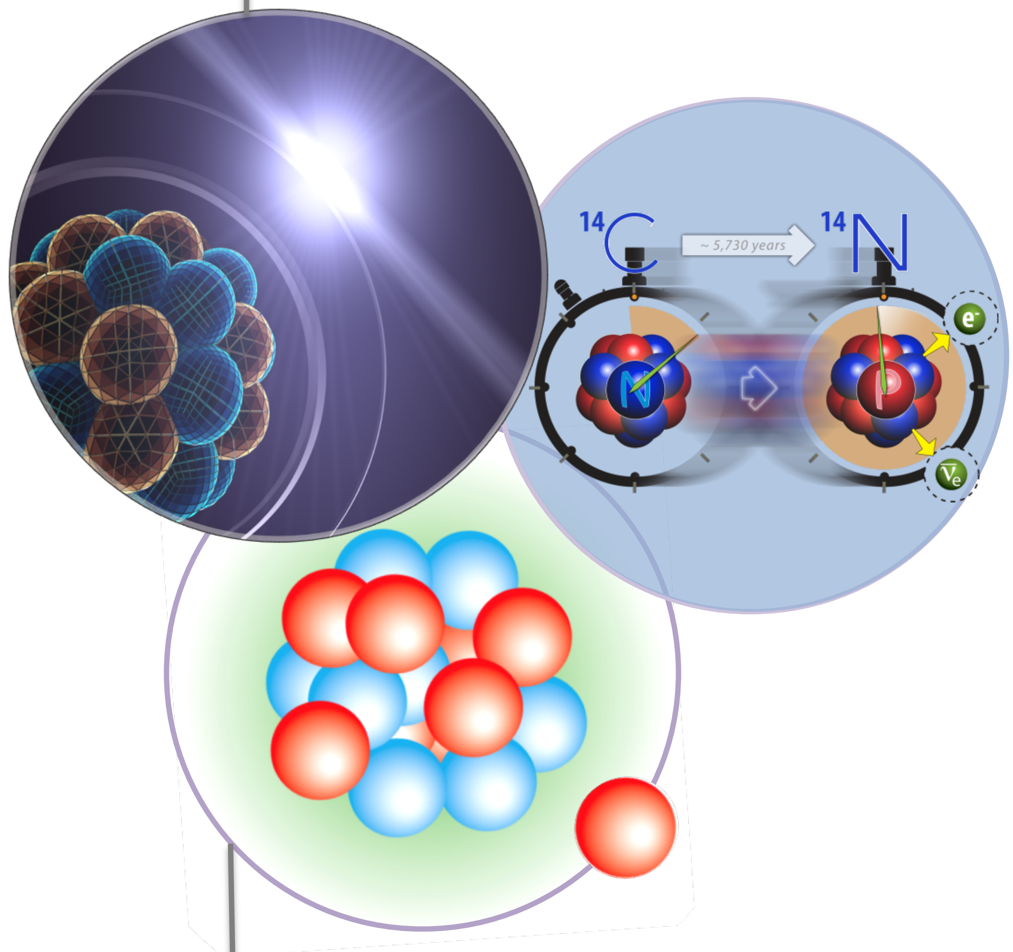
# Current status and challenges of ab-initio computations of nuclei





**Gaute Hagen**

**Oak Ridge National Laboratory**


INT workshop on "Nuclear Physics from Lattice QCD"

INT, May 5th, 2016


U.S. DEPARTMENT OF ENERGY

NUCLEI
Nuclear Computational Low-Energy Initiative

BSF
United States – Israel
Binational Science Foundation

OAK RIDGE NATIONAL LABORATORY
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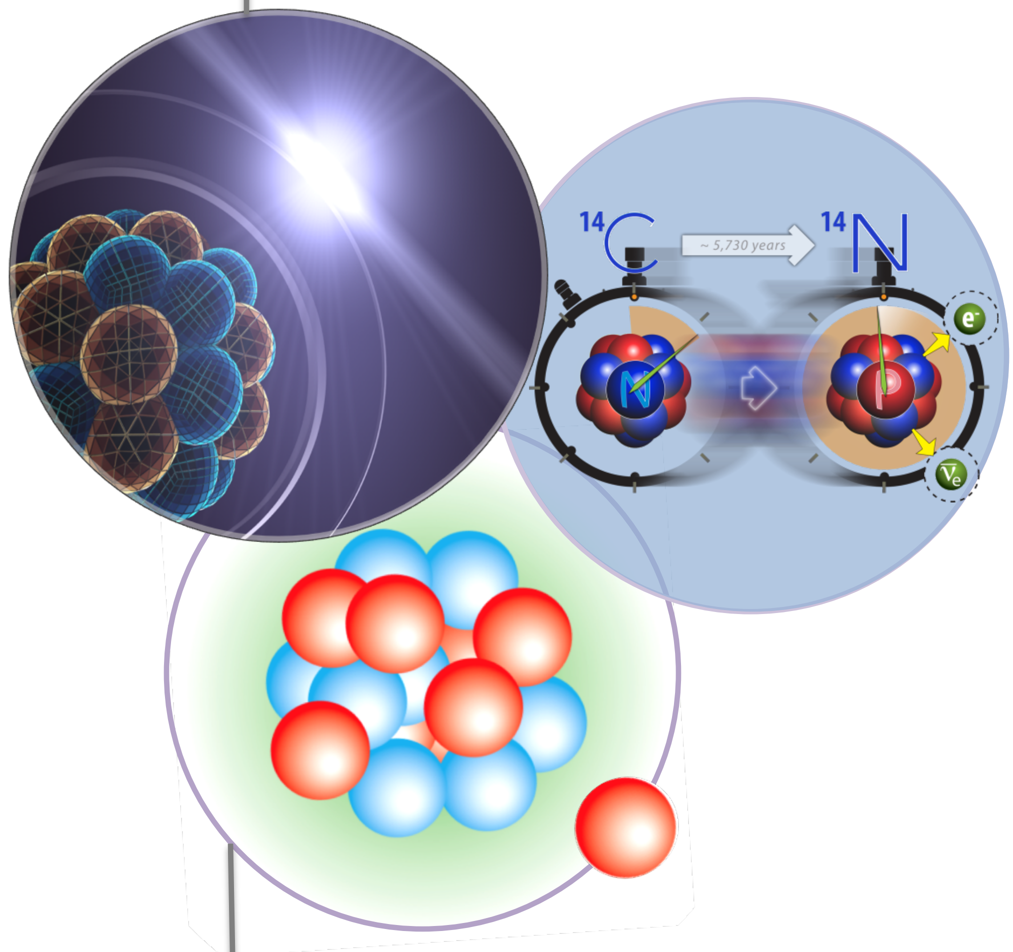
# Computing “real nuclei” from “pseudo EFT” interactions





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# Collaborators

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

@ MSU: W. Nazarewicz

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

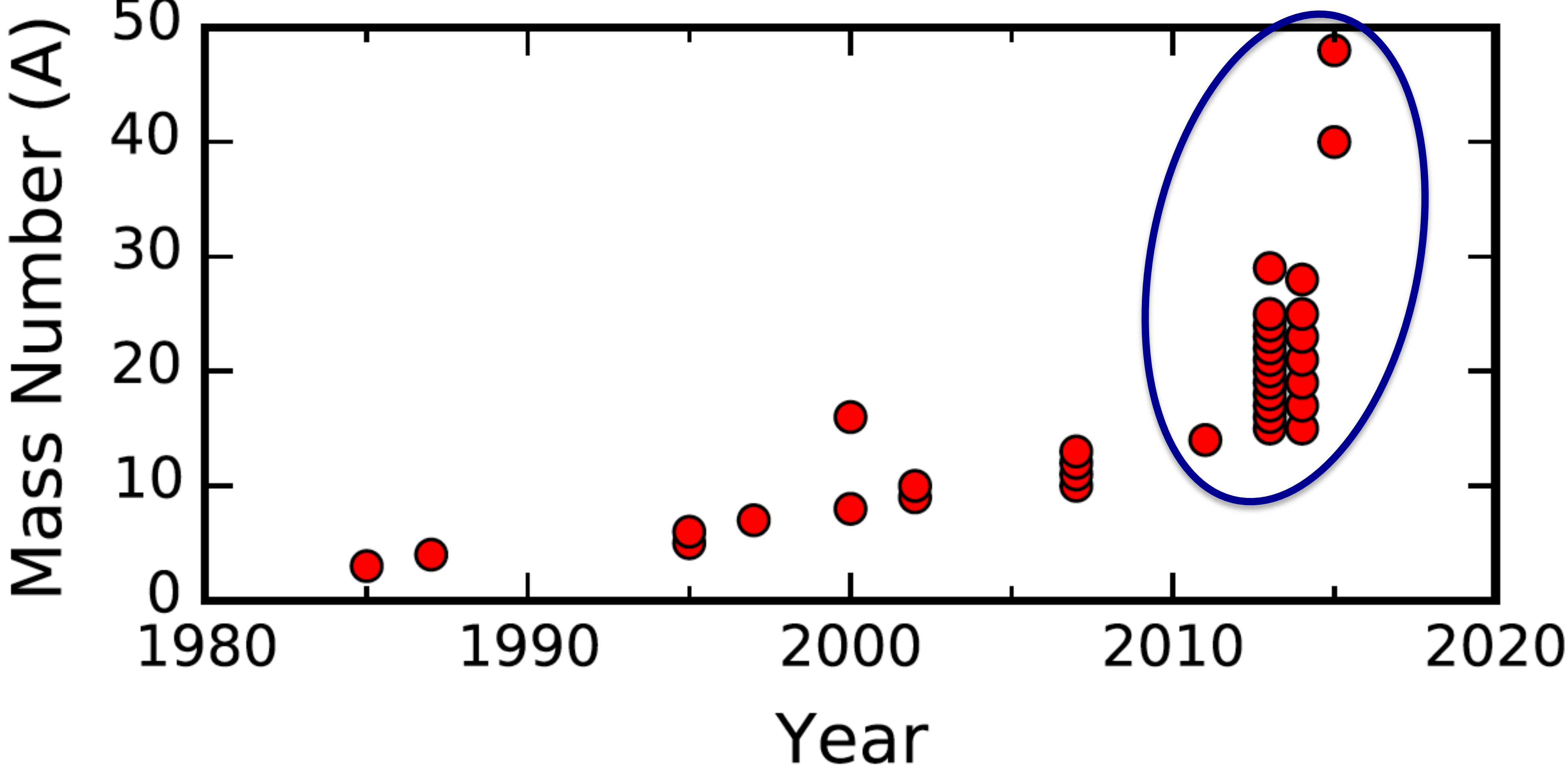
# Outline

- Challenges and status of ab initio computations of nuclei
- Accurate binding energies and radii from a chiral interaction
- The neutron radius and dipole polarizability of $^{48}Ca$
- Unexpected large charge radii of $^{52}Ca$ questions its magicity
- Structure of $^{78}Ni$ from first principles computations
- Role of continuum on shell structure of neutron-rich calcium isotopes

# 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, …)

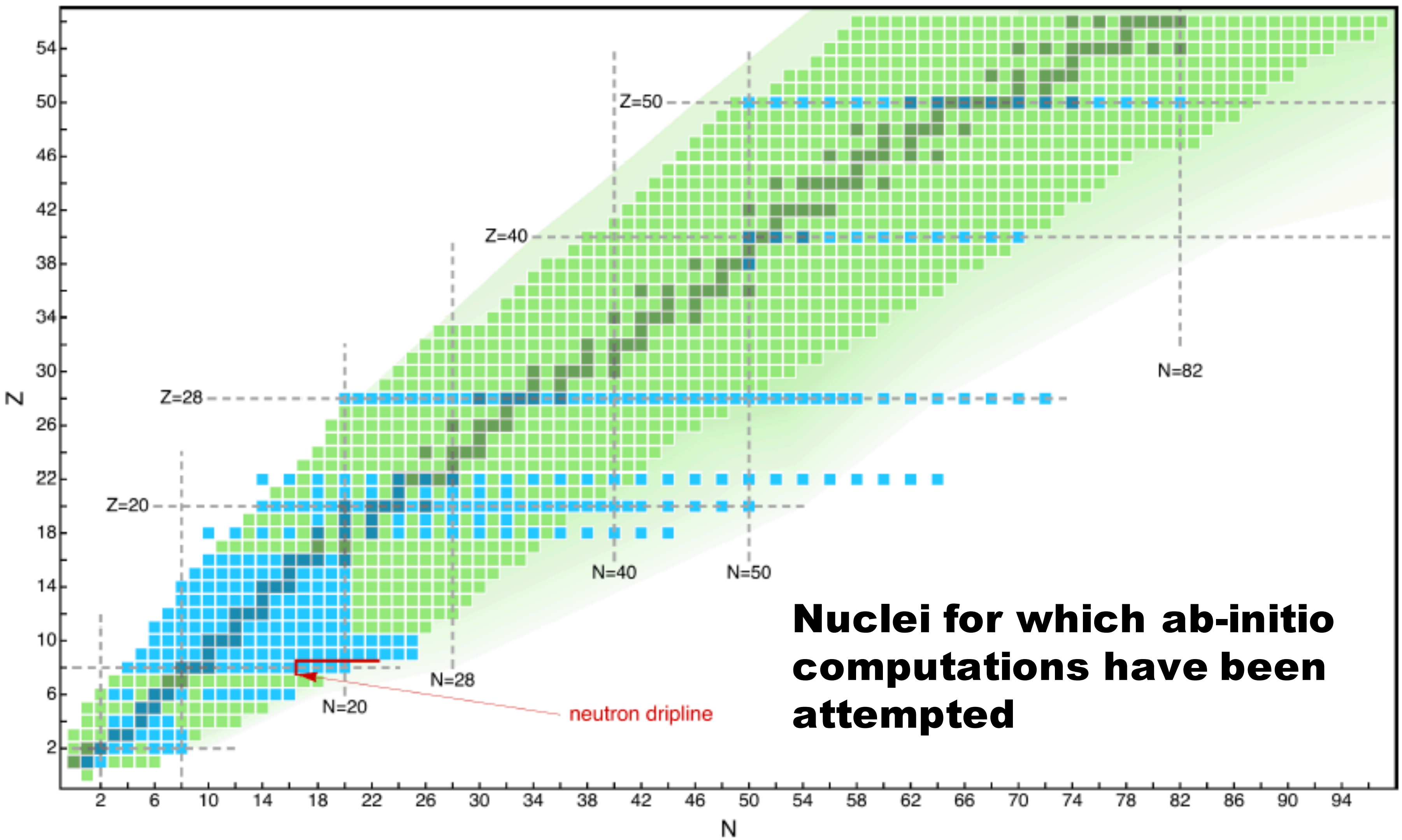
**Application of ideas from EFT and renormalization group** ($V_{low-k}$, Similarity Renormalization Group, …)




Computational capabilities exceed accuracy of available interactions

[Binder *et al*, Phys. Lett. B 736 (2014) 119]

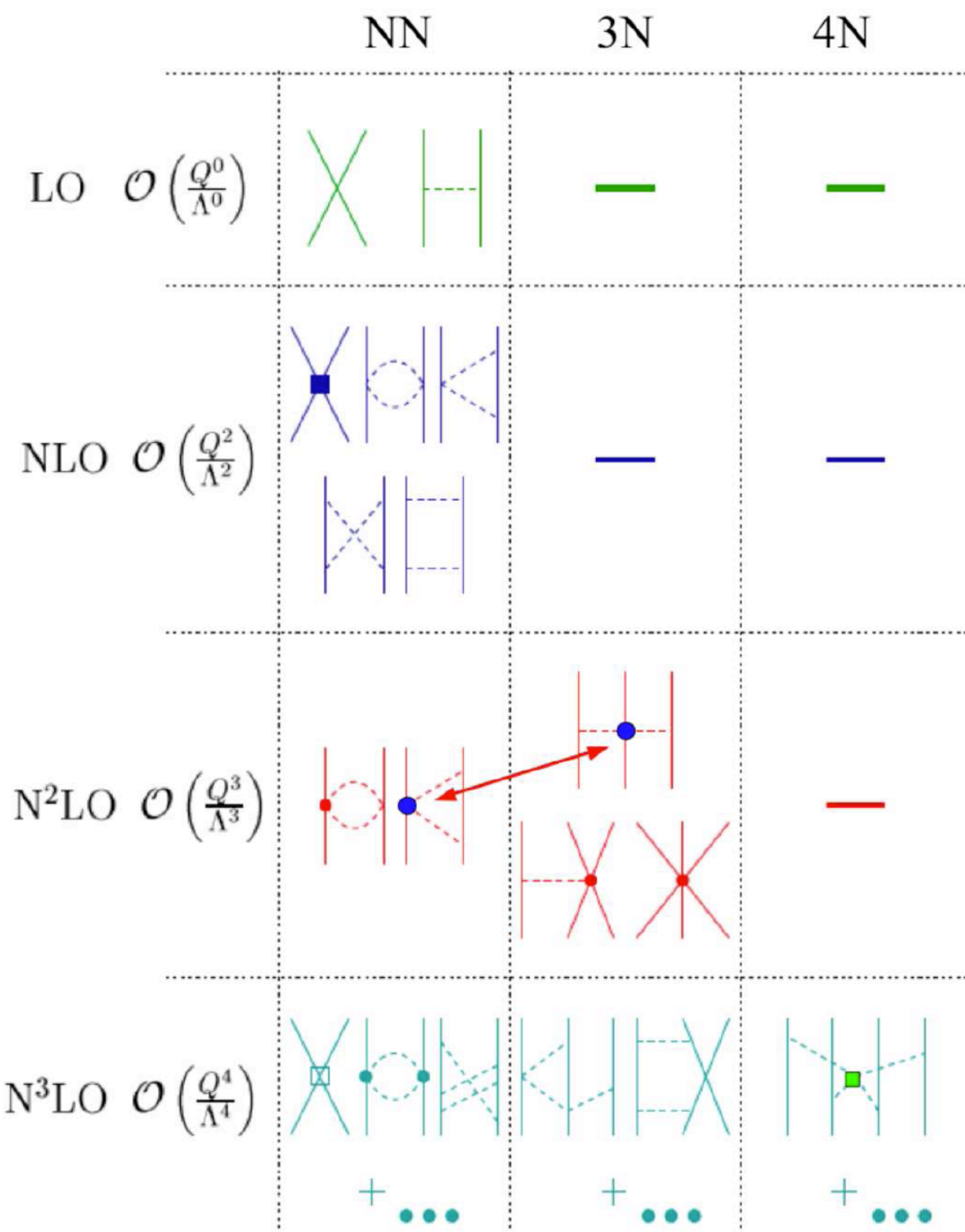
# Reach of ab-initio computations of nuclei




H. Hergert *et al*, Physics Reports 621, 165-222 (2016)

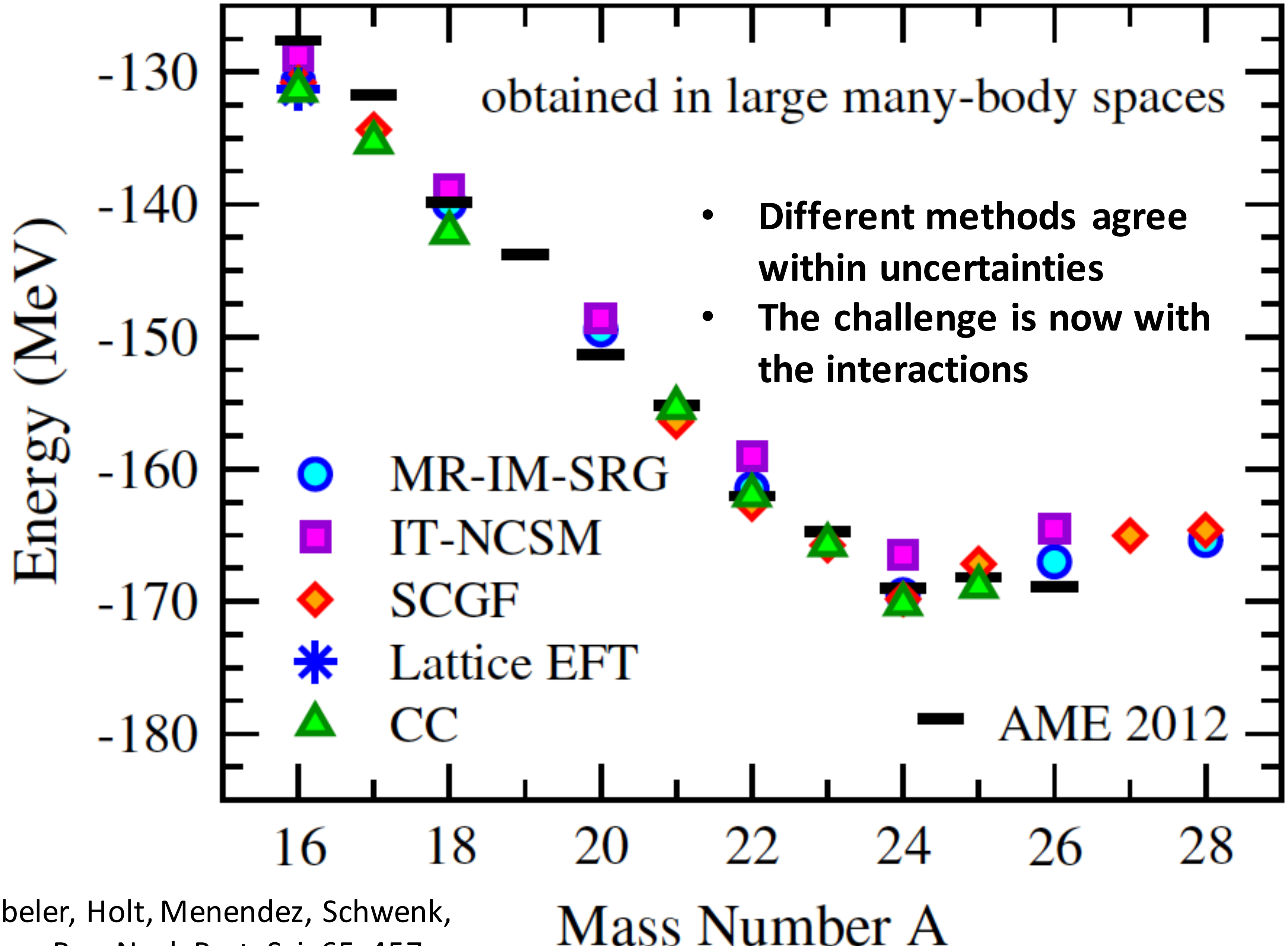
# Nuclear forces from chiral effective field theory

[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; …]
- 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 2013]
- Improved understanding and handling via renormalization group transformations [Bogner et al 2003; Bogner et al 2007]
- Problem: Not RG invariant. Different power counting schemes underway

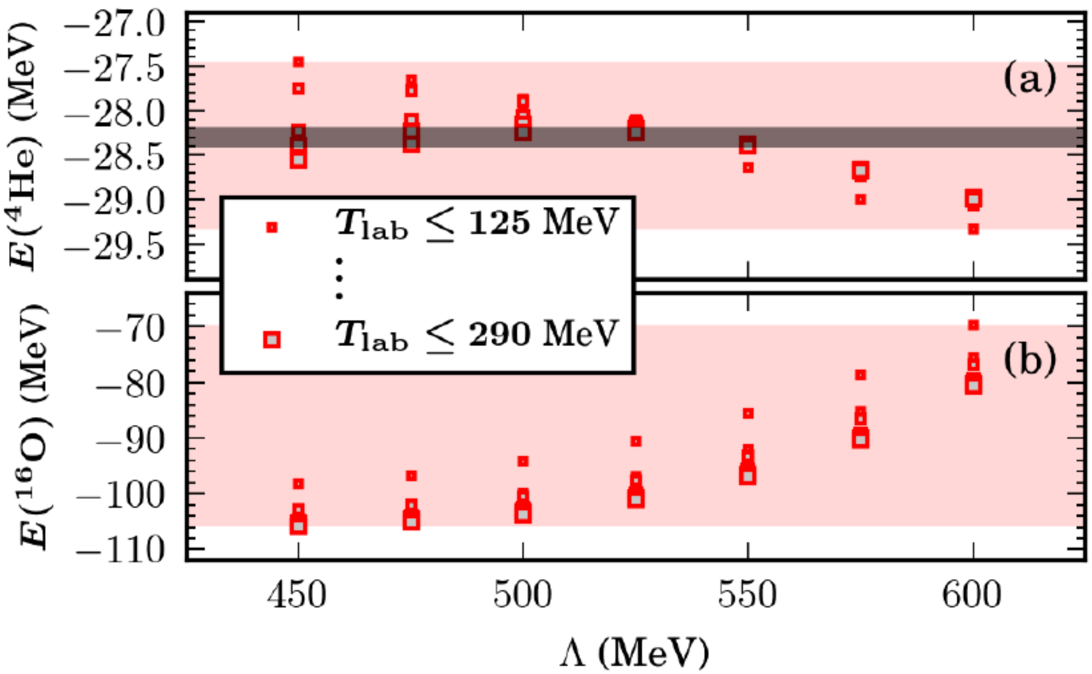
# Oxgyen chain with interactions from chiral EFT




- **Different methods agree within uncertainties**
- **The challenge is now with the interactions**

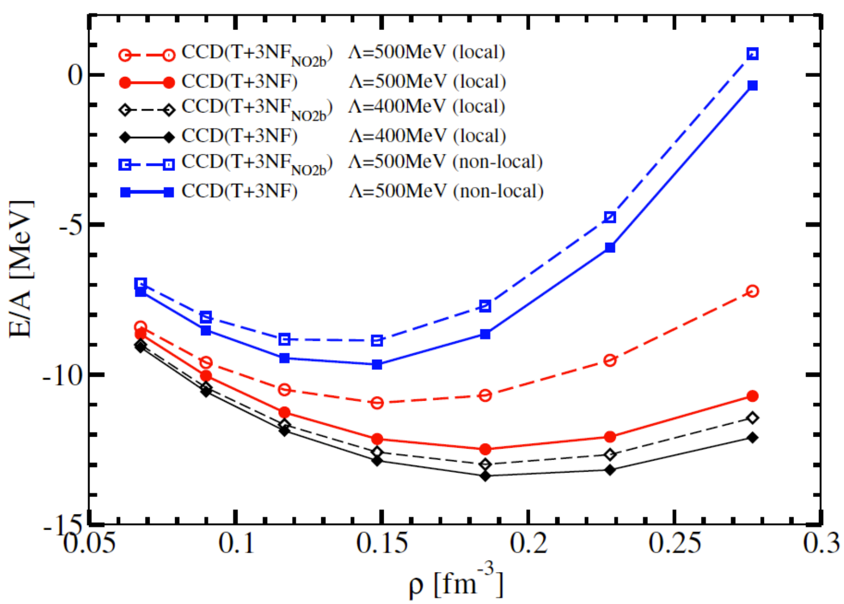
Hebeler, Holt, Menendez, Schwenk, Annu. Rev. Nucl. Part. Sci. 65, 457 (2015)

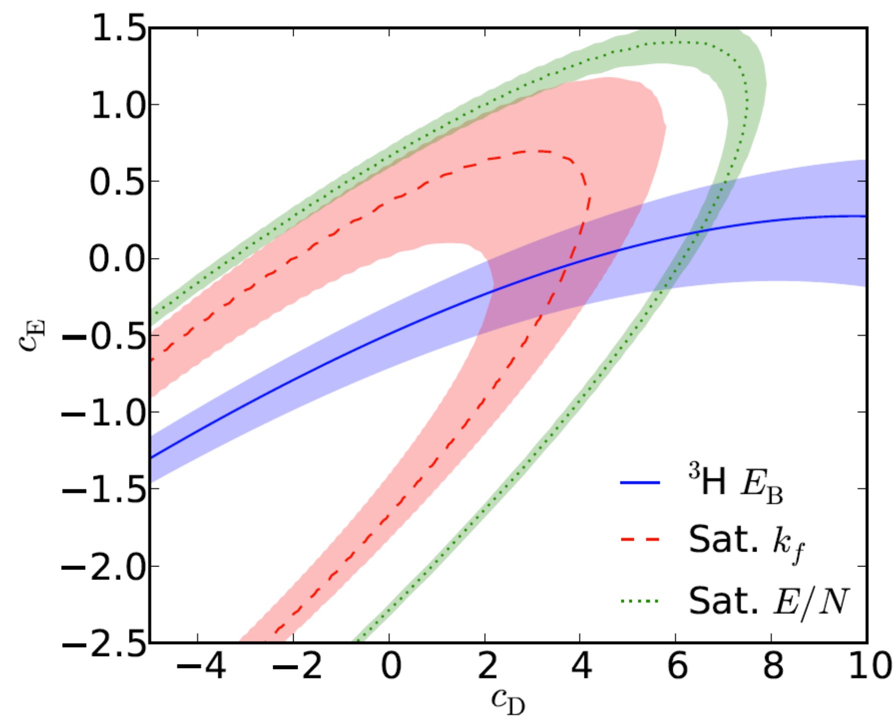
# Nuclear saturation is finely tuned



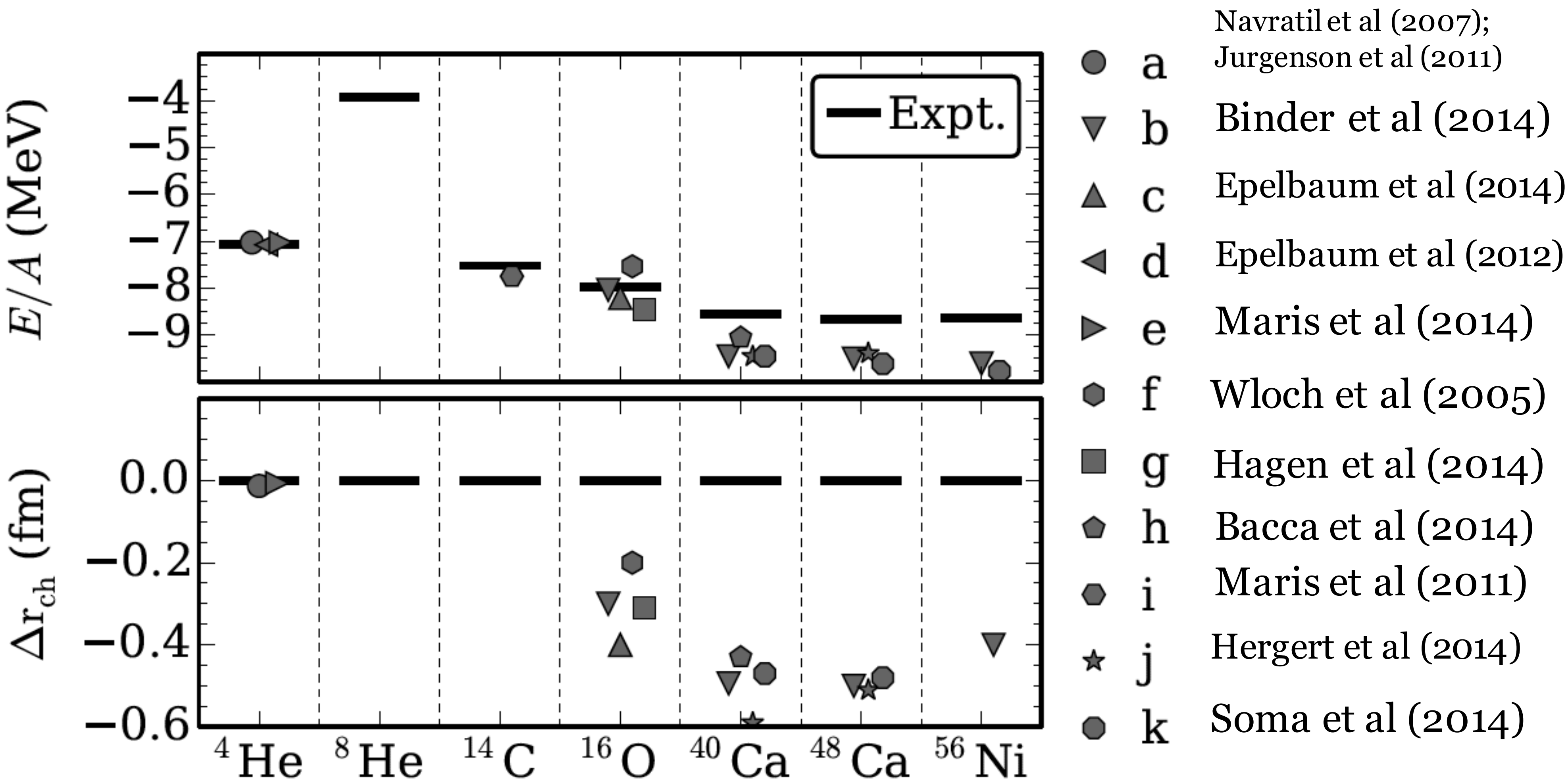

- A 4% change in the binding energy of $^4$He yields a 15% change in $^{16}$O [B. Carlsson, A. Ekström, C. Forssén *et al.*, PRX **6**, 011019 (2016)].
- Regulator dependence in saturation properties of nuclear matter
- Not possible to simultaneously describe nuclear matter light nuclei by only adjusting $c_E$ and $c_D$ of 3NF

G. Hagen *et al.*, PRC 89 014319 (2013)]



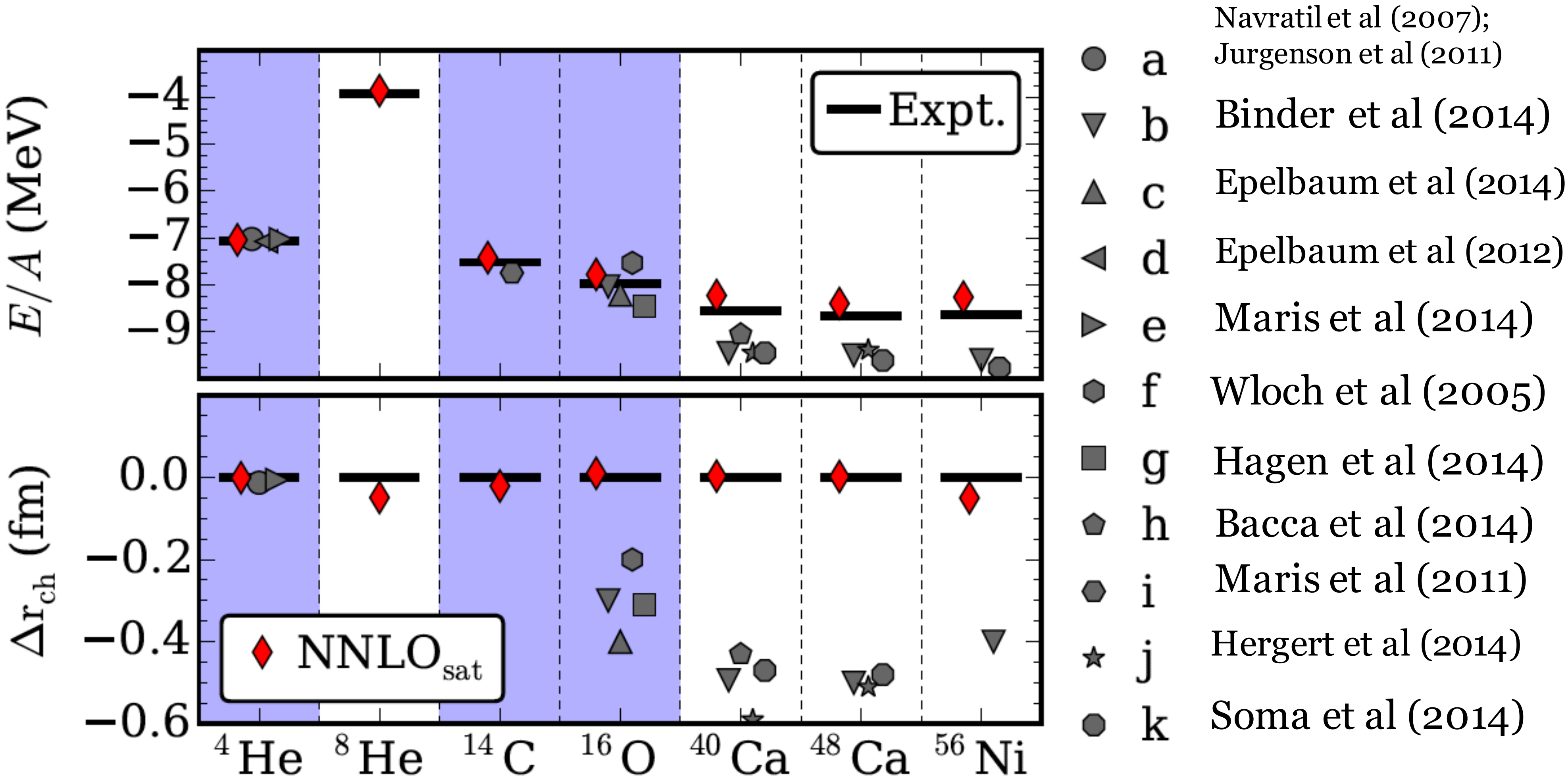



# Accurate nuclear binding energies and radii from a chiral interaction




- 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



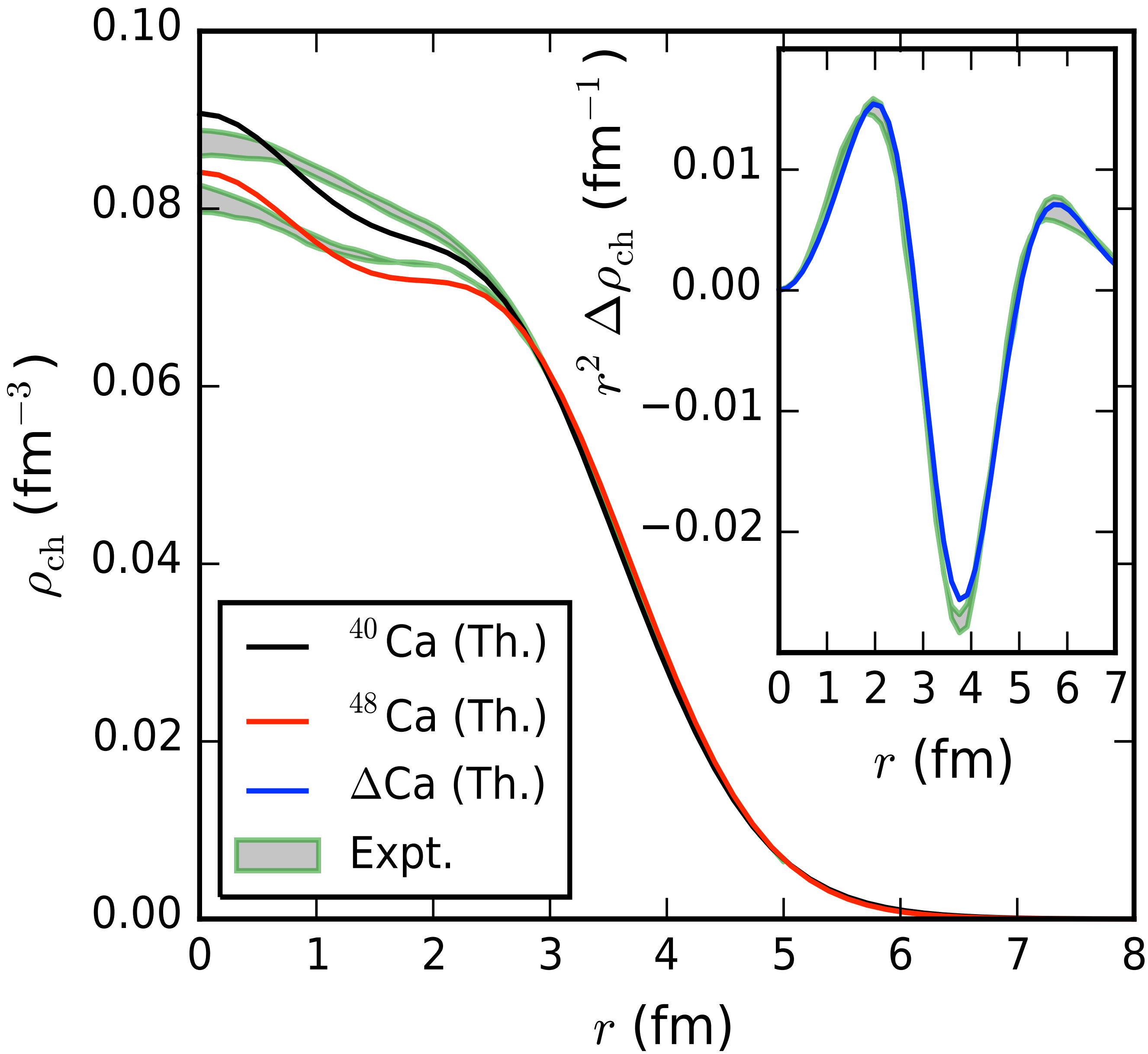

**Solution**: Simultaneous optimization of NN and 3NFs
Include charge radii and binding energies of $^3$H, $^{3,4}$He, $^{14}$C, $^{16}$O in the optimization ($NNLO_{sat}$)

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

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

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

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



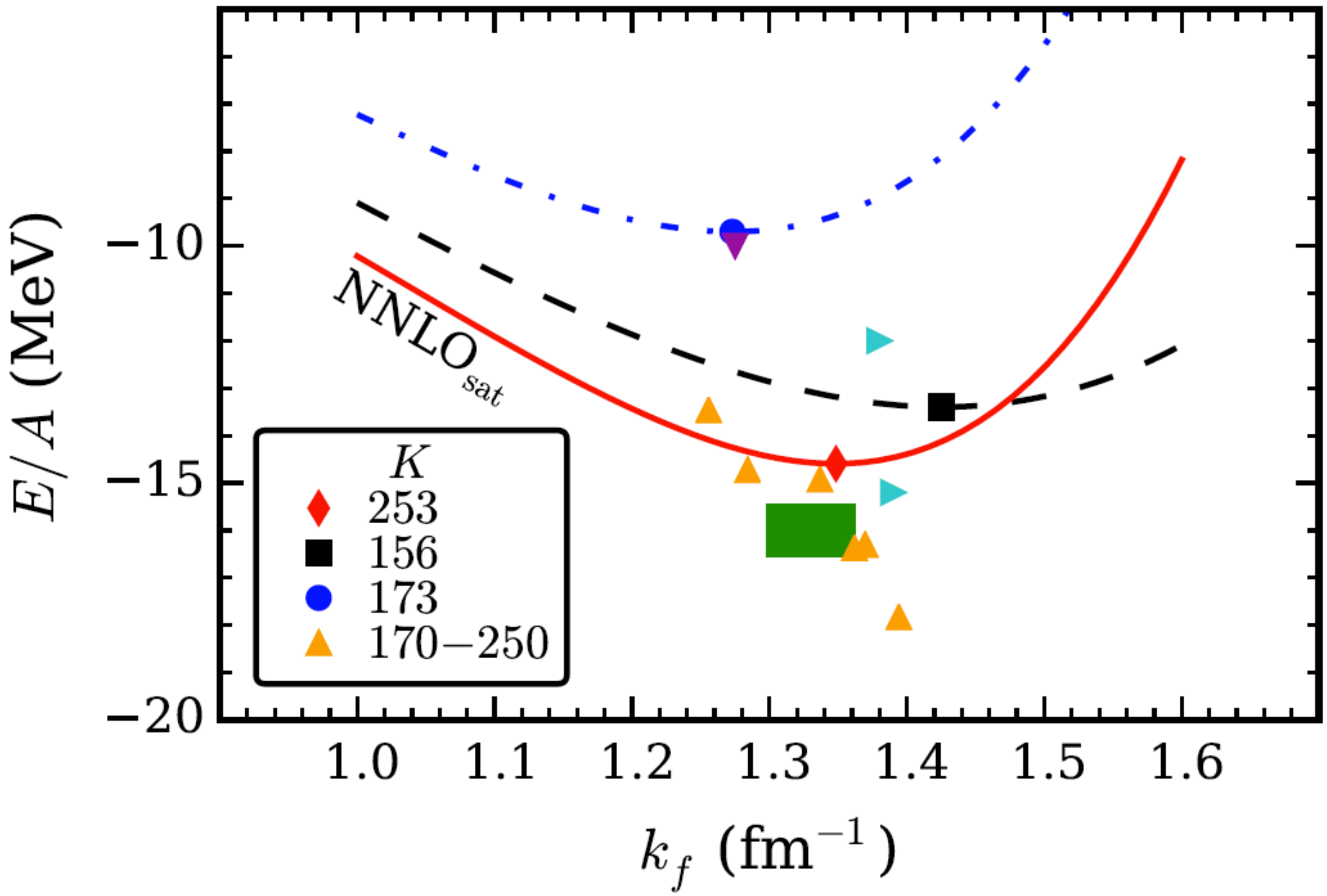

Electric charge distributions have been a long-standing problem for *ab initio* theory.

$BE$(Th) = 404(3) MeV
$BE$(Exp) = 416 MeV

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

# Nuclear matter from $NNLO_{sat}$

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



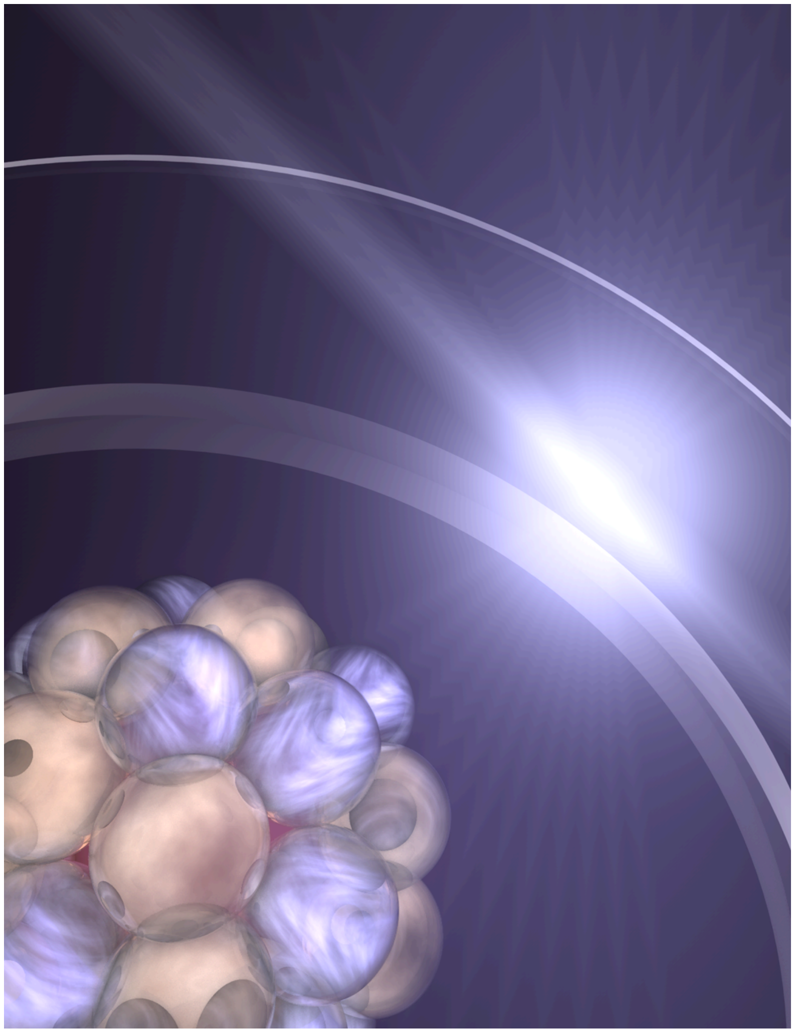

Nuclear matter saturation curves for $NNLO_{sat}$ and other interactions.

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

▲ **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

# What is the neutron skin of $^{48}$Ca



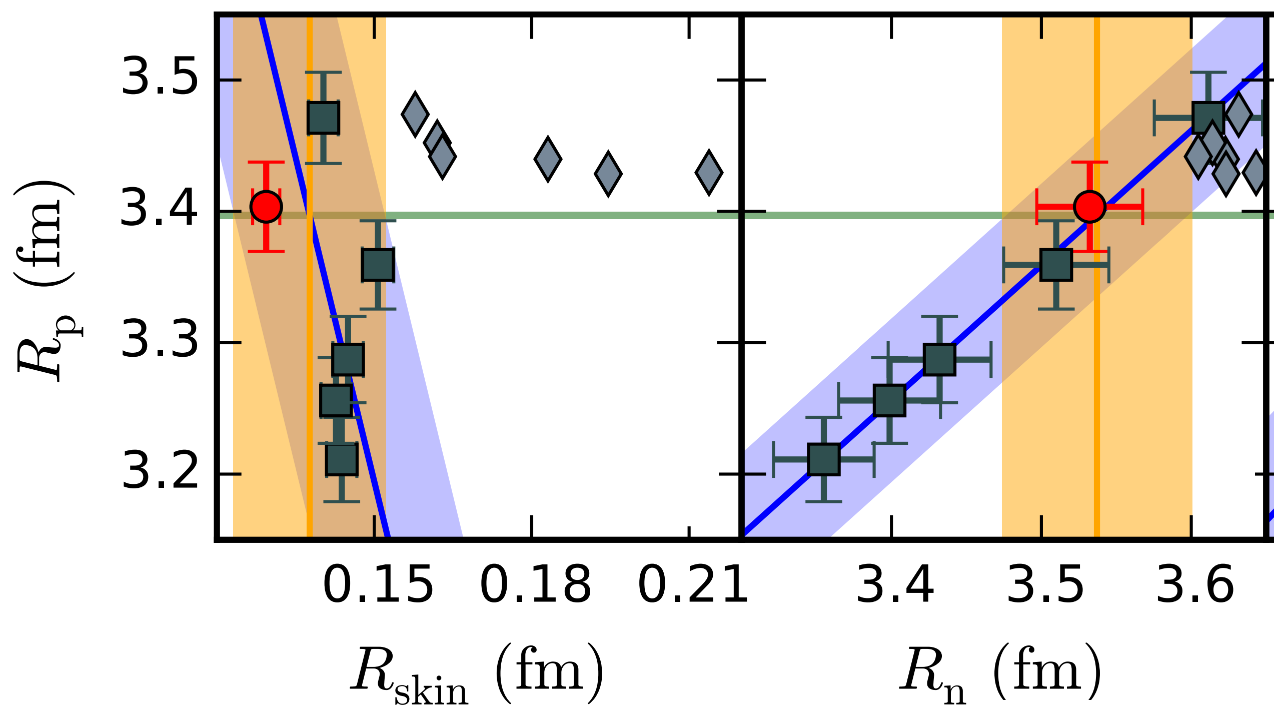
**Neutron skin** = Difference between radii of neutron and proton distributions

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 radius and skin of $^{48}$Ca

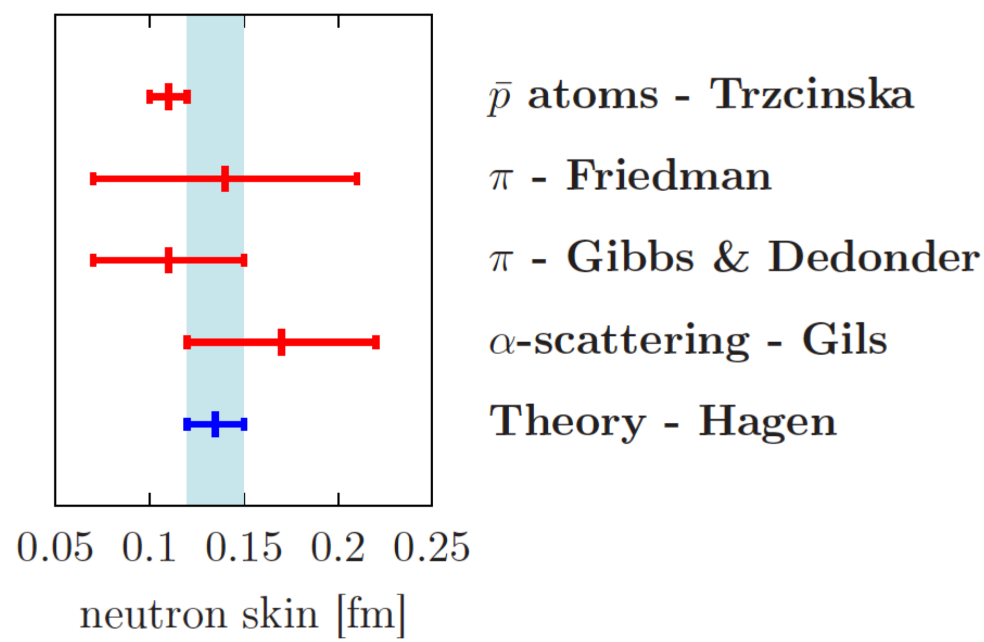



G. Hagen *et al*, Nature Physics **12**, 186–190 (2016)

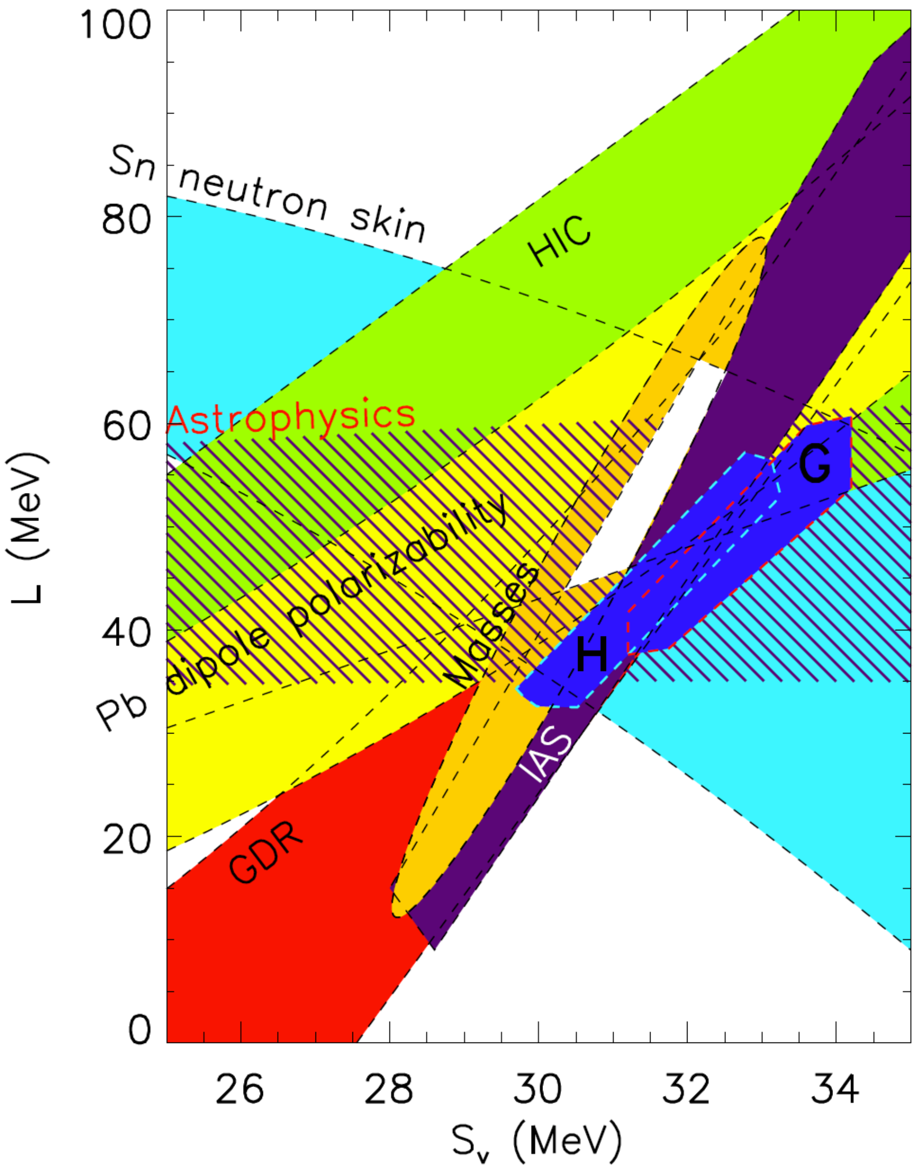
Uncertainty estimates from family of chiral interactions.

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

- Neutron skin significantly smaller than in DFT
- Neutron skin almost independent of the employed Hamiltonian
- Our prediction is consistent with existing data

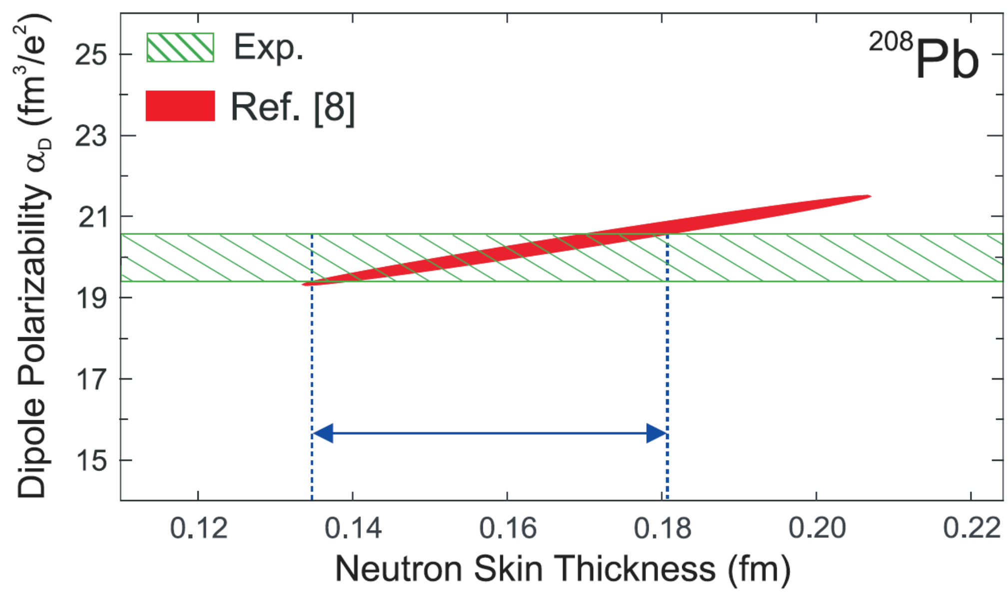


# Neutron radii and dipole polarizabilities




Lattimer & Lim 2013; Lattimer & Steiner 2014

Brown, PRL 2000, Piekarewicz & Horowitz, PRL 2001; Furnstahl, NPA 2002; Reinhard & Nazarewicz, PRC 2010; Piekarewicz et al., PRC 2012; Horowitz et al, PRC 2012; …

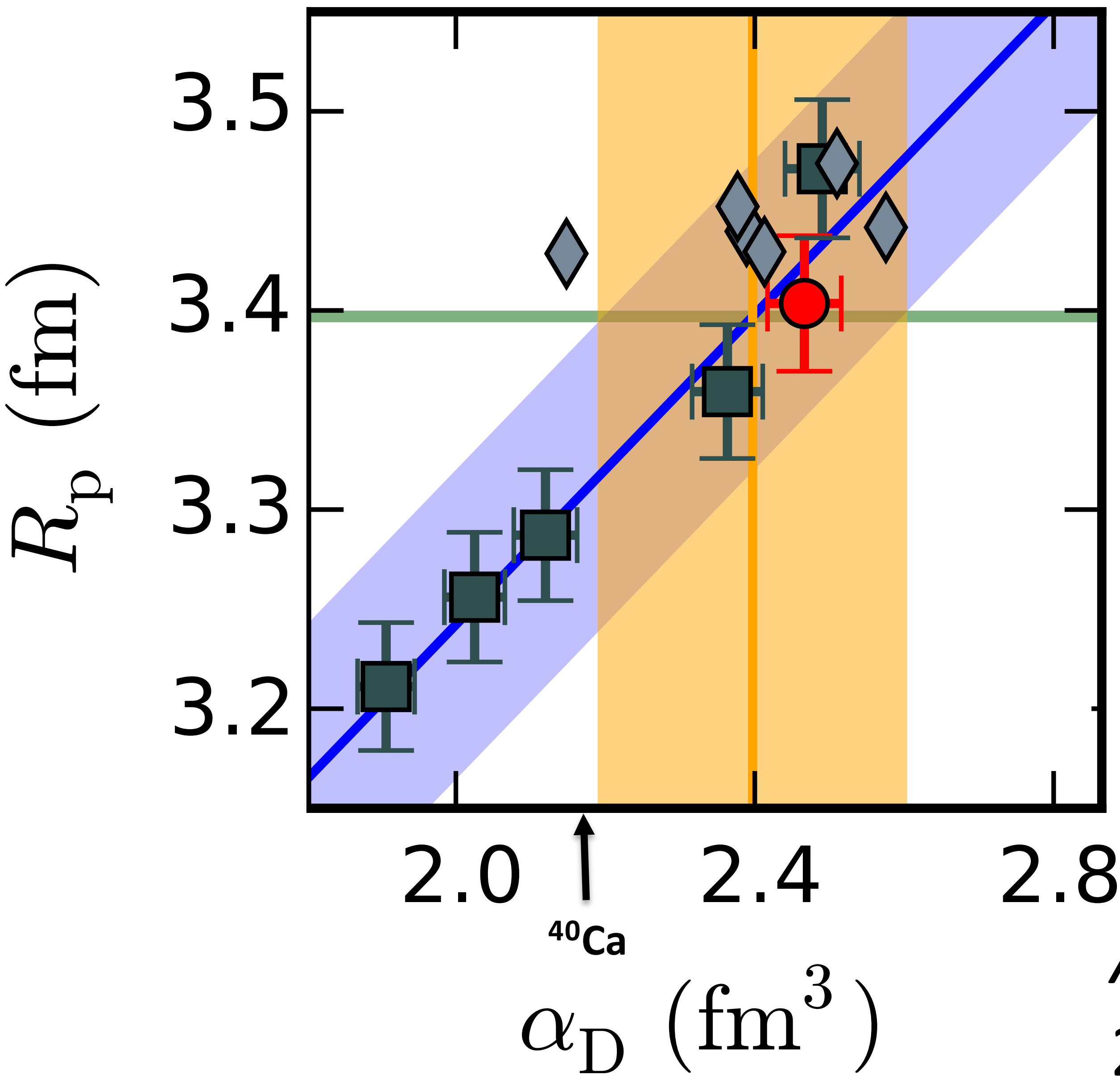



**$\alpha_D$**: $^{208}$Pb by Tamii et al, PRL 2011; $^{68}$Ni by Rossi et al, PRL 2013; $^{120}$Sn by Hashimoto et al. (2015); $^{48}$Ca coming soon …

**$R_n$**: $^{208}$Pb by Abrahamyan et al, PRL 2012; Tarbert et al, PRL 2013; $^{48}$Ca planned …

# 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:

$2.19 \lesssim \alpha_D \lesssim 2.60$ fm$^3$

# Large charge radii questions magicity of $^{52}$Ca

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

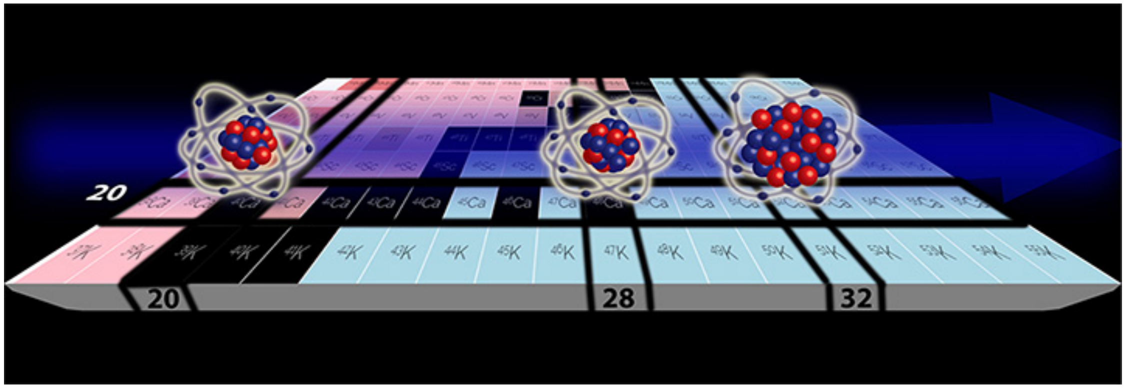
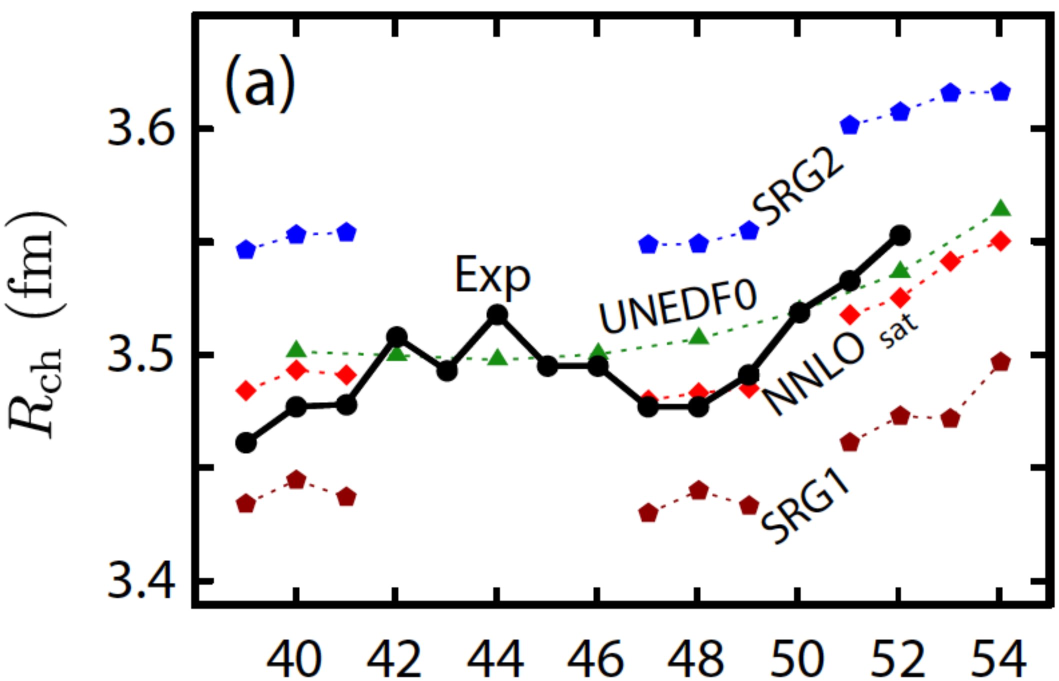
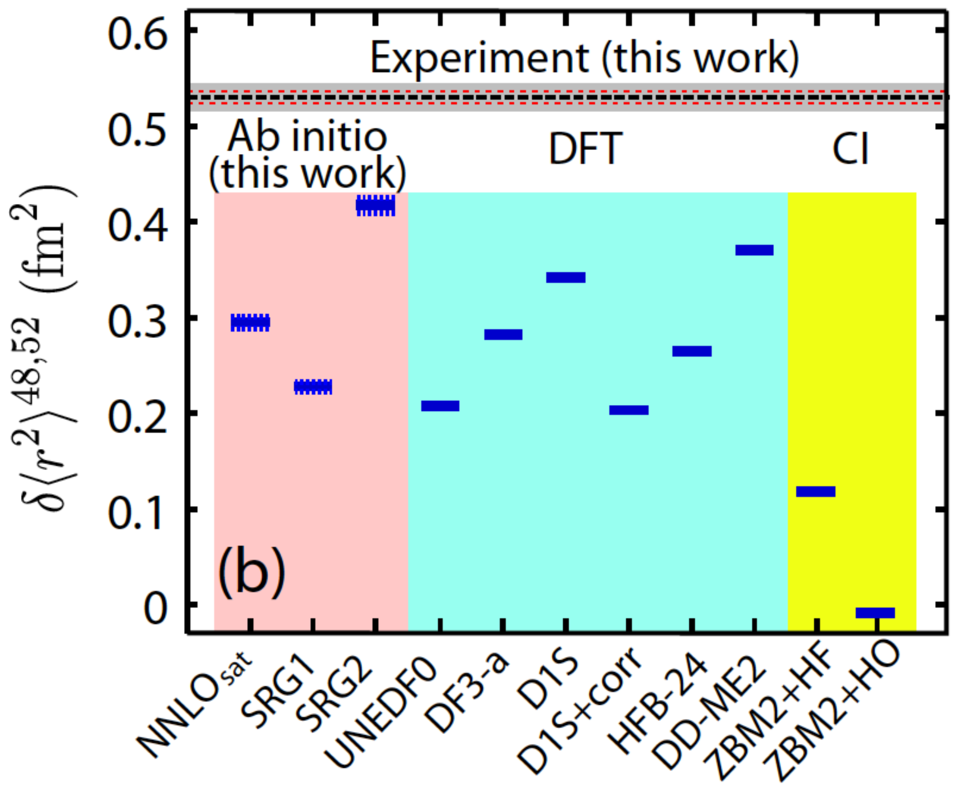


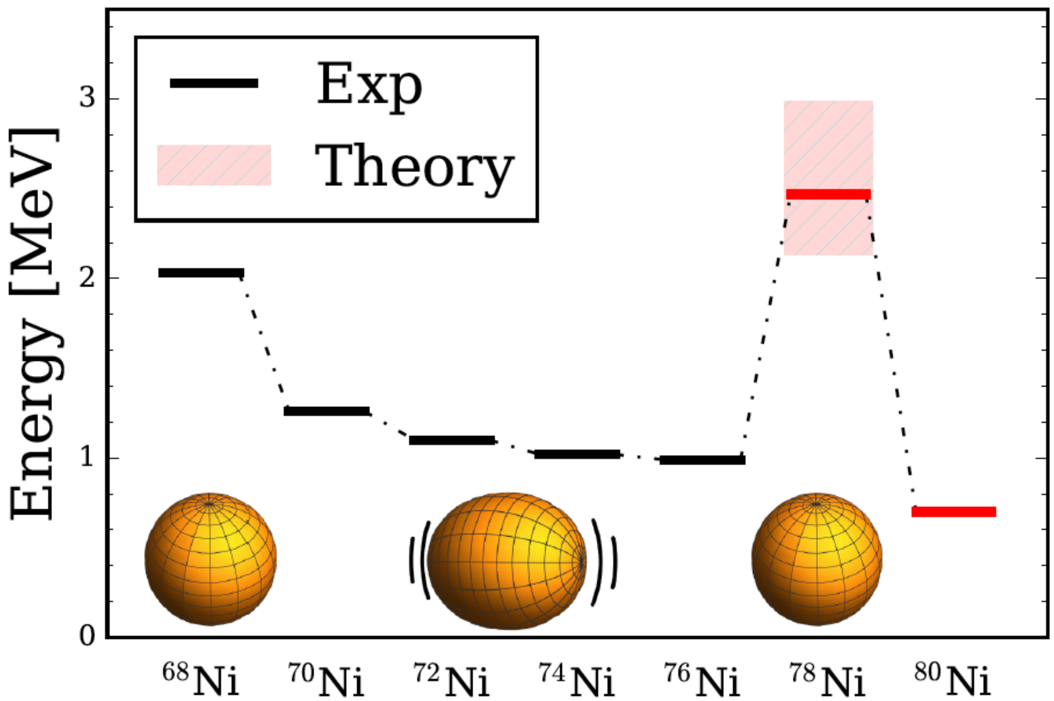

Image: COLLAPS Collaboration/Ronald Fernando Garcia Ruiz.

- Charge radii of $^{49,51,52}$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



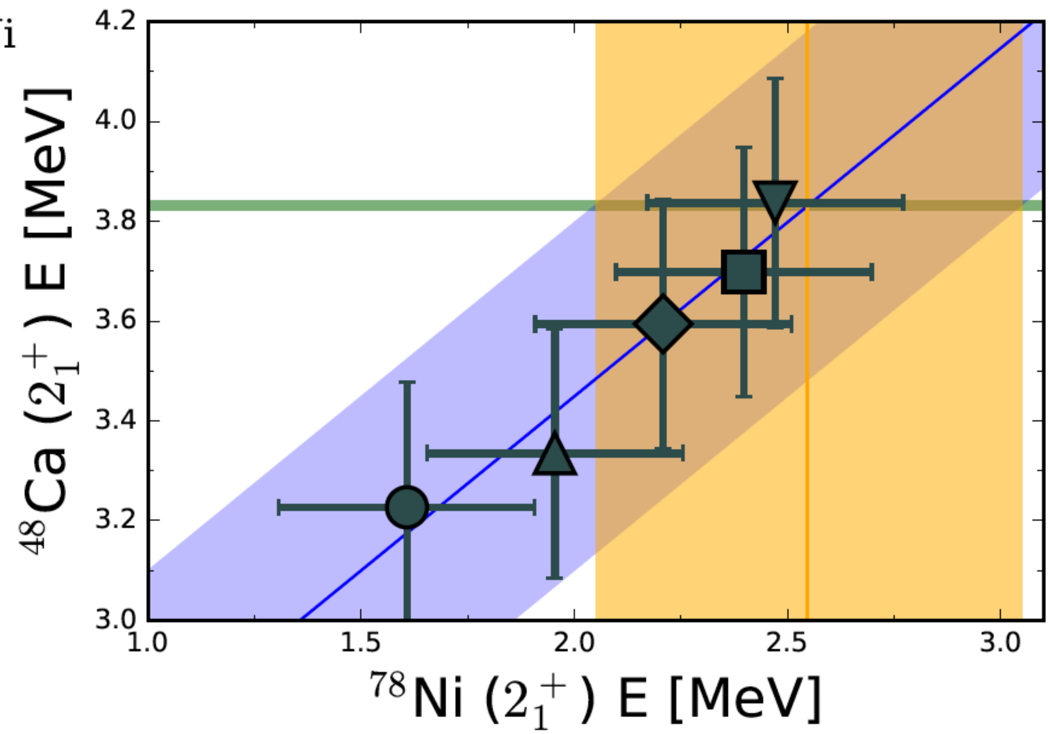
# Structure of $^{78}$Ni from first principles




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

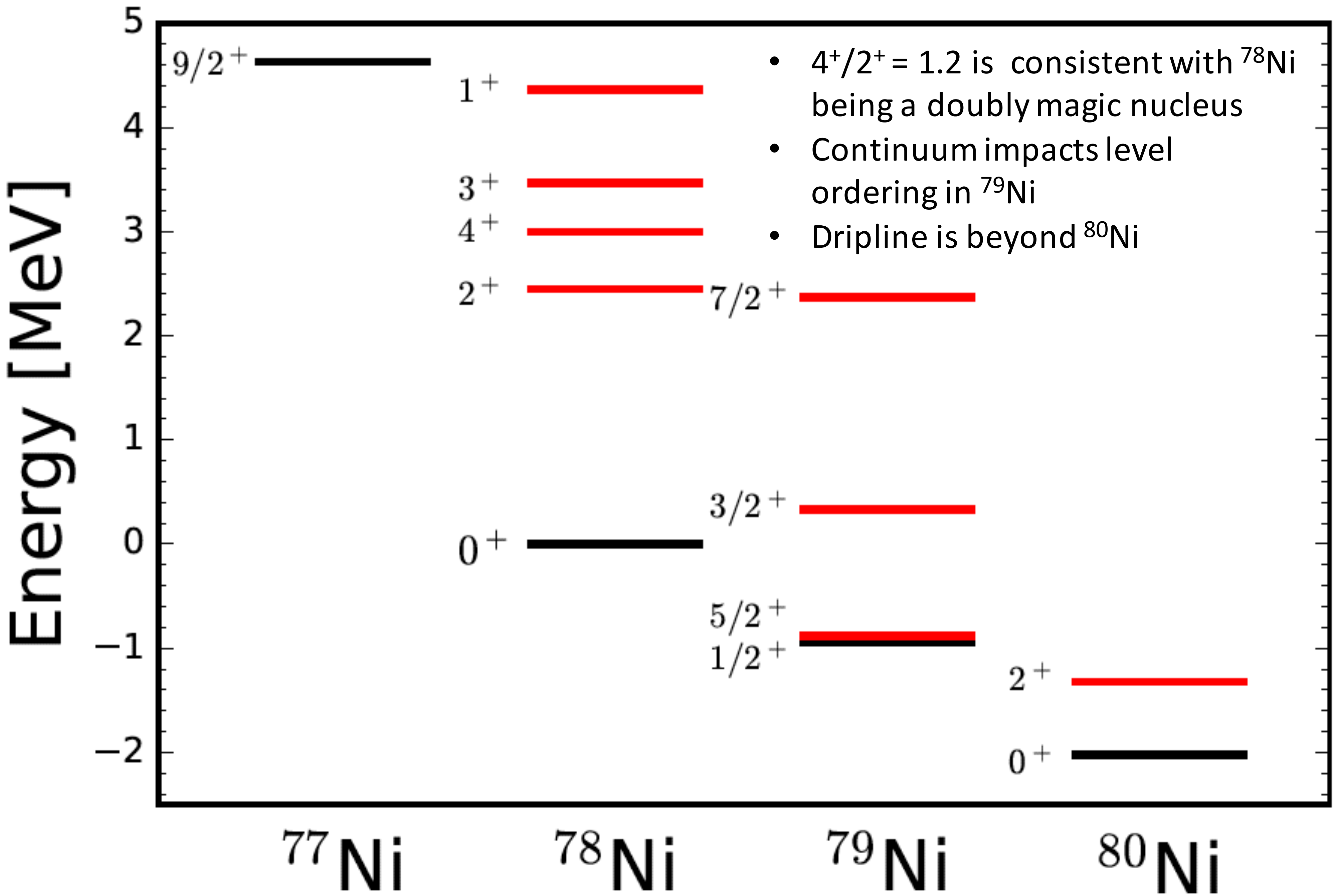
A measurement of this state has been made at RIBF, RIKEN
R. Taniuchi *et al.*, in preparation

- 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



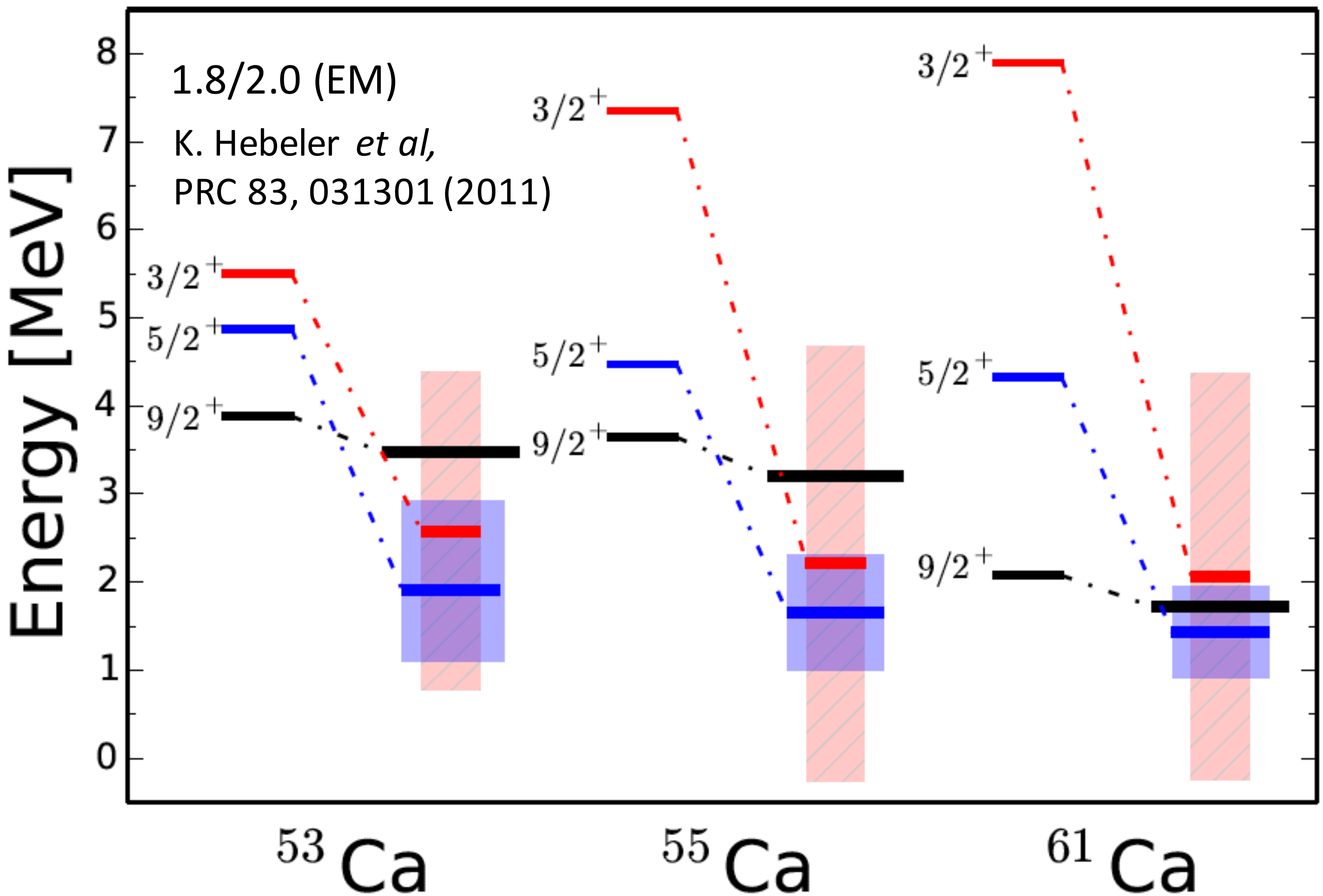

G. Hagen, G. R. Jansen, and T. Papenbrock
arXiv (2016)

# Excited states in $^{78}$Ni and its neighbors



# Role of continuum on unbound states in calcium isotopes

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



# Summary

- Exciting times in nuclear theory:
  - explosion of many-body solvers
  - many new developments regarding interactions and currents
- $NNLO_{sat}$ a pragmatic approach to the problem of nuclear saturation
- Neutron skin, dipole polarizability in $^{48}Ca$, and charge radii of neutron-rich calciums
- Structure of neutron-rich $^{78}Ni$ suggest it is doubly magic
  - predictions for soon-to-be measured quantities
  - charge radii in neutron-rich calcium isotopes not well understood
- How to address the problem of finetuned interactions, regulator dependencies and saturation in nuclei?
- Explore new power counting schemes?
- Computation of heavy nuclei from Hamiltonian based methods
- Propagation of uncertainties from the interaction to the nuclear many-body problem on the horizon
- Quantifying systematic uncertainties associated with truncations in ab-initio methods is still a challeng