Recent progress and open questions in ab initio simulations of nuclei

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Ab initio vs. effective approach

Ab initio approach

A-body Hamiltonian

$H = T + V^{2\text{N}} + V^{3\text{N}} + \ldots + V^{A\text{N}}$

← $H|\Psi_k^A\rangle = E_k^A|\Psi_k^A\rangle$ → A-body wave-function

➟ Solve many-body Schrödinger equation in a controlled, systematically improvable way

Effective approach

Two main options

- Reduce active Hilbert space → Interacting shell model
- Simplify $|\Psi_k^A\rangle$ → Energy density functional

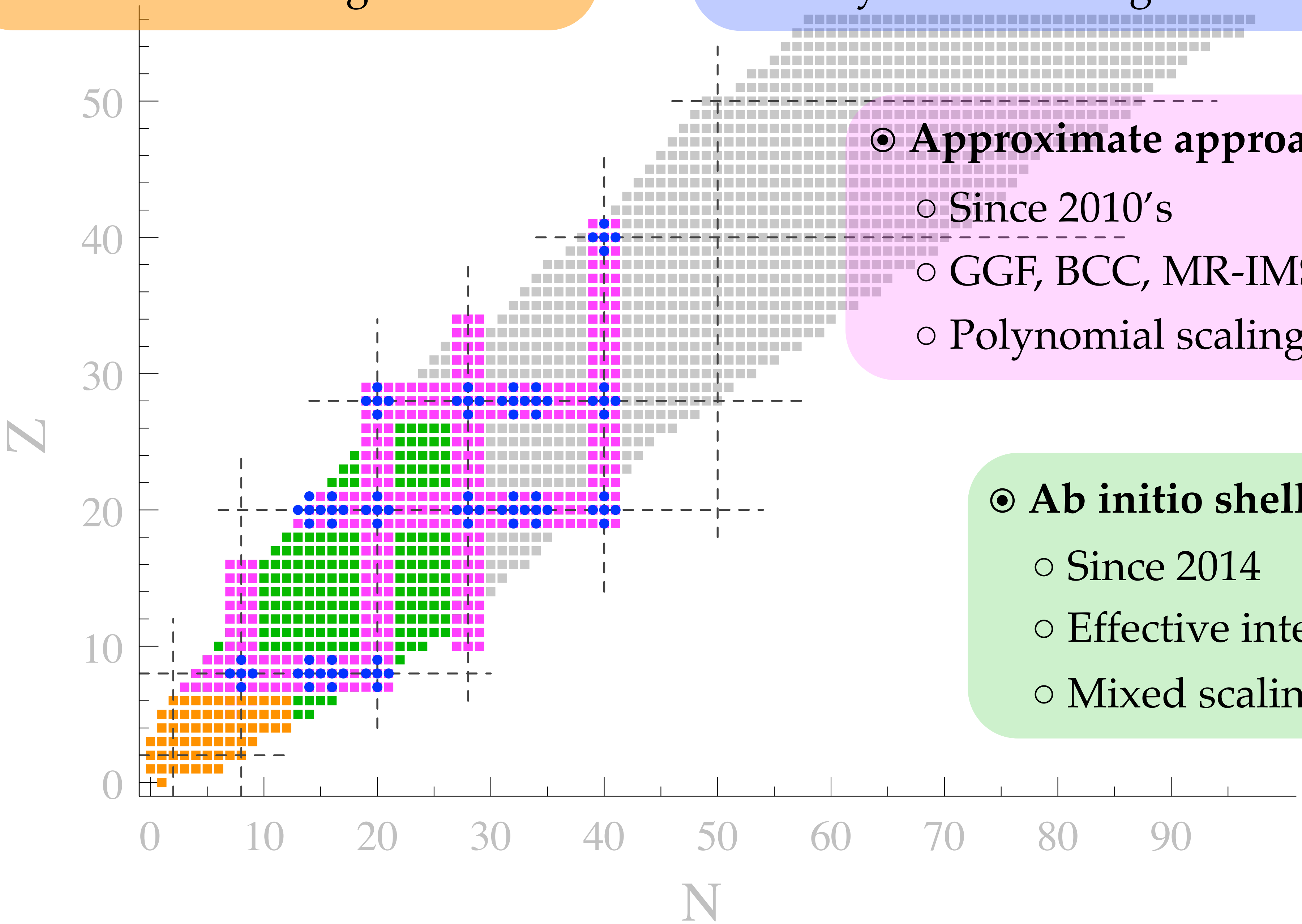
→ $H^{\text{eff}}|\Psi^{\text{eff}}\rangle = E|\Psi^{\text{eff}}\rangle$

	Ab initio	**Shell model**	**EDF**
Accuracy	🌤️	☀️	🌤️
Reach across the mass table	🌧️	🌧️	☀️
Predictive power / error estimate	🌦️	🌧️	🌧️

Evolution of ab initio nuclear chart

- **"Exact" approaches**
  - Since 1980's
  - Monte Carlo, CI, …
  - Factorial scaling

- **Approximate approaches for closed-shell nuclei**
  - Since 2000's
  - SCGF, CC, IMSRG
  - Polynomial scaling



- **Approximate approaches for open-shells**
  - Since 2010's
  - GGF, BCC, MR-IMSRG
  - Polynomial scaling

- **Ab initio shell model**
  - Since 2014
  - Effective interaction via CC/IMSRG
  - Mixed scaling

Self-consistent Green's function approach

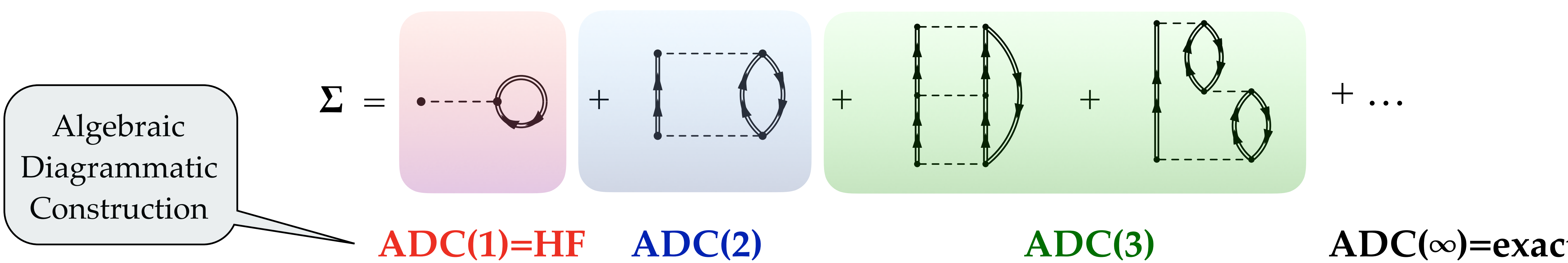
- **Solution of the *A*-body Schrödinger equation** $H|\Psi_k^A\rangle = E_k^A|\Psi_k^A\rangle$ **achieved by**

  1) Rewriting it in terms of **1-, 2-, …. *A*-body objects** $G_1 = G$, $G_2, \ldots G_A$ (**Green's functions**)

  2) Expanding these objects in perturbation (in practise **G** ➟ **one-body observables**, etc..)

  ○ **Self-consistent** schemes resum (infinite) subsets of perturbation-theory contributions

- **Self-energy expansion**



- **Access a variety of quantities**

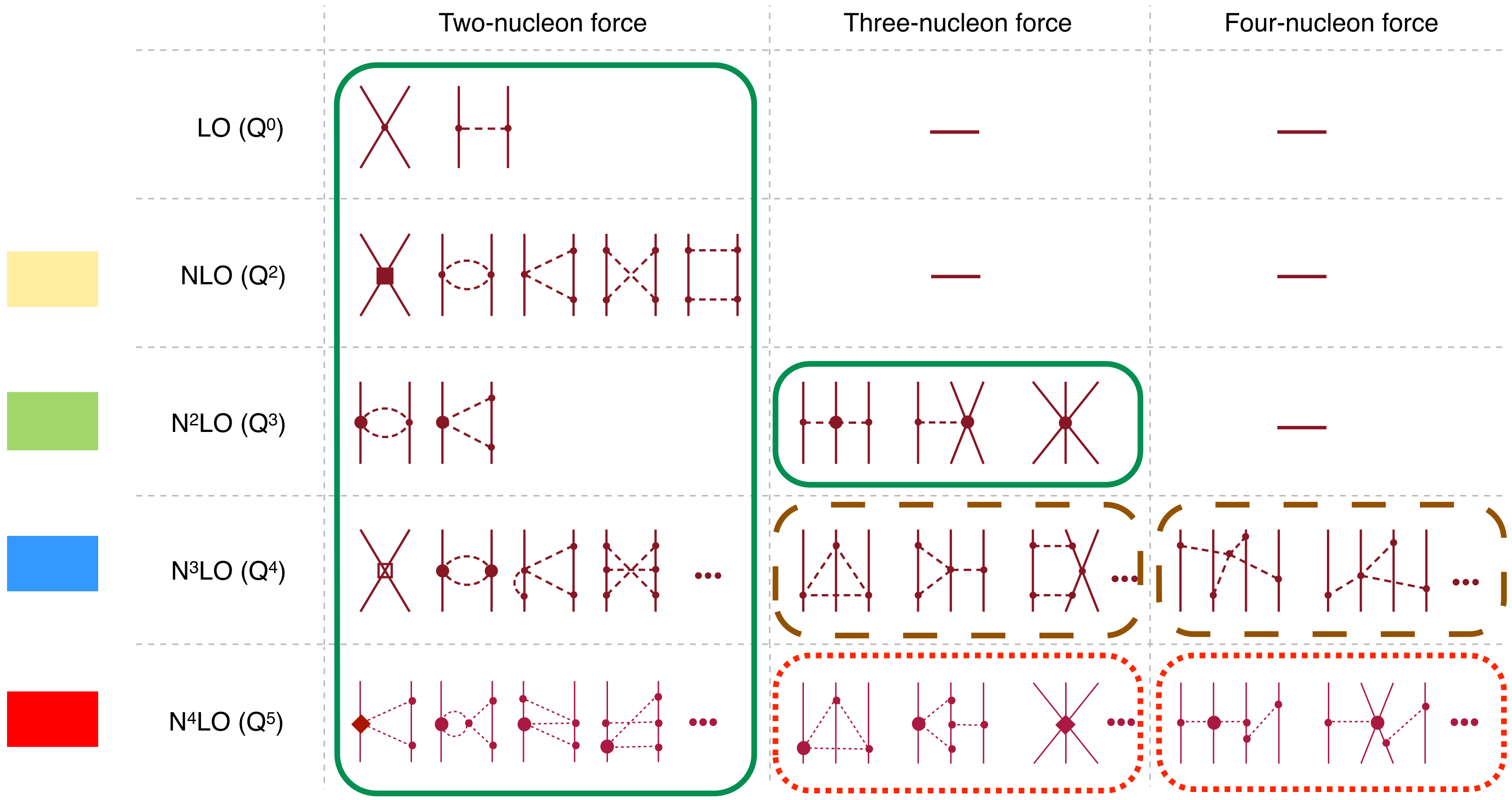
  ○ One-body GF → Ground-state properties of even-even *A* + spectra of odd-even neighbours

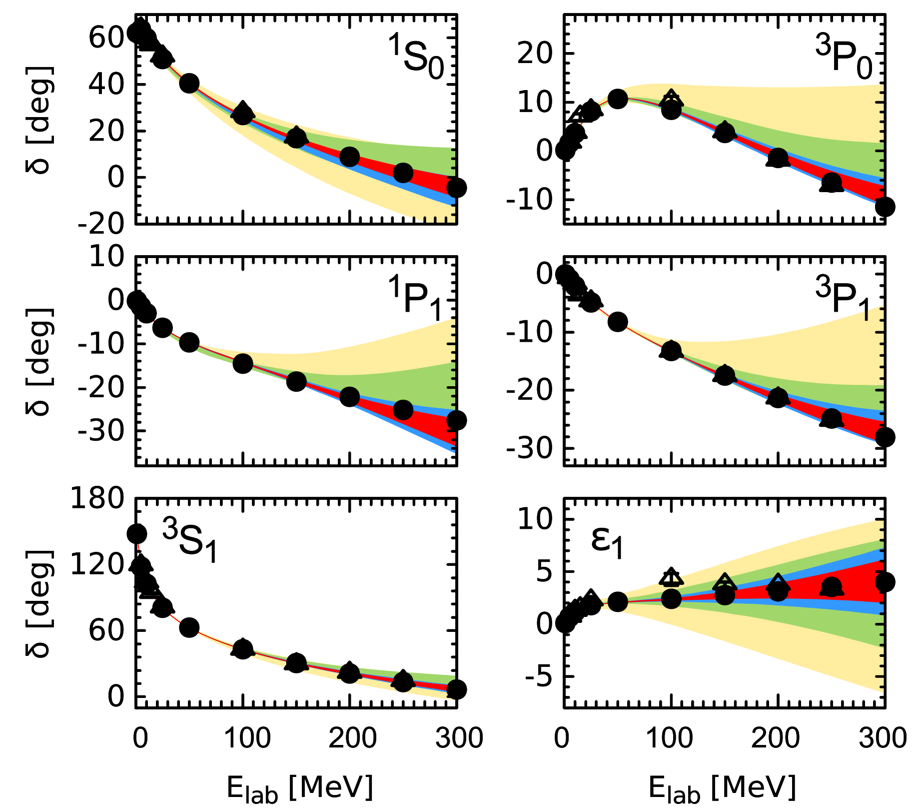
  ○ Two-body GF → Excited spectrum of even-even *A*

  ○ Self-energy → Optical potential for nucleon-nucleus scattering

Chiral effective field theory & nuclear interactions

- Chiral EFT provides a **systematic** framework to construct *A*N interactions (*A*=2, 3, …)
- Main features:
  - High-energy physics unresolved → **soft potentials** → improved many-body convergence
  - Many-body forces and currents consistently derived
  - A **theoretical error** can be, in principle, assigned to each order in the expansion

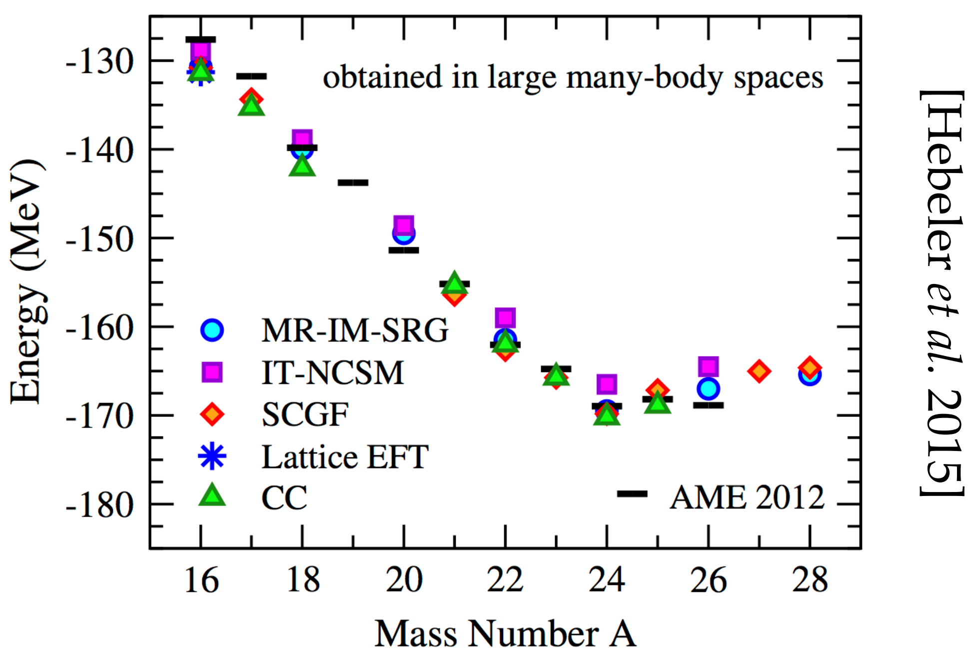




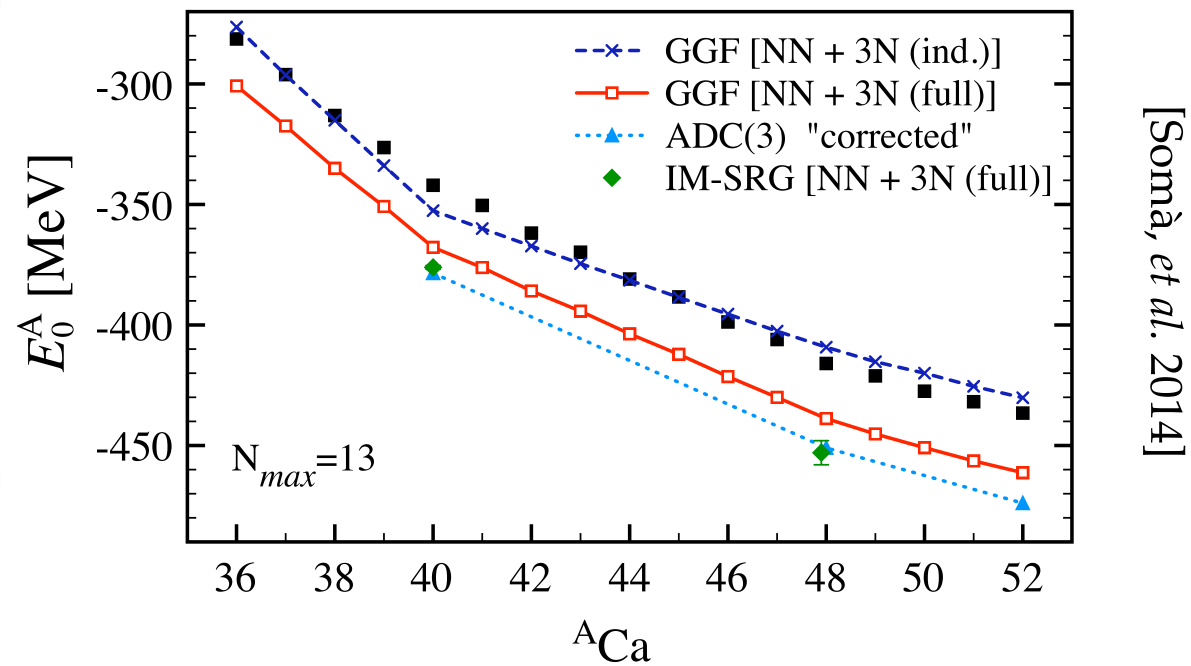
[Meißner 2016]

➪ **Ideally: apply to the many-nucleon system (and propagate the theoretical error)**

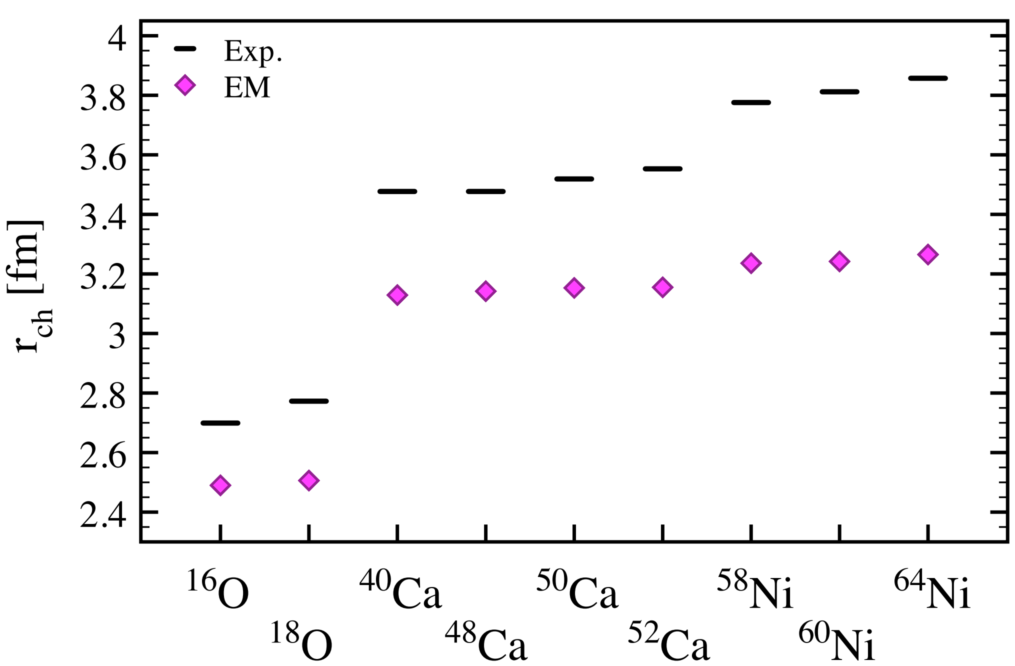
N3LO *NN* + 3*N* (400) interaction



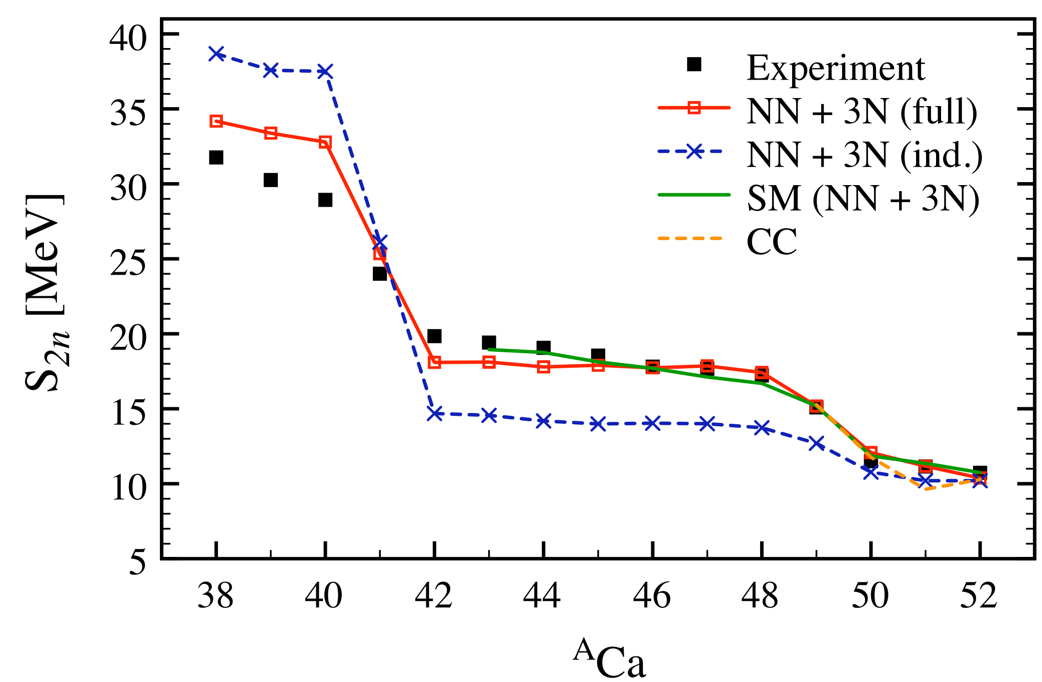
✓ **Successful benchmarks**



✗ **Overbinding**



✗ **Radii underestimated**



✓ **Differential quantities OK**

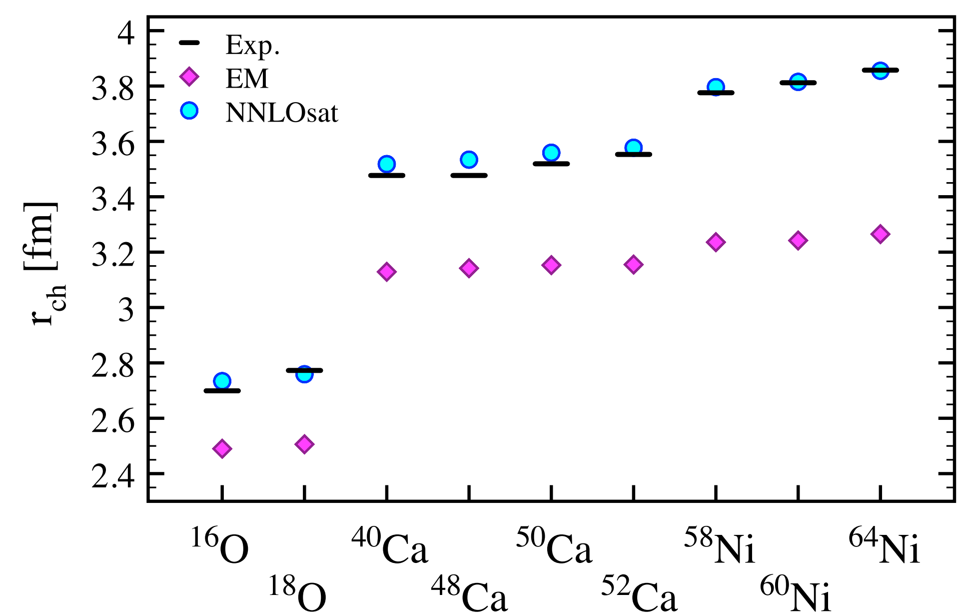
NNLO$_{sat}$ interaction

- **Development of a new ChEFT-inspired Hamiltonian: NNLO$_{sat}$**
  - Simultaneous fit of low-energy constants in 2- and 3-body sectors
  - Data from light nuclei included in fit of low-energy constants

[Ekström *et al.* 2015]

TABLE I. Binding energies (in MeV) and charge radii (in fm) for ^{3}H, ^{3,4}He, ^{14}C, and ^{16,22,23,24,25}O employed in the optimization of NNLO$_{sat}$.

	$E_{g.s.}$	Expt. [69]	r_{ch}	Expt. [65,66]
^{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)		



[Somà, *et al.* unpublished]

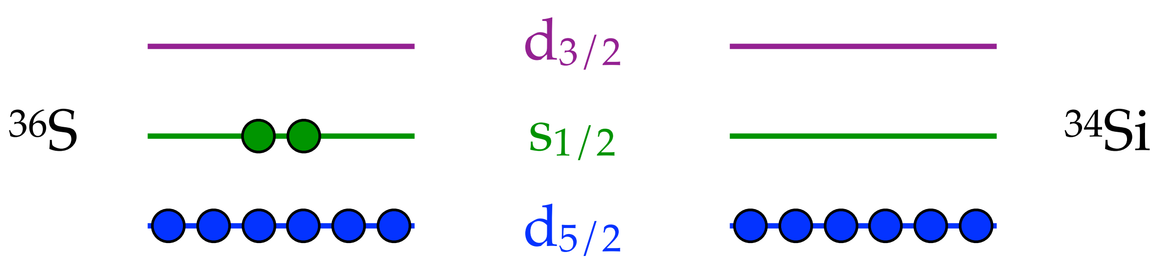
- **Generated debate in the community**
  - Is it really ab initio?
  - What about associated (EFT) uncertainties?
  - How should we fix the parameters of the interaction?
  - *Optimistic* view: NNLO$_{sat}$ indicates that ChEFT strategy is feasible

The case of ^{34}Si

- **Unconventional depletion** (“bubble”) in the centre of ρ_{ch} conjectured for certain nuclei
- **Purely quantum mechanical effect**
  - $\ell = 0$ orbitals display radial distribution peaked at $r = 0$
  - $\ell \neq 0$ orbitals are instead suppressed at small r
  - Vacancy of s states ($\ell = 0$) embedded in larger-ℓ orbitals might cause central depletion
- **Conjectured associated effect on spin-orbit splitting**
  - Non-zero derivative at the interior
  - Spin-orbit potential of “non-natural” sign
  - Reduction of (energy) splitting of low-ℓ spin-orbit partners

- Bubbles predicted for hyper-heavy nuclei [Dechargé *et al.* 2003]
- In light/medium-mass nuclei the **most promising candidate is ^{34}Si**

[Todd-Rutel *et al.* 2004, Khan *et al.* 2008, …]



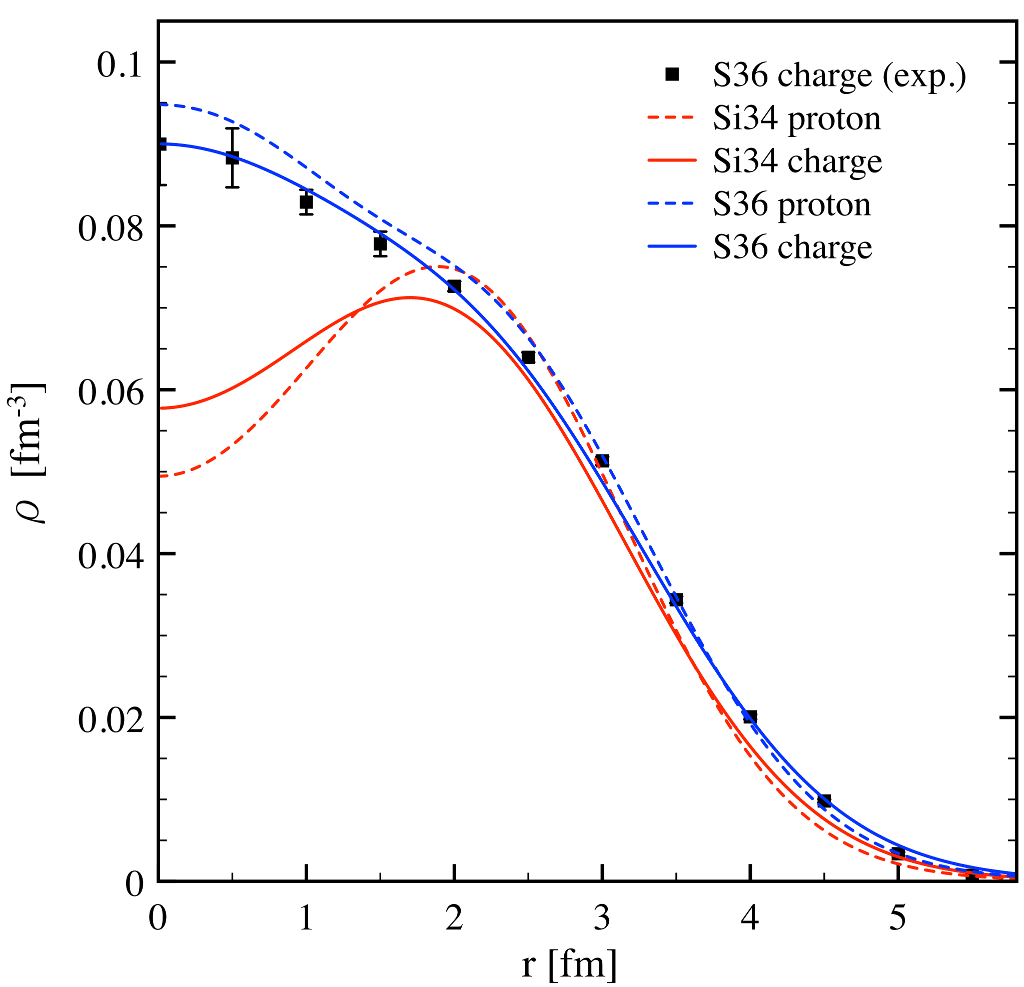
The case of ^{34}Si

⦿ Good reproduction of g.s. properties

E [MeV]	ADC(1)	ADC(2)	ADC(3)	Experiment
^{34}Si	-84.481	-274.626	-282.938	-283.427
^{36}S	-90.007	-296.060	-305.767	-308.714

$\langle r^2_{ch} \rangle^{1/2}$	ADC(1)	ADC(2)	ADC(3)	Experiment
^{34}Si	3.270	3.189	3.187	-
^{36}S	3.395	3.291	3.285	3.2985 ± 0.0024

⦿ **Mild central depletion predicted**



➪ Charge density computed via folding with the finite charge of the proton

➪ Folding smears out central depletion

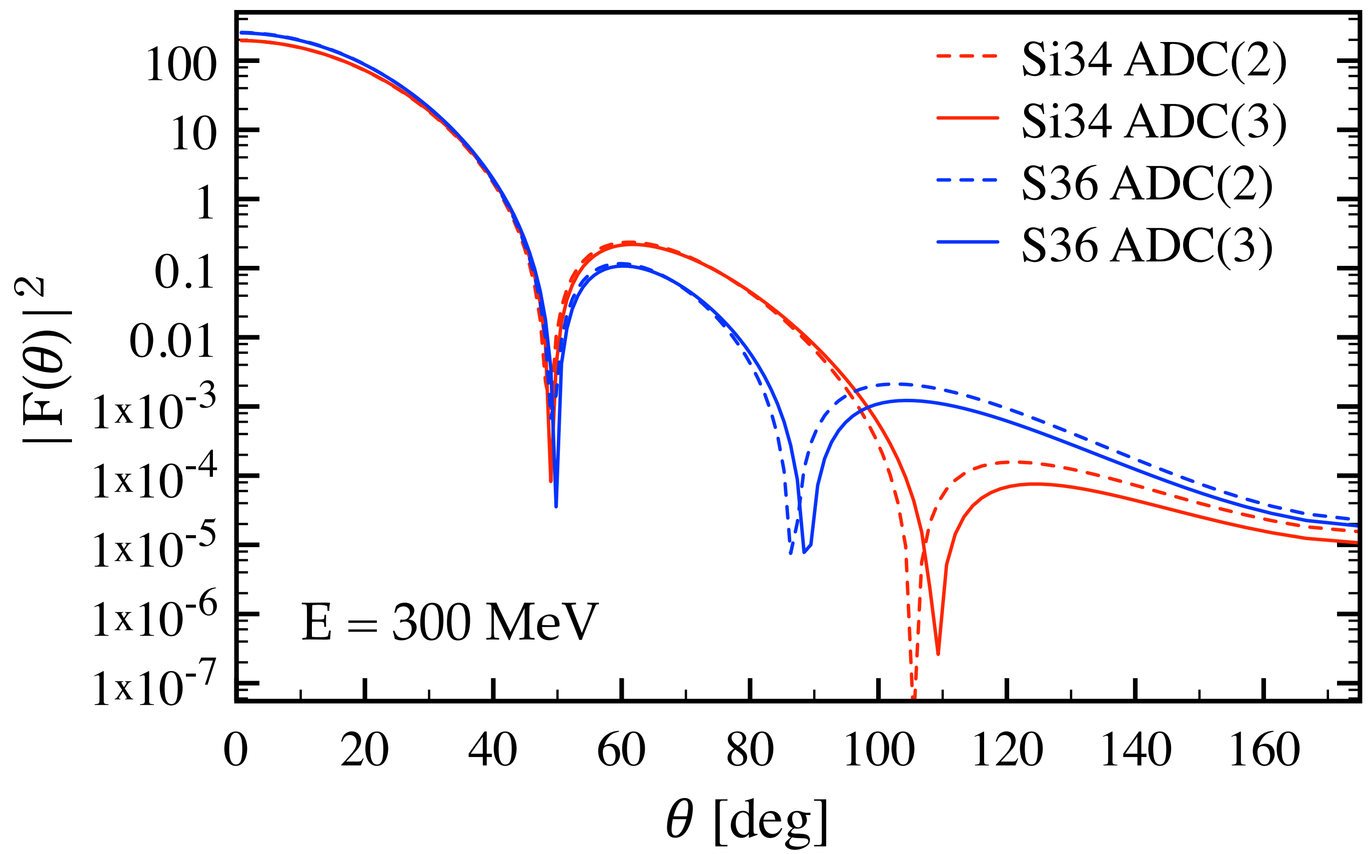
➪ Excellent agreement with experimental charge distribution of ^{36}S

[Duguet *et al.* 2017]

The case of ^{34}Si

- Charge form factor measured in (e,e) experiments sensitive to bubble structure?

$$F(q) = \int d\vec{r} \rho_{\rm ch}(r) e^{-i\vec{q}\cdot\vec{r}} \quad \text{and} \quad q = 2p \sin\theta/2$$



○ Central depletion reflects in larger F(θ) for angles θ>70° and shifted 2nd minimum

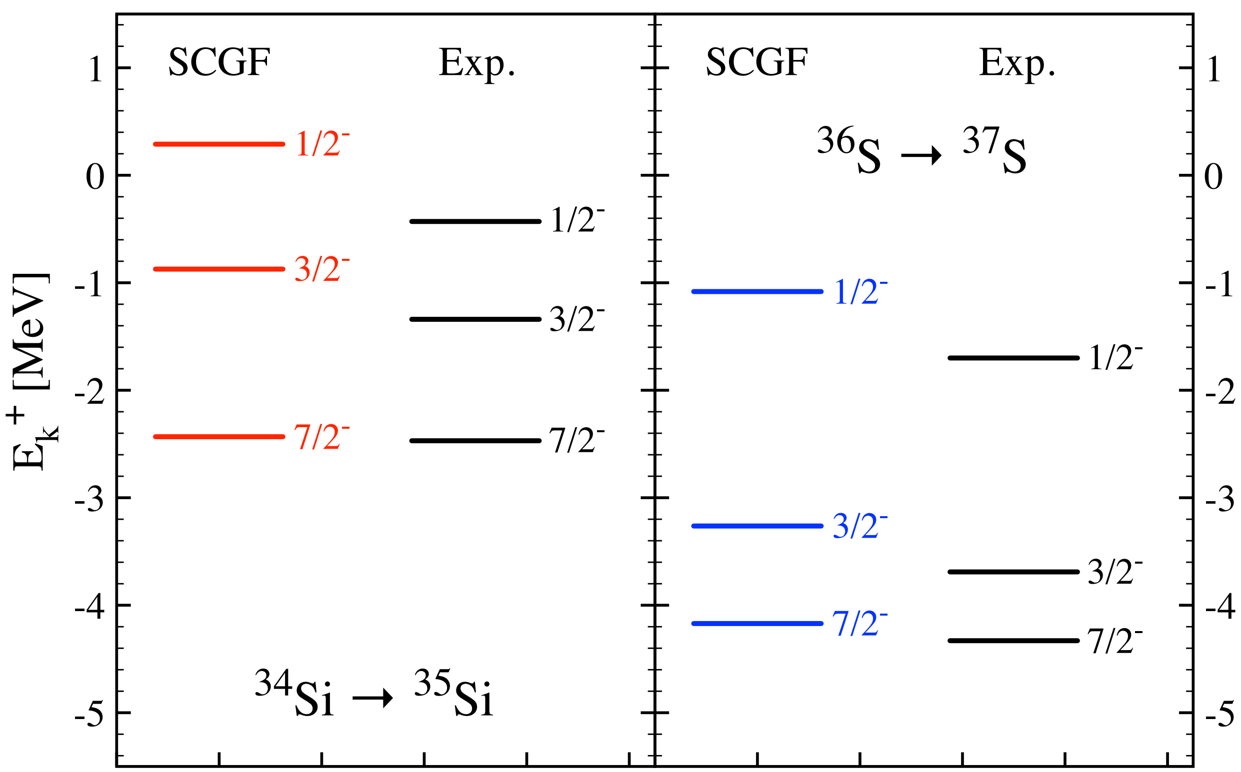
○ **Future electron scattering experiments might be able to see its fingerprints**

The case of ^{34}Si

⦿ Addition and removal spectra compared to **transfer** and **knock-out reactions**

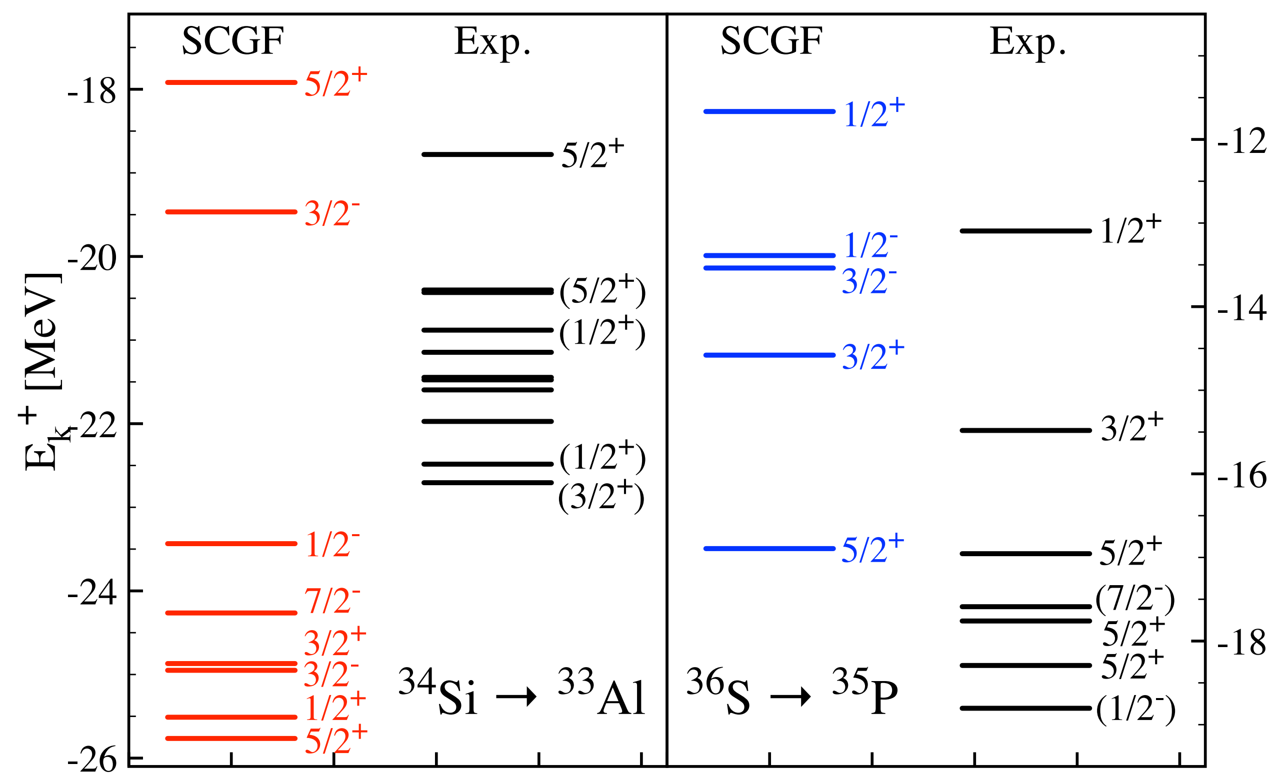
One-neutron addition

Exp. data: [Thorn *et al.* 1984] [Eckle *et al.* 1989] [Burgunder *et al.* 2014]



One-proton knock-out

Exp. data: [Khan *et al.* 1985] [Mutschler *et al.* 2016 (PRC)] [Mutschler *et al.* 2016 (Nature Phys.)]

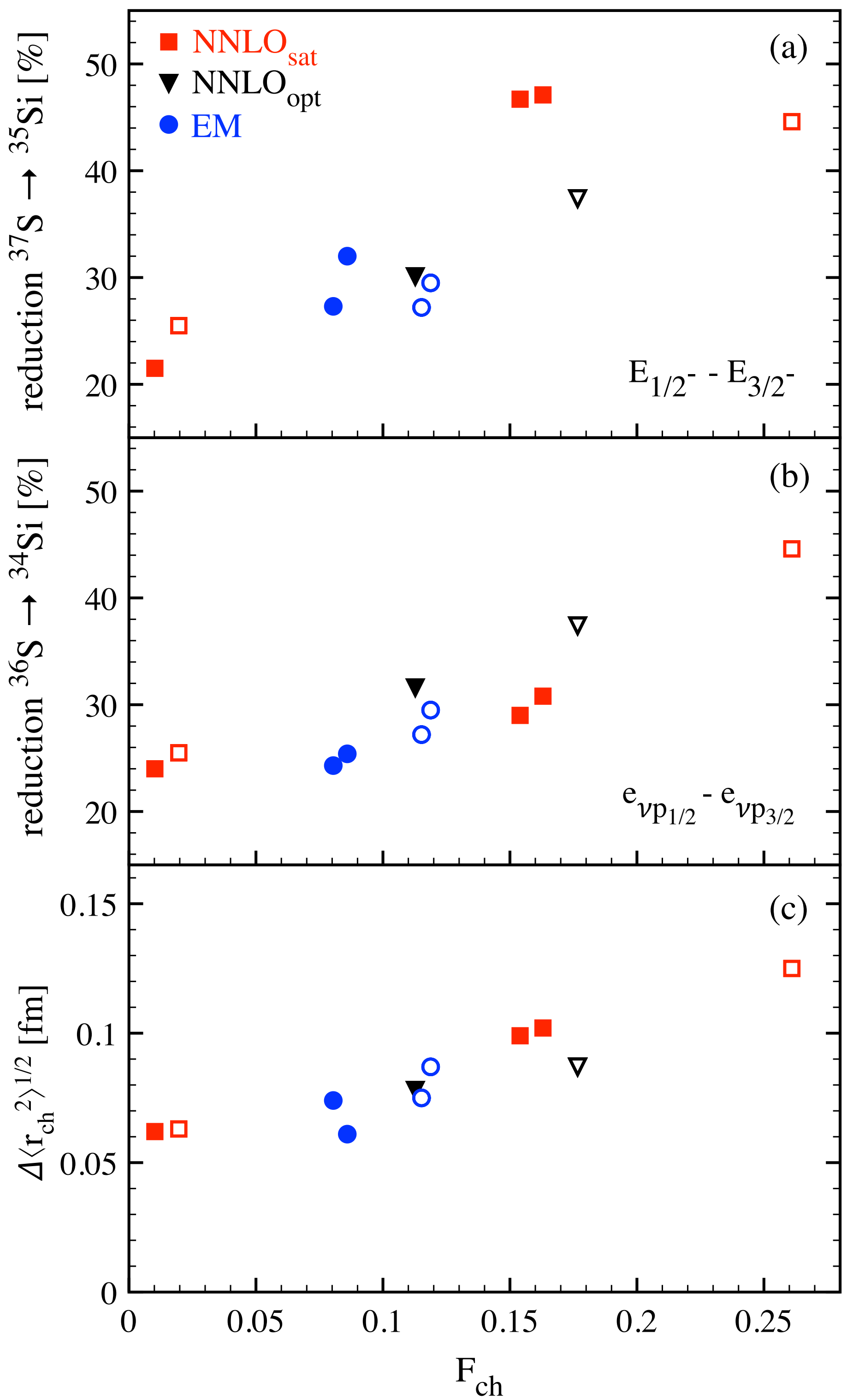


○ Good agreement for one-neutron addition, to a lesser extent for one-proton removal

○ **Reduction of $E_{1/2^-}$ - $E_{3/2^-}$ spin-orbit splitting (unique in the nuclear chart!) well reproduced**

The case of ^{34}Si

⦿ **Correlation** between bubble structure and reduction of spin-orbit splitting?



Separation energies

○ Different *H*s lead to very different depletions

○ Calculations support existence of a correlation

Effective single-particle energies

○ Lower reduction of s.o. splitting

○ Linear correlation holds also for ESPEs

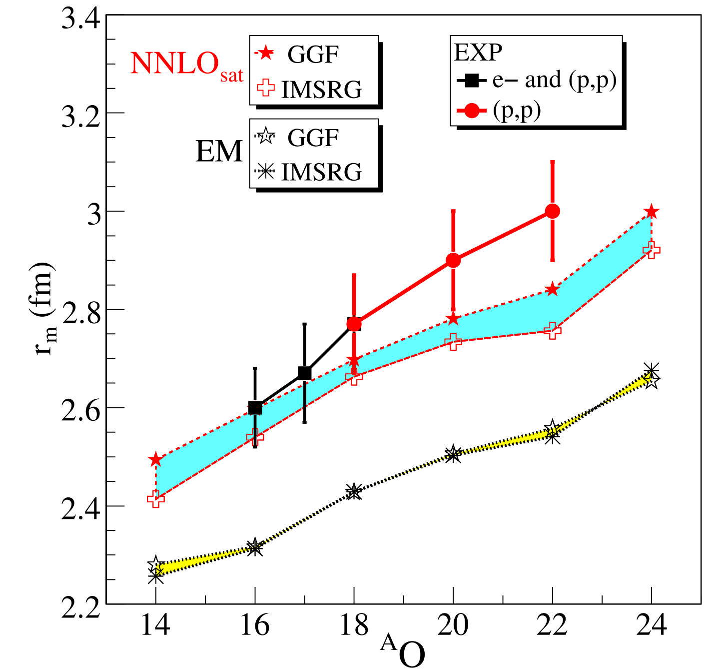
Charge radius difference (^{36}S-^{34}Si)

○ Radius difference also correlates with F_{ch}

○ Motivation for measuring ^{34}Si radius

N3LO *NN* + 3*N* (LNL) interaction

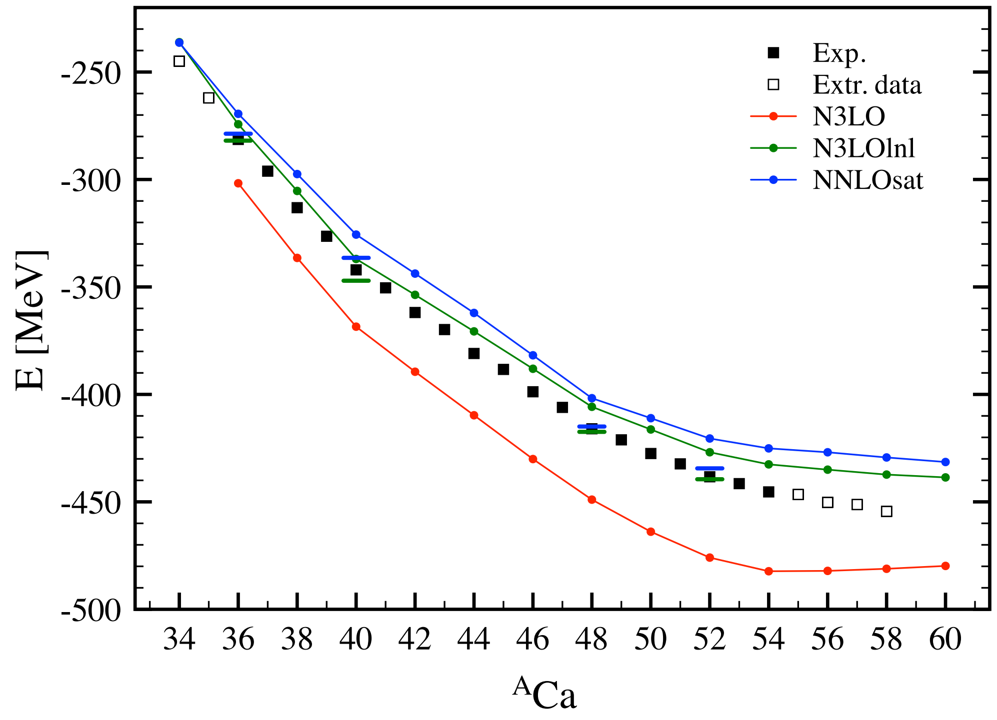
- **Is NNLO$_{sat}$ the end of the story?**
  - Description of *NN* phase shifts and light nuclei
  - Issues with symmetry energy? Spectra of medium-mass nuclei?
  - Technical issues (strong 3N, SRG induces substantial 4N forces)

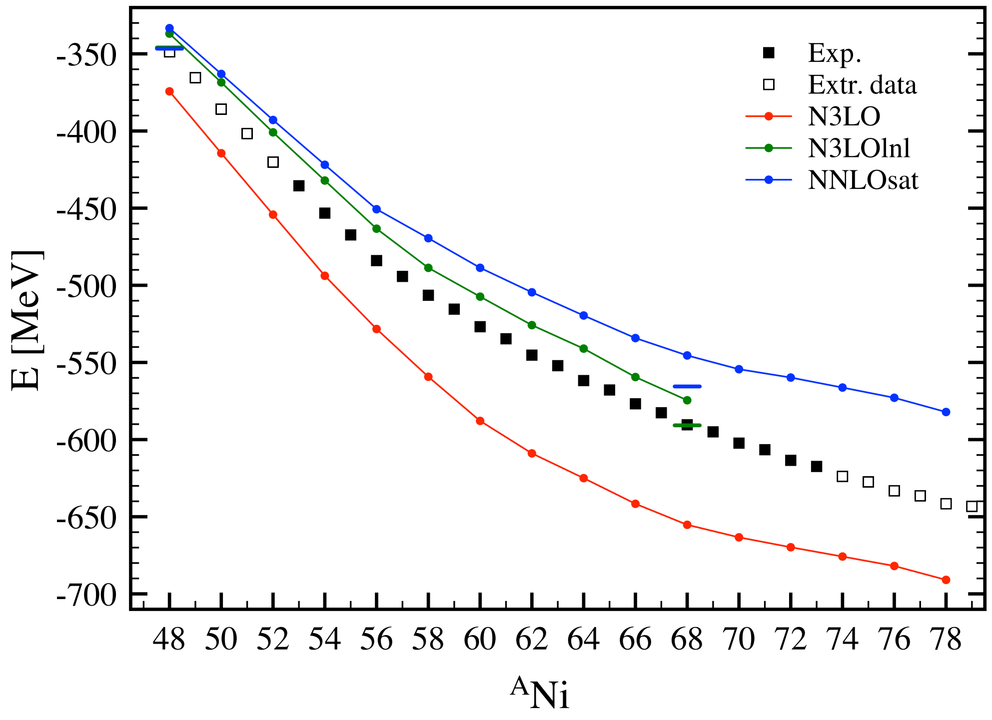


[Lapoux, *et al.* 2016]

- **Novel version of the 'standard' N3LO interaction**
  - "Local/nonlocal" (LNL) regulators [Navrátil 2018]
  - Improves on overbinding and spectra
  - However, radii still slightly underestimated

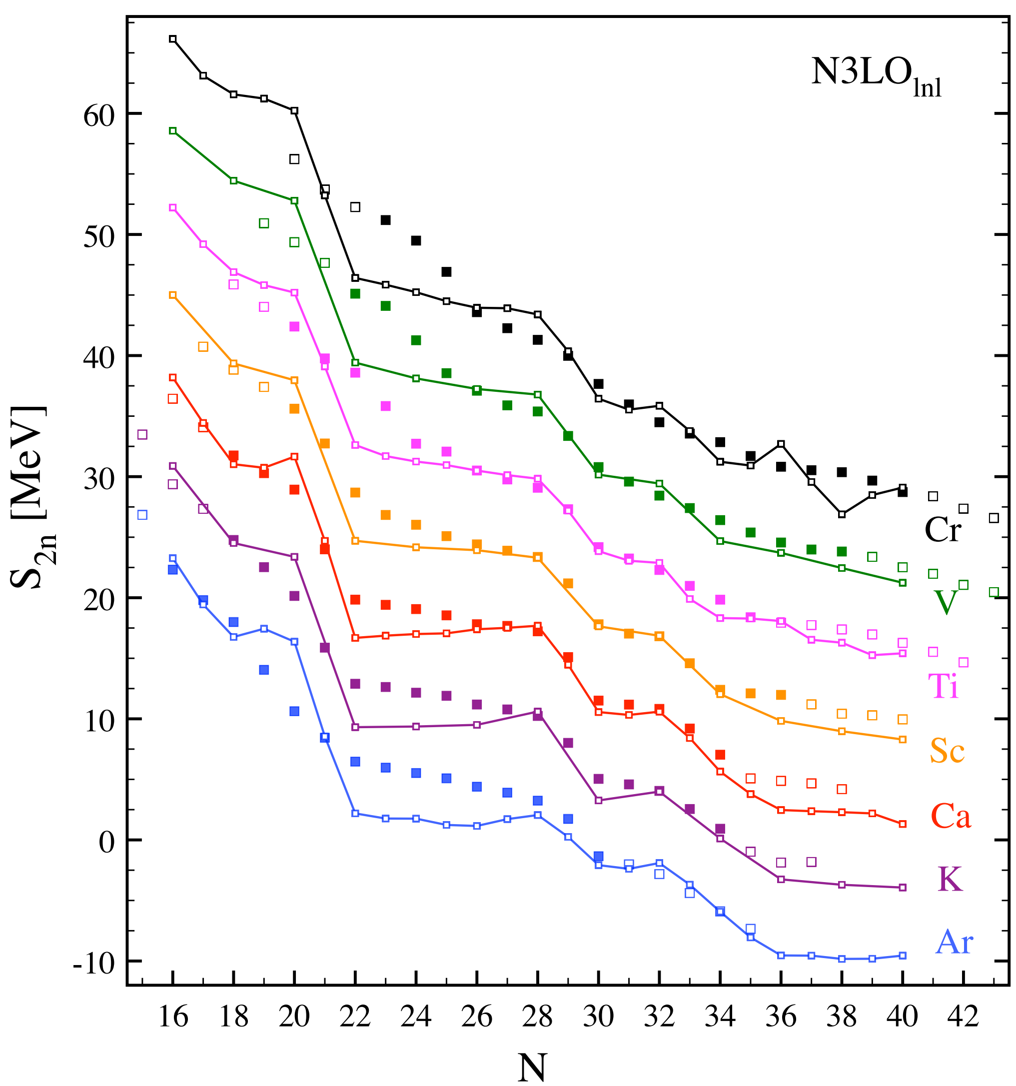
[Somà, *et al.* in preparation]

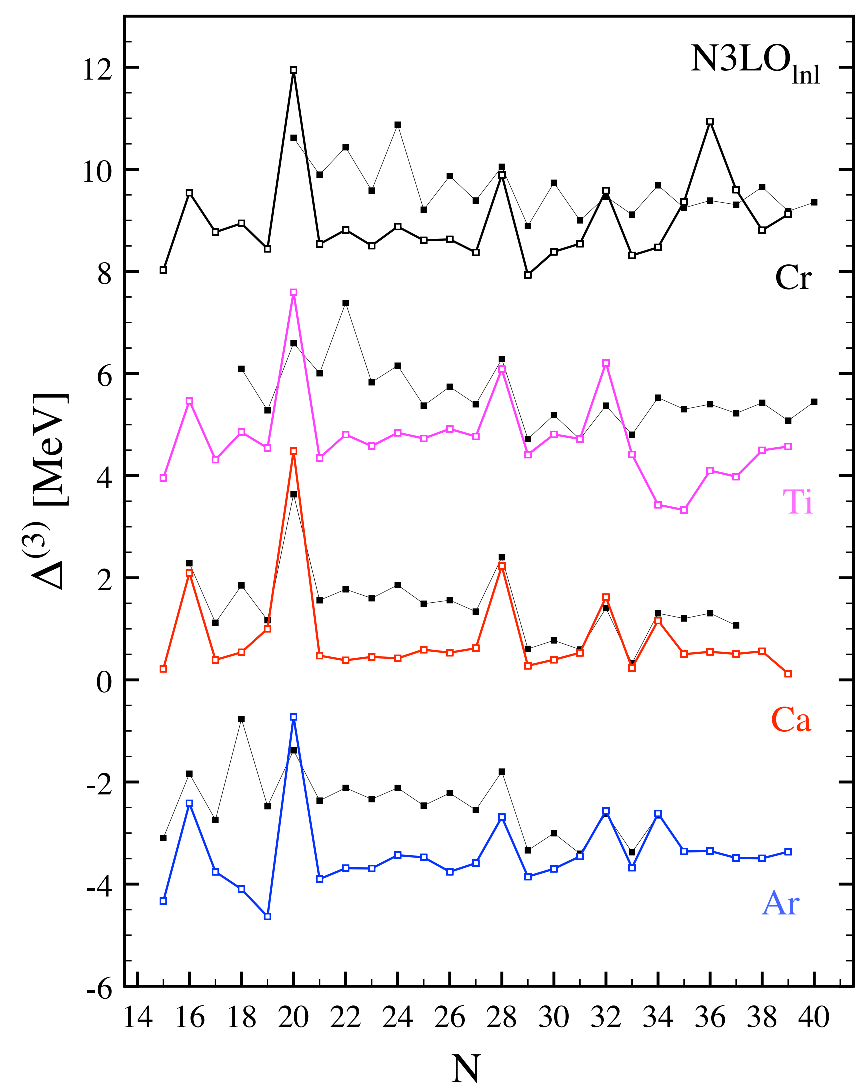




Systematics in mid-mass nuclei

- **Systematic investigation of *Z*=18-24 region**
  - *N*=20 gap overestimated, good performance for *N*>28
  - Weak pairing in *N*=20-28, good reproduction in *N*=28-34





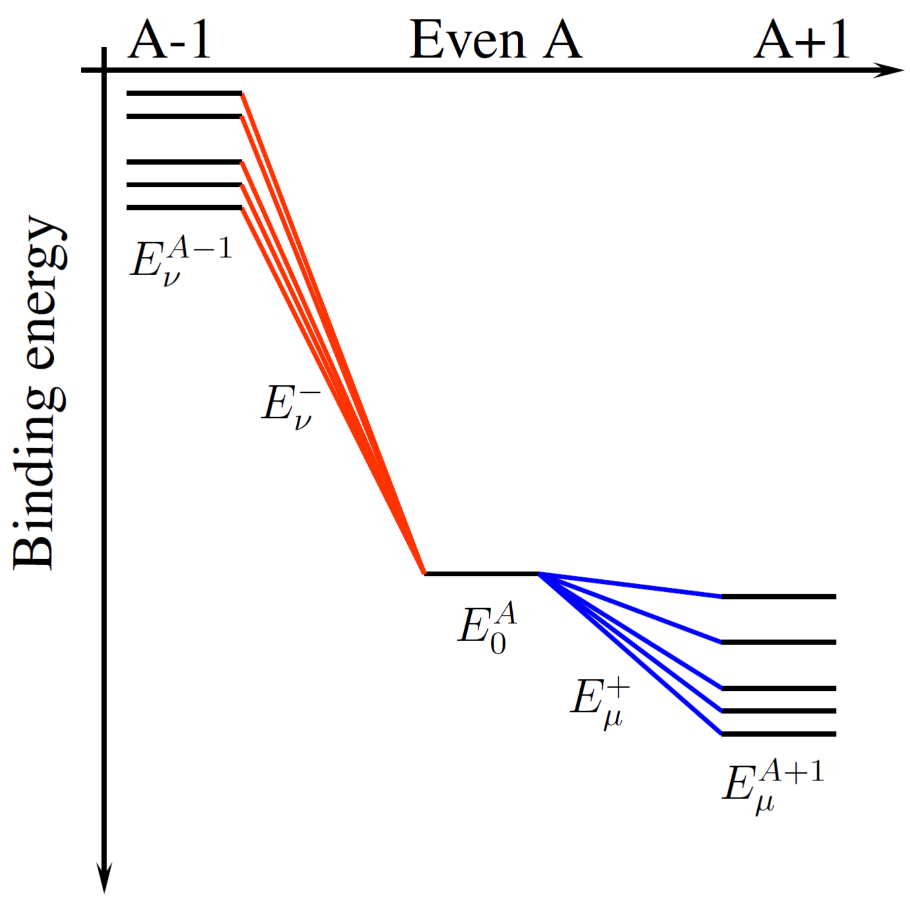
[Somà, *et al.* in preparation]

Spectral representation

$$G_{ab}(z) = \sum_{\mu} \frac{U_a^{\mu} (U_b^{\mu})^*}{z - E_{\mu}^{+} + i\eta} + \sum_{\nu} \frac{(V_a^{\nu})^* V_b^{\nu}}{z - E_{\nu}^{-} - i\eta}$$

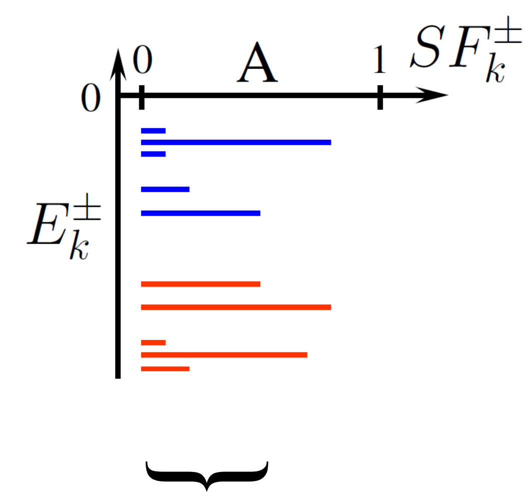
Separation energies

$$E_{\mu}^{+} \equiv E_{\mu}^{A+1} - E_0^A$$
$$E_{\nu}^{-} \equiv E_0^A - E_{\nu}^{A-1}$$



Spectral strength distribution

$$\mathcal{S}(z) = \sum_{\mu \in \mathcal{H}_{A+1}} SF_{\mu}^{+}\, \delta(z - E_{\mu}^{+}) + \sum_{\nu \in \mathcal{H}_{A-1}} SF_{\nu}^{-}\, \delta(z - E_{\nu}^{-})$$



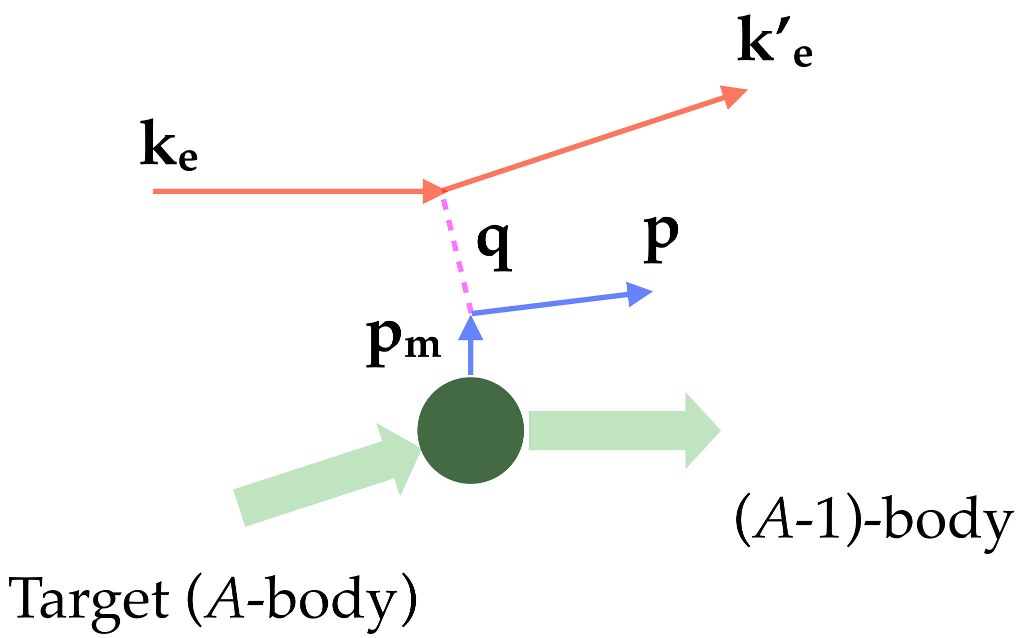
Spectroscopic factors

$$SF_{\mu}^{+} \equiv \mathrm{Tr}_{\mathcal{H}_1}\left[\mathbf{S}_{\mu}^{+}\right] = \sum_{a \in \mathcal{H}_1} \left|U_{\mu}^{a}\right|^2$$

$$SF_{\nu}^{-} \equiv \mathrm{Tr}_{\mathcal{H}_1}\left[\mathbf{S}_{\nu}^{-}\right] = \sum_{a \in \mathcal{H}_1} \left|V_{\nu}^{a}\right|^2$$

Spectral strength in experiments

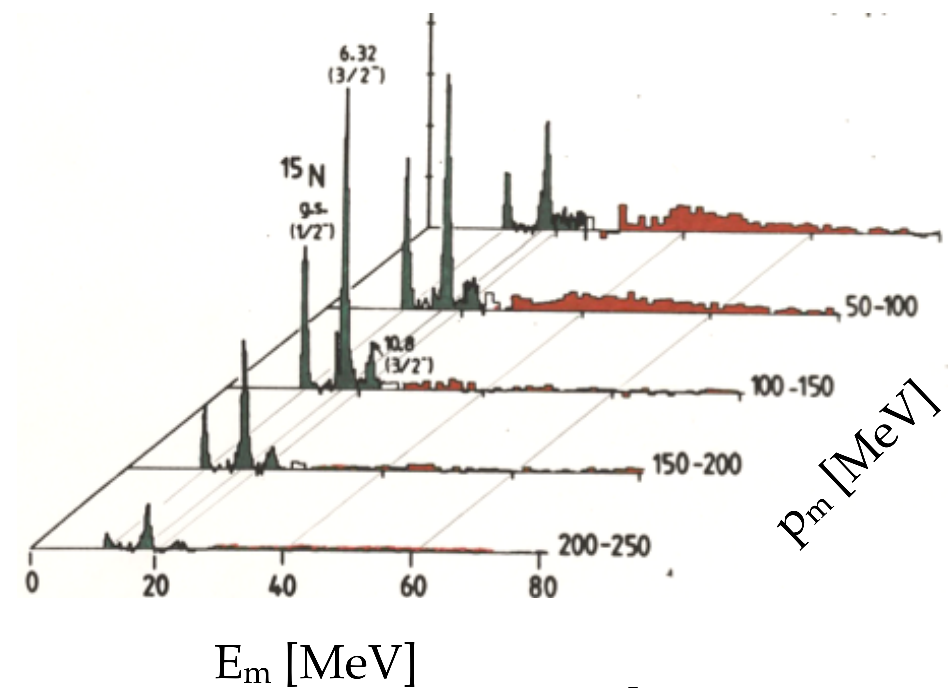
- Clean connection to (*e,e′p*) experiments



- Measuring **q** and **p** gives information on $\mathbf{p_m}$
- Similarly for missing energy E_m
- Spectral strength distribution ↔ $P(p_m, E_m)$

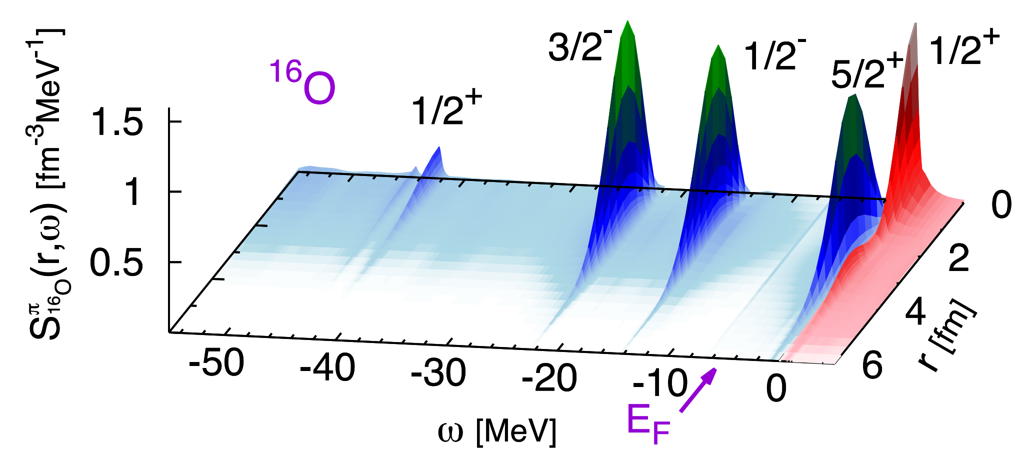
- Spectroscopy via knockout / transfer exp.

Results from (e,e′p) on ¹⁶O (ALS in Saclay)



[Mougey *et al*. 1980]

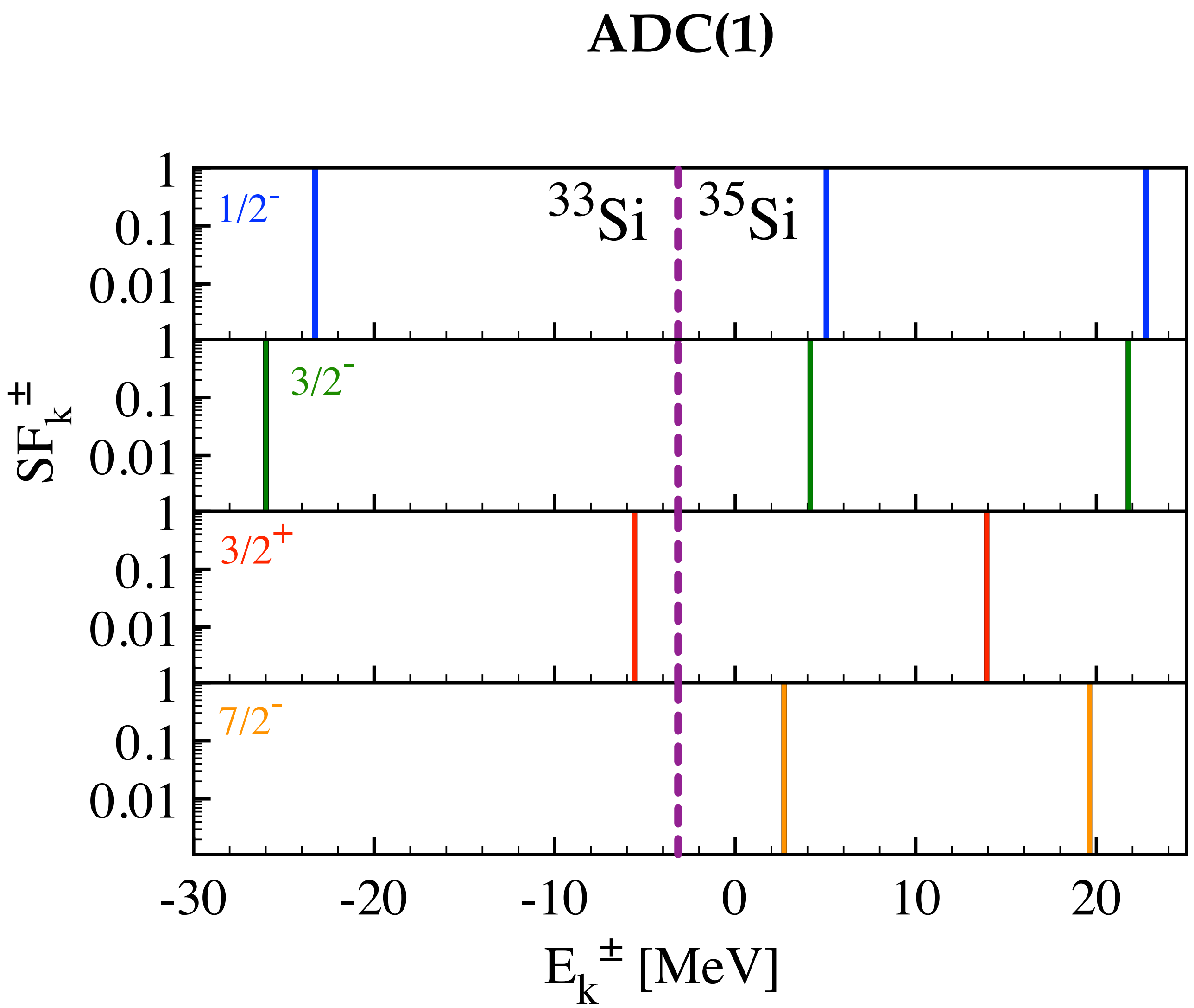
SCGF calculations



[Cipollone *et al*. 2015]

Spectral strength distribution

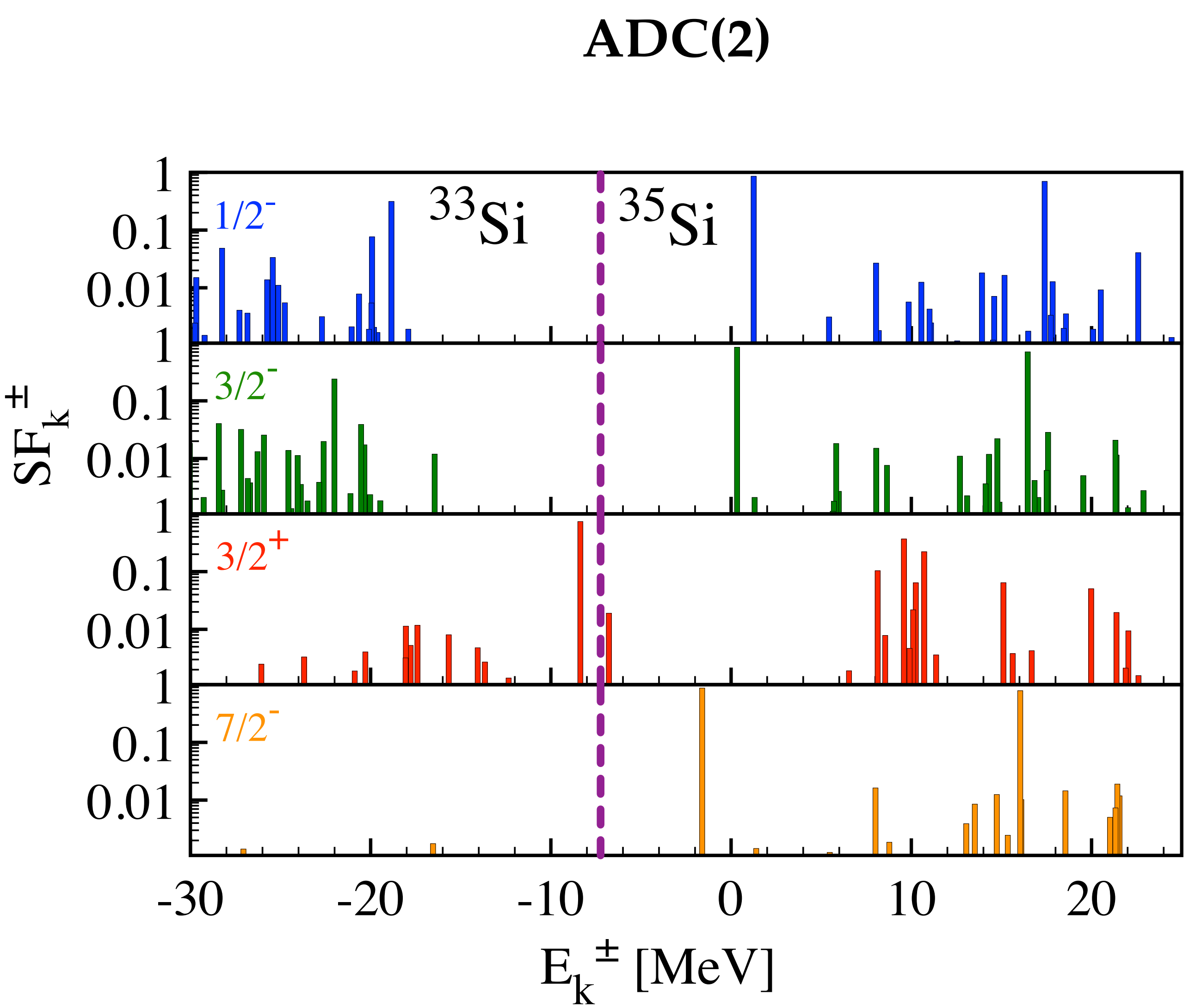
- ^{34}Si neutron addition & removal strength



- Independent-particle picture

Spectral strength distribution

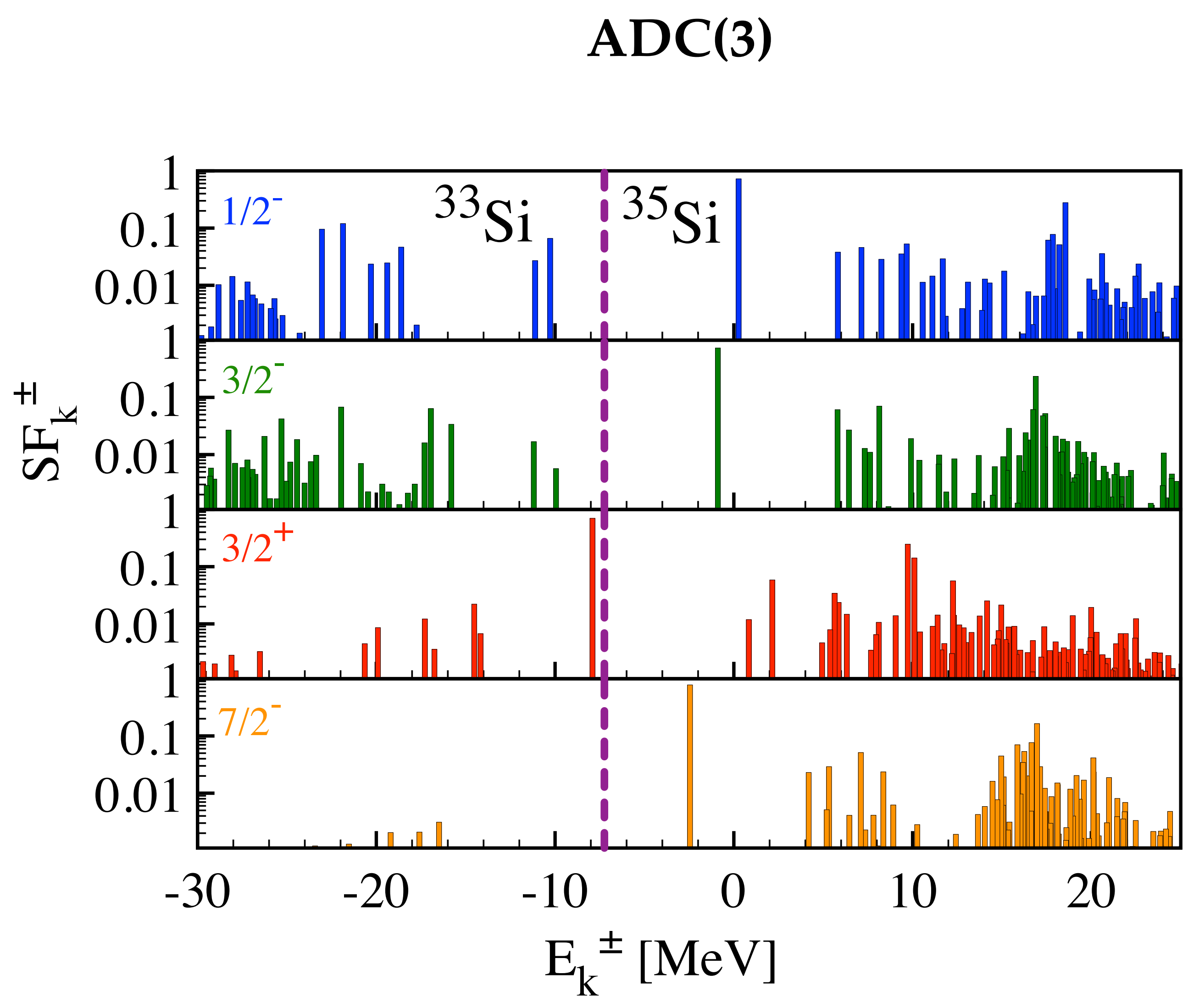
- ^{34}Si neutron addition & removal strength



- Second-order dynamical correlations fragment IP peaks

Spectral strength distribution

⊙ ^{34}Si neutron addition & removal strength

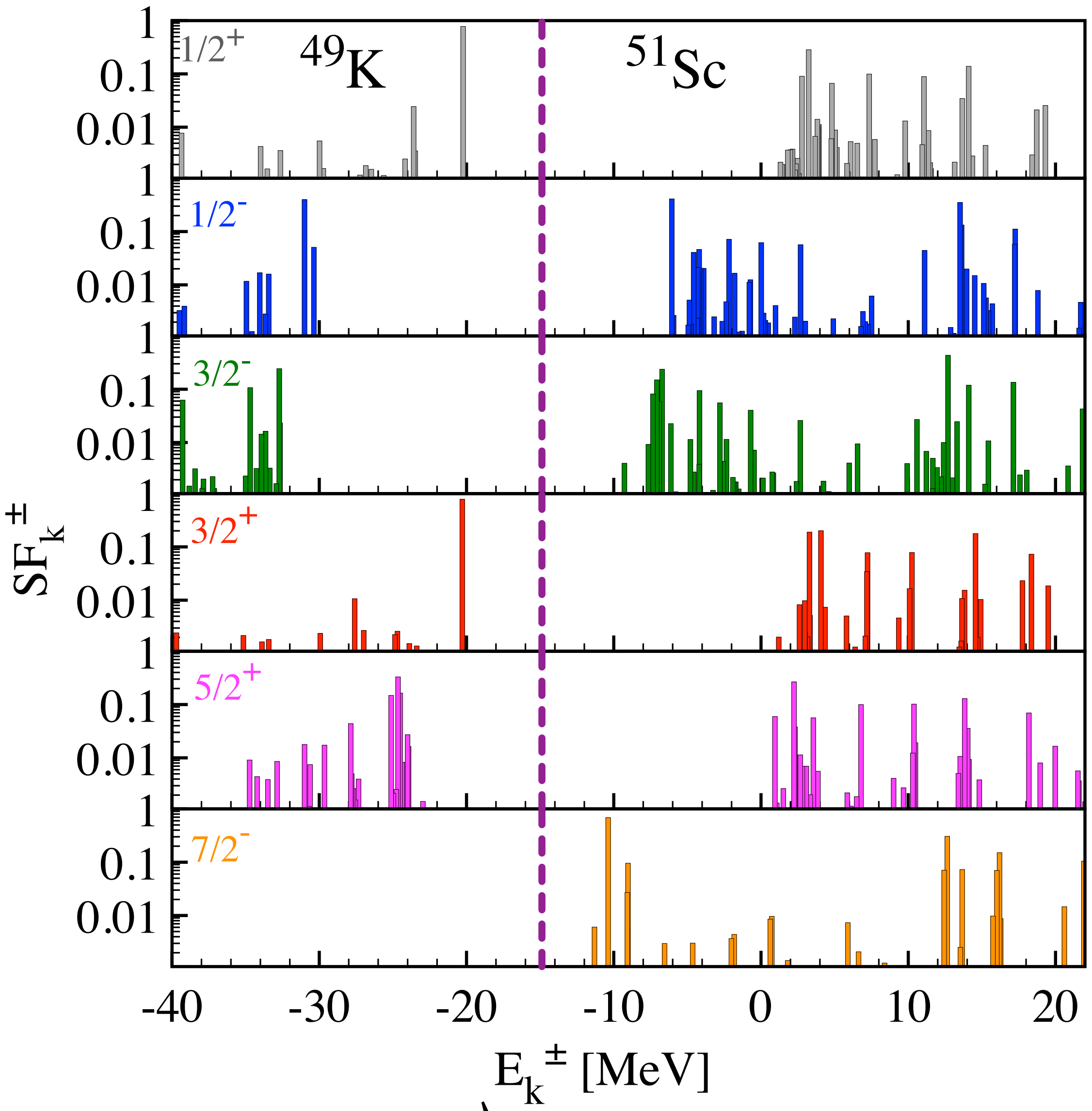


○ Third-order compresses the spectrum (main peaks)

○ Further fragmentation is generated

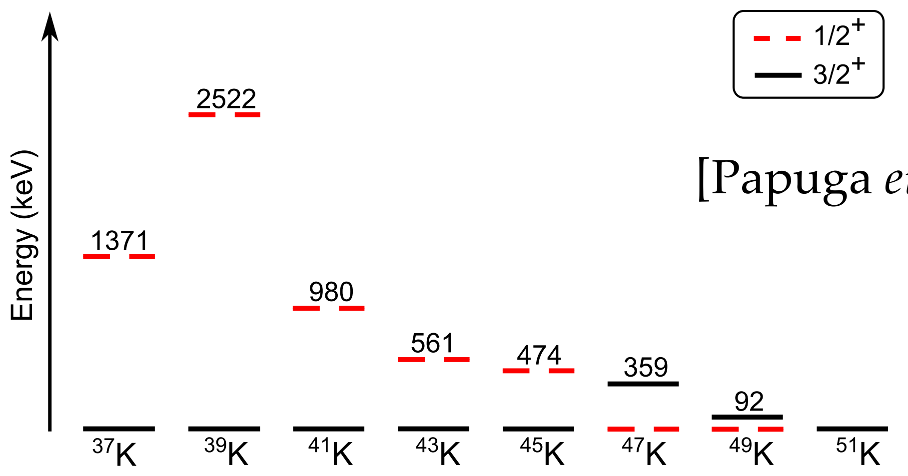
K spectra

➪ **K spectra show interesting g.s. spin inversion and re-inversion**

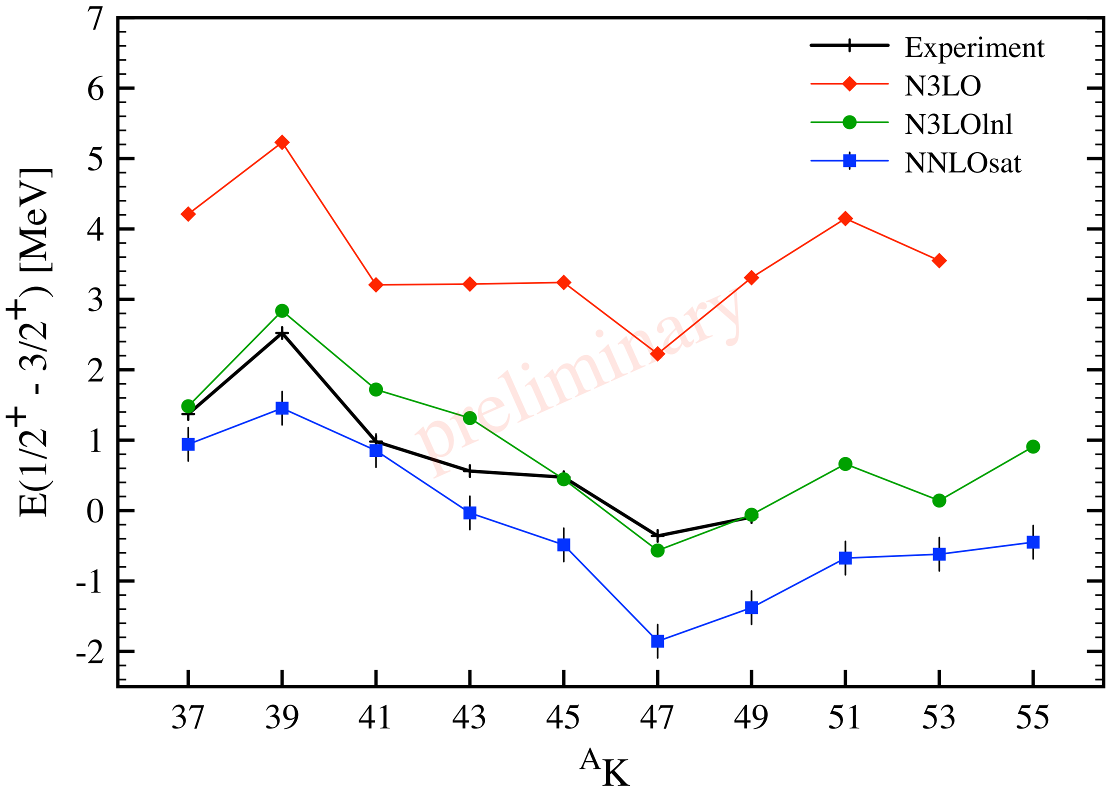


One-proton addition and removal from ^{50}Ca

Laser spectroscopy COLLAPS @ ISOLDE



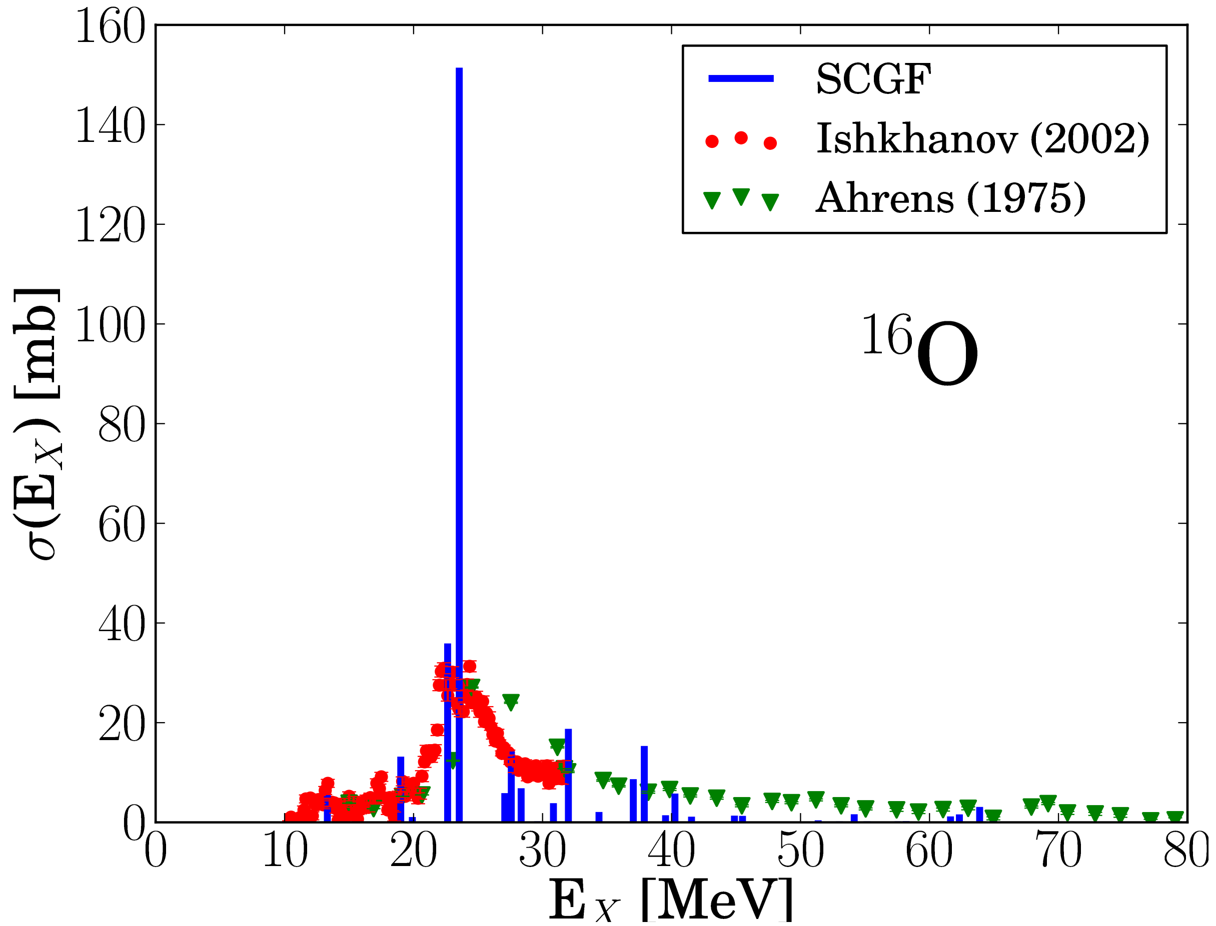
[Papuga *et al.* 2013]

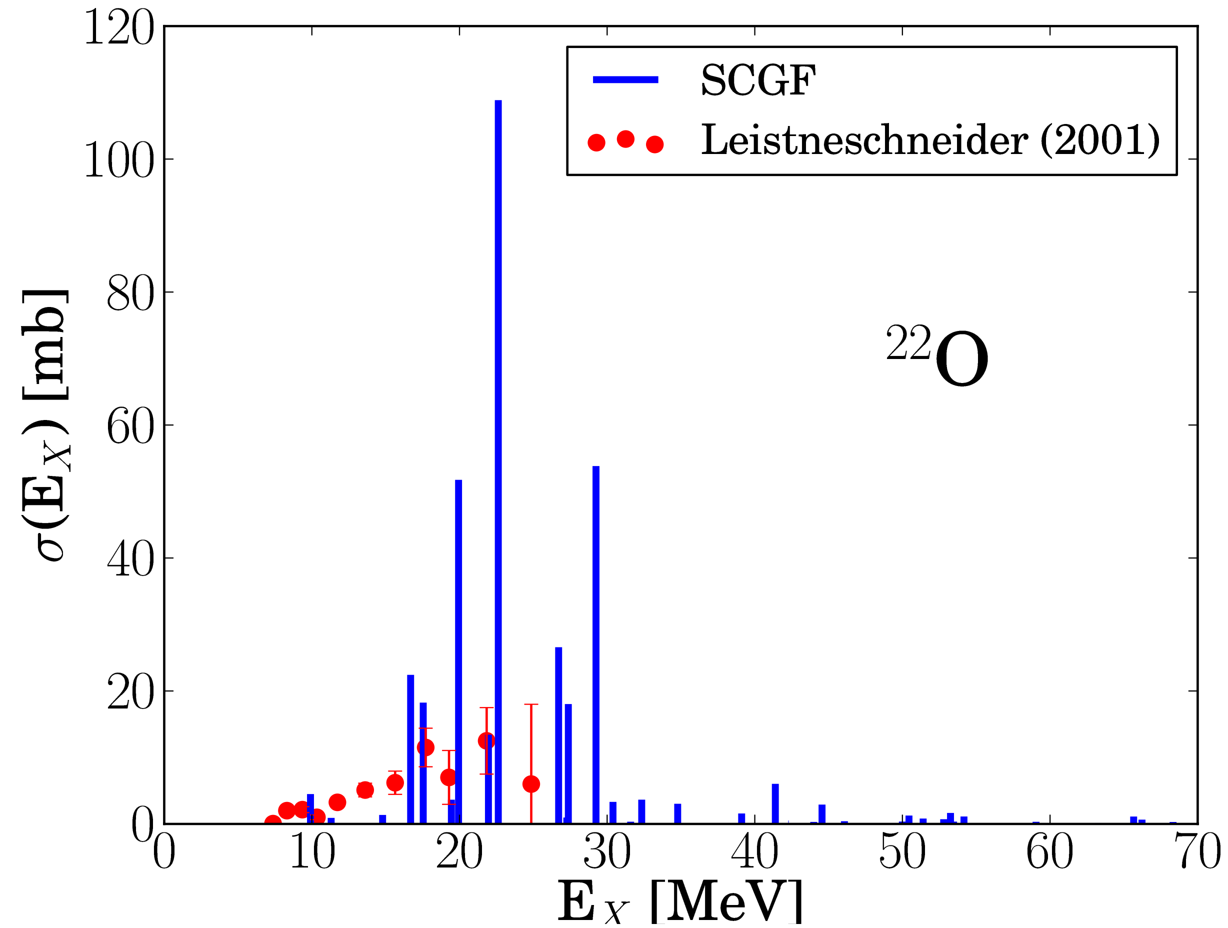


Electromagnetic response

⦿ Computed σ from RPA response vs. σ from photoabsorption and Coulomb excitation

[Raimondi *et al.* in preparation]





○ GDR position of ^{16}O well reproduced

○ Hint of a soft dipole mode in ^{22}O

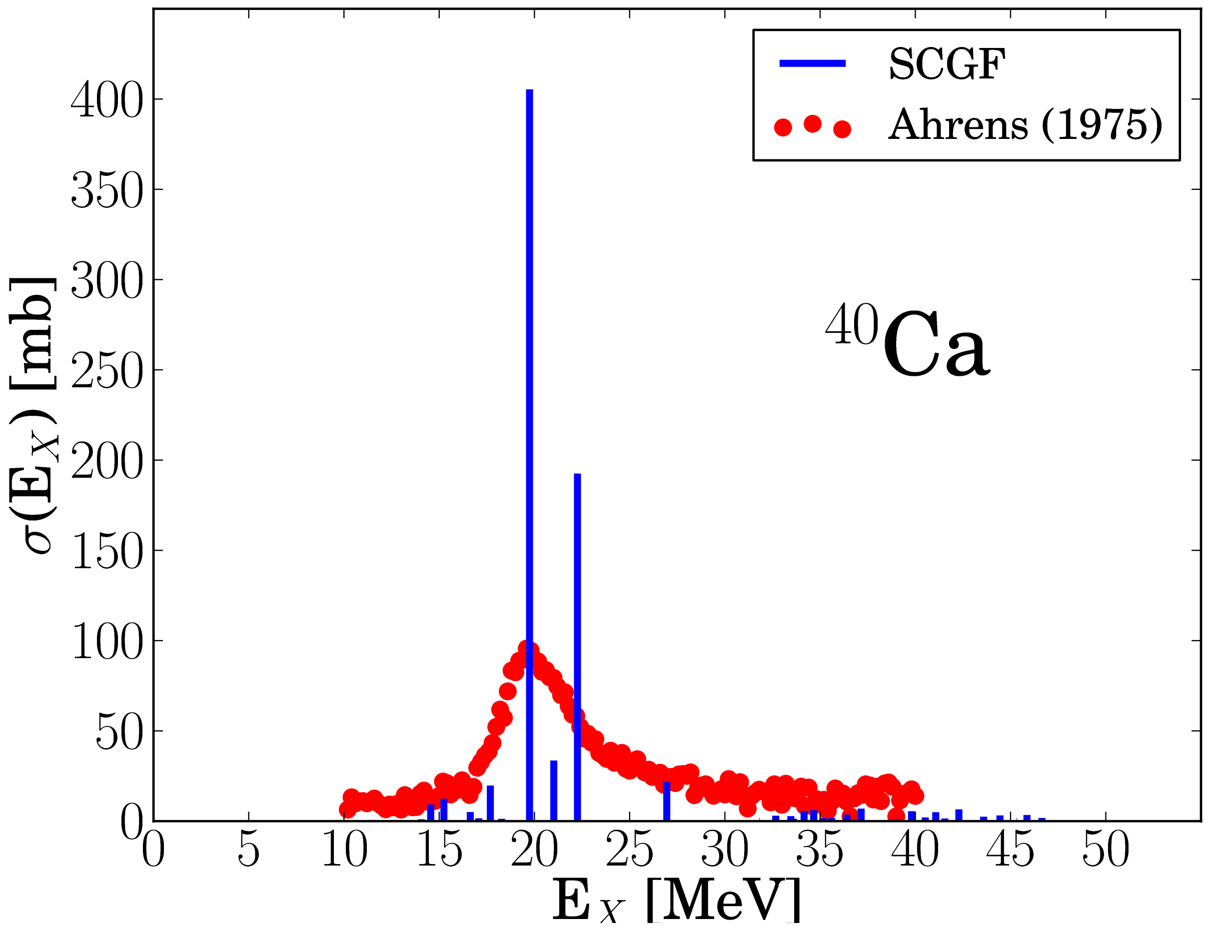
○ Comparison with CC LIT results for α_D

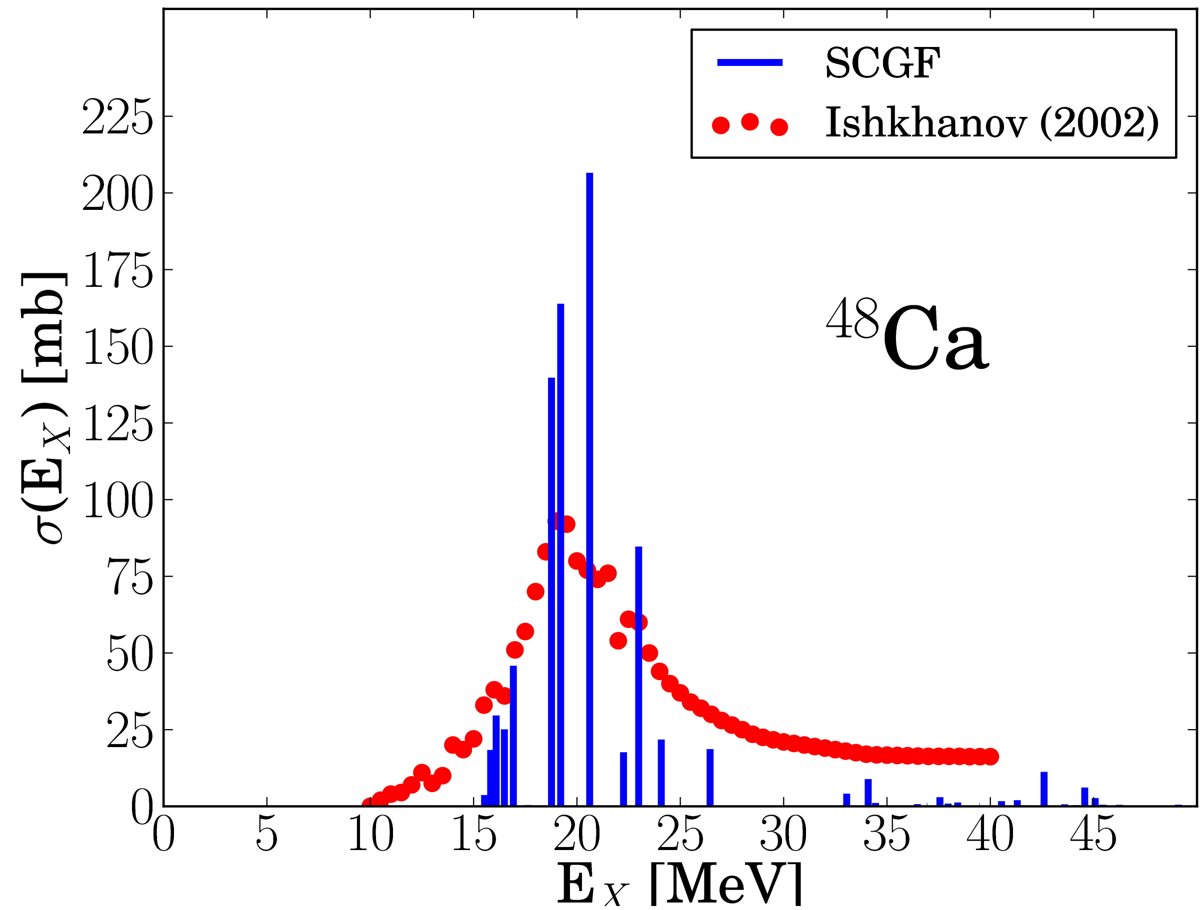
Dipole polarizability α_D (fm^3)			
Nucleus	SCGF	CC/LIT	Exp
^{16}O	0.50	0.57(1)	0.585(9)
^{22}O	0.72	0.86(4)	0.43(4)

Electromagnetic response

- Computed σ from RPA response vs. σ from photoabsorption and Coulomb excitation

[Raimondi *et al.* in preparation]





- GDR positions reproduced
- Total sum rule OK but poor strength distribution
- Comparison with CC LIT results for α_D

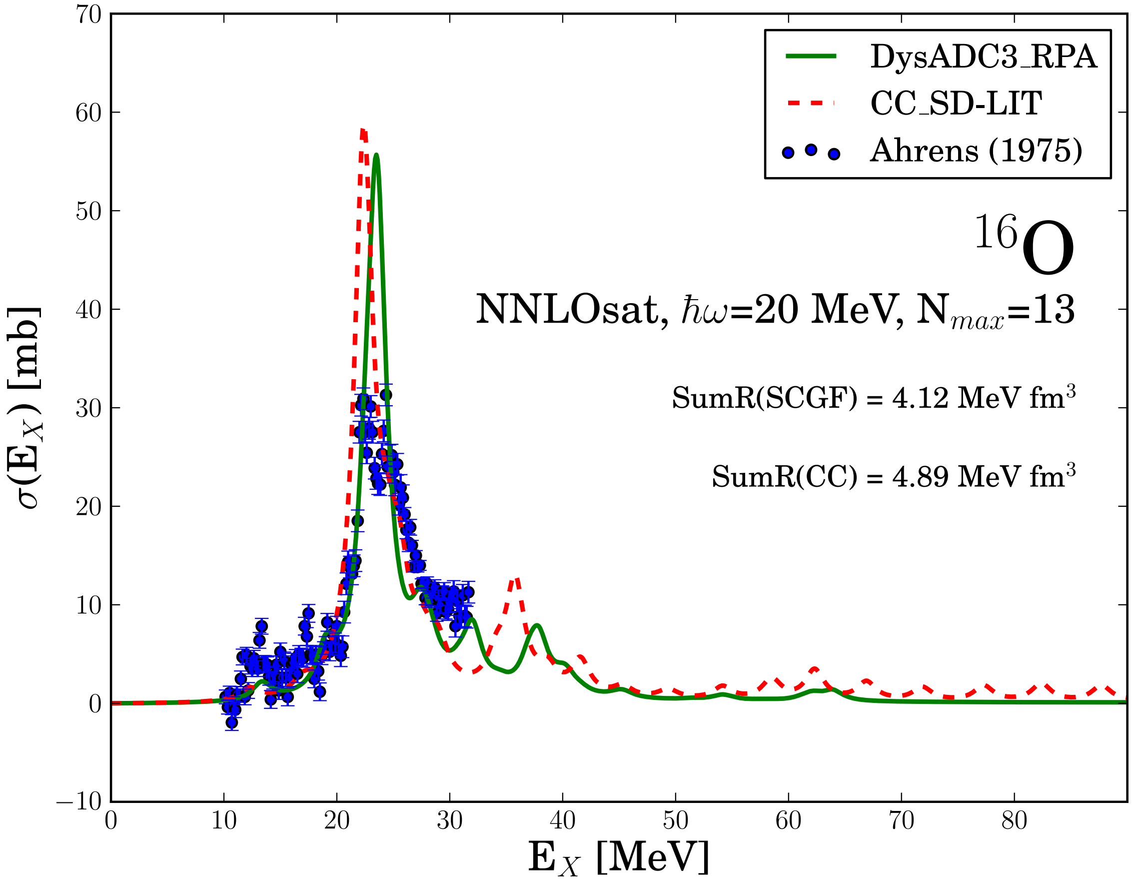
Dipole polarizability α_D (fm^3)

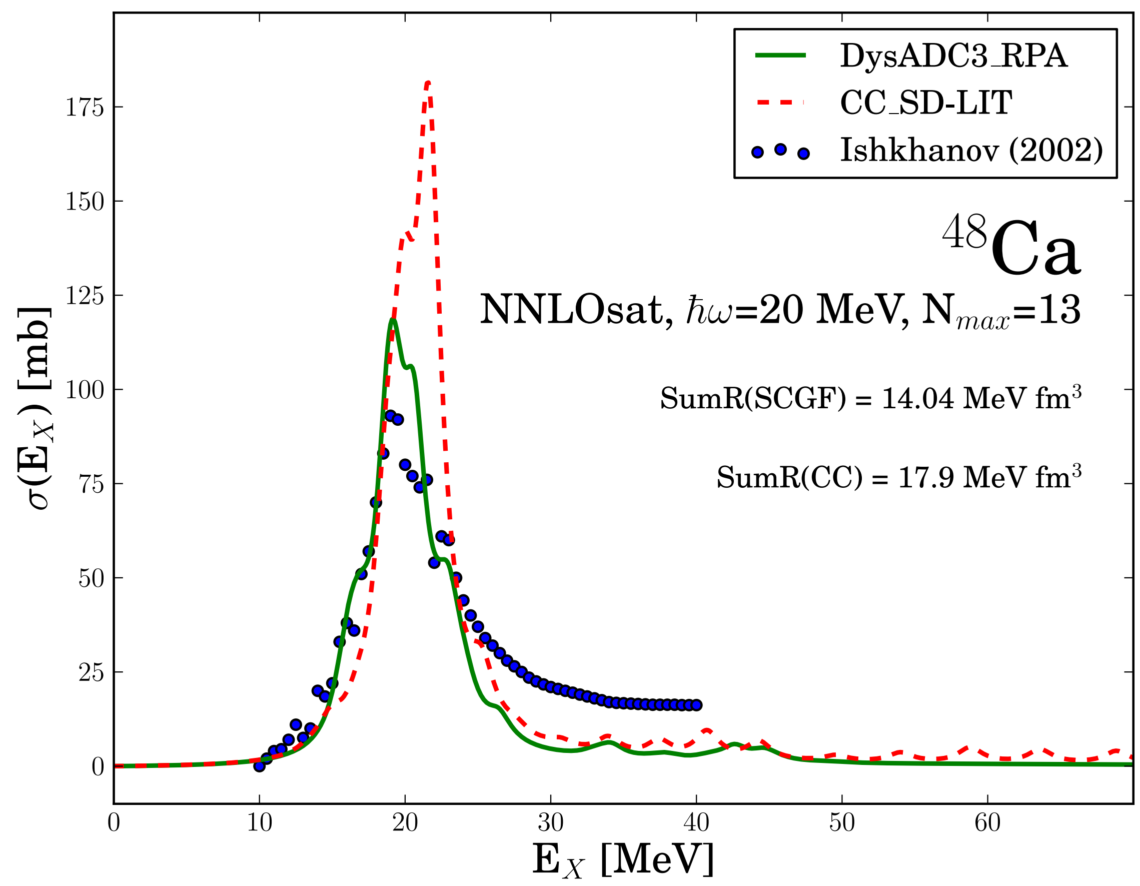
Nucleus	SCGF	CC/LIT	Exp
^{40}Ca	1.79	1.47 $(1.87)_{thresh}$	1.87(3)
^{48}Ca	2.08	2.45	2.07(22)

Electromagnetic response

⊙ Comparison with coupled-cluster Lorentz integral transform (CC-LIT)

[Raimondi *et al.* in preparation]



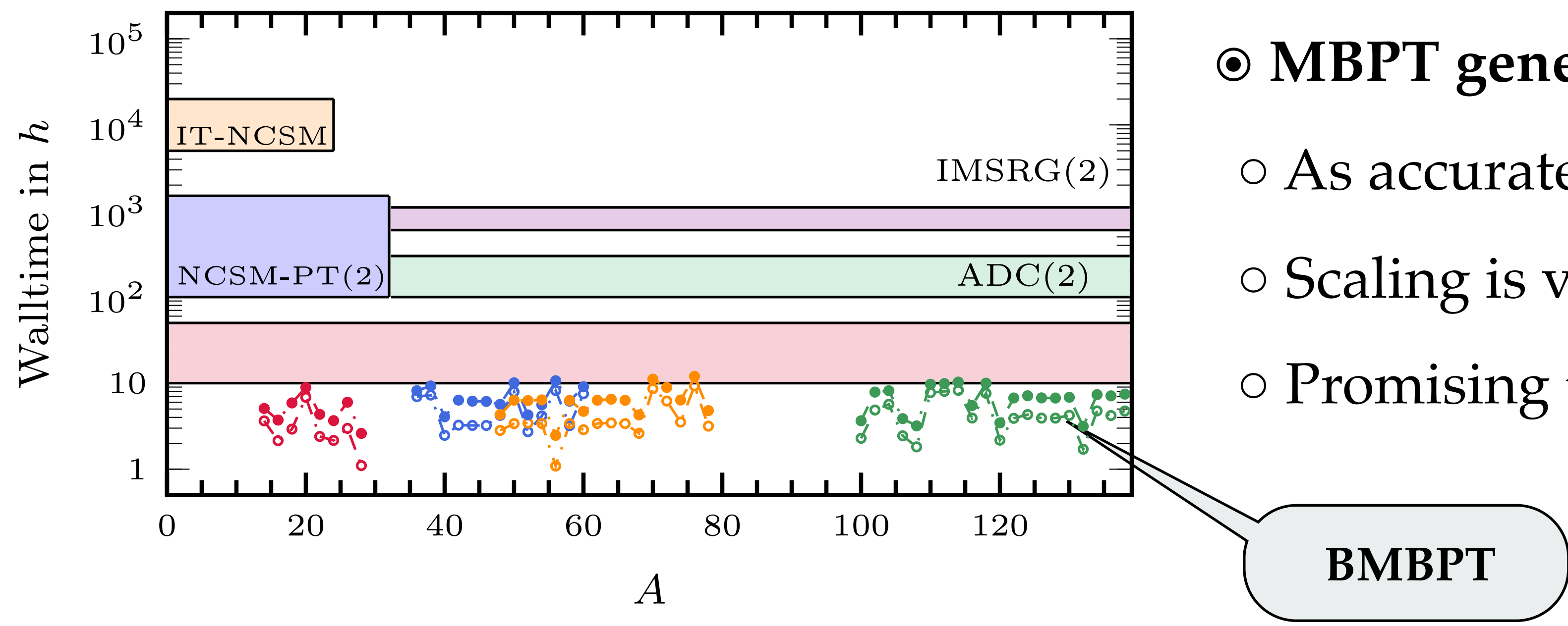


○ Different ways of including correlations

GF → RPA (first-order 2-body correlator) on top of fully correlated reference state

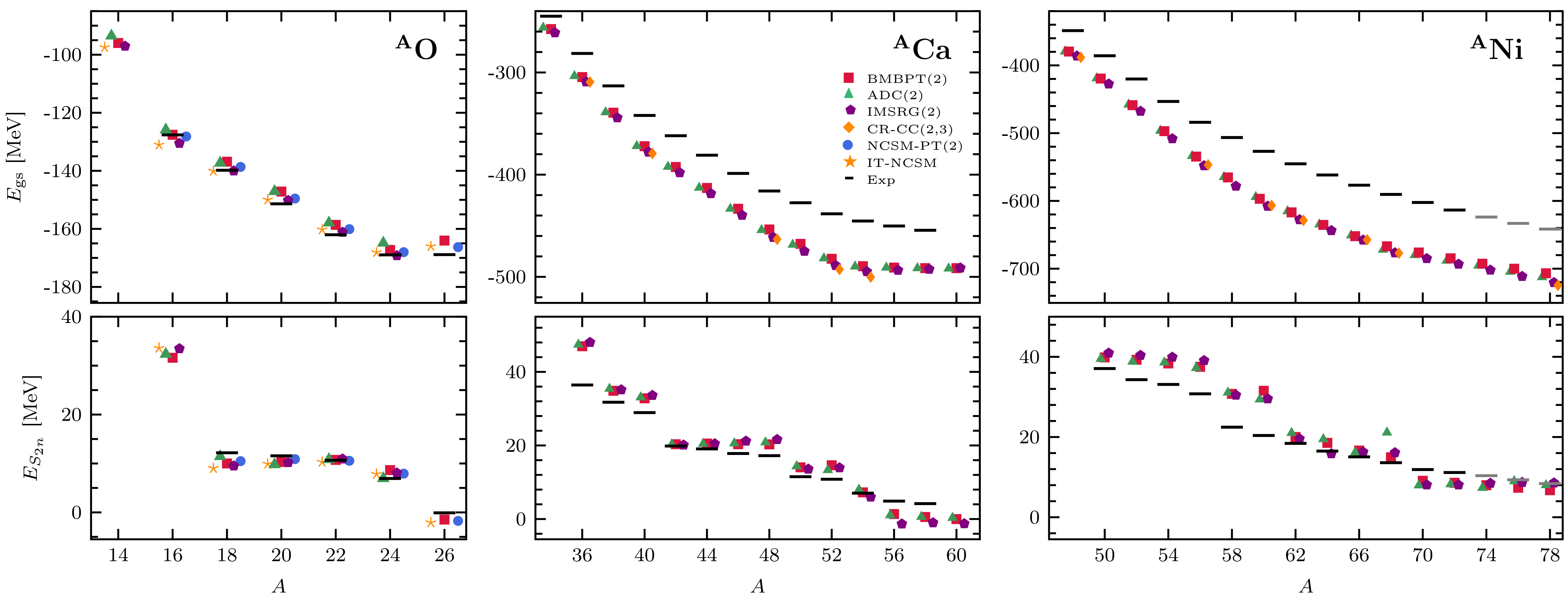
CC → SD (analogous to second RPA) on top of HF reference state

Bogolyubov many-body perturbation theory



- **MBPT generalised to open-shell nuclei**
  - As accurate as non-perturbative methods for soft H
  - Scaling is very favourable
  - Promising tool for diagnostic

[Tichai, Arthuis, *et al.* (in preparation)]



Conclusions

- **Many-body formalism well grounded**
  - Closed- & open-shell nuclei, g.s. observables & spectroscopy, …
  - Two-body propagators to be implemented to access spectroscopy of even-even systems

- **At present, interactions constitute main source of uncertainty**
  - ChEFT is undergoing intense development, facing fundamental & practical issues
  - *Pragmatic* strategy: interaction performs well over good range of nuclei & observables

- **Extension of ab initio simulations to heavy nuclei**
  - Mid-mass region of the nuclear chart being scrutinised
  - Computational challenges ahead: work in progress and more smart ideas needed