The No Core Shell Model with a Core: Deriving the Shell Model Microscopically
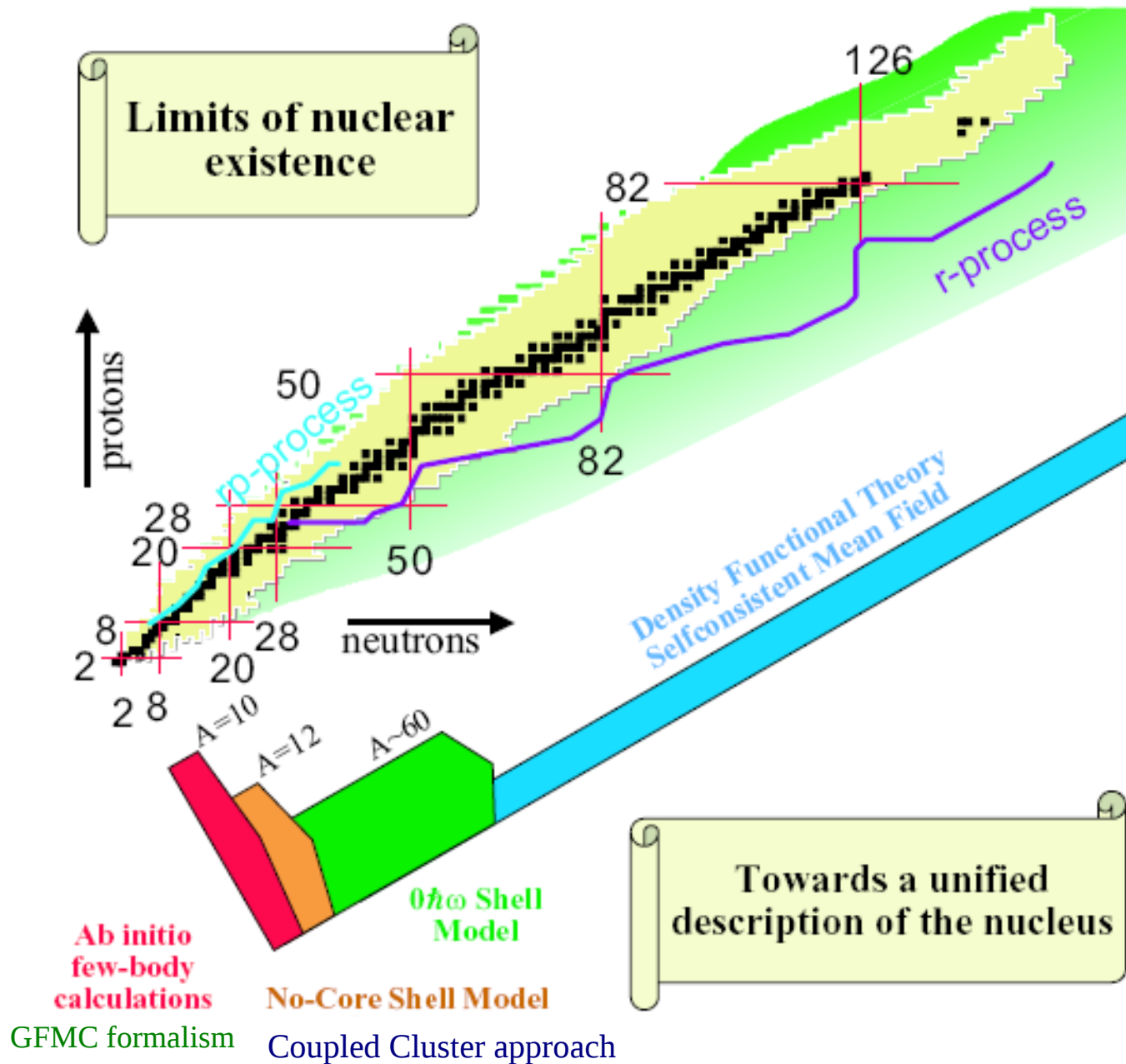
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Limits of nuclear existence

126

82

r-process

protons

50

rp-process

82

28
20

50

8
2

8   28

20

neutrons

2   8

A=10

A=12

A~60

Density Functional Theory
Selfconsistent Mean Field

0ℏω Shell
Model

Towards a unified
description of the nucleus

Ab initio
few-body
calculations

No-Core Shell Model

GFMC formalism   Coupled Cluster approach

OUTLINE

I. Overview of the *Ab Initio* Shell Model with a Core Approach

From few-body to many-body

Using the NCSM to calculate the shell model input

**_Ab initio_
No Core Shell Model**

Core Shell Model

Realistic NN & NNN forces

Effective interactions in cluster approximation ←→ **effective interactions for valence nucleons**

Diagonalization of many- body Hamiltonian

Diagonalization of the Hamiltonian for valence nucleons

Many-body experimental data

$N'_{max} = 0$

$P'H'_{eff}P'$

N_{max}

P   Q

P

Q

H

OLS

OLS

$PH_{eff}P$
NCSM

$PH_{eff}Q = 0$

$QH_{eff}P = 0$

$QH_{eff}Q$
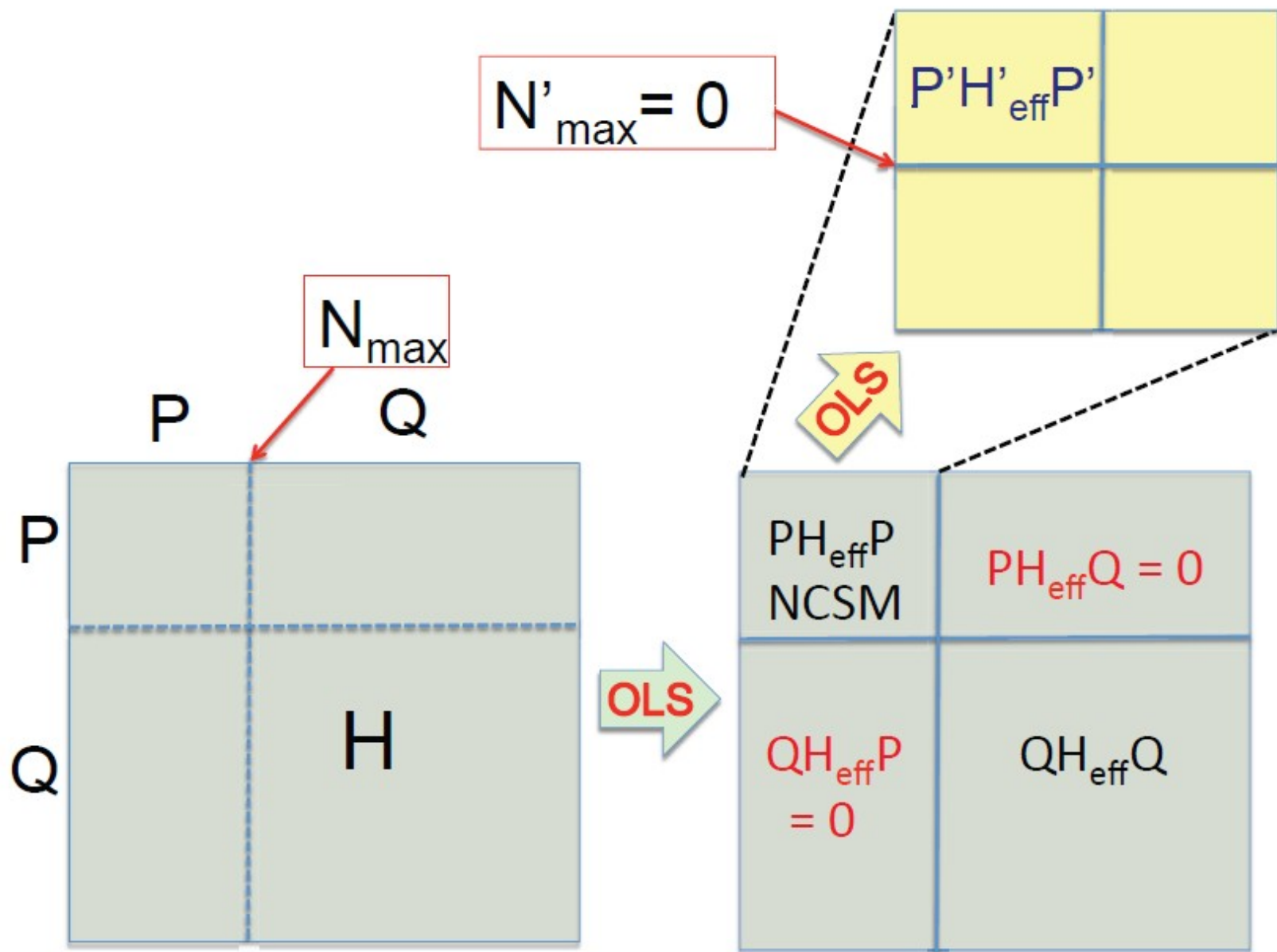
Effective interaction in a projected model space

$$H\Psi_\alpha = E_\alpha \Psi_\alpha \quad \text{where} \quad H = \sum_{i=1}^{A} t_i + \sum_{i \leq j}^{A} v_{ij}.$$

$$\mathcal{H}\Phi_\beta = E_\beta \Phi_\beta$$

$$\Phi_\beta = P\Psi_\beta$$

P is a projection operator from S into $\mathcal{S}$

$$< \tilde{\Phi}_\gamma | \Phi_\beta > = \delta_{\gamma\beta}$$

$$\mathcal{H} = \sum_{\beta \epsilon S} |\Phi_\beta > E_\beta < \tilde{\Phi}_\beta|$$

Effective Hamiltonian for NCSM

Solving $\boxed{\mathrm{H}^{\Omega}_{A,\,a=2}\,\Psi_{a=2} = \mathrm{E}^{\Omega}_{A,\,a=2}\,\Psi_{a=2}}$

in "infinite space" $2n+l = 450$ relative coordinates

$P + Q = 1$;   P – model space;   Q – excluded space;

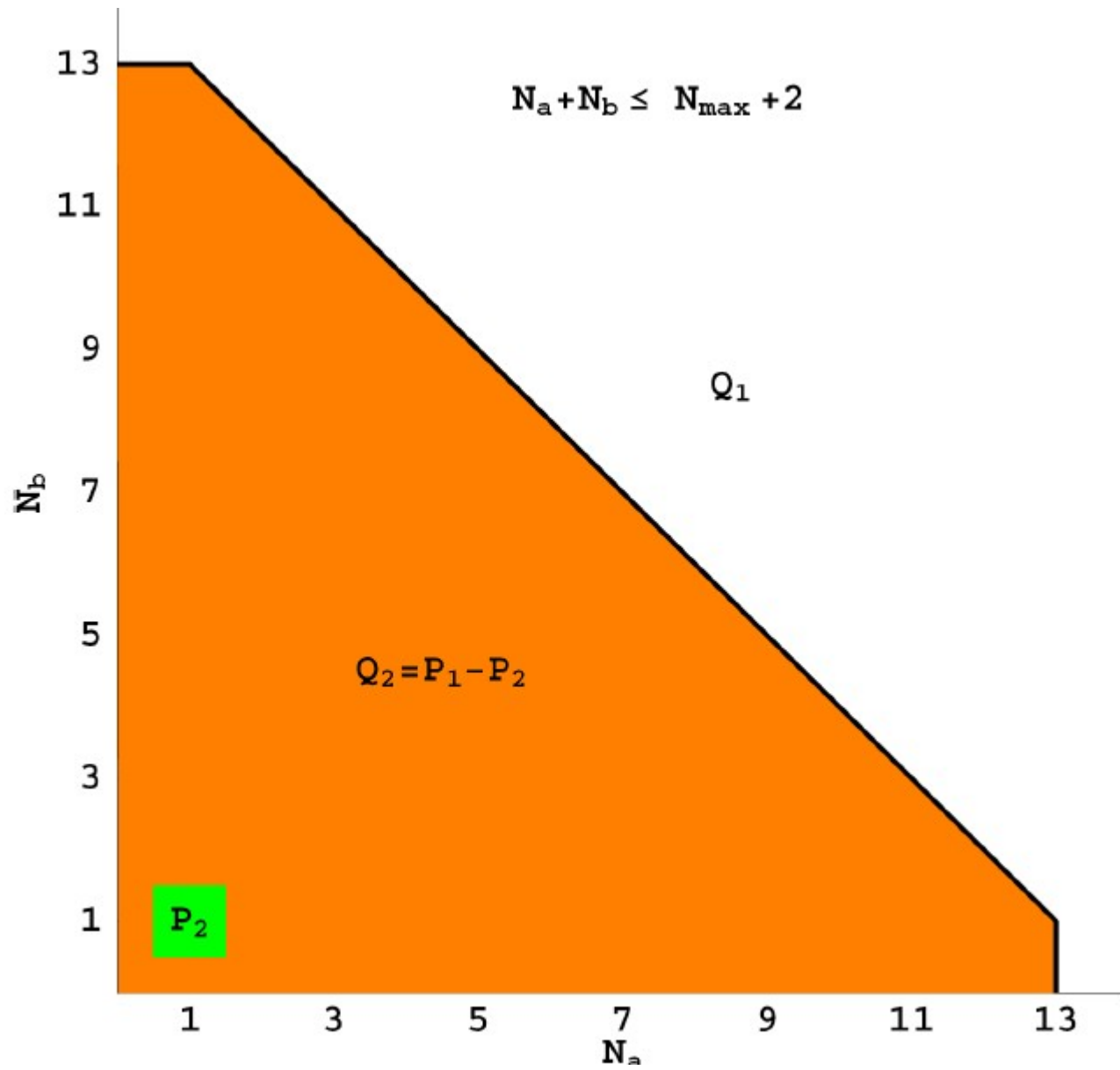$$E^{\Omega}_{A,2} = U_2 H^{\Omega}_{A,2} U_2^{\dagger} \qquad U_2 = \begin{pmatrix} U_{2,P} & U_{2,PQ} \\ U_{2,QP} & U_{2,Q} \end{pmatrix} \qquad E^{\Omega}_{A,2} = \begin{pmatrix} E^{\Omega}_{A,2,P} & 0 \\ 0 & E^{\Omega}_{A,2,Q} \end{pmatrix}$$

$$H^{N_{\max},\Omega,\mathrm{eff}}_{A,2} = \frac{U^{\dagger}_{2,P}}{\sqrt{U^{\dagger}_{2,P} U_{2,P}}} E^{\Omega}_{A,2,P} \frac{U_{2,P}}{\sqrt{U^{\dagger}_{2,P} U_{2,P}}}$$

Two ways of convergence:

1) For $P \to 1$ and fixed a: $H^{\mathrm{eff}}_{A,a=2} \to H_A$

2) For $a \to A$ and fixed P: $H^{\mathrm{eff}}_{A,a} \to H_A$

Ab-initio shell model with a core

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We construct effective two- and three-body Hamiltonians for the p-shell by performing $12\hbar\Omega$ ab initio no-core shell model (NCSM) calculations for $A = 6$ and 7 nuclei and explicitly projecting the many-body Hamiltonians onto the $0\hbar\Omega$ space. We then separate these effective Hamiltonians into inert core, one- and two-body contributions (also three-body for $A = 7$) and analyze the systematic behavior of these different parts as a function of the mass number A and size of the NCSM basis space. The role of effective three- and higher-body interactions for $A > 6$ is investigated and discussed.

P. Navratil, M. Thoresen and B.R.B., Phys. Rev. C 55, R573 (1997)

FORMALISM

1. Perform a large basis NCSM for a core + 2N system, e.g., 18^F.

2. Use Okubo-Lee-Suzuki transformation to project these results into a single major shell to obtain effective 2-body matrix elements.

3. Separate these 2-body matrix elements into a core term, single-particle energies and residual 2-body interactions, i.e., the standard input for a normal Shell Model calculation.

4. Use these values for performing SM calculations in that shell.

How to calculate the Shell Model 2-body effective interaction:

Two ways of convergence:

1) For $P \to 1$ and fixed a: $H^{eff}_{A,a=2} \to H_A$: previous slide

2) For $a_1 \to A$ and fixed P_1: $H^{eff}_{A,a1} \to H_A$

$P_1 + Q_1 = P$; P_1 - small model space; Q_1 - excluded space;

$$\mathcal{H}^{N_{1,\max},N_{\max}}_{A,a_1} = \frac{U^{A,\dagger}_{a_1,P_1}}{\sqrt{U^{A,\dagger}_{a_1,P_1} U^A_{a_1,P_1}}} E^{N_{\max},\Omega}_{A,a_1,P_1} \frac{U^A_{a_1,P_1}}{\sqrt{U^{A,\dagger}_{a_1,P_1} U^A_{a_1,P_1}}}$$

Valence Cluster Expansion

$N_{1,\max} = 0$ space (p-space) ; $a_1 = A_c + a_v$; a_1 - order of cluster;

A_c - number of nucleons in core; a_v - order of valence cluster;

$$\mathcal{H}^{0,N_{\max}}_{A,a_1} = \sum_{k}^{a_v} V^{A,A_c+k}_k$$

II. Results: a.) sd-shell nuclei

Ab initio effective interactions for *sd*-shell valence nucleons

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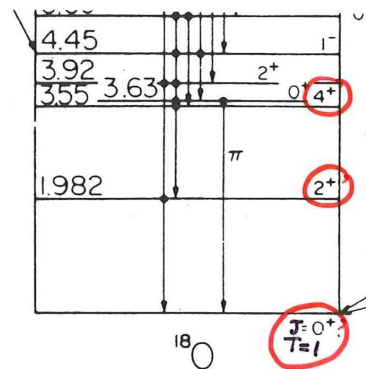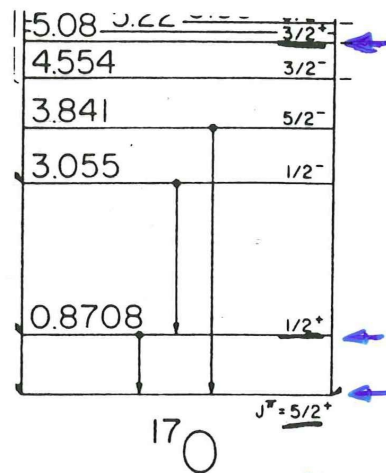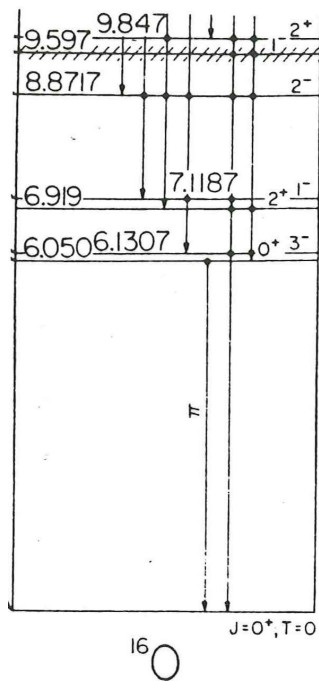[4] *Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Moscow 119991, Russia*
[5] *Pacific National University, 136 Tikhookeanskaya st., Khabarovsk 680035, Russia*
(Dated: February 3, 2015)

We perform *ab initio* no core shell model calculations for $A = 18$ and 19 nuclei in a $4\hbar\Omega$, or $N_{\max} = 4$, model space using the effective JISP16 and chiral N3LO nucleon-nucleon potentials and transform the many-body effective Hamiltonians into the $0\hbar\Omega$ model space to construct the A-body effective Hamiltonians in the *sd*-shell. We separate the A-body effective Hamiltonians with $A = 18$ and $A = 19$ into inert core, one- and two-body components. Then, we use these core, one- and two-body components to perform standard shell model calculations for the $A = 18$ and $A = 19$ systems with valence nucleons restricted to the *sd*-shell. Finally, we compare the standard shell model results in the $0\hbar\Omega$ model space with the exact no core shell model results in the $4\hbar\Omega$ model space for the $A = 18$ and $A = 19$ systems and find good agreement.

Empirical Single-Particle Energies

^{16}O — $J = 0^+, T = 0$

- 9.847 — 2^+
- 9.597 — 1^-
- 8.8717 — 2^-
- 7.1187
- 6.919 — 2^+ 1^-
- 6.1307 — 3^-
- 6.050 — 0^+
- π

^{17}O — $J^\pi = 5/2^+$

- 5.08 / 5.22 — $3/2^+$
- 4.554 — $3/2^-$
- 3.841 — $5/2^-$
- 3.055 — $1/2^-$
- 0.8708 — $1/2^+$
- π

^{18}O — $J = 0^+$, $T = 1$

- 4.45 — 1^-
- 3.92 — 2^+
- 3.63
- 3.55 — 0^+ 4^+
- 1.982 — 2^+
- π

$$\mathcal{E}_{0d_{5/2}} = 0.0 \text{ MeV}$$

$$\mathcal{E}_{1s_{1/2}} = 0.87 \text{ MeV}$$

$$\mathcal{E}_{0d_{3/2}} = 5.08 \text{ MeV}$$

$$H^{sd}\left(\Psi\right)^{sd} = \left\{ \sum_{i}^{sd} \mathcal{E}_i + \upsilon_{eff}^{sd} \right\}\left(\Psi\right)^{sd}$$

$$\left\{ H_0 + \upsilon_{eff}^{sd} \right\}\left(\Psi\right)^{sd} = E^{sd}\left(\Psi\right)^{sd}$$

Input: The results of N_max = 4 and hw = 14 MeV NCSM calculations

TABLE II: Proton and neutron single-particle energies (in MeV) for JISP16 effective interaction obtained for the mass of $A = 18$ and $A = 19$.

j_i	$A = 18$ $E_{core} = -115.529$			$A = 19$ $E_{core} = -115.319$		
	$\frac{1}{2}$	$\frac{5}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	$\frac{5}{2}$	$\frac{3}{2}$
$\epsilon_{j_i}^n$	-3.068	-2.270	6.262	-3.044	-2.248	6.289
$\epsilon_{j_i}^p$	0.603	1.398	9.748	0.627	1.419	9.774

TABLE III: Proton and neutron single-particle energies (in MeV) for chiral N3LO effective interaction obtained for the mass of $A = 18$ and $A = 19$.

j_i	$A = 18$ $E_{core} = -118.469$			$A = 19$ $E_{core} = -118.306$		
	$\frac{1}{2}$	$\frac{5}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	$\frac{5}{2}$	$\frac{3}{2}$
$\epsilon_{j_i}^n$	-3.638	-3.042	3.763	-3.625	-3.031	3.770
$\epsilon_{j_i}^p$	0.044	0.690	7.299	0.057	0.700	7.307

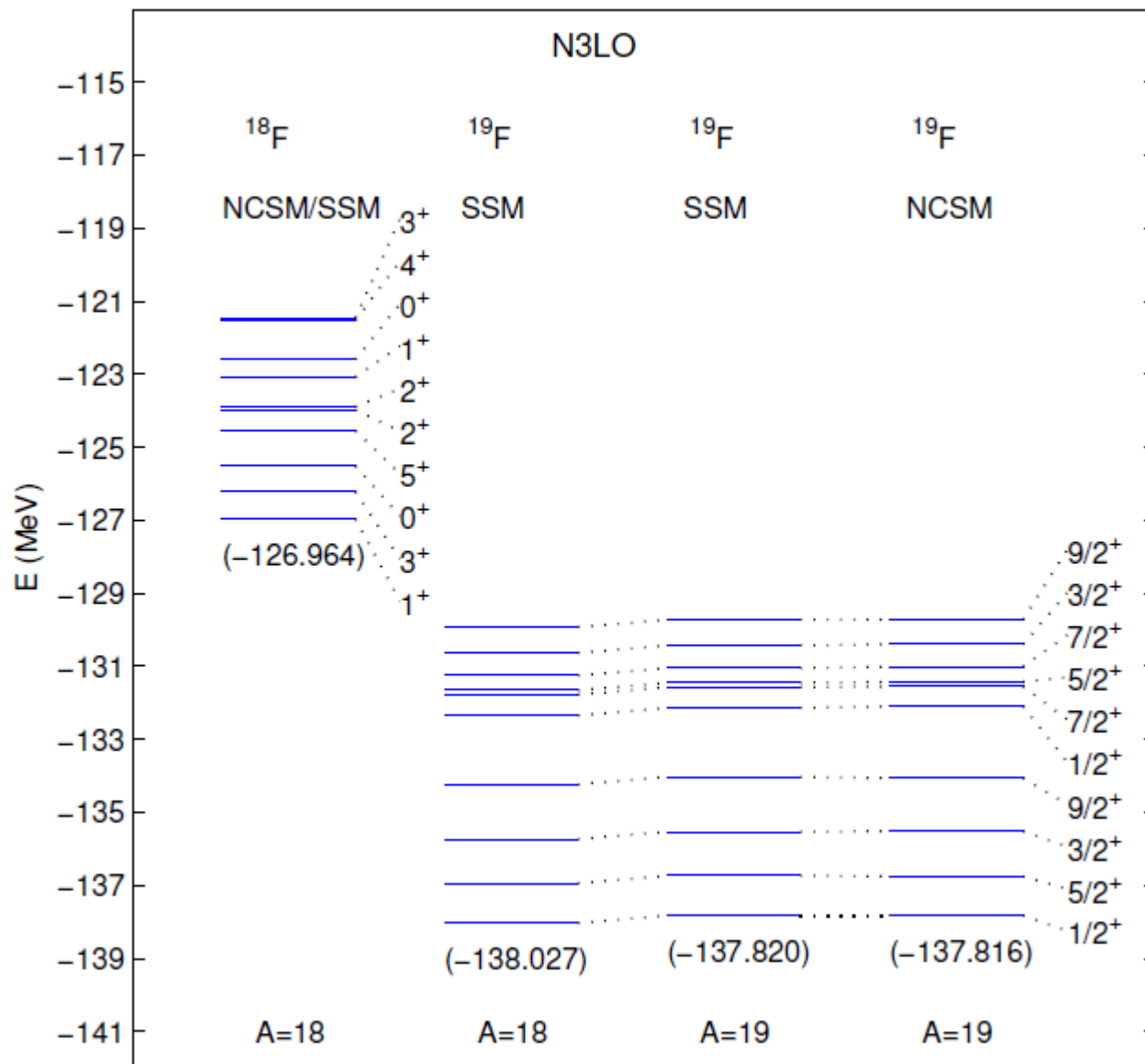|	A = 18	A = 19	
Coupled Cluster, E_core: Idaho NN N3LO + 3N N2LO	-130.462	-130.056	from G.R. Jansen et al. PRL 113, 142502 (2014)
IM-SRG, E_core: Idaho NN N3LO + 3N N2LO	-130.132	-129.637	from H. Hergert private comm.

No-Core Shell-Model Approach

- Next, add CM harmonic-oscillator Hamiltonian

$$H_{CM}^{HO} = \frac{\vec{P}^2}{2Am} + \frac{1}{2}Am\Omega^2\vec{R}^2 \;; \quad \vec{R} = \frac{1}{A}\sum_{i=1}^{A}\vec{r}_i \,, \quad \vec{P} = Am\dot{\vec{R}}$$
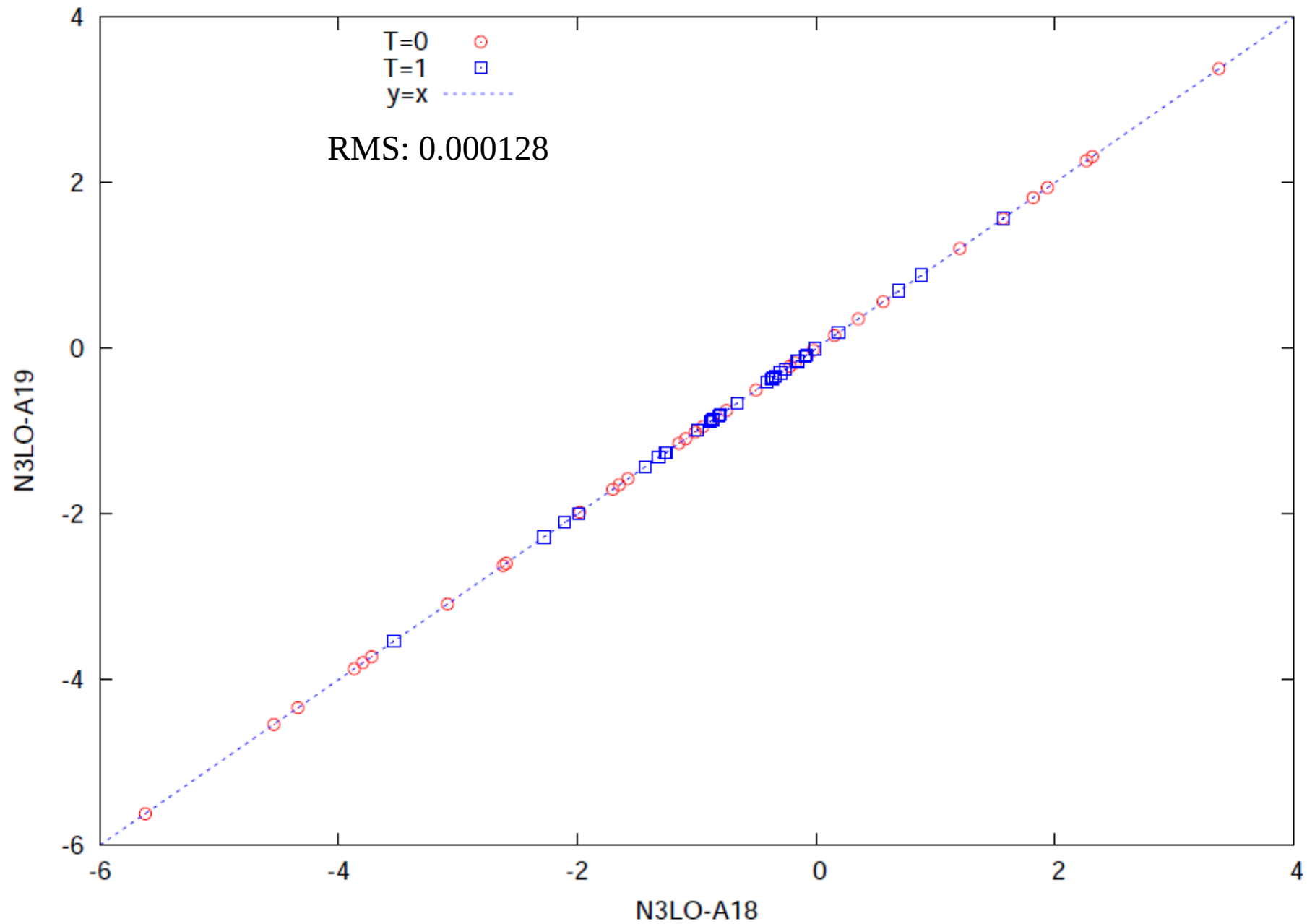
To H_A, yielding

$$H_A^{\Omega} = \sum_{i=1}^{A}\left[\frac{\vec{p}_i^2}{2m} + \frac{1}{2}m\Omega^2\vec{r}_i^2\right] + \sum_{i<j=1}^{A}\underbrace{\left[V_{NN}(\vec{r}_i - \vec{r}_j) - \frac{m\Omega^2}{2A}(\vec{r}_i - \vec{r}_j)^2\right]}_{v_{ij}}$$

Defines a basis (*i.e.* HO) for evaluating $\qquad v_{ij}$

N3LO

E (MeV)

-115

-117

-119

-121

-123

-125

-127

-129

-131

-133

-135

-137

-139

-141

^{18}F
NCSM/SSM

(−126.964)

3^+
4^+
0^+
1^+
2^+
2^+
5^+
0^+
3^+
1^+

^{19}F
SSM

(−138.027)

^{19}F
SSM

(−137.820)

^{19}F
NCSM

(−137.816)

$9/2^+$
$3/2^+$
$7/2^+$
$5/2^+$
$7/2^+$
$1/2^+$
$9/2^+$
$3/2^+$
$5/2^+$
$1/2^+$

A=18   A=18   A=19   A=19

PRELIMINARY RESULT

RMS: 0.000128

II. Results: b) Fluorine isotopes

Survey of the Fluorine isotopes

1. Calculate the Fluorine isotopes using the same set of effective TBMEs, which are very weakly A-dependent, e.g., those determined from the N3LO NN interaction, to test how well they reproduce data trends.

2. Approximate the effect of 3NFs by replacing our theoretical single-particle energies with the theoretical ones obtained in the IM-SRG calculations of S.R. Stroberg et al. *

3. Compare our results for 18,20,22,24 F with those obtained with the IM-SRG approach* using an EFT N3LO NN plus N2LO NNN interaction and with experiment.

* S.R. Stroberg et al., arXiv Nucl-th 1511.02802 (2015)
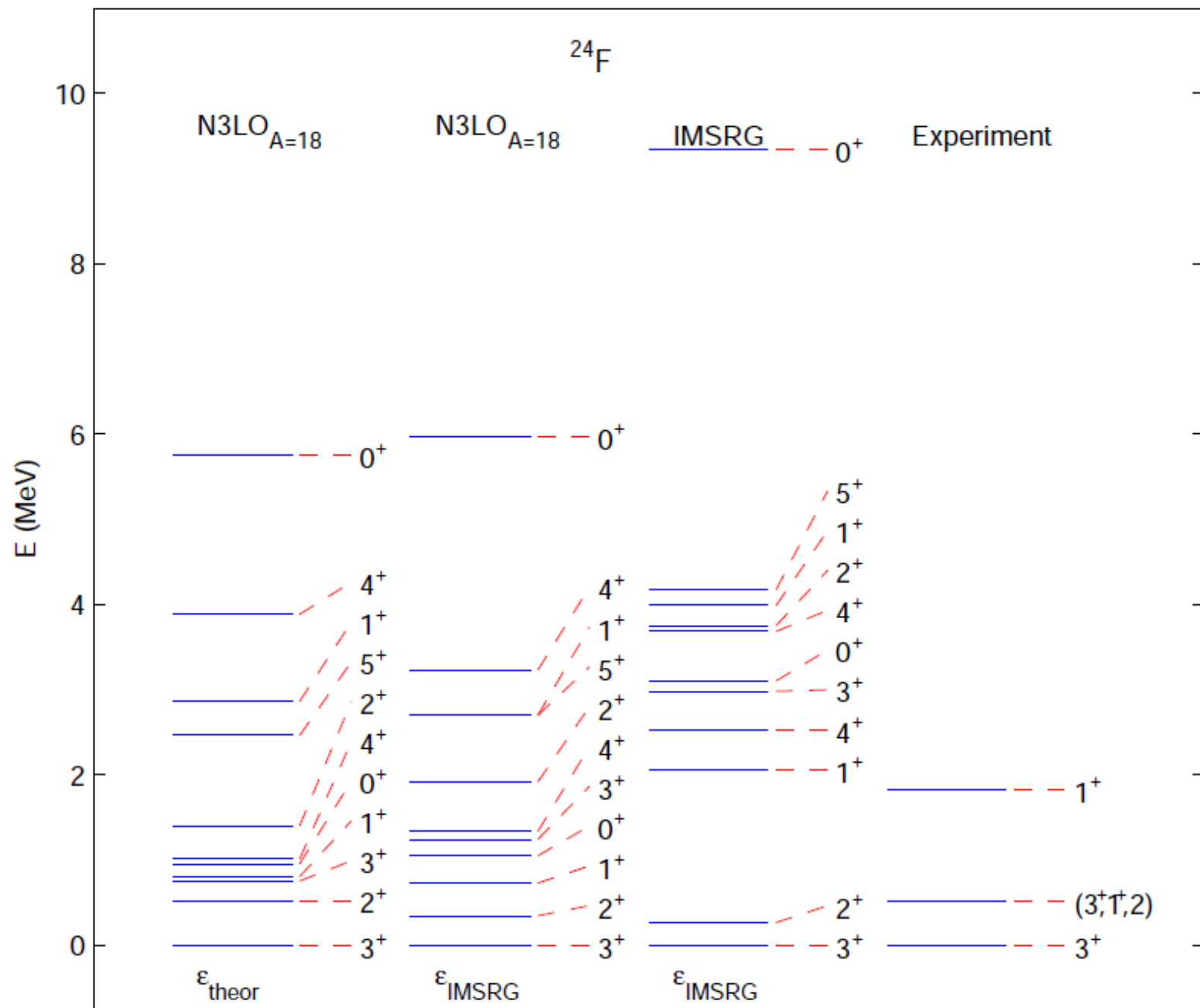
Preliminary Results

TABLE I: The single-particle energies (in MeV) used in the standard shell model calculations of F isotopes. (n) and (p) represent neutron and proton, respectively.

j_i	$\frac{1}{2}$	$\frac{5}{2}$	$\frac{3}{2}$	
JISP16$_{A=18}$ (^{17}O) : (n)	-3.068	-2.270	6.262	
JISP16$_{A=18}$ (^{17}F) : (p)	0.603	1.398	9.748	
USDA	-3.0612	-3.9436	1.9798	*
USDB	-3.2079	-3.9257	2.1117	
IM-SRG (^{17}O) : (n)	-3.089	-4.643	2.940	**
IM-SRG (^{17}F) : (p)	0.255	-0.909	6.035	

* B.A. Brown & W.A. Richter, PRC 74, 034315 (2006)

** S.R. Stroberg, et al., arXiv Nucl-th 1511.02802
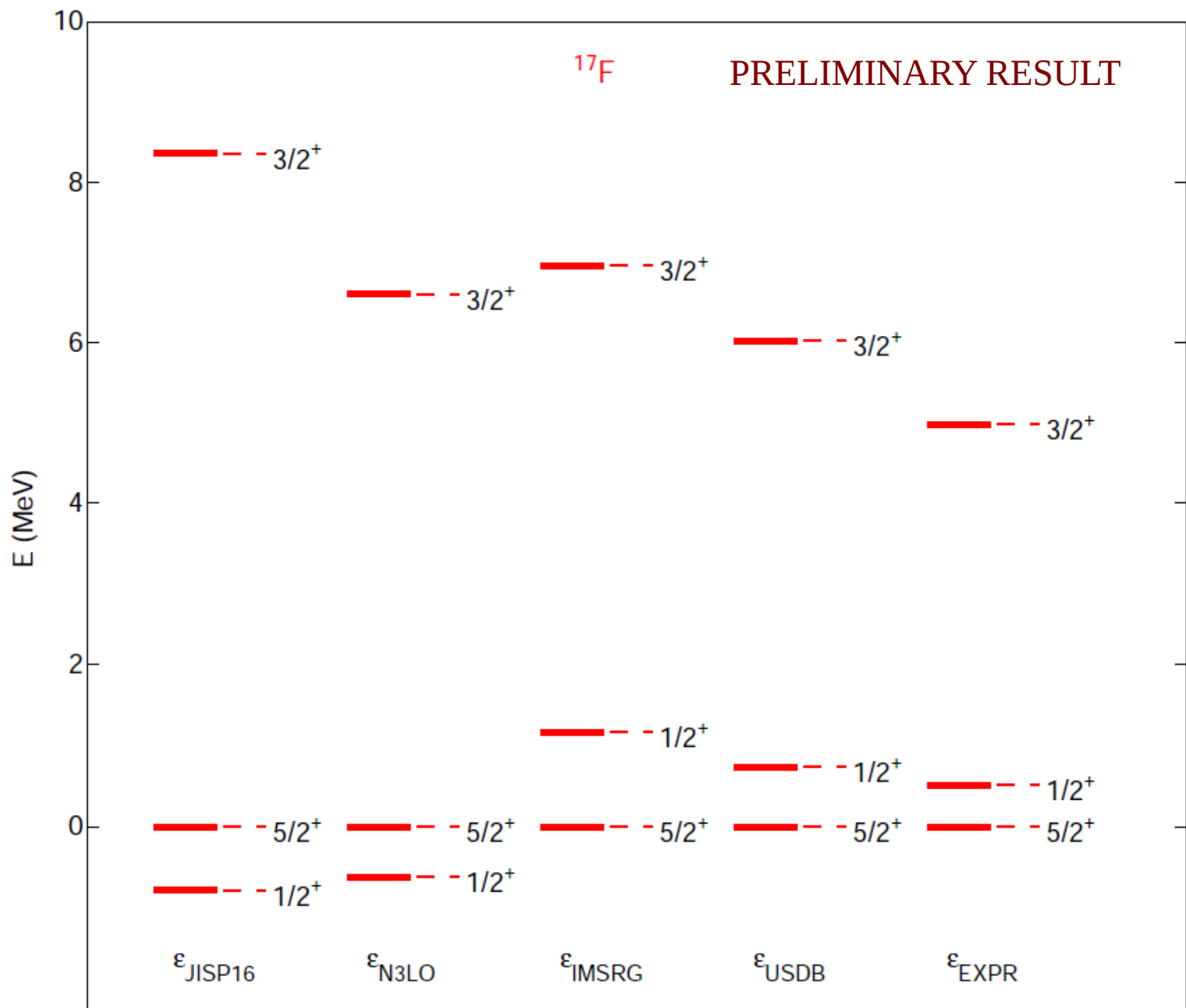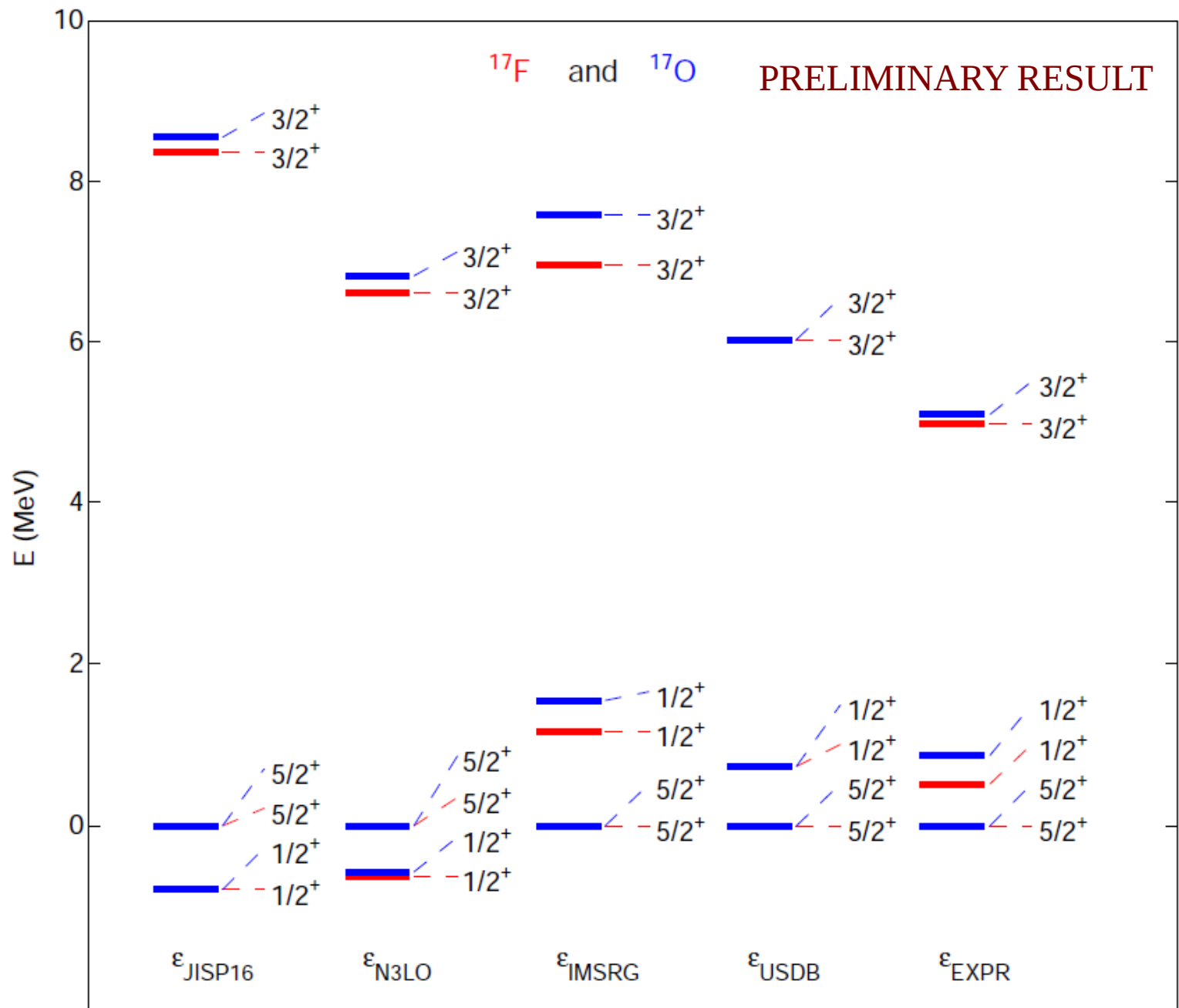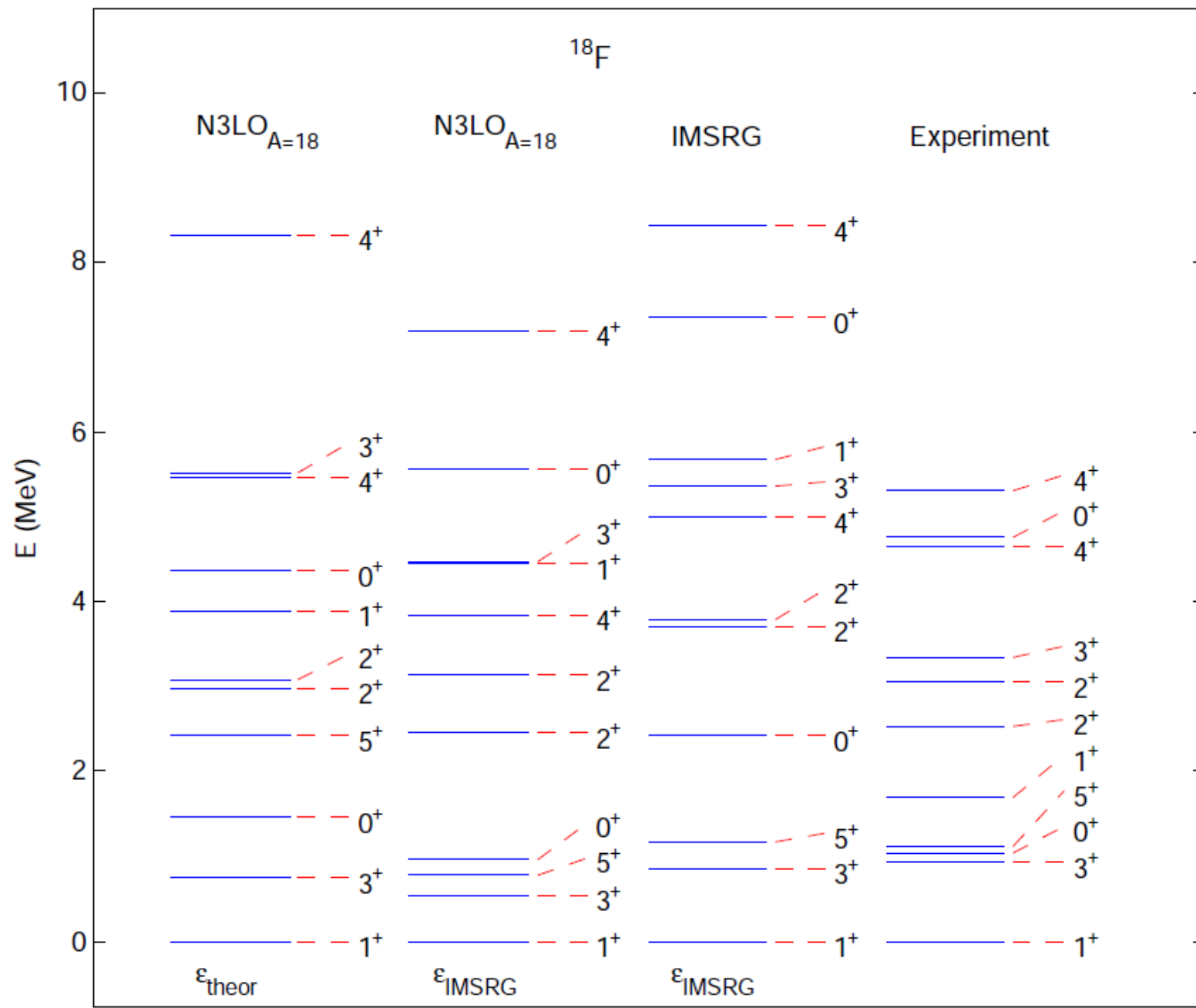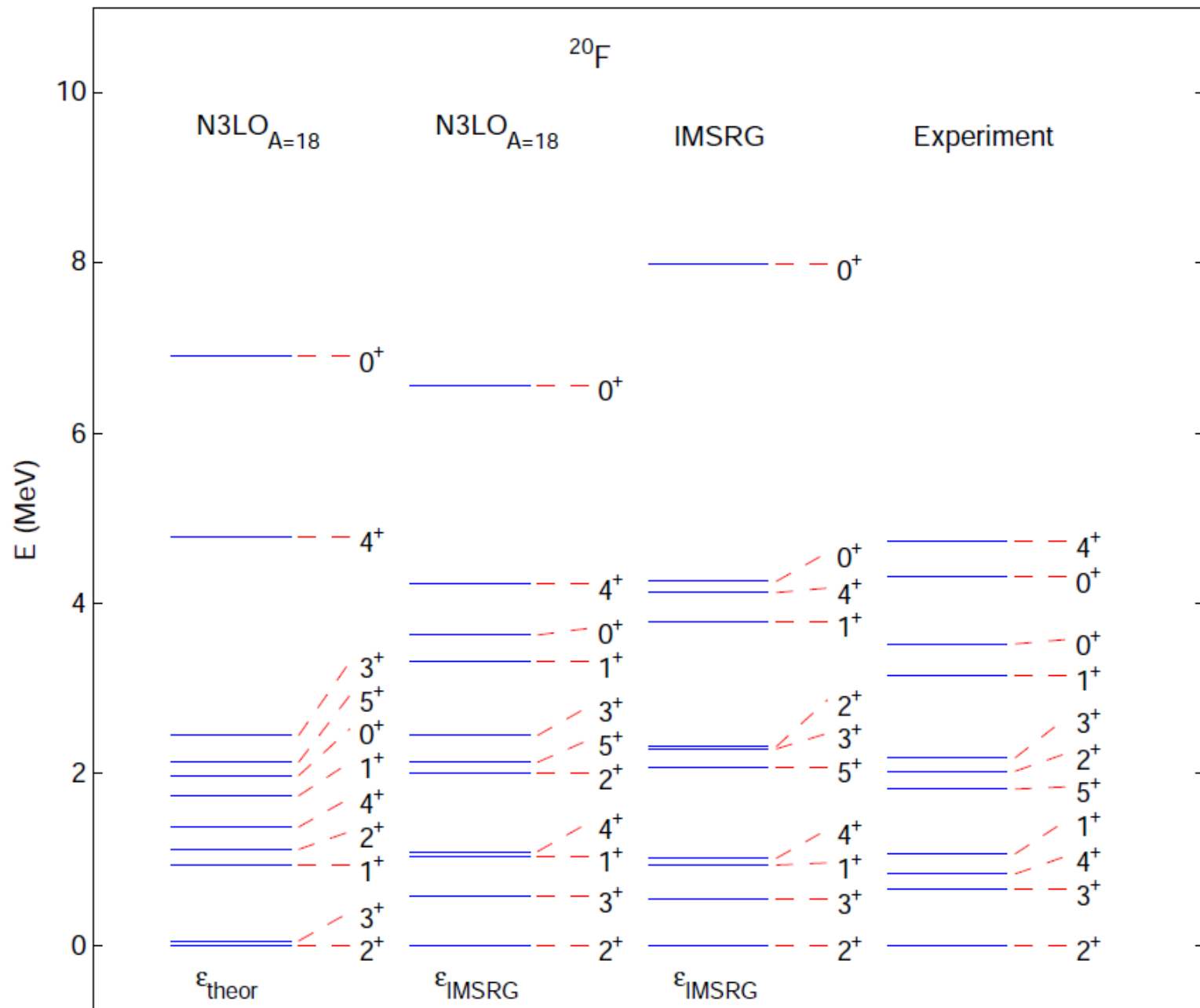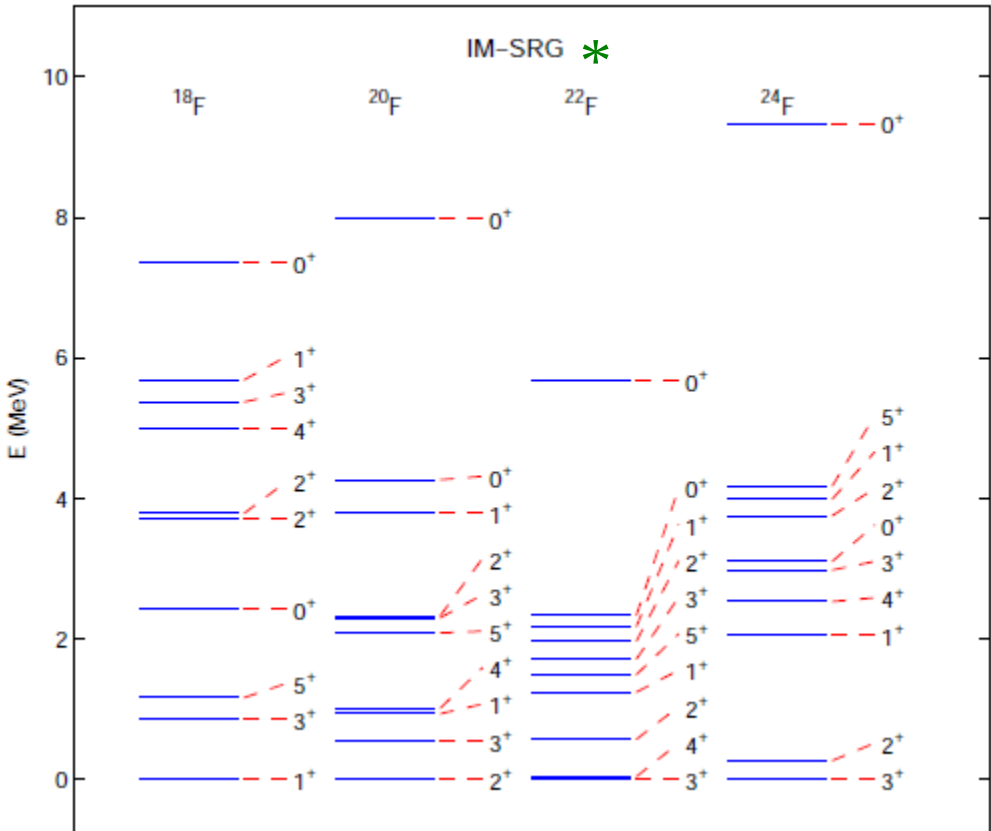
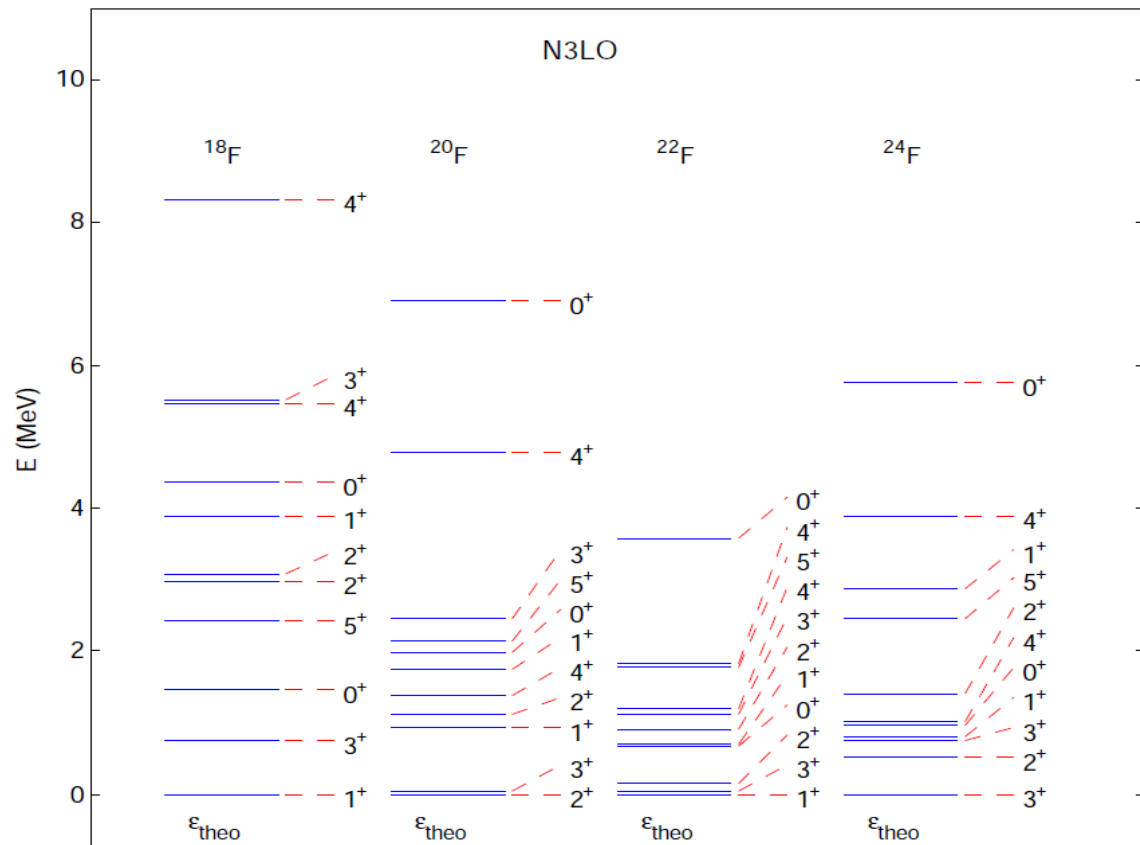^{17}F and ^{17}O   PRELIMINARY RESULT

PRELIMINARY RESULT

PRELIMINARY RESULT

PRELIMINARY RESULT

^{22}F
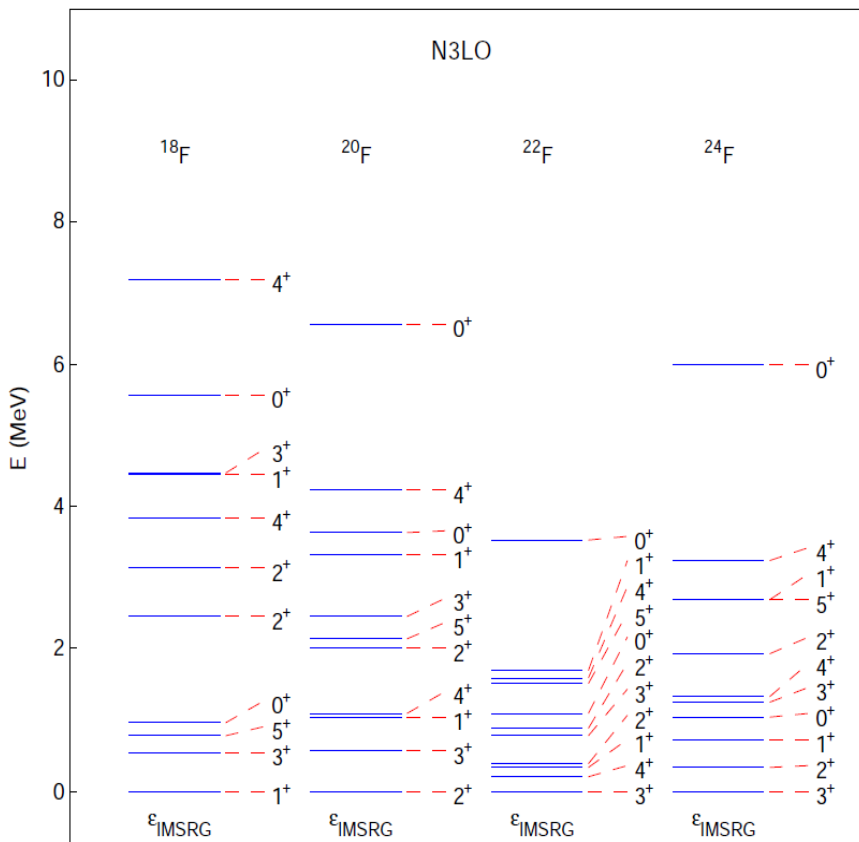
PRELIMINARY RESULT

^{24}F
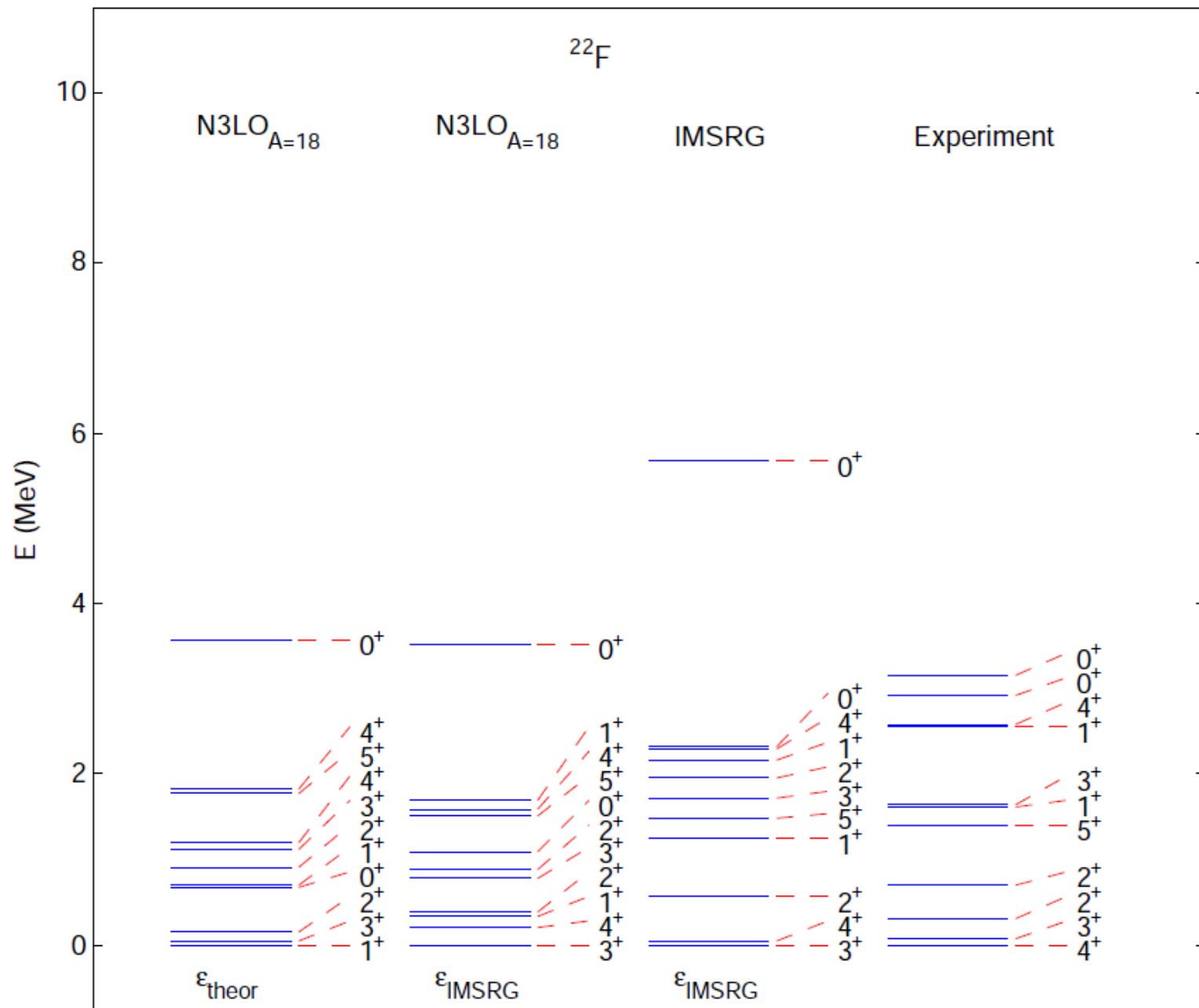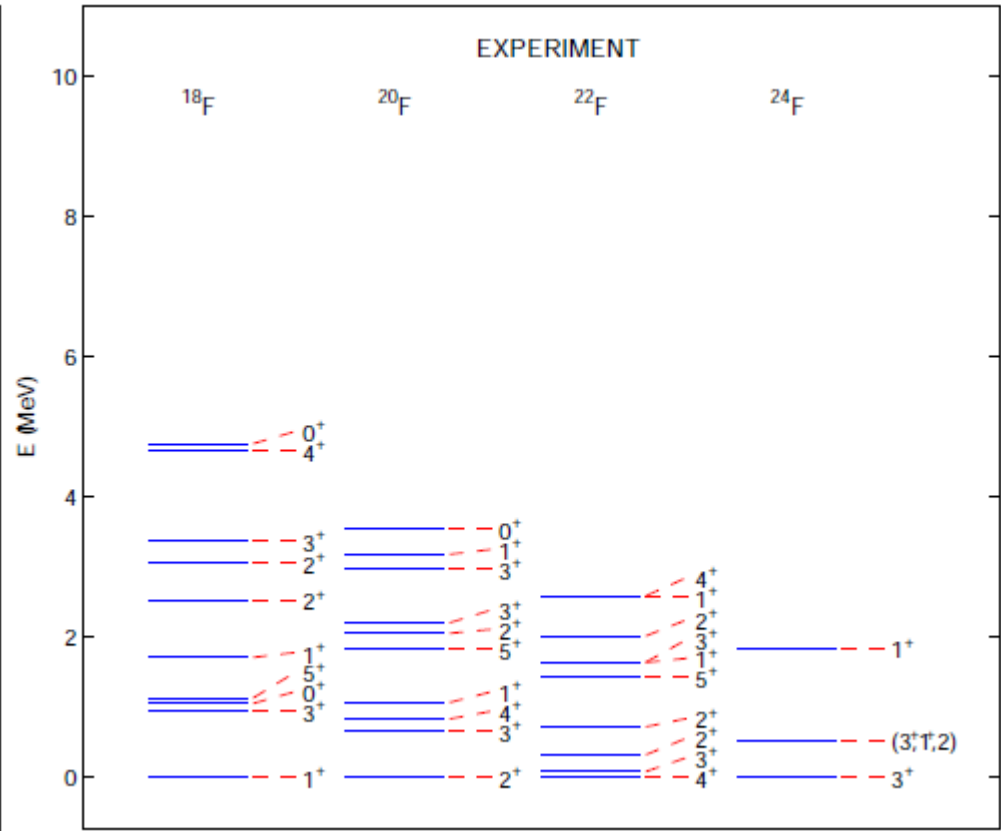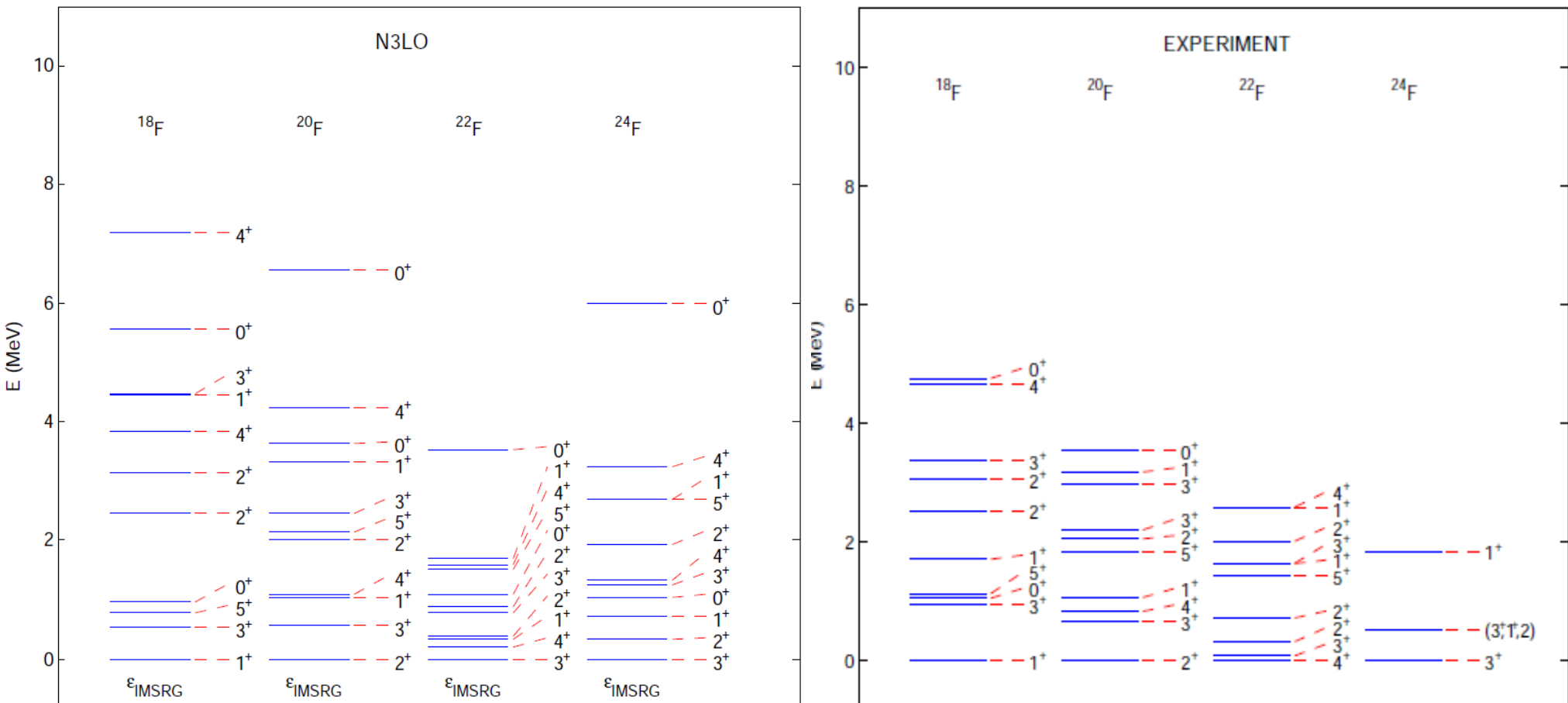
* S.R. Stroberg, et al., arXiv Nucl-th 1511.02802

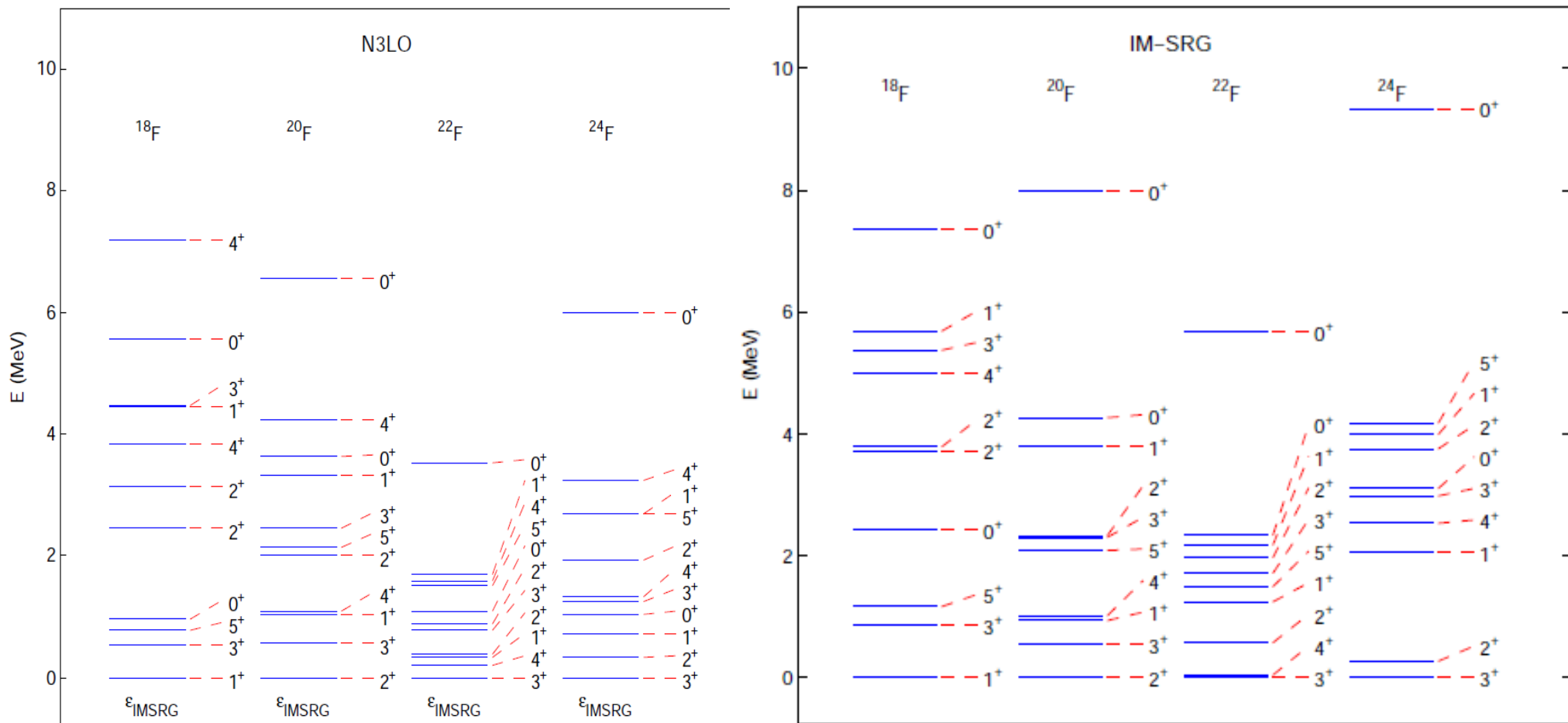## N3LO + IMSRG spe vs N3LO + theoretical spe

PRELIMINARY RESULTS

N3LO + IMSRG spe vs Experiment

PRELIMINARY RESULTS


N3LO + IMSRG spe vs IM-SRG

SUMMARY AND OUTLOOK

1. The interactions and approaches used in this study reproduced the gross trends and features of the experimental data for the 18,20,22,24 F isotopes.

2. Replacing our theoretical s.p. energies with those obtained in the IM-SRG calculations of Stroberg et al. to approximate the effects of a NNN interaction, in general, improved the agreement with experiment.

3. The overall, reasonable agreement with experiment obtained using the IM-SRG approach with an EFT N3LO NN and N2LO NNN suggests that the trends in our results should continue to improve as we improve the interactions used and increase the size of our model space for our NCSM calculations.

4. The current results support the hypothesis that a single A-independent set of effective TBMEs can explain the trends in the F isotopes.
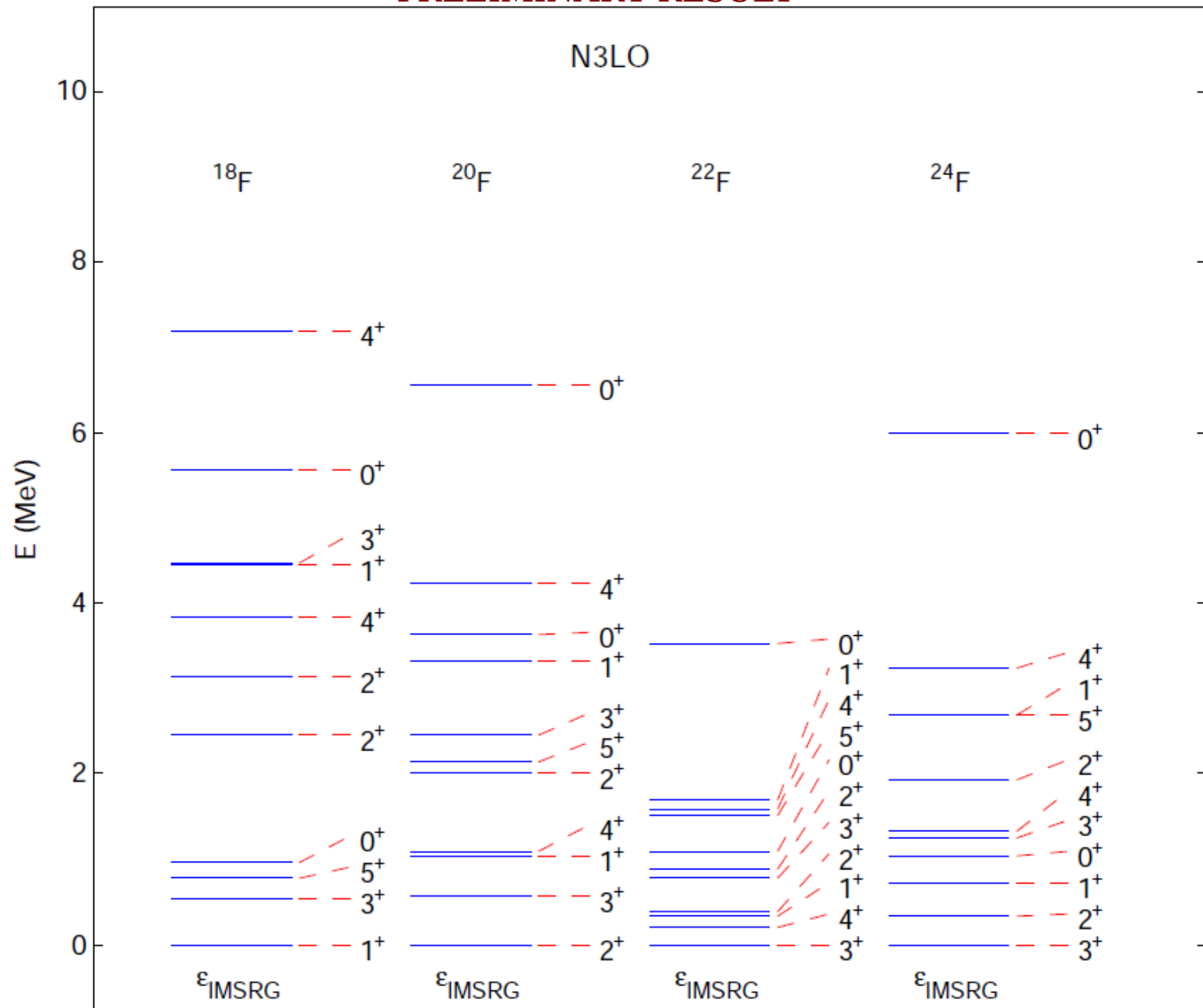
OUTLOOK: Plan to perform further calculations implementing the changes outlined above.

N3LO
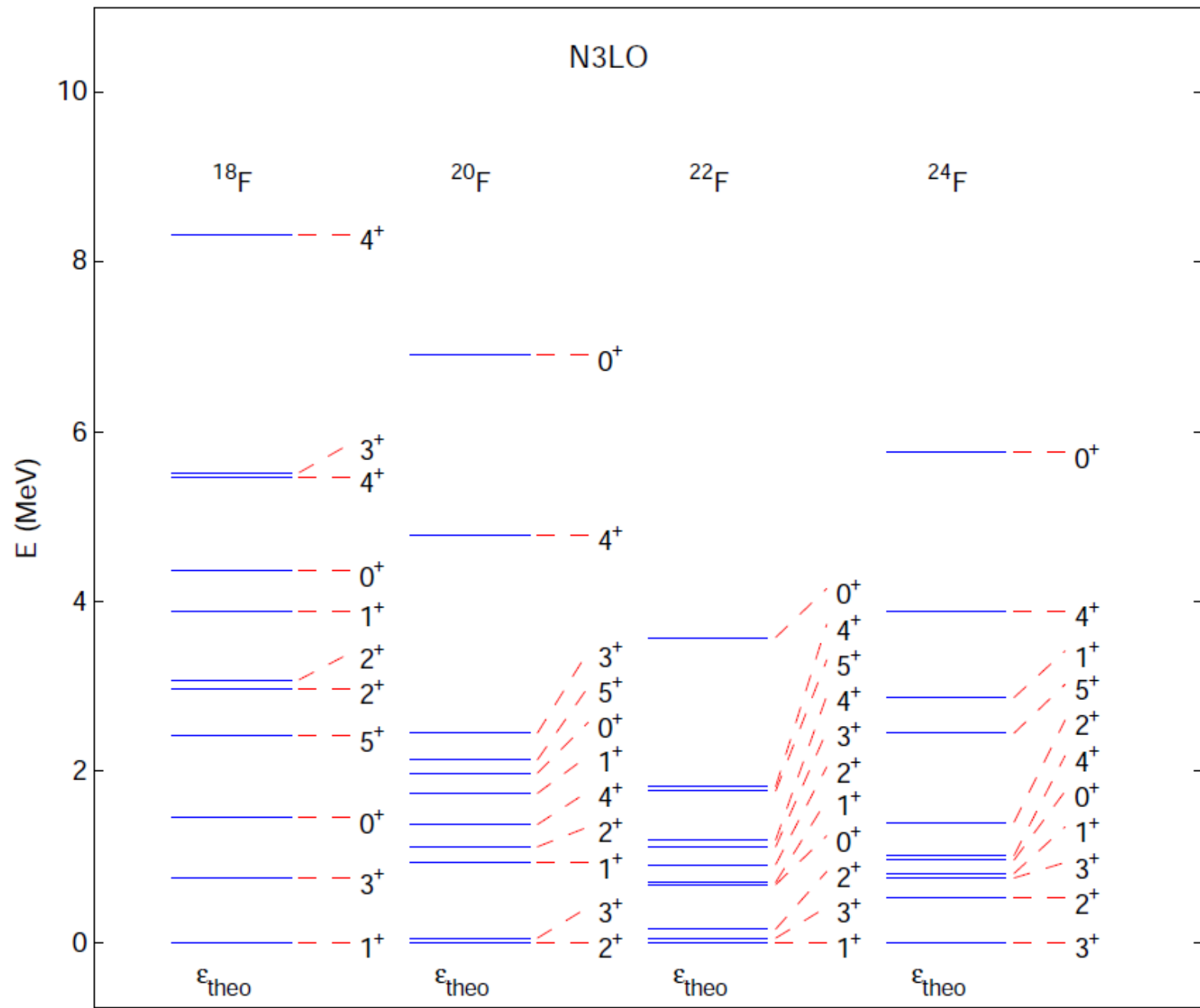
PRELIMINARY RESULT

Two-body VCE for ^{6}Li

$$\mathcal{H}^{0,N_{\max}}_{A=6,a_1=6} = V_0^{6,4} + V_1^{6,5} + V_2^{6,6}$$

Need NCSM results in $N_{\max}$ space for ^{4}He ^{5}He ^{5}Li ^{6}He ^{6}Li ^{6}Be

With effective interaction for A=6 !!! $H^{N_{\max},\Omega,\text{eff}}_{A=6,2}$

3-body Valence Cluster approximation for A>6

$$\mathcal{H}_{A,a_1=7}^{0,N_{\max}} = V_0^{A,4} + V_1^{A,5} + V_2^{A,6} + V_3^{A,7}$$

Need NCSM results in N$_{max}$ space for

^{4}He ^{5}He ^{5}Li ^{6}He ^{6}Li ^{6}Be ^{7}He ^{7}Li ^{7}B ^{7}Be

With effective interaction for A !!!

$$H_{A,2}^{N_{\max},\Omega,\text{eff}}$$

Construct 3-body interaction in terms of 3-body matrix elements: Yes

$$V_3^{A,7} = \mathcal{H}_{A,7}^{0,N_{\max}} - \mathcal{H}_{A,6}^{0,N_{\max}}$$