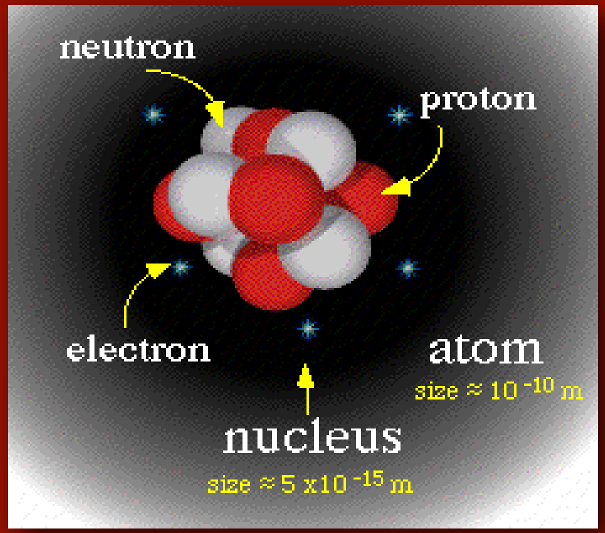
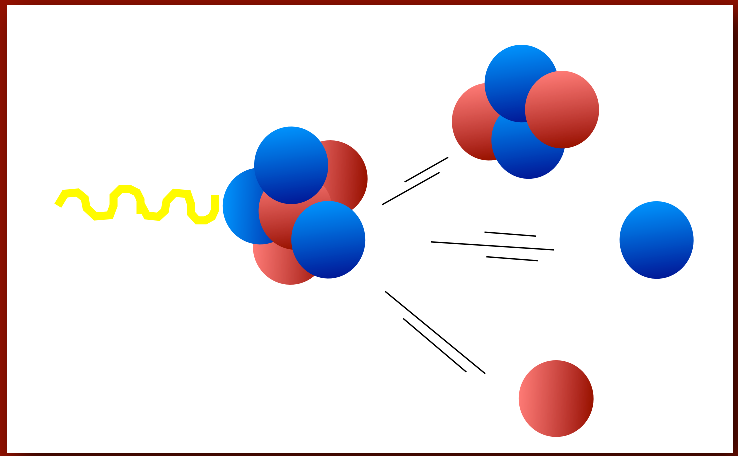
Ab initio computations of the electric dipole polarizability

Sonia Bacca | Theory Department | TRIUMF

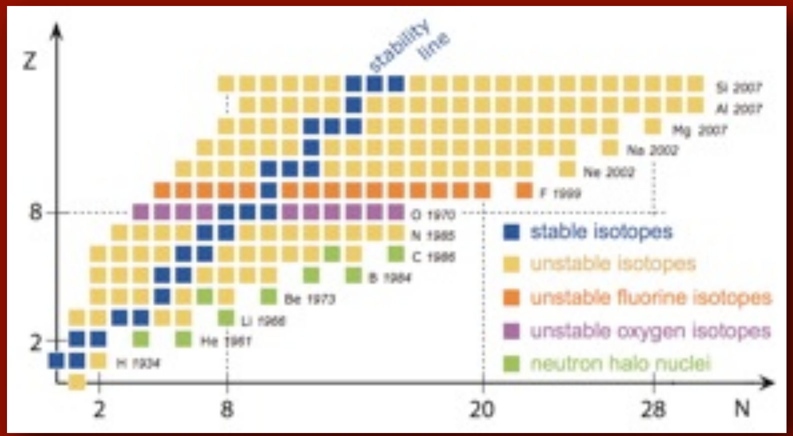
NSKIN2016 Workshop, Mainz, May 23 2016



The Atomic Nucleus



Electroweak Reactions



Nuclear Chart

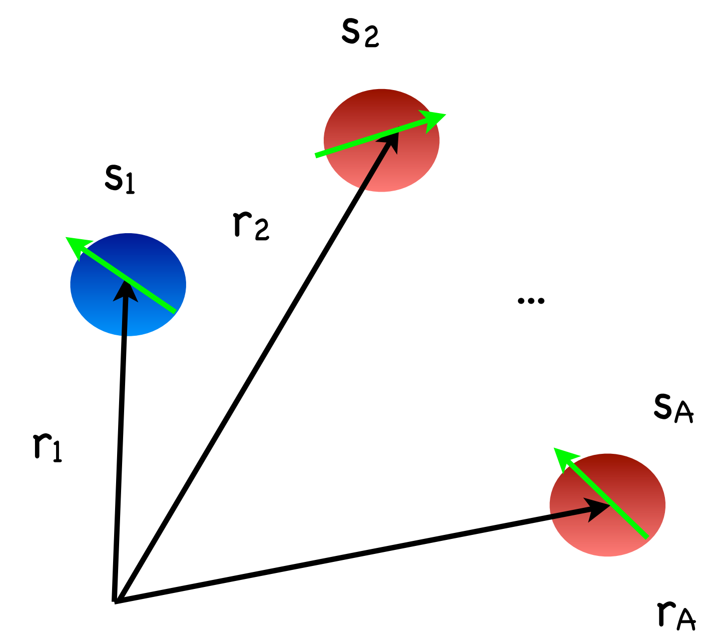
“Ab-initio” methods

- Start from neutrons and protons as building blocks (centre of mass coordinates, spins, isospins)

- Solve the non-relativistic quantum mechanical problem of A-interacting nucleons

$$H|\psi_i\rangle = E_i|\psi_i\rangle$$

$$H = T + V_{NN}(\Lambda) + V_{3N}(\Lambda) + \ldots$$

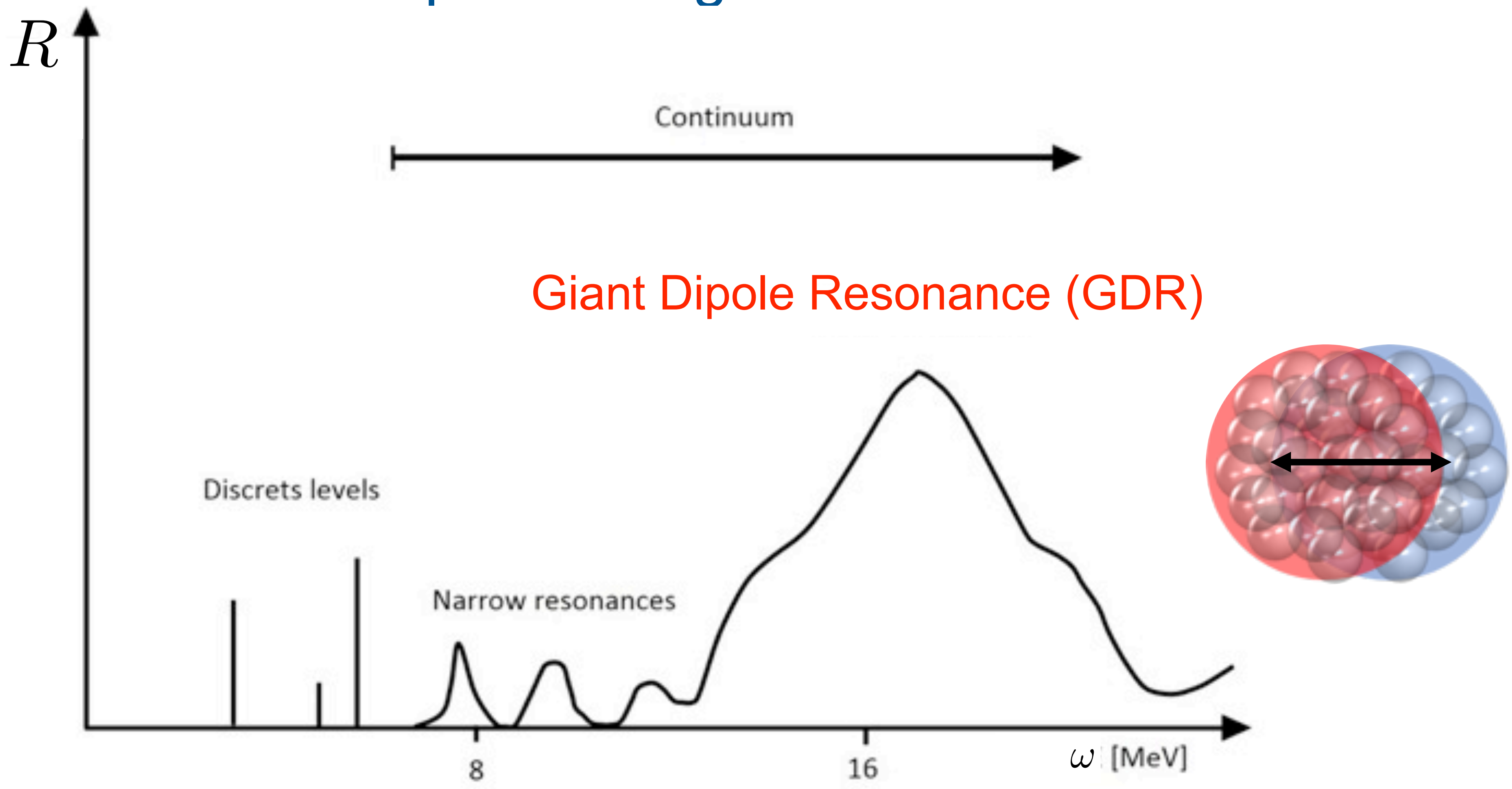


- Find numerical solutions with no approximations or controllable approximations (error bars)

- Calculate low-energy observables and compare with experiment to test nuclear forces and provide predictions for future experiments or quantity that cannot be measured

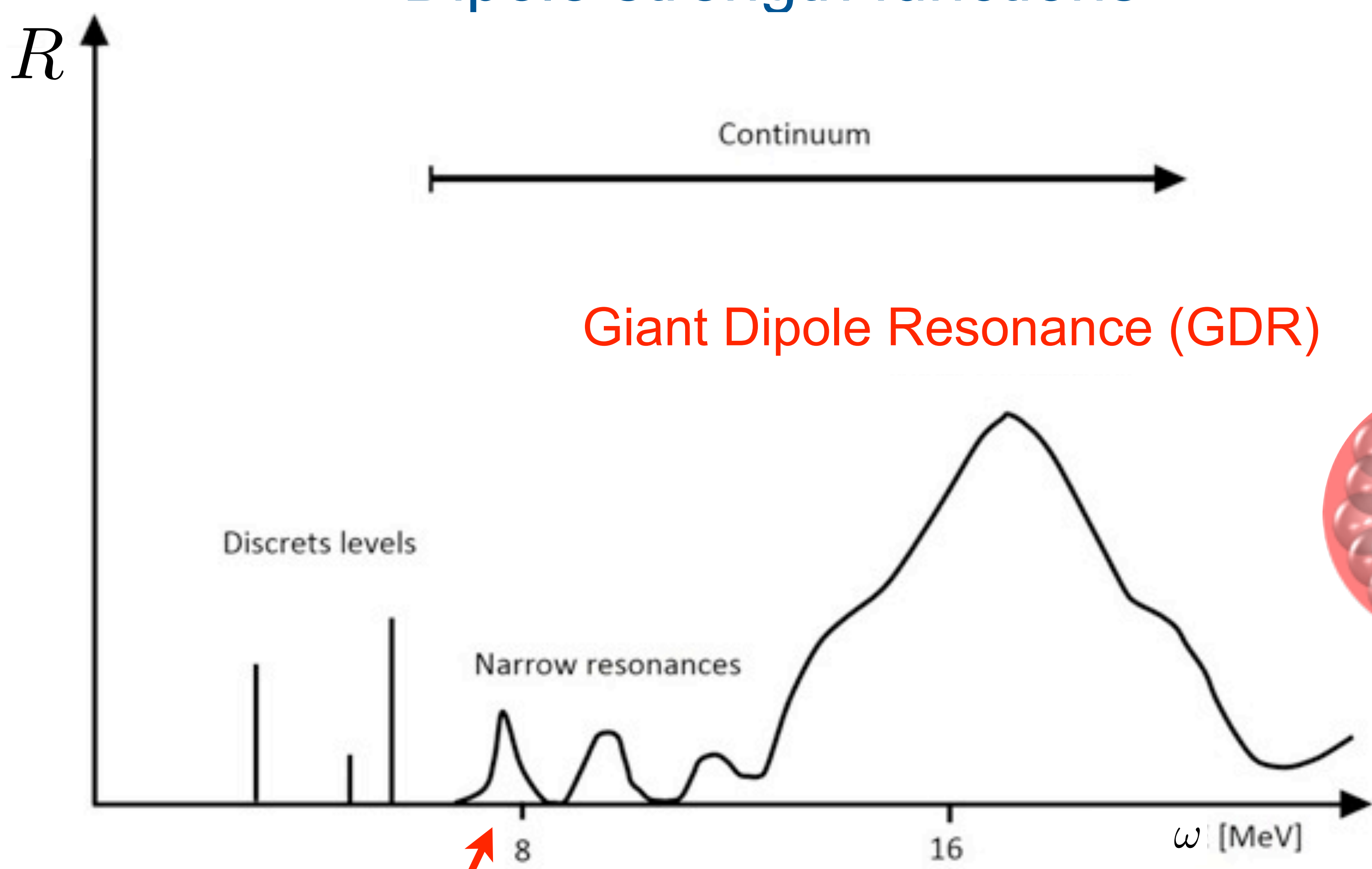
Observables

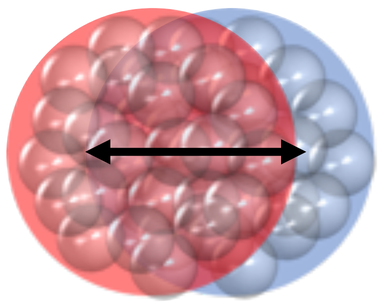
Dipole strength functions

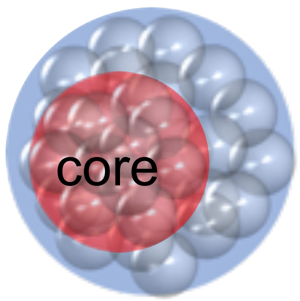


Observables

Dipole strength functions







Pigmy dipole resonance (PDR) in neutron-rich nuclei

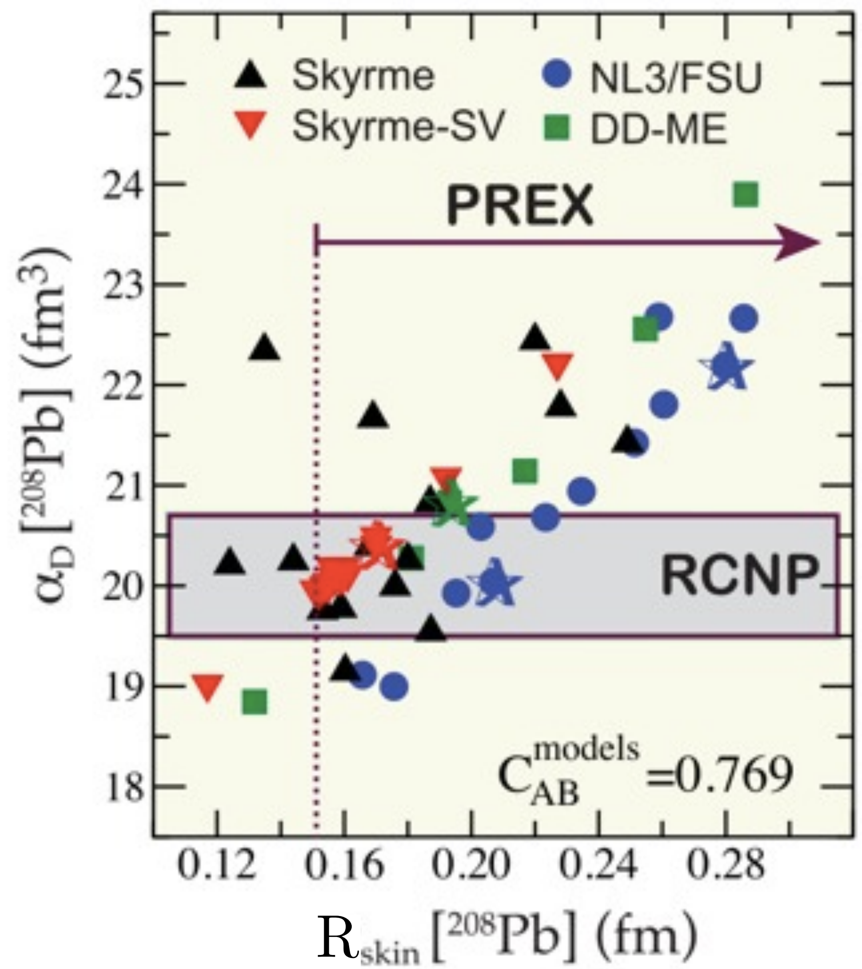
Electric dipole polarizability

$$\alpha_D = 2\alpha \int_{\omega_{ex}}^{\infty} d\omega \frac{R(\omega)}{\omega}$$ ⇨ PDR enhances the polarizability

Polarizability

Why is it important to NSKIN2016?

- It has been shown to correlate with neutron skin thickness in Density Functional Theory
- Learn about equation of state of asymmetric nuclear matter



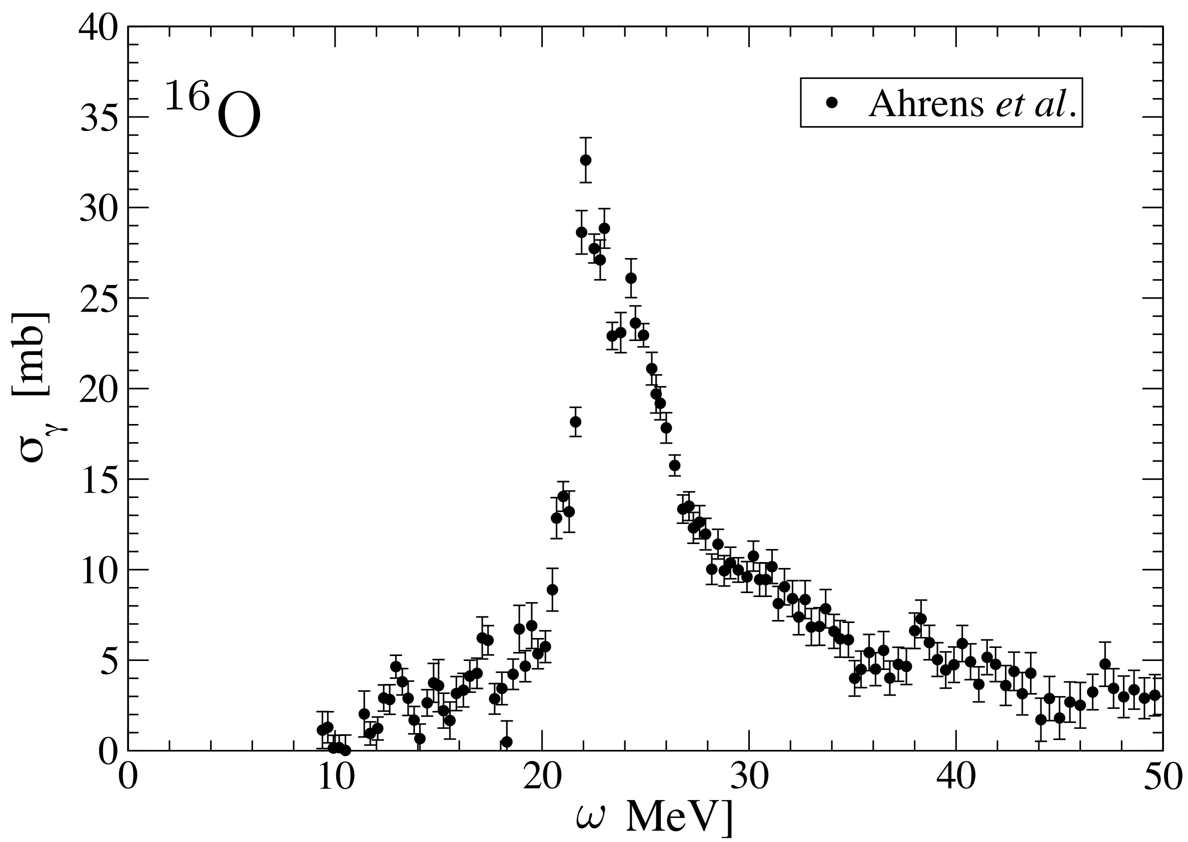
Phys. Rev. C **85**, 041302(R) (2012)

What can we tell from ab-initio calculations?

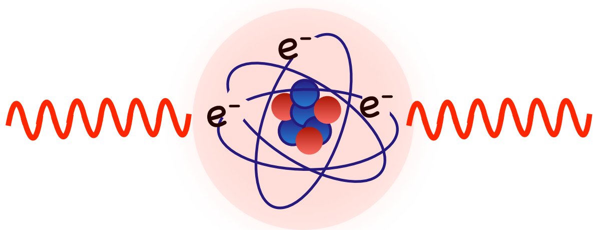
Experimental status

Stable Nuclei

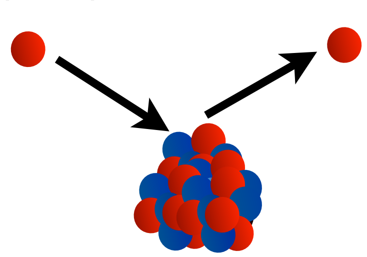
We have data on ~180 stable nuclei
Giant dipole resonances



From photoabsorption experiments

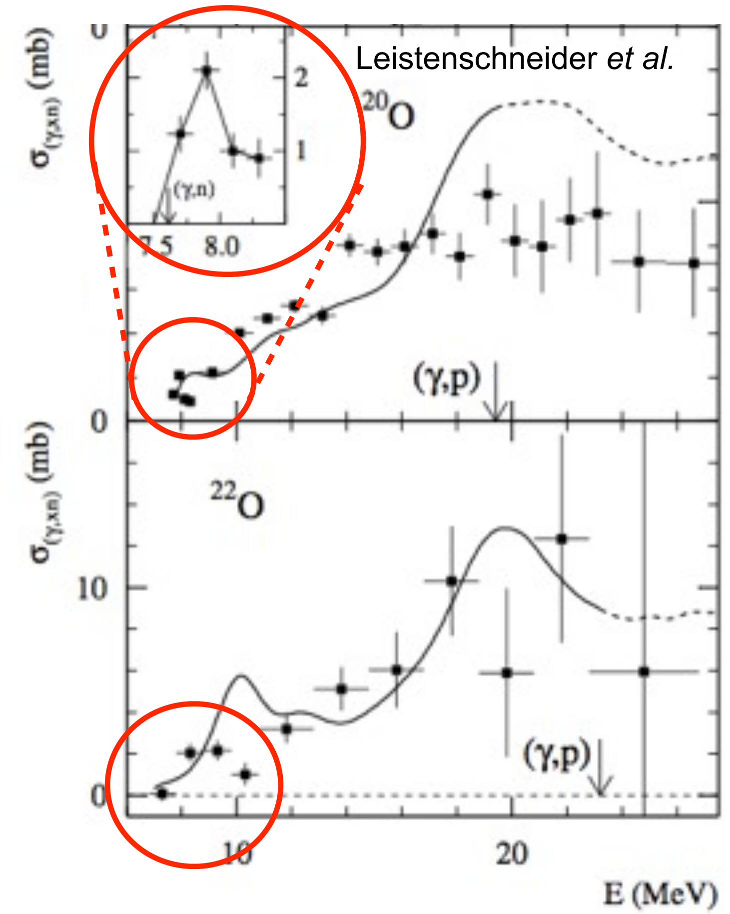


(p,p') experiments

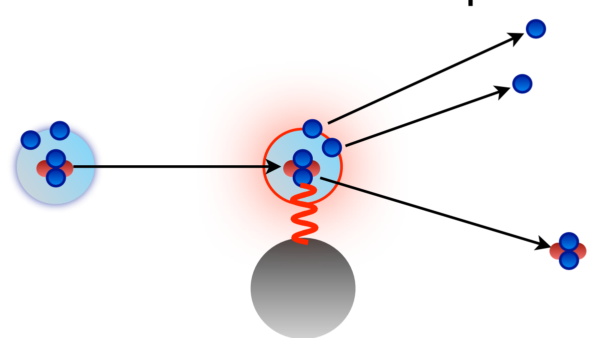


Unstable Nuclei

Fewer data, pigmy dipole resonances



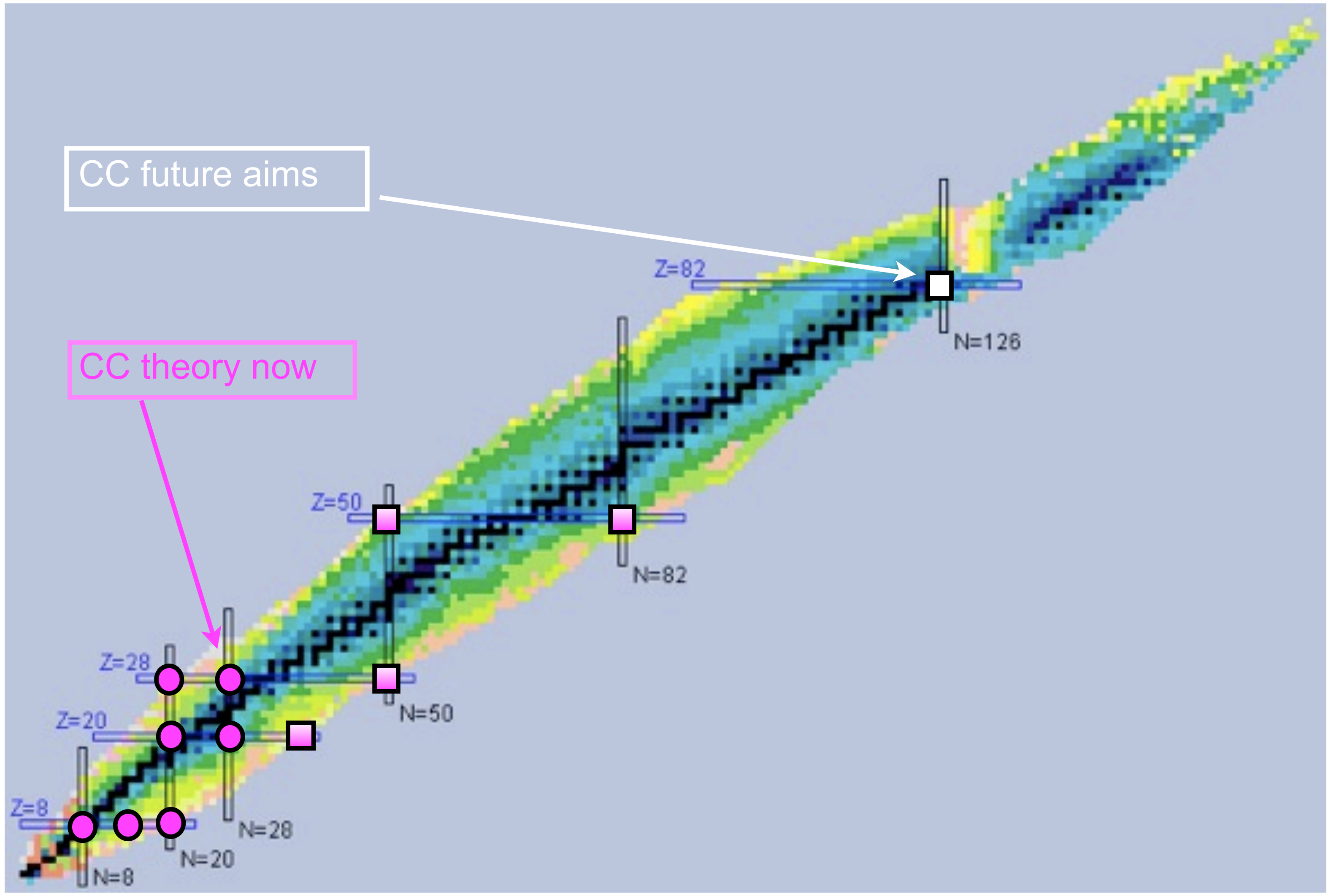
From Coulomb excitation experiments



Do we see the emergence of collective motions from first principle calculations?

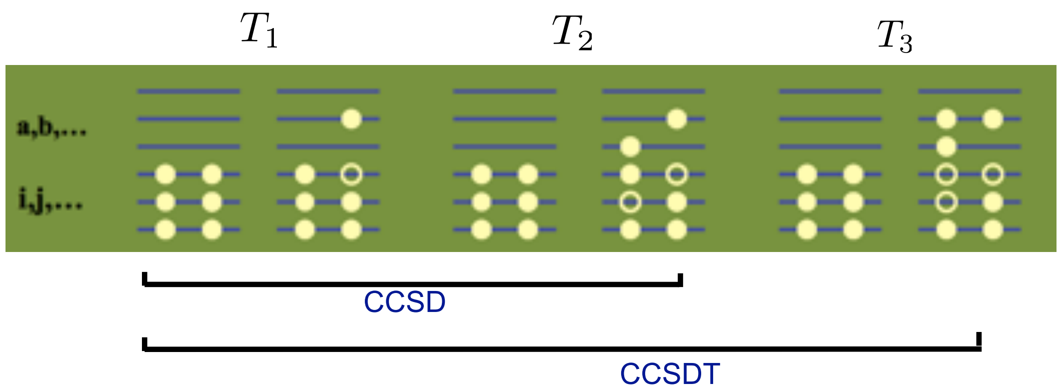
Coupled-cluster theory

Many-body method that can extend the frontiers of ab-initio calculations to heavier and neutron nuclei



$$|\psi_0(\vec{r}_1, \vec{r}_2, ..., \vec{r}_A)\rangle = e^T |\phi_0(\vec{r}_1, \vec{r}_2, ..., \vec{r}_A)\rangle$$

$$T = \sum T_{(A)}$$ cluster expansion

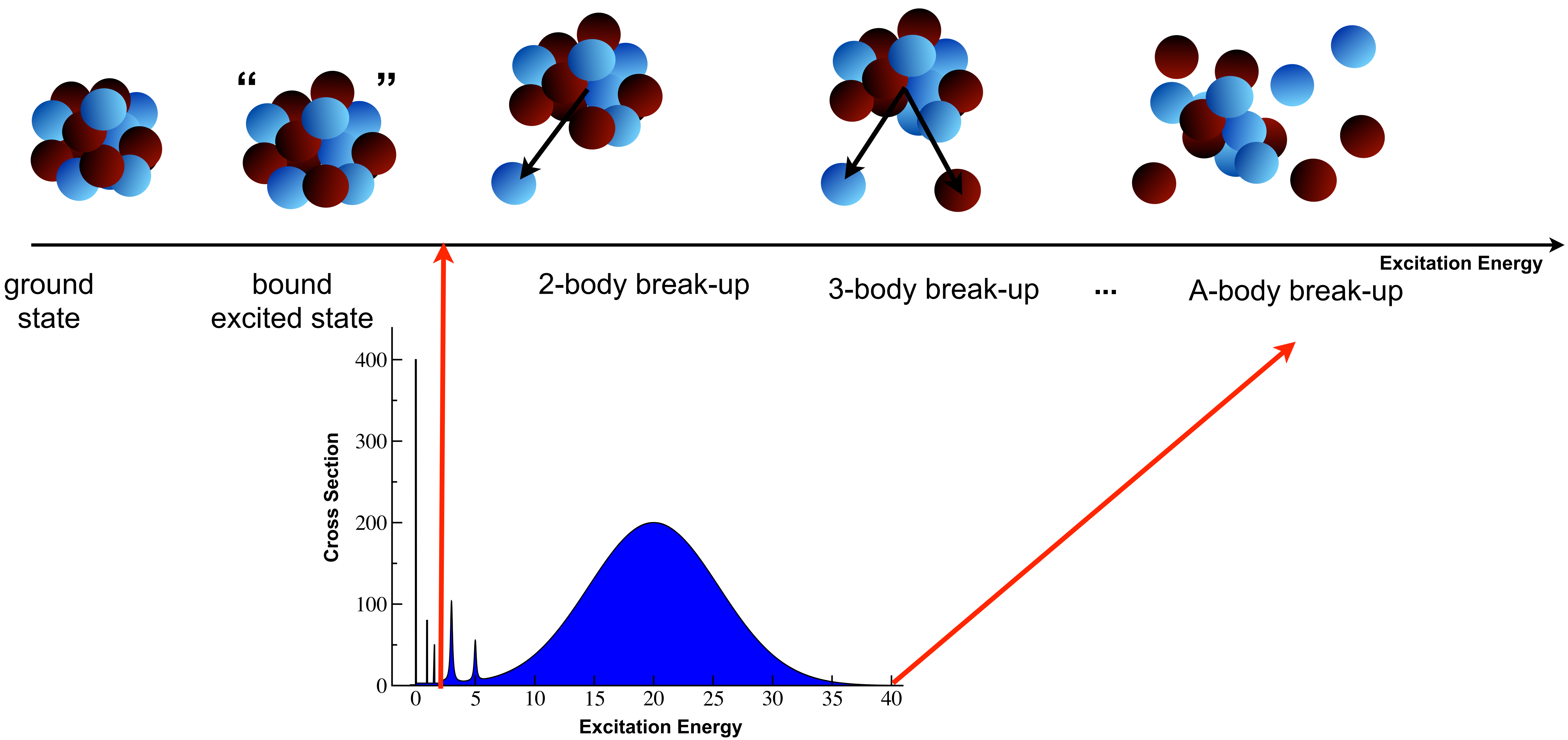


Work by ORNL group, TUD group. Mature theory for bound states, but what about break-up reactions?

The problem of the continuum

$$R(\omega) = \sum\!\!\!\!\!\!\!\int_f \left| \left\langle \psi_f \middle| \Theta \middle| \psi_0 \right\rangle \right|^2 \delta(E_f - E_0 - \omega)$$

Depending on ω, many channels may be involved

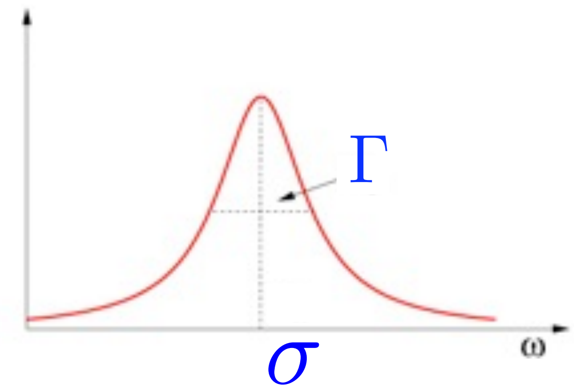


Lorentz Integral Transform

Efros *et al.*, Nucl.Part.Phys. **34** (2007) R459

Response in the continuum

$$R(\omega) = \sum_f \left| \left\langle \psi_f \middle| \Theta \middle| \psi_0 \right\rangle \right|^2 \delta(E_f - E_0 - \omega)$$



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

$$(H - E_0 - \sigma + i\Gamma) \, | \, \tilde{\psi} \rangle = \Theta \, | \, \psi_0 \rangle$$

- Due to imaginary part Γ the solution $|\tilde{\psi}\rangle$ is unique
- Since the r.h.s. is finite, then $|\tilde{\psi}\rangle$ has bound state asymptotic behaviour

You can use any good bound state method! e.g. Hyperspherical Harmonics,
No Core Shell Model,
Coupled Cluster Theory

$$L(\sigma, \Gamma) \xrightarrow{\text{inversion}} R(\omega)$$ with all channels and final state interaction

LIT with Coupled Cluster Theory

Reduce the continuum problem to a bound-state problem

$$L(\sigma,\Gamma) = \int d\omega \frac{R(\omega)}{(\omega-\sigma)^2+\Gamma^2} = \left\langle \tilde{\psi} | \tilde{\psi} \right\rangle < \infty$$

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

Merging the Lorentz integral transform method with coupled-cluster theory :
New many-body method to extend *ab initio* calculations of em reactions to medium-mass-nuclei

S.B. *et al.*, Phys. Rev. Lett. **111**, 122502 (2013)

$$(\bar{H} - E_0 - \sigma + i\Gamma)|\tilde{\Psi}_R\rangle = \bar{\Theta}|\Phi_0\rangle$$

$$\bar{H} = e^{-T} H e^{T}$$

$$\bar{\Theta} = e^{-T} \Theta e^{T}$$

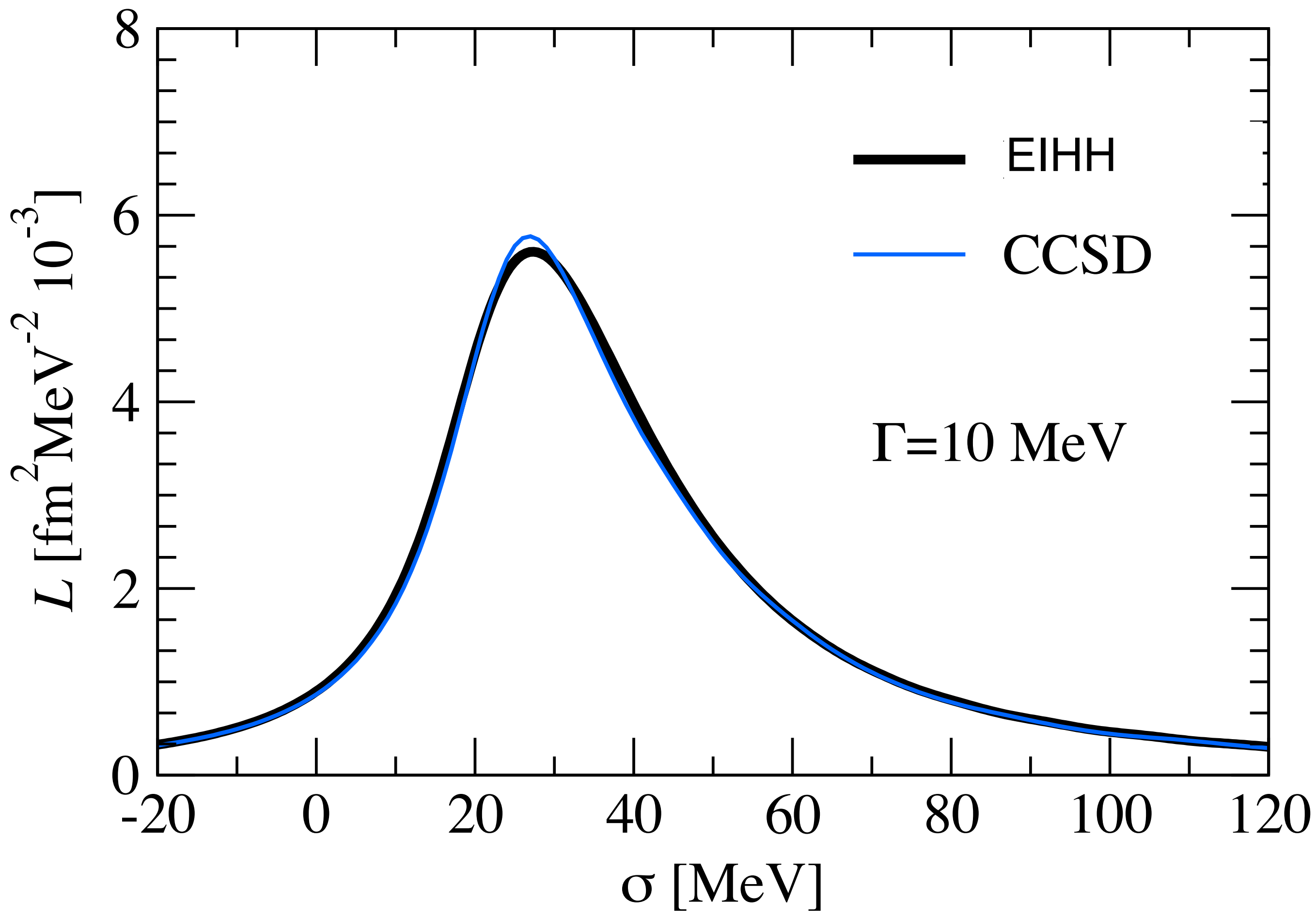
$$|\tilde{\Psi}_R\rangle = \hat{R}|\Phi_0\rangle$$

Presently implemented at CCSD level

LIT with Coupled Cluster Theory

Validation for ^{4}He

Comparison of CCSD with exact hyperspherical harmonics (EIHH) with NN forces at N^{3}LO

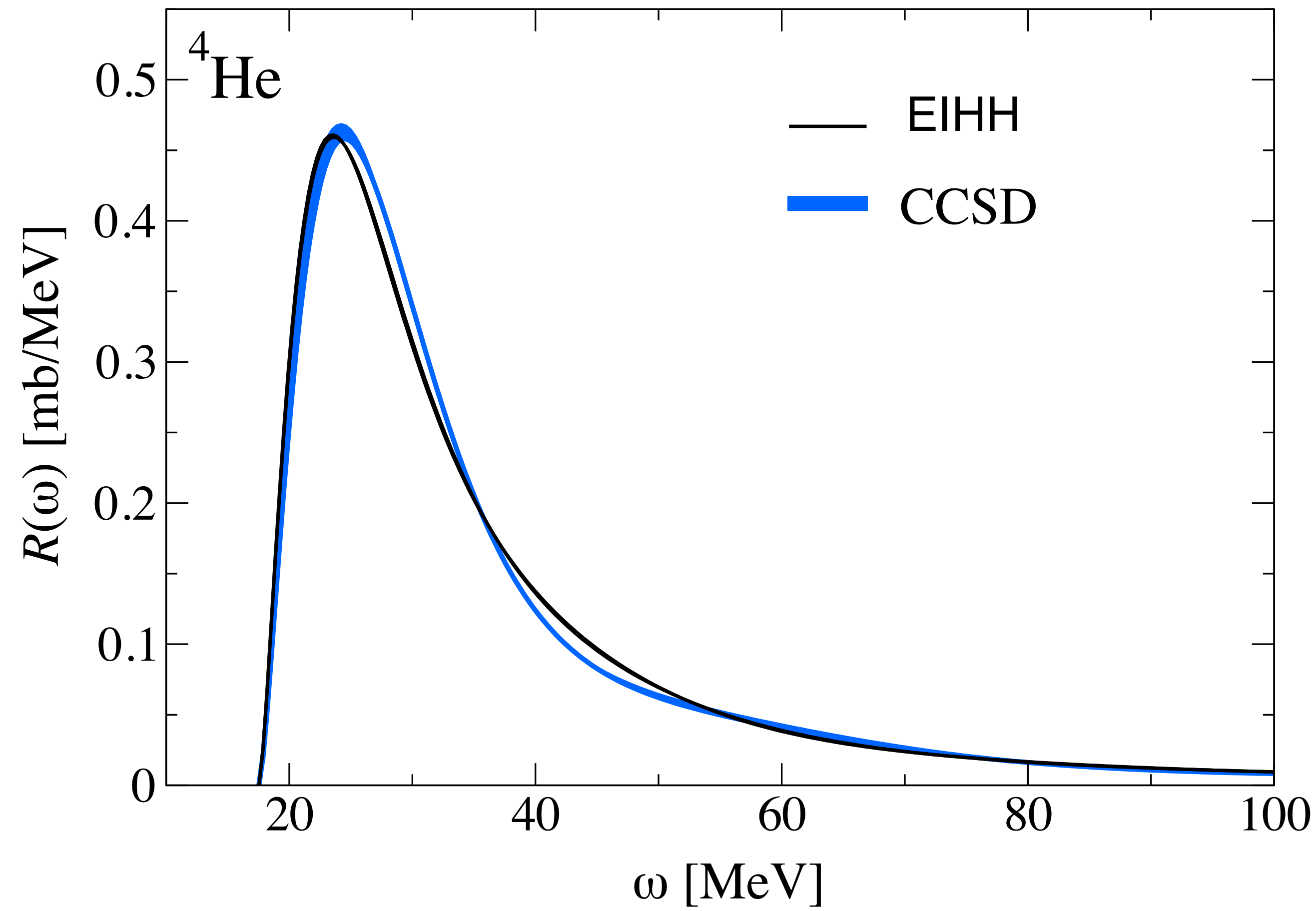


Inversion of the LIT

Ansatz

$$R(\omega) = \sum_i^{I_{\max}} c_i \chi_i(\omega, \alpha) \Rightarrow L(\sigma, \Gamma) = \sum_i^{I_{\max}} c_i \mathcal{L}[\chi_i(\omega, \alpha)]$$

Least square fit of the coefficients c_i to reconstruct the response function



The comparison with exact theory is very good!

Polarizability with Coupled Cluster Theory

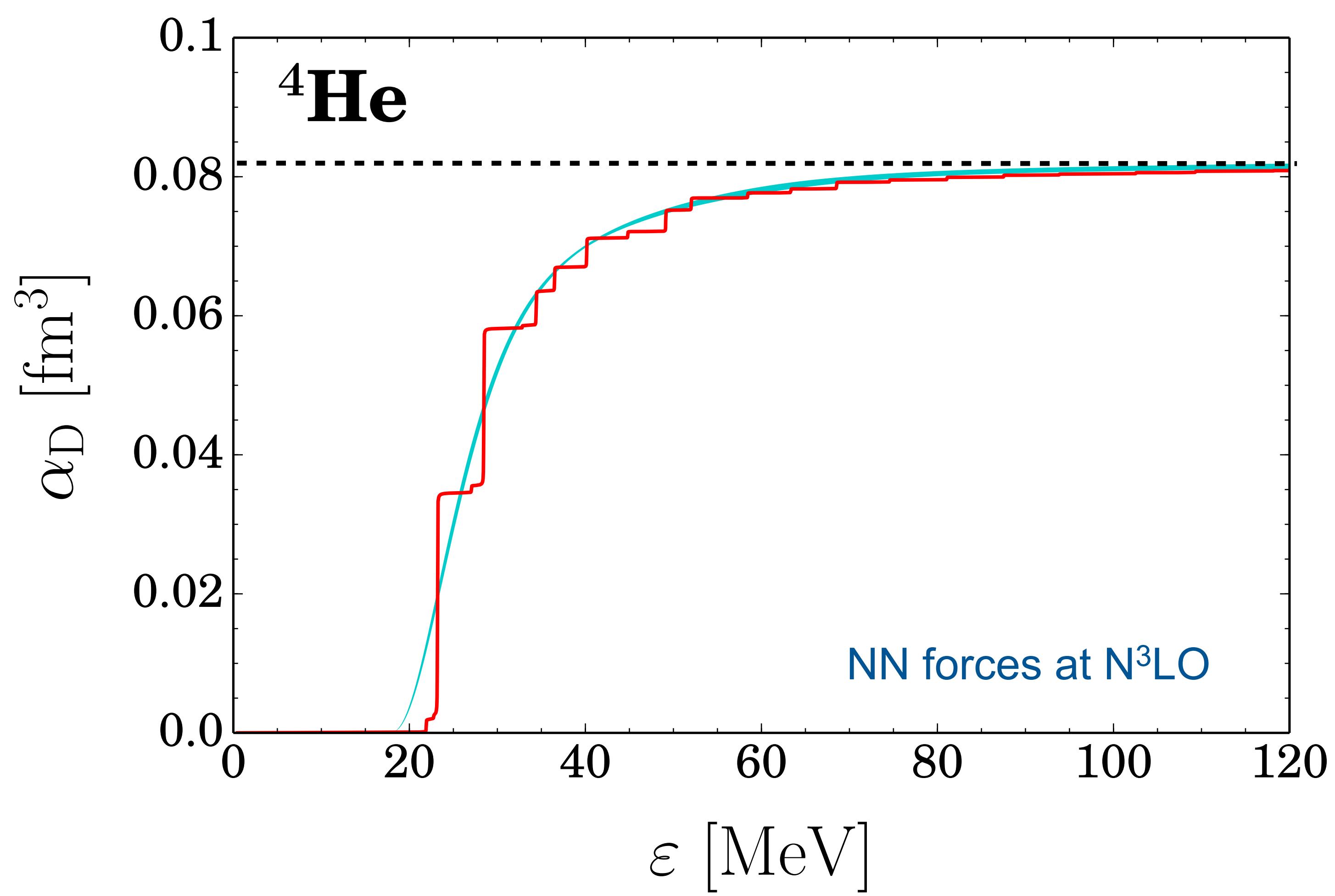
- If one can invert the LIT, one can integrate the response function $\alpha_D = 2\alpha \int_{\omega_{th}}^{\varepsilon} d\omega \frac{R(\omega)}{\omega}$

- To stably invert the LIT, one needs a very accurate calculation. Alternatively one can exploit the properties of the kernel

$$L(\sigma,\Gamma) = \int d\omega \frac{R(\omega)}{(\omega - \sigma)^2 + \Gamma^2}$$

$$L(\sigma,\Gamma \to 0) = \int d\omega R(\omega)\delta(\omega - \sigma) = R(\sigma)$$

$$\alpha_D = 2\alpha \int_0^{\varepsilon} d\sigma \frac{L(\sigma,\Gamma \to 0)}{\sigma}$$

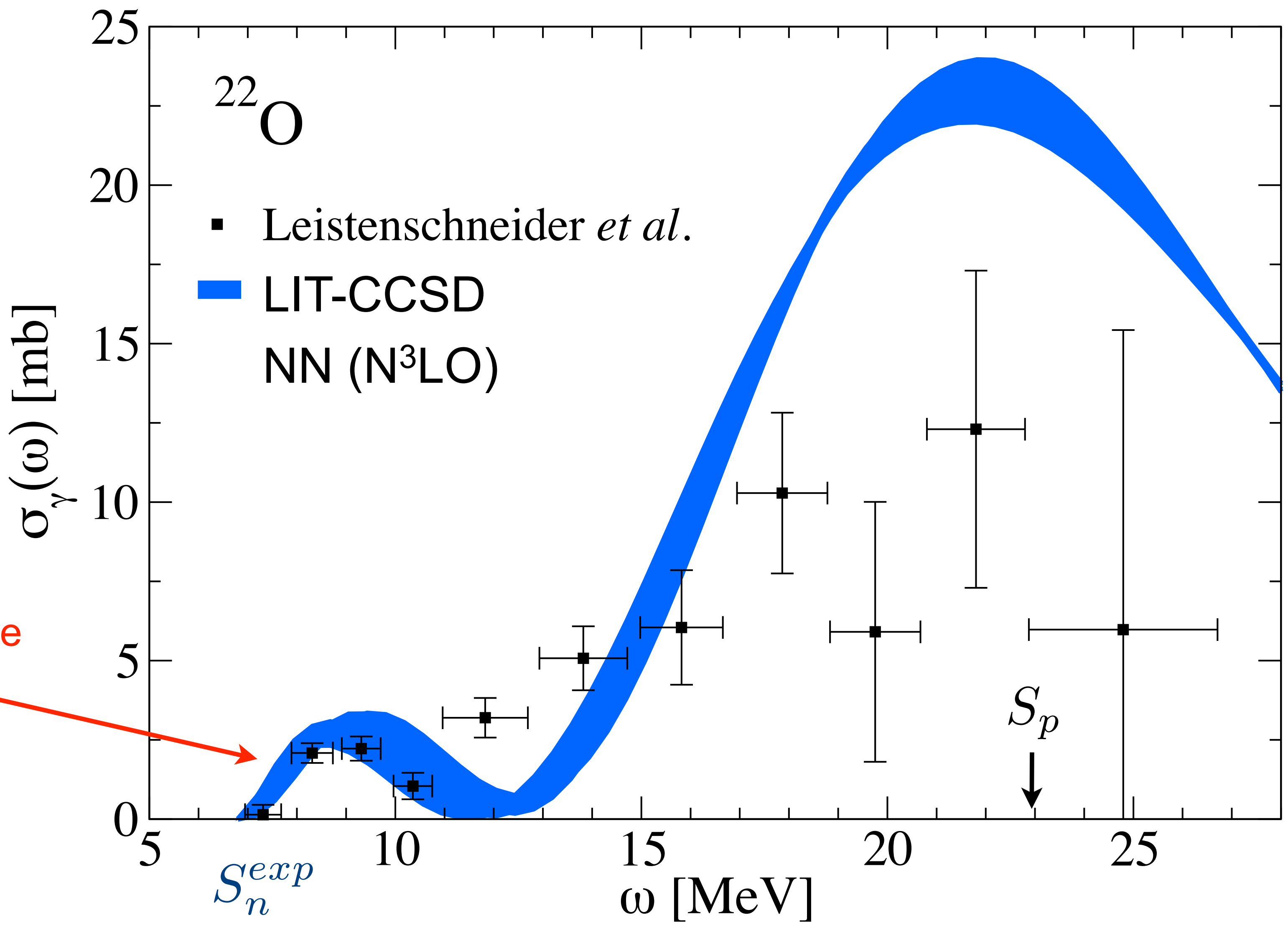


Results

With Mirko Miorelli, PhD student at UBC

Addressing neutron-rich nuclei

PRC **90**, 064619 (2014)

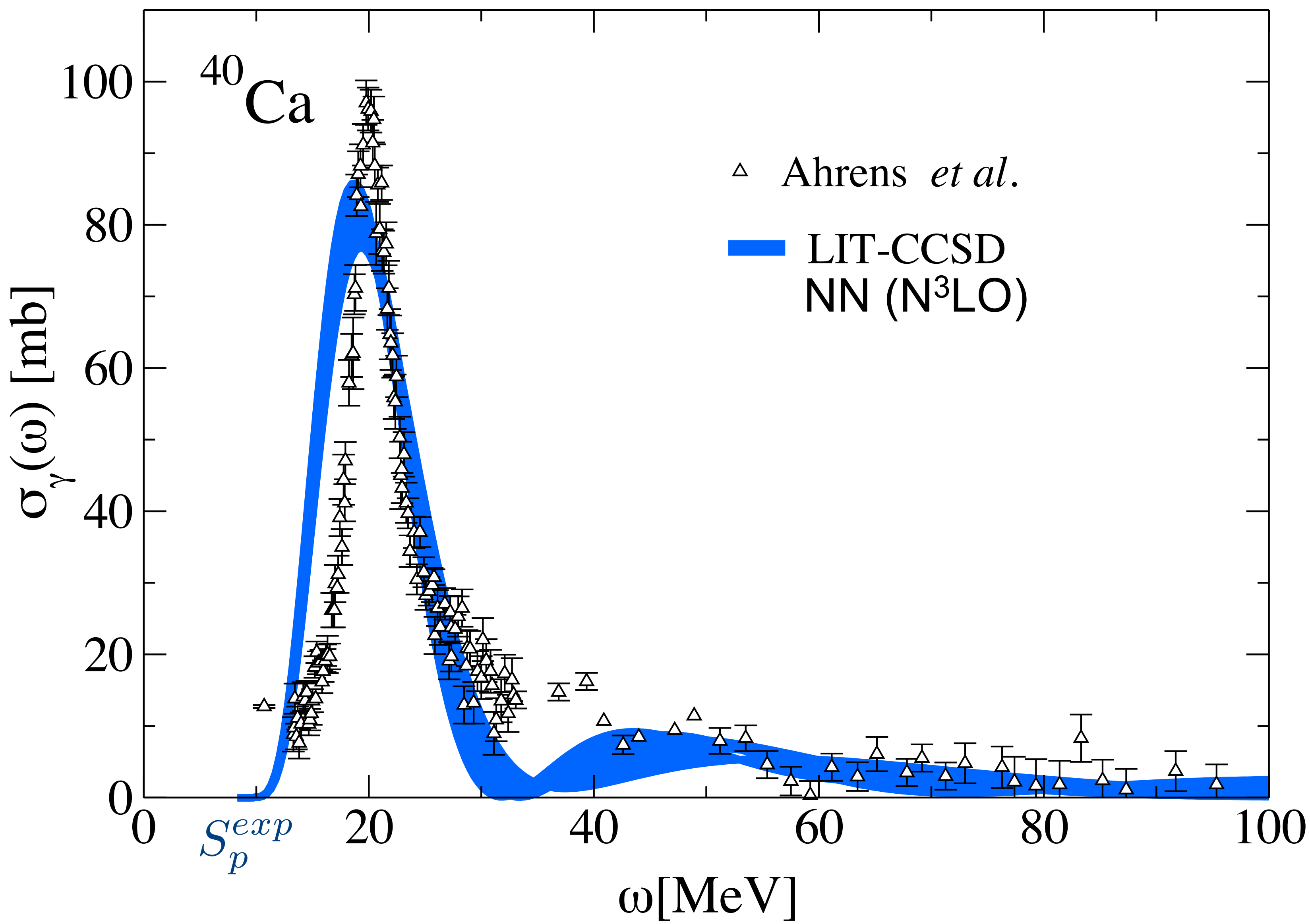


Soft Dipole Mode

Ab-initio theory describes the soft dipole mode

Extension to heavier nuclei

PRC **90**, 064619 (2014)

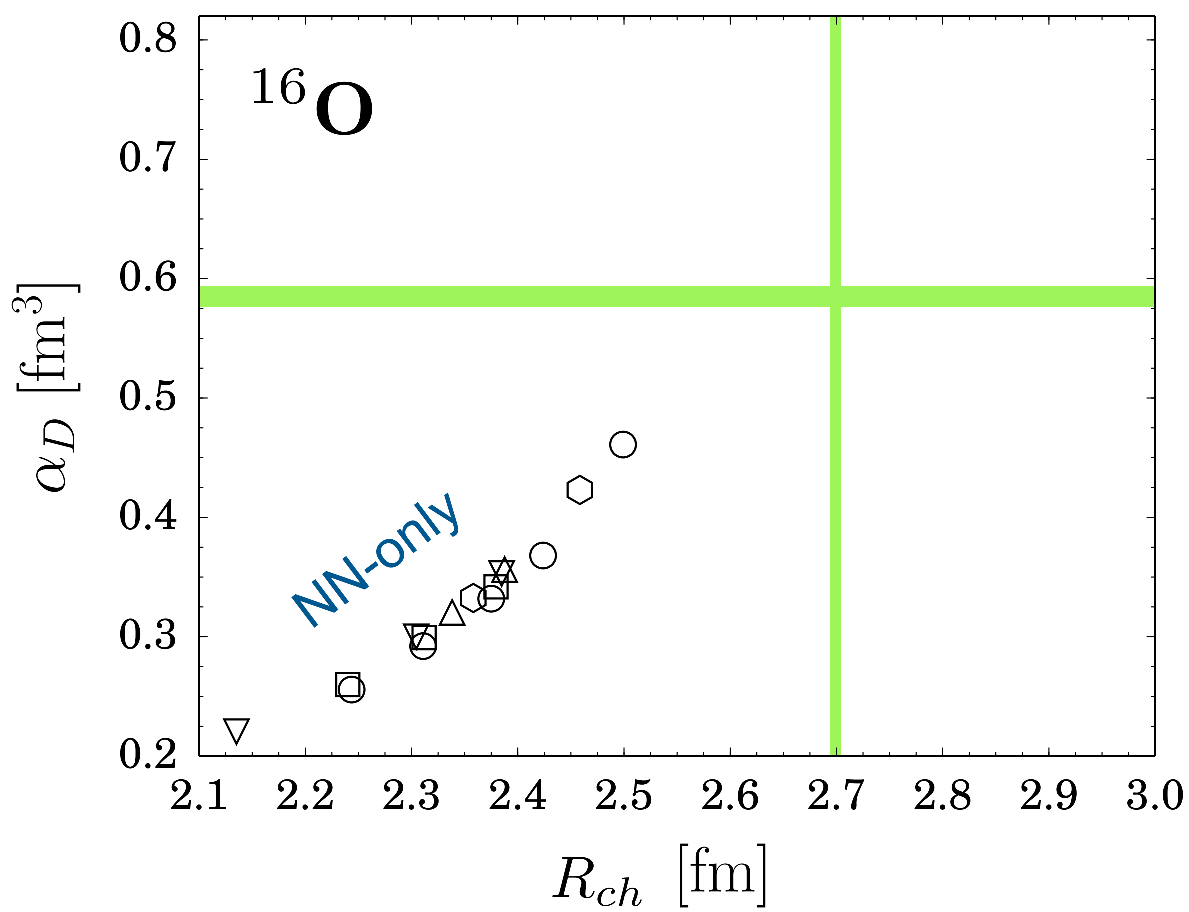


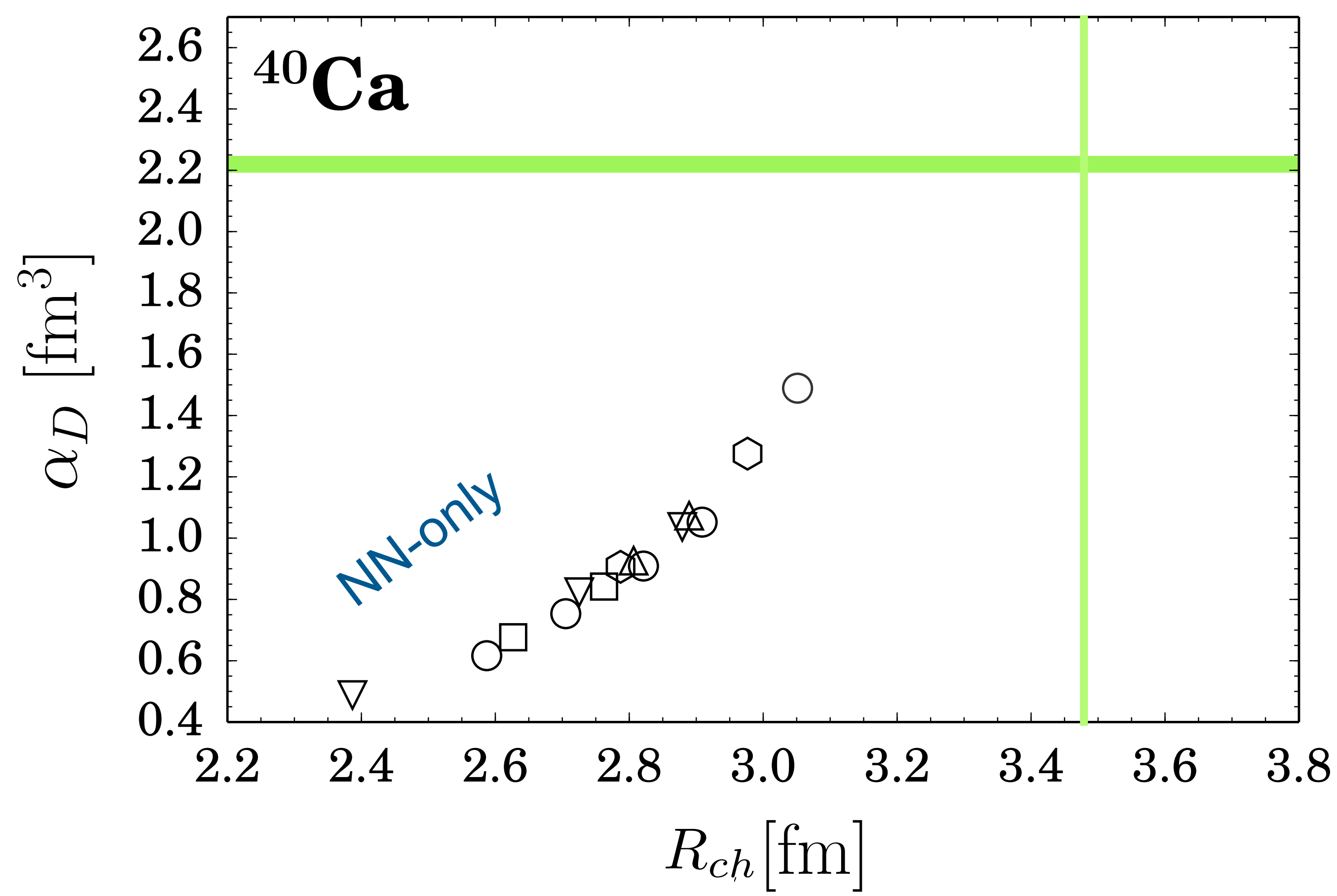
➡ The GDR is observed in ab-initio calculations

Study of Correlations

Medium-mass nuclei with NN interactions

arXiv:1604.05381



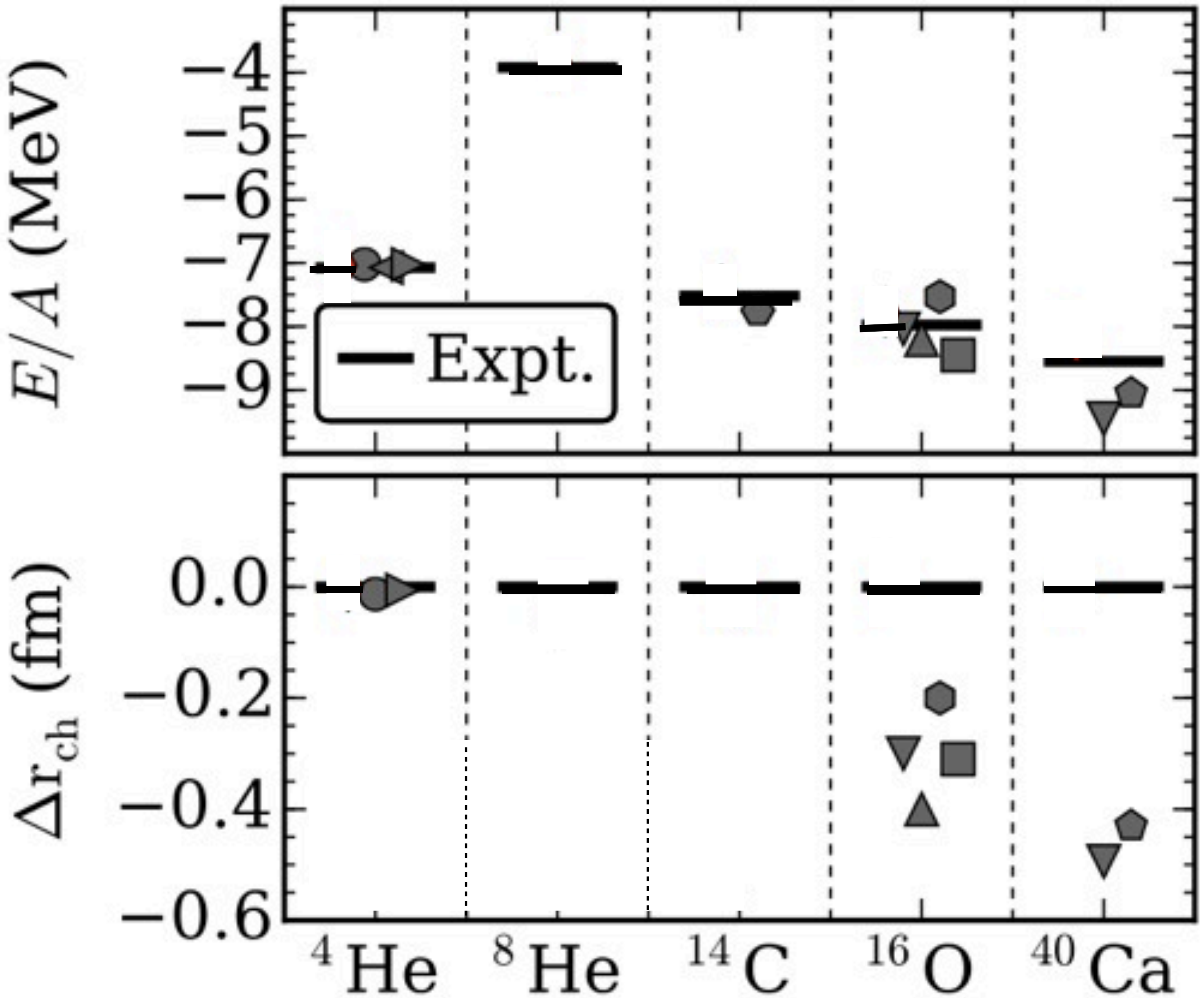


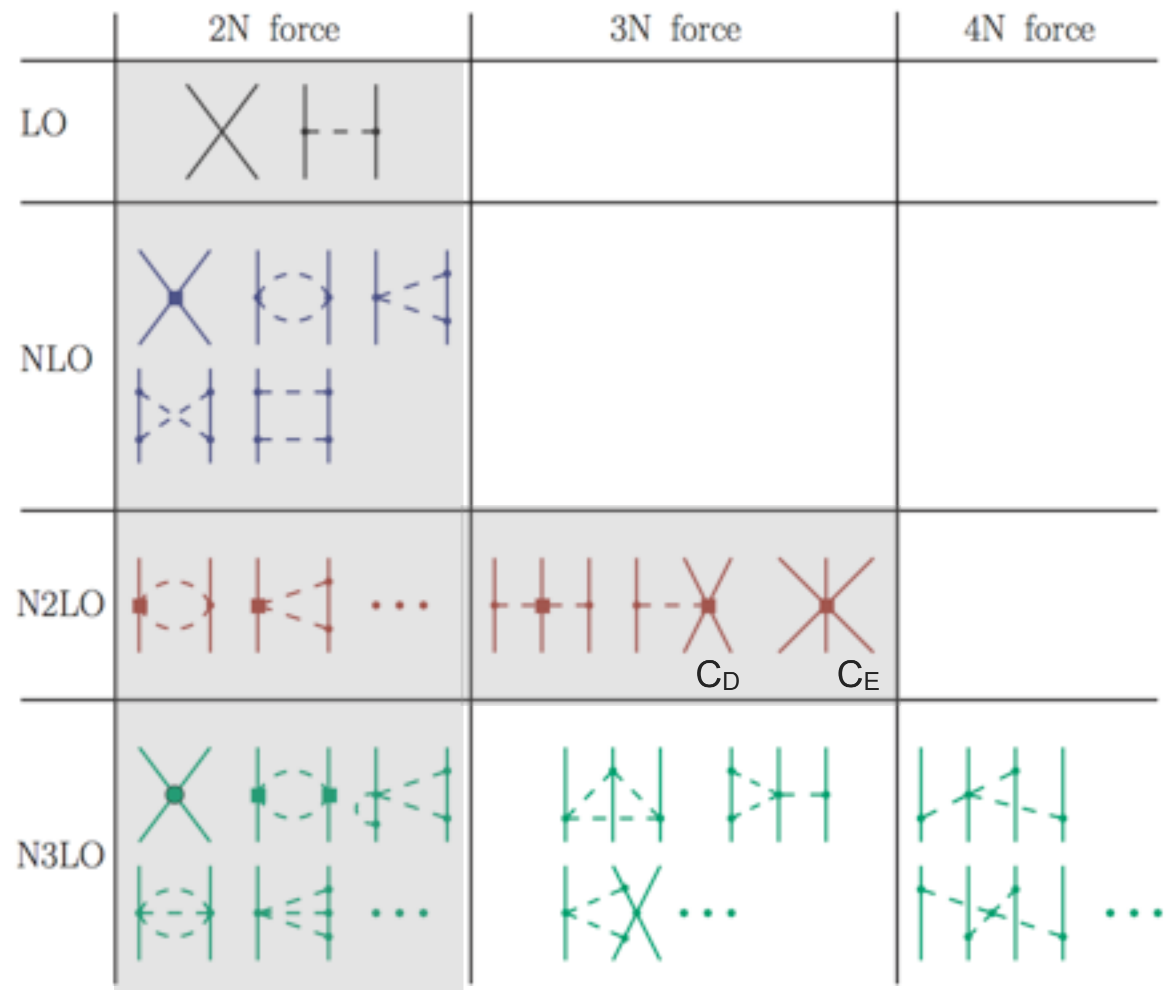
Strong correlations of polarizability with charge radii

Underestimating both radii and polarizability

Including three-nucleon forces

We need accurate interactions able to reproduce both energies and radii





Tuesday, 24 May, 16

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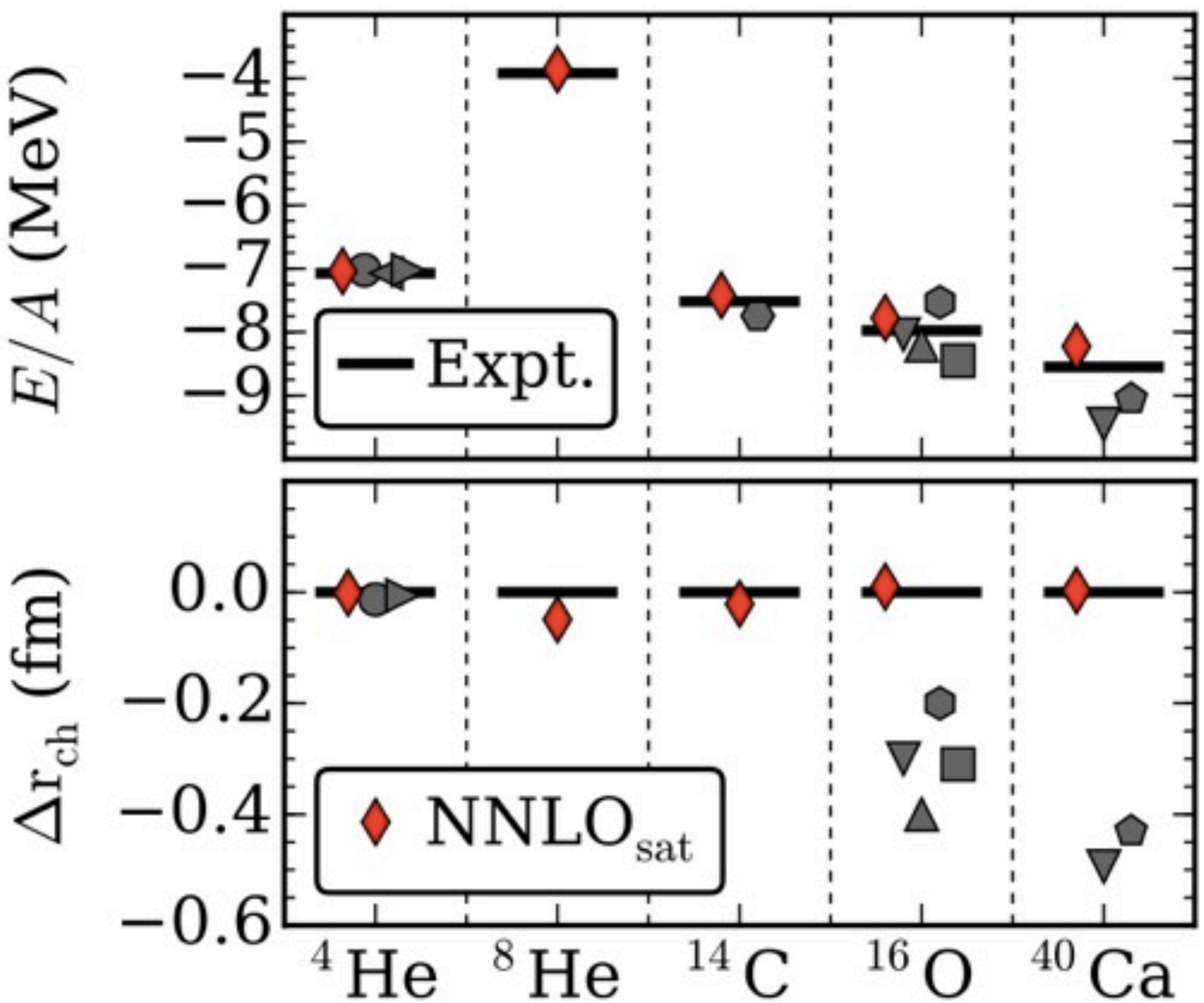
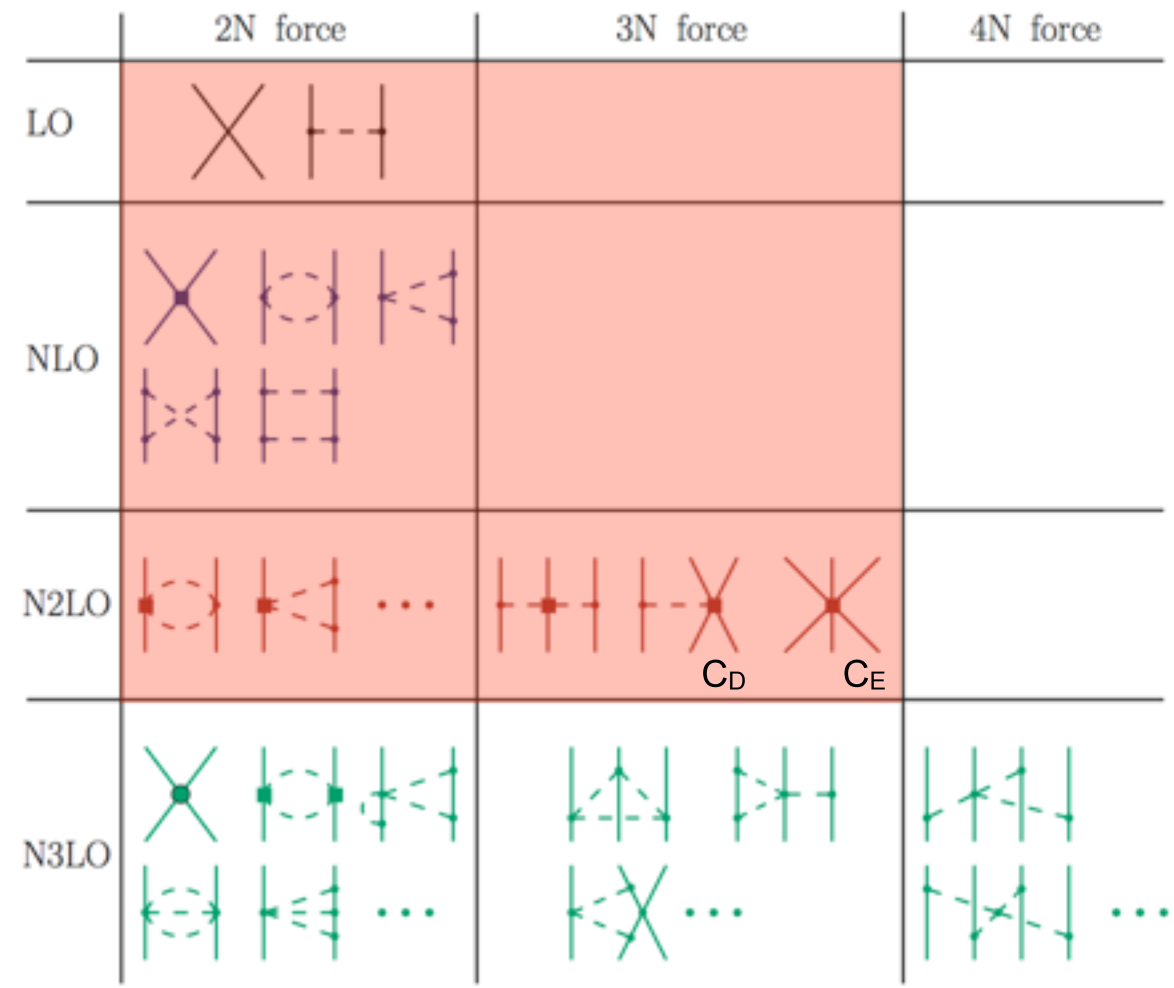




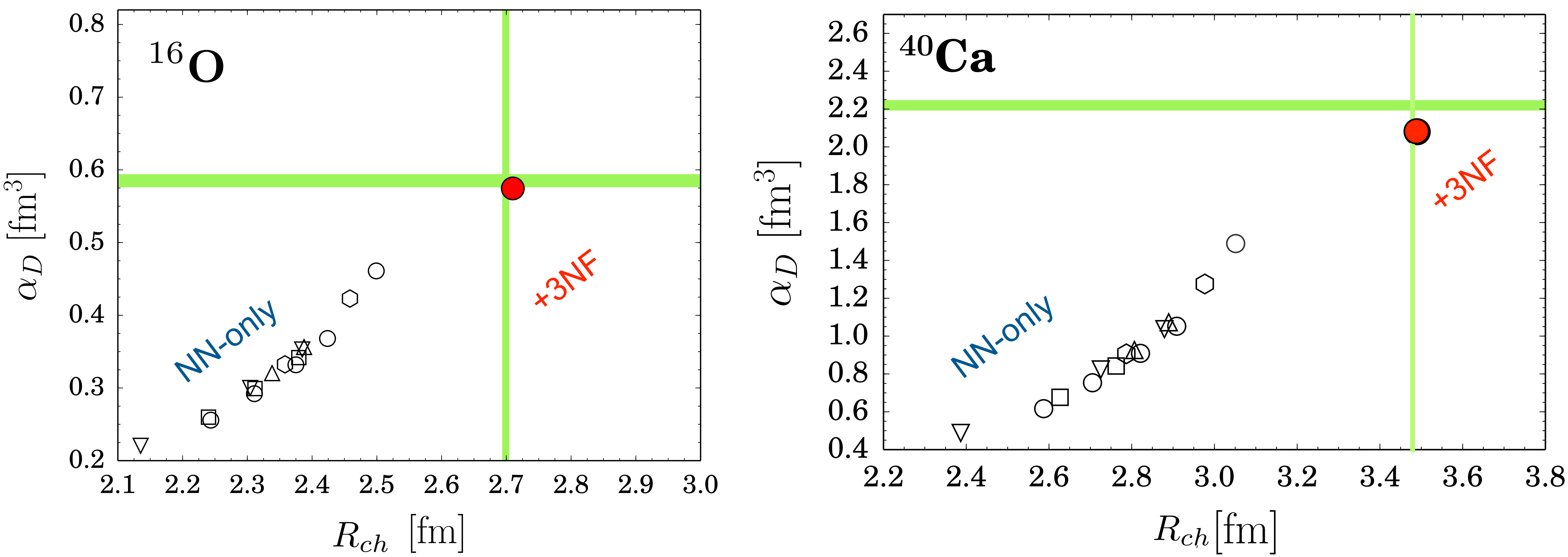
Include radii in the fit of LEC for the three-body force

New Paradigm: **NNLO$_{sat}$**: Fit of all LEC at N^{2}LO on NN data and nuclear radii Phys. Rev. C **91**, 051301(R) (2015)

Study of Correlations

Medium-mass nuclei with NN + 3NF interactions

arXiv:1604.05381

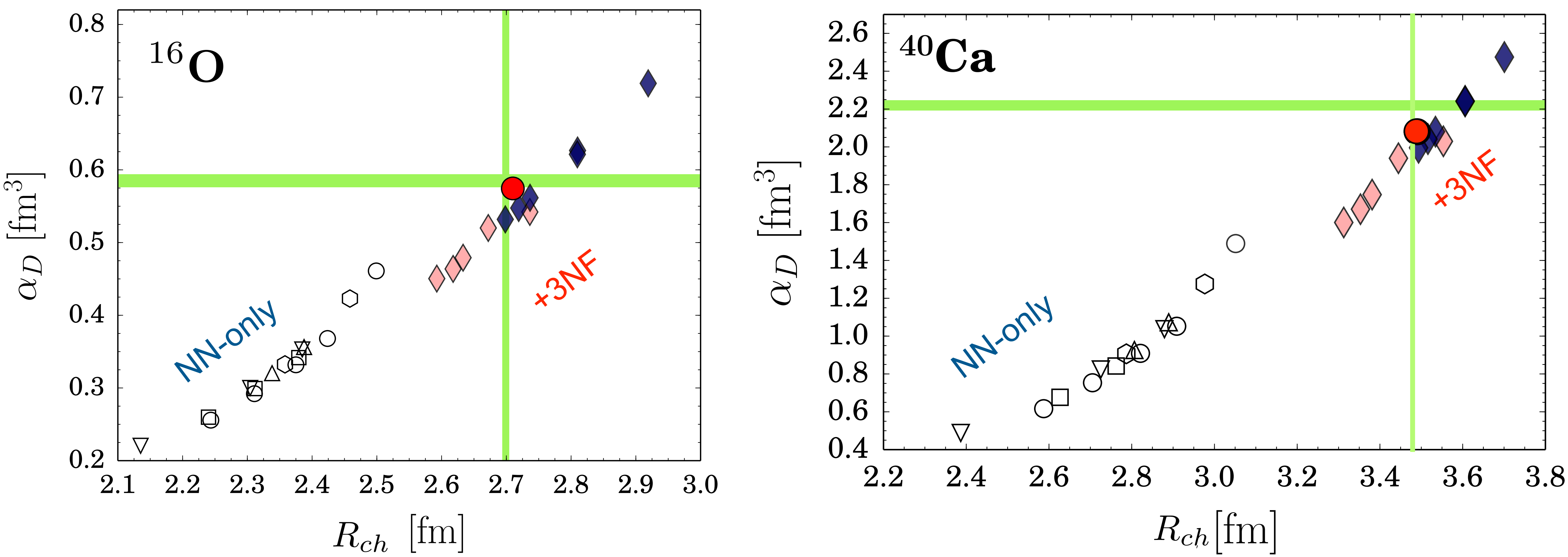


● A. Ekström *et al.*, Phys. Rev. C91, 051301 (2015) N2LOsat

Study of Correlations

Medium-mass nuclei with NN + 3NF interactions

arXiv:1604.05381



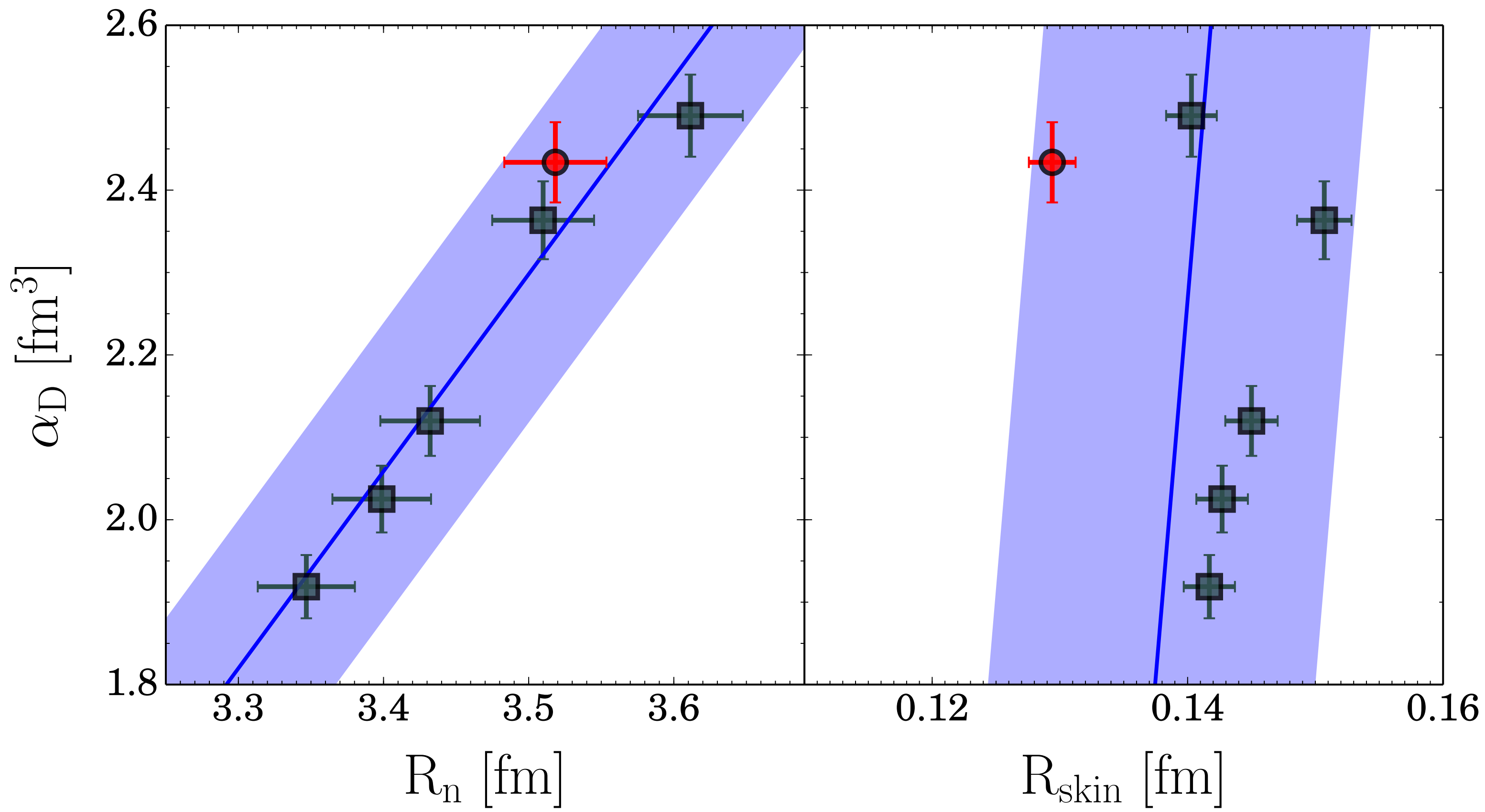
- A. Ekström *et al.*, Phys. Rev. C91, 051301 (2015) N2LOsat
- K. Hebeler *et al.*, Phys. Rev. C83, 031301 (2011)
- B. Carlson *et al.*, Phys. Rev. X 6, 011019 (2016)

Much better agreement with experimental data
Variation of Hamiltonian can be used to assess the theoretical error bar

TRIUMF

Results for ^{48}Ca

Nature Physics **12**, 186-190 (2016)

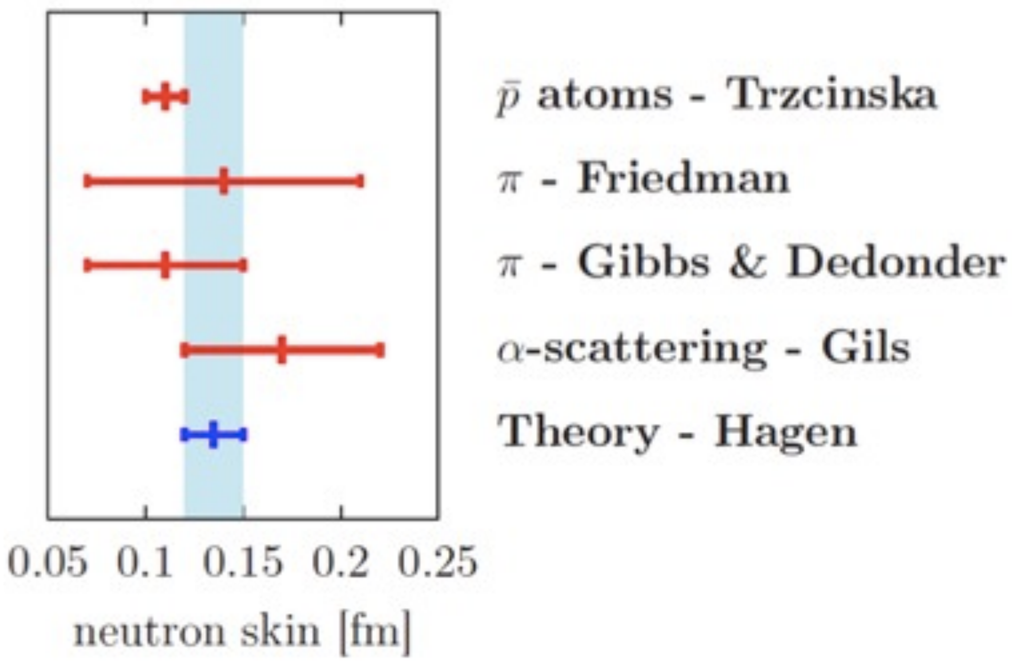


$NNLO_{sat}$

Soft NN(N^{3}LO)+3N(N^{2}LO) Hebeler *et al.*

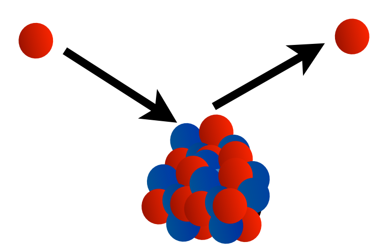
R_{skin} much smaller than predictions from DFT, but consistent with data

R_{skin} will be measured at JLab by CREX



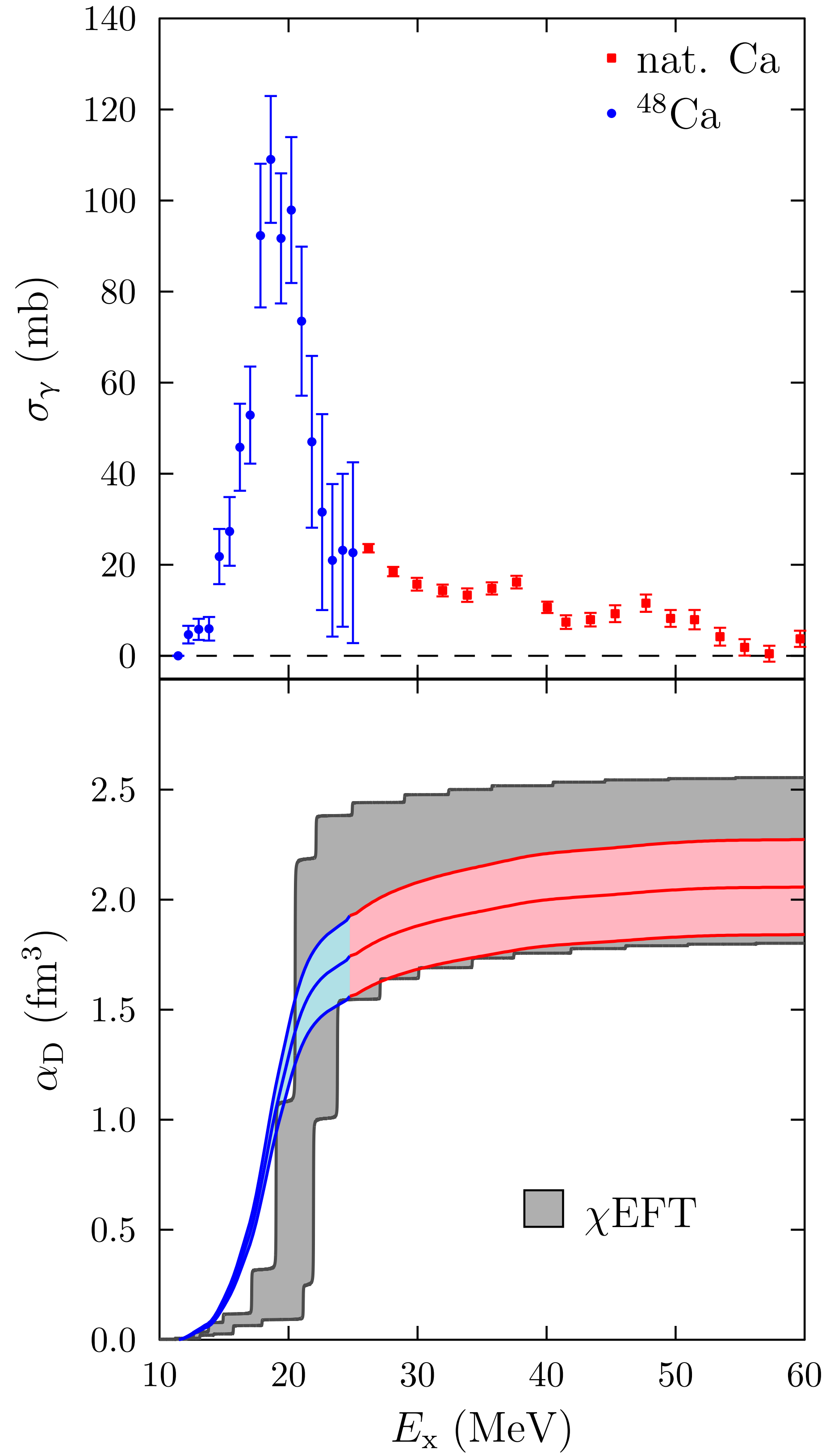
Results for ^{48}Ca

(p,p') experiments

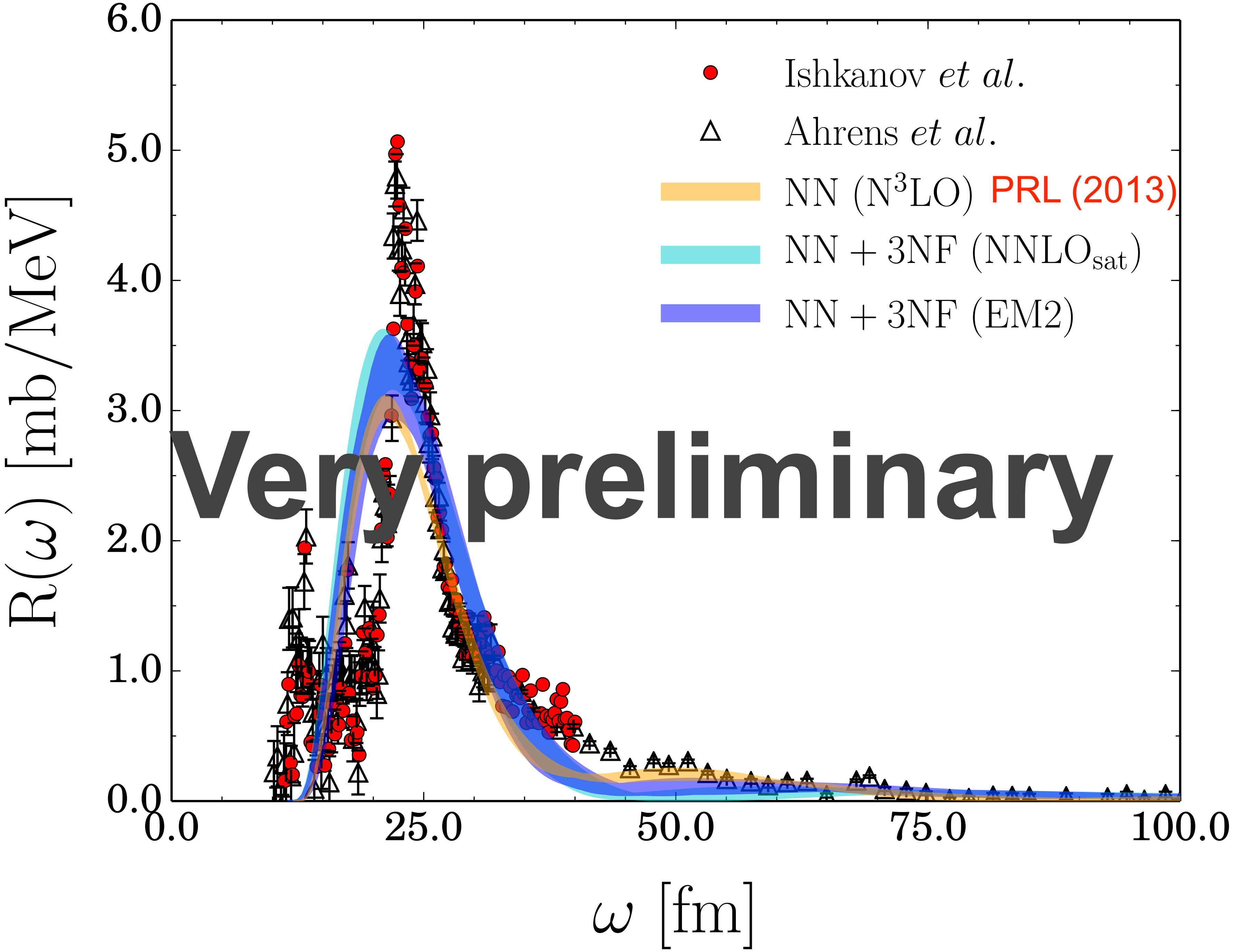


Osaka-Darmstadt collaboration
See talk by von Neumann-Cosel

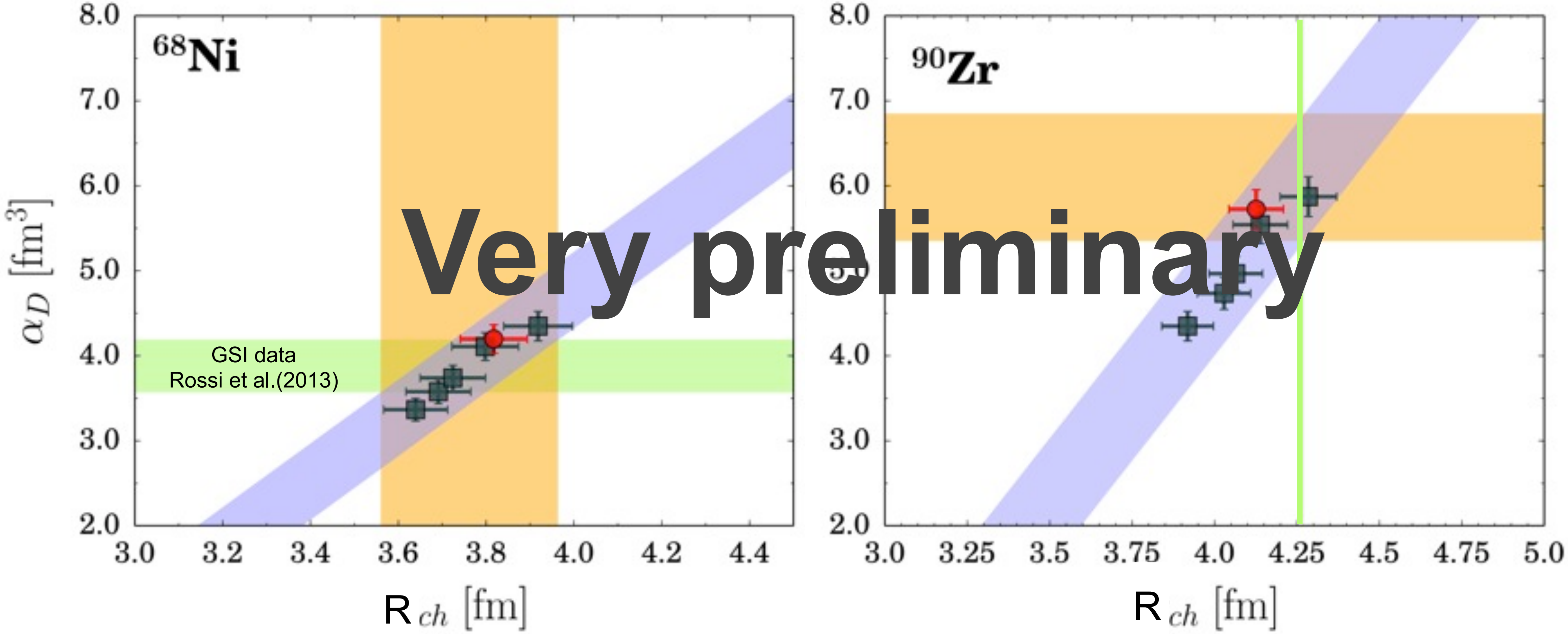
χEFT band includes various interactions with 3NF



Dipole Strength of ^{16}O



Pushing the mass limits...



^{64}Ni $R_{ch} = 3.8572$ fm

Consistent with DFT calculations, Roca-Maza (2015)
$\alpha_D \approx 5.65 \text{ fm}^3$

Outlook

- Ab-initio theory is able to provide predictions for neutron-skin and other observables strongly correlated to it

- Improvements of the theory include addressing the role of triples in CC and further investigating the dependence on the Hamiltonians

Thanks to my collaborators

National Research Council Canada

CINP ICPN Canadian Institute of Nuclear Physics Institut canadien de physique nucléaire

NSERC CRSNG

Thank you for your attention!