Oxygen and Fluorine isotopes from coupled cluster theory

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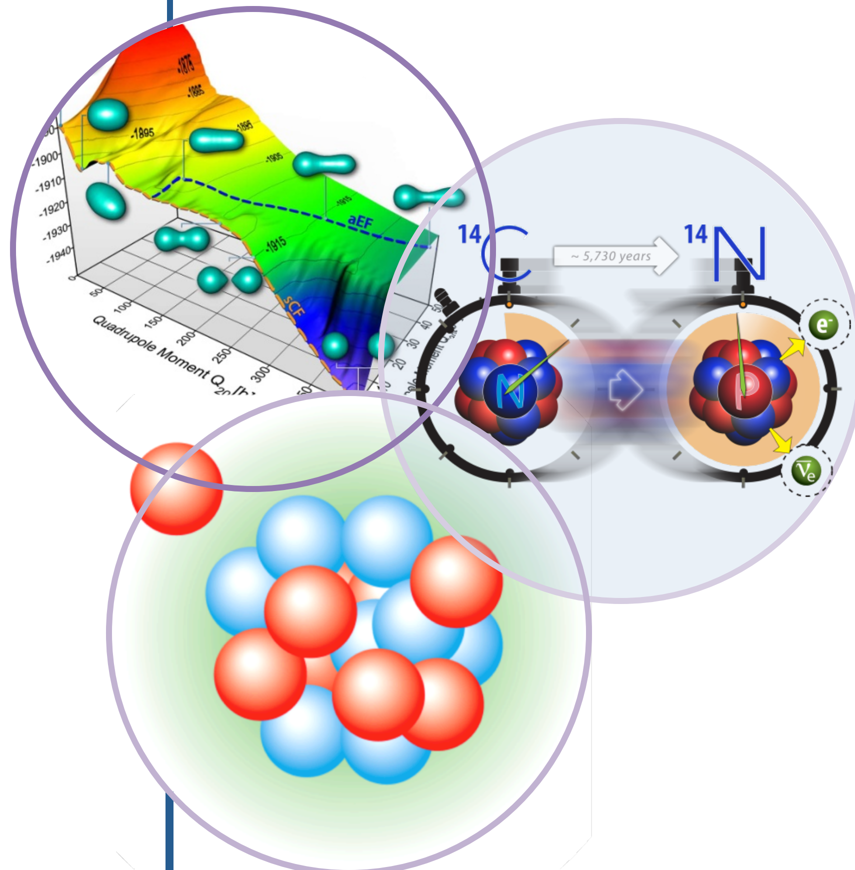

TRIUMF Workshop
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U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY
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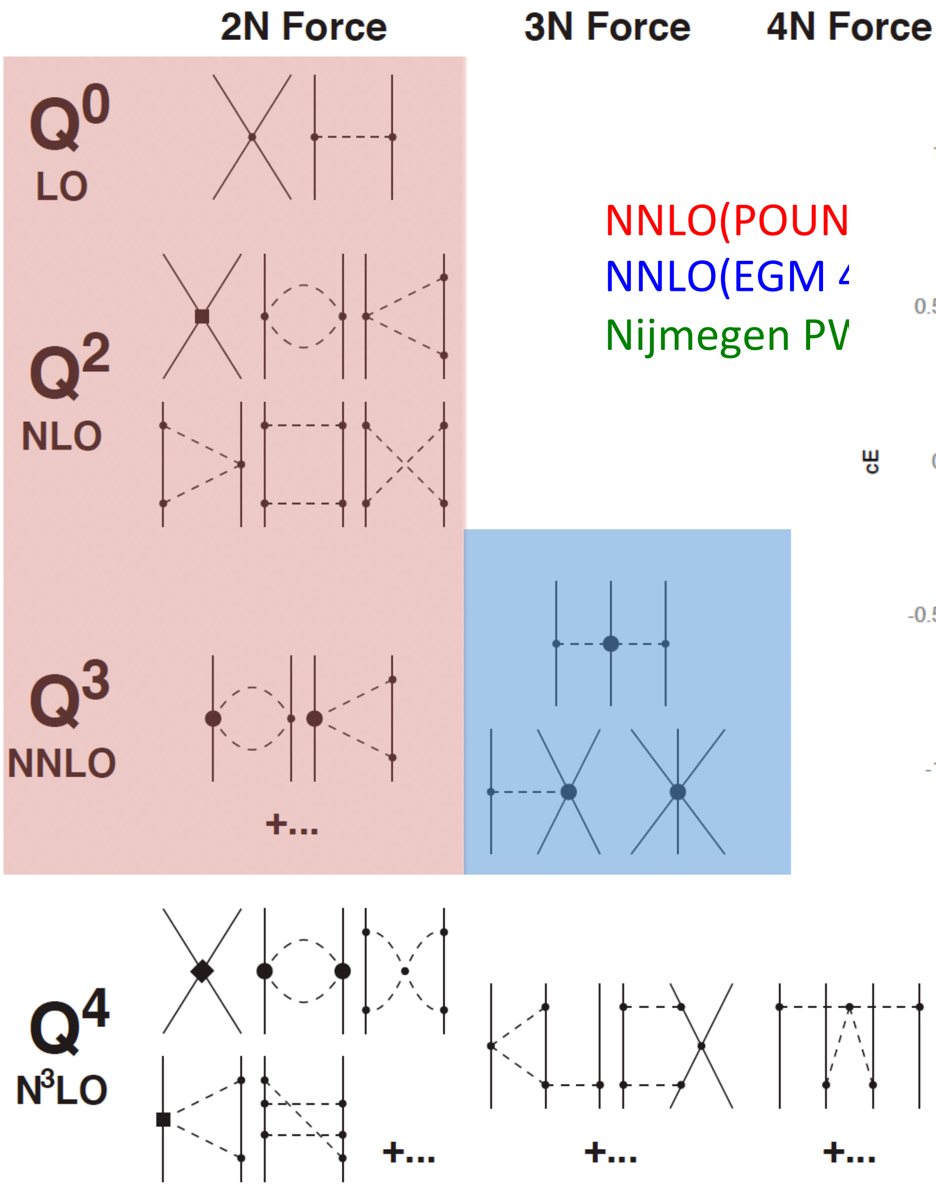
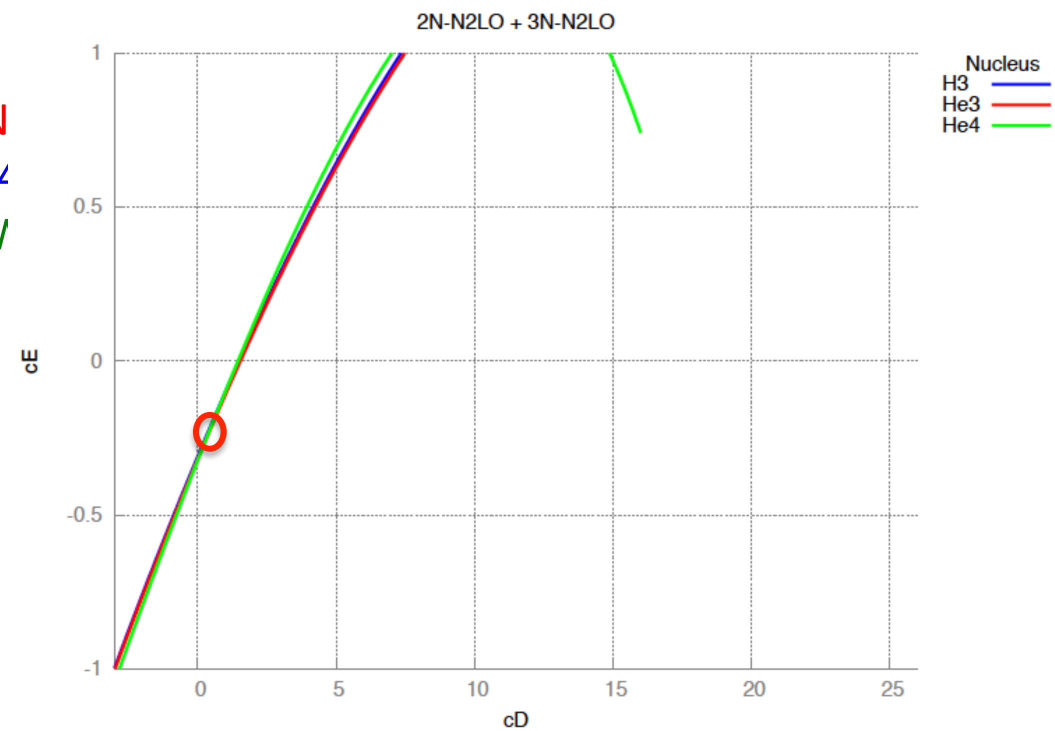
Outline

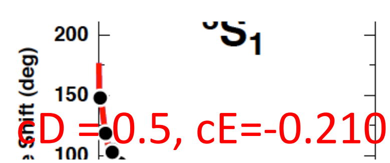
1. Interactions from chiral EFT, open quantum systems and Coupled-Cluster theory
2. Structure of oxygen isotopes from N2LO(POUNDerS)
3. Role of continuum and three-nucleon forces in neutron rich oxygen and fluorine isotopes
4. Inelastic photo induced reactions from Coupled-Cluster theory
5. First principle calculation of the giant-dipole resonance in Oxygen-16

Interactions from chiral effective field theory



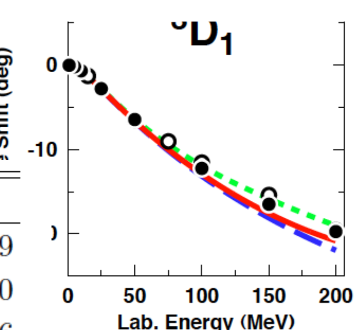
NNLO(POUN
NNLO(EGM 4
Nijmegen PV



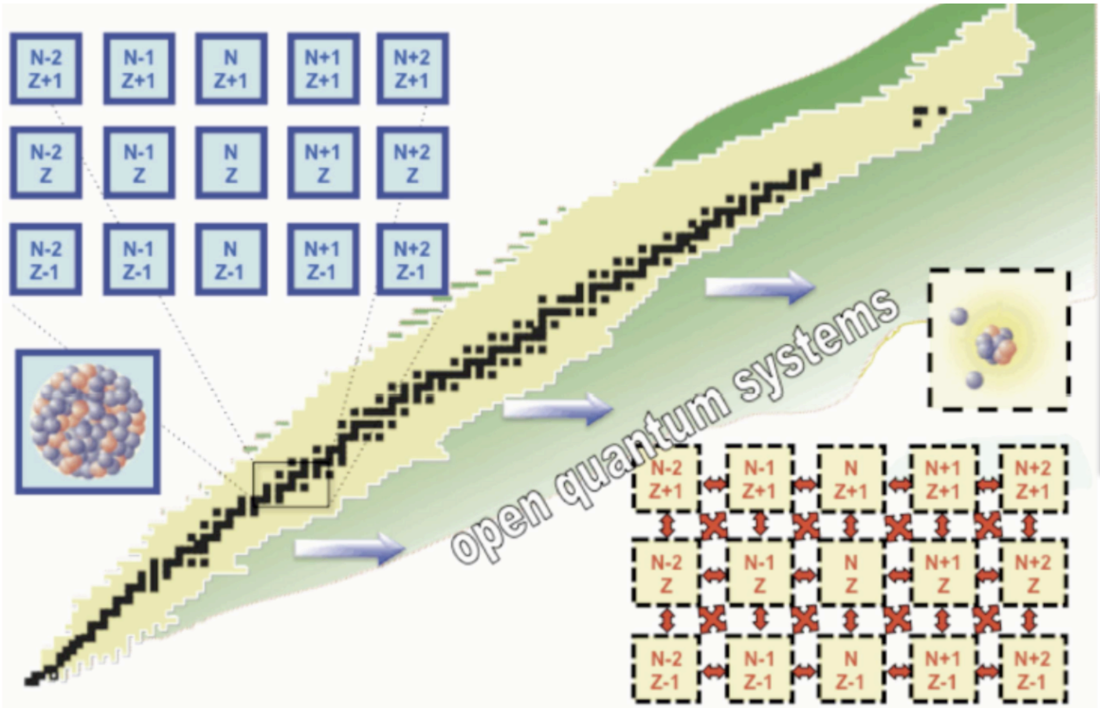


cD =0.5, cE=-0.210

	^3H	^3He	^4He
NNLO	-8.249	-7.501	-27.759
NNLO+NNN	-8.470	-7.723	-28.290
Experiment	-8.482	-7.717	-28.296



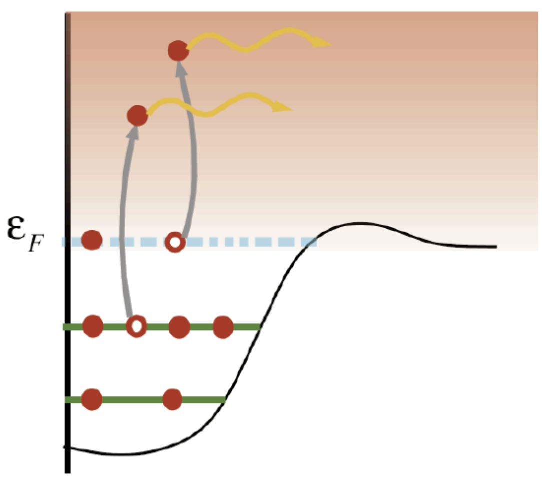
Physics of nuclei at the edges of stability

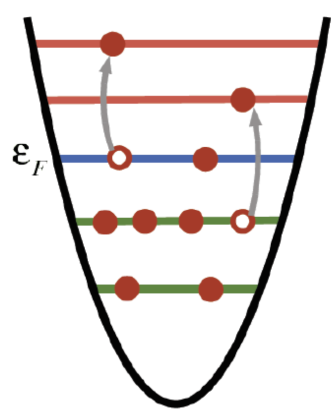


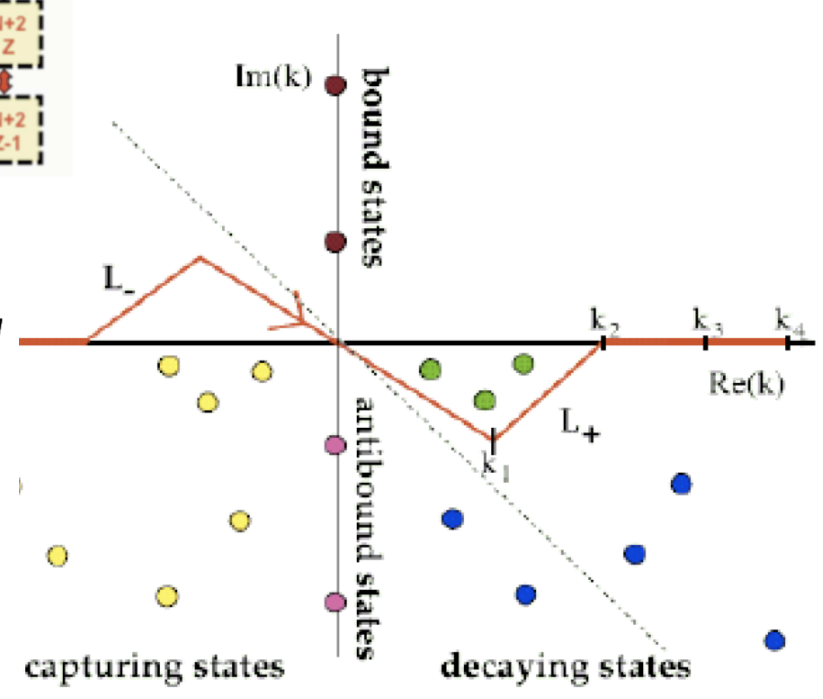
The Berggren completeness treats bound, resonant and scattering states on equal footing.

Has been successfully applied in the shell model in the complex energy plane to light nuclei. For a review see

N. Michel et al J. Phys. G 36, 013101 (2009).







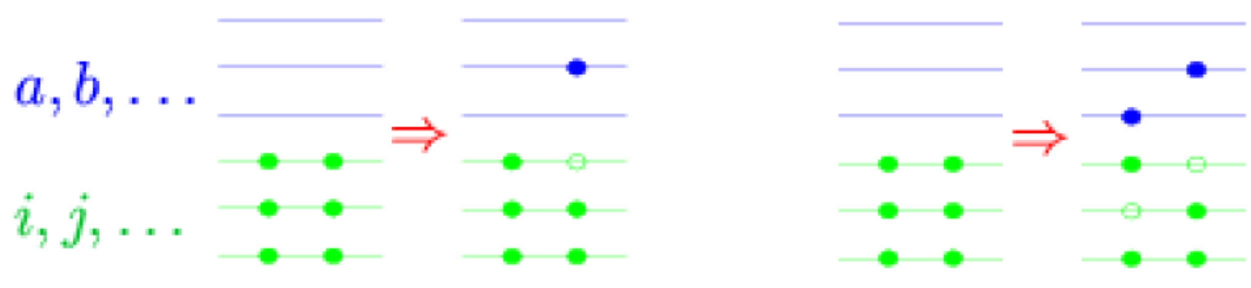
Coupled-cluster method (in CCSD approximation)

Ansatz:

$$
\begin{aligned}
|\Psi\rangle &= e^{T}|\Phi\rangle \\
T &= T_1 + T_2 + \ldots \\
T_1 &= \sum_{ia} t_i^a a_a^\dagger a_i \\
T_2 &= \sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i
\end{aligned}
$$

- ☺ Scales gently (polynomial) with increasing problem size o^2u^4 .
- ☺ Truncation is the only approximation.
- ☺ Size extensive (error scales with A)
- ☹ Most efficient for doubly magic nuclei

Correlations are *exponentiated* 1p-1h and 2p-2h excitations. Part of np-nh excitations included!



Coupled cluster equations

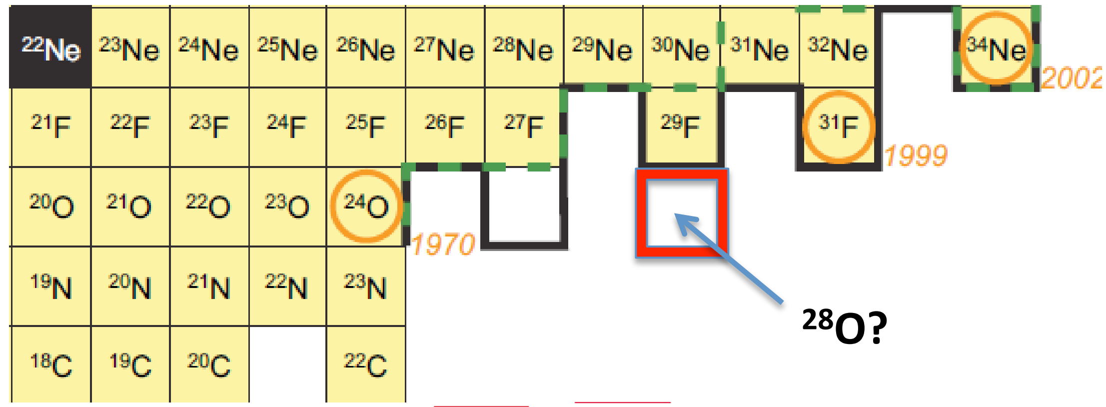
$$
\begin{aligned}
E &= \langle\Phi|\overline{H}|\Phi\rangle \\
0 &= \langle\Phi_i^a|\overline{H}|\Phi\rangle \\
0 &= \langle\Phi_{ij}^{ab}|\overline{H}|\Phi\rangle \\
\overline{H} &\equiv e^{-T}He^{T} = \left(He^{T}\right)_c = \left(H + HT_1 + HT_2 + \frac{1}{2}HT_1^2 + \ldots\right)_c
\end{aligned}
$$

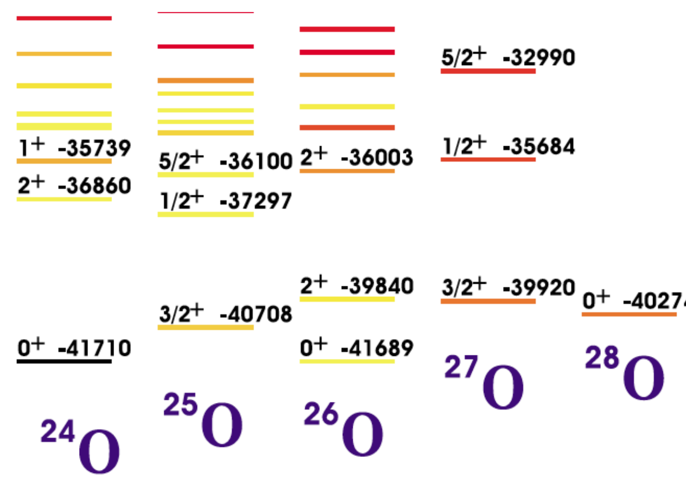
Alternative view: CCSD generates similarity transformed Hamiltonian with no 1p-1h and no 2p-2h excitations.

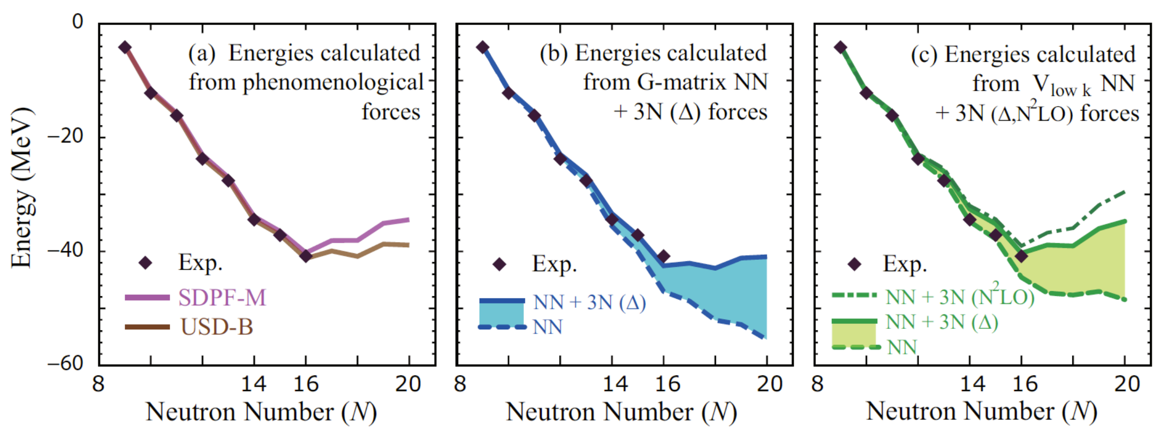
Is ^{28}O a bound nucleus?

Experimental situation

- "Last" stable oxygen isotope ^{24}O
- ^{25,26}O unstable (Hoffman et al 2008, Lunderberg et al 2012)
- ^{28}O not seen in experiments
- ^{31}F exists (adding on proton shifts drip line by 6 neutrons!?)



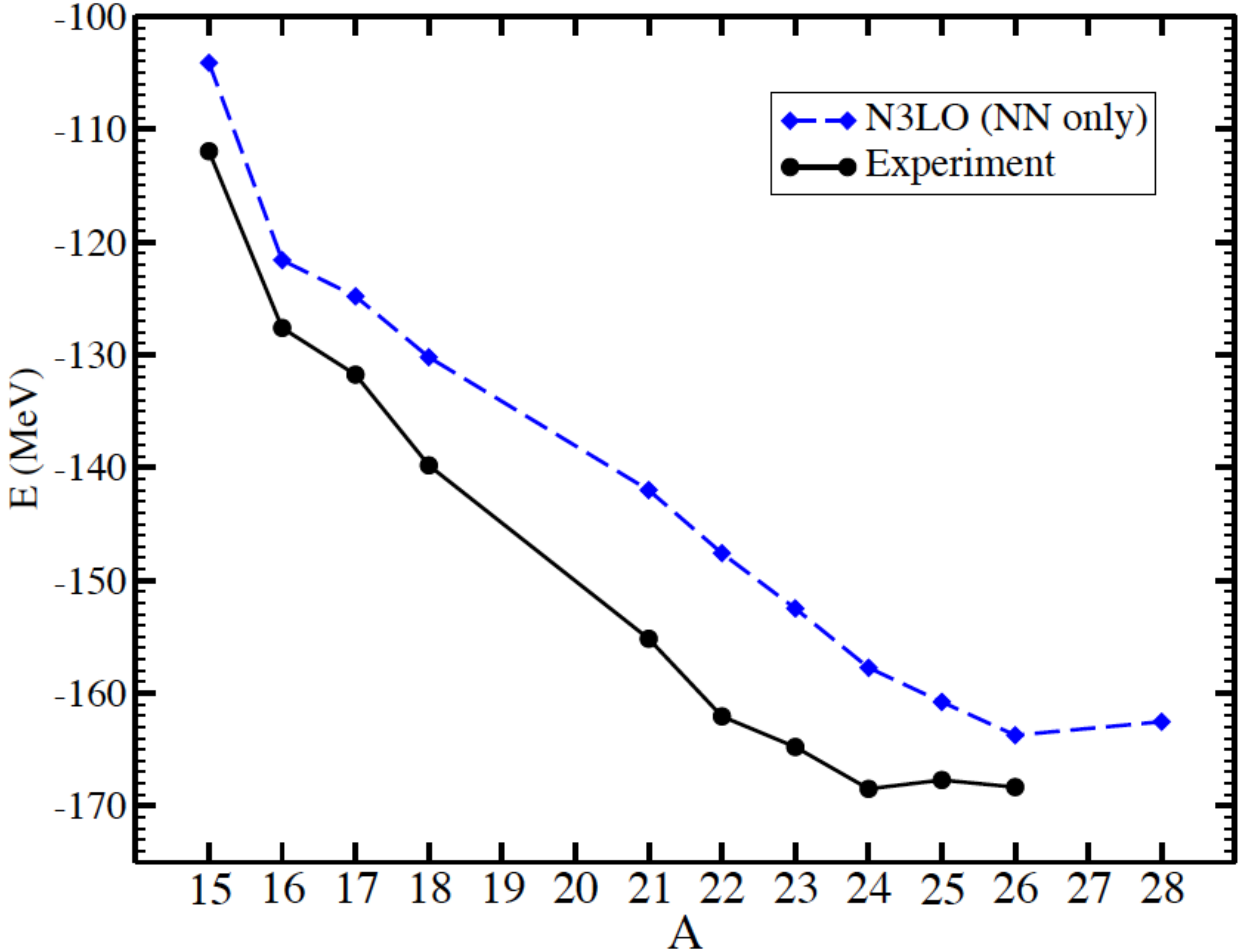




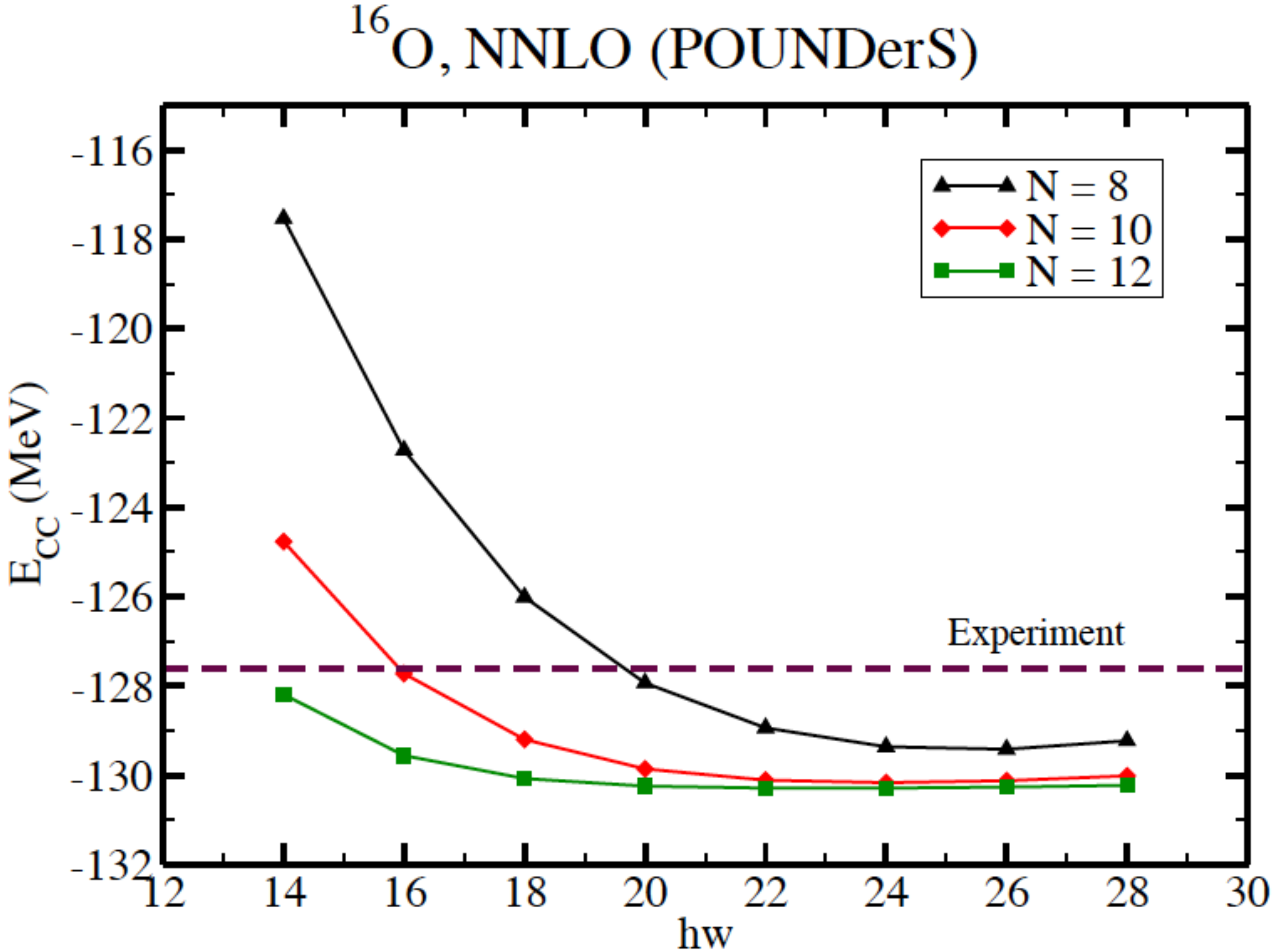
Continuum shell model with HBUSD interaction predict ^{28}O unbound. A. Volya and V. Zelevinsky PRL (2005)

Shell model (sd shell) with monopole corrections based on three-nucleon force predicts 2nd O as last stable isotope of oxygen. [Otsuka, Suzuki, Holt, Schwenk, Akaishi, PRL (2010), arXiv:0908.2607]

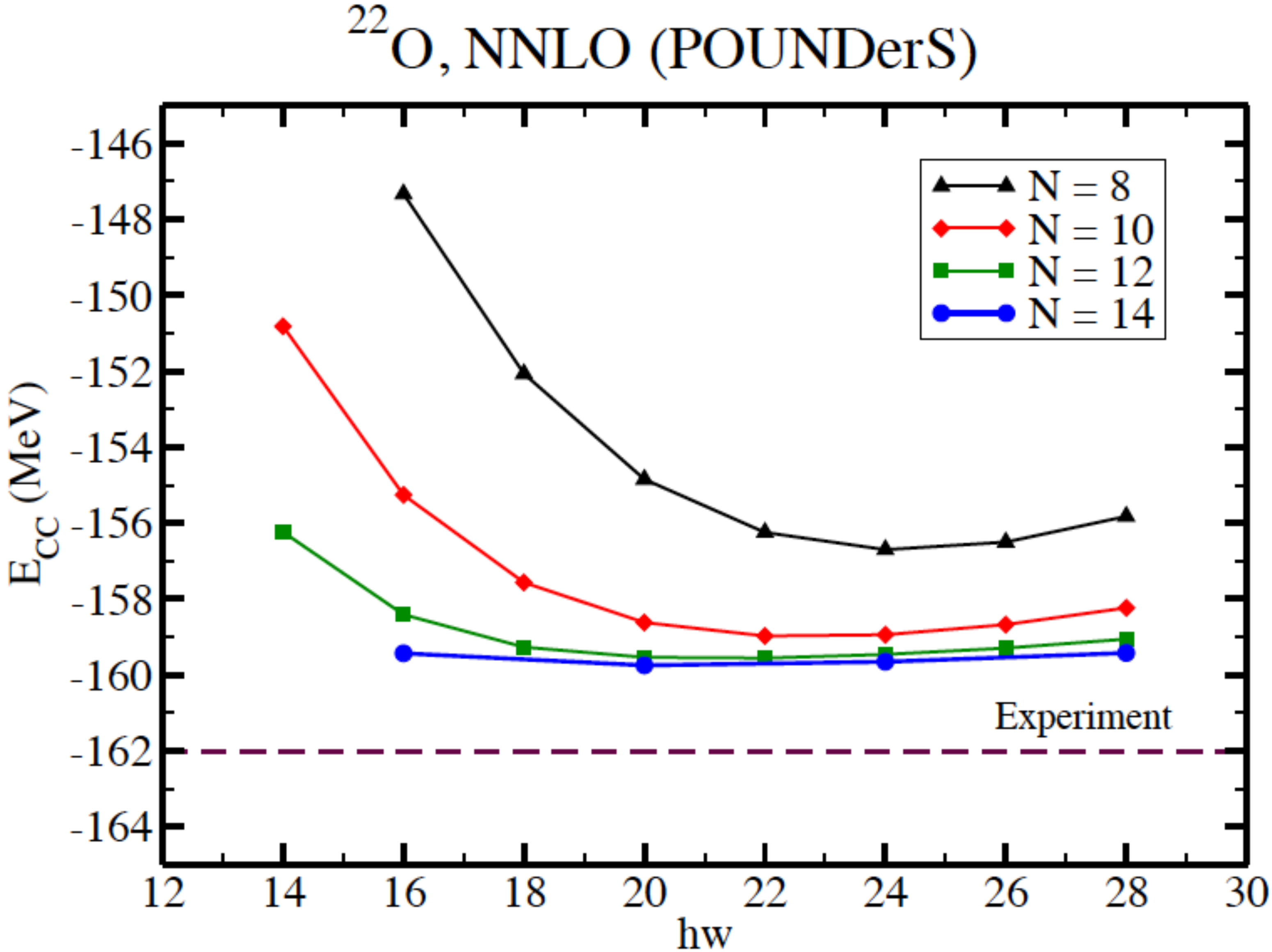
Oxygen isotopes from chiral interactions (NN only)



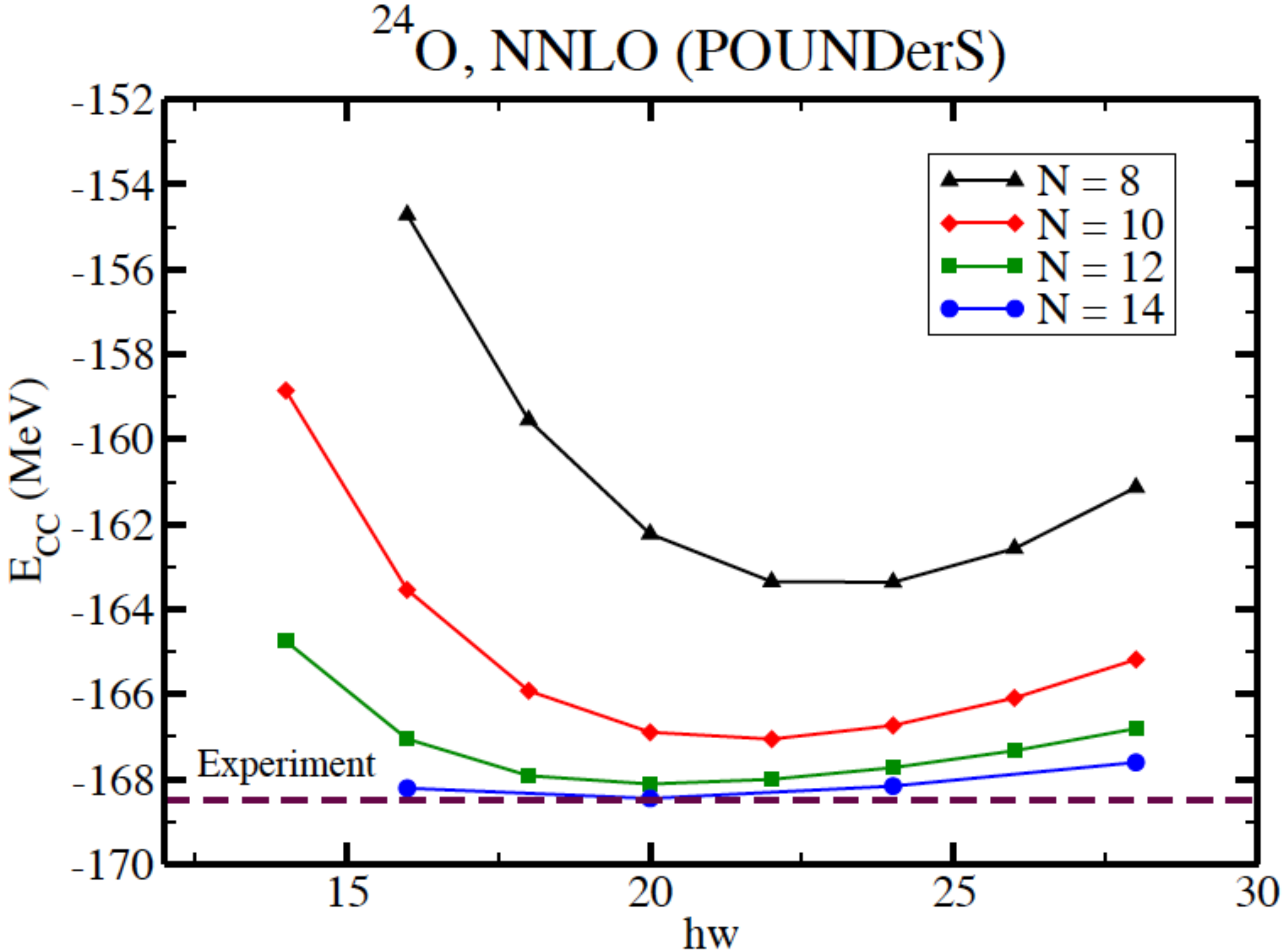
Oxygen isotopes from chiral interactions (NN only)



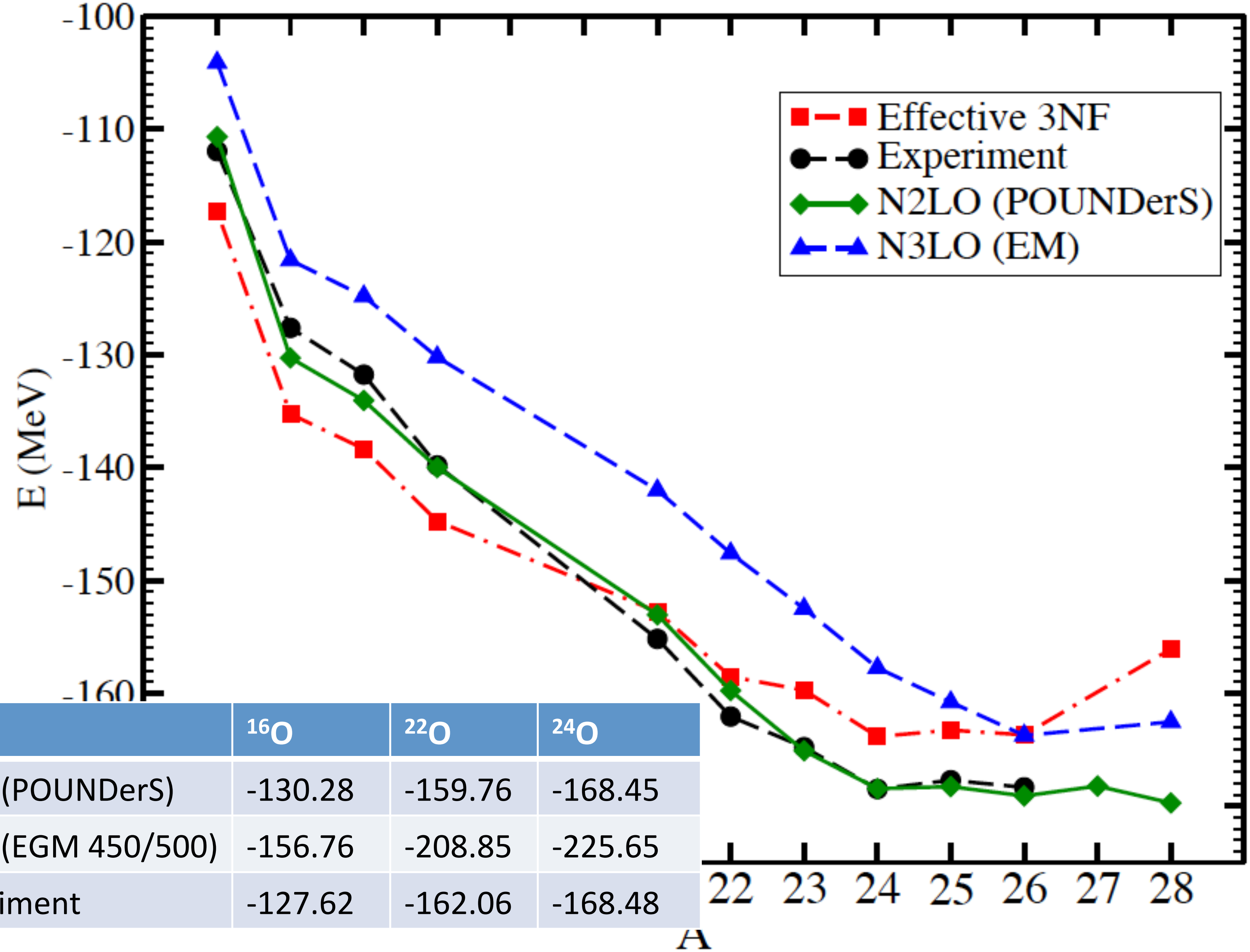
Oxygen isotopes from chiral interactions (NN only)



Oxygen isotopes from chiral interactions (NN only)

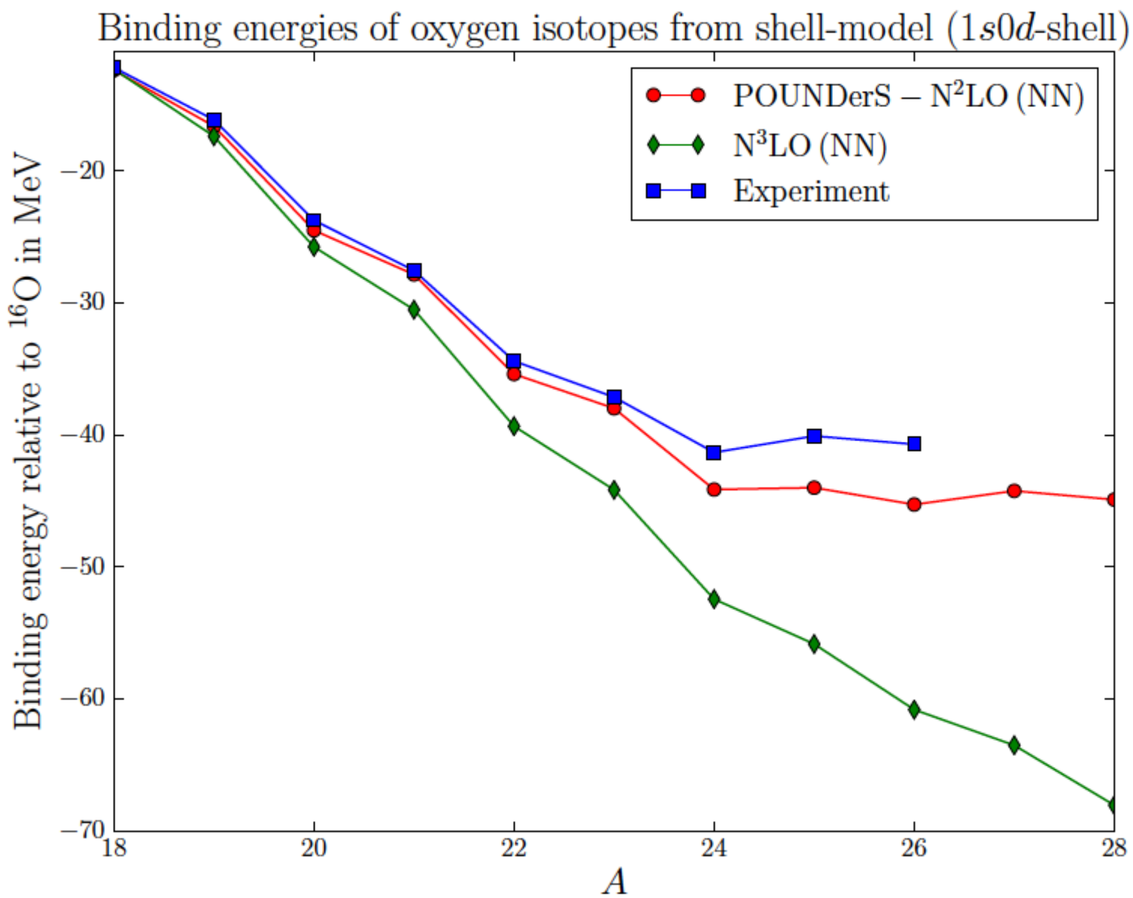


Oxygen isotopes from chiral interactions



	^{16}O	^{22}O	^{24}O
NNLO(POUNDerS)	-130.28	-159.76	-168.45
NNLO(EGM 450/500)	-156.76	-208.85	-225.65
Experiment	-127.62	-162.06	-168.48

Shell model calculations of oxygen from chiral interactions

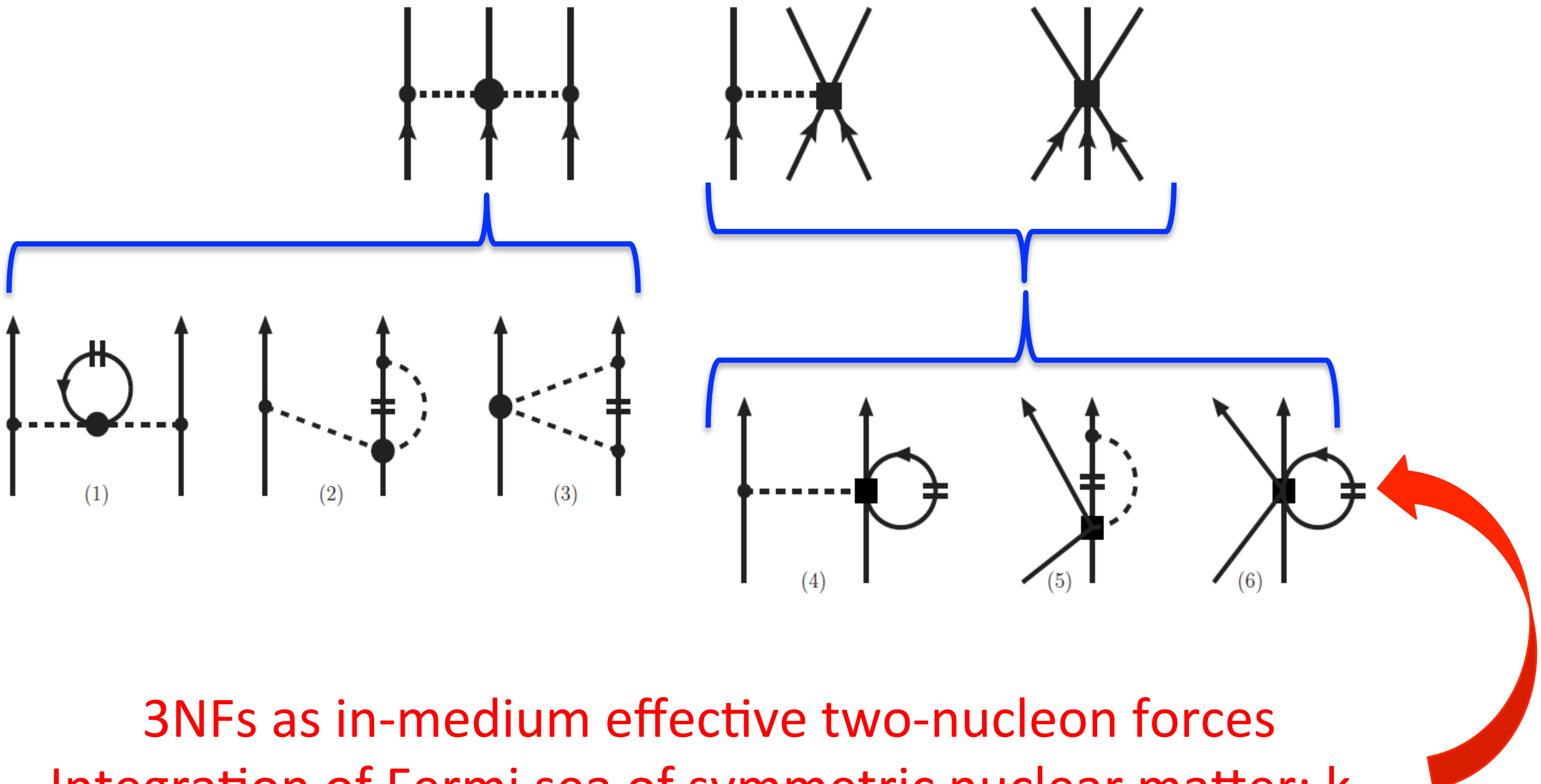


- Shell model calculations done in s-d model space
- Effective interaction from g-matrix and third order perturbation theory.
- Folded diagrams to infinite order
- hw = 14MeV, N = 12 for intermediate excitations.

1. NNLO(POUNDerS) gives remarkable agreement with experiment, and the dripline in oxygen is correctly placed at ^{24}O.
2. **Two-body forces alone get the structure to leading order right!**

Including the effects of 3NFs (approximation!)

[J.W. Holt, Kaiser, Weise, PRC 79, 054331 (2009); Hebeler & Schwenk, PRC 82, 014314 (2010)]



3NFs as in-medium effective two-nucleon forces

Integration of Fermi sea of symmetric nuclear matter: k_F

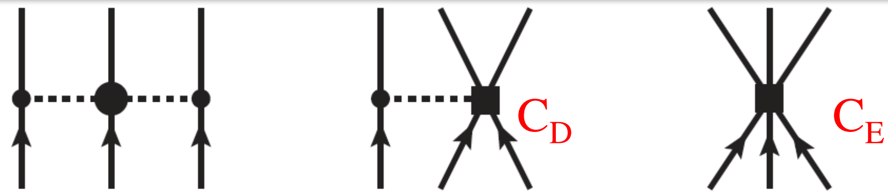
Parameters: For Oxygen we use k_F=1.05 fm^{-1}, c_E=0.71, c_D=-0.2 from binding energies of $^{16,22}O$, for Calcium we use k_F = 0.95 fm^{-1}, c_E = 0.735, c_D = -0.2 from binding energy of ^{40}Ca and ^{48}Ca (The parameters c_D, c_E differ from values proposed for light nuclei)

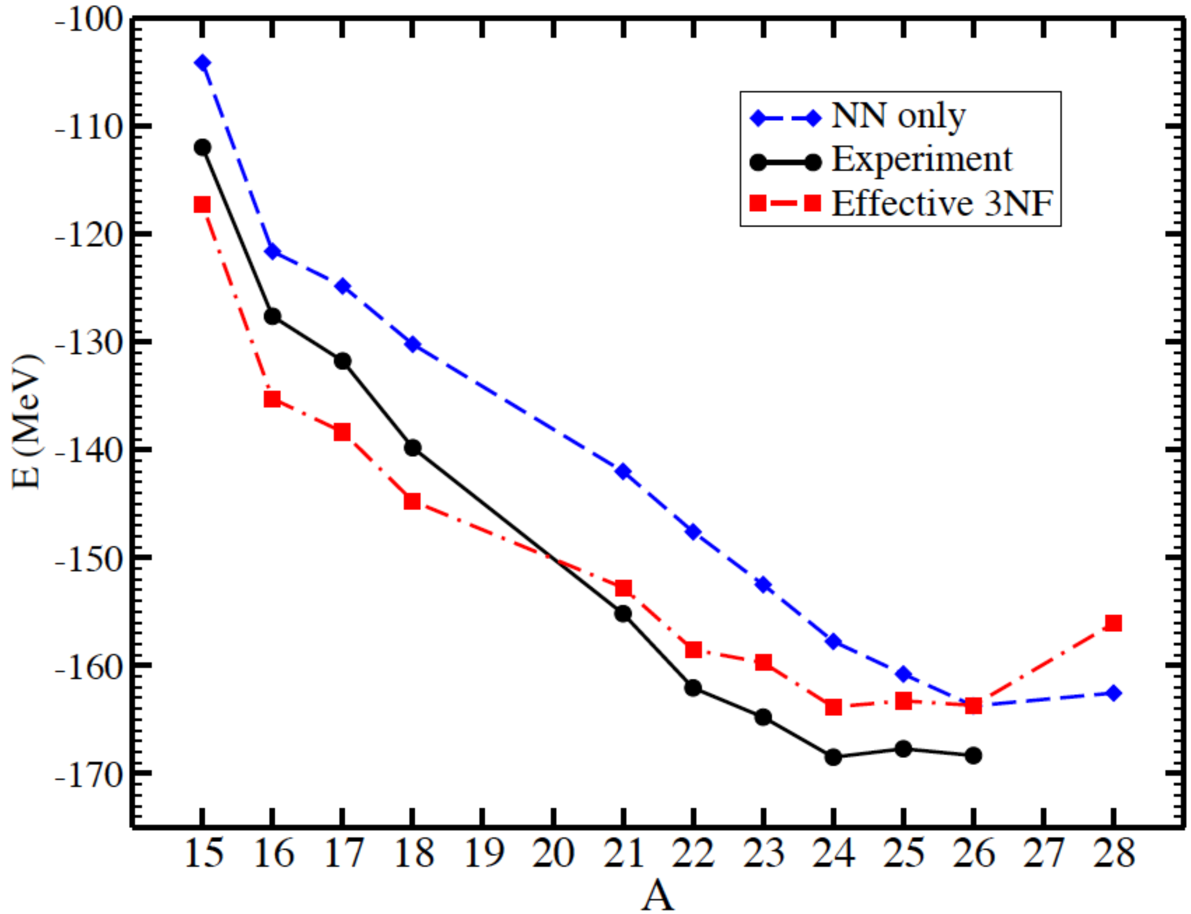
Oxygen isotopes from chiral interactions

1. Effective 3NF place dripline at ^{25}O.
2. Odd-even staggering is well reproduced.
3. ^{26}O unbound by ~100keV, **Lunderberg et al., Phys. Rev. Lett. 108 (2012) 142503**
4. ^{28}O unbound, with a width of ~2MeV

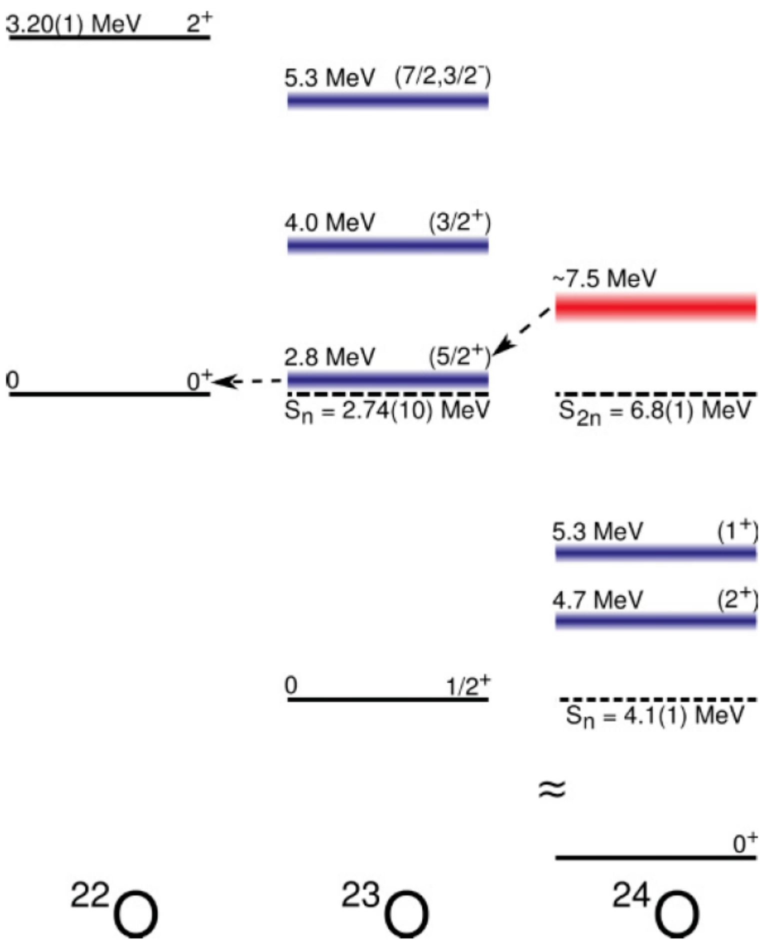
G. Hagen, M. Hjorth-Jensen, G. R. Jansen, R. Machleidt, T. Papenbrock, Phys. Rev. Lett. 108, 242501 (2012).

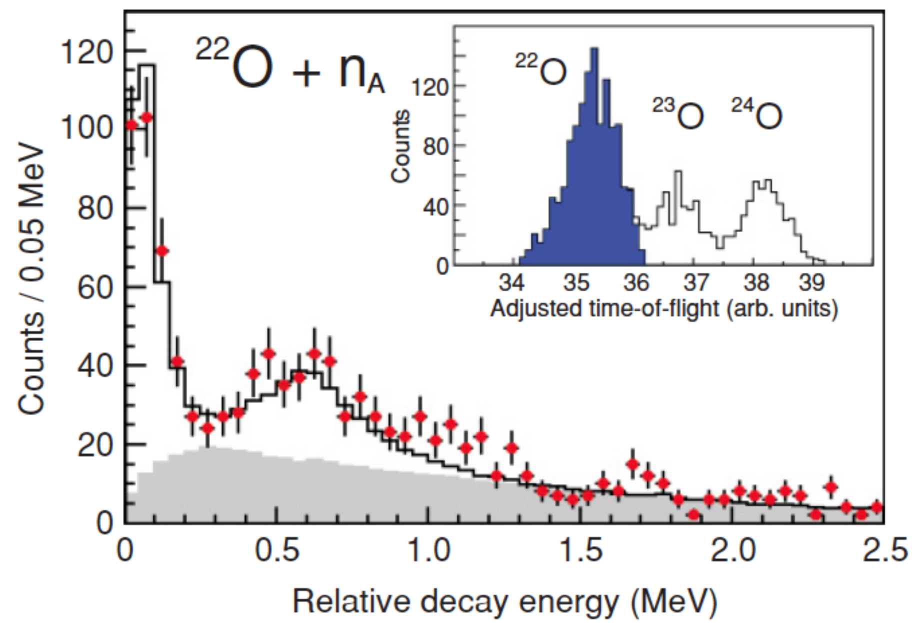
Chiral three-nucleon force at order N2LO. k_f=1.05fm^{-1}, C_D = 0.2, C_E = 0.71 (k_f and c_E fitted to to the binding Energy of ^{16}O and ^{22}O).





Resonances in neutron rich oxygen-24

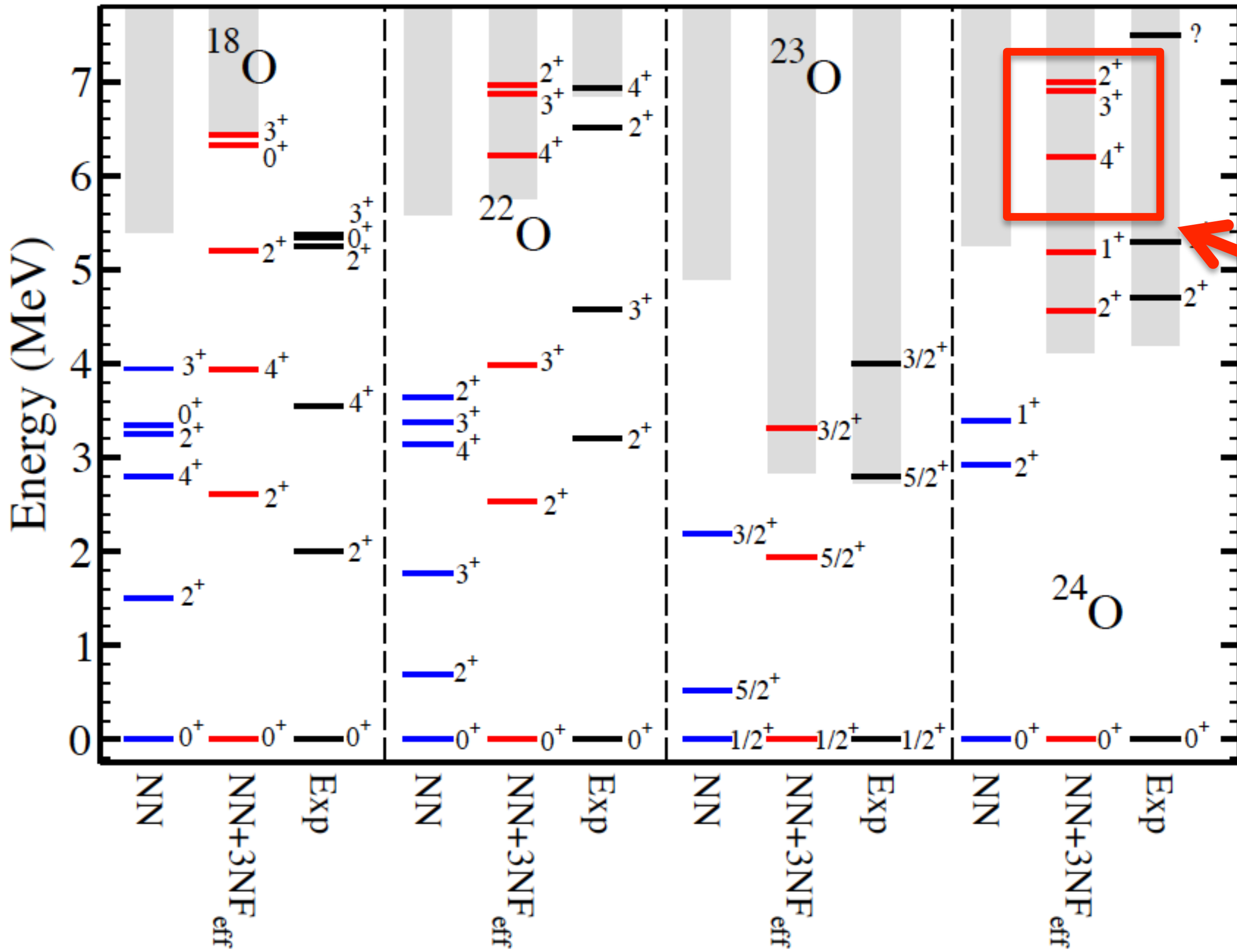




C. R. Hoffman et al Phys. Rev. C **83**, 031303(R) (2011)

- Knockout reaction of ^{26}F reveal a resonance above the two-neutron threshold in ^{24}O
- No spin and parity assigned of this state
- A challenge for microscopic theory to address these states

Oxygen isotopes from chiral interactions



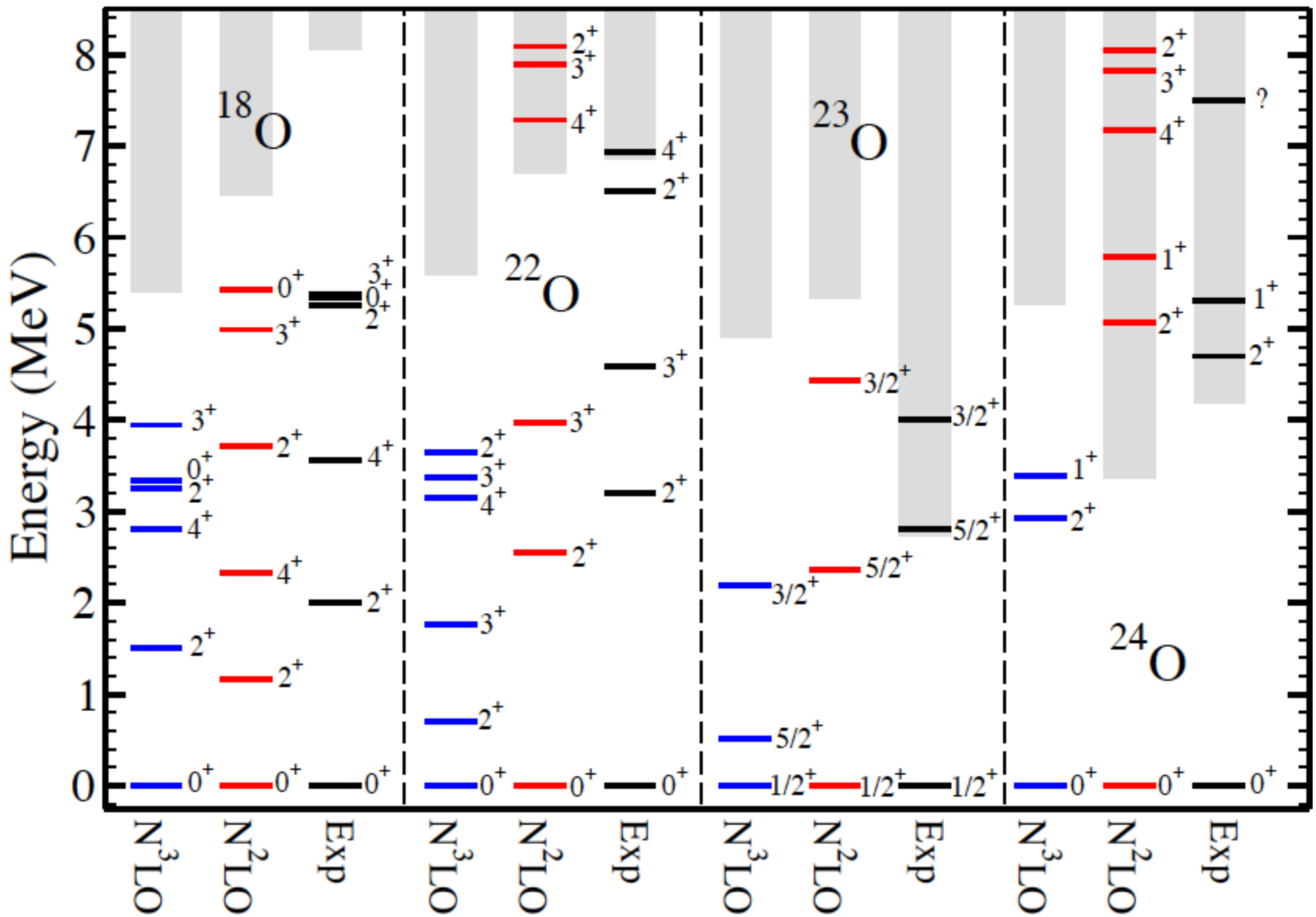
The effects of three-nucleon forces decompress the spectra and brings it in good agreement with experiment.

We find several states (4^+,3^+,2^+) near the observed peak at ~7.5MeV in ^{24}O
C. R. Hoffman et al
Phys. Rev. C **83**, 031303 (2011)

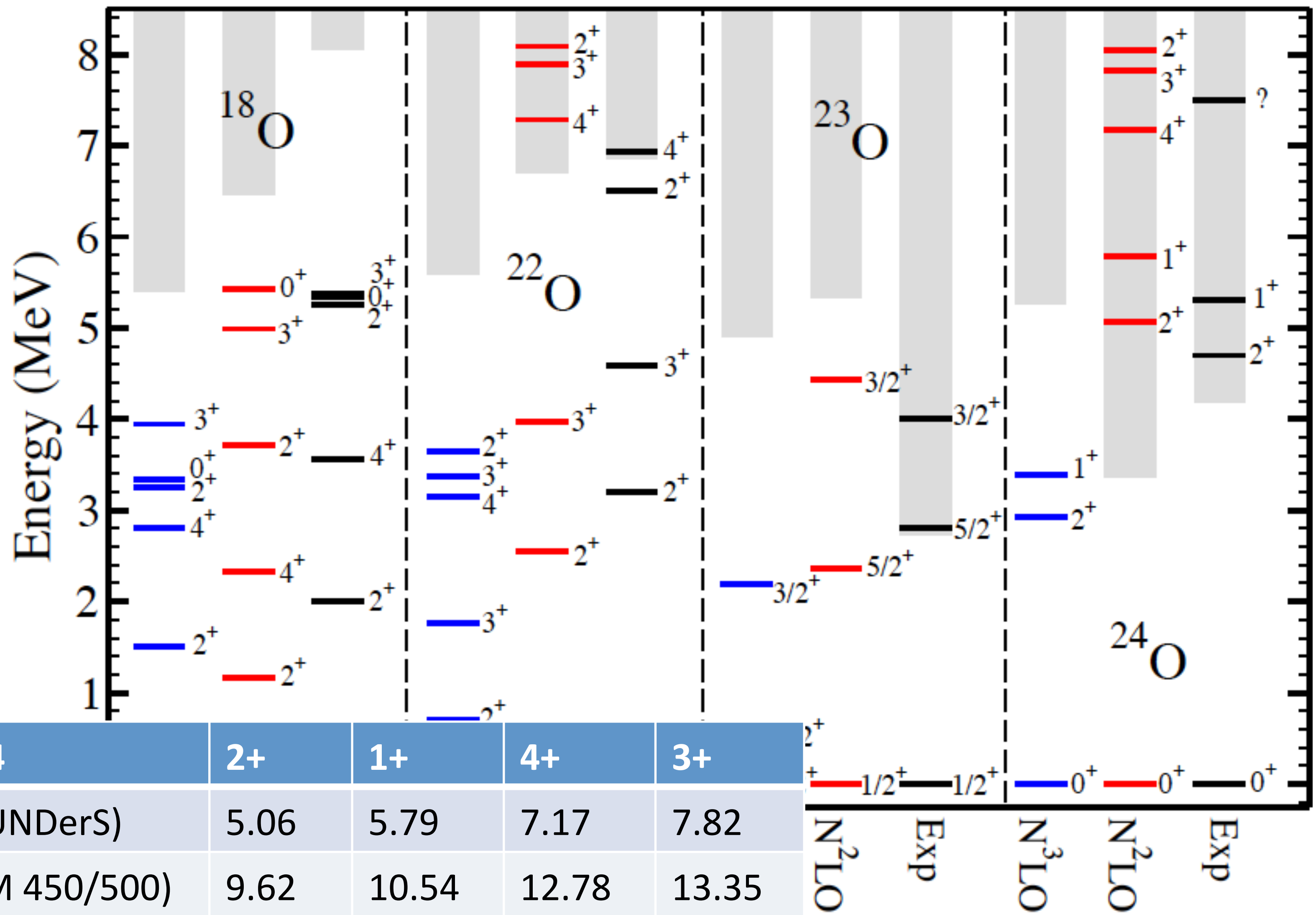
J^π	2_1^+	1_1^+	4_1^+	3_1^+	2_2^+	1_2^+
$E_{\rm CC}$	4.56	5.2	6.2	6.9	7.0	8.4
$E_{\rm Exp}$	4.7(1)	5.33(10)				
$\Gamma_{\rm CC}$	0.03	0.04	0.005	0.01	0.04	0.56
$\Gamma_{\rm Exp}$	$0.05^{+0.21}_{-0.05}$	$0.03^{+0.12}_{-0.03}$				

Hagen, Hjorth-Jensen, Jansen, Machleidt, T. Papenbrock, Phys. Rev. Lett. 108, 242501 (2012).

Excited states in oxygen isotopes from NNLO(POUNDerS)

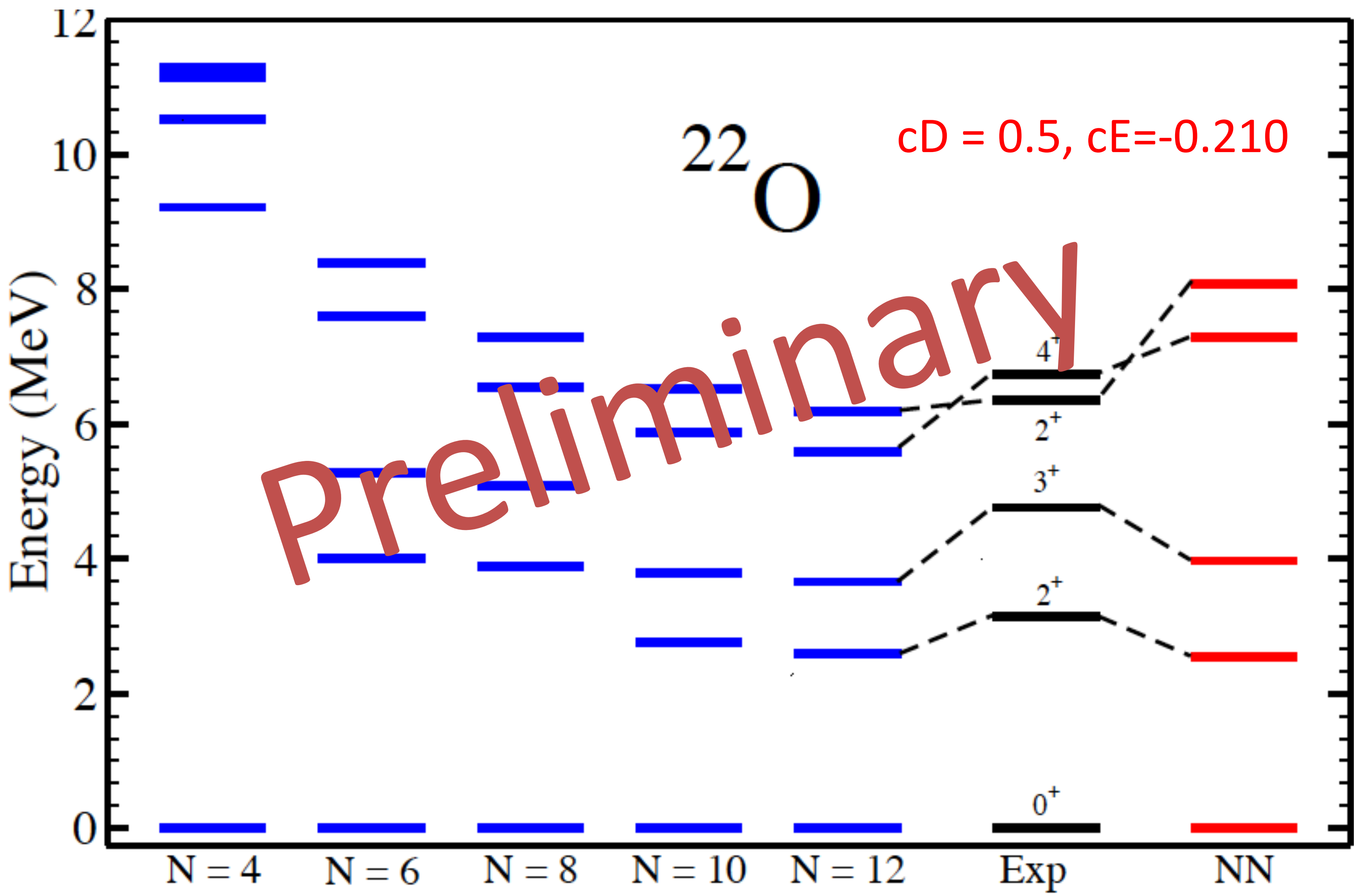


Excited states in oxygen isotopes from NNLO(POUNDerS)



Oxygen-24	2+	1+	4+	3+
NNLO(POUNDerS)	5.06	5.79	7.17	7.82
NNLO(EGM 450/500)	9.62	10.54	12.78	13.35
Experiment	4.7	5.3	?	?

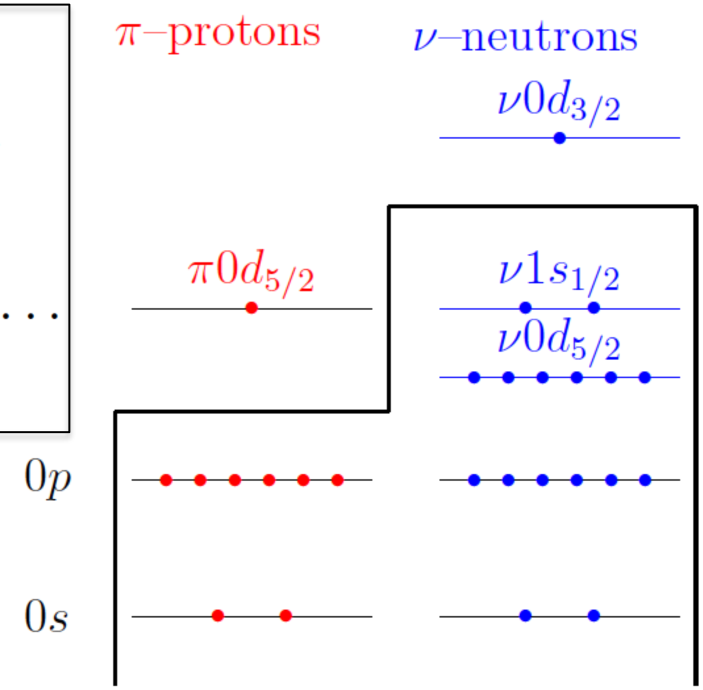
Excited states in Oxygen-22 with NN + 3NF from N2LO(POUNDerS)



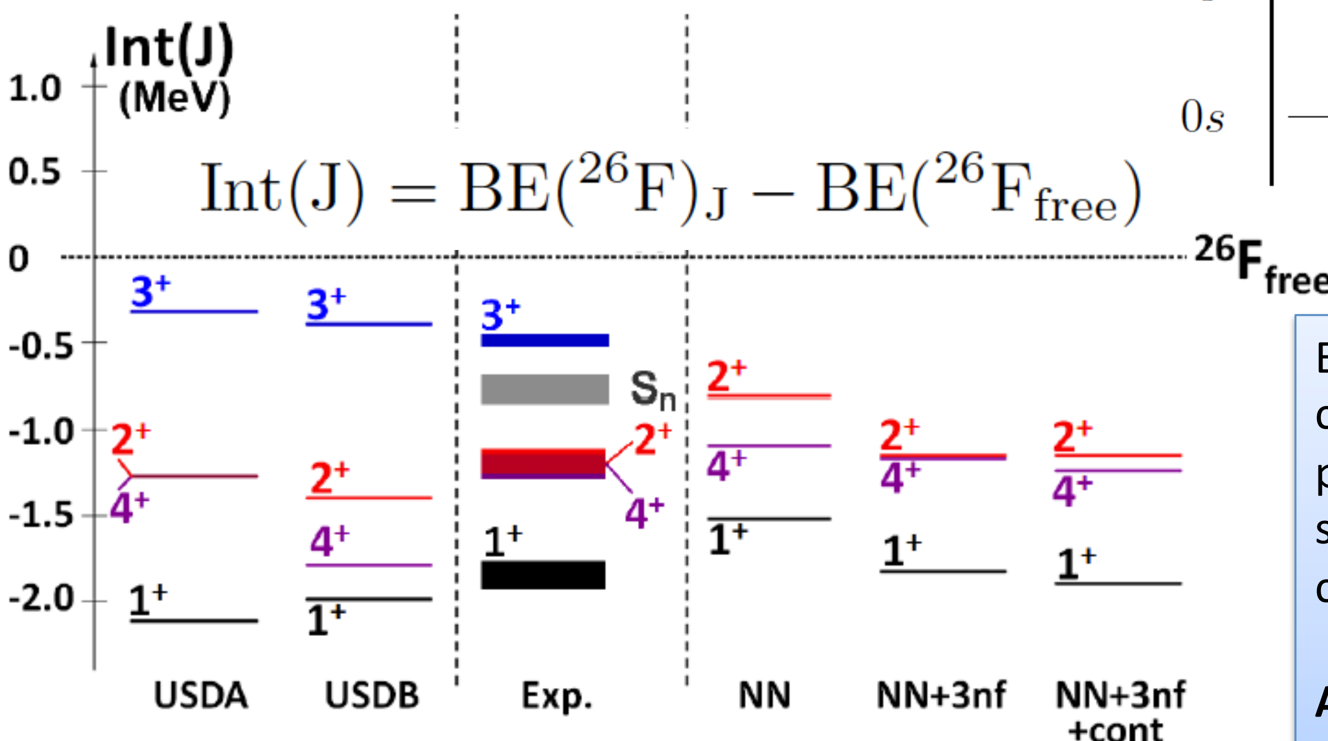
Computing open-shell Fluorine-26

$$(\bar{H}\hat{R}_\mu^{(A\pm2)})_C|\Phi_0\rangle = \omega_\mu \hat{R}_\mu^{(A\pm2)}|\Phi_0\rangle$$

$$\hat{R}^{(A+2)} = \frac{1}{2}\sum_{ba} r^{ab} a_a^\dagger a_b^\dagger + \frac{1}{6}\sum_{iabc} r_i^{abc} a_a^\dagger a_b^\dagger a_c^\dagger a_i + \ldots$$



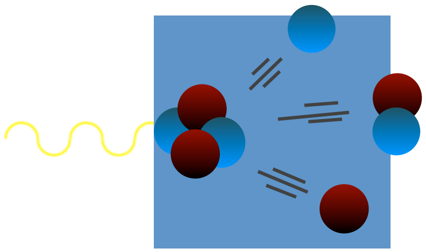
$$\mathrm{Int(J)} = \mathrm{BE}(^{26}\mathrm{F})_\mathrm{J} - \mathrm{BE}(^{26}\mathrm{F}_{\mathrm{free}})$$



Experimental spectra in ^{26}F compared with phenomenological USD shell-model calculations and coupled-cluster calculations

A. Lepailleur et al, PRL 110 082502 (2013)

Break-up observables for medium-mass nuclei?



Cross section is related to the Response Function in the continuum

$$R(\omega) = \sum\!\!\!\!\!\!\int_f \left| \left\langle \psi_f \left| \hat{O} \right| \psi_0 \right\rangle \right|^2 \delta(E_f - E_0 - \omega)$$

Cannot be calculated beyond 3-body break-up even for A=4

Solution: Lorentz Integral Transform method   Efros *et al*.,J. Phys. G: Nucl. Part. Phys. 34 (2007)

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

$$(H - E_0 - \sigma + i\Gamma) \mid \tilde{\psi} \rangle = \hat{O} \mid \psi_0 \rangle$$

Bound-state-like object
Need bound state technique to calculate it

So far used mostly with Hyperspherical Harmonics, limit the mass number to $A \lessapprox 8$

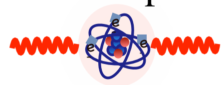
LIT+CC can possibly extend calculations of inelastic reactions into medium-mass nuclei!

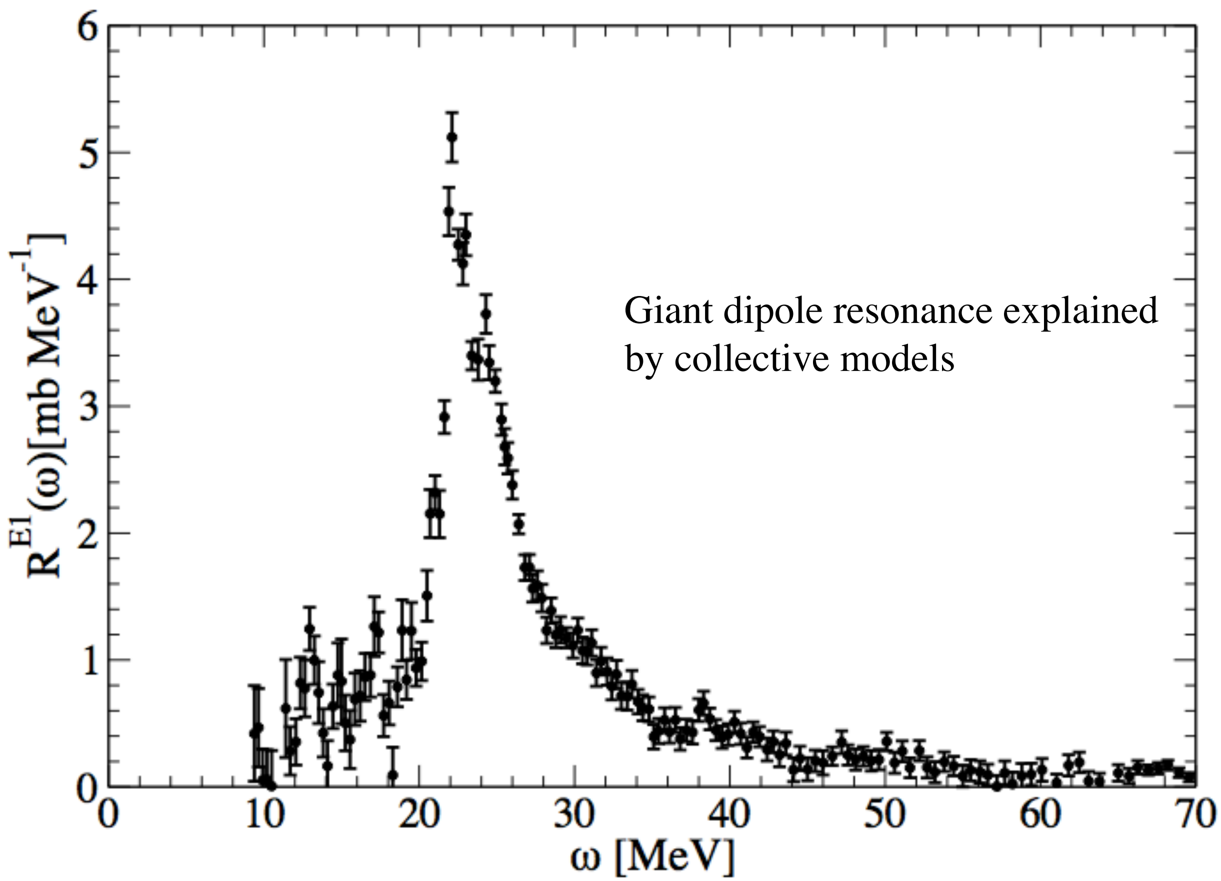
Physics Goal: Describe the collective giant dipole resonance of ^{16}O from first principles

Break-up observables for medium-mass nuclei?

Photo-absorption on ^{16}O: Ahrens *et al.*, NPA **251** (1975) 479 $\sigma_\gamma = \frac{4\pi^2\alpha}{3}\omega R^{E1}(\omega)$

- Inclusive cross section from Mainz: attenuation experiment on natural target due to absorption of bremsstrahlung photons

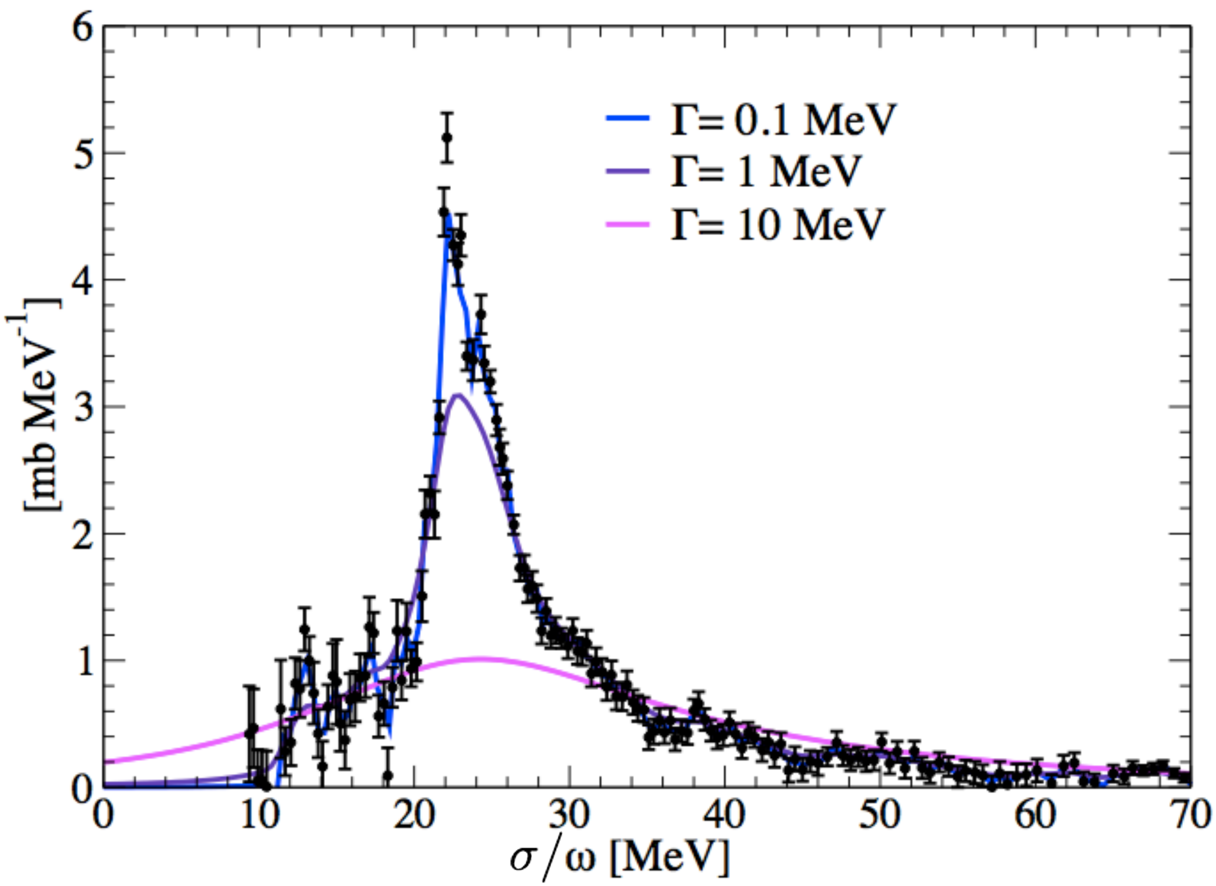




Data still wait for a microscopic interpretation

Break-up observables for medium-mass nuclei?

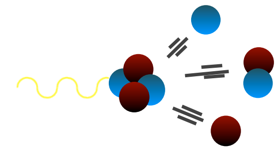
LIT of data $$\frac{\Gamma}{\pi}\int d\omega \frac{R(\omega)}{(\omega-\sigma)^2+\Gamma^2}$$



Shape of data is preserved.

It is like changing the resolution of the data to Γ

LIT with Coupled Cluster Theory



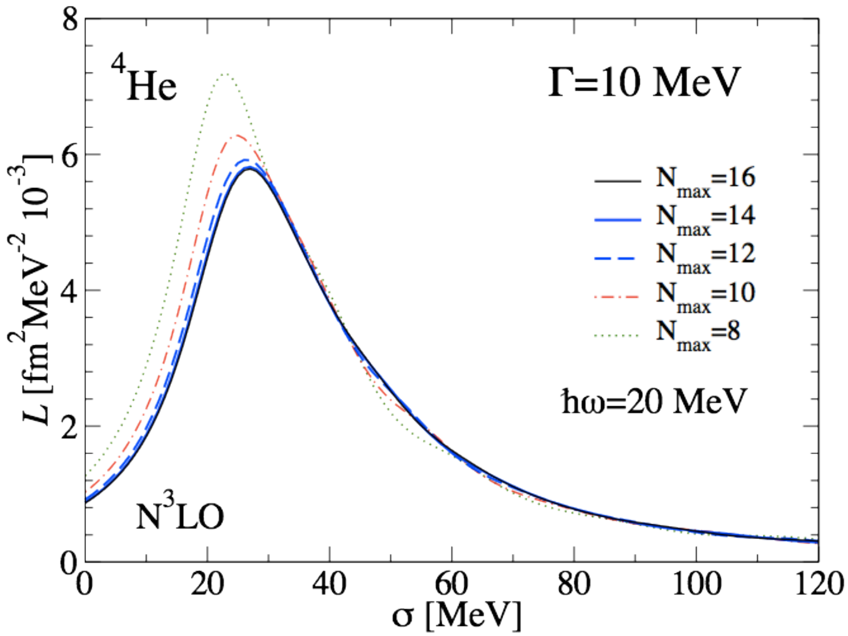
$$L(\sigma,\Gamma) = \int d\omega \frac{R(\omega)}{(\omega-\sigma)^2+\Gamma^2}$$

$$L(\sigma,\Gamma) = \left\langle \tilde{\Psi} | \tilde{\Psi} \right\rangle \rightarrow \left\langle \tilde{\Psi}_L | \tilde{\Psi}_R \right\rangle = \langle \Phi_0 L(z) | R(z^*) \Phi_0 \rangle \quad \text{with} \quad z = E_0 + \sigma + i\Gamma$$

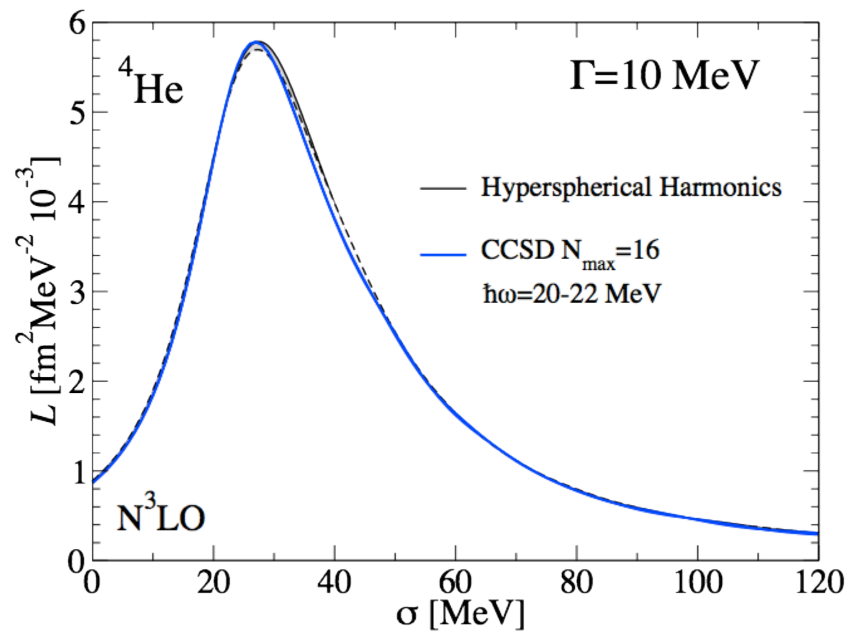
$$R_0 + \sum_{ia} R_i^a \hat{c}_a^\dagger \hat{c}_i + \sum_{ijab} R_{ij}^{ab} \hat{c}_a^\dagger \hat{c}_b^\dagger \hat{c}_j \hat{c}_i + \ldots$$

LIT of Dipole response functions with NN forces derived from χEFT

Convergence of CCSD in model space

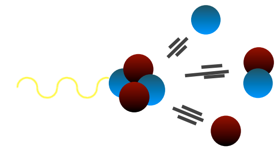


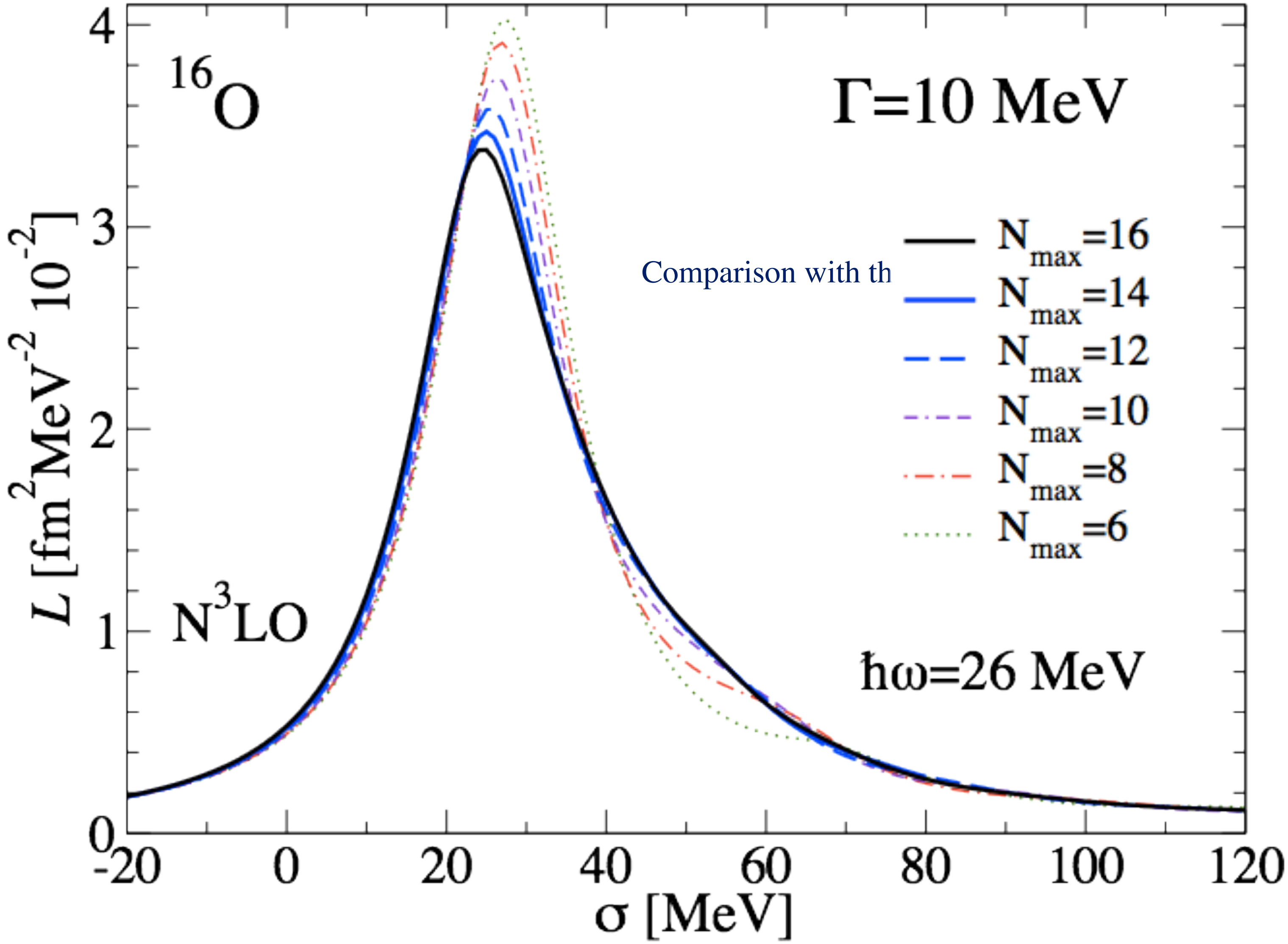
Benchmark with exact theory



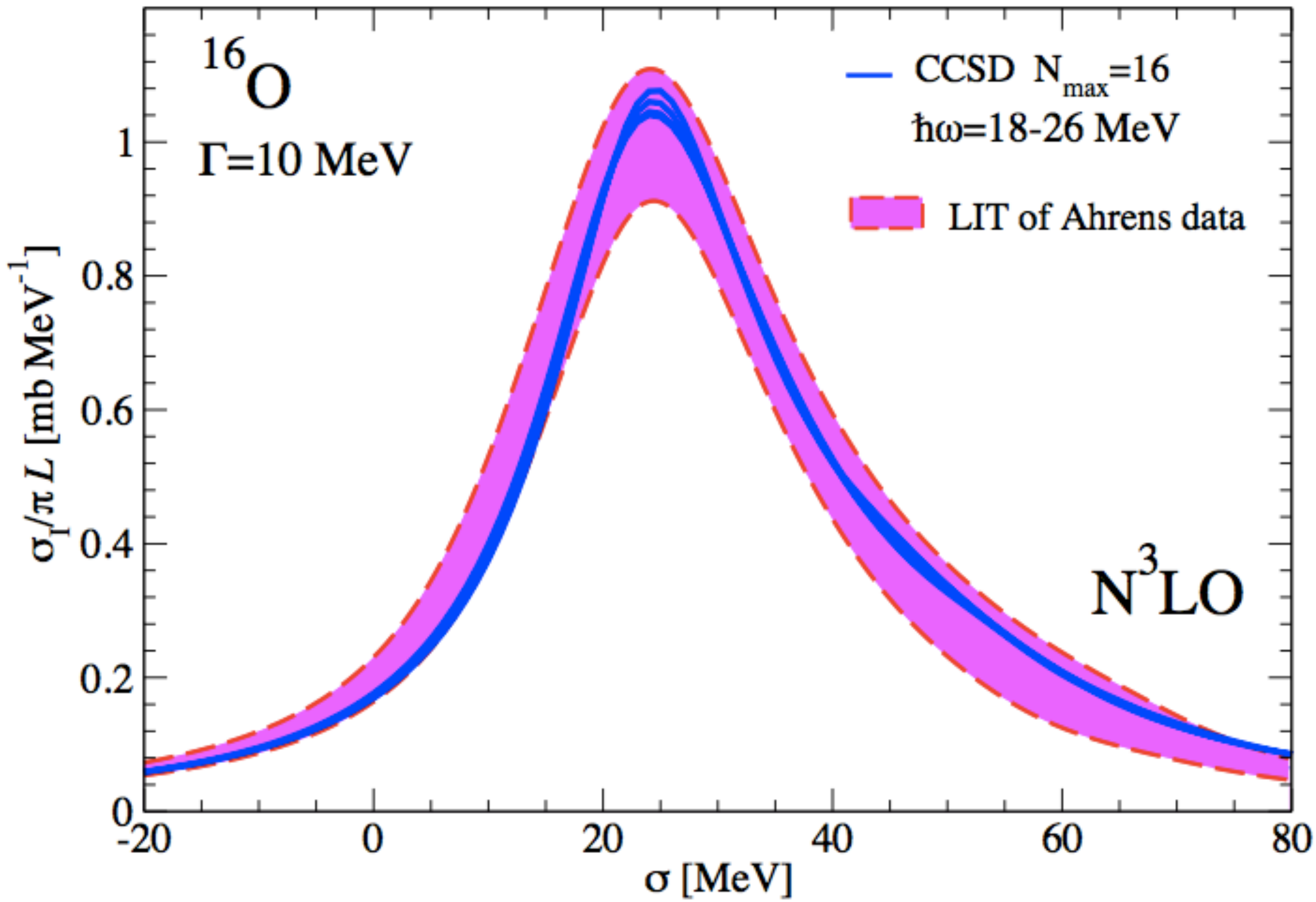
The comparison is very good!

Giant Dipole Resonance of ^{16}O with LIT-CCSD





Giant Dipole Resonance of ^{16}O with LIT-CCSD



Summary

1. Interactions from Chiral EFT probed in nuclei
2. NNLO(POUNDerS) get nuclear structure right to leading order.
3. Remarkable agreement with experiment for oxygen isotopes using NN forces only
4. Predict spin and parity of newly observed resonance peak in ^{24}O.
5. Developed coupled-cluster theory for inelastic photo induced reactions
6. First principle calculation of the giant-dipole resonance in Oxygen-16