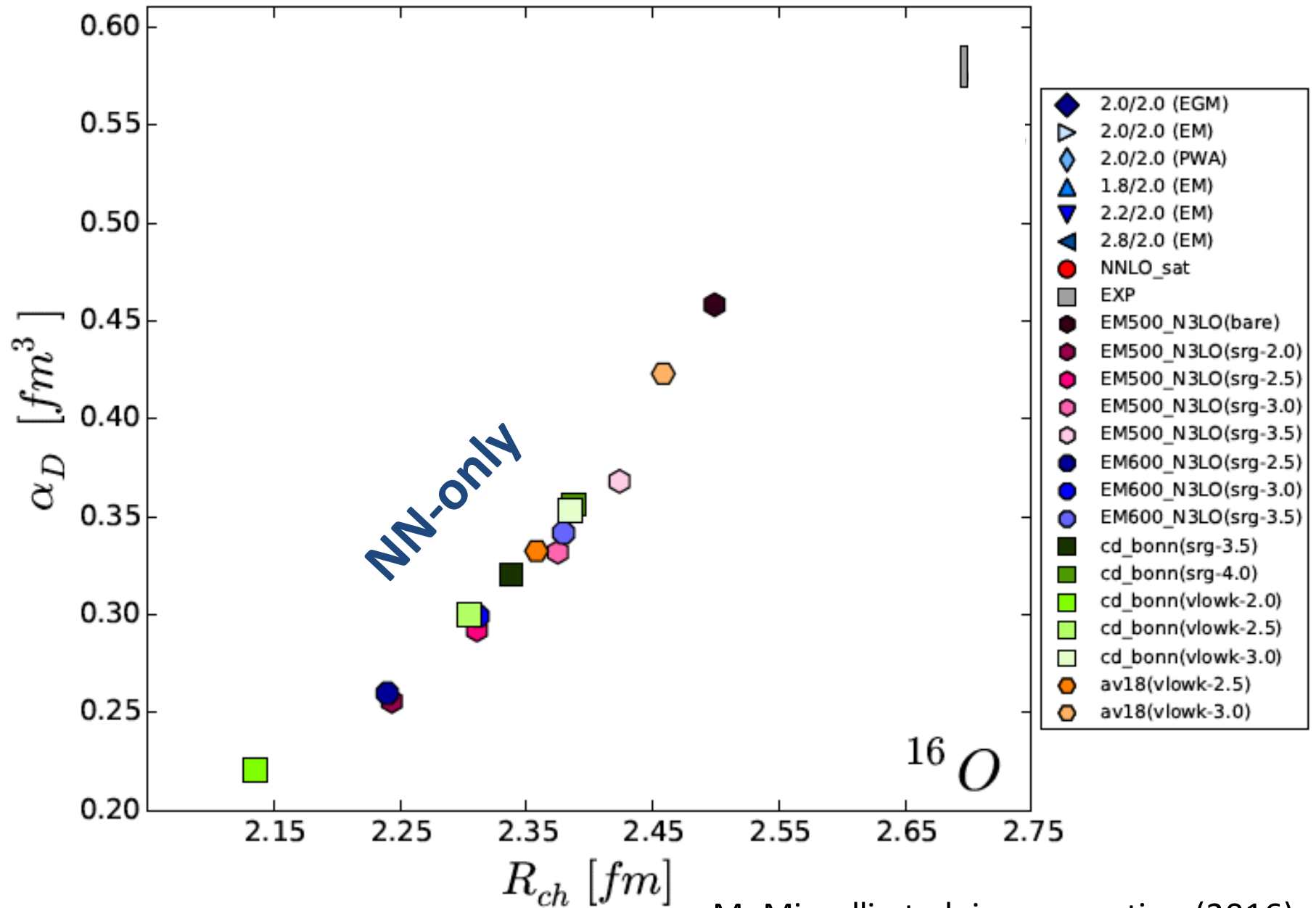


Image: COLLAPS Collaboration/Ronald Fernando Garcia Ruiz.

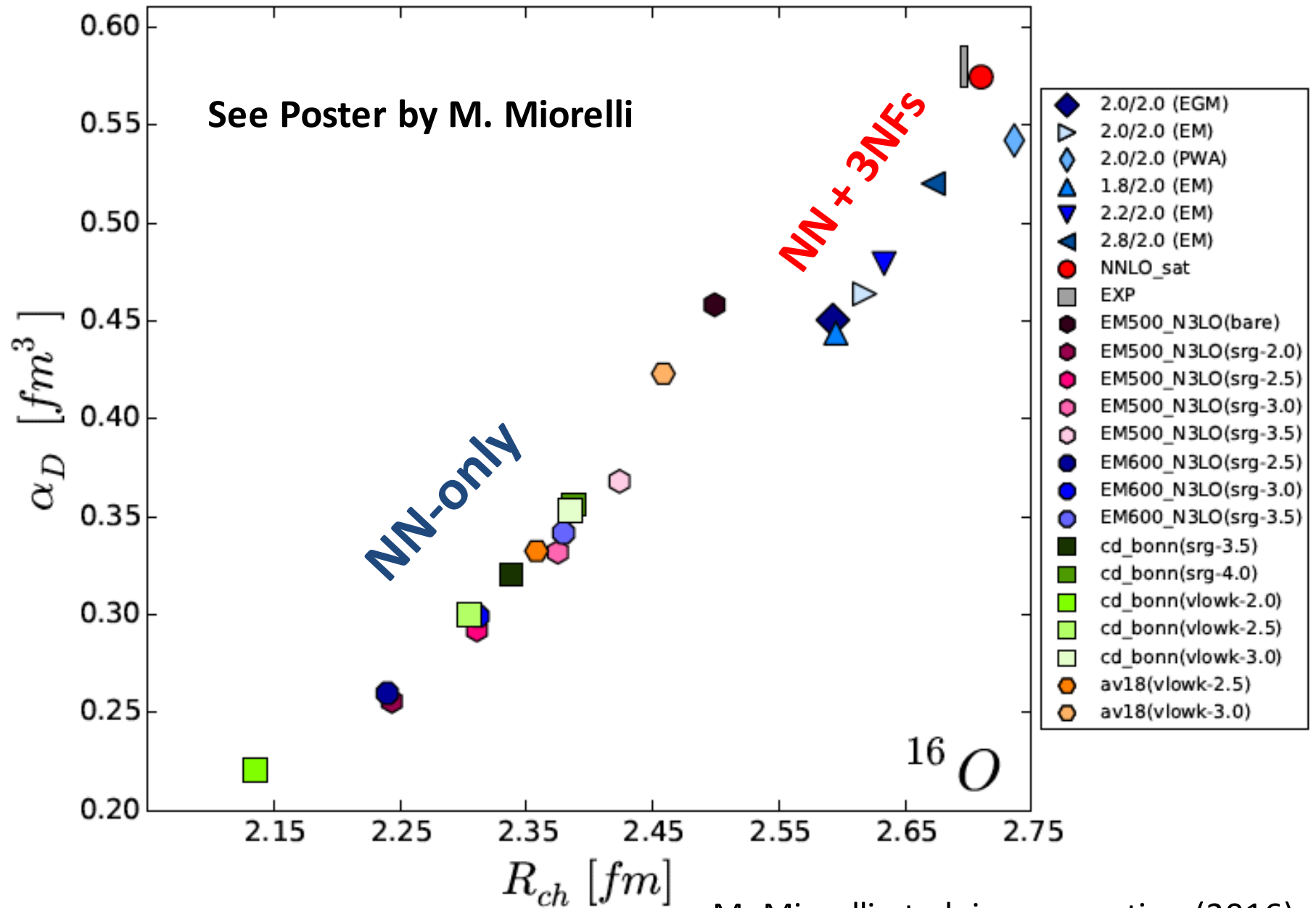
- Charge radii of $^{49,51,52}\text{Ca}$, obtained from laser spectroscopy experiments at ISOLDE, CERN
- Unexpected large charge radius questions the magicity of ^{52}Ca
- Theoretical models all underestimate the charge radius
- Ab-initio calculations reproduce the trend of charge radii



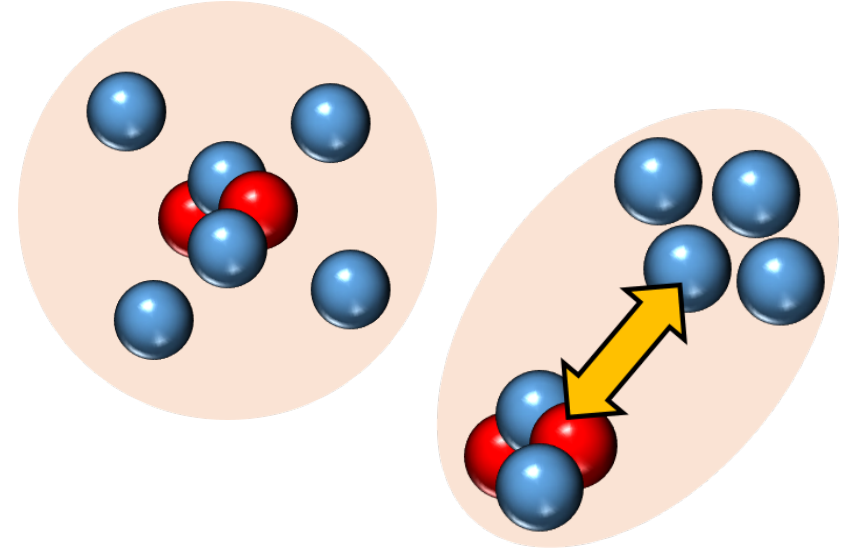
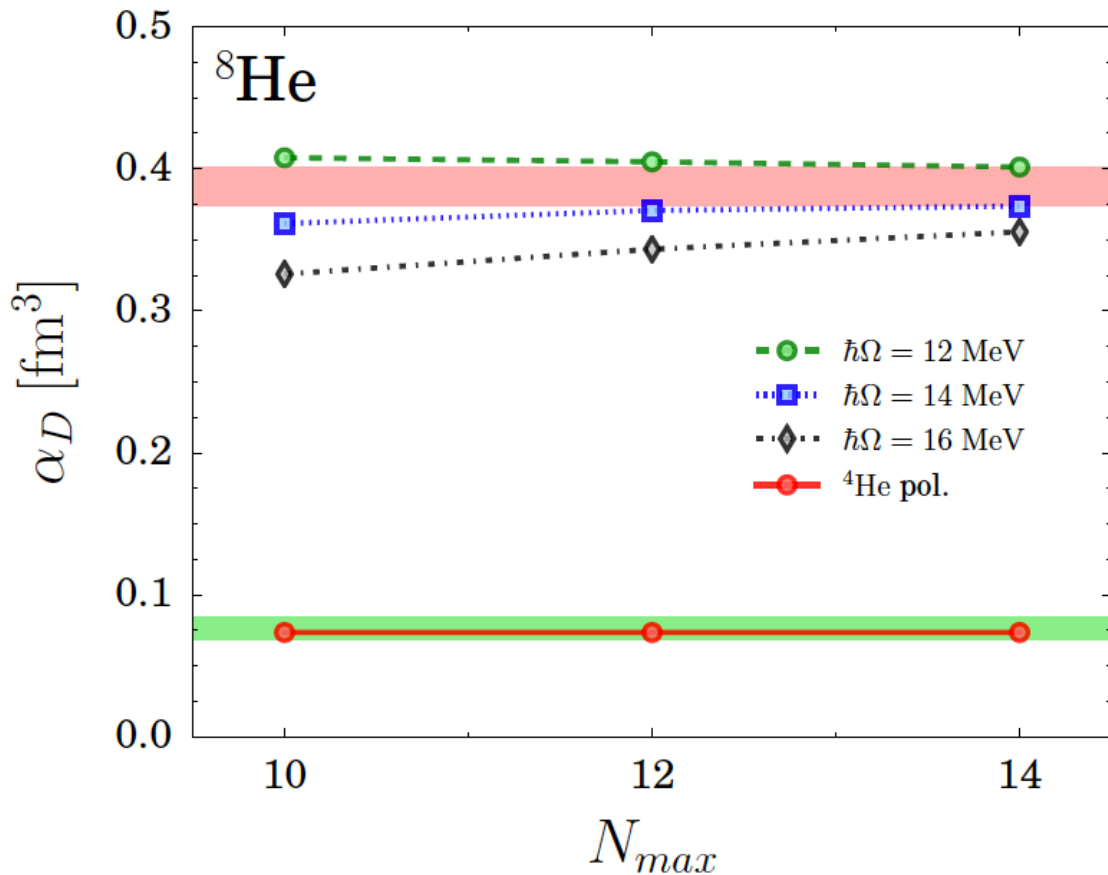
Dipole polarizability of ^{16}O : The role of three-nucleon forces



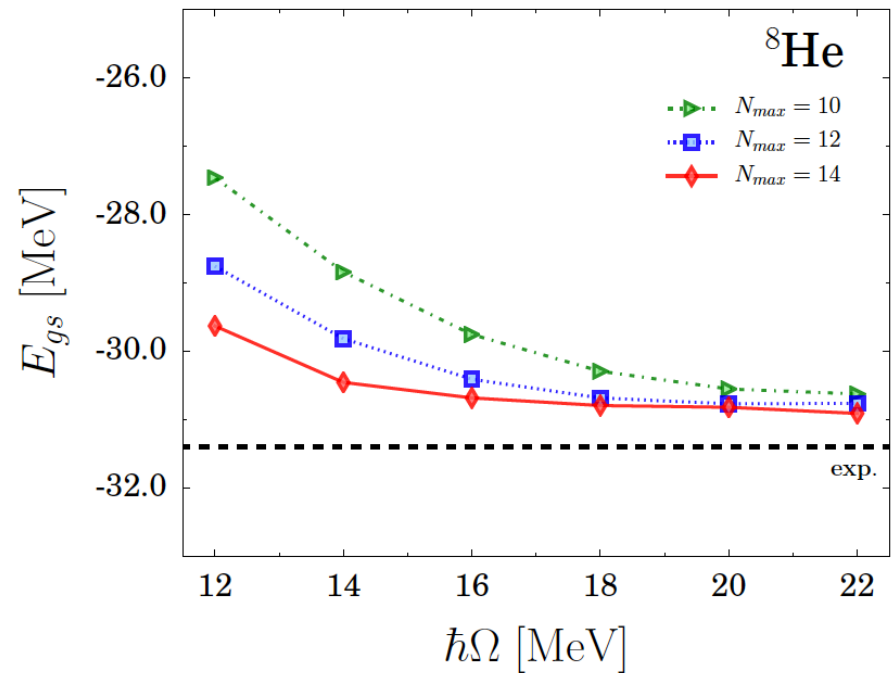
Dipole polarizability of ^{16}O : The role of three-nucleon forces



A “giant” pygmy resonance in ^8He

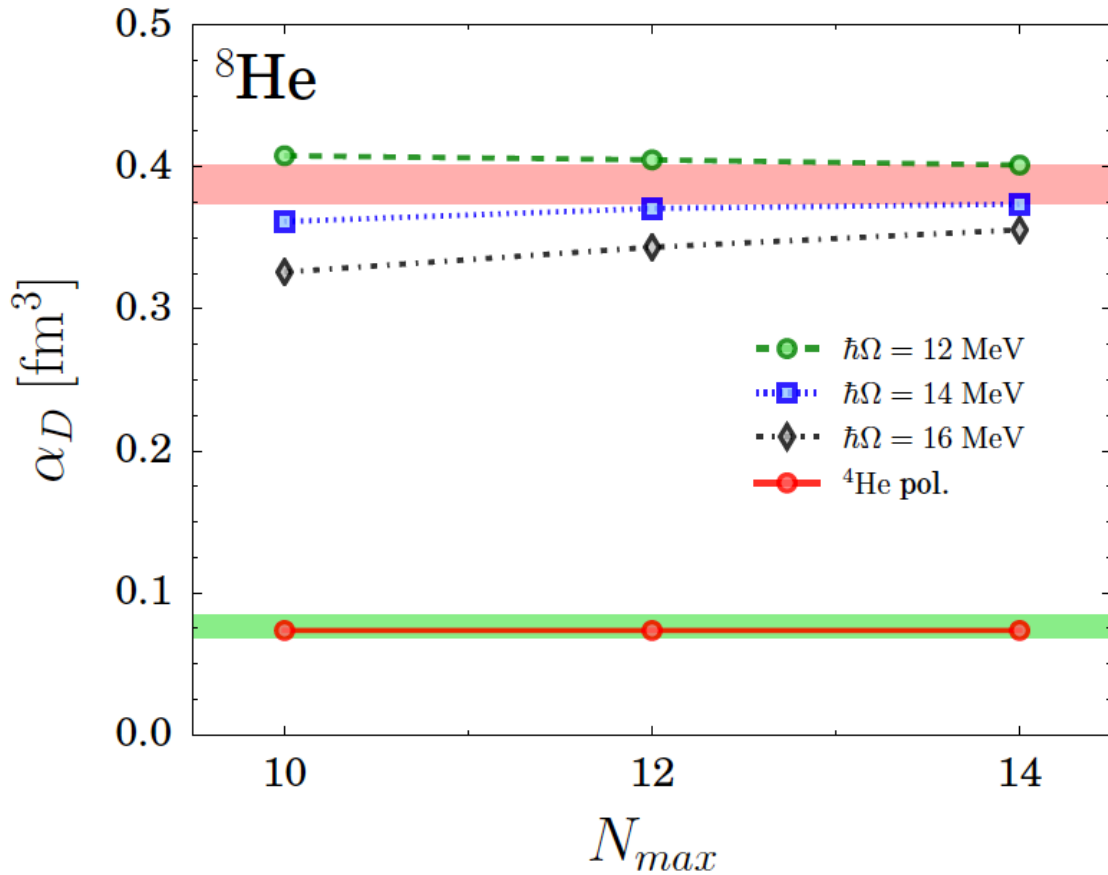


- BE and charge radius of ^8He reproduced with NNLO_{sat}
- A large neutron radius $R_n = 2.57(2)$ fm gives a neutron skin $R_{\text{skin}} = 0.8$ fm
- R_{skin} of ^8He is 2-4 times larger than the R_{skin} of ^{208}Pb

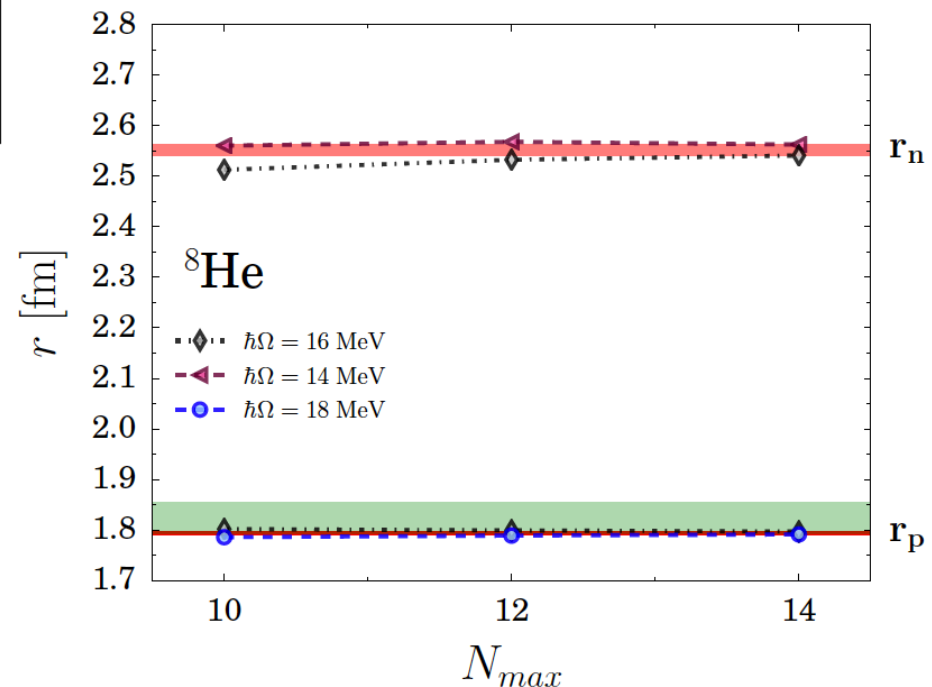
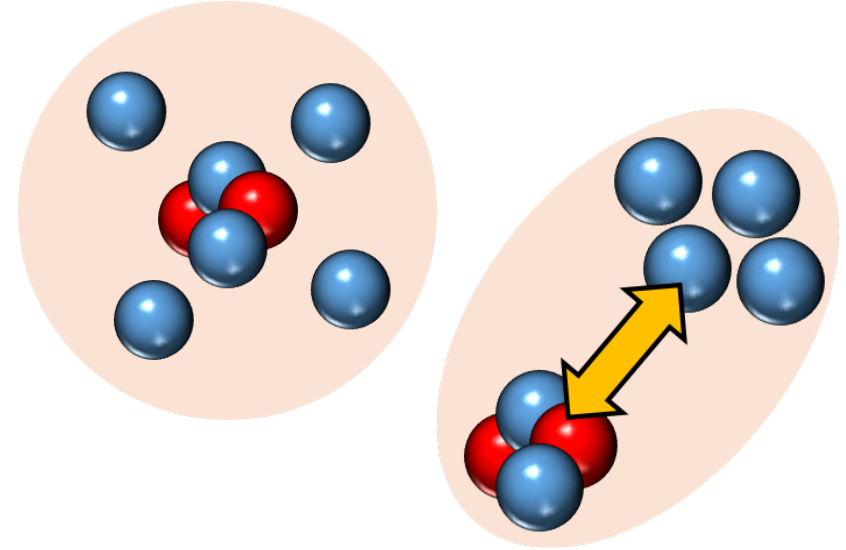


M. Miorelli et al, in preparation (2016)

A “giant” pygmy resonance in ^8He



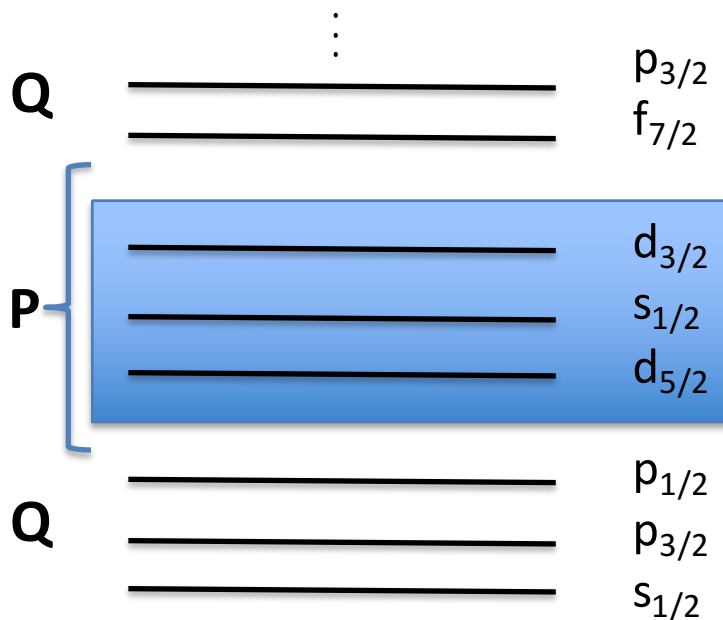
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M. Miorelli et al, in preparation (2016)

Coupled-cluster effective interactions (CCEI)

- 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.



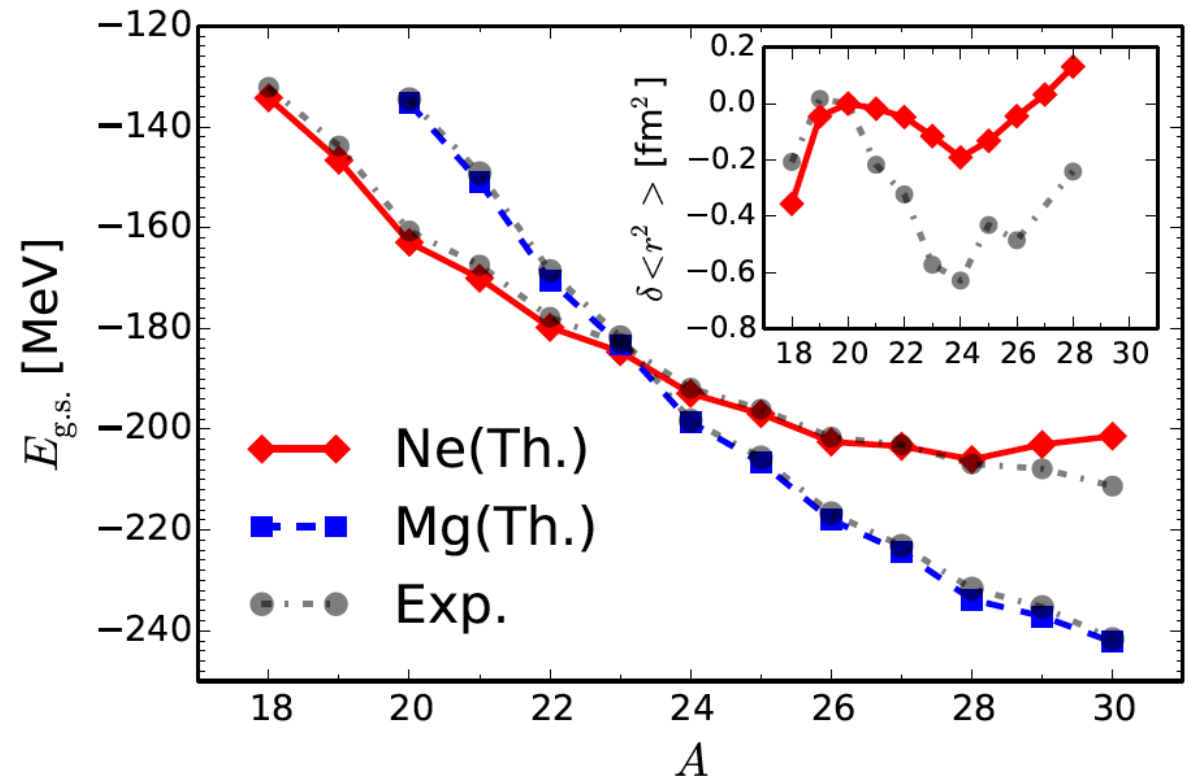
- Diagonalize the effective hamiltonian in the valence space.

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

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

See Talks by M. Schuster

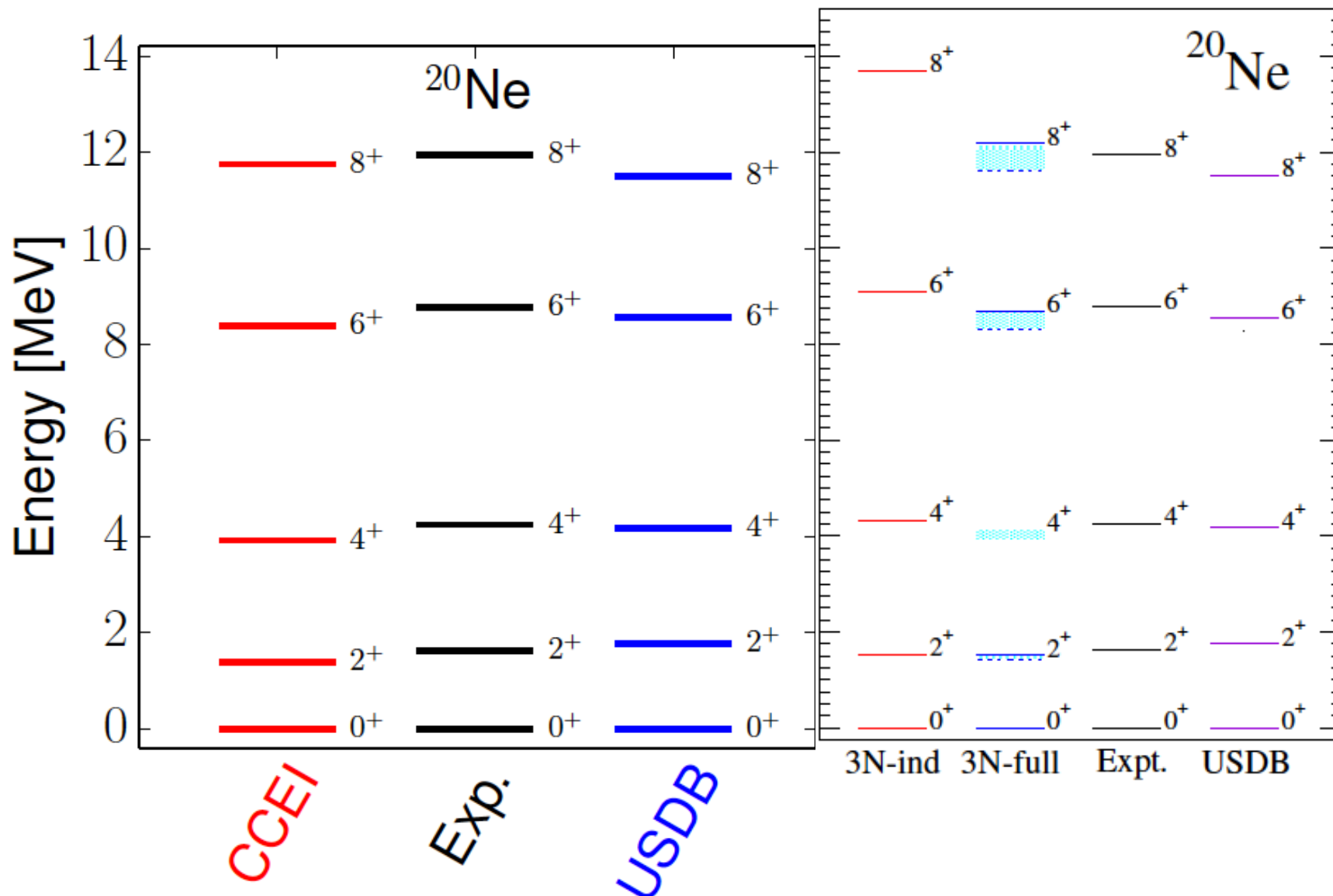
S. R. Stroberg and B. Barrett



Deformed sd-shell nuclei from CCEI

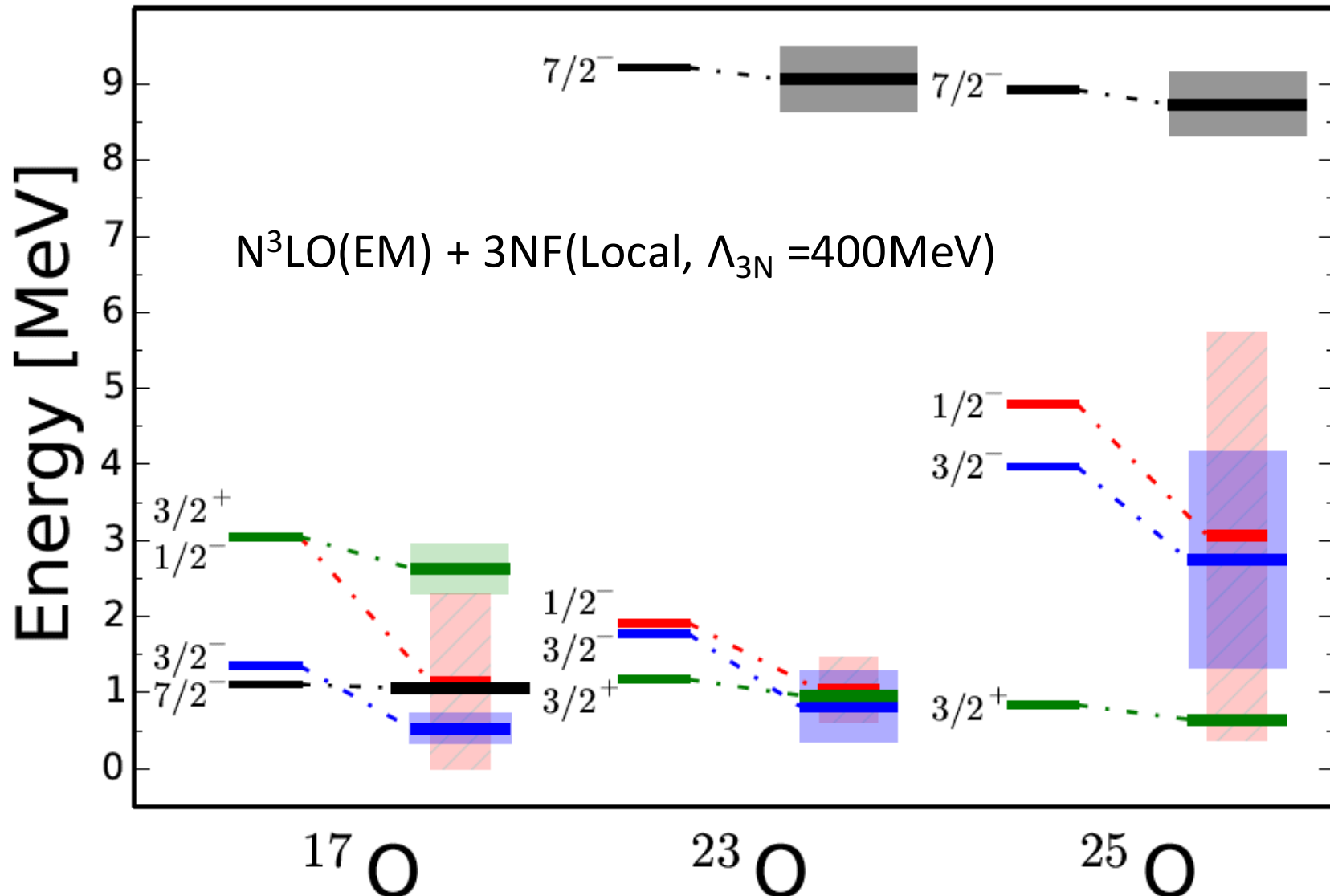
G. R. Jansen, A. Signoracci, GH, P. Navratil arXiv:1511.00757 (2015).

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



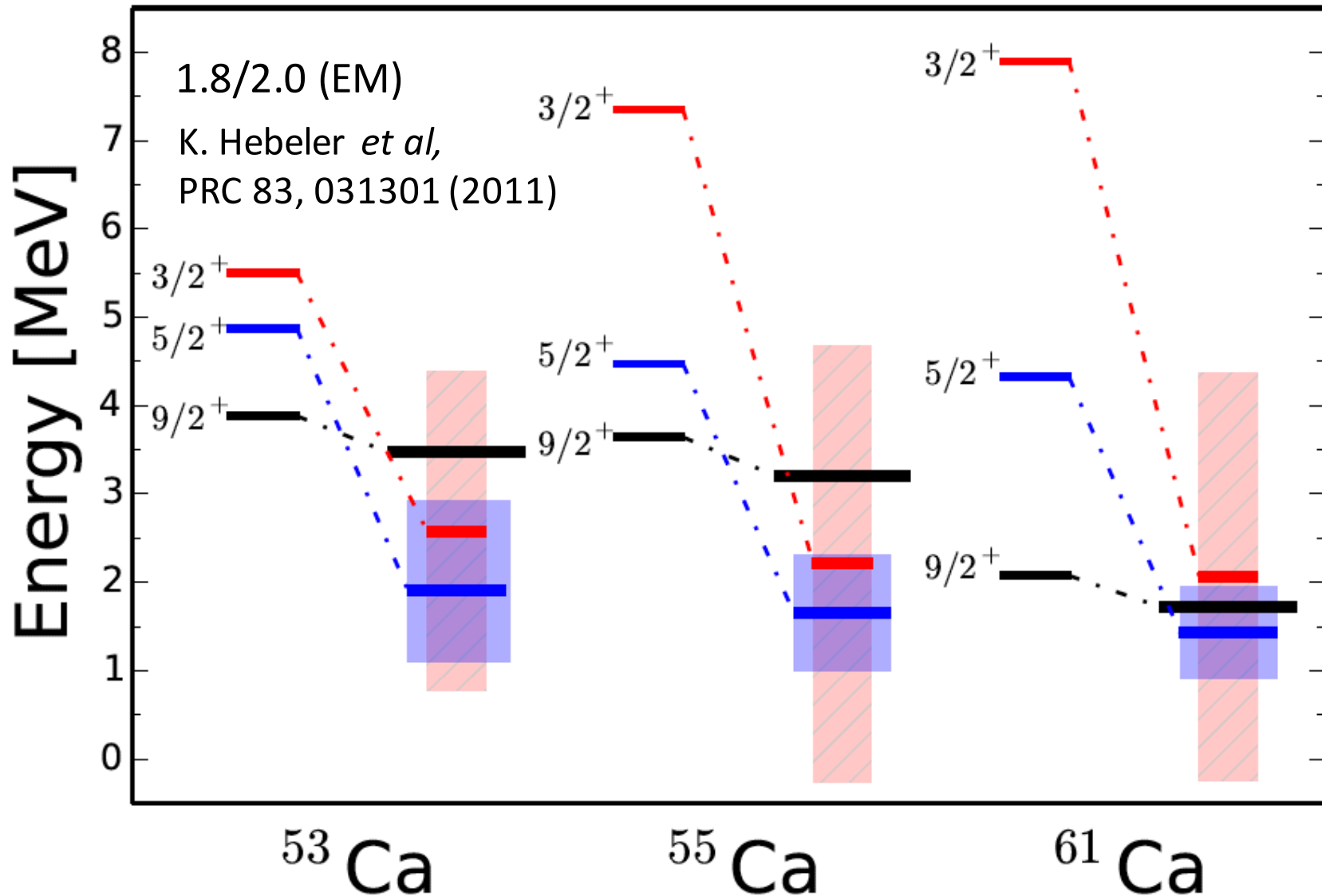
Role of continuum on unbound states in oxygen isotopes

G. Hagen *et al*, arXiv:1601.08203 (2016).



Role of continuum on unbound states in oxygen isotopes

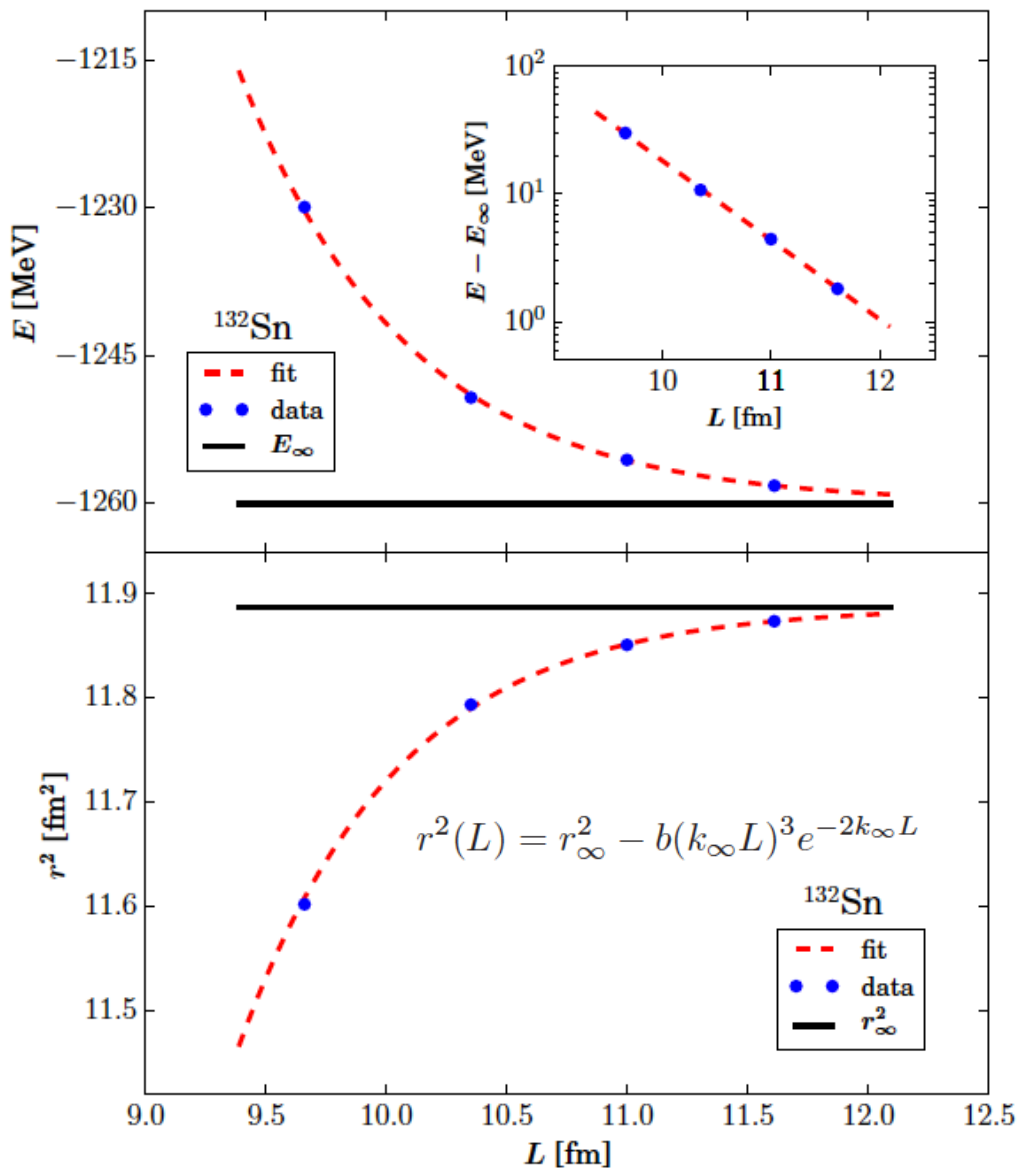
G. Hagen *et al*, arXiv:1601.08203 (2016).



Towards ab-initio computations of heavy nuclei with HO-EFT

$$E(L) = E_\infty + ae^{-2k_\infty L}$$

S. Binder *et al*, arXiv:1512.03802 (2015)



N_{\max}	^4He	^{16}O	^{40}Ca	^{90}Zr	^{132}Sn
	E_{CCSD} [MeV]				
10	-31.57	-142.89	-402.0	-918.4	-1230.0
12	-31.57	-142.92	-402.4	-923.1	-1249.3
14	-31.57	-142.93	-402.5	-924.6	-1255.6
16	-31.57	-142.93	-402.5	-925.1	-1258.3
∞	-31.57	-142.93	-402.5	-925.4	-1260.1
exp	-28.30	-127.62	-342.1	-783.9	-1102.9
	r^2 [fm 2]				
10	1.78	4.14	6.58	9.70	11.60
12	1.78	4.15	6.60	9.77	11.79
14	1.78	4.15	6.60	9.80	11.85
16	1.78	4.15	6.61	9.82	11.88
∞	1.78	4.15	6.61	9.83	11.89
exp	2.12	6.60	11.41	17.57	21.57

- Rapid convergence of BEs and radii in medium mass and heavy nuclei
- IR extrapolations with no UV contamination
- Next step: NNLO $_{\text{sat}}$ in HO-EFT

Summary

- Predictions for neutron skin and dipole polarizability of ^{48}Ca
- Unexpected large radii in ^{52}Ca questions its magicity and poses a challenge for theory
- Developed non-perturbative shell-model interactions for the shell-model with application to deformed nuclei
- Prediction of “giant” pygmy resonance in ^8He
- Impact of continuum on unbound states in oxygen and calcium
- Towards heavy nuclei with HO-EFT

Family of chiral interactions

G. Hagen et al, in preparation (2015)

Interaction	BE	S_n	Δ	R_{ch}	R_W	S_v	L
NNLO _{sat}	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			