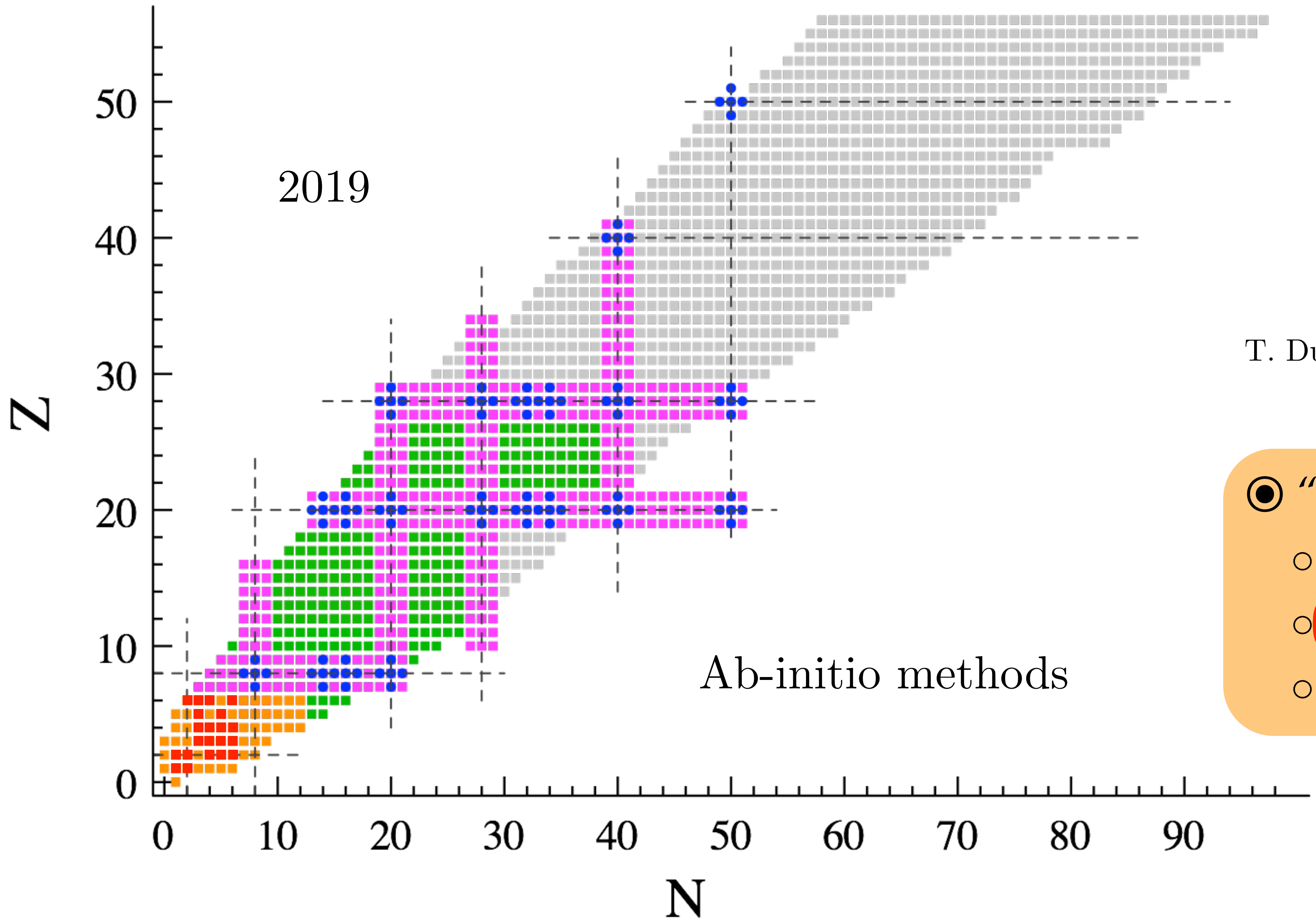
Quantum Monte Carlo calculations of nuclear charge radii

Diego Lonardoni, FRIB Theory Fellow

Laser spectroscopy as a tool for nuclear theories, CEA-Saclay, October 11, 2019

Goal: predict the emergence of nuclear properties and structure from first principles



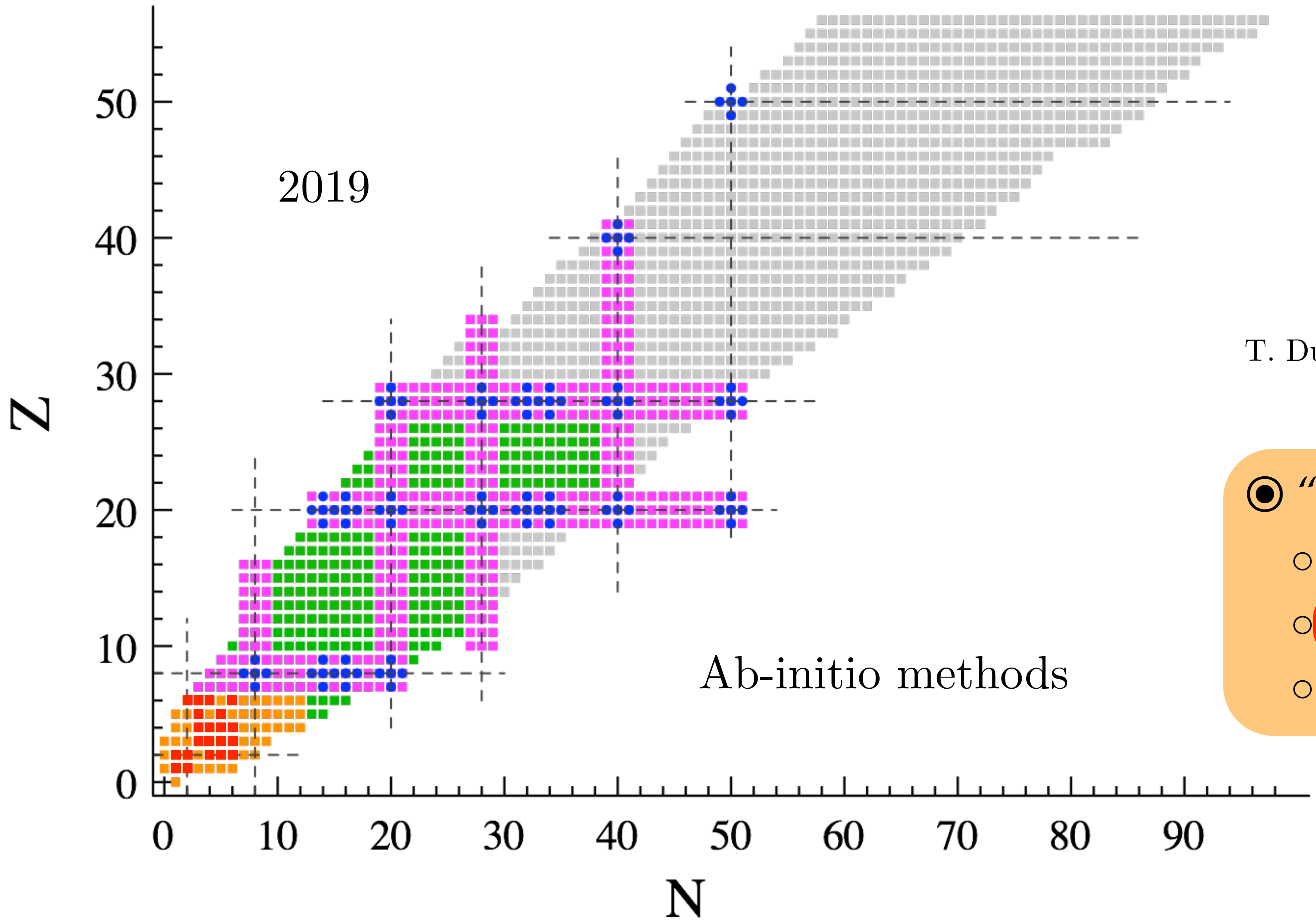
T. Duguet's talk @ CEA-Saclay, Oct 7th, 2019

- "Exact" methods
  - Since 1980's
  - Monte Carlo, CI, ...
  - Factorial / exponential scaling

2015: "standard" Quantum Monte Carlo (QMC) calculations (VMC, GFMC)

- Scaling: exponential
- Nuclear Hamiltonians: phenomenological

Goal: predict the emergence of nuclear properties and structure from first principles



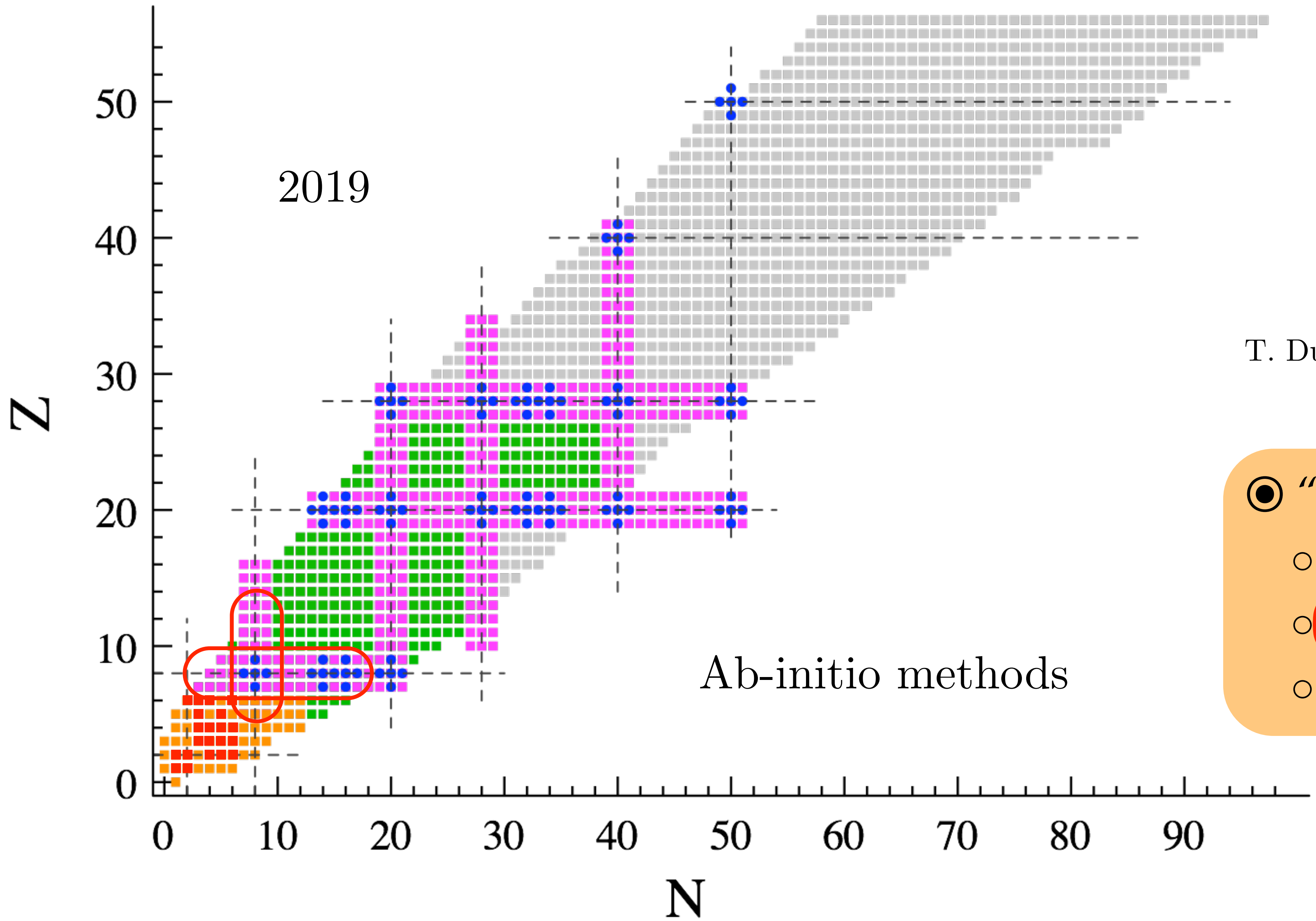
T. Duguet's talk @ CEA-Saclay, Oct 7th, 2019

- "Exact" methods
  - Since 1980's
  - Monte Carlo, CI, …
  - Factorial / exponential scaling

2016-2018: "standard" Quantum Monte Carlo (QMC) calculations (VMC, GFMC)

- Scaling: exponential
- Nuclear Hamiltonians: phenomenological + local chiral interactions

***Goal*:** predict the emergence of nuclear properties and structure from first principles



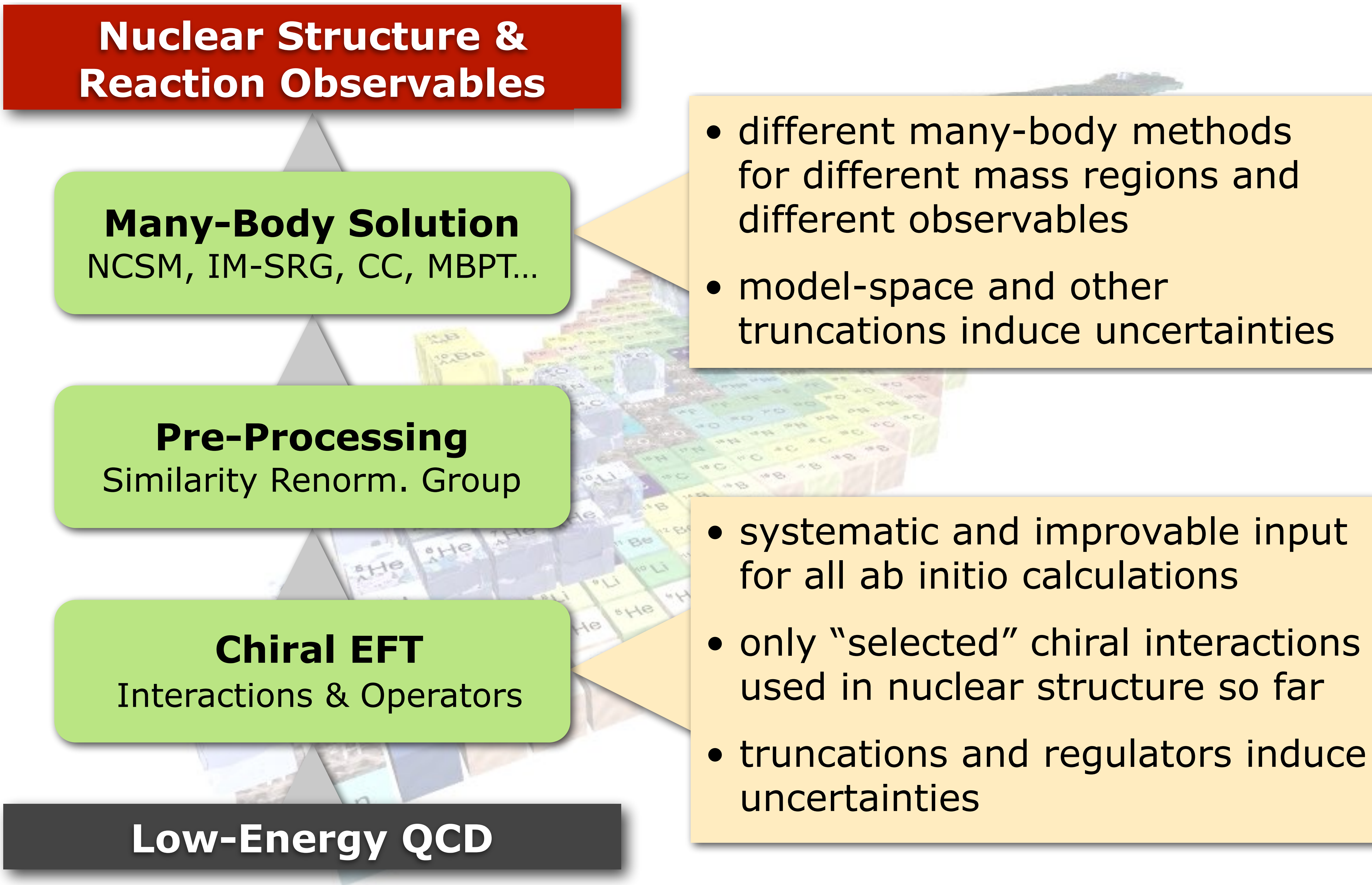
T. Duguet's talk @ CEA-Saclay, Oct 7th, 2019

- "Exact" methods
  - Since 1980's
  - Monte Carlo, CI, …
  - Factorial/exponential scaling

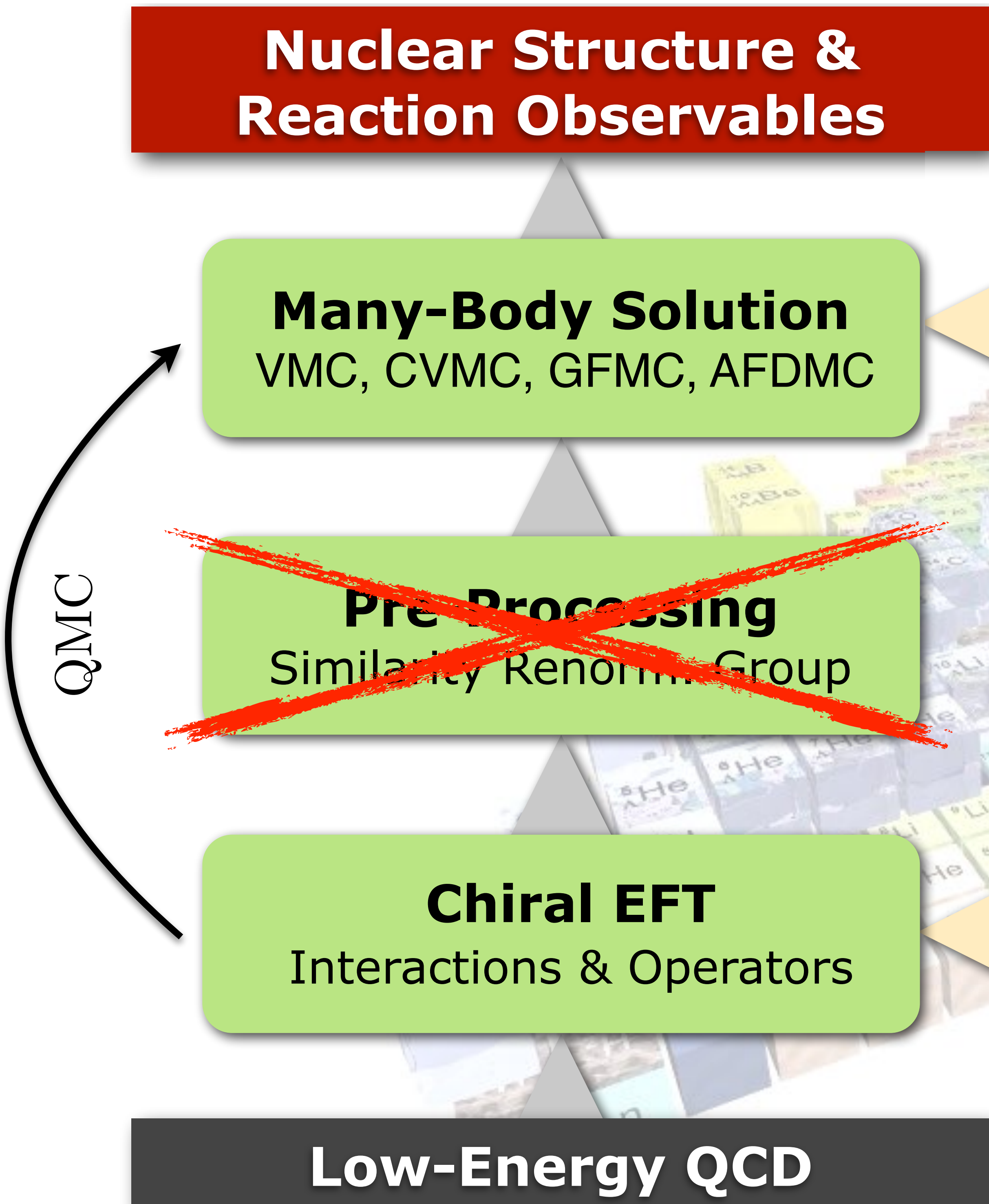
2018: "alternative" QMC calculations (AFDMC)

- Scaling: polinomial
- Nuclear Hamiltonians: local chiral interactions (Δ-less)

Goal: predict the emergence of nuclear properties and structure from first principles



Goal: predict the emergence of nuclear properties and structure from first principles

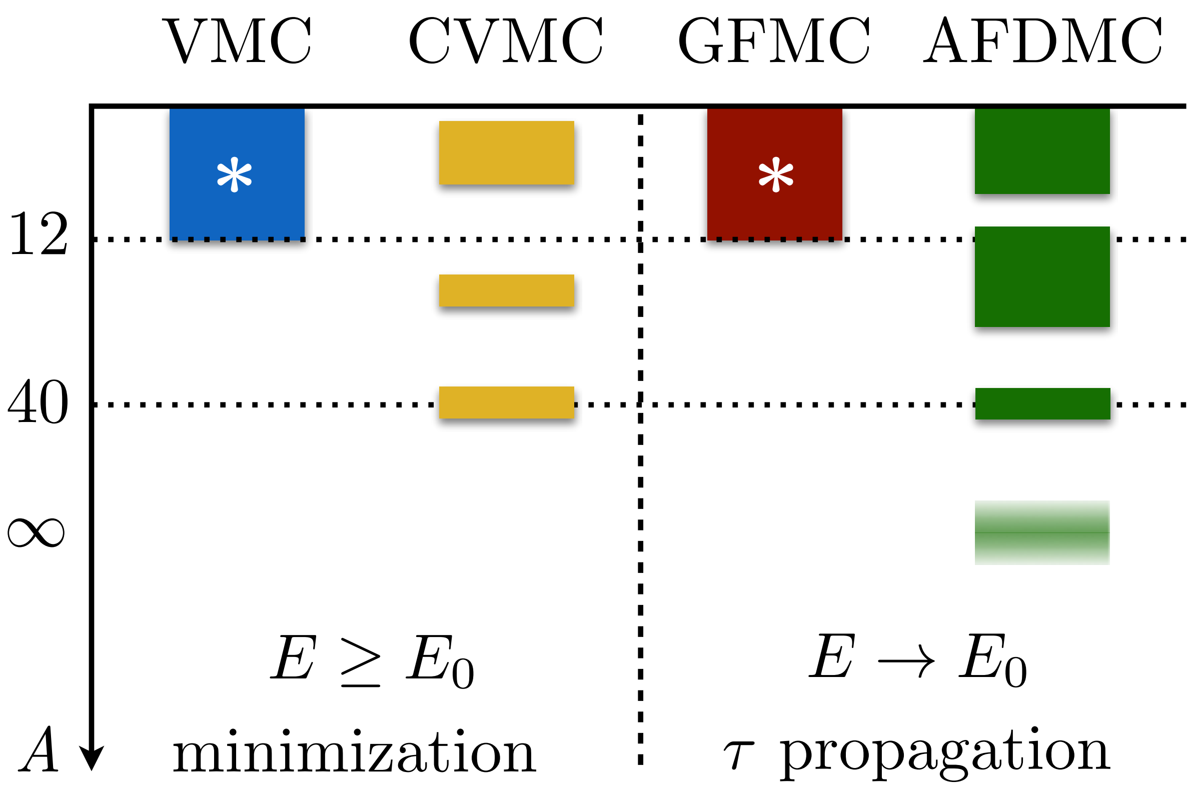


- different many-body methods for different mass regions and different observables
- ~~model-space and other truncations induce uncertainties~~
- statistical uncertainties (systematically improvable)

- systematic and improvable input for all ab initio calculations
- only "selected" chiral interactions used in nuclear structure so far
- truncations and regulators induce uncertainties

Quantum Monte Carlo methods

Idea: solve the many-body problem for correlated systems in a non perturbative fashion



(C)VMC GFMC AFDMC	light systems	$A \leq 12$
CVMC AFDMC	light to medium-mass nuclei	$A \sim 50$
AFDMC	infinite matter	$A \to \infty$

Pros:

- *Ab-initio*: microscopic "exact" approach, bare interactions
- Fully correlated many-body wave functions
- Stochastic method: errors quantifiable and systematically improvable $\sigma \sim 1/\sqrt{\mathcal{N}}$

Cons:

- Limitations in the systems and/or in the interaction to be used
- Can be computationally expensive

Quantum Monte Carlo methods

$$|\Psi_T\rangle = \mathcal{F}\,|\Phi\rangle$$

- $|\Phi\rangle$ long-range, low-momentum component (mean-field)
- $\mathcal{F}$ short-range, high-momentum component

1. VMC: variational search of optimal parameters for $|\Psi_T\rangle$

$$\text{minimize:}\quad E_V = \frac{\langle\Psi_T|H|\Psi_T\rangle}{\langle\Psi_T|\Psi_T\rangle} \geq E_0 \longrightarrow \text{NLopt, SR, LM}$$

2. DMC: propagation in imaginary time

$$|\Psi(\tau)\rangle = e^{-(H-E_0)\tau}|\Psi_T\rangle$$

$$= \sum_{n=0}^{\infty} e^{-(E_n-E_0)\tau} c_n|\psi_n\rangle \xrightarrow{\tau\to\infty} c_0|\psi_0\rangle \quad \text{(ground state)} \qquad \tau = \mathcal{M}d\tau \qquad \mathcal{M} \gg 1, \quad d\tau \ll 1$$

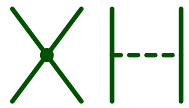
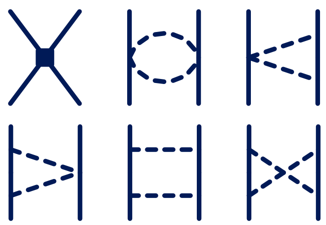
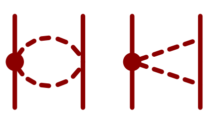
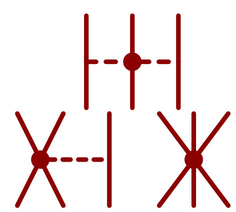
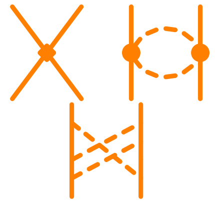
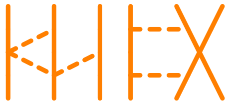
GFMC: sample of spatial degrees of freedom, full spin-isospin structure

scaling $\sim 2^A \binom{A}{Z}$

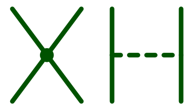
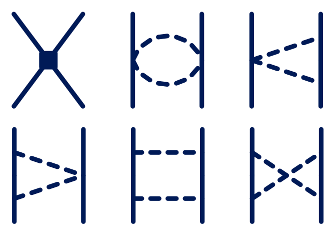
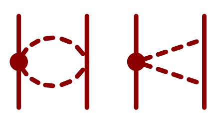
AFDMC: sample of both spatial and spin-isospin degrees of freedom

scaling $\sim A^n$ (currently n=4)

Nuclear Hamiltonians: chiral interactions

		NN	NNN	NNNN
LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^0$		—	—
NLO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^2$		—	—
N^2LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^3$			—
N^3LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^4$	 $+\cdots$	 $+\cdots$	$\cdots$

Nuclear Hamiltonians: chiral interactions

	NN
LO $\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^0$	
NLO $\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^2$	
N^2LO $\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^3$	

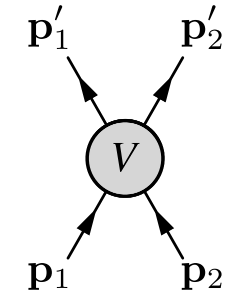
local in coordinate space

↓

good for QMC

Regularization schemes for nuclear interactions (here: NN)

Separation of long- and short-range physics



$$\mathbf{p} = (\mathbf{p}_1 - \mathbf{p}_2)/2$$
$$\mathbf{p}' = (\mathbf{p}_1' - \mathbf{p}_2')/2$$
$$\mathbf{Q} = (\mathbf{p}_1 - \mathbf{p}_1')$$

nonlocal

$$V_{\mathrm{NN}}(\mathbf{p},\mathbf{p}') \to \exp\left[-\left((p^2+p'^2)/\Lambda^2\right)^n\right] V_{\mathrm{NN}}(\mathbf{p},\mathbf{p}')$$

Epelbaum, Glöckle, Meissner, NPA 747, 362 (2005)
Entem, Machleidt, PRC 68, 041001 (2003)

local (momentum space)

$$V_{\mathrm{NN}}(\mathbf{Q}) \to \exp\left[-(Q^2/\Lambda^2)^n\right] V_{\mathrm{NN}}(\mathbf{Q})$$

cf. Navratil, Few-body Systems 41, 117 (2007)

local (coordinate space)

$$V^{\pi}_{\mathrm{NN}}(\mathbf{r}) \to \left(1 - \exp\left[-\left(r^2/R^2\right)^n\right]\right) V^{\pi}_{\mathrm{NN}}(\mathbf{r})$$
$$\delta(\mathbf{r}) \to \alpha_n \exp\left[-(r^2/R^2)^n\right]$$

Gezerlis et. al, PRL, 111, 032501 (2013)

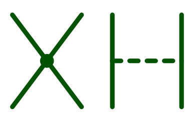
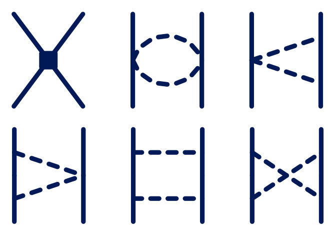
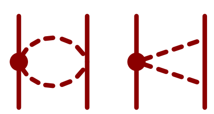
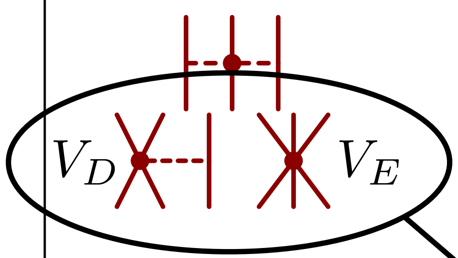
semi-local

$$V^{\pi}_{\mathrm{NN}}(\mathbf{r}) \to \left(1 - \exp\left[-\left(r^2/R^2\right)\right]\right)^n V^{\pi}_{\mathrm{NN}}(\mathbf{r})$$
$$\delta(\mathbf{r}) \to C \to \exp\left[-\left((p^2+p'^2)/\Lambda^2\right)^n\right] C$$

Epelbaum et. al, PRL, 115, 122301 (2015)

K. Hebeler's talk @ INT 19-2a, July 1st, 2019

Nuclear Hamiltonians: chiral interactions

		NN	*NNN*
LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^0$		—
NLO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^2$		—
N^2LO	$\mathcal{O}\left(\frac{Q}{\Lambda_b}\right)^3$		

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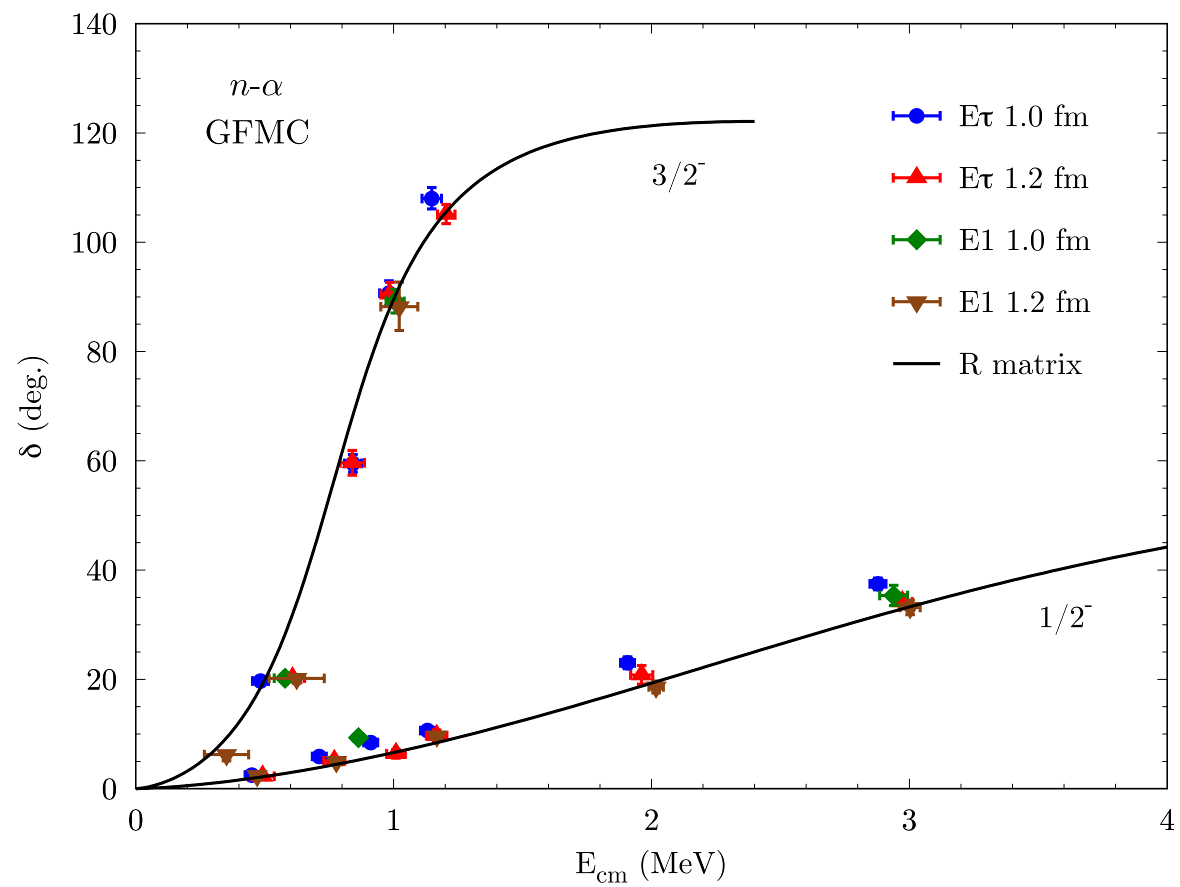
good for QMC

J.E. Lynn *et al.*, PRL **116**, 062501 (2016)
D.L. *et al.*, PRC **97**, 044318 (2018)



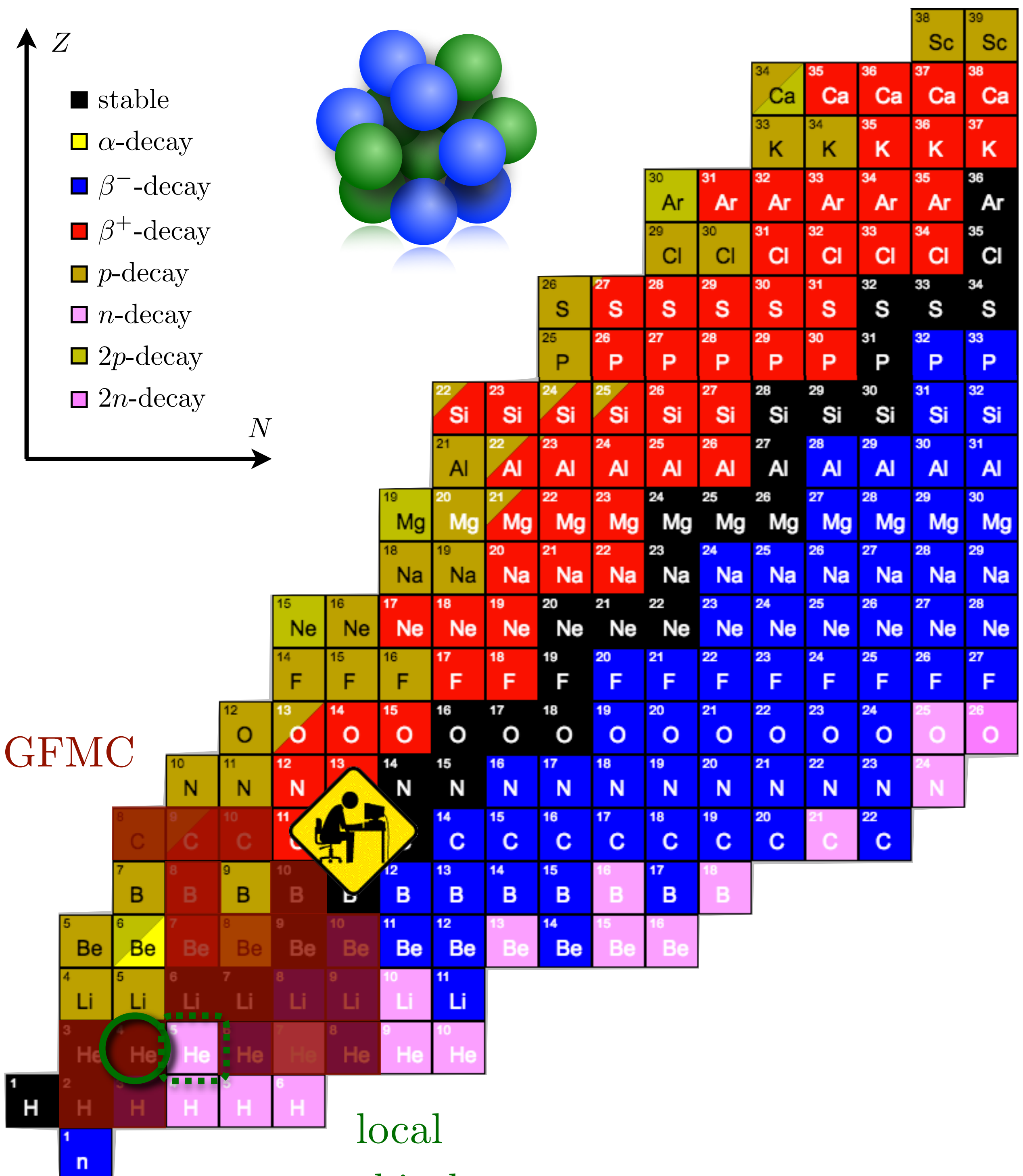
local chiral potentials at N^2LO

- 2b LECs fit to *NN* phase shifts
- 3b LECs fit to (GFMC):
  - ✓ ^{4}He binding energy
  - ✓ n-α scattering phase shifts

↓

info on $T = \frac{3}{2}$ and spin-orbit physics

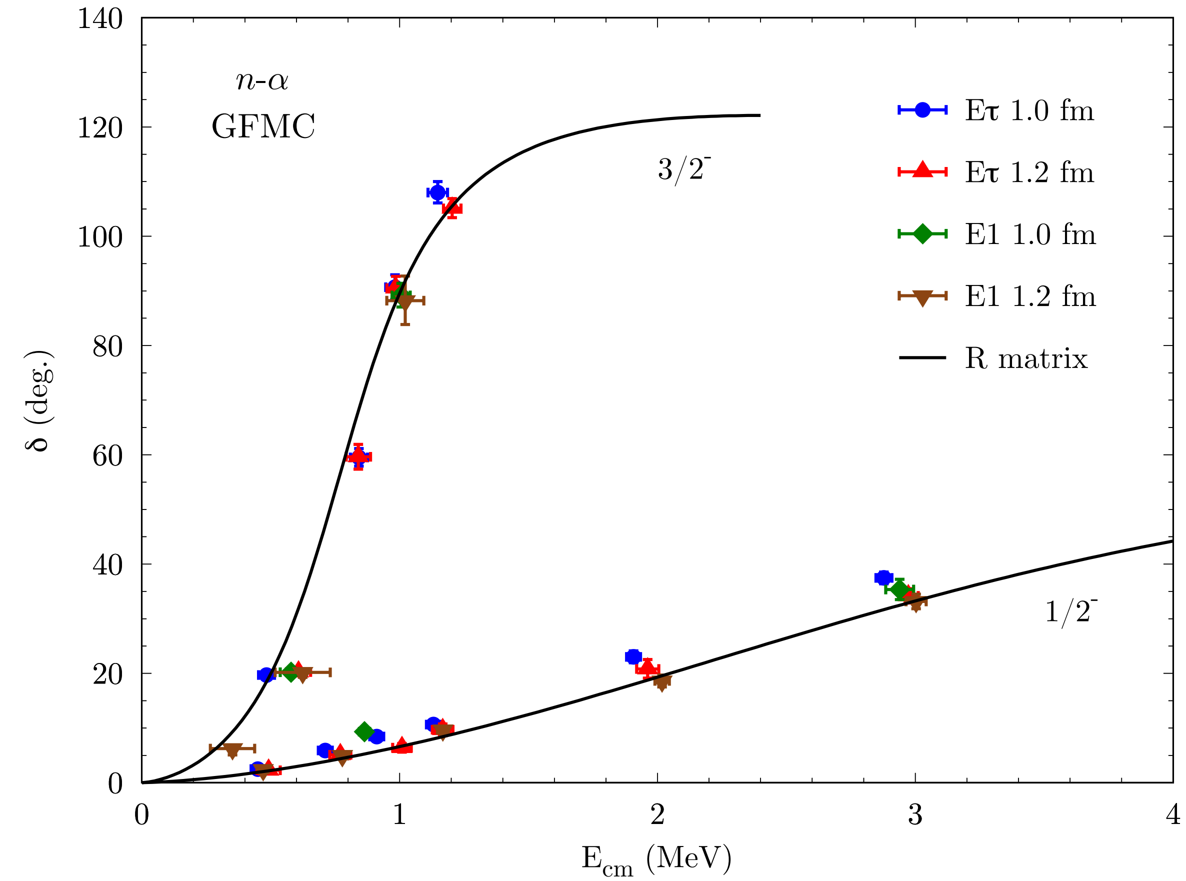
QMC & local chiral interactions



GFMC

local chiral

AV18+3b (UIX, IL7)



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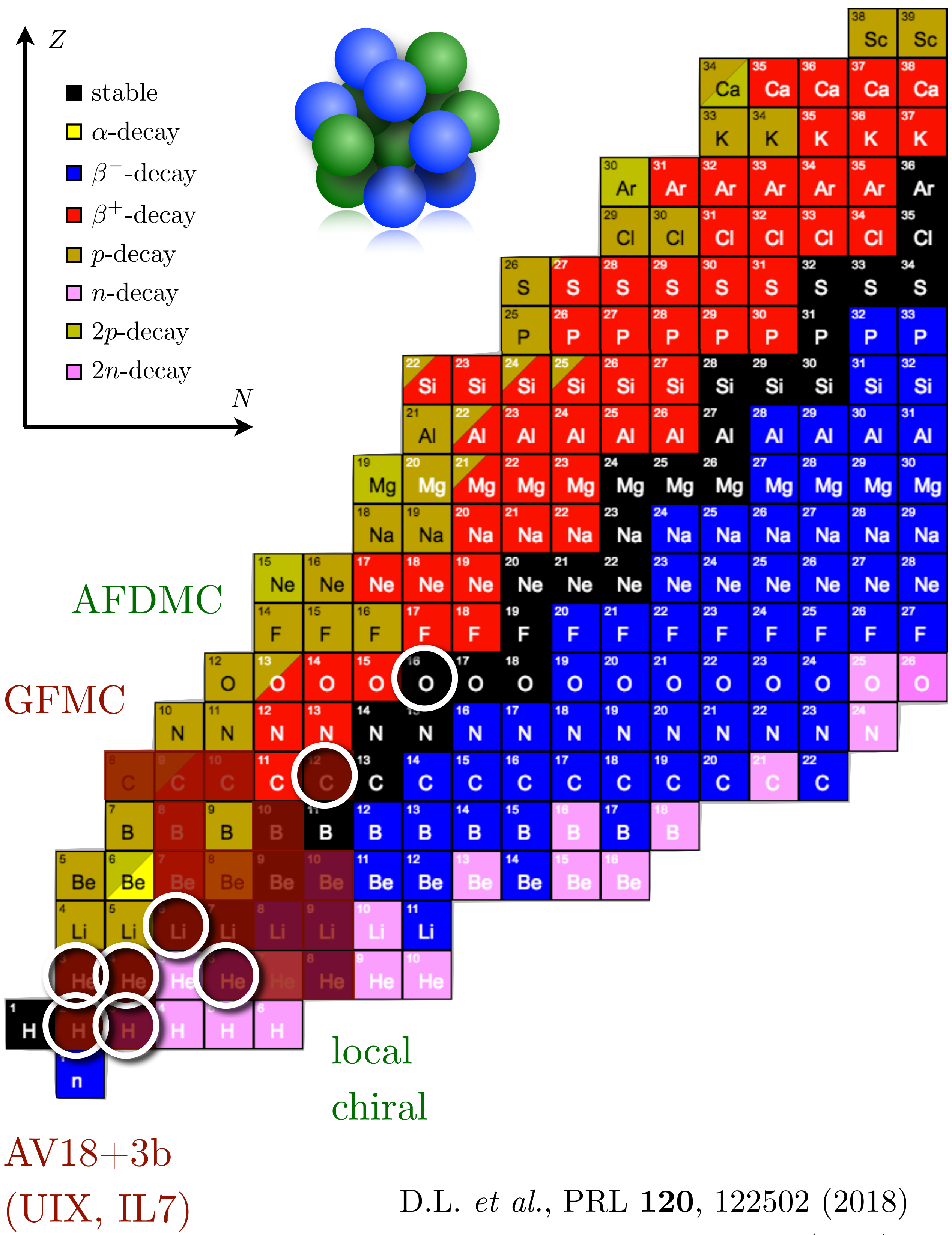

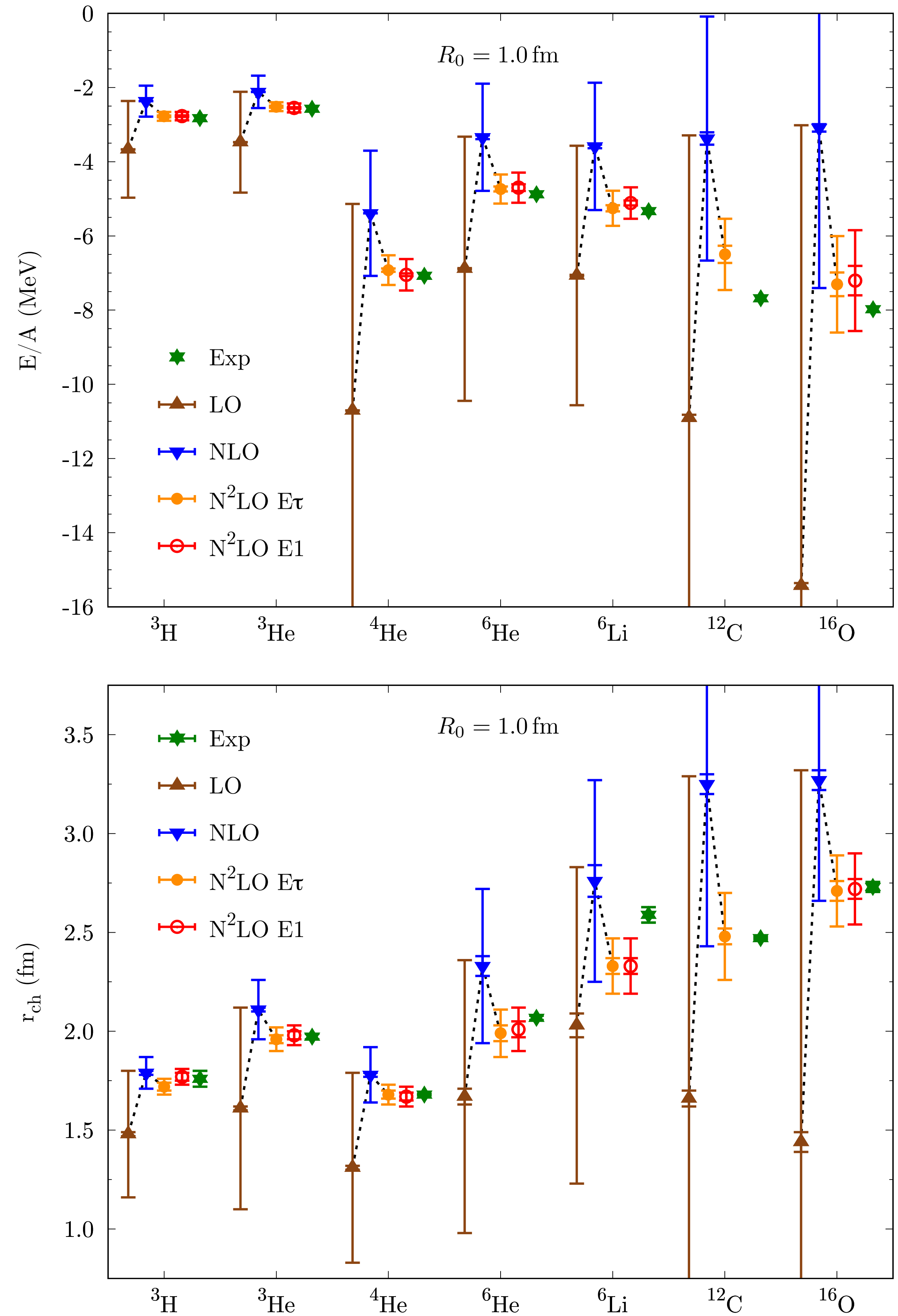

D.L. *et al.*, PRL **120**, 122502 (2018)

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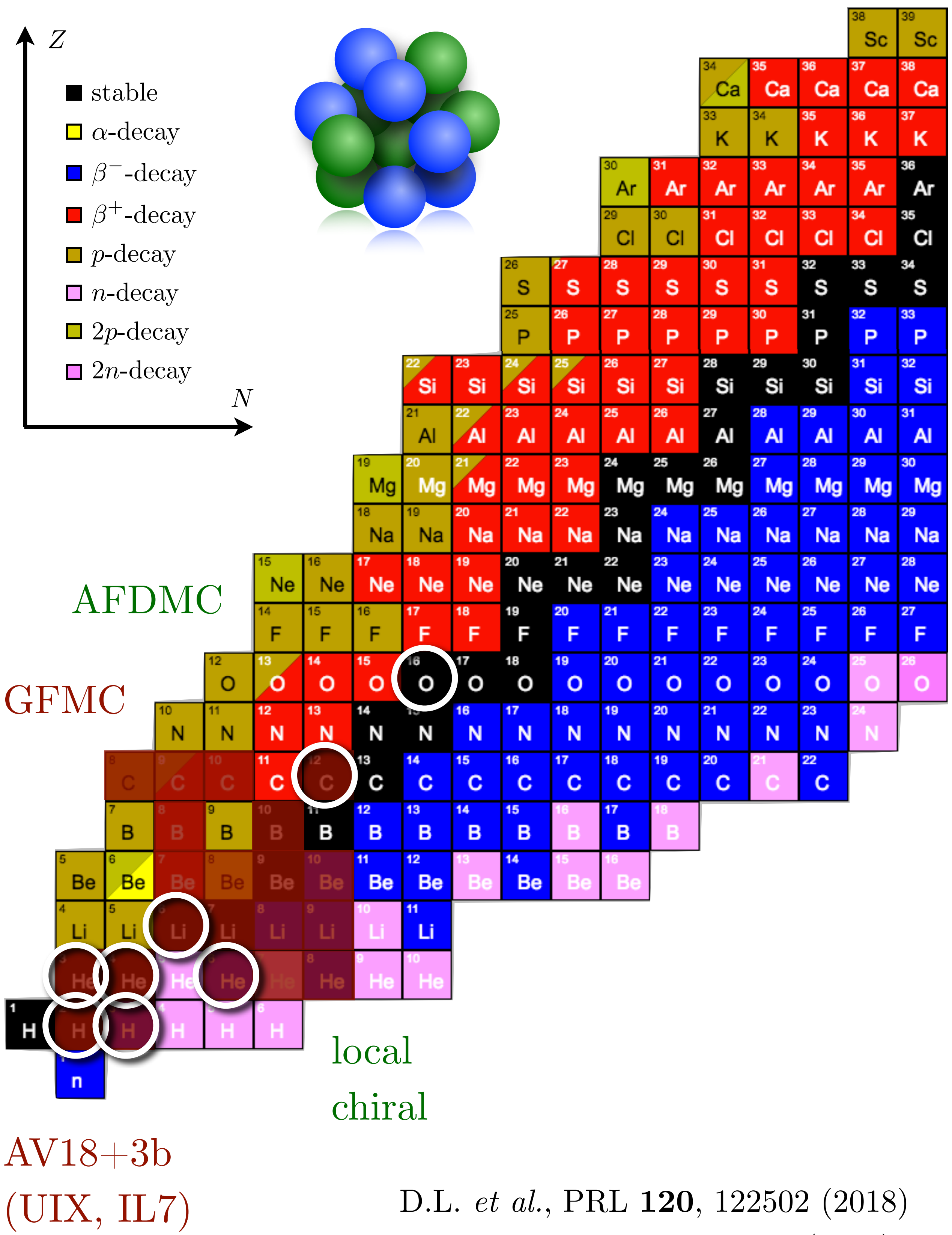

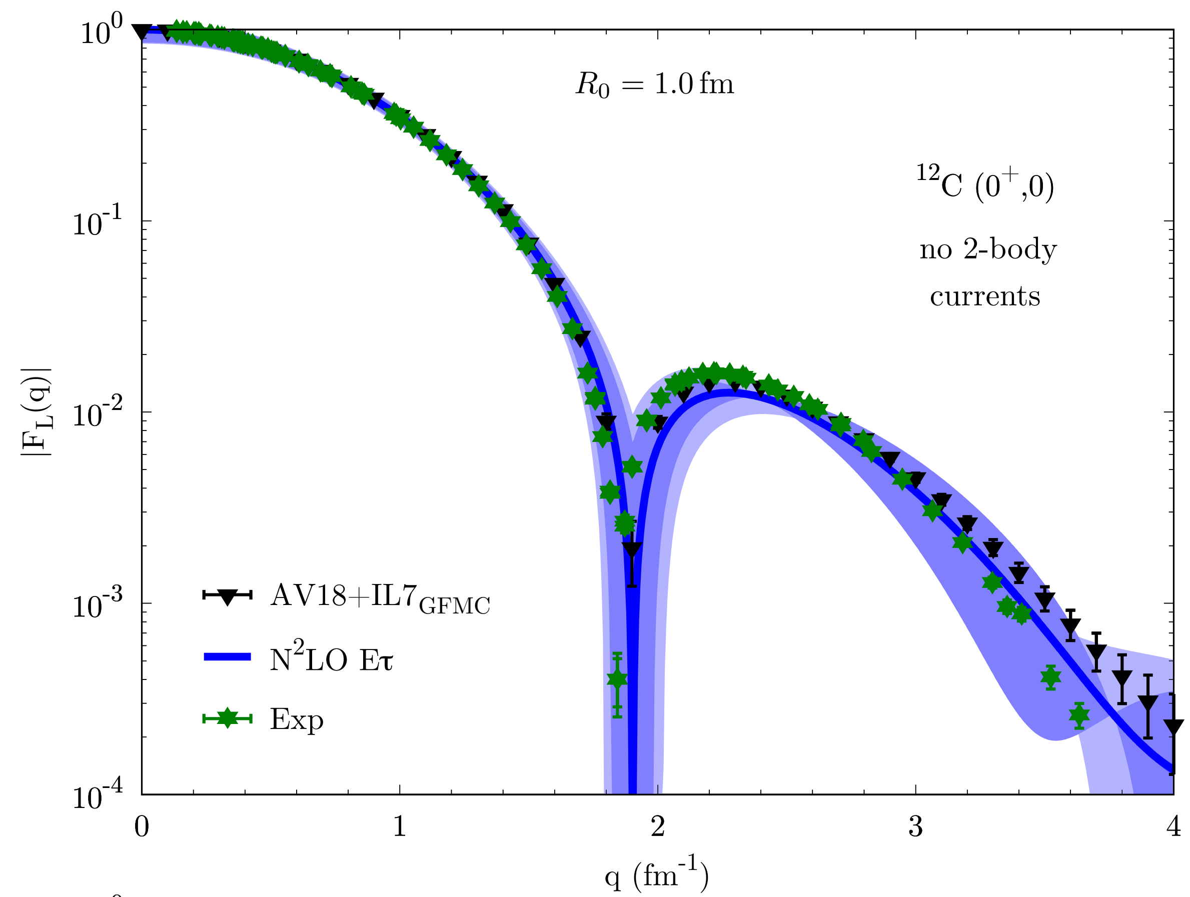

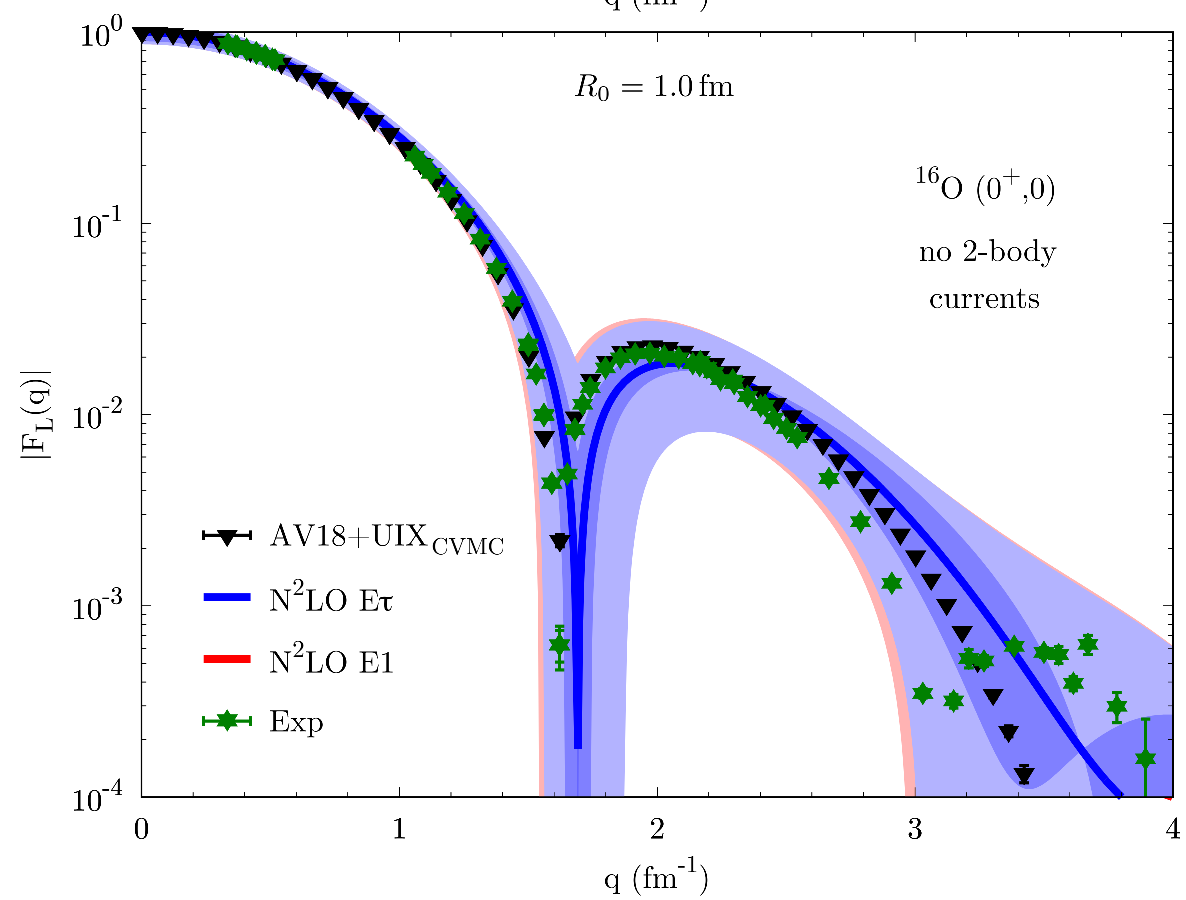

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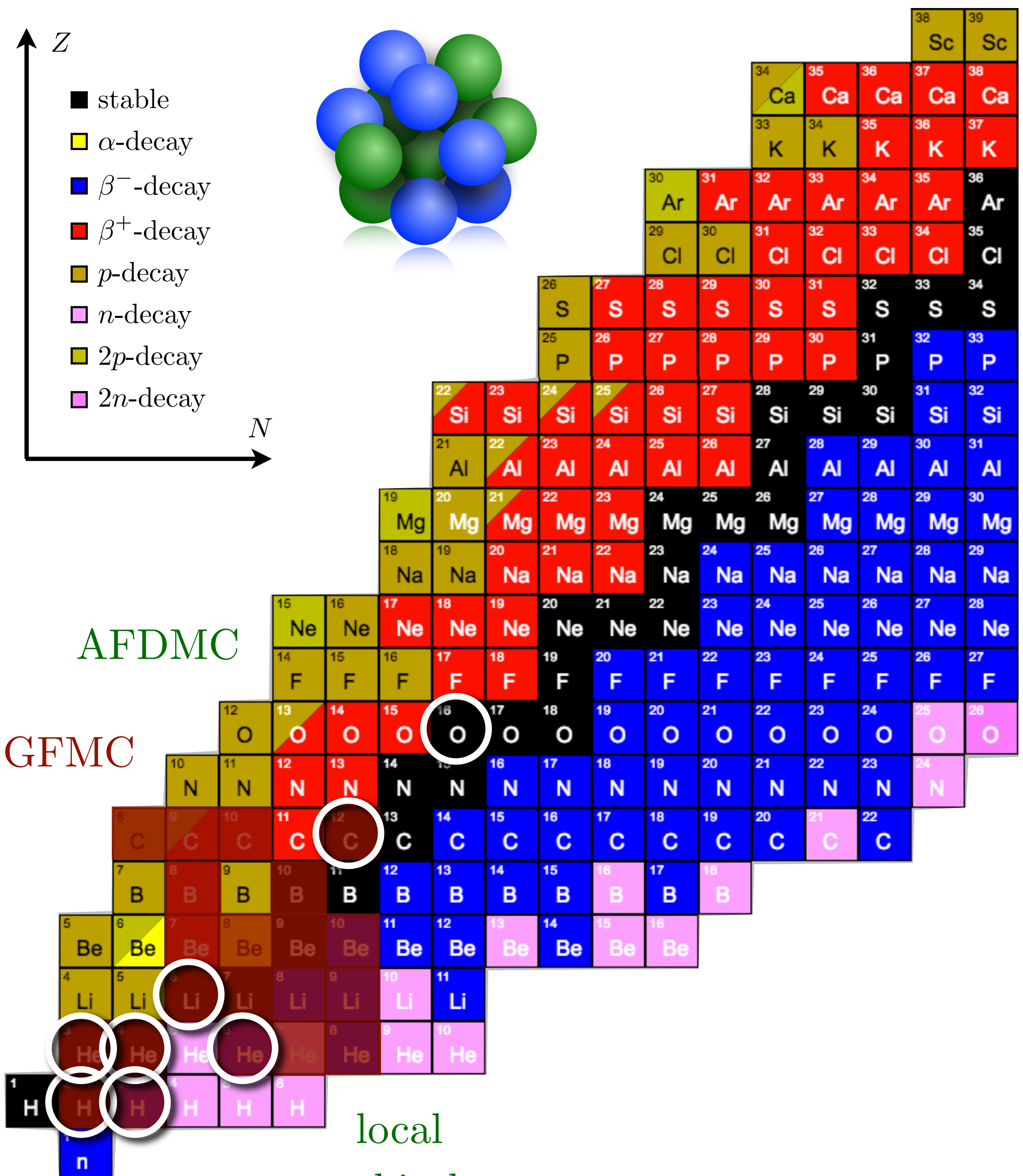
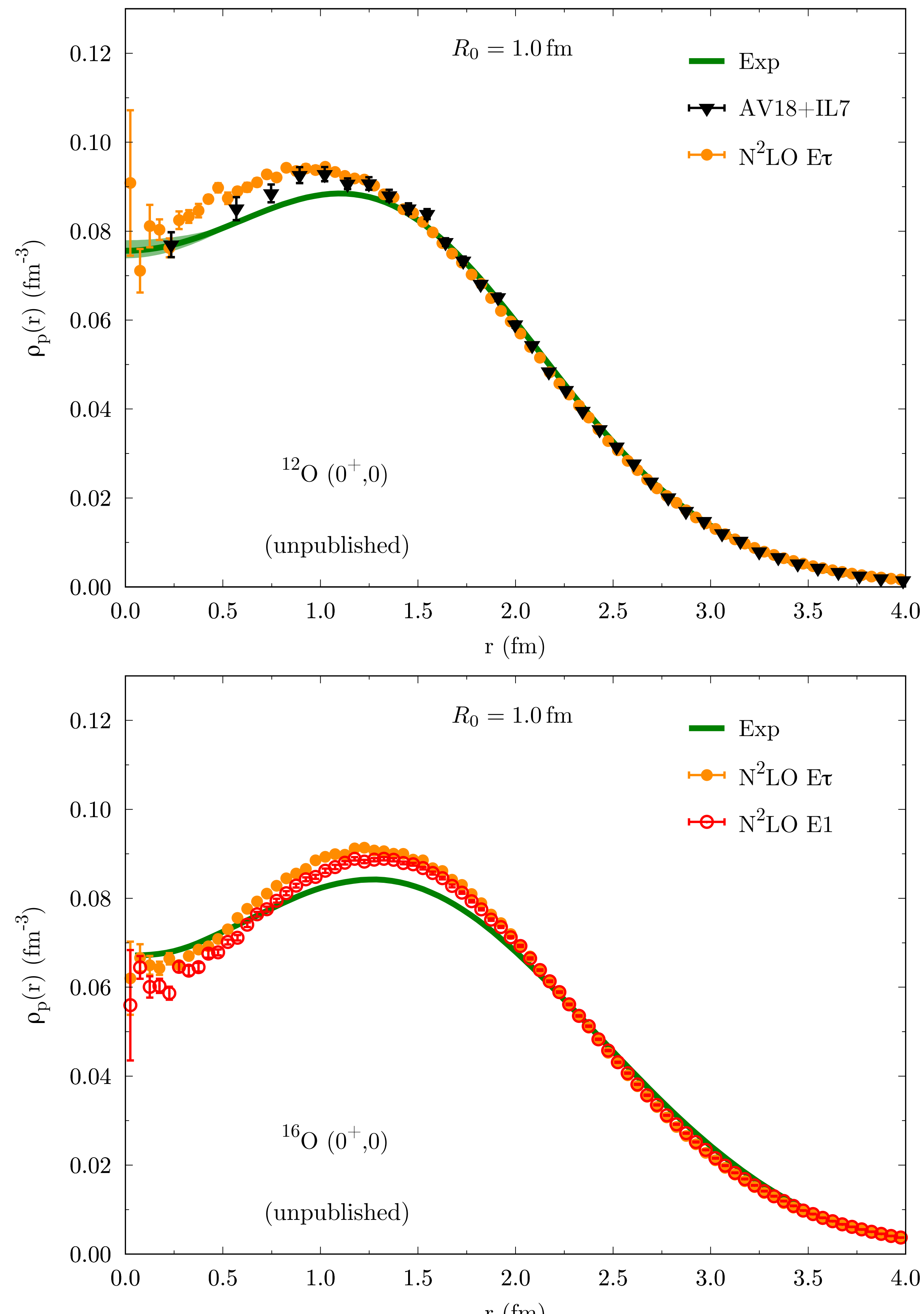


AV18+3b
(UIX, IL7)



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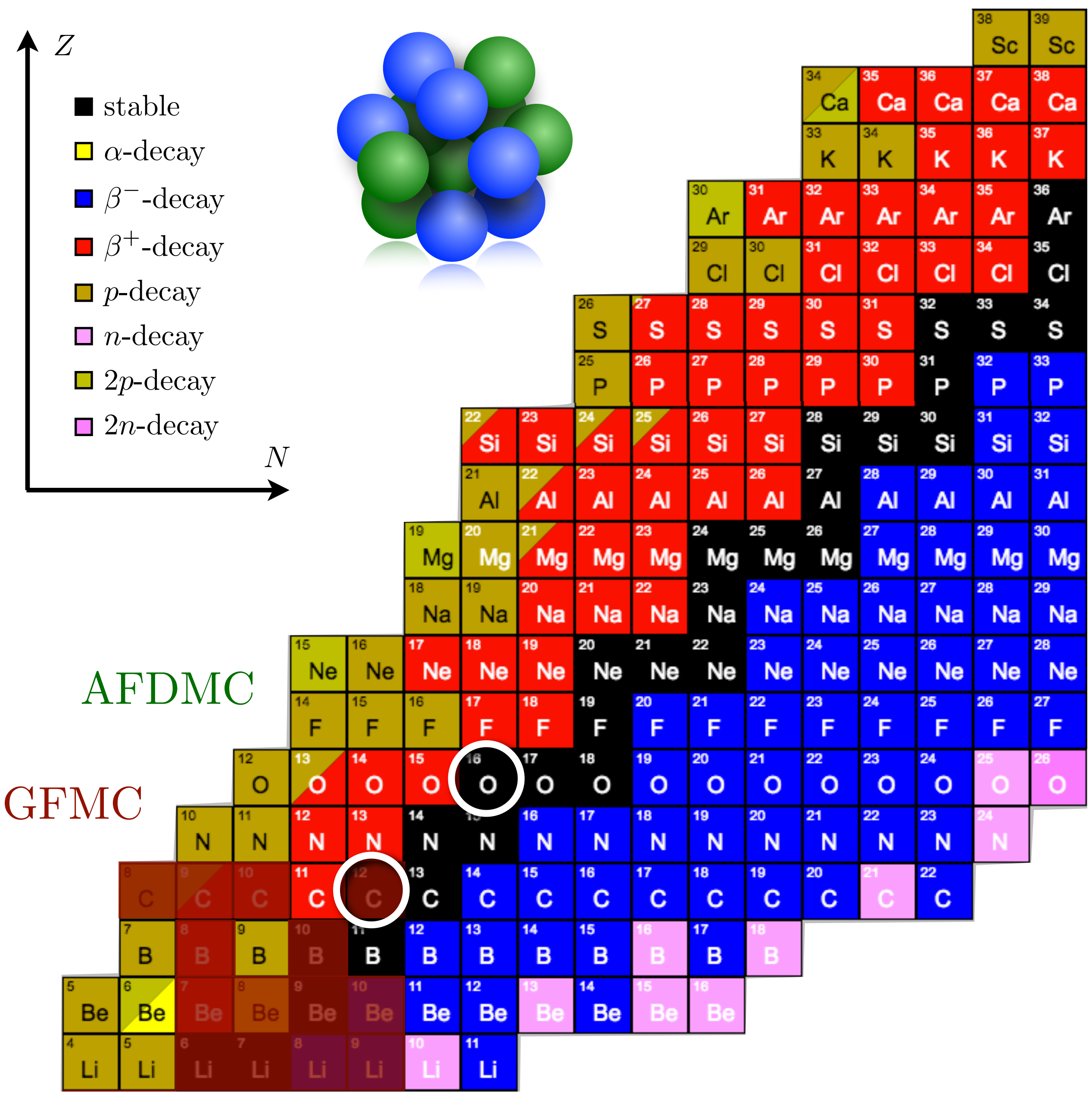


R. Cruz-Torres, D.L. *et al.*, arXiv:1907.03658 [nucl-th]
J.E. Lynn, D.L. *et al.*, arXiv:1903.12587 [nucl-th]
R. Cruz-Torres, D.L. *et al.*, PLB **797**, 134890 (2019)
S.H. Lim, D.L. *et al.*, PRC **99**, 044904 (2019)
D.L. *et al.*, PRC **98**, 014322 (2018)
D.L. *et al.*, PRC **97**, 044318 (2018)
D.L. *et al.*, PRL **120**, 122502 (2018)

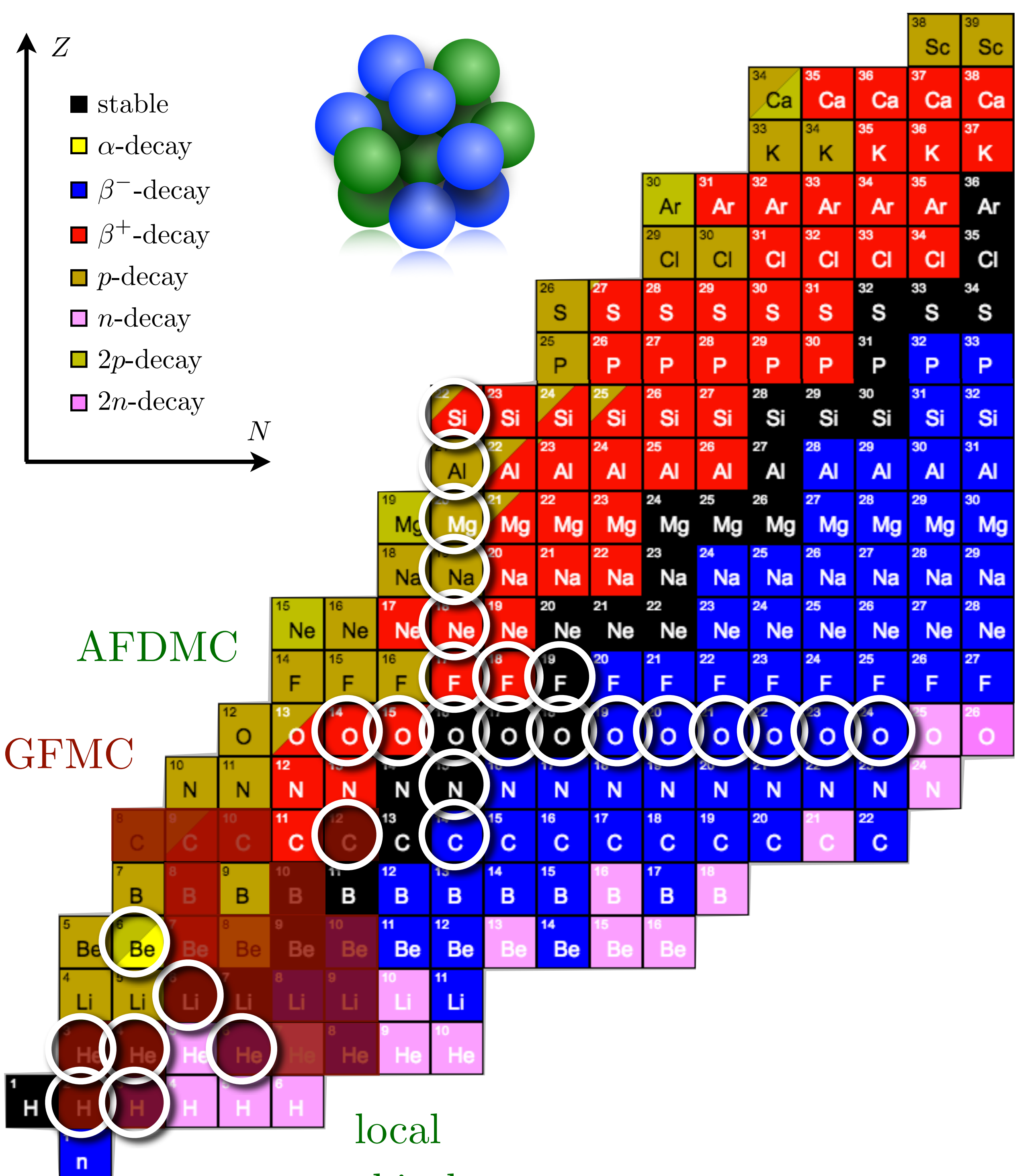
direct calculation:

- binding energies (& operators)
- nucleon radii
- single- & two-nucleon coordinate-space densities
- single- & two-nucleon momentum-space densities

derived quantities:

- charge radii
- nucleon skins
- charge form factors
- Coulomb sum rules
- short-range correlation scaling factor
- slope of the EMC effect
- “nuclear contacts”
- geometries for heavy ion collisions
- (beta-decay matrix elements)

QMC & local chiral interactions

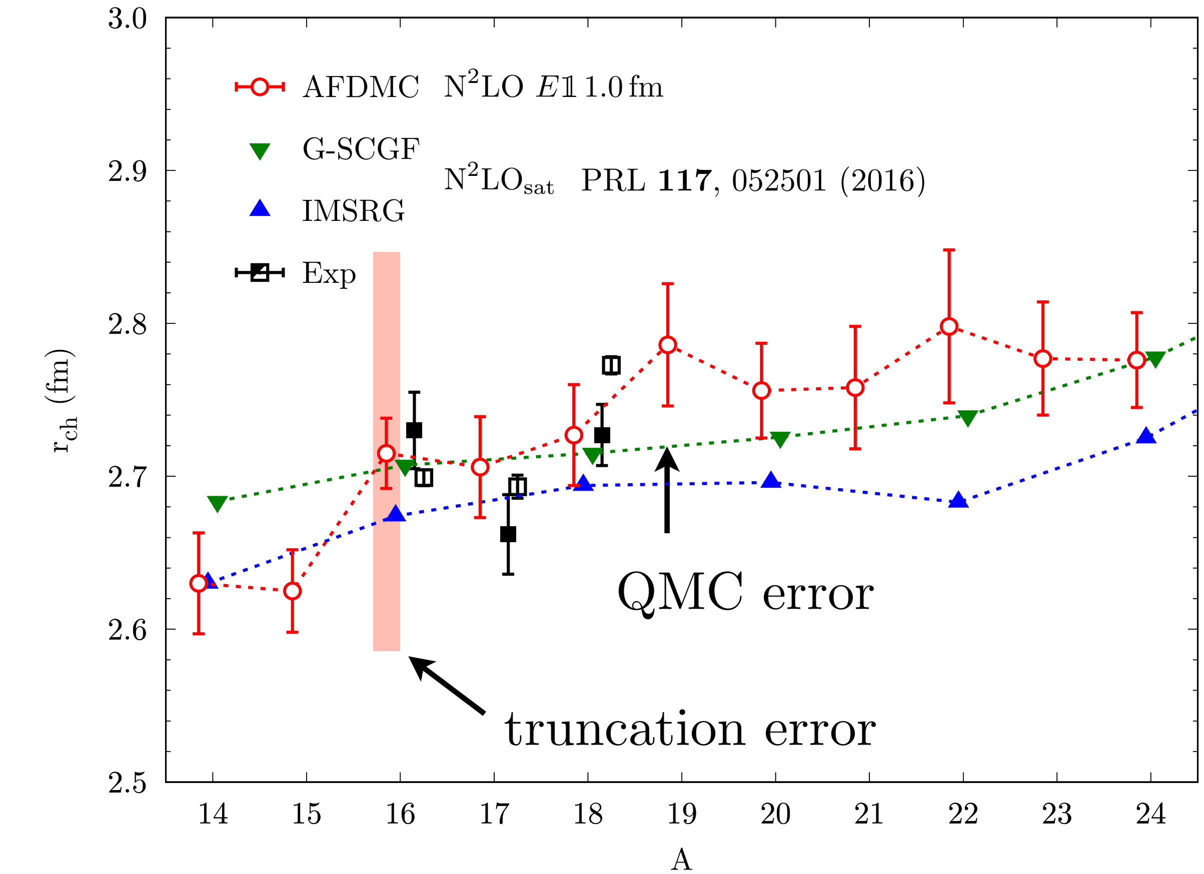


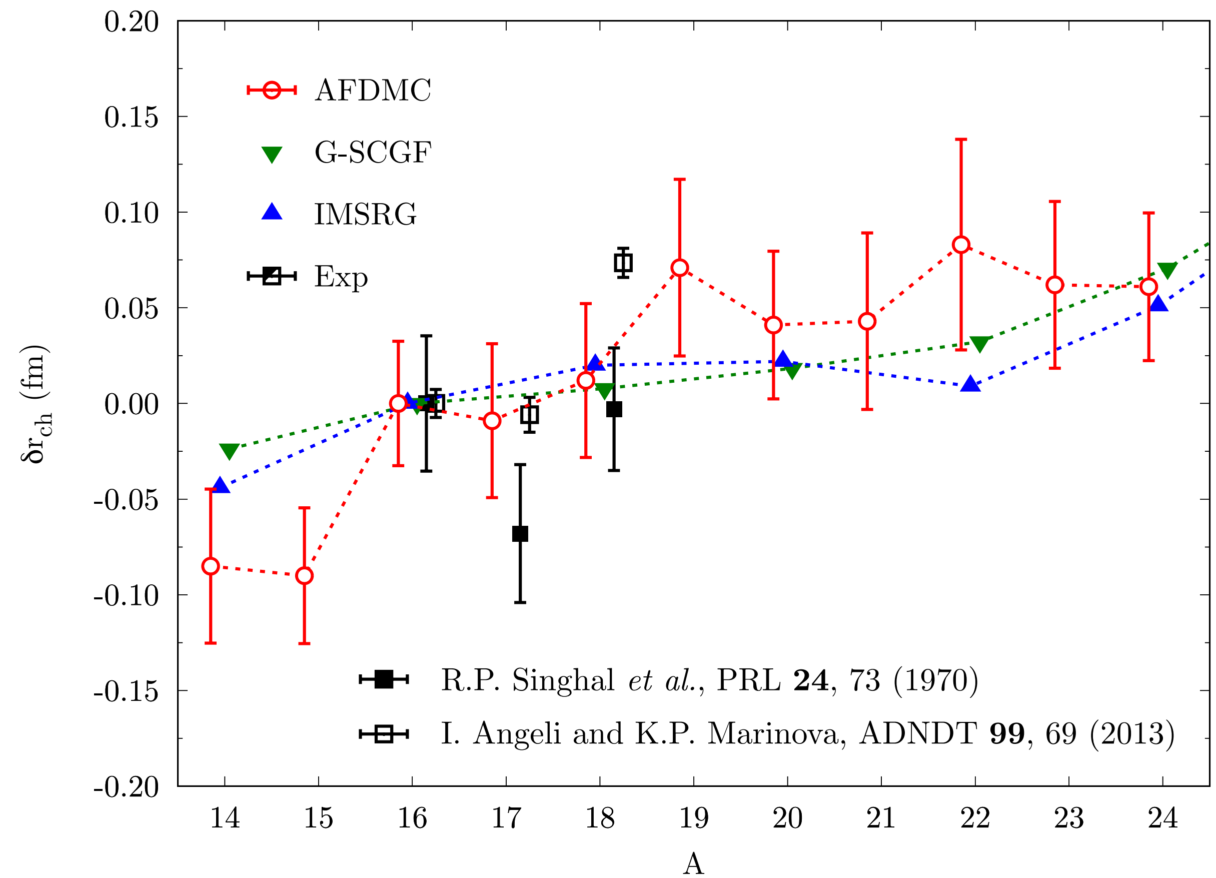
AFDMC

GFMC

local chiral

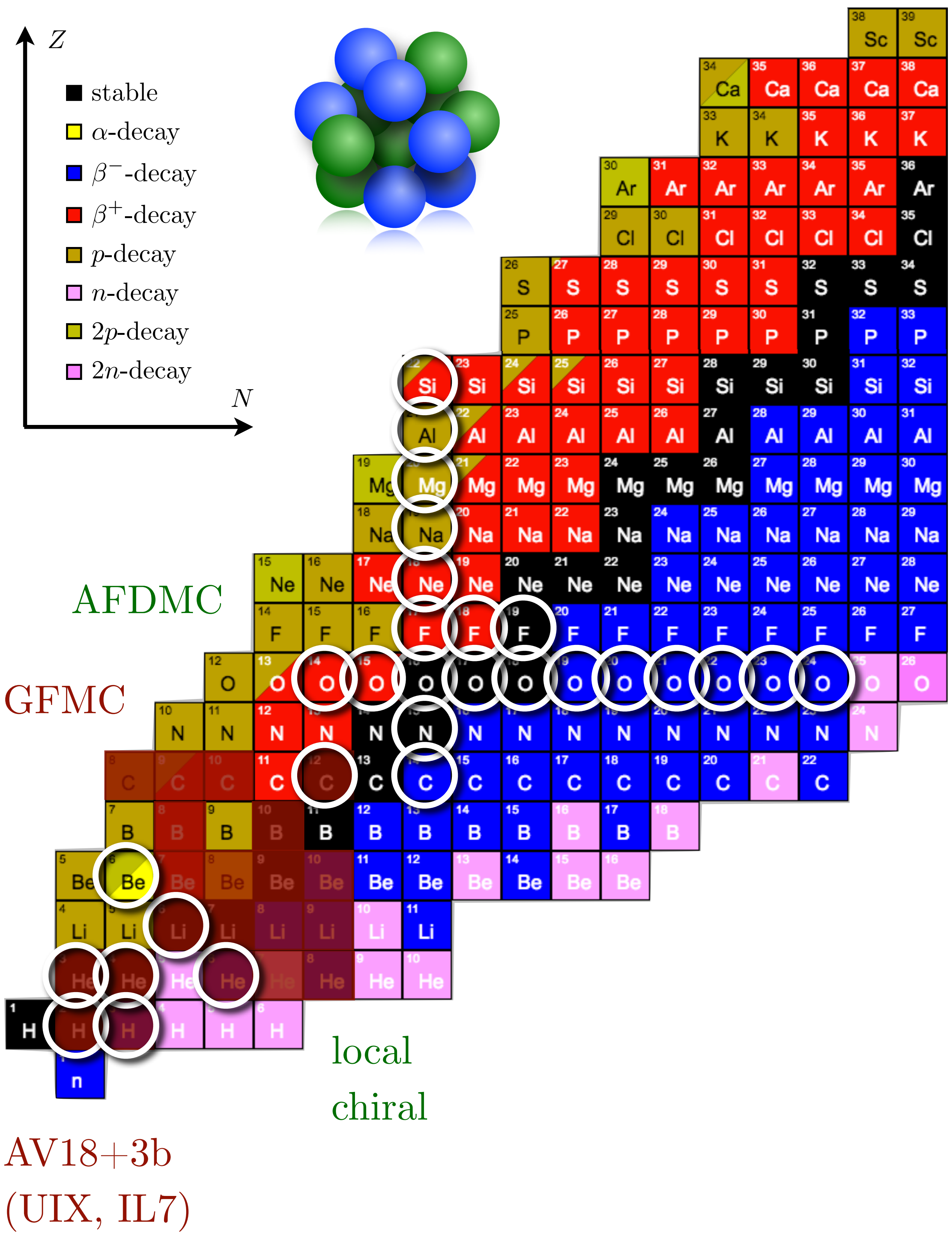
AV18+3b (UIX, IL7)

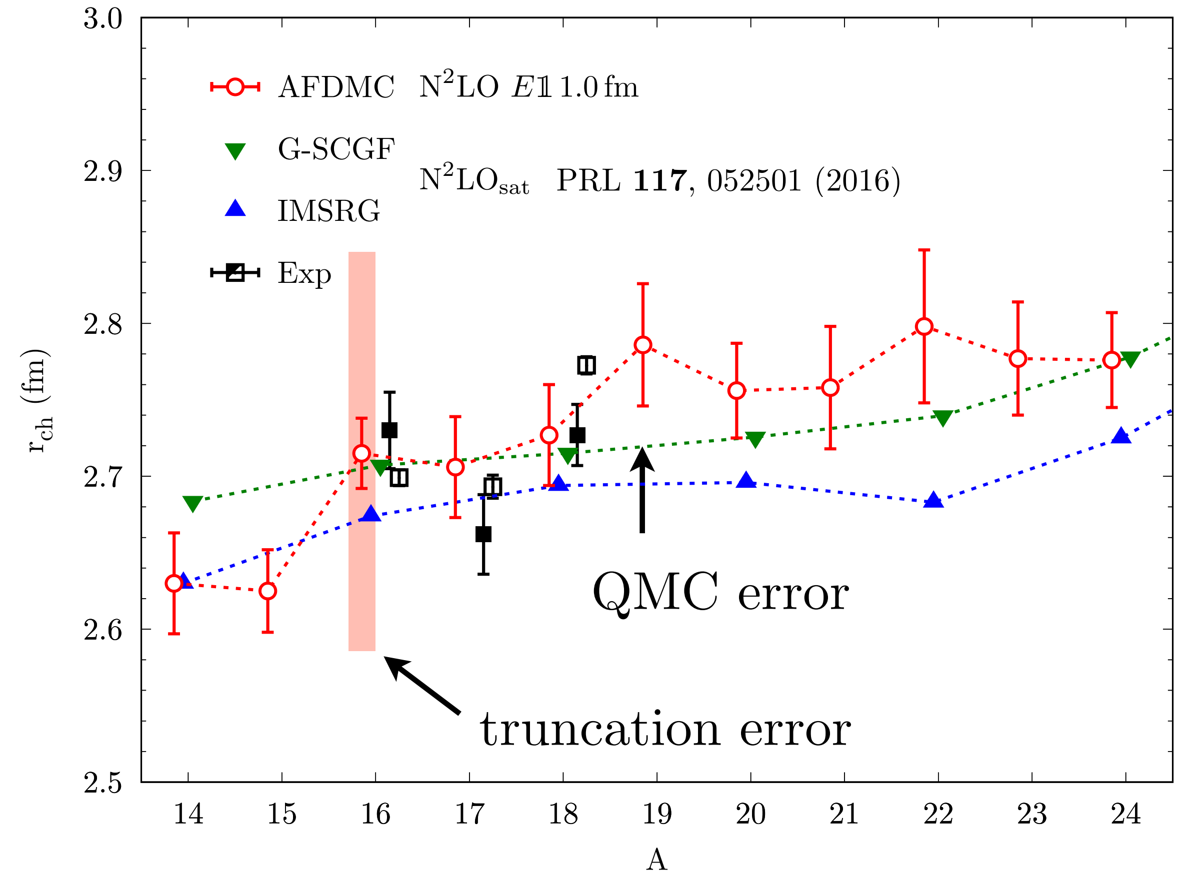




preliminary!!

QMC & local chiral interactions

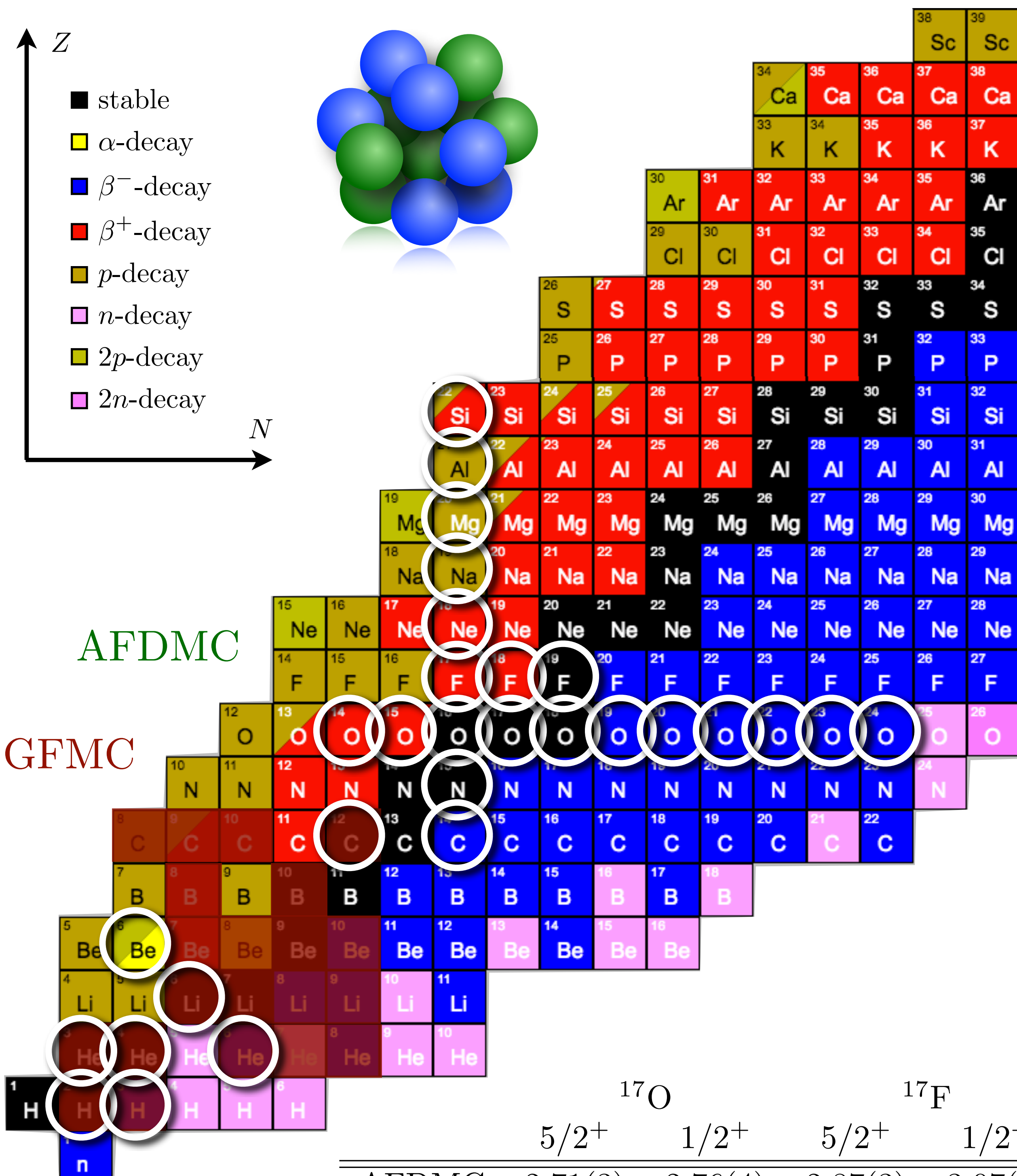




$^{A}Z\ (J^\pi, T)$	AFDMC	Exp.	
^{12}C $(0^+, 0)$	2.48(4)	2.47(1)	*e*-scattering
^{14}C $(0^+, 1)$	2.48(4)	2.56(5)	*e*-scattering
		2.50(2)	muonic X-ray
^{15}N $(\frac{1}{2}^-, \frac{1}{2})$	2.58(5)	2.58(3)	*e*-scattering
		2.61(1)	*e*-scattering
→ ^{17}F $(\frac{5}{2}^+, \frac{1}{2})$	2.87(5)	–	
^{18}F $(1^+, 0)$	3.03(8)	–	
^{19}F $(\frac{1}{2}^+, \frac{3}{2})$	3.01(7)	2.90(2)	*e*-scattering
		2.90(1)	muonic X-ray
^{18}Ne $(0^+, 1)$	3.06(6)	2.97(8)	ref ^{20}Ne (e^-)
		2.97(3)	ref ^{20}Ne (μ)

preliminary!!

QMC & local chiral interactions



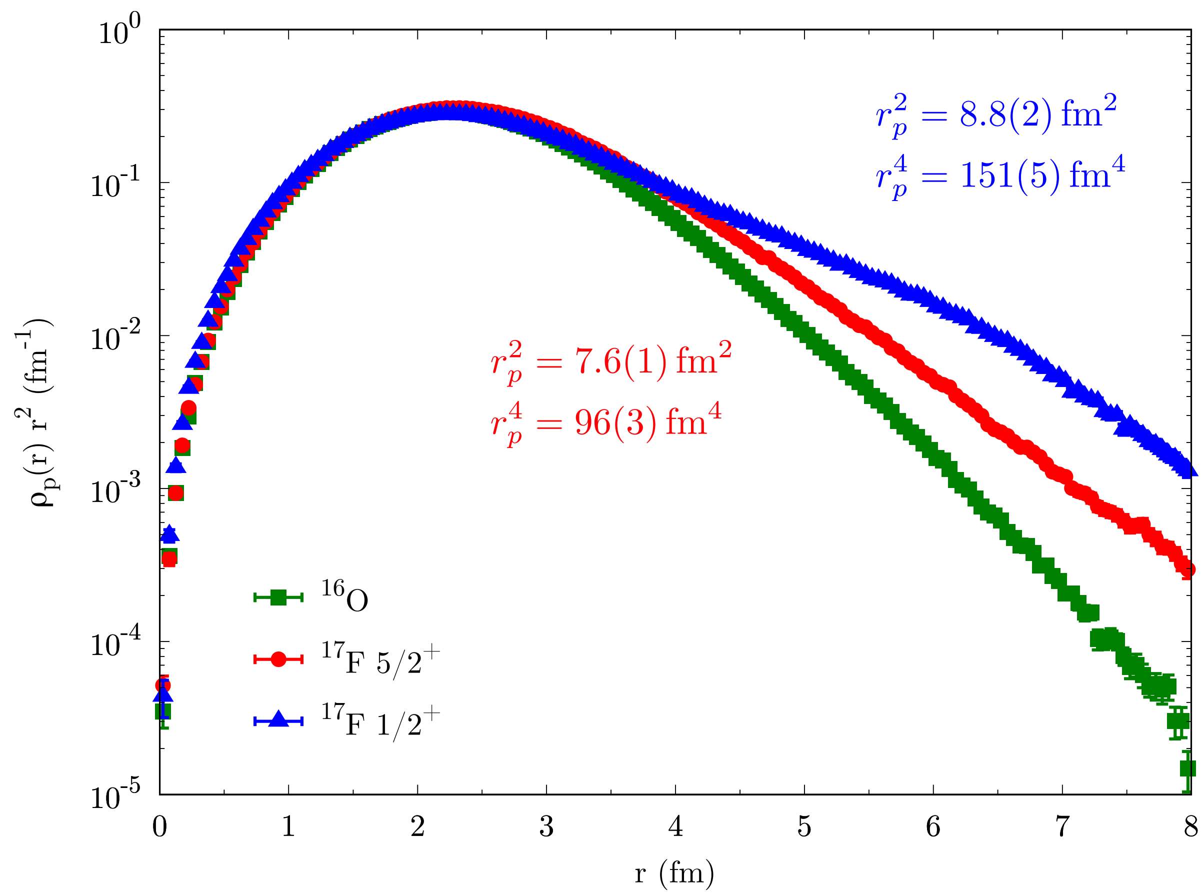
AFDMC

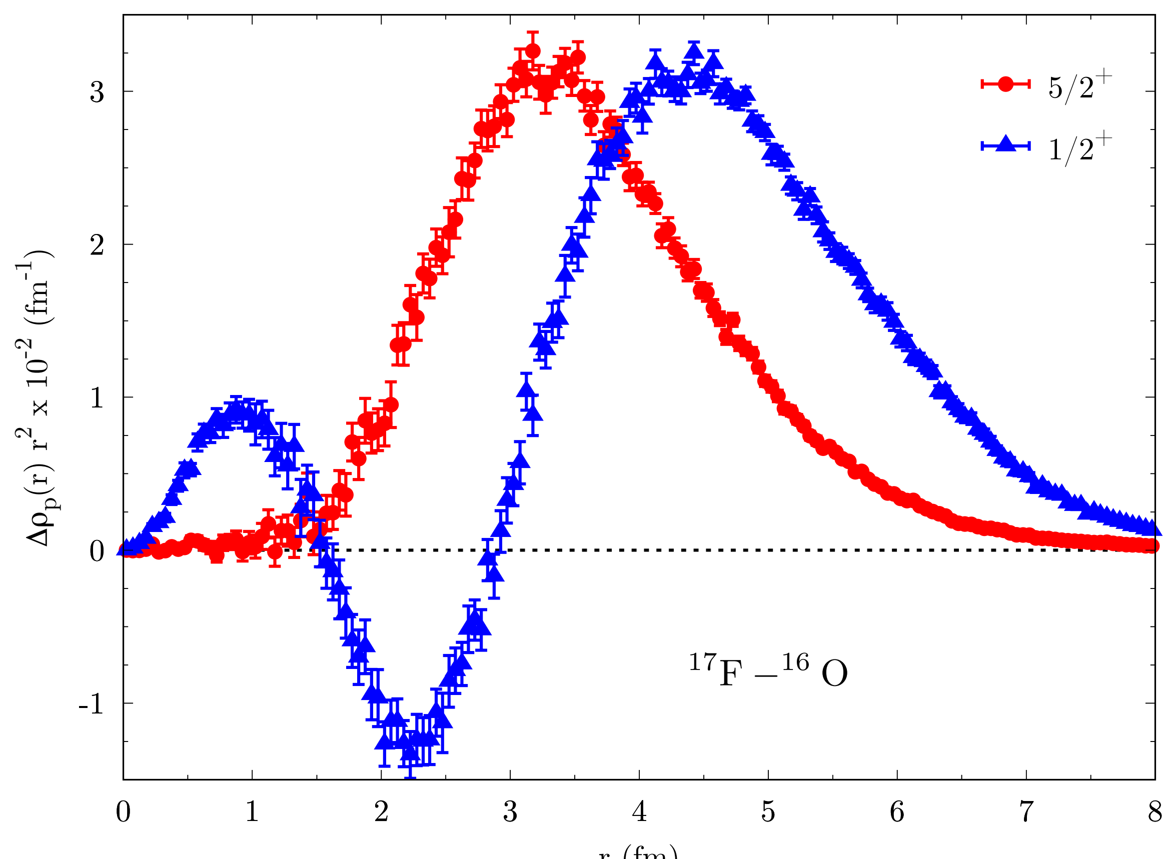
GFMC

AV18+3b
(UIX, IL7)

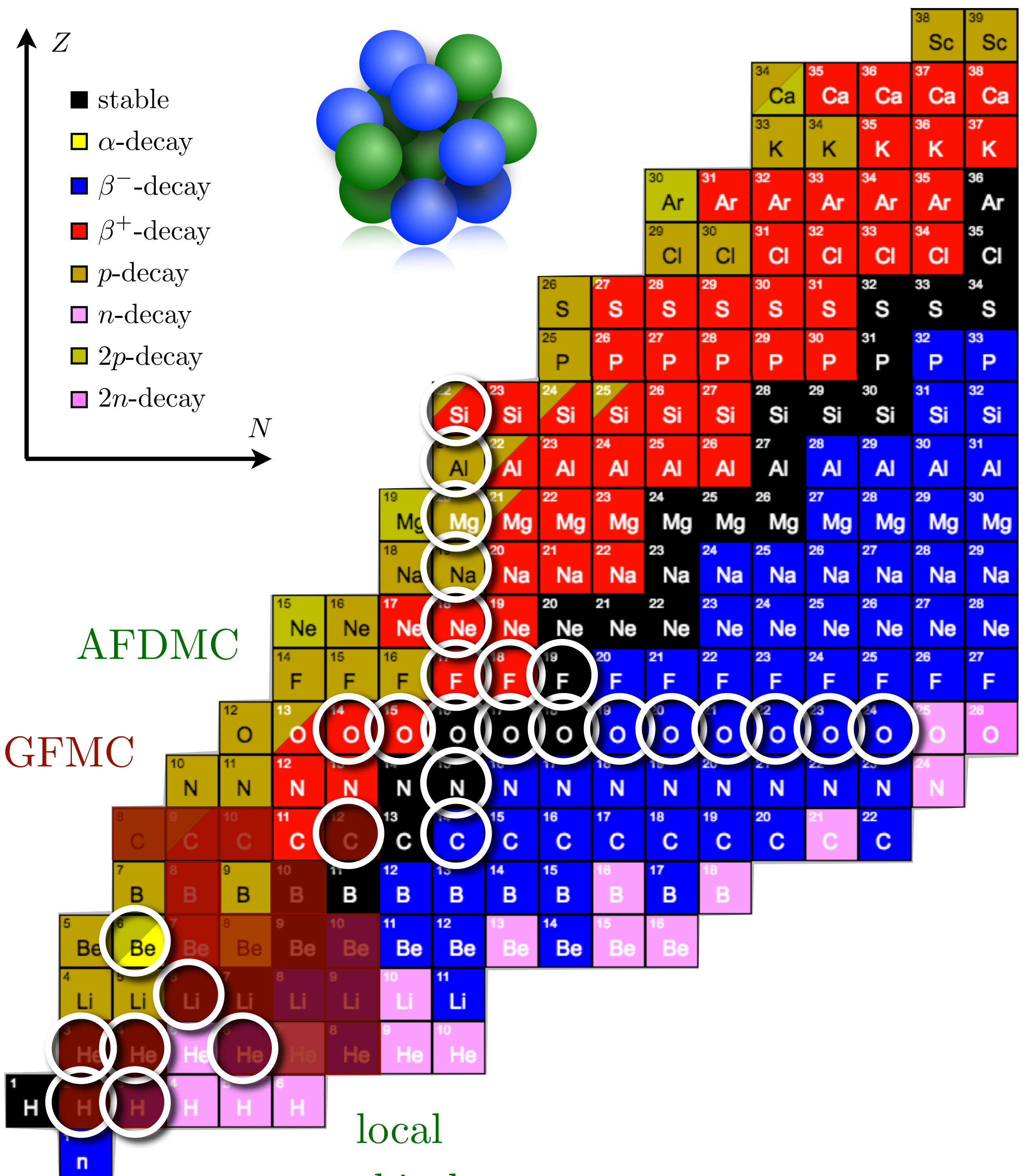
	^{17}O		^{17}F	
	$5/2^+$	$1/2^+$	$5/2^+$	$1/2^+$
AFDMC	2.71(3)	2.76(4)	2.87(3)	3.07(4)
Exp.	2.66(3)	–	–	–
	2.69(1)	–	–	–

preliminary!!





QMC & local chiral interactions



AFDMC

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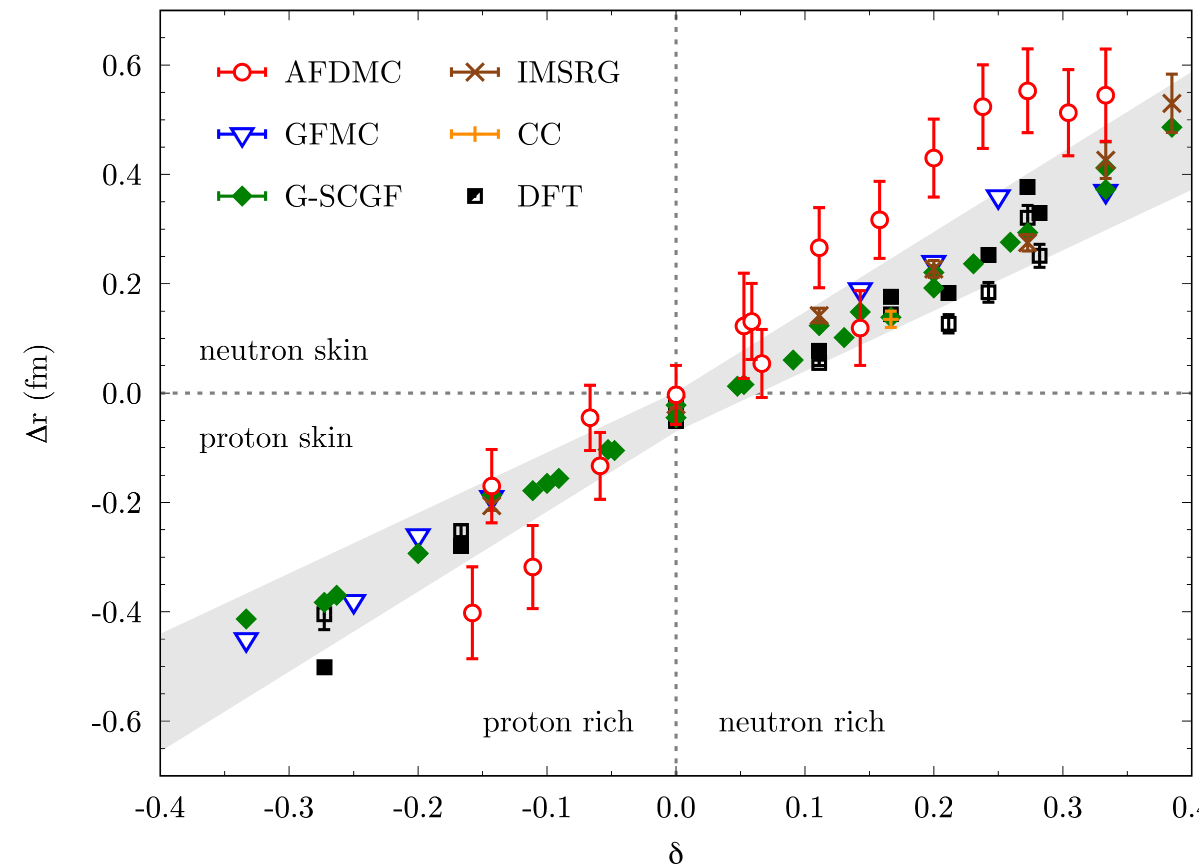

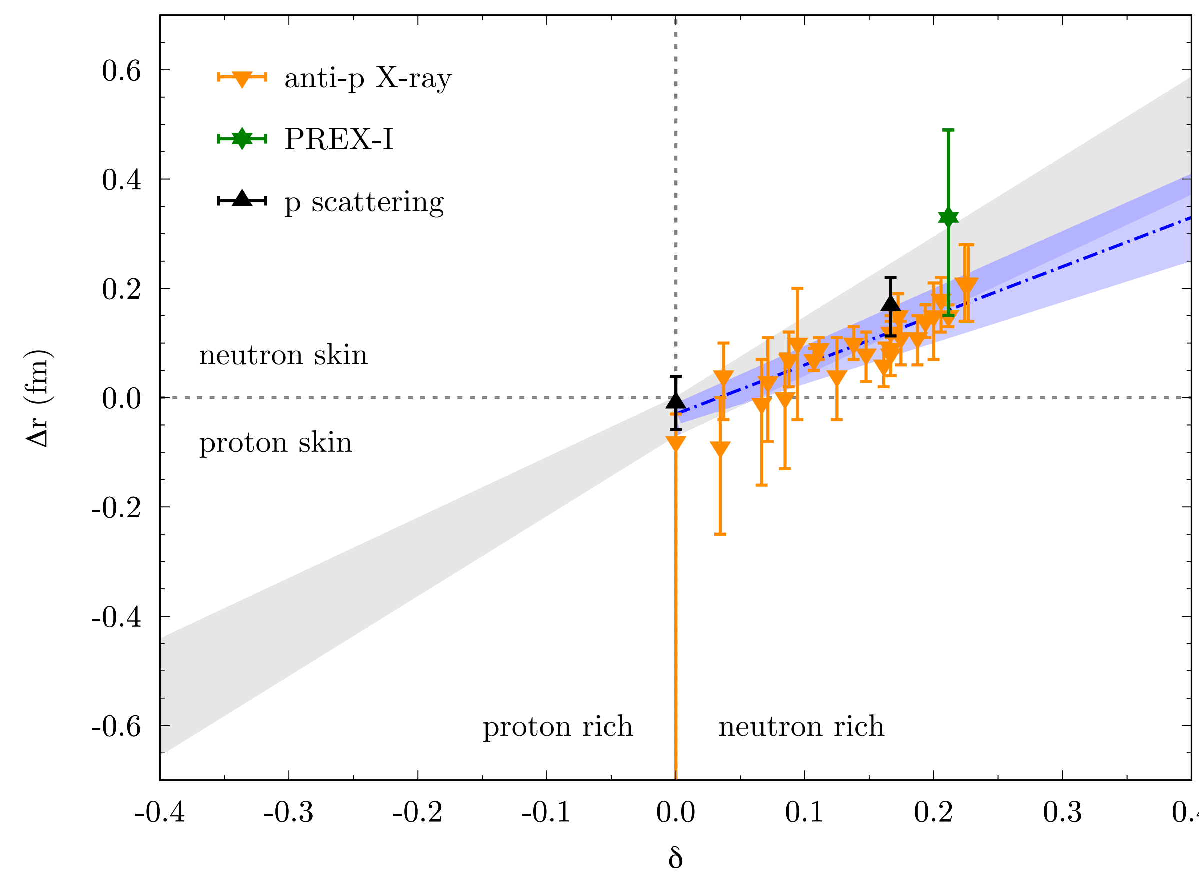

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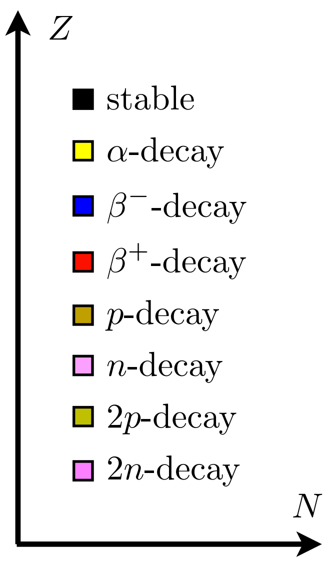
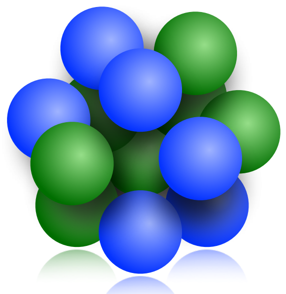
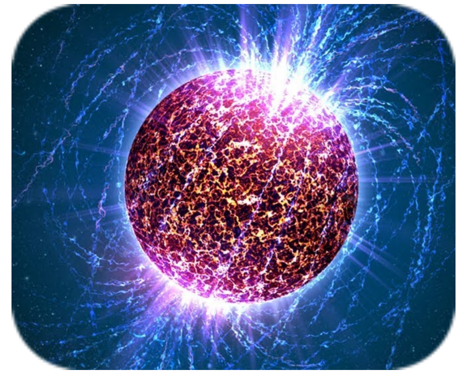
QMC & local chiral interactions

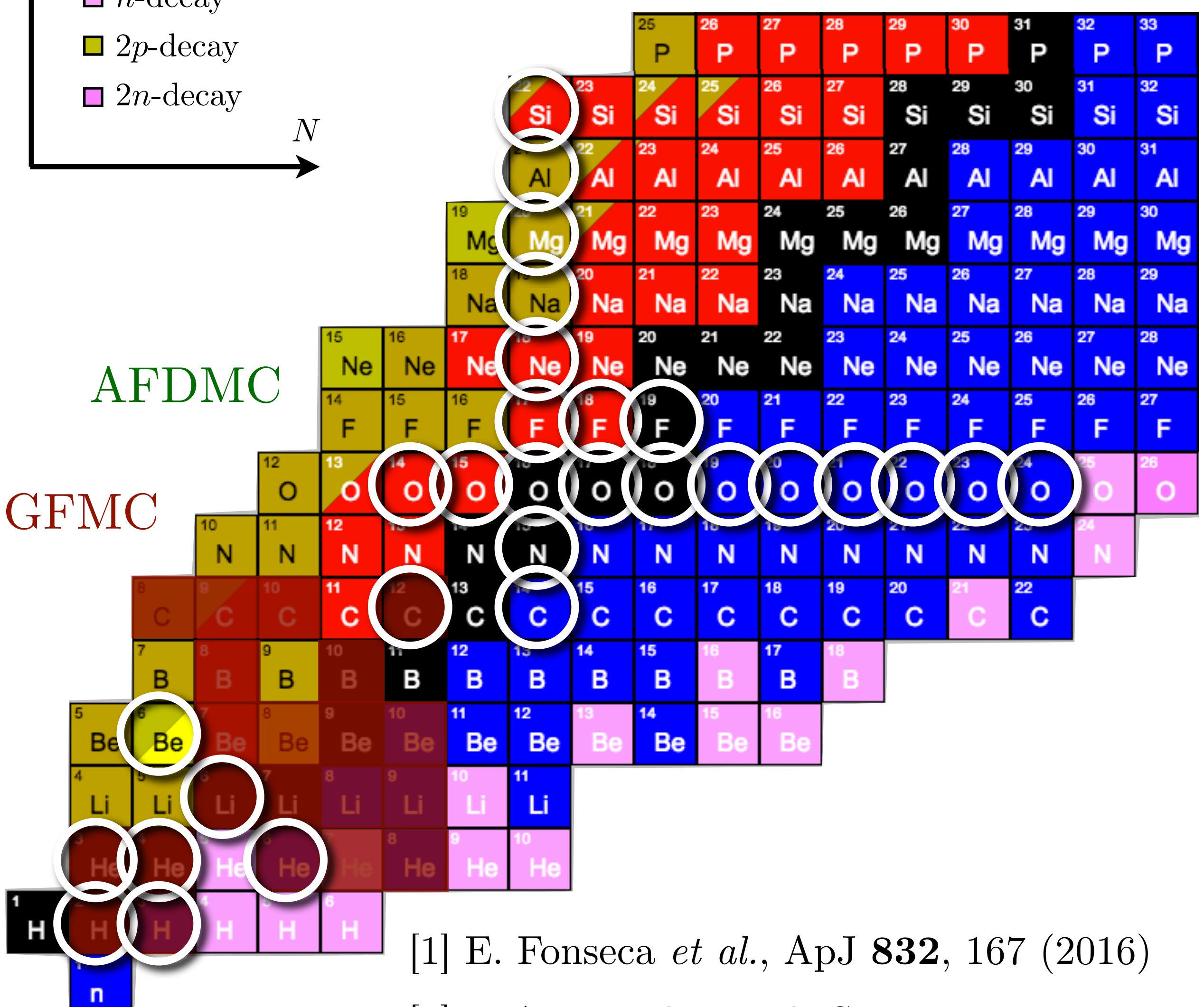






AFDMC

GFMC



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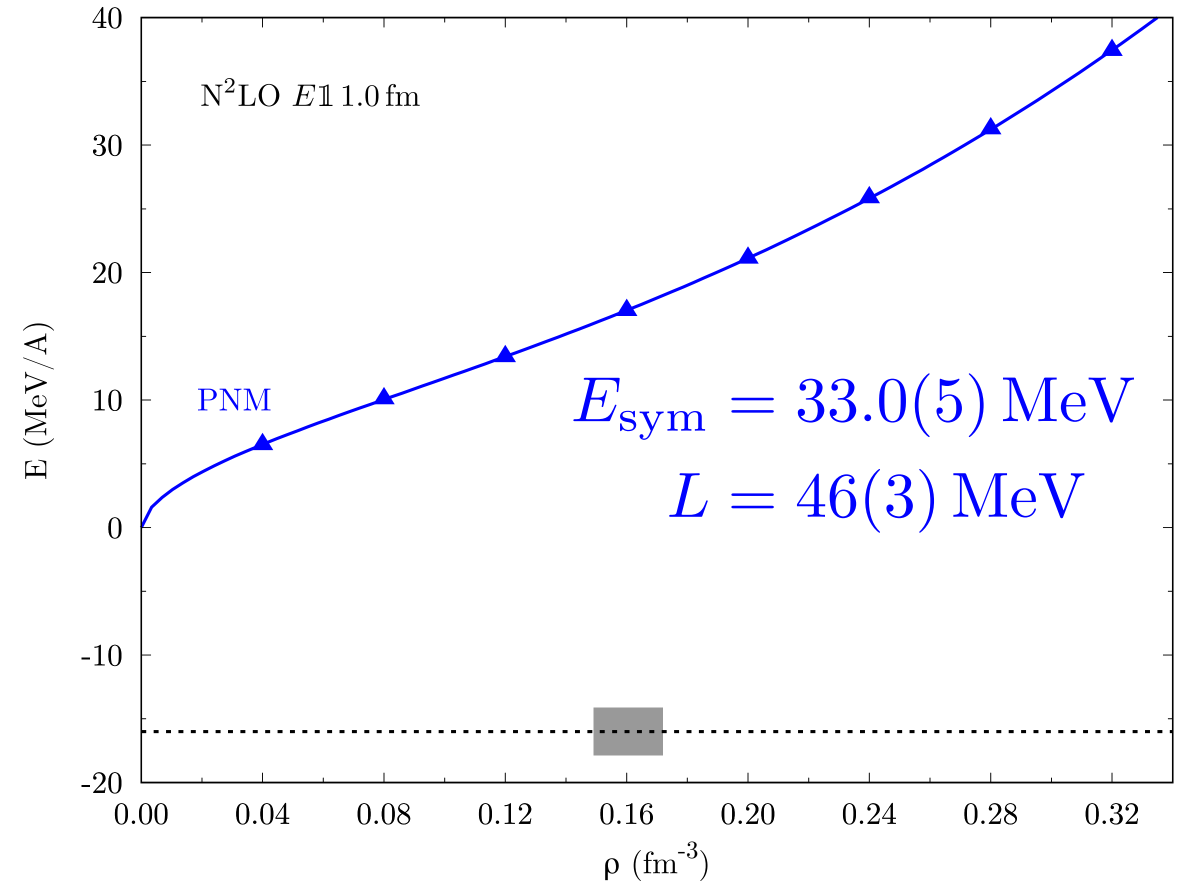
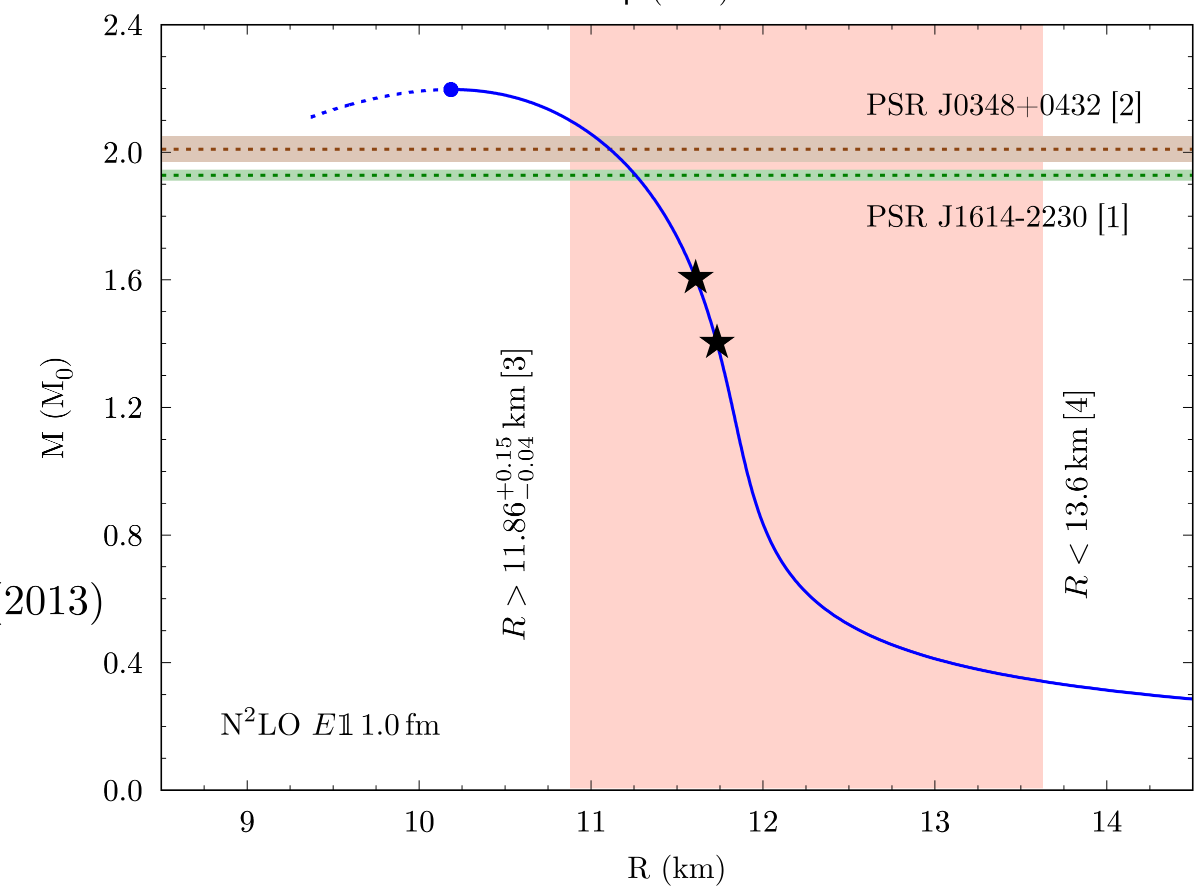
(UIX, IL7)





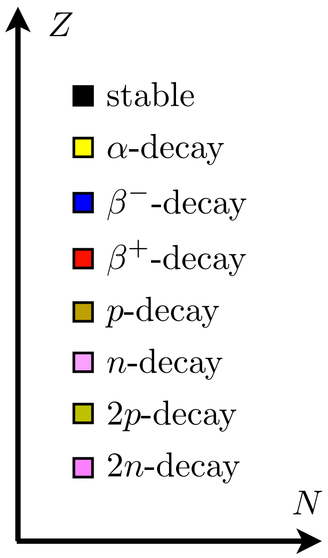
[1] E. Fonseca *et al.*, ApJ **832**, 167 (2016)

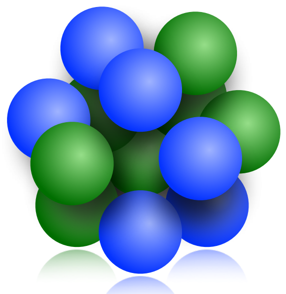
[2] J. Antoniadis *et al.*, Science **340**, 1233232 (2013)

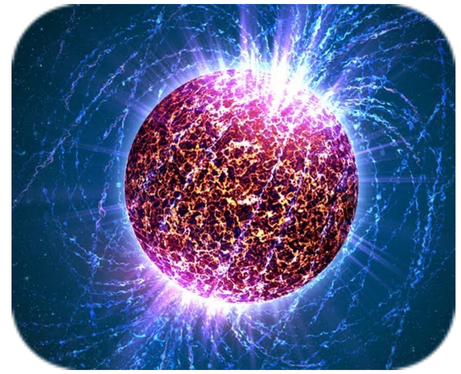
[3] A. Bauswein *et al.*, ApJ **850**, L34 (2017)

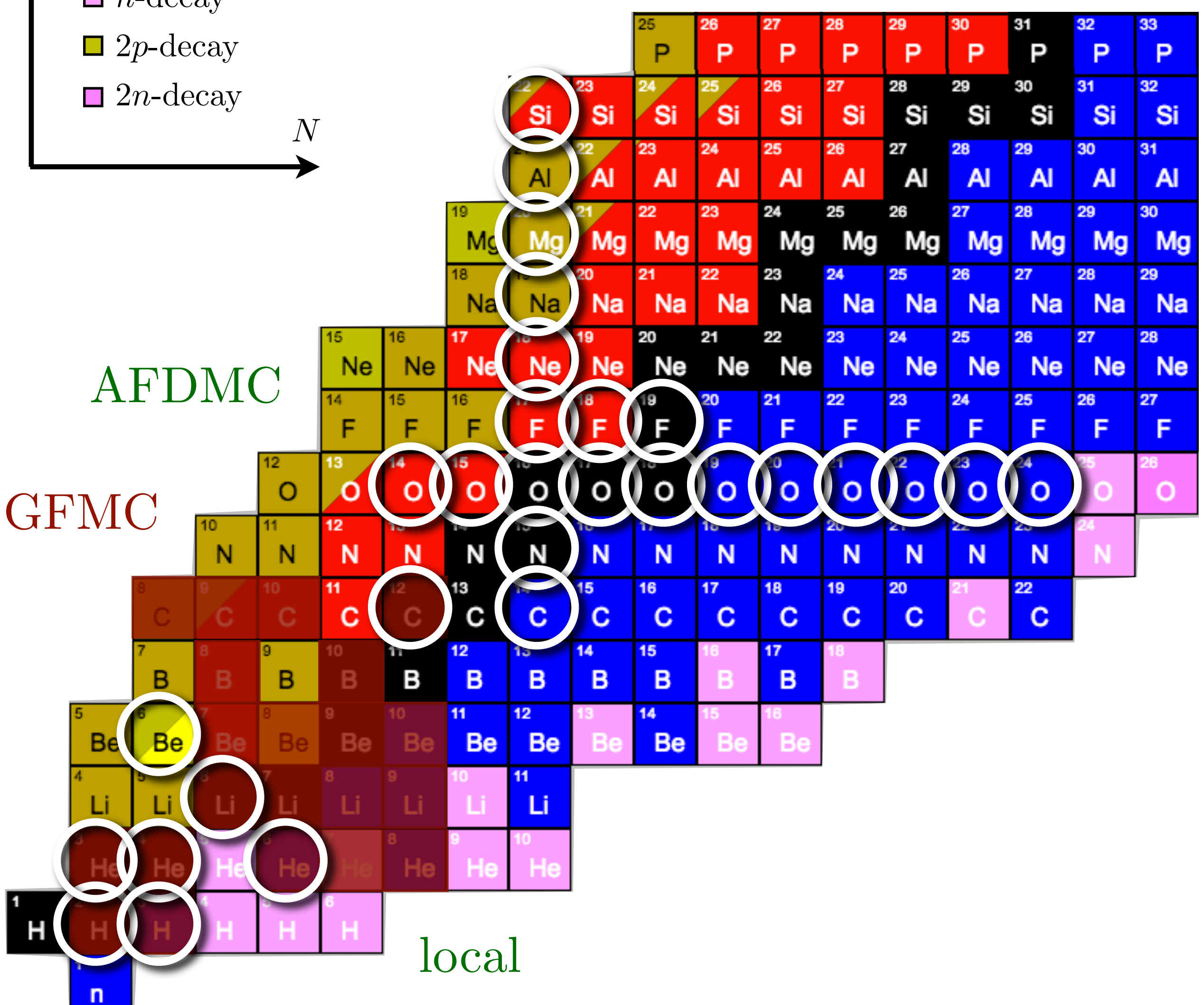
[4] E. Annala *et al.*, PRL **120**, 172703 (2017)

QMC & local chiral interactions



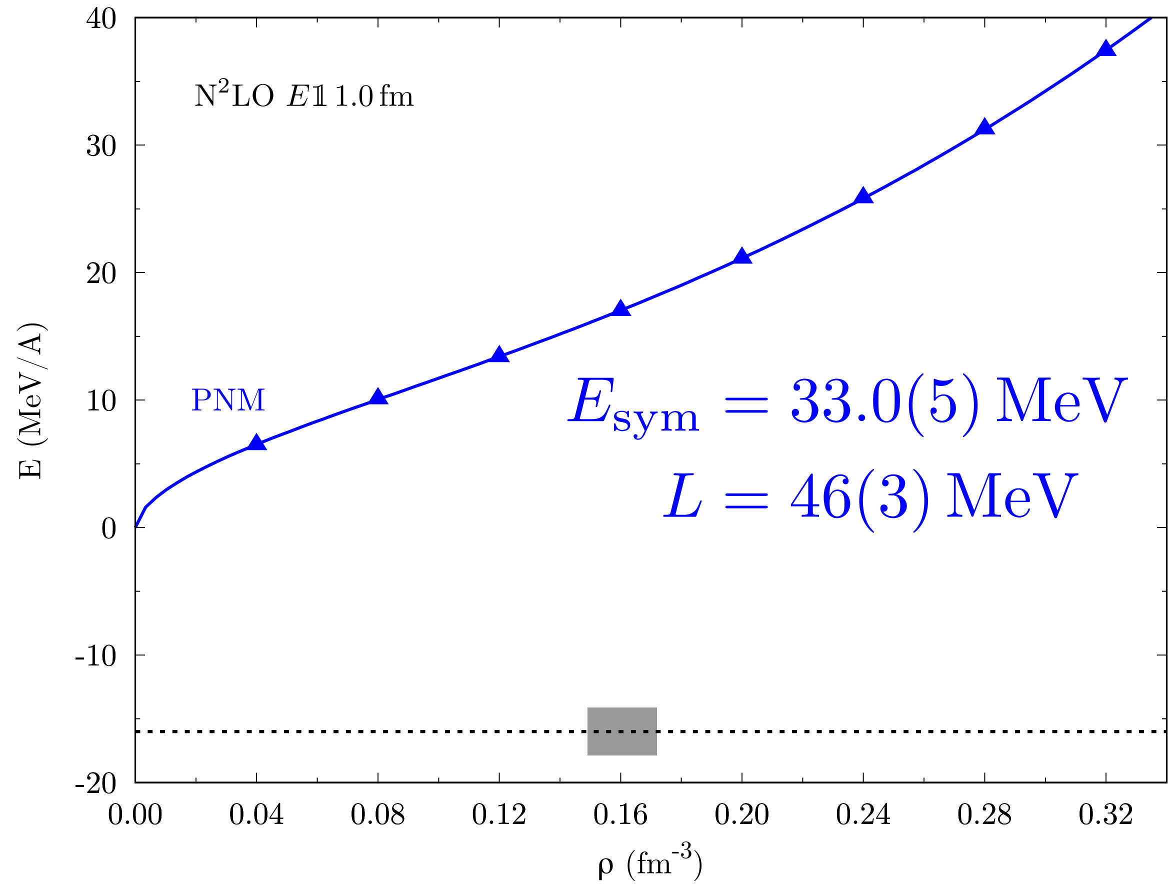


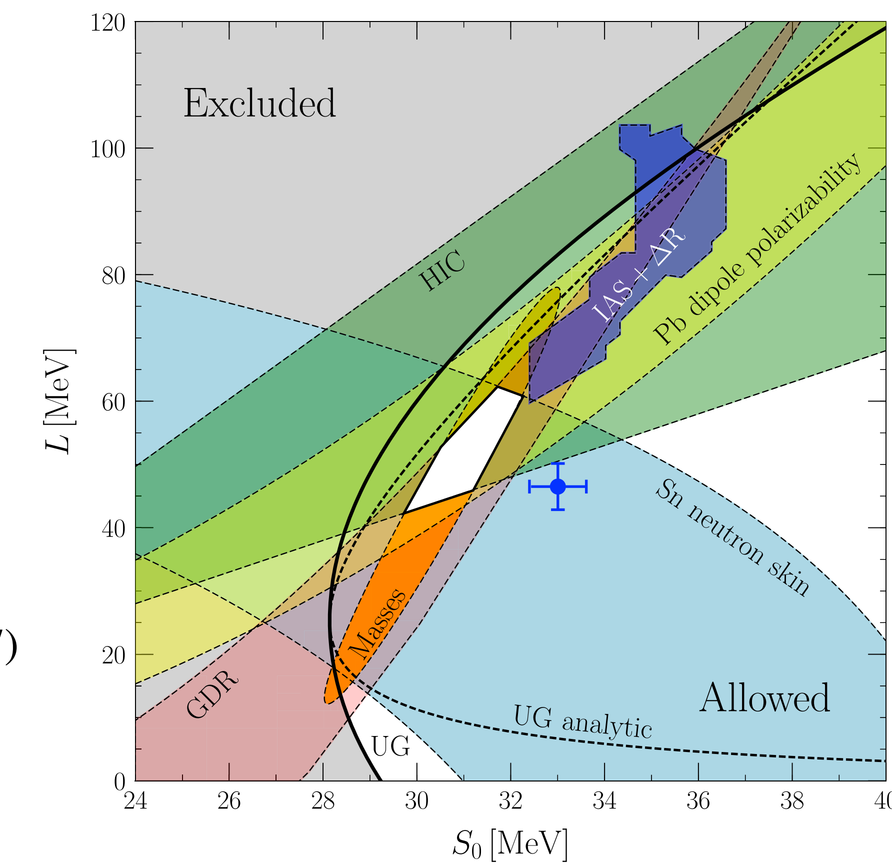




local chiral

AV18+3b (UIX, IL7)

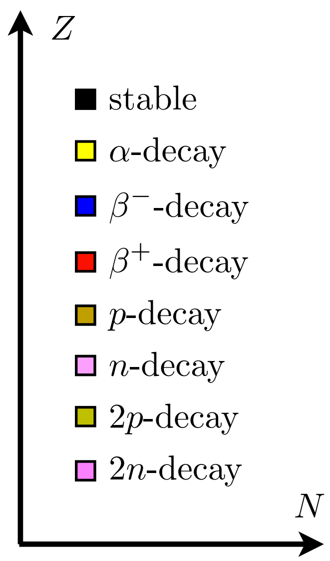


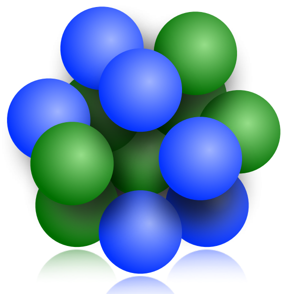


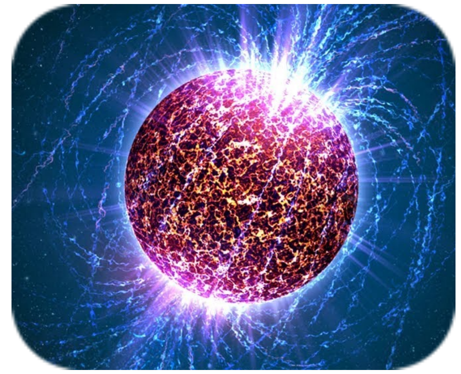
I. Tews *et al.*, ApJ **848**, 105 (2017)

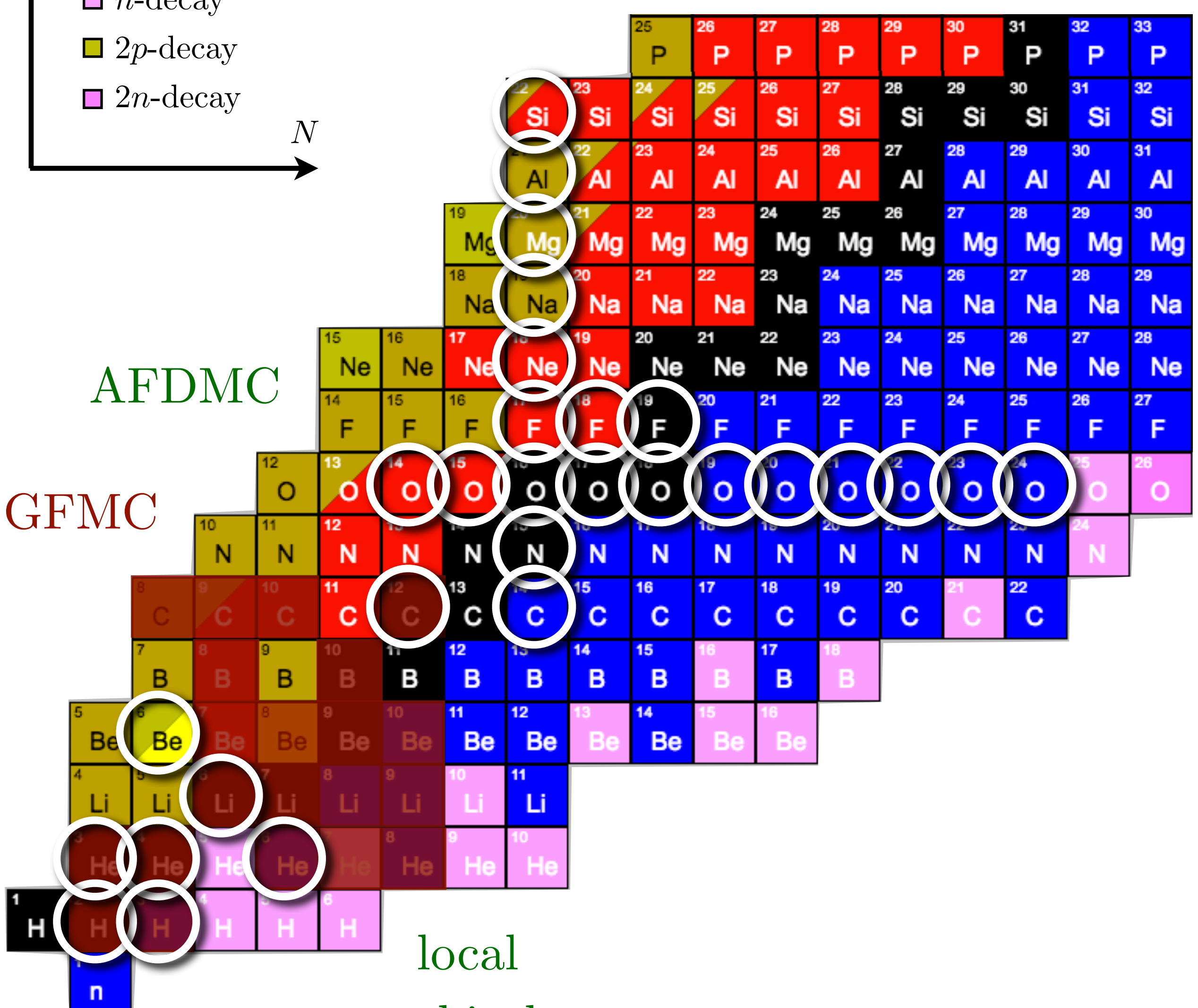
preliminary!!

QMC & local chiral interactions



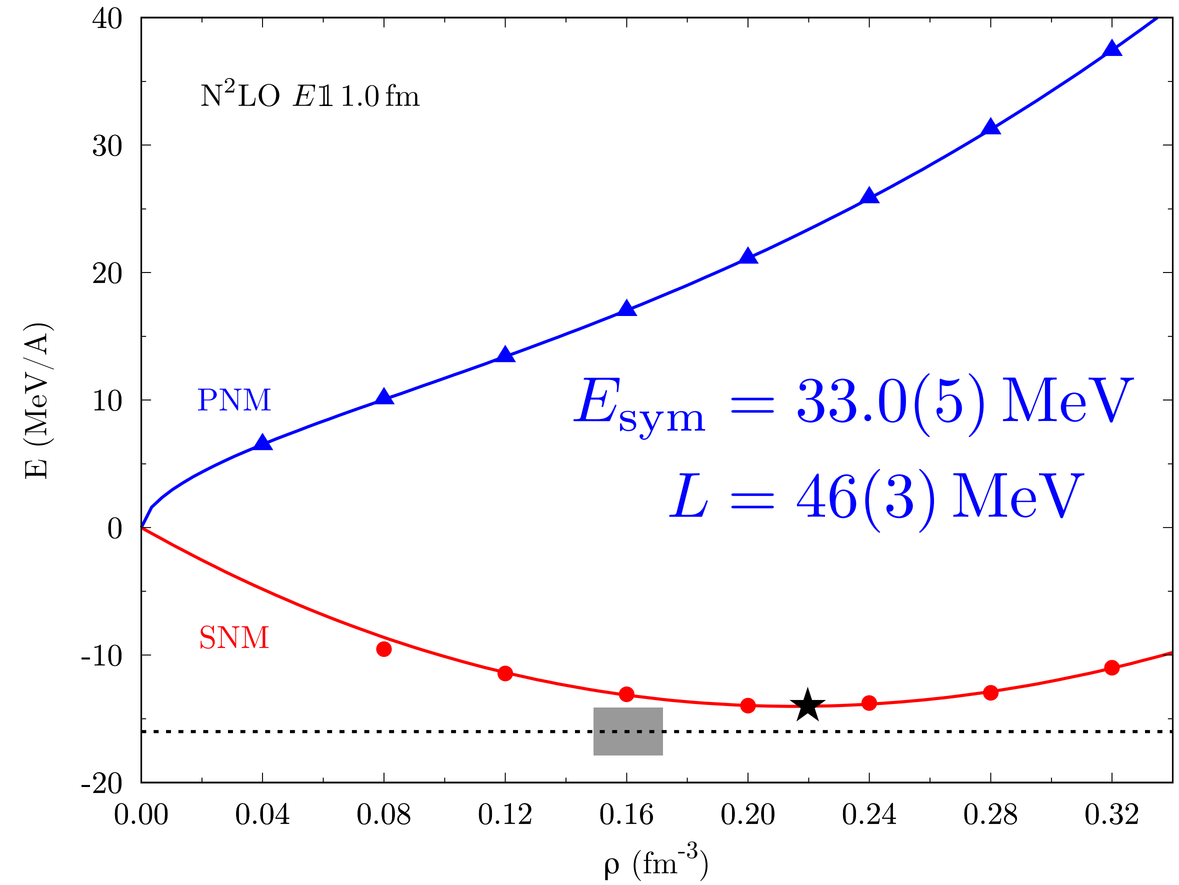






local chiral

AV18+3b (UIX, IL7)



$$E_{\rm SNM}(\rho) = E_0 + \frac{K_0}{18}\left(\frac{\rho-\rho_0}{\rho_0}\right)^2 + \frac{Q_0}{162}\left(\frac{\rho-\rho_0}{\rho_0}\right)^3 + O\left(\frac{\rho-\rho_0}{\rho_0}\right)^4$$

$$E_0 = -14.0(1)\ \mathrm{MeV}$$

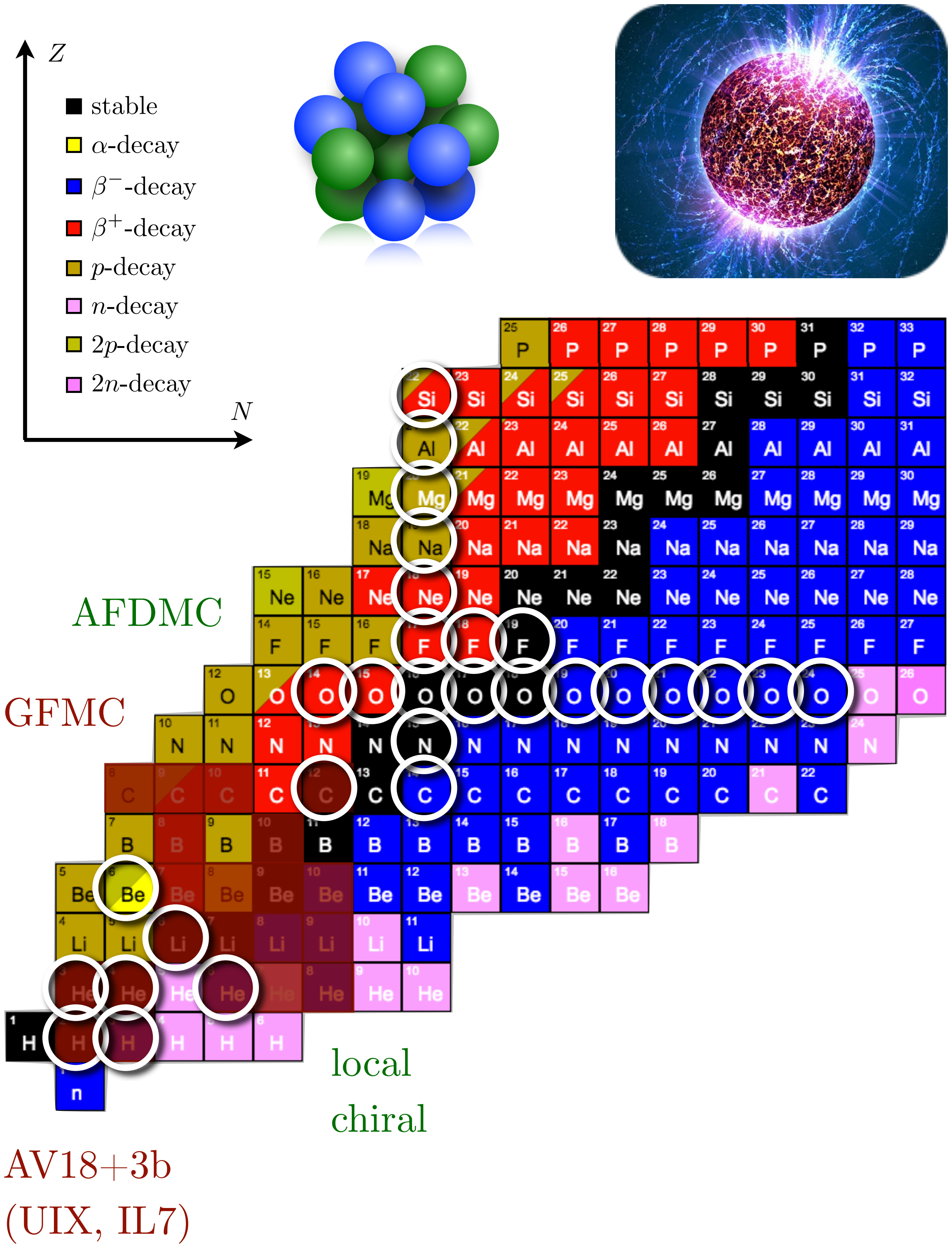
$$\rho_0 = 0.22(2)\ \mathrm{fm}^{-3}$$

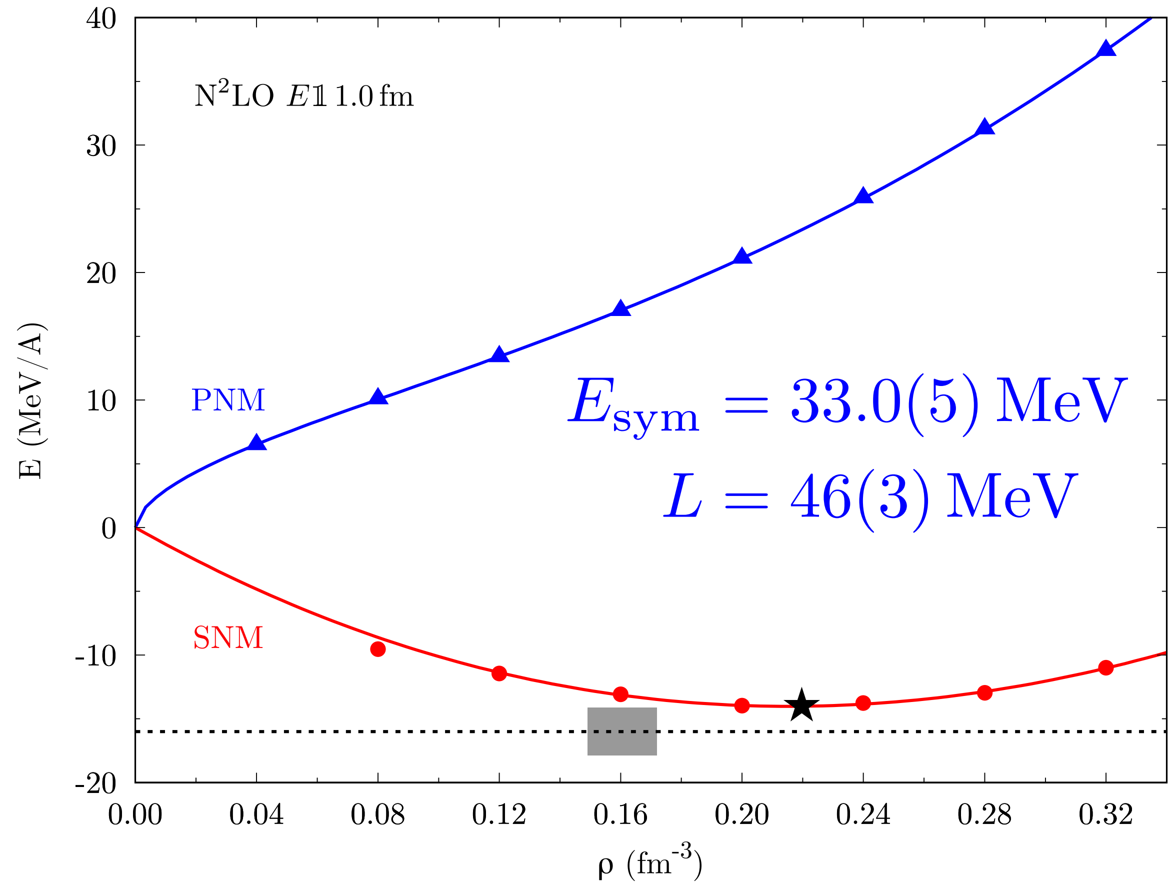
$$K_0 = 236(10)\ \mathrm{MeV}$$

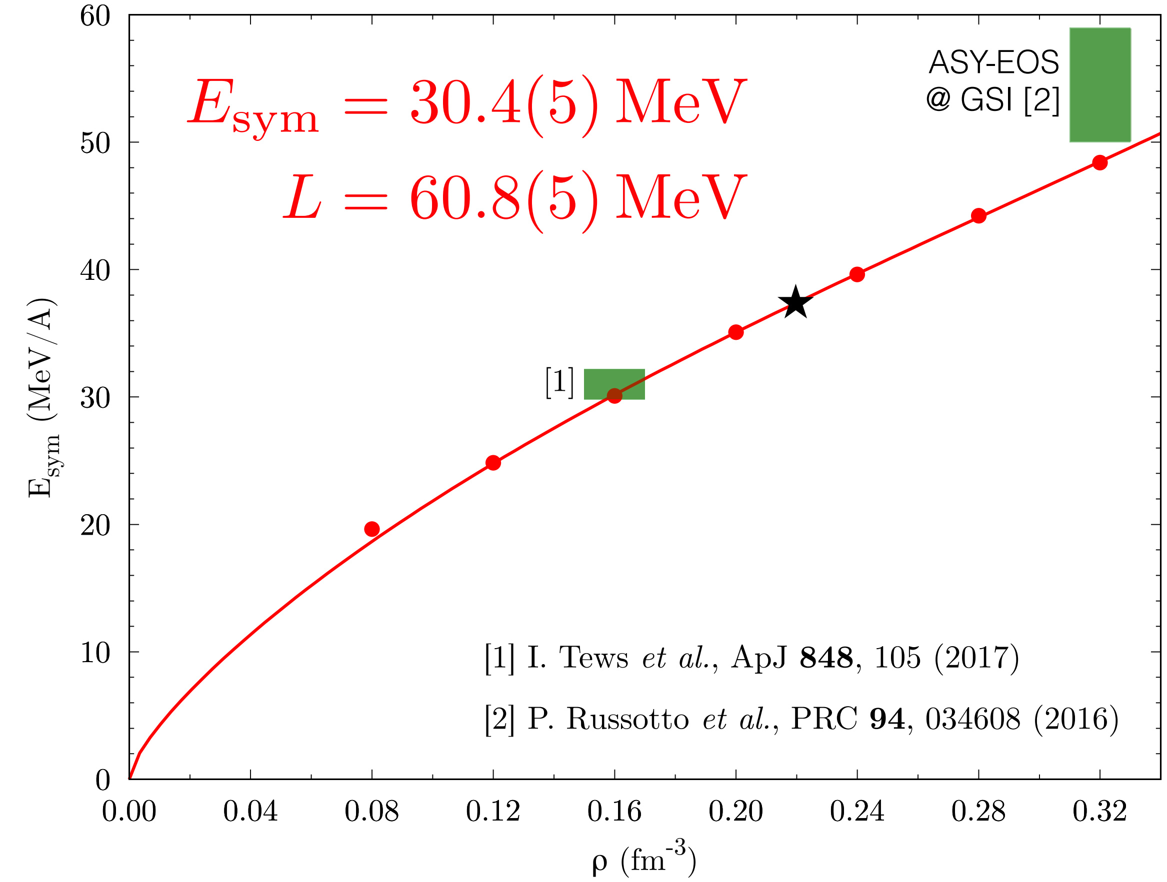
$$Q_0 = -144(100)\ \mathrm{MeV}$$

preliminary!!

QMC & local chiral interactions

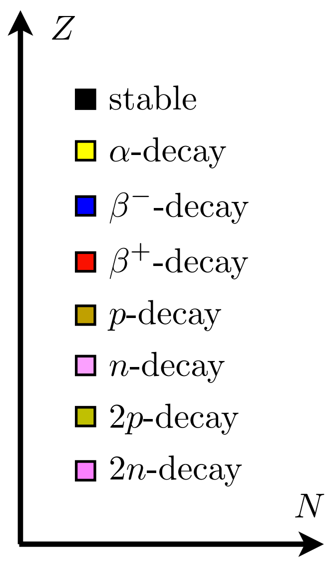


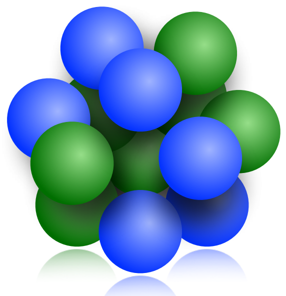


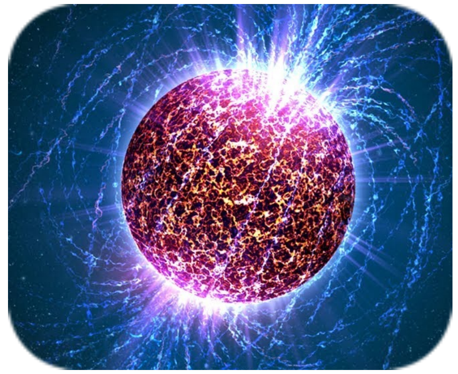


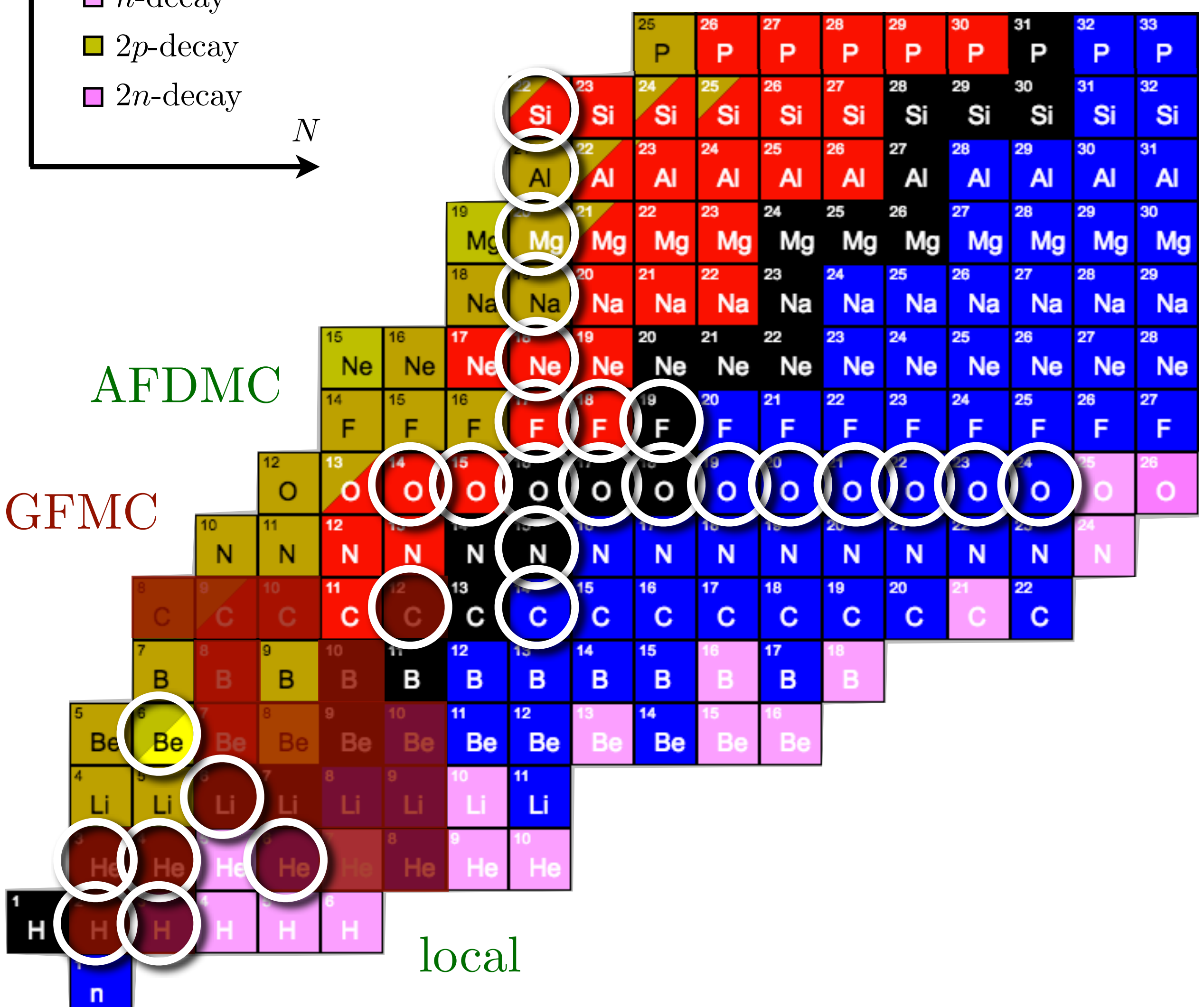
preliminary!!

QMC & local chiral interactions







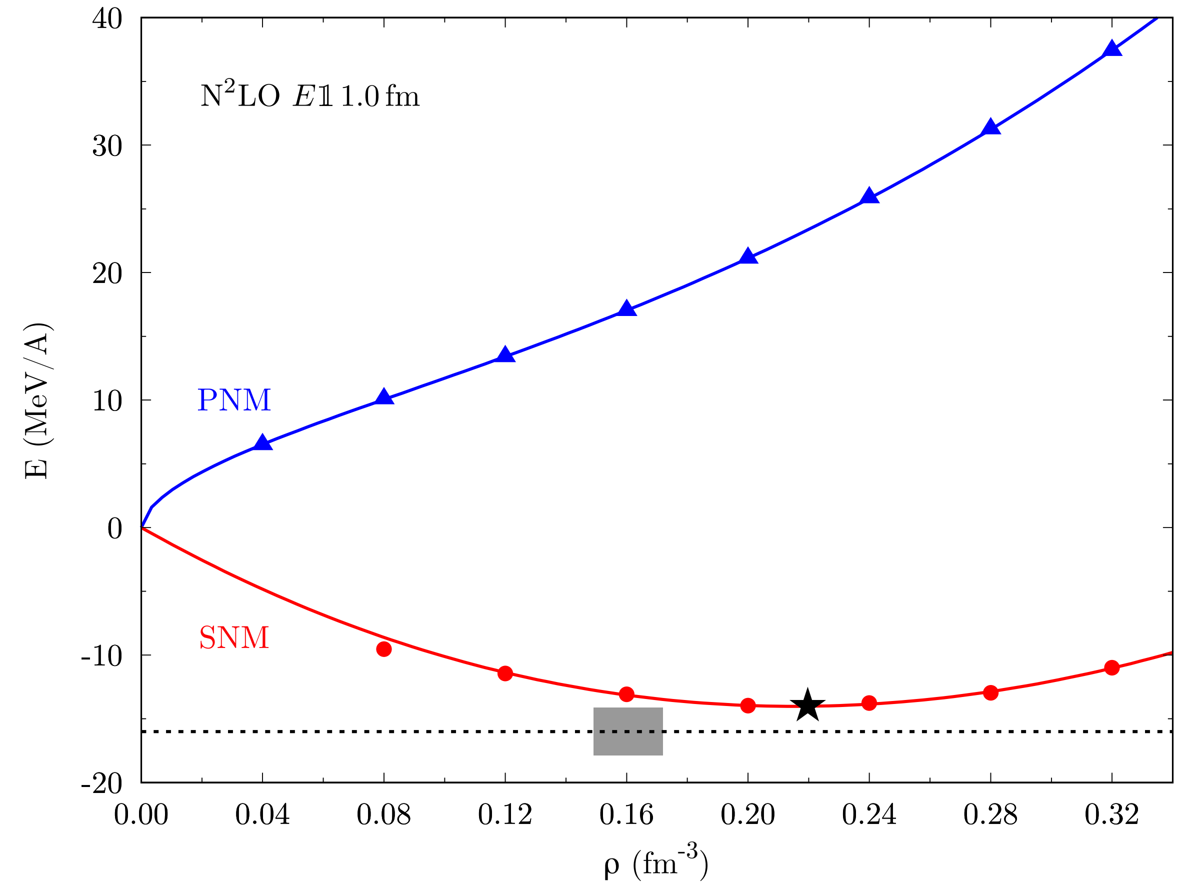


AFDMC

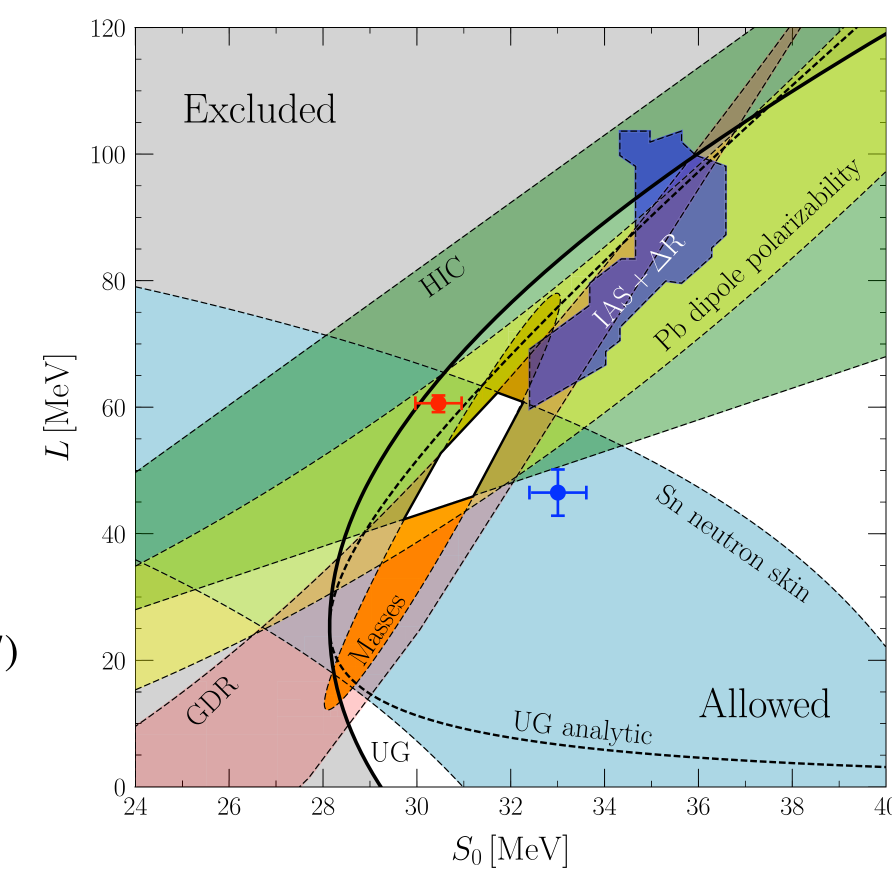
GFMC

local chiral

AV18+3b
(UIX, IL7)

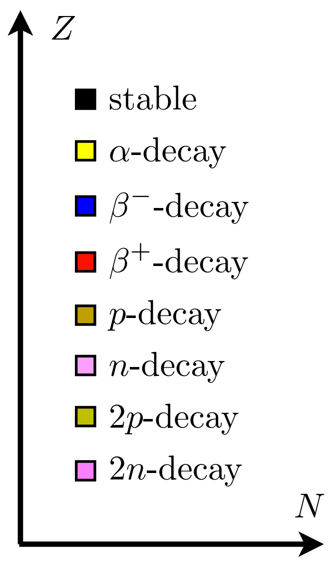


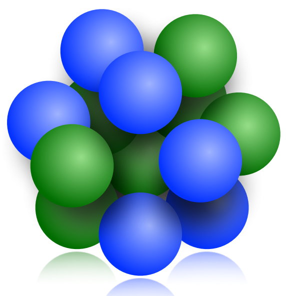
I. Tews *et al.*, ApJ **848**, 105 (2017)

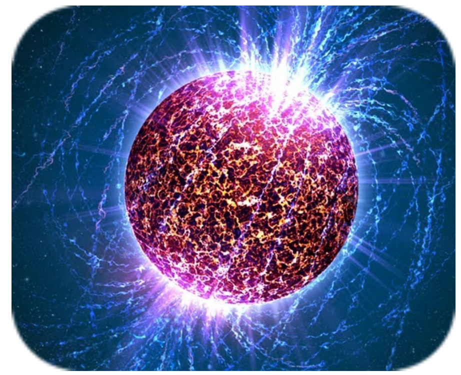


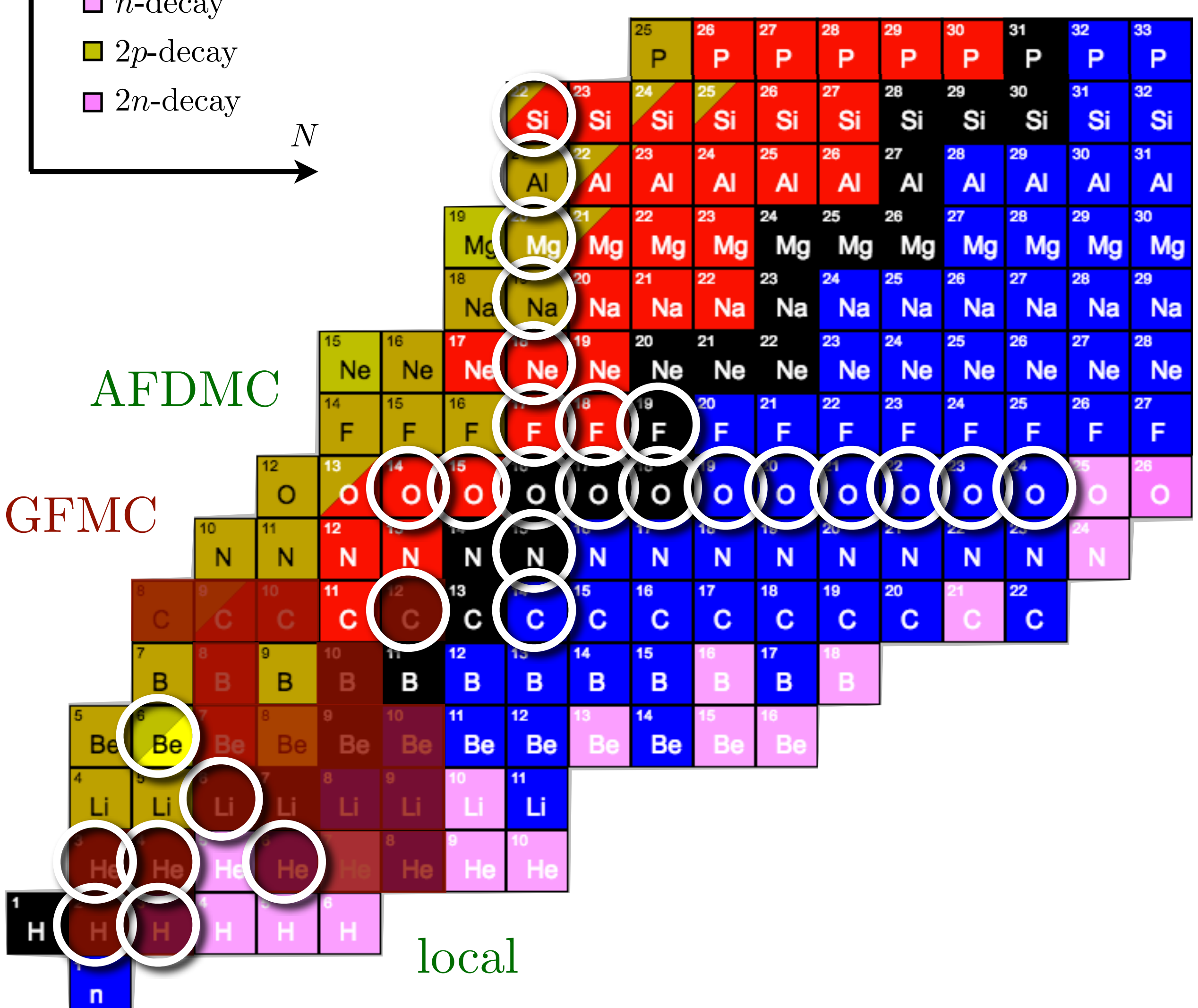
preliminary!!

QMC & local chiral interactions







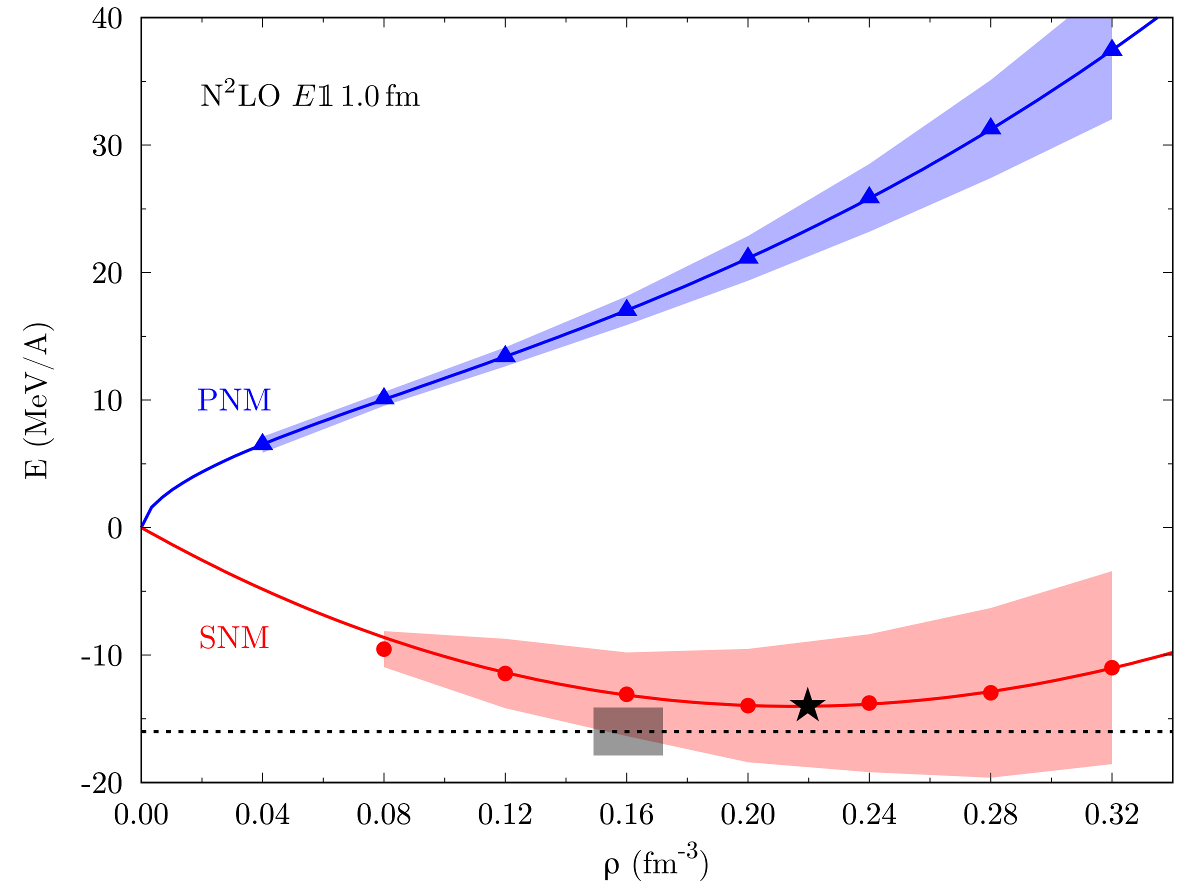


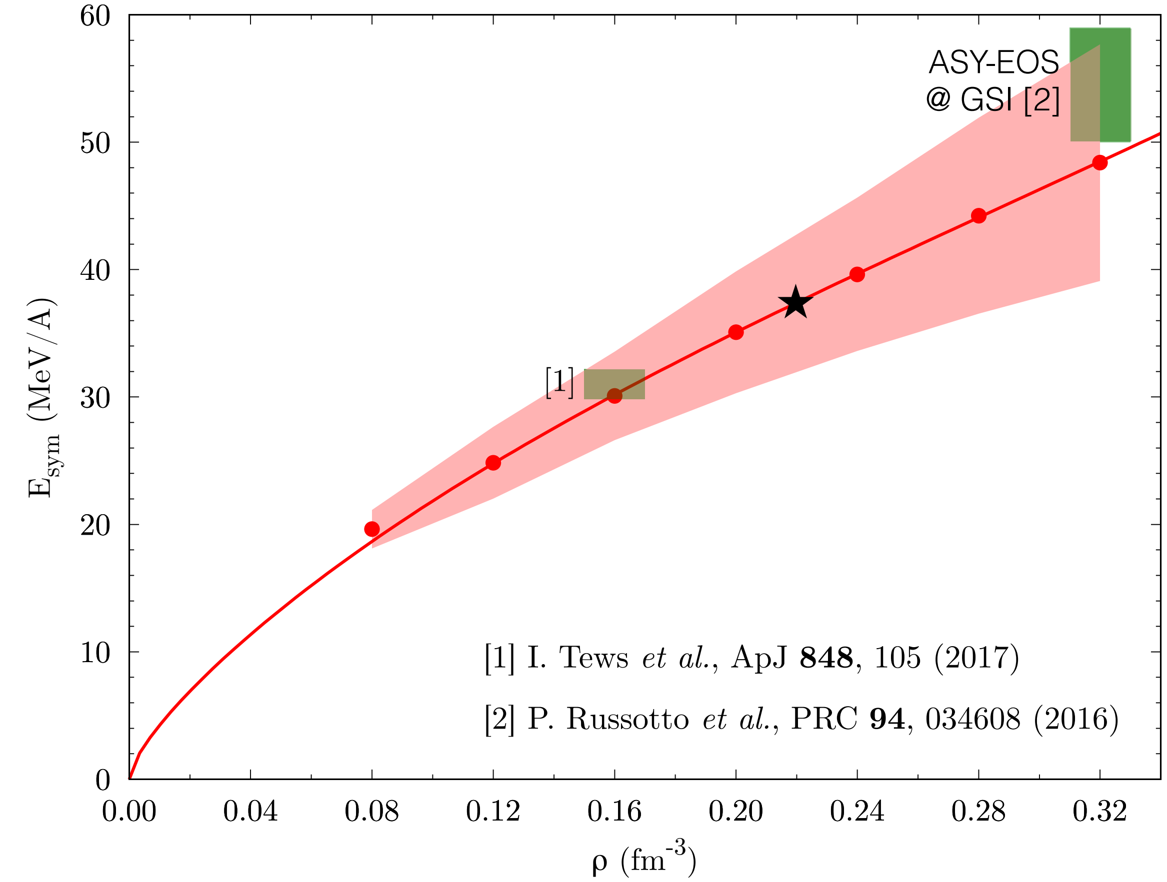
AFDMC

GFMC

local chiral

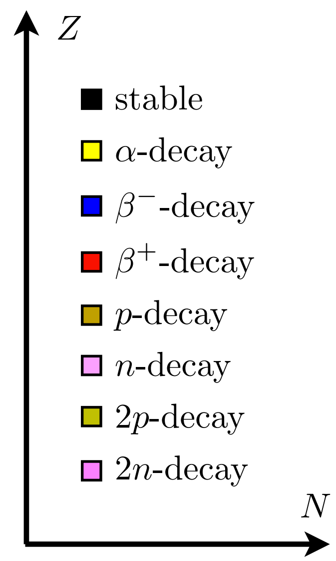
AV18+3b (UIX, IL7)

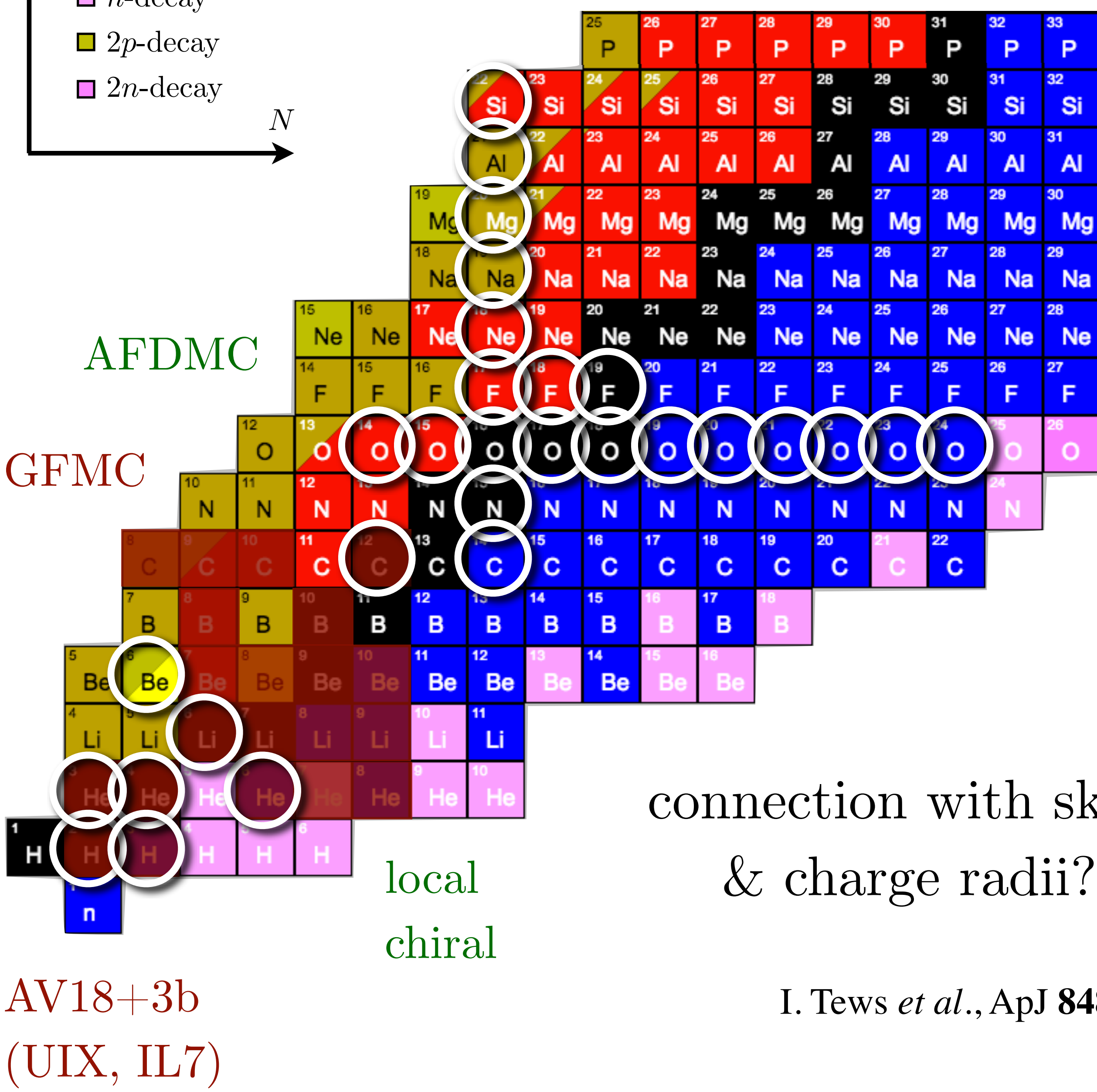


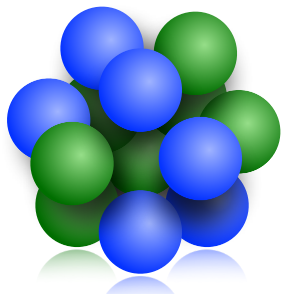


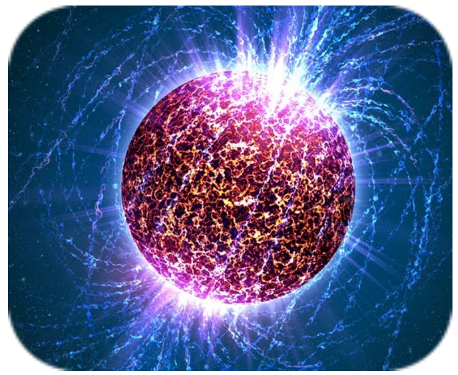
preliminary!!

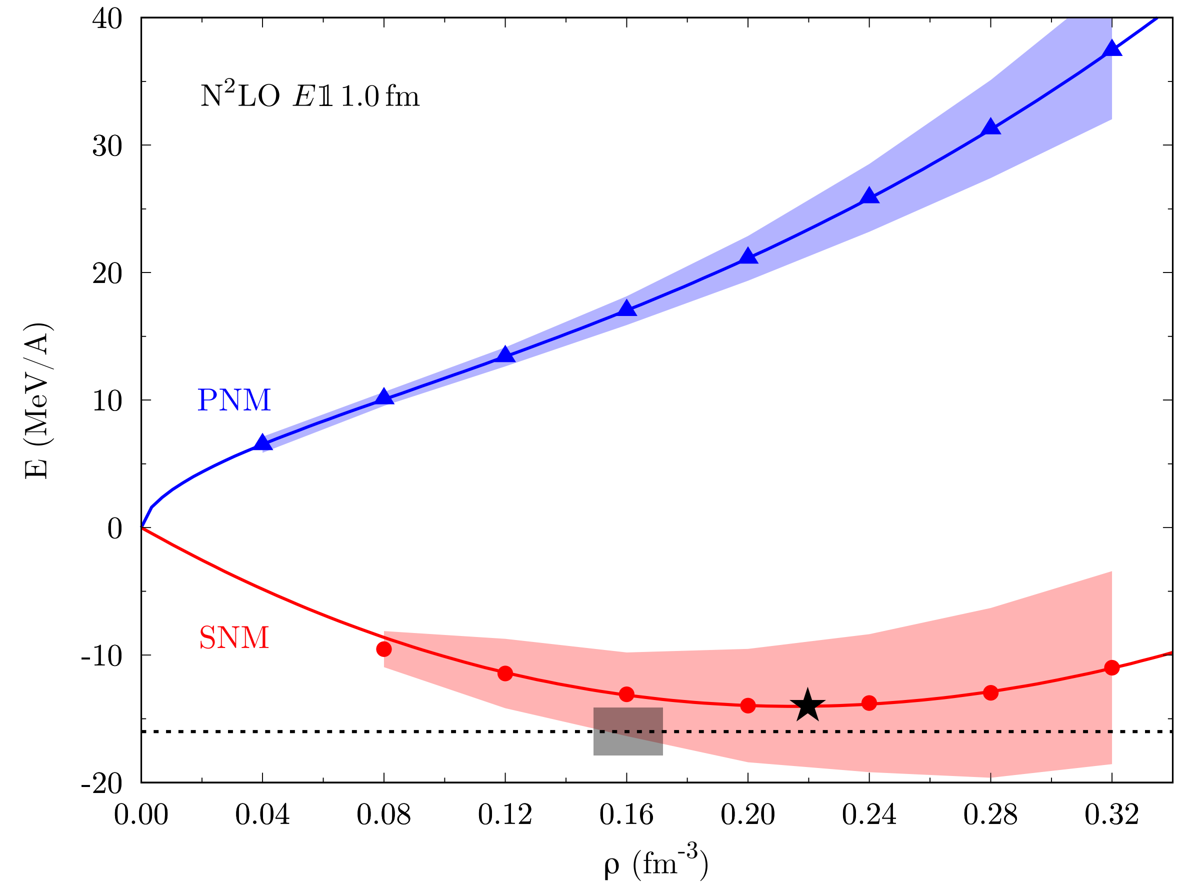
QMC & local chiral interactions

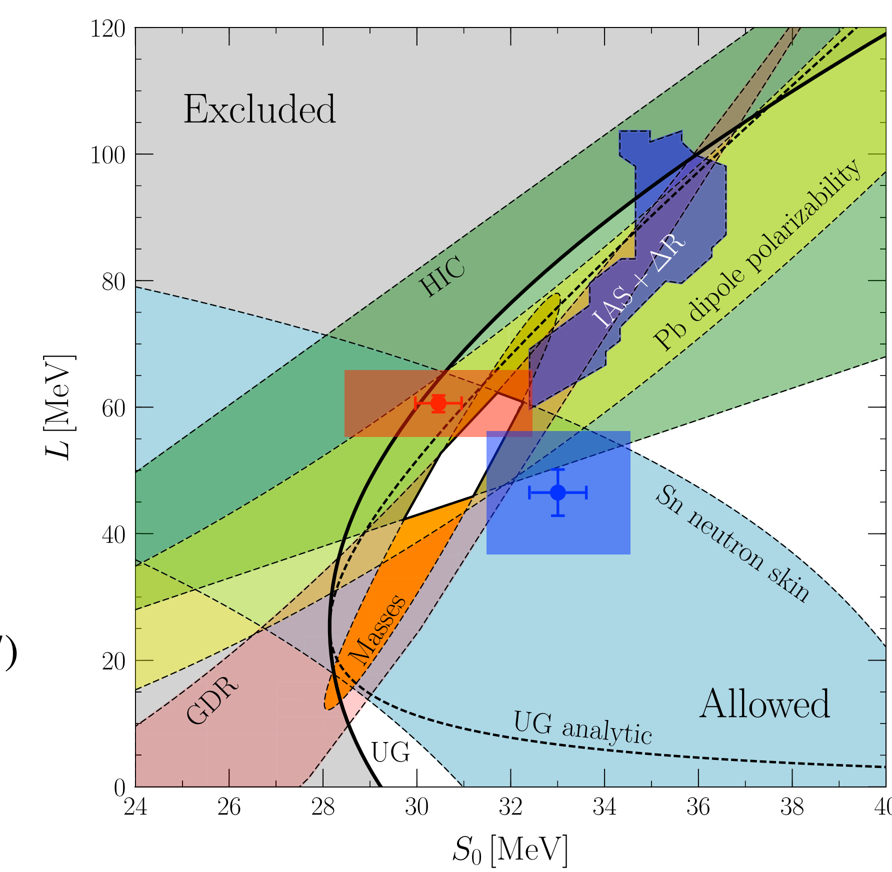










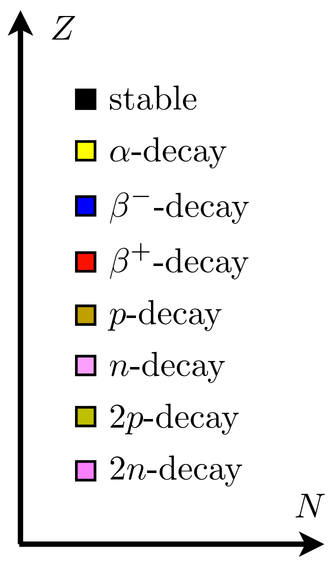


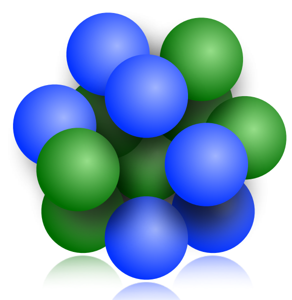
connection with skins
& charge radii?

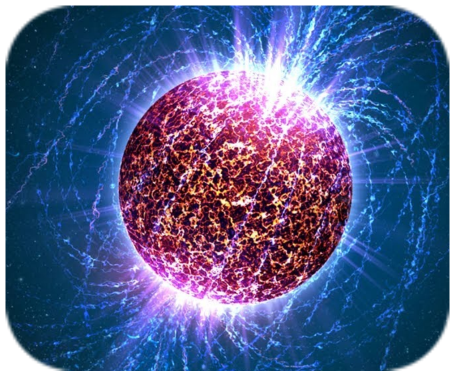
I. Tews *et al.*, ApJ **848**, 105 (2017)

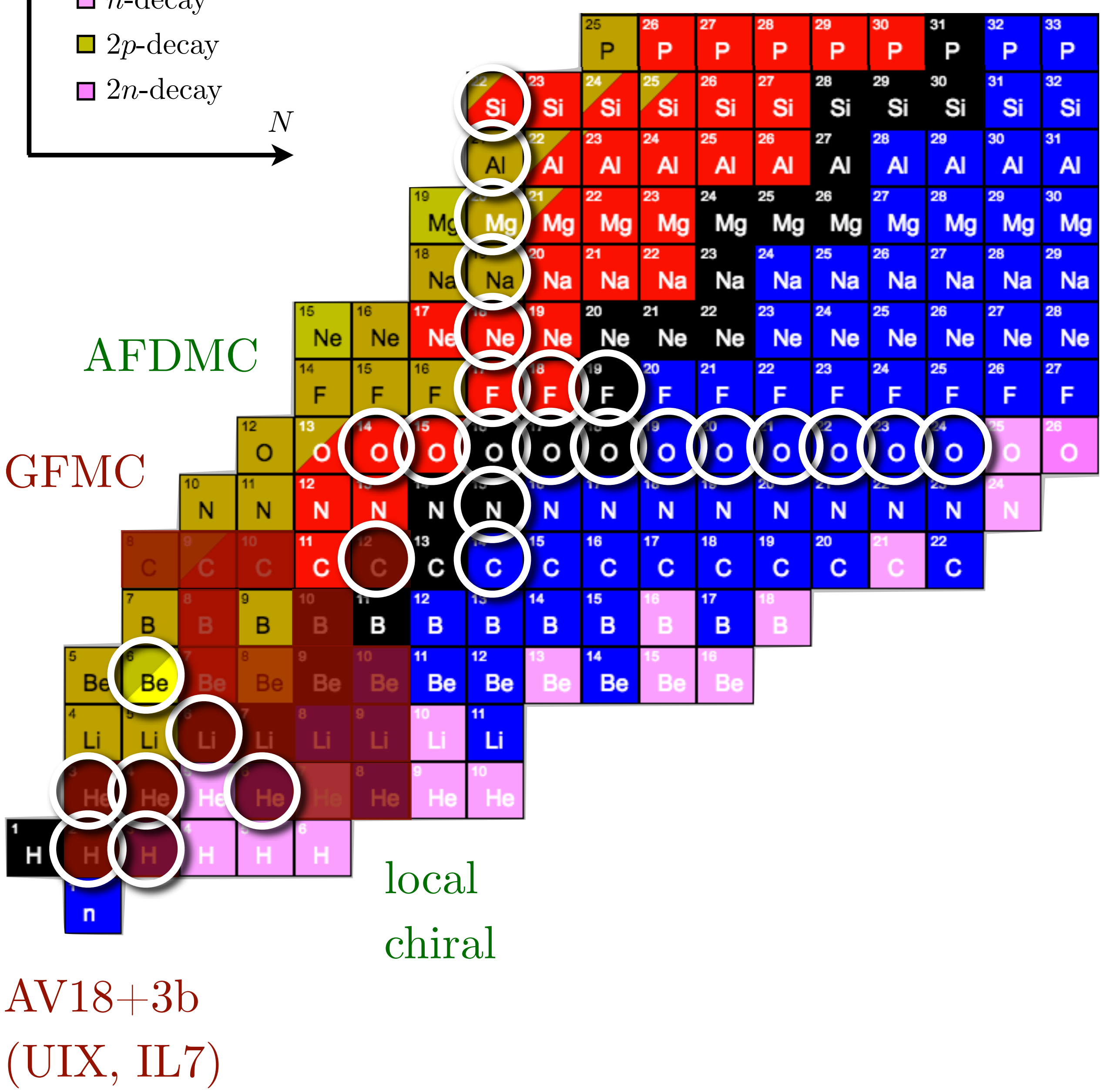
preliminary!!

Summary



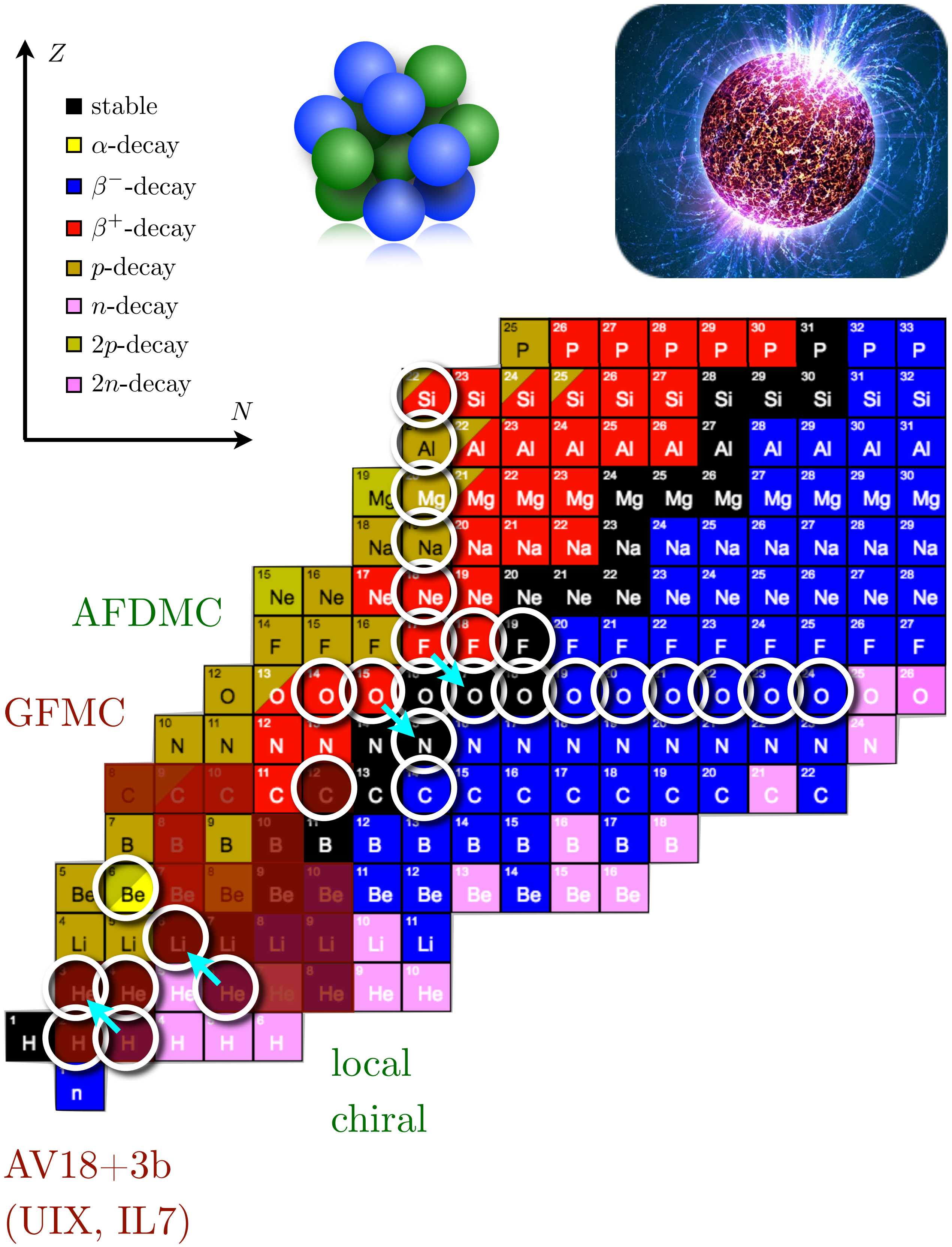






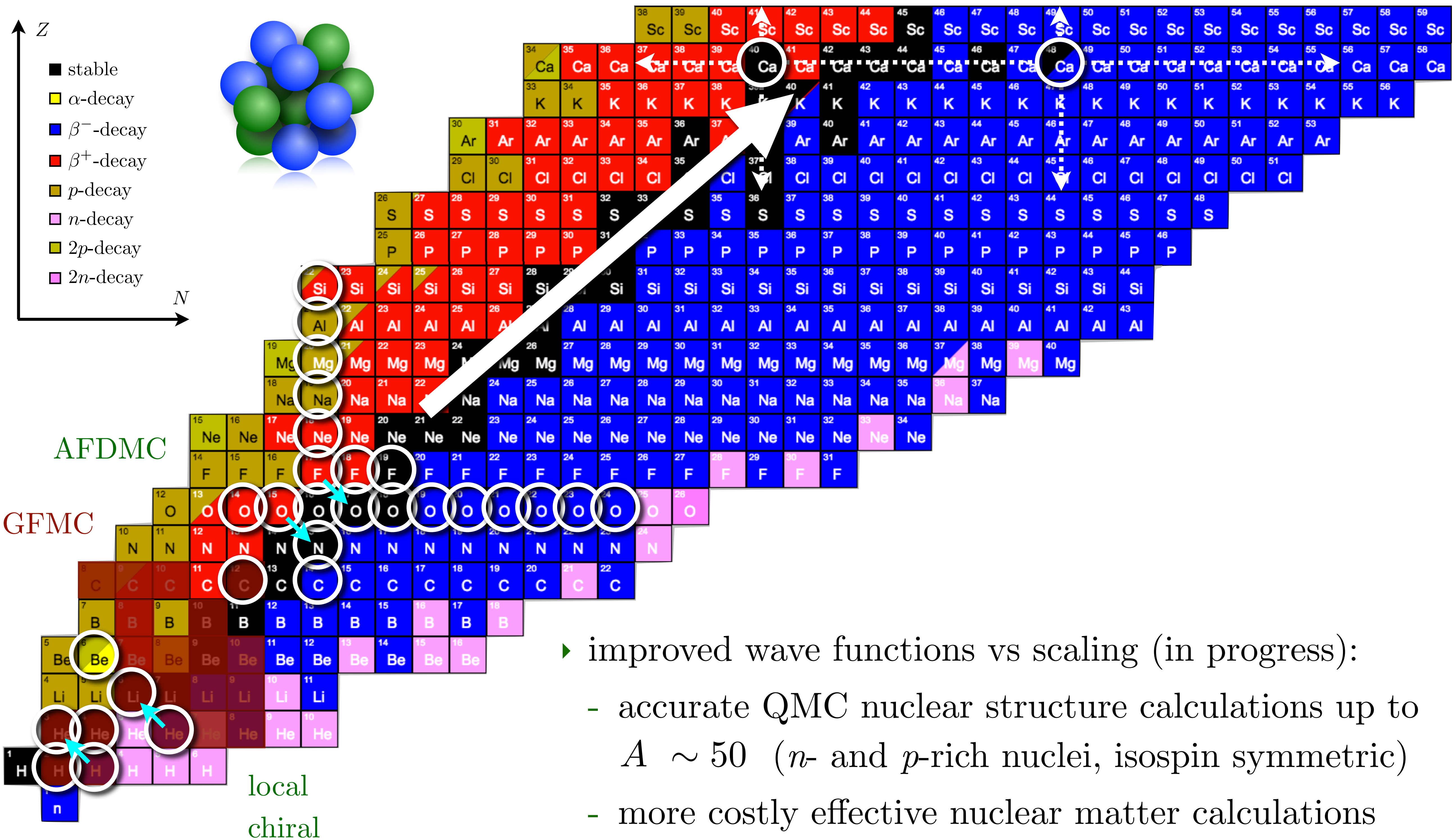
- advances in QMC techniques and the integration of local chiral potentials largely extend the range of applicability of QMC methods
- calculations for both nuclei and infinite matter can be carried out using the same algorithm, the same bare Hamiltonians, the "same" wave functions, and a comprehensive uncertainty estimation can be provided
- chiral interactions fit to few-body observables can simultaneously describe the physics of nuclei and infinite matter
- charge radii, nucleon skins, and other structural properties of nuclei up to (at least) A=24 can be calculated
- connections between radii, skins, the symmetry energy and its slope can be consistently investigated

Perspectives



- construction of harder coordinate-space local chiral potentials @ N^2LO for QMC (in progress). Next: N^3LO ?
- implementation of coordinate-space Δ-full chiral potentials in AFDMC (2-body ok, 3-body in progress)
- derivation and implementation of consistent 2-body currents in AFDMC, both Δ-less and Δ-full (in progress) *Example:* β-decay matrix elements, magnetic moments, transitions?

Perspectives



AV18+3b
(UIX, IL7)

- improved wave functions vs scaling (in progress):
  - accurate QMC nuclear structure calculations up to $A \sim 50$ (n- and p-rich nuclei, isospin symmetric)
  - more costly effective nuclear matter calculations
  - inherit the light-nuclei QMC "technology" and export it to the medium-mass range

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In collaboration with:

- C. Barbieri, Uni of Surrey, UK
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- W. Detmold, MIT
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- A. Schmidt, MIT
- K.E. Schmidt, Arizona State Uni
- V. Somà, Uni Paris-Saclay, France
- *L. Tang*, JLab
- I. Tews, LANL
- X.B. Wang, Huzhou Uni, China
- R. Weiss, Hebrew Uni, Israel
- R.B. Wiringa, ANL
- and more ...