Coupled cluster calculations of heavy and rare isotopes

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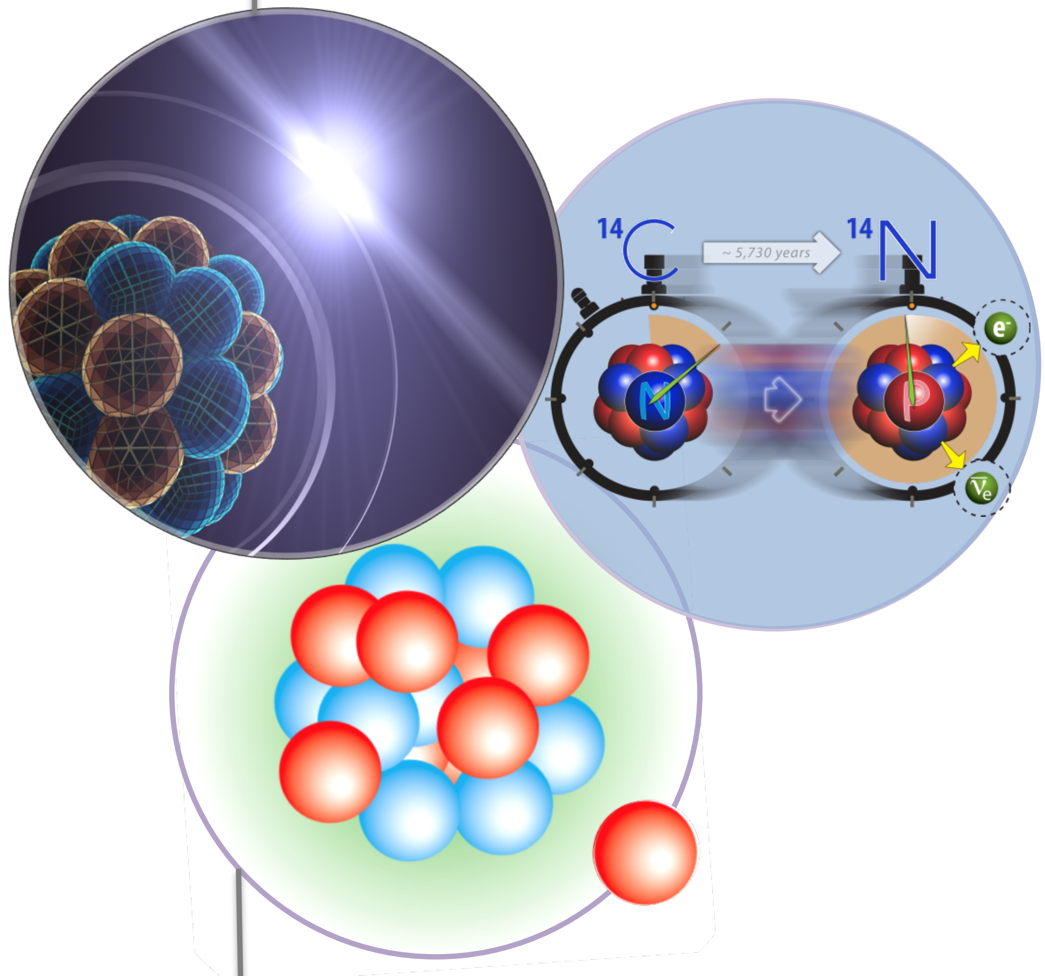
Oak Ridge National Laboratory

TRIUMF, March 2nd, 2017



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

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@ MSU/ U Oslo: M. Hjorth-Jensen

@ Trento: G. Orlandini

@ TRIUMF: S. Bacca, J. Holt, **M. Miorelli**, P. Navratil, **S. R. Stroberg**

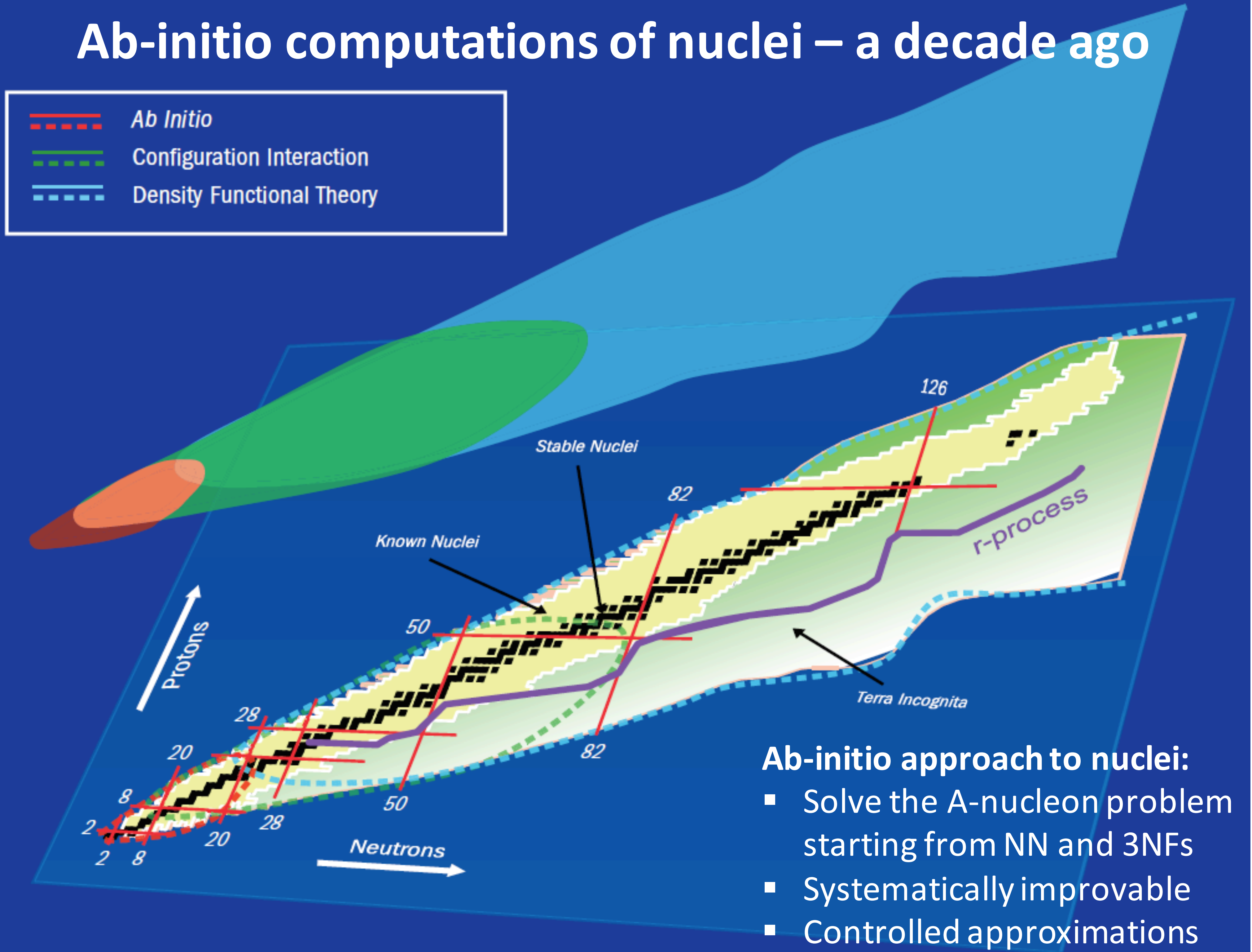
@ TU Darmstadt: **C. Drischler**, **C. Stumpf**, K. Hebeler, R. Roth, A. Schwenk, **J. Simonis**

@ LLNL: **K. Wendt**

Outline

- The neutron skin and dipole polarizability of ^{48}Ca and ^{68}Ni
- Structure of ^{78}Ni
- Structure and decay of ^{100}Sn
- Gamow-Teller response in ^{132}Sn
- Optical potentials from coupled-cluster theory

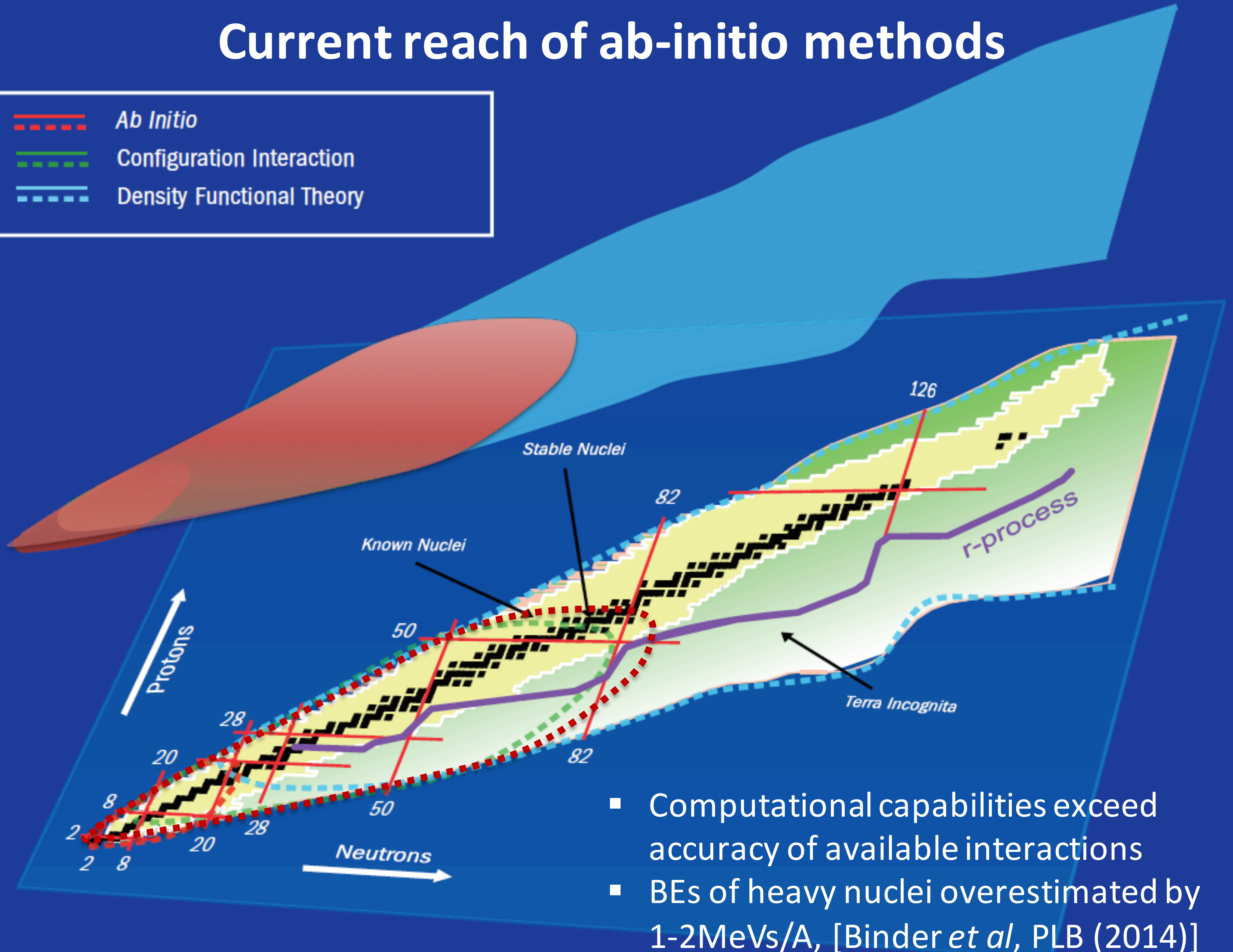
Ab-initio computations of nuclei – a decade ago



Ab-initio approach to nuclei:

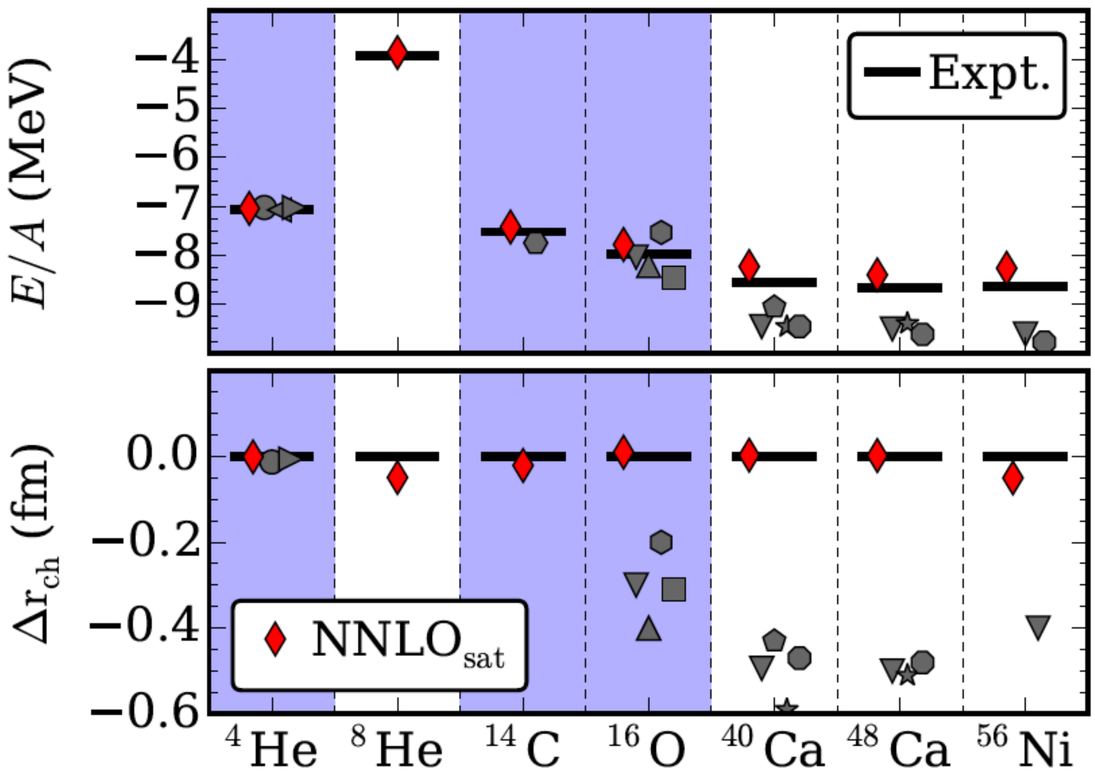
- Solve the A-nucleon problem starting from NN and 3NFs
- Systematically improvable
- Controlled approximations

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)]

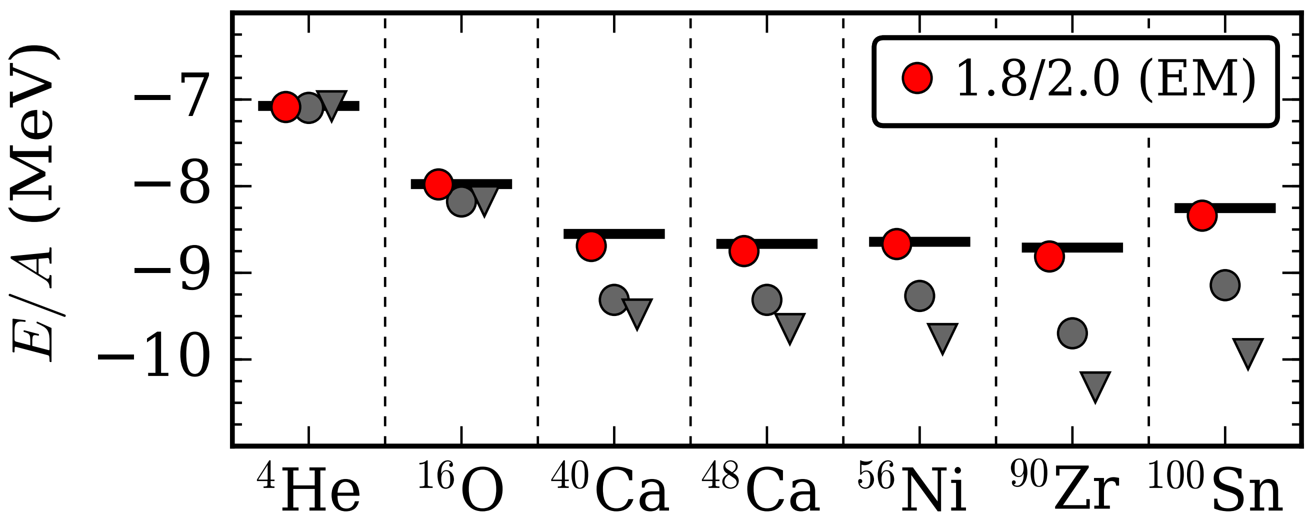
Two remarkable interactions from chiral EFT: $\mathrm{NNLO}_{\mathrm{sat}}$ & 1.8/2.0 (EM)



$\mathrm{NNLO}_{\mathrm{sat}}$: Accurate radii and BEs

- 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
- Harder interaction: difficult to converge beyond ^{56}Ni

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

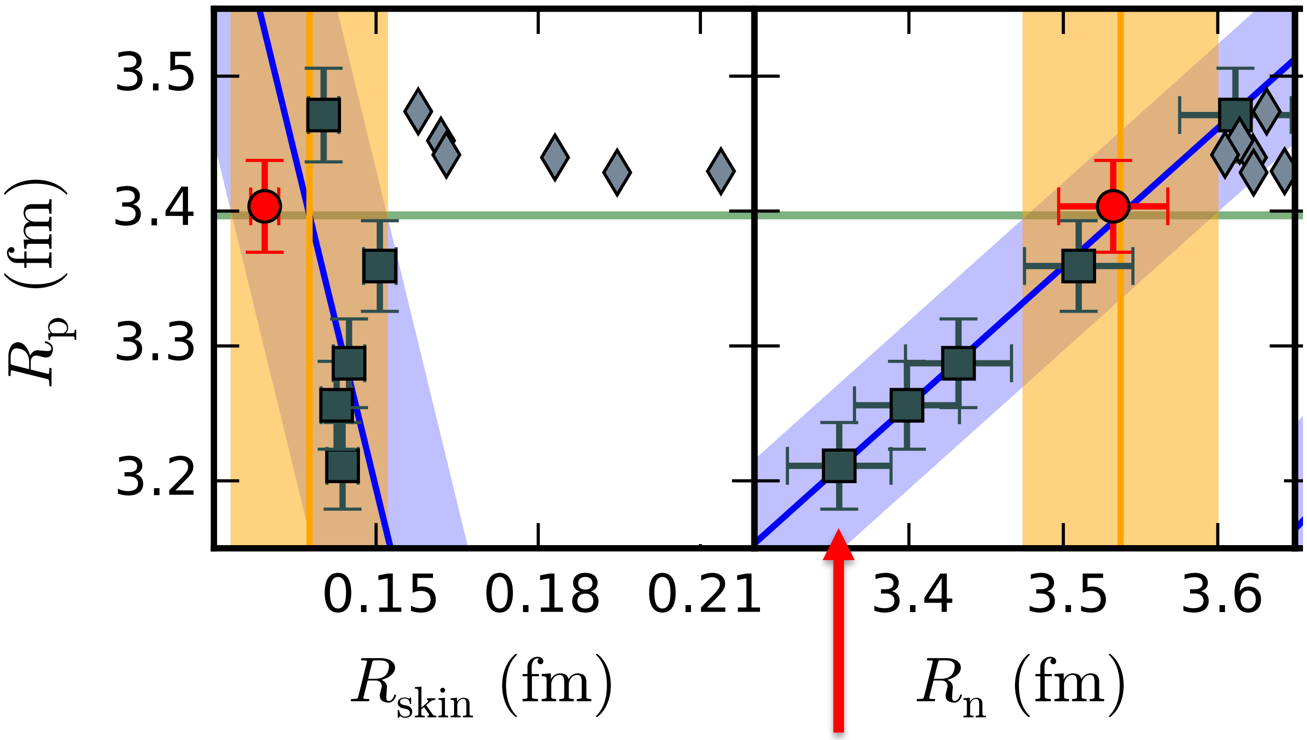


1.8/2.0(EM): Accurate BEs

Soft interaction: SRG NN from Entem & Machleidt with 3NF from chiral EFT

1.8/2.0 (EM) from K. Hebeler *et al* PRC (2011). The other chiral NN + 3NFs are from Binder et al, PLB (2014)

Neutron radius and skin of ^{48}Ca



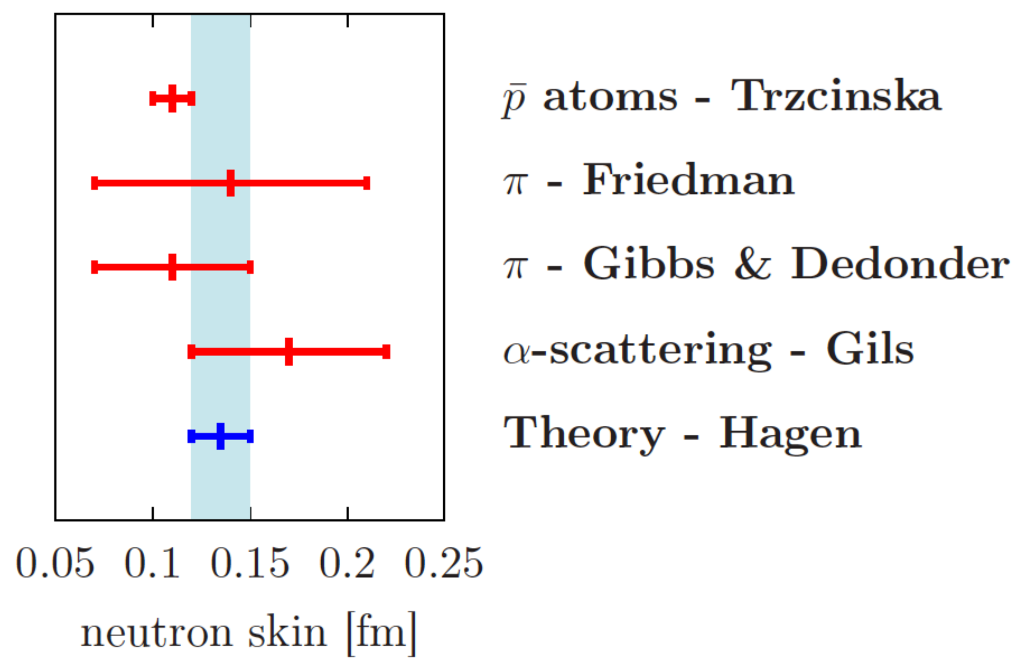
1.8/2.0 (EM)

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

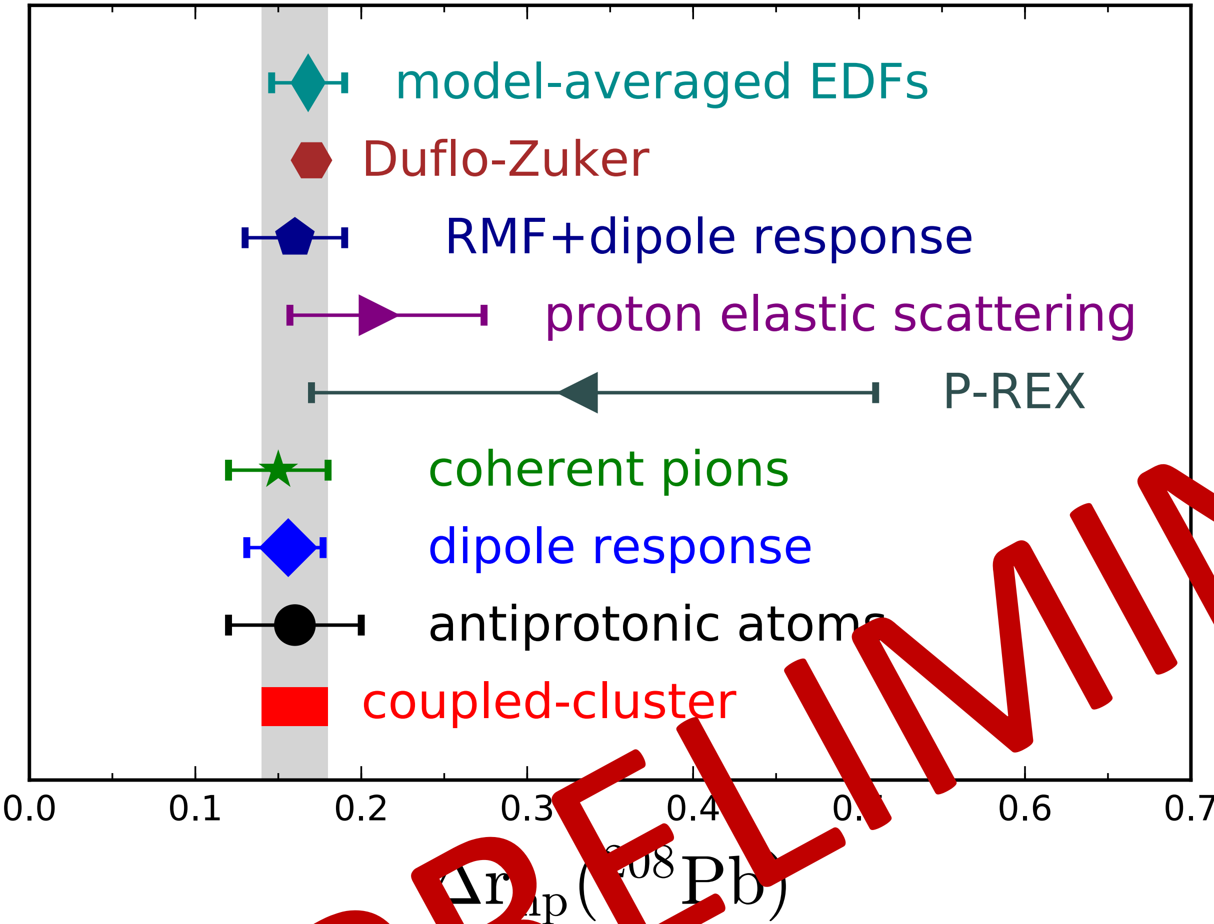
Uncertainty estimates from family of chiral interactions: K. Hebeler *et al* PRC (2011)

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

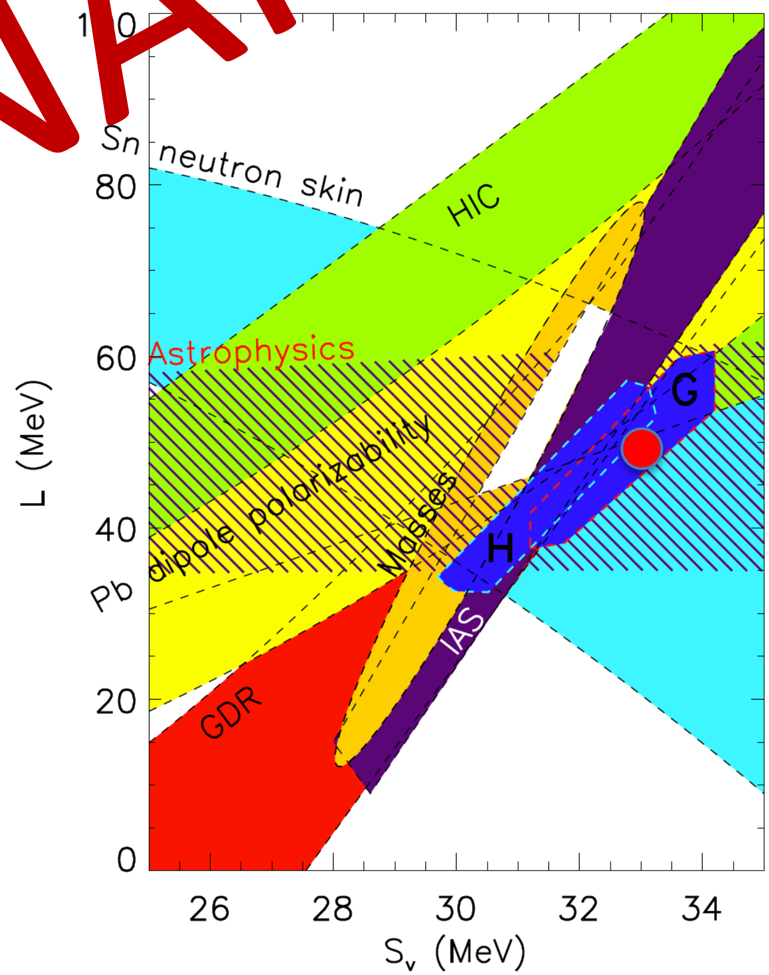
- Neutron skin significantly smaller than in DFT
- Neutron skin almost independent of the employed Hamiltonian
- Our predictions for ^{48}Ca are consistent with existing data



Neutron skin of ^{208}Pb

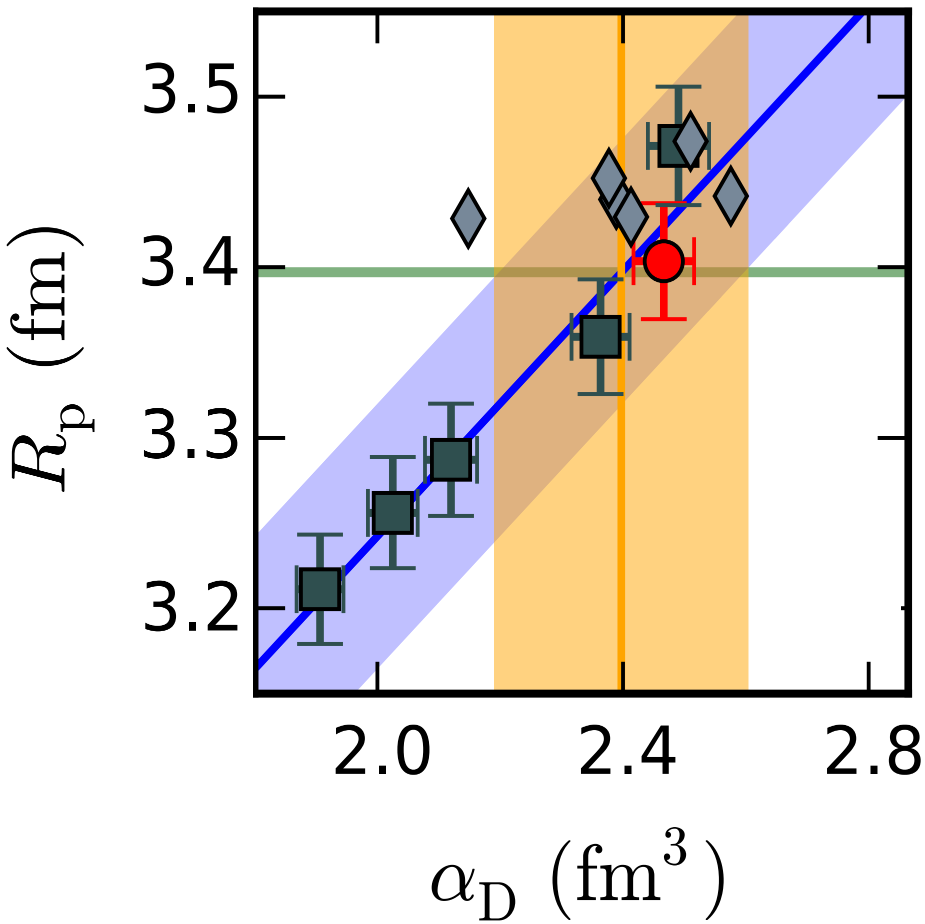


- Differences in radii converges more rapidly
- BE/A = 7.6(3) MeV in good agreement with data 7.87MeV



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

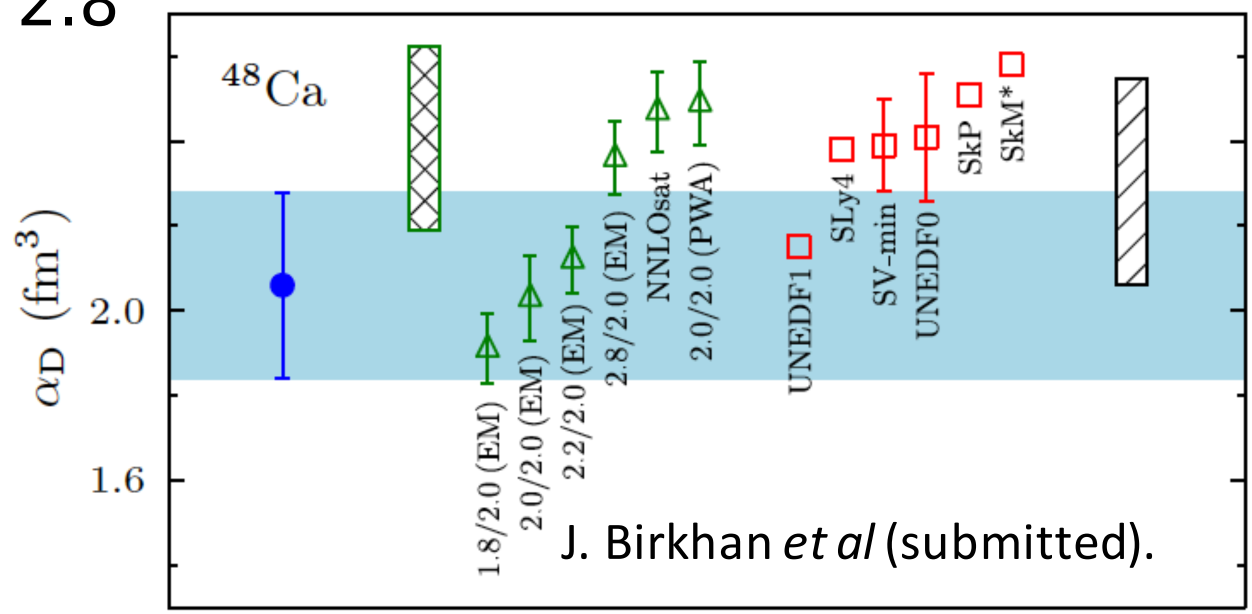
Dipole polarizability of ^{48}Ca



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



J. Birkhan *et al* (submitted).

Large charge radii questions magicity of ^{52}Ca

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

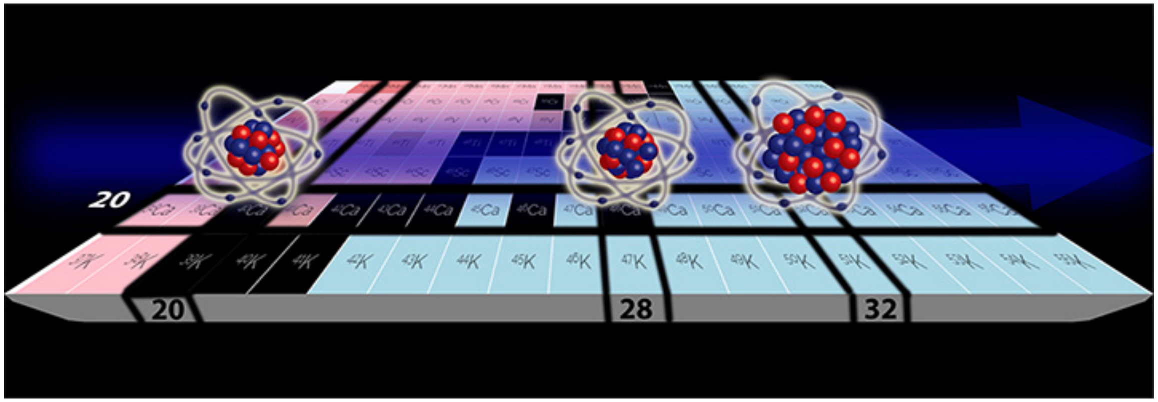
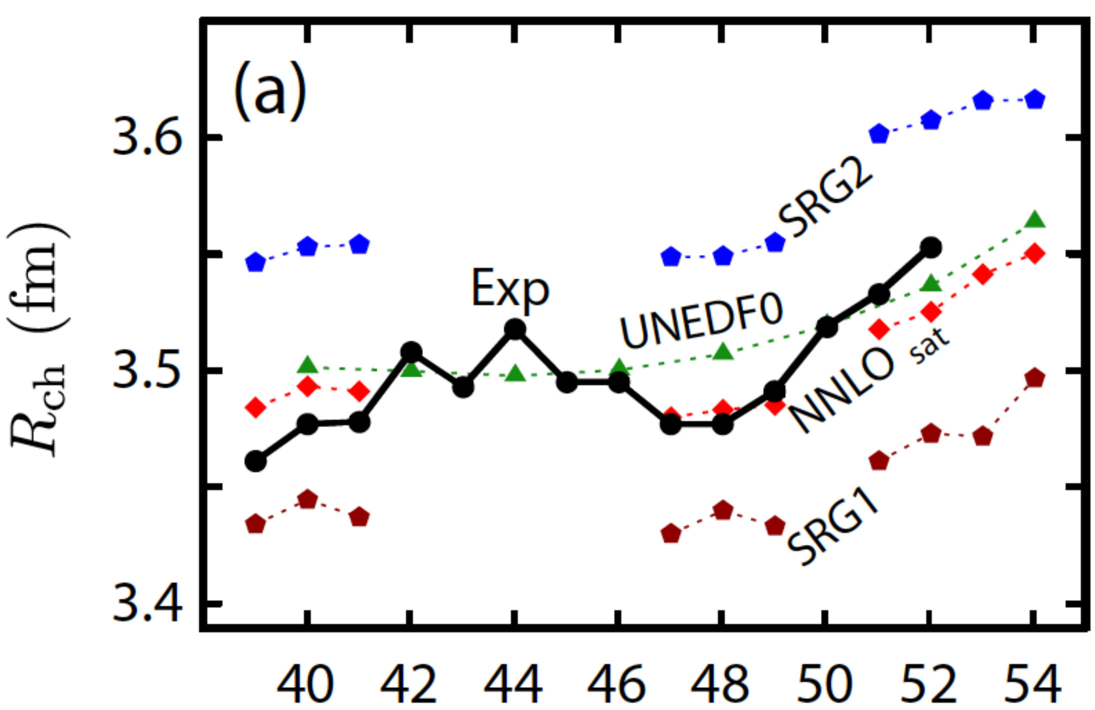
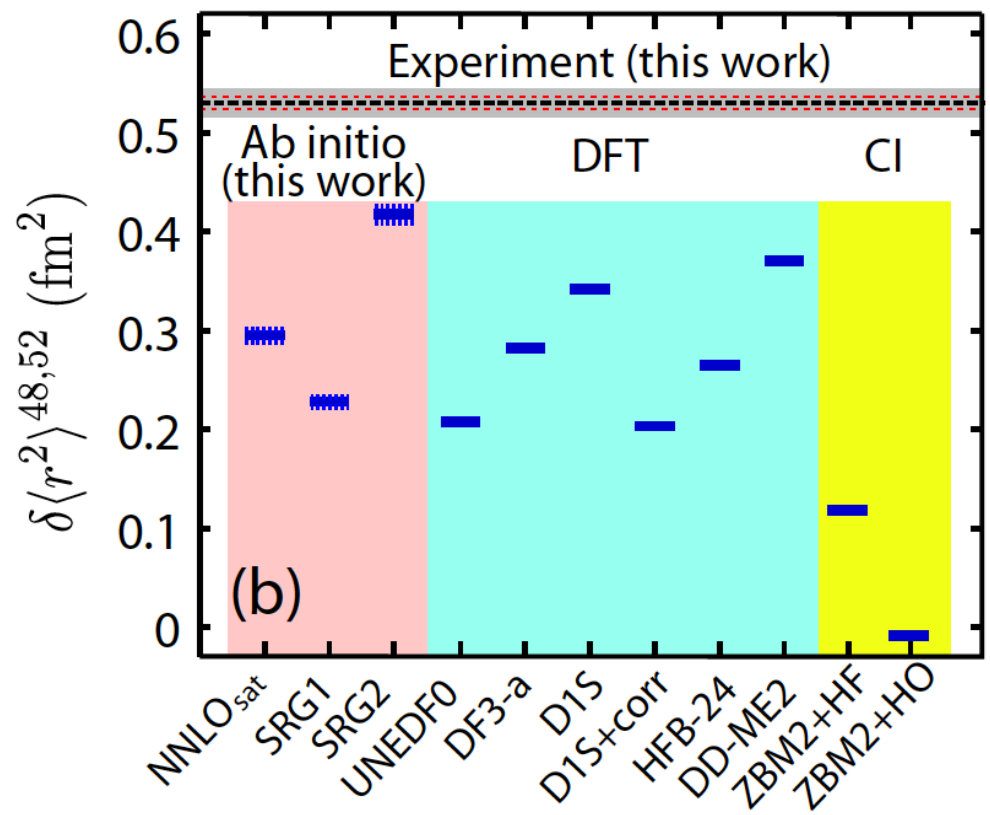


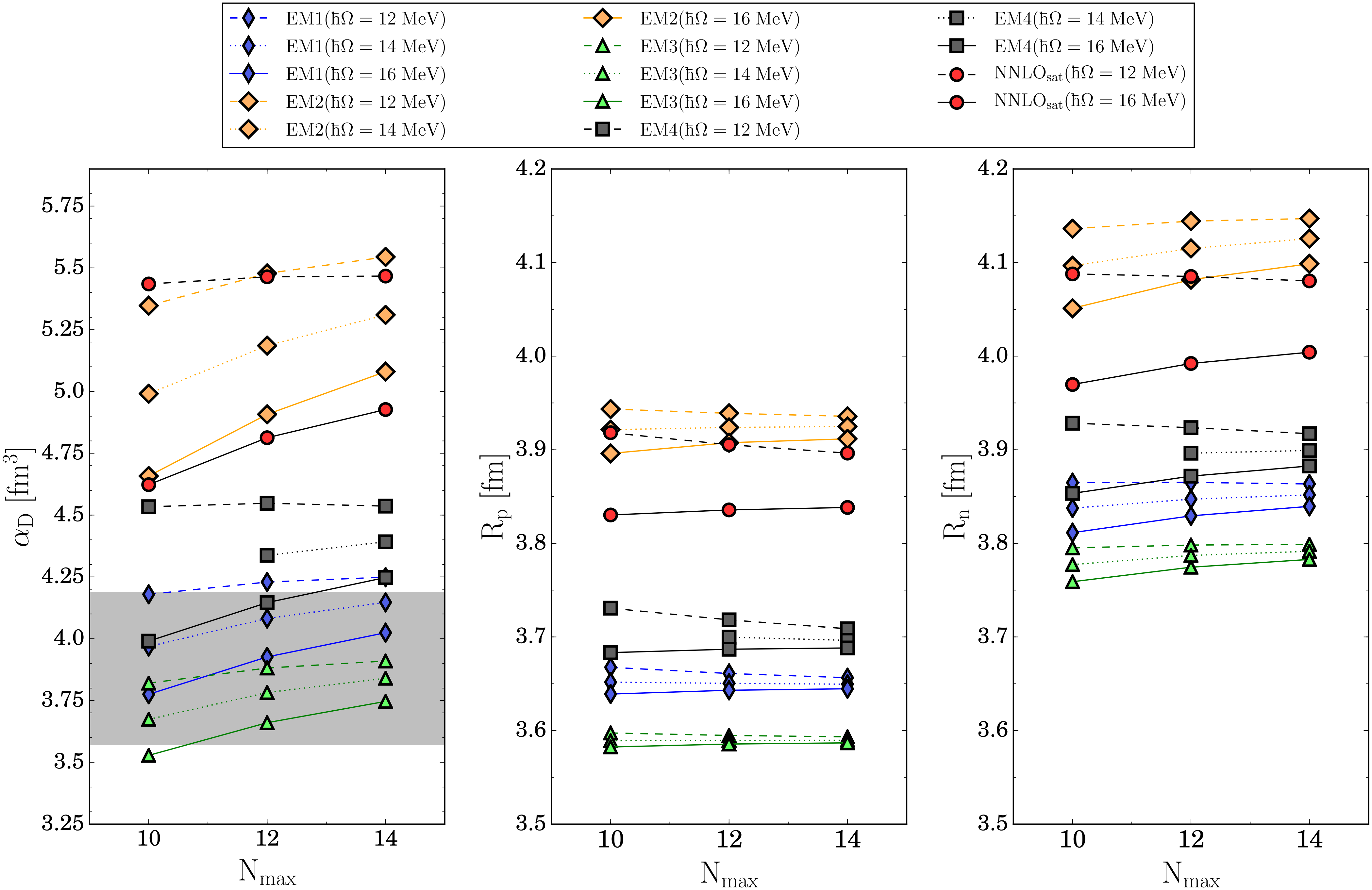
Image: COLLAPS Collaboration/Ronald Fernando Garcia Ruiz.

- 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

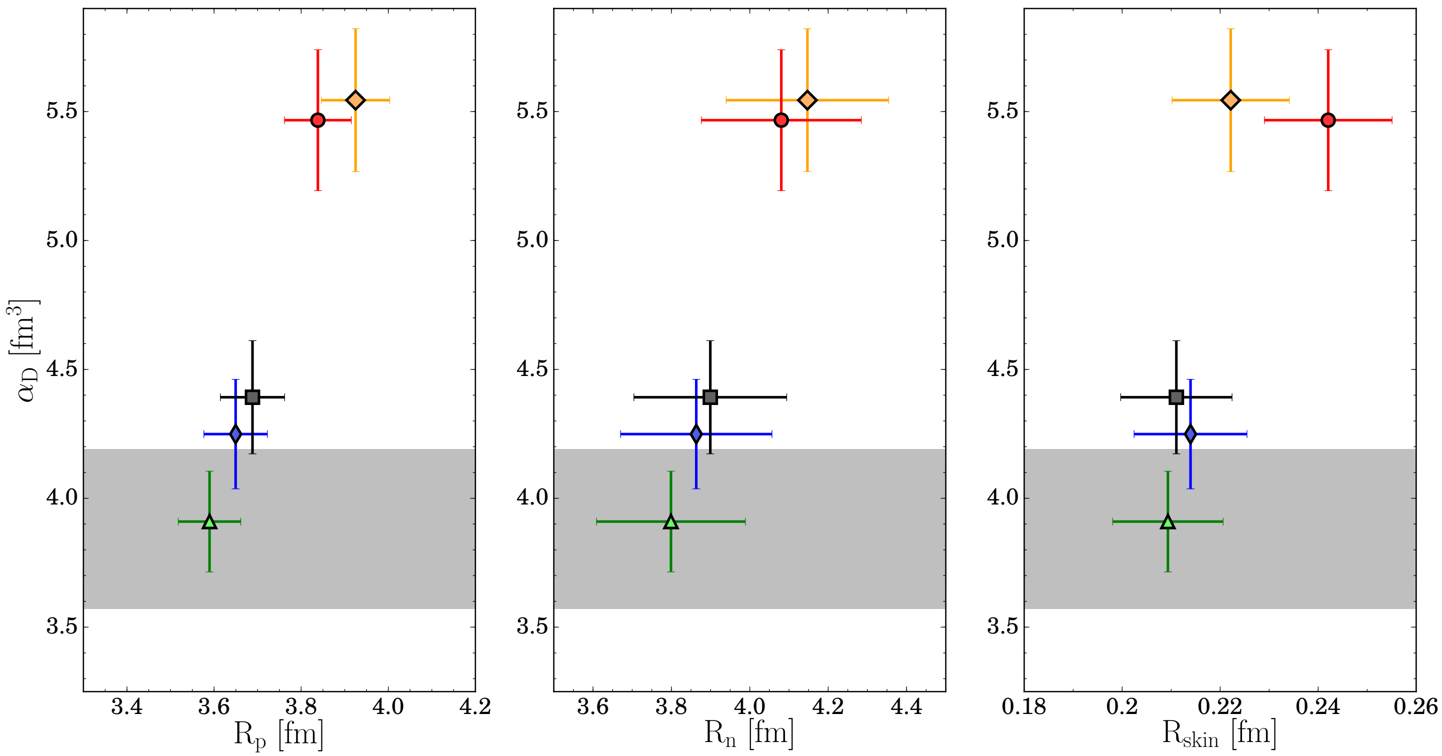




Neutron skin/dipole polarizability of ^{68}Ni



Neutron skin/dipole polarizability of ^{68}Ni



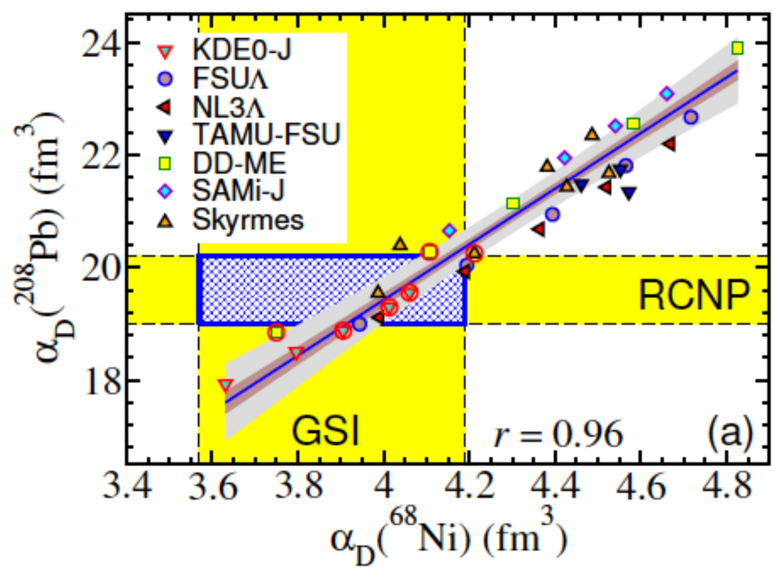
- Charge radii have been measured by the the COLLAPS collaboration at ISOLDE, CERN
- Neutron skin significantly larger than RPA results

Self consistent RPA results based on large set of EDFs from X. Roca-Maza Phys. Rev. C 92, 064304 (2015)

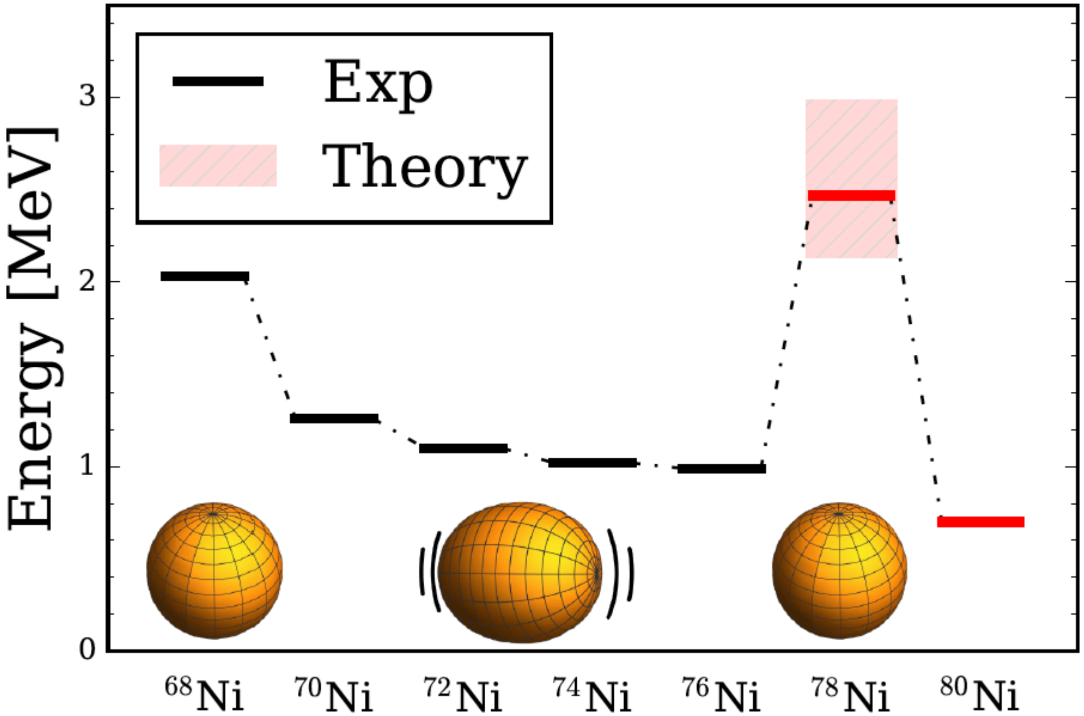
Measuremet of dipole strength in ^{68}Ni:

D. Rossi et al, PRL 111 242503 (2013)

Nucleus	Δr_{np} (a)	Δr_{np} (b)	Δr_{np} (c)
^{68}Ni	0.15–0.19	0.18 ± 0.01	0.16 ± 0.04
^{120}Sn	0.12–0.16	0.14 ± 0.02	0.12 ± 0.04
^{208}Pb	0.13–0.19	0.16 ± 0.02	0.16 ± 0.03



Structure of ^{78}Ni from first principles

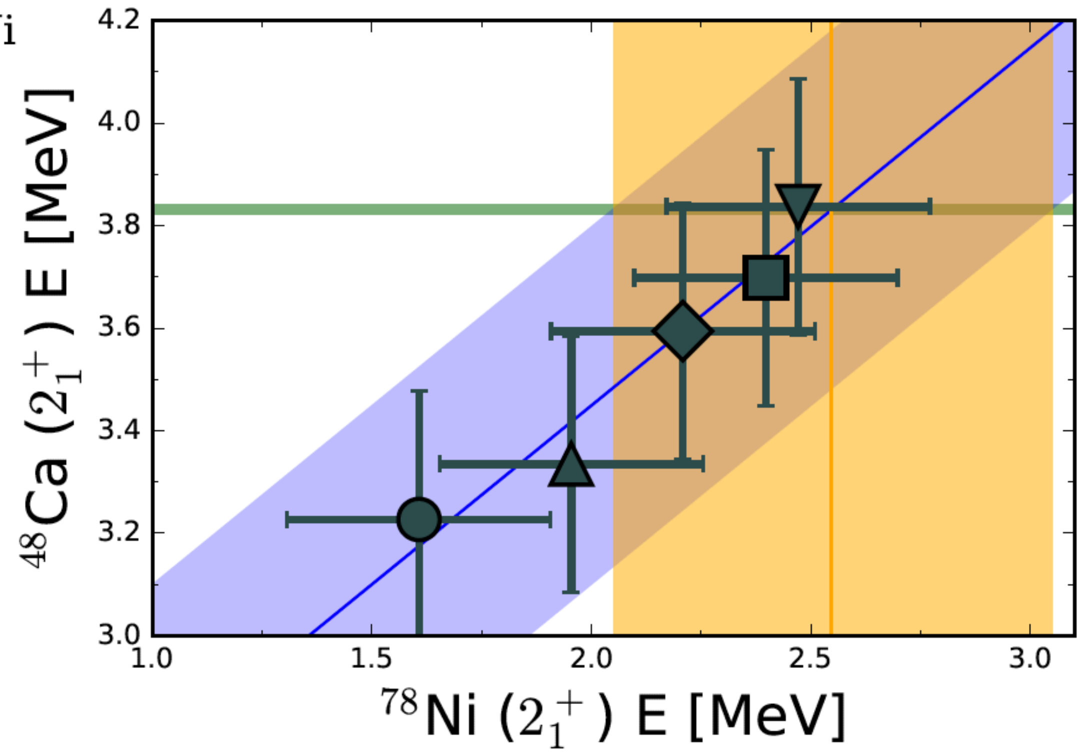


A high 2^+ energy in ^{78}Ni indicates that this nucleus is doubly magic

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.*, PRL 117, 272501 (2016)

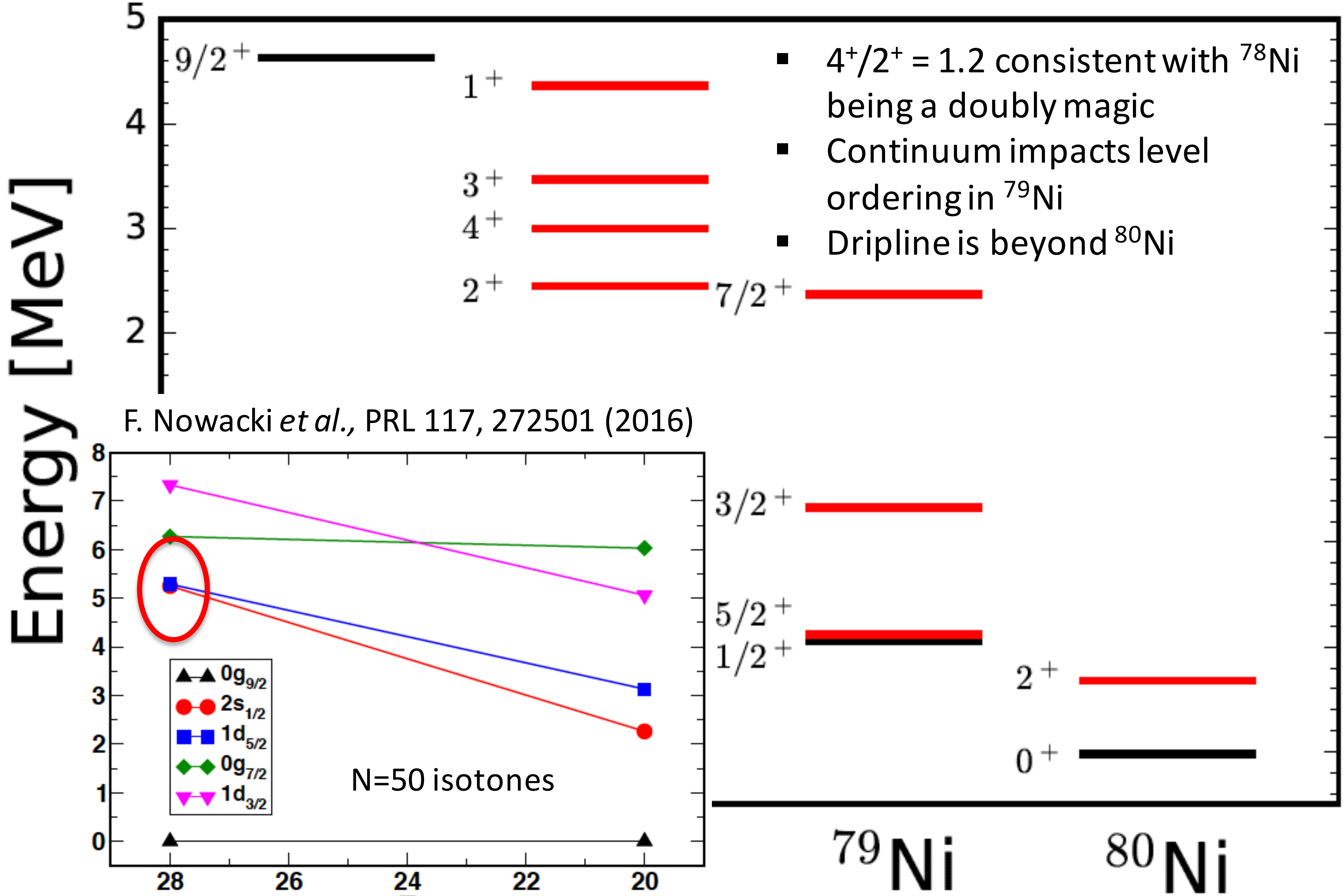
- From an observed correlation we predict the 2^+ excited state in ^{78}Ni using the experimental data for the 2^+ state in ^{48}Ca
- Similar correlations have been observed in other nuclei, e.g. Tjon line in light nuclei



G. Hagen, G. R. Jansen, and T. Papenbrock
Phys. Rev. Lett. **117**, 172501 (2016)

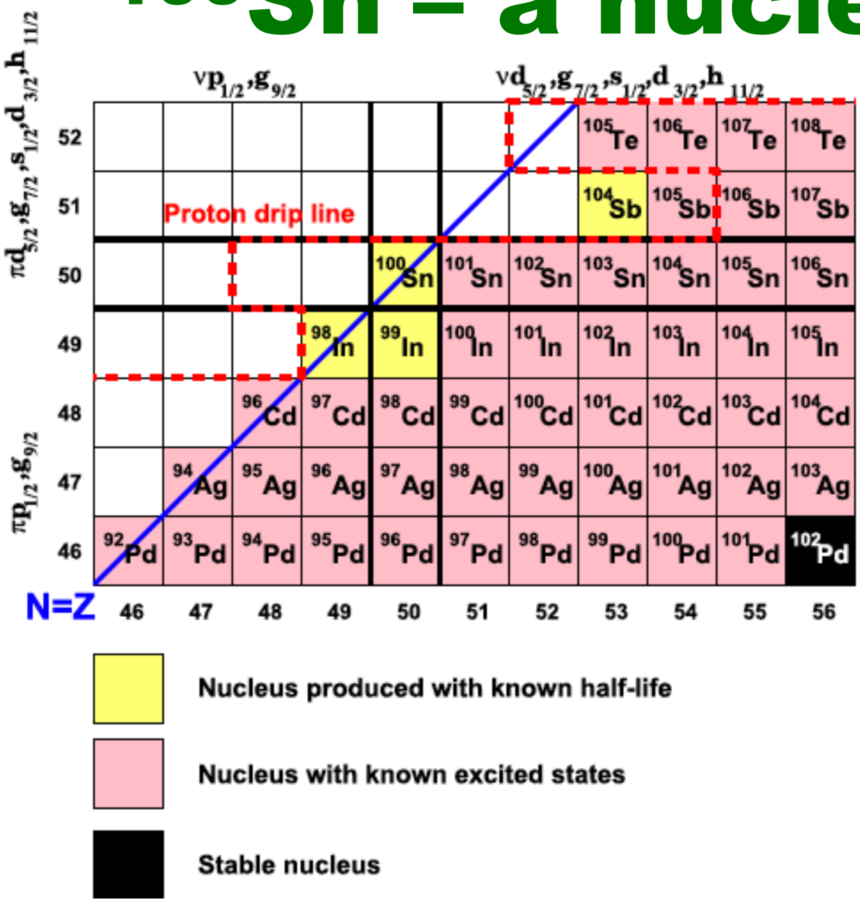
Excited states in ^{78}Ni and its neighbors

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

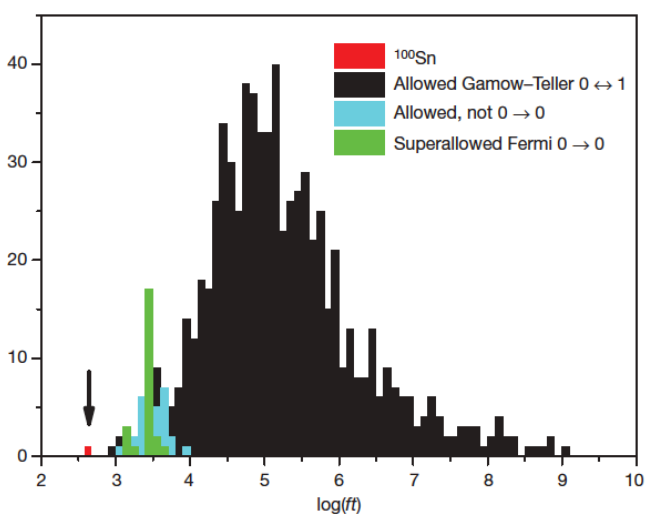


F. Nowacki *et al.*, PRL 117, 272501 (2016)

^{100}Sn – a nucleus of superlatives



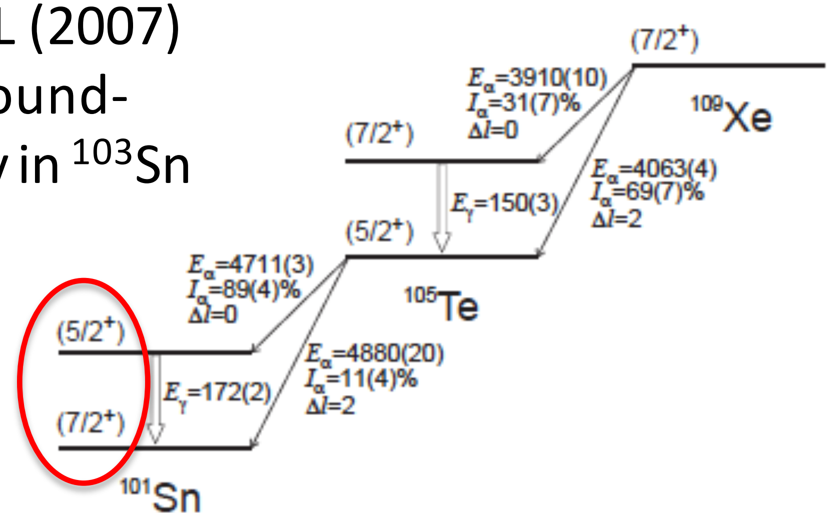
- Heaviest self-conjugate doubly magic nucleus
- Largest known strength in allowed nuclear β-decay
- In the closest proximity to the proton dripline
- At the endpoint of the rapid proton capture process (Sn-Sb-Te cycle)
- Unresolved controversy regarding s.p. structure of ^{101}Sn



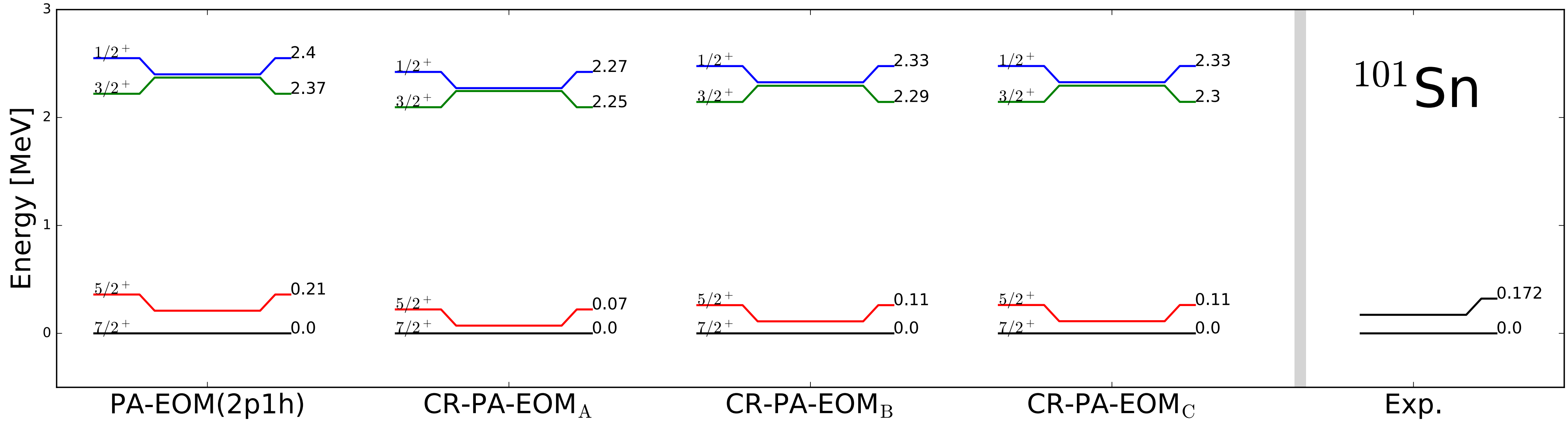
Hinke et al, Nature (2012)

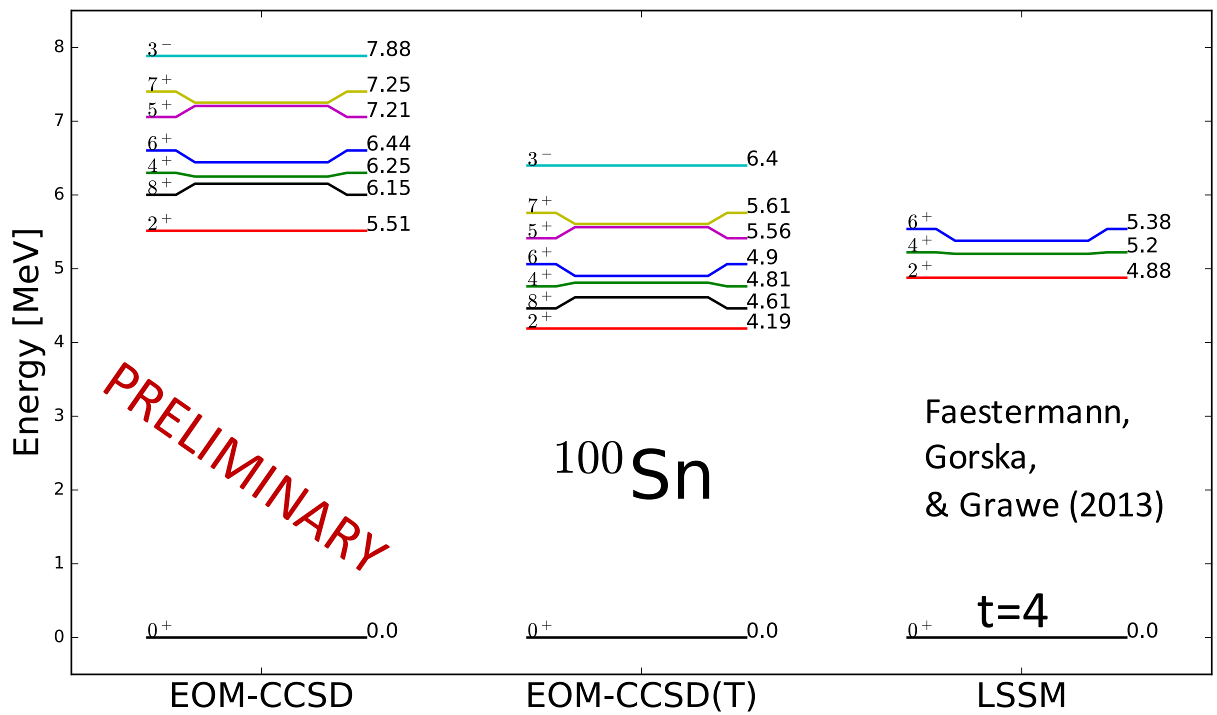
Sewernyiak et al PRL (2007) predicted a 5/2+ ground-state as presumably in ^{103}Sn

Darby et al, PRL (2010)



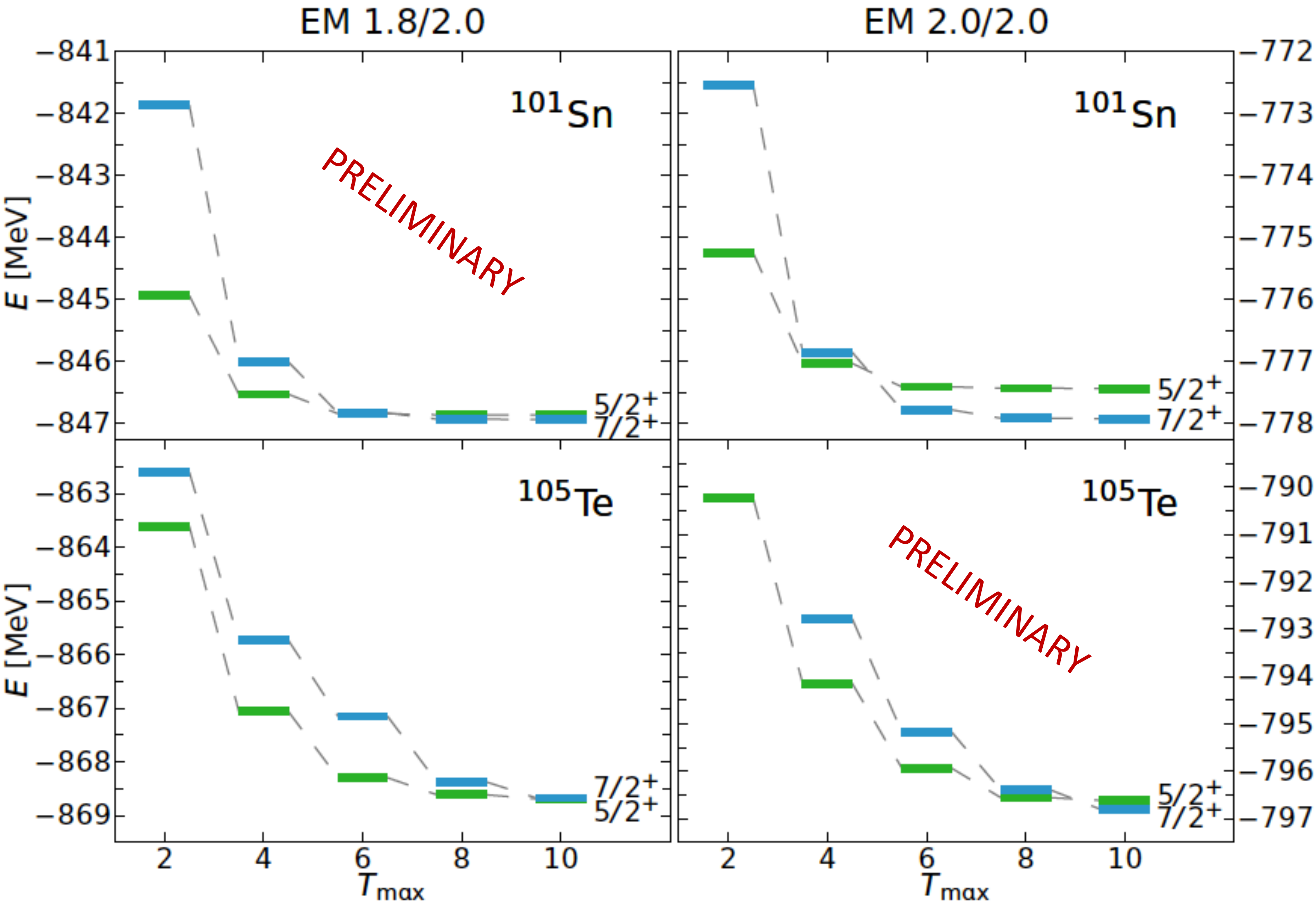
Structure of the ligthest tin isotopes





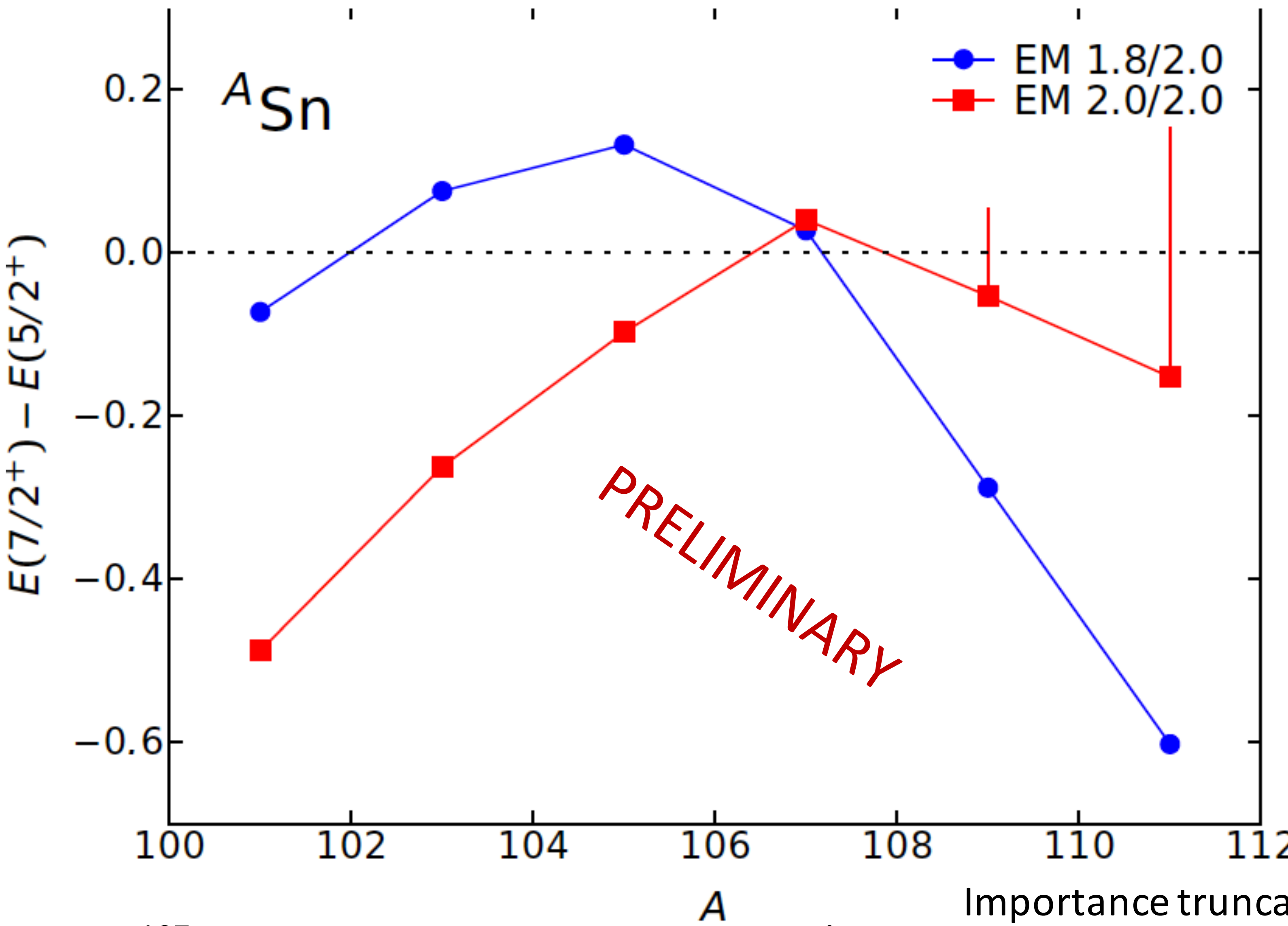
- High 2^+ energy in ^{100}Sn
- Predict $7/2^+$ ground-state in ^{101}Sn
- Experimental splitting between $7/2^+$ and $5/2^+$ reproduced
- Ground-state spins of $^{101-121}$Sn will be measured at CERN (CRIS collaboration)

Structure of the ligthest tin isotopes



Importance truncated CI results from **C. Stumpf** and R. Roth, valence space effective interactions from **S. R. Stroberg** and J. Holt.

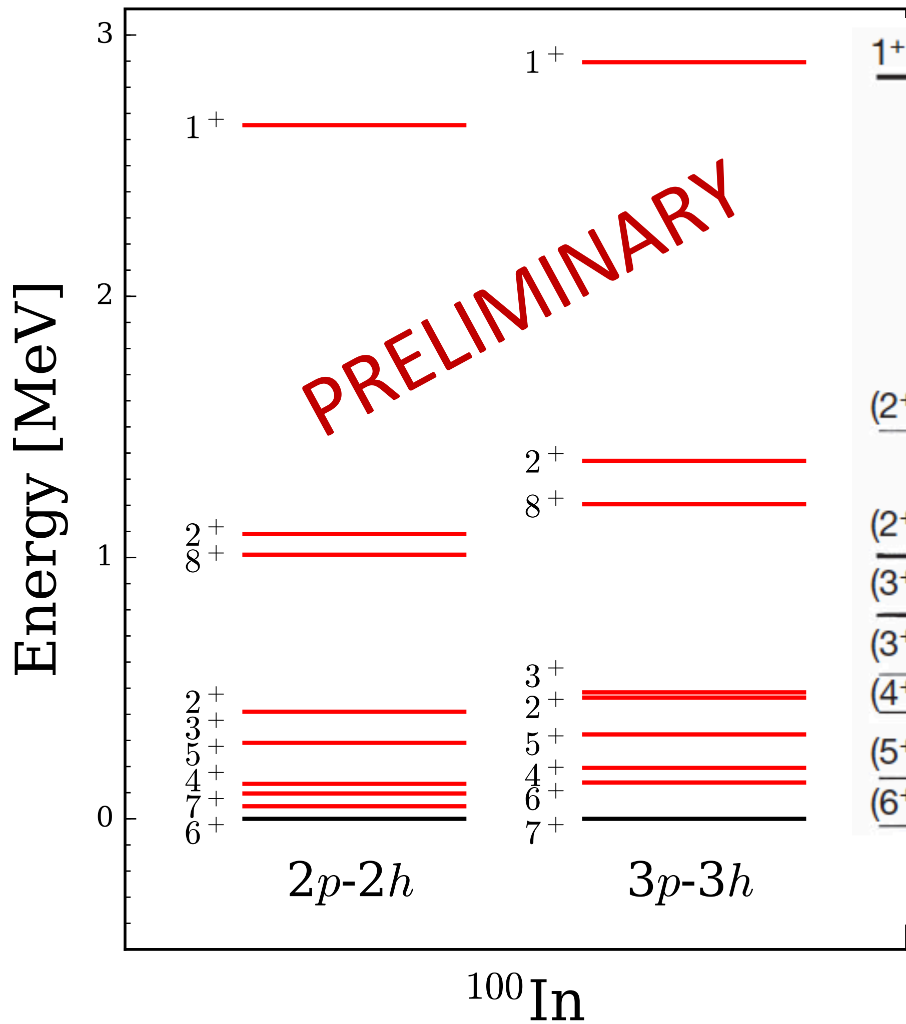
Structure of the ligthest tin isotopes

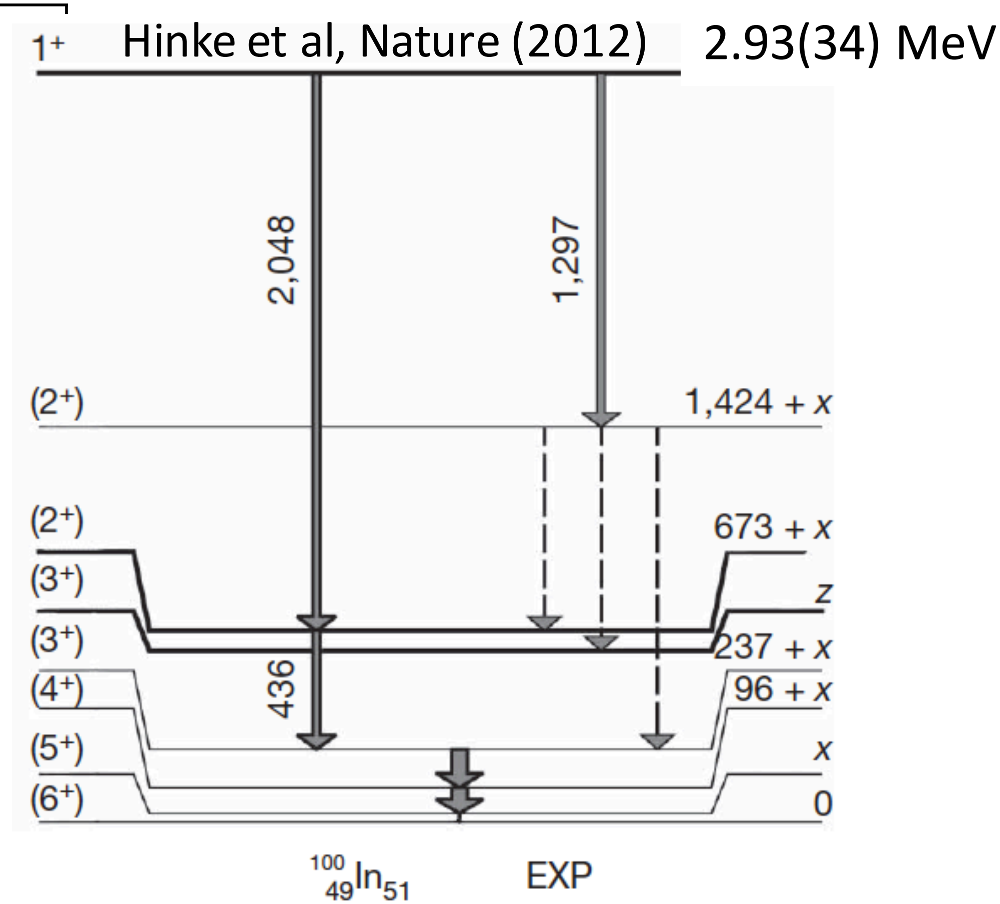


G.s. spin of ^{107}Sn correctly predicted to be 5/2+
[G. Cerizza et al Phys. Rev. C **93**, 021601 (2016)]

Importance truncated CI results from **C. Stumpf** and R. Roth, valence space effective interactions from **S. R. Stroberg** and J. Holt.

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





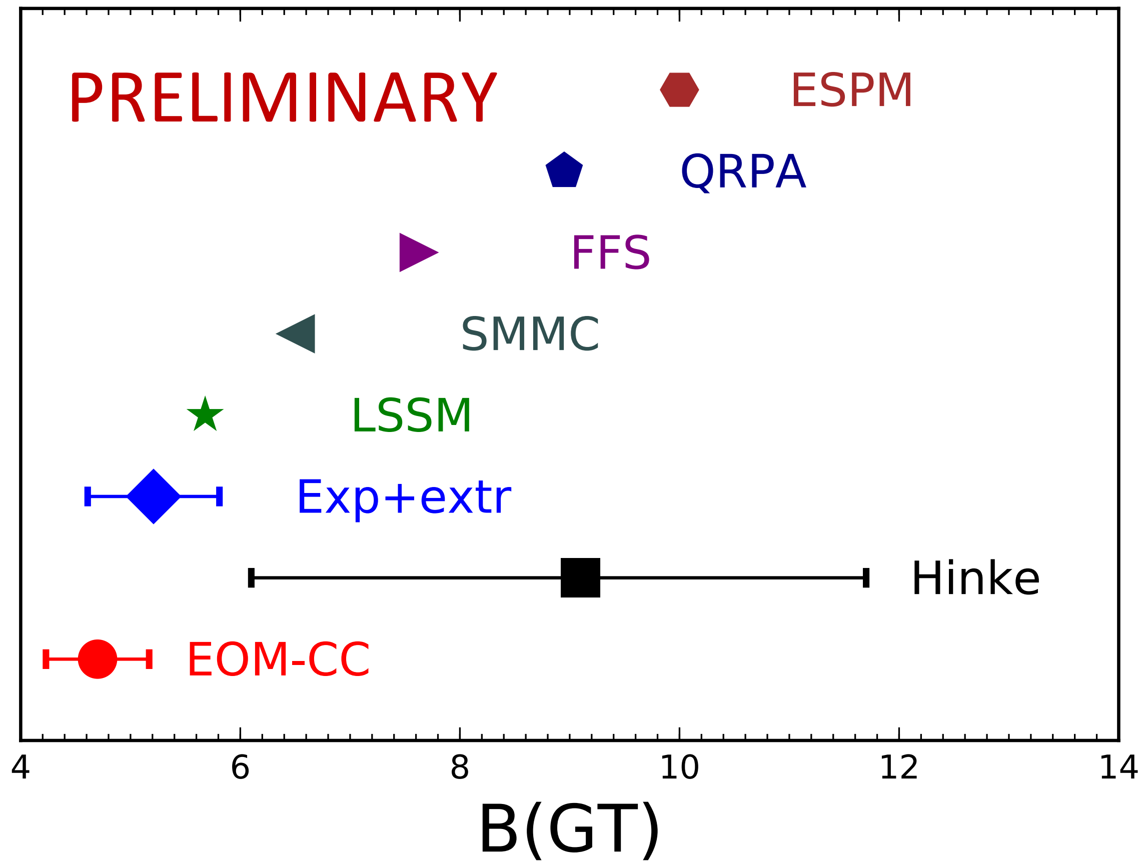
- Reproduce known 1^+ state at 2.93(34) MeV
- Predict a 7^+ ground-state for ^{100}In
- Ground-state spin of ^{100}In can be measured by CRIS collab. at CERN

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

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

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



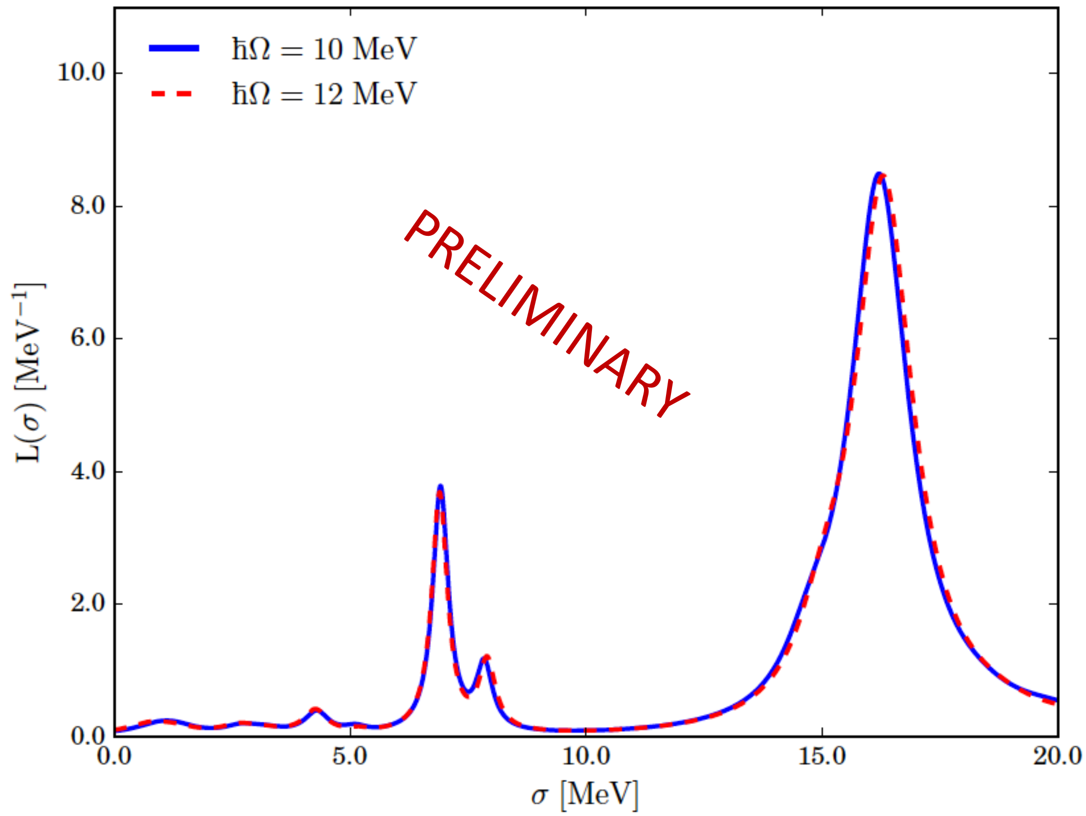
Hinke et al, Nature (2012)

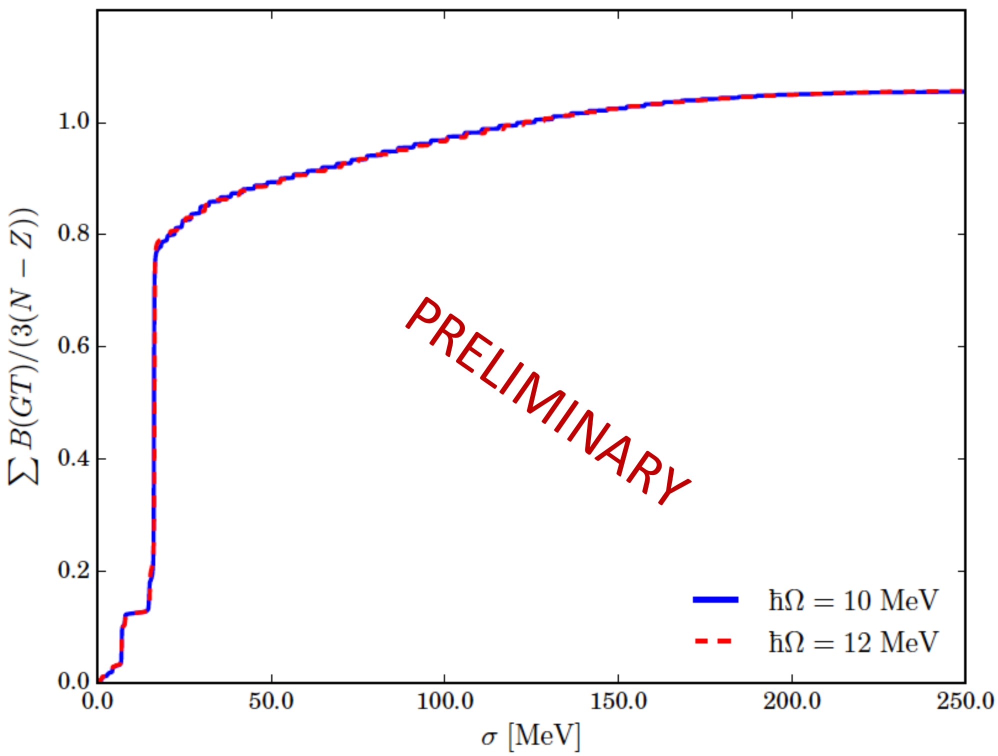
Model	Ref	unquenched	quenched
ESPM	[30]	17.78	10.00
MCSM	[8]	10.3	6.5
QRPA	[9]	8.95	
FFS	[9]	7.63	
extrapol.	[10]	9.8	5.2
SM+corr.	[7]	14.2	
LSSM	this work	~ 13.90	~ 7.82
LSSM (only 1_1^+)	this work	10.10	5.68

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

Gamow-Teller response in ^{132}Sn

- Prediction for the Gamow-Teller strength in ^{132}Sn
- Strengths has been measured at RIKEN
- Results show that high energy tail is important to exhaust the sum rule





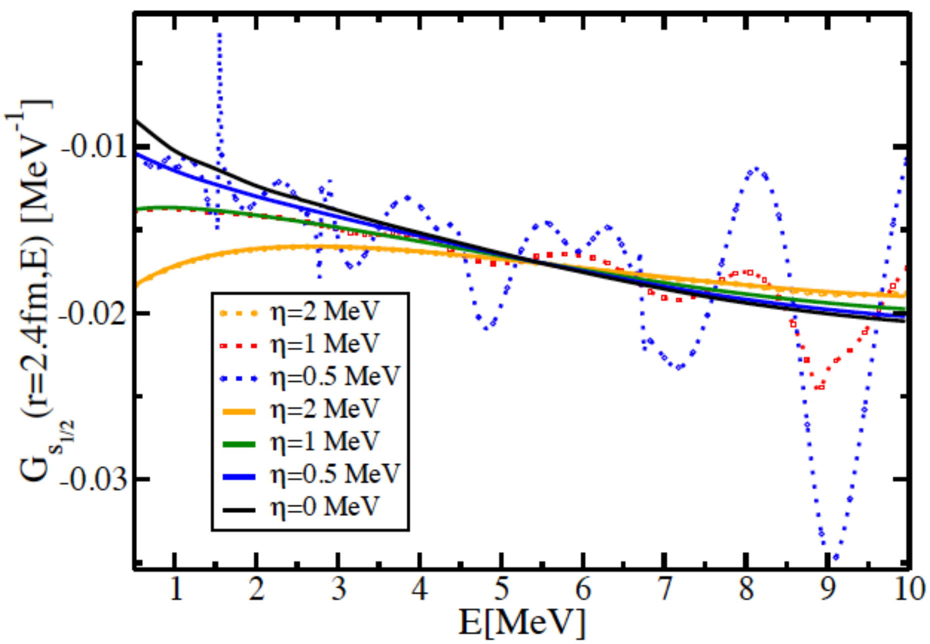
- Role of two-body currents on quenching on sum rule and Gamow Teller strengths will be examined

Optical potentials from coupled-cluster theory

J. Rotureau et al, Phys. Rev. C 95, 024315 (2017)

Coupled-cluster Green's function:

$$G^{CC}(\alpha,\beta,E) \equiv \langle\Phi_{0,L}|\overline{a_\alpha}\frac{1}{E-(\overline{H}-E^A_{gs})+i\eta}\overline{a^\dagger_\beta}|\Phi_0\rangle + \langle\Phi_{0,L}|\overline{a^\dagger_\beta}\frac{1}{E-(E^A_{gs}-\overline{H})-i\eta}\overline{a_\alpha}|\Phi_0\rangle$$



Imaginary part of the neutron s-wave Green's function

- Green's function solved via the Lanczos technique (continued fractions)
- Using a Berggren basis allows stable results for eta –> 0

Inverting the Dyson equation we obtain the self-energy:

$$\Sigma^*(E) = [G^{(0)}(E)]^{-1} - G^{-1}(E)$$

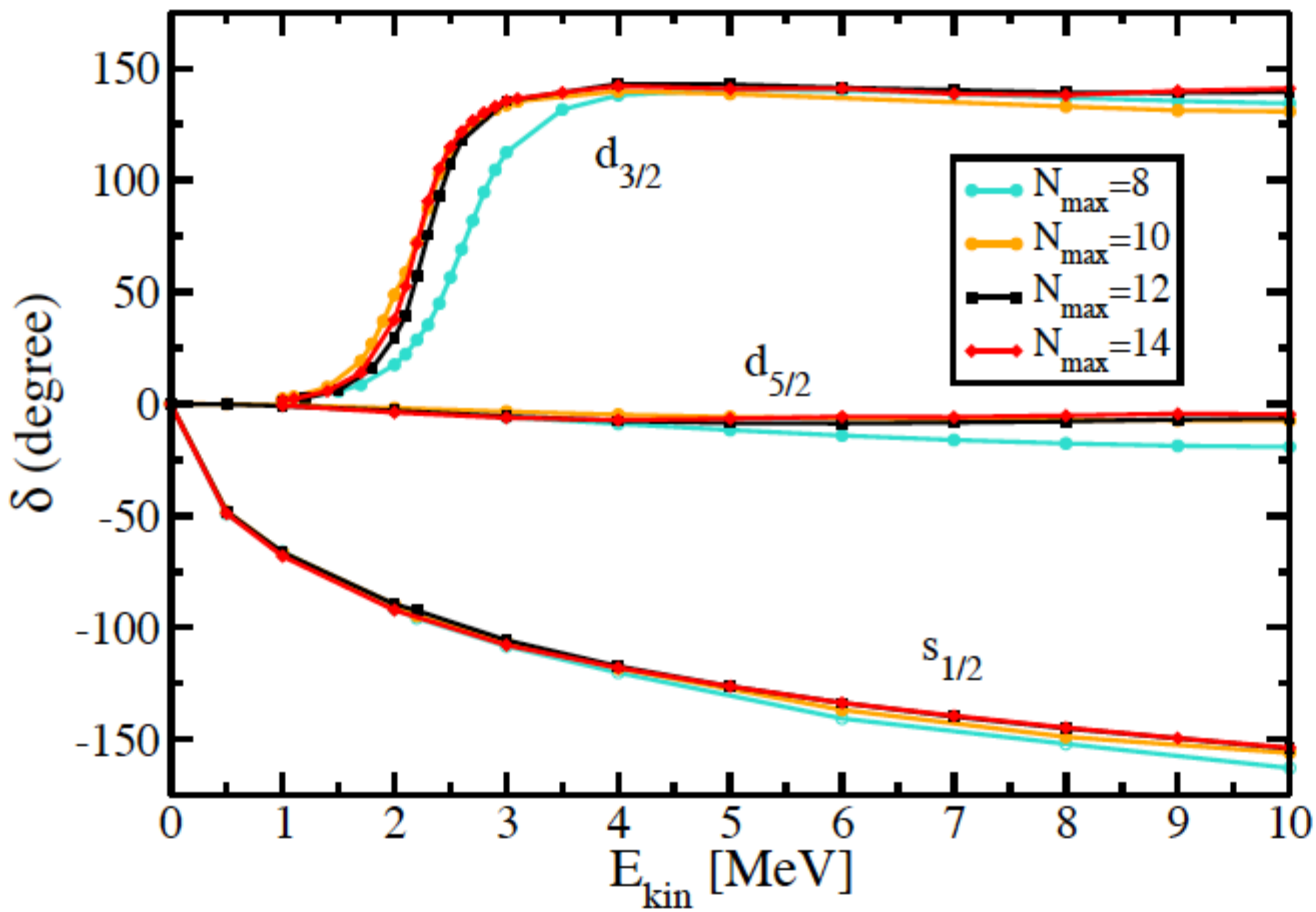
Scattering phase shifts are obtained by the solving the equation:

$$-\frac{\hbar^2}{2\mu}\nabla^2\xi(\mathbf{r}) + \int d\mathbf{r}'\Sigma'(\mathbf{r},\mathbf{r}',E^+)\xi(\mathbf{r}') = E^+\xi(\mathbf{r})$$

See also talk by Andrea Idini, and C. Barbieri and B. K Jennings Phys.Rev. C72 (2005) 014613

Neutron elastic scattering on ^{16}O with $NNLO_{opt}$

J. Rotureau et al, Phys. Rev. C 95, 024315 (2017)



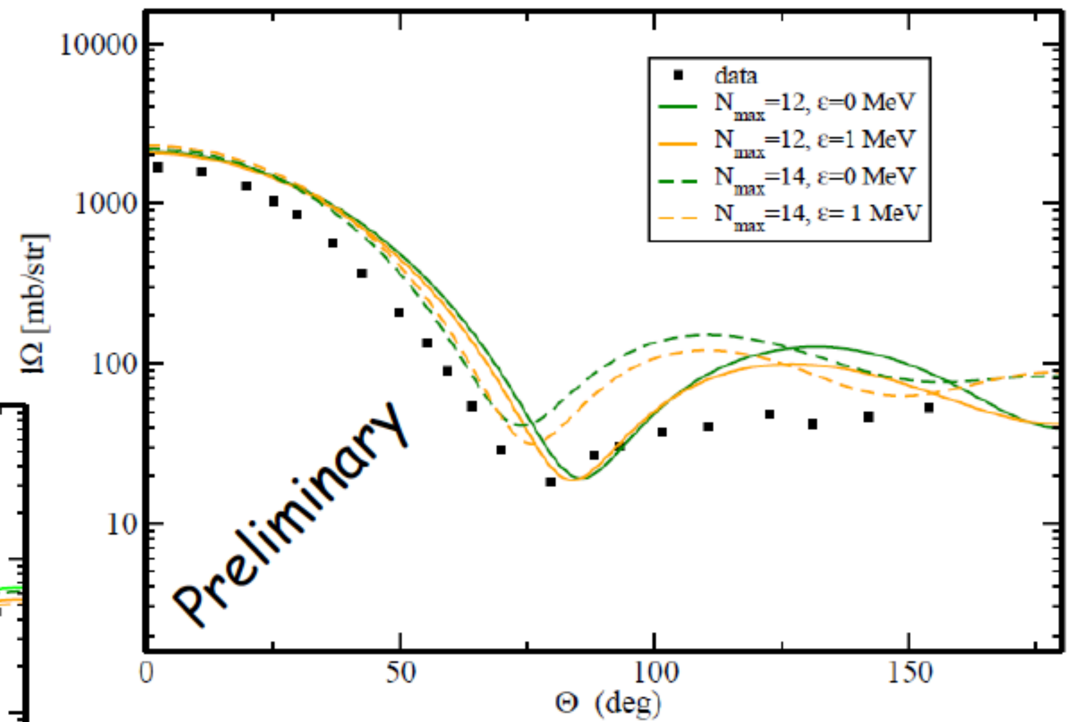
Consistent results between computed phase shifts and resonances computed directly in the Berggren basis via PA-EOMCCSD

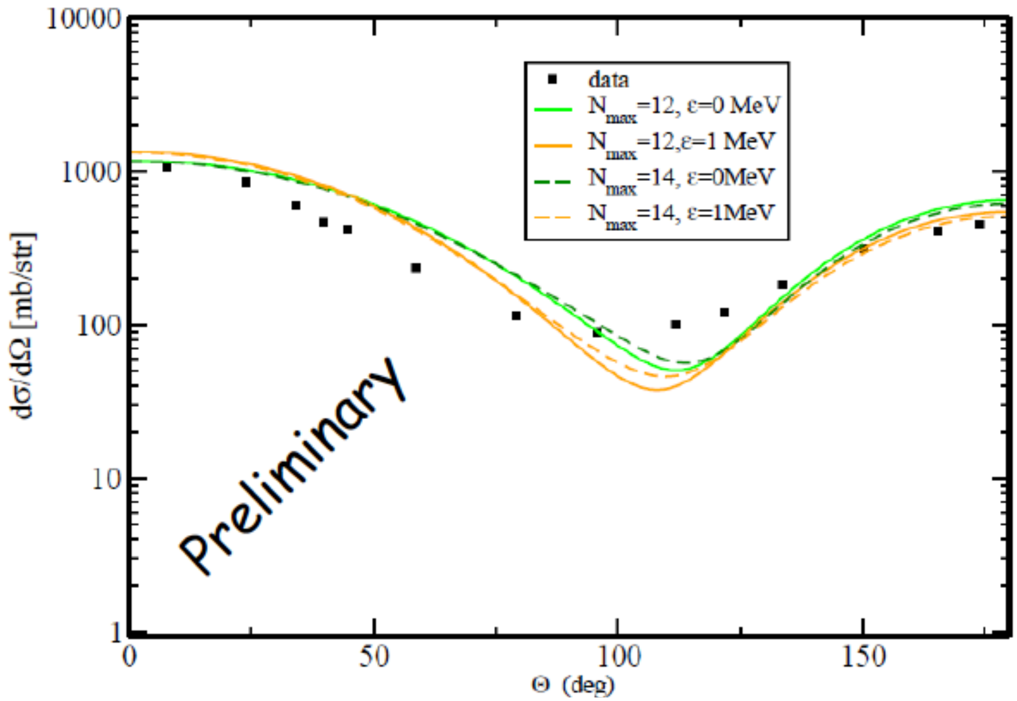
$N_{\max}$	$E(5/2^+)$	$E(1/2^+)$	$E(3/2^+)$
8	-4.35	-2.62	2.68-i0.32
10	-4.49	-2.73	2.24-i0.25
12	-4.56	-2.76	2.34-i0.21
14	-4.57	-2.80	2.26-i0.12

Neutron elastic scattering on ^{40}Ca

- Diffraction minima in good agreement with data
- Cross section overestimated due to lack of absorption (e.g. 0^+ state in ^{40}Ca too high)
- Using a Berggren basis allows for stable results as ε –> 0.

$^{40}Ca(n,n)^{40}Ca$, E_{lab} =5.3 MeV



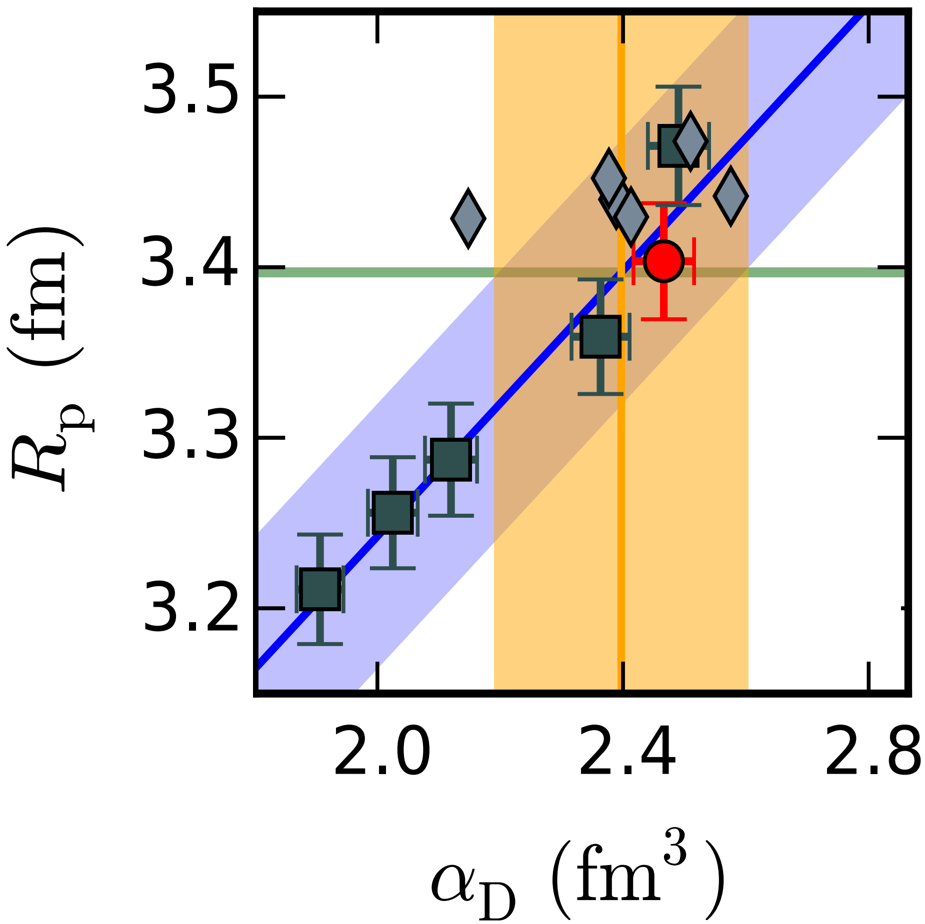


$^{40}Ca(n,n)^{40}Ca$, E_{lab} =2.1 MeV

Summary

- Prediction of dipole polarizability of ^{48}Ca consistent with data
- Predictions for dipole polarizability and neutron skin of ^{68}Ni
- ^{78}Ni is predicted to be doubly magic
- Structure and decay of ^{100}Sn
- Gamow-Teller response of ^{132}Sn
- Optical potentials from coupled-cluster theory – promising first results for ^{40}Ca+n with NNLO$_{sat}$

Dipole polarizability of ^{48}Ca



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

Ab-initio prediction from correlation with R_p:
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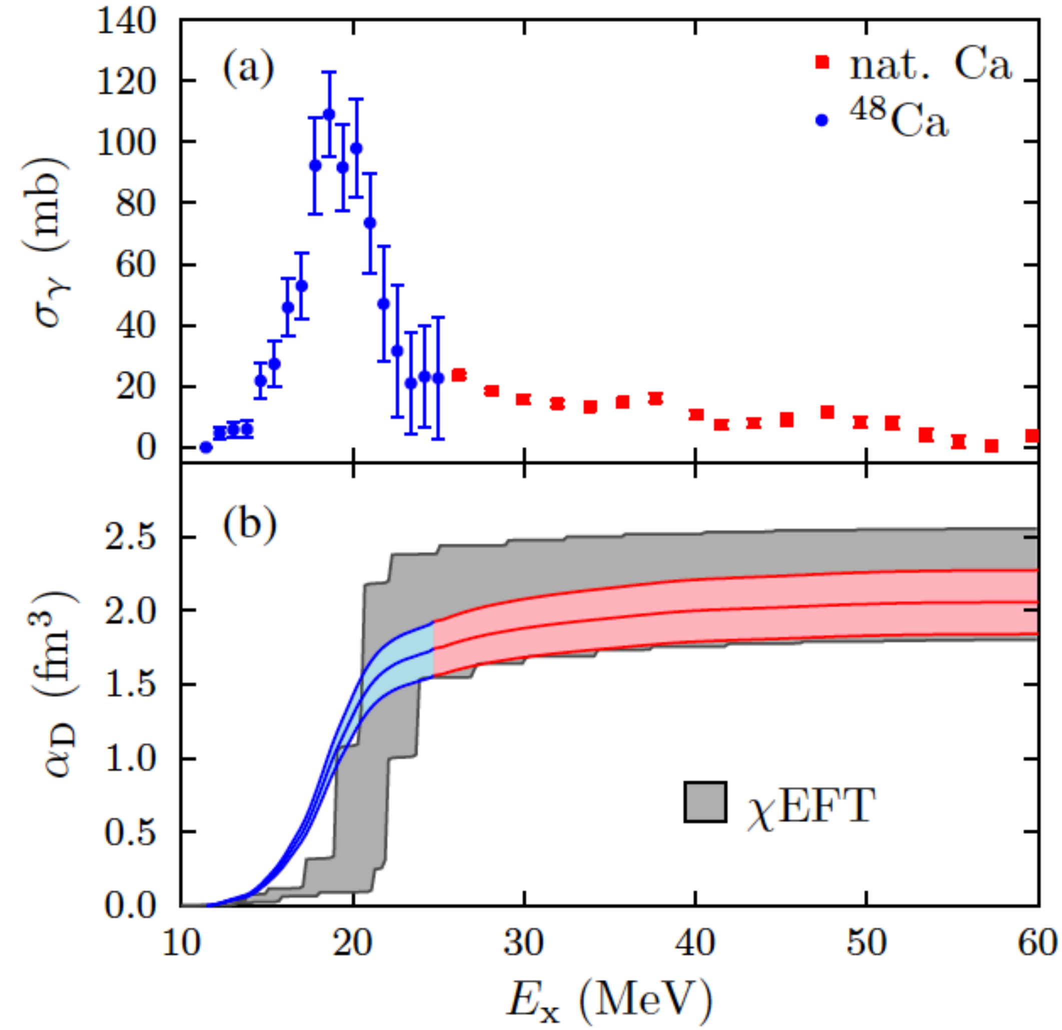
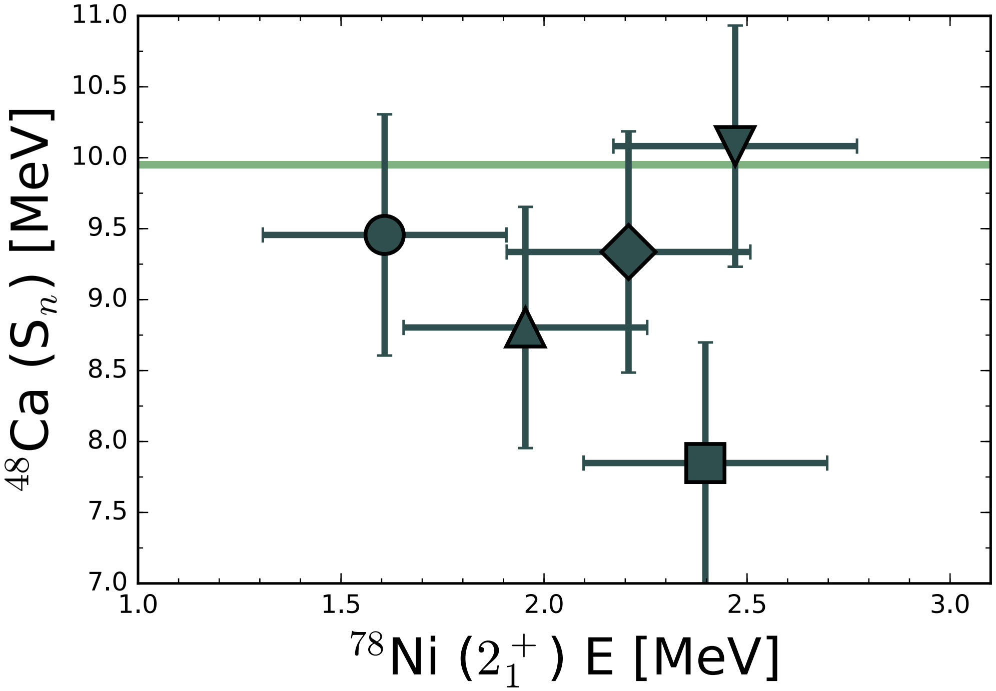


J. Birkhan *et al* (submitted).

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^+