Microscopically Calculated Shell-Model Effective TBMEs in the sd-Shell

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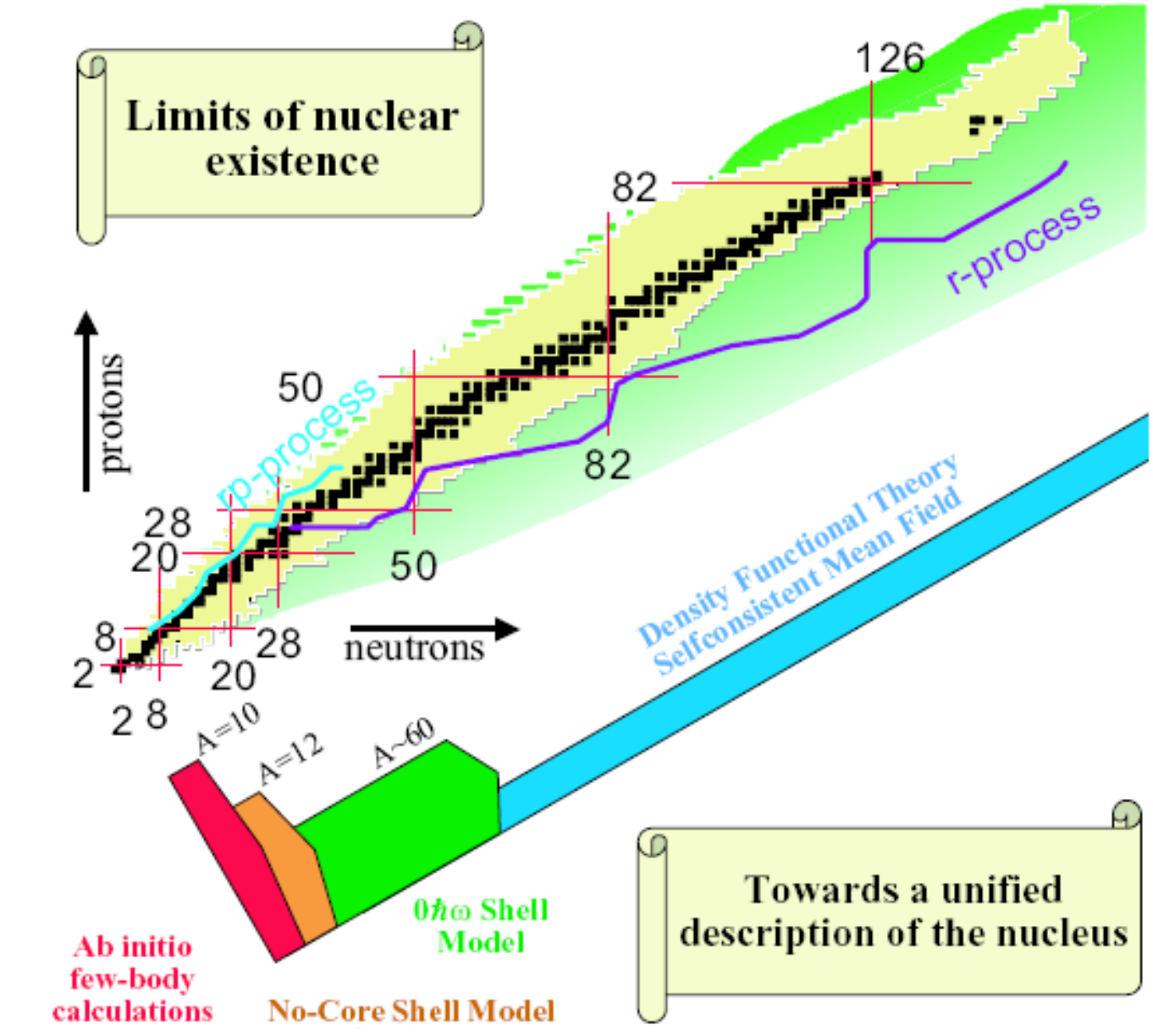

Limits of nuclear existence
126
82
82
50
50
28
20
28
20
8
2
2 8
protons
neutrons
rp-process
r-process
Density Functional Theory
Selfconsistent Mean Field
A=10
A=12
A~60
0ħω Shell Model
Towards a unified description of the nucleus
Ab initio few-body calculations
GFMC formalism
No-Core Shell Model
Coupled Cluster approach
IM-SRG

OUTLINE

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

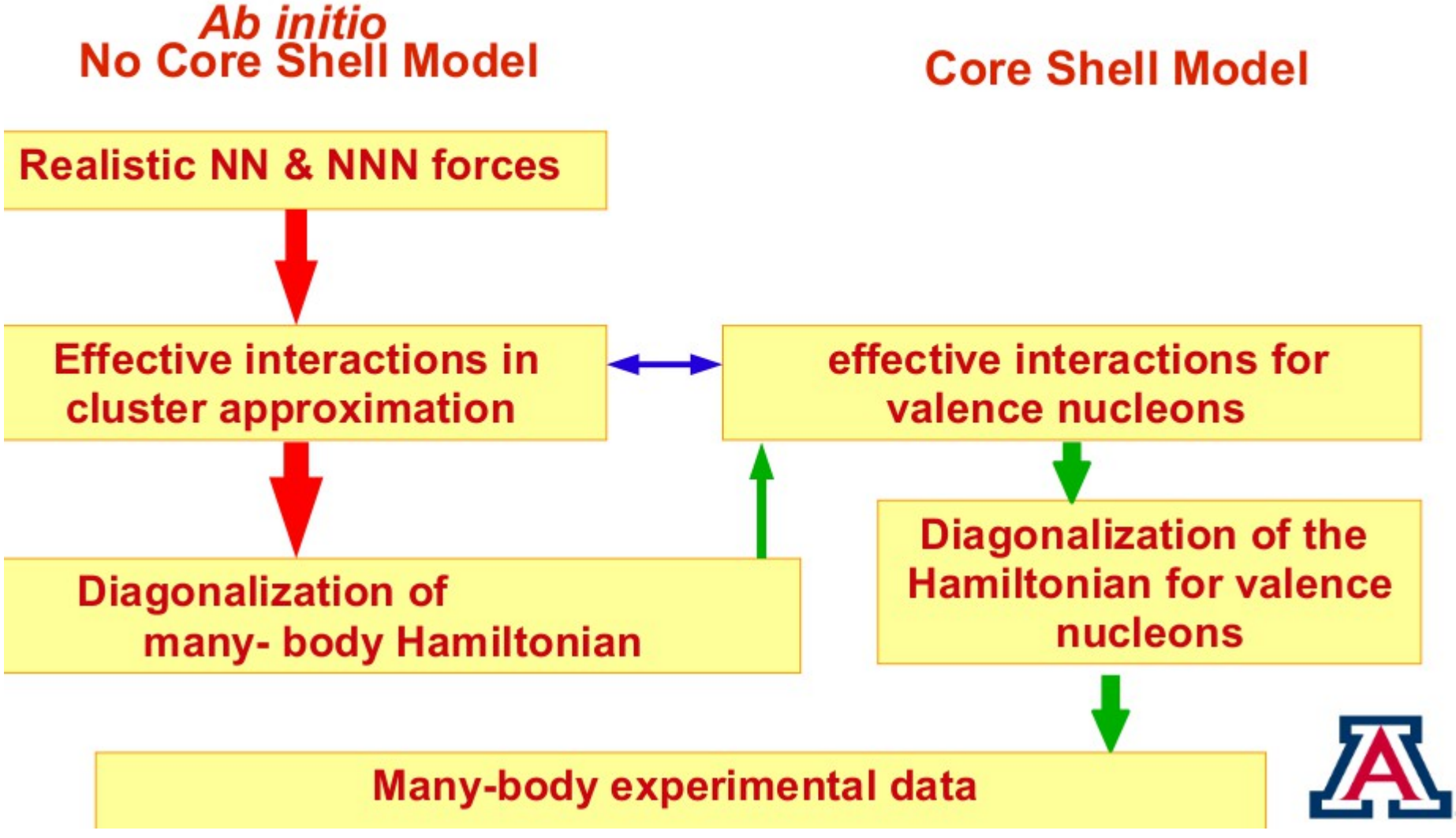
II. Results:
- a.) General sd-shell
- b.) Fluorine isotopes
- c.) Effective Interactions Comparisons

III. Summary/Outlook

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



Effective interaction in a projected model space

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

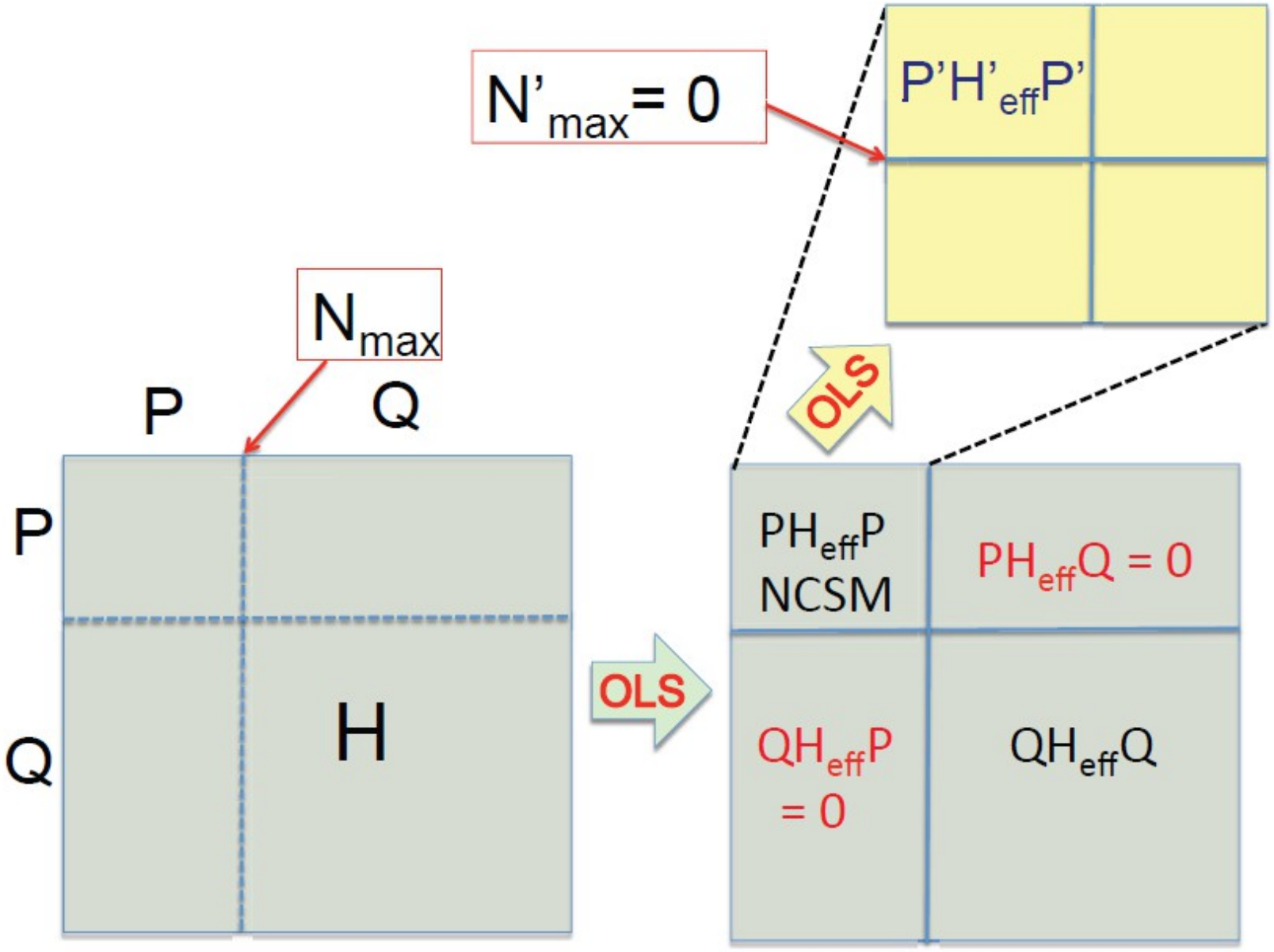
$$\mathcal{H}\Phi_\beta = E_\beta \Phi_\beta$$

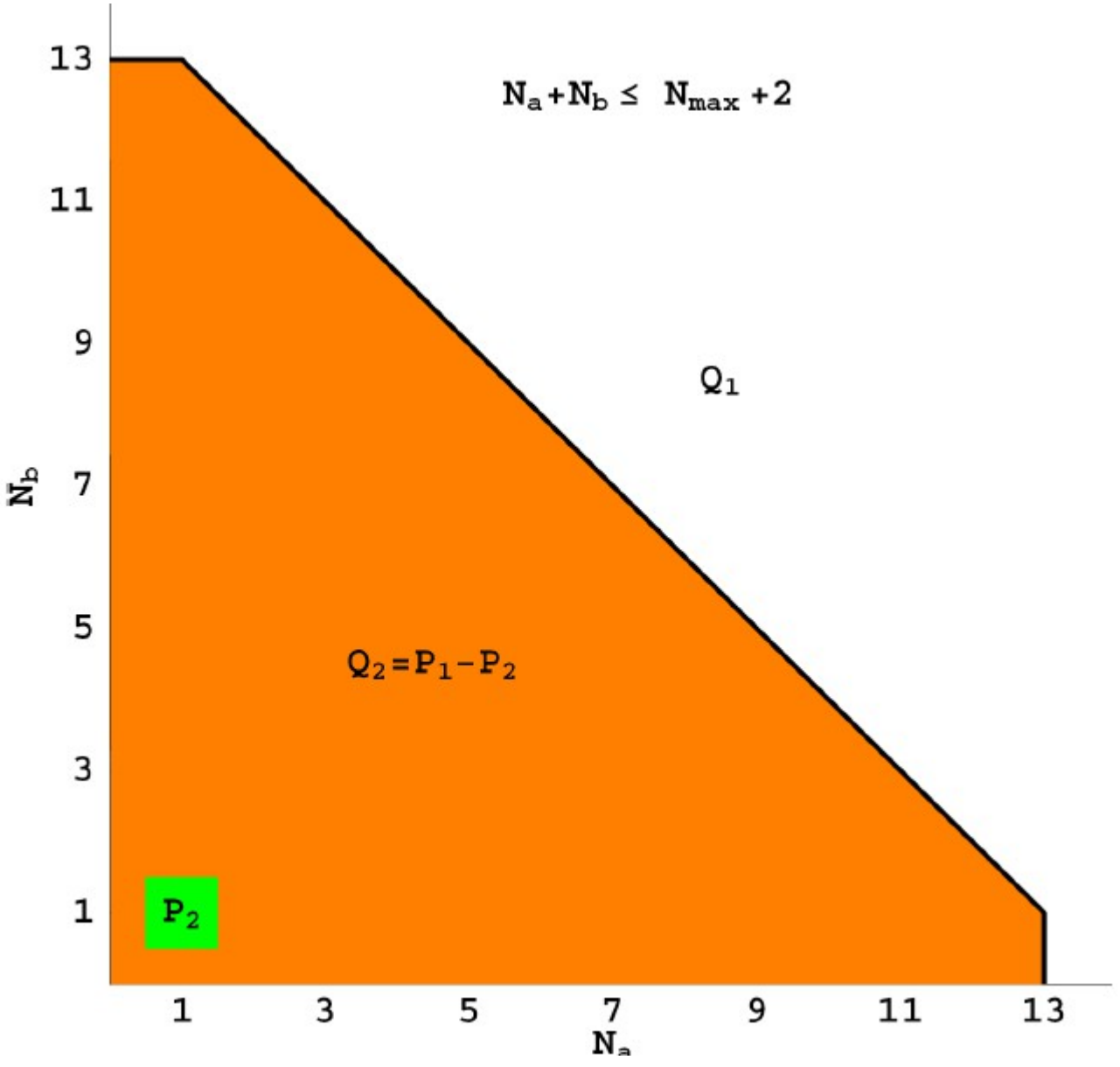
$$\Phi_\beta = P\Psi_\beta$$

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

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

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


N'max = 0
P'H'effP'
Nmax
P
Q
P
Q
H
OLS
OLS
PHeffP
NCSM
PHeffQ = 0
QHeffP
= 0
QHeffQ


$N_a+N_b \leq N_{max}+2$
Q_1
$Q_2=P_1-P_2$
P_2
13
11
9
7
5
3
1
N_b
1
3
5
7
9
11
13
N_a

PHYSICAL REVIEW C **78**, 044302 (2008)

Ab-initio shell model with a core

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(Received 20 June 2008; published 10 October 2008)

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.

DOI: 10.1103/PhysRevC.78.044302 PACS number(s): 21.10.Hw, 21.60.Cs, 23.20.Lv, 27.20.+n

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.

II. Results: a.) sd-shell nuclei

Phys. Rev. C 91, 064301 (2015)

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

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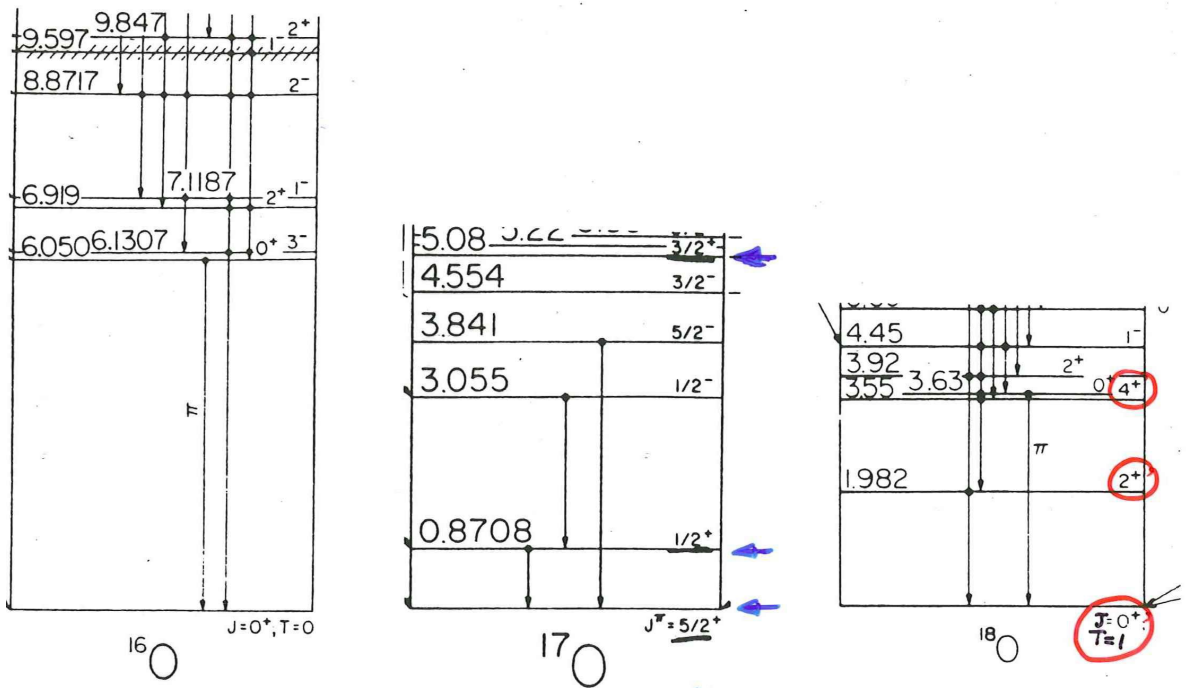
(Dated: February 3, 2015)

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.

ArXiv: Nucl-th 1502.00700

Empirical Single-Particle Energies



$\varepsilon_{od_{5/2}} = 0.0$ MeV

$\varepsilon_{1s_{1/2}} = 0.87$ MeV

$\varepsilon_{od_{3/2}} = 5.08$ MeV

$$H^{sd}(I^{\pi}T)^{sd} = \left\{ \sum_i^{sd} \varepsilon_i + v_{eff}^{sd} \right\} (I^{\pi}T)^{sd}$$

$$\{H_0 + v_{eff}^{sd}\}(I^{\pi}T)^{sd} = E^{sd}(I^{\pi}T)^{sd}$$

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 $A = 19$.

	$A = 18$ $E_{\rm core} = -115.529$			$A = 19$ $E_{\rm core} = -115.319$		
j_i	$\frac{1}{2}$	$\frac{5}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	$\frac{5}{2}$	$\frac{3}{2}$
$\epsilon^n_{j_i}$	-3.068	-2.270	6.262	-3.044	-2.248	6.289
$\epsilon^p_{j_i}$	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 $A = 19$.

	$A = 18$ $E_{\rm core} = -118.469$			$A = 19$ $E_{\rm core} = -118.306$		
j_i	$\frac{1}{2}$	$\frac{5}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	$\frac{5}{2}$	$\frac{3}{2}$
$\epsilon^n_{j_i}$	-3.638	-3.042	3.763	-3.625	-3.031	3.770
$\epsilon^p_{j_i}$	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

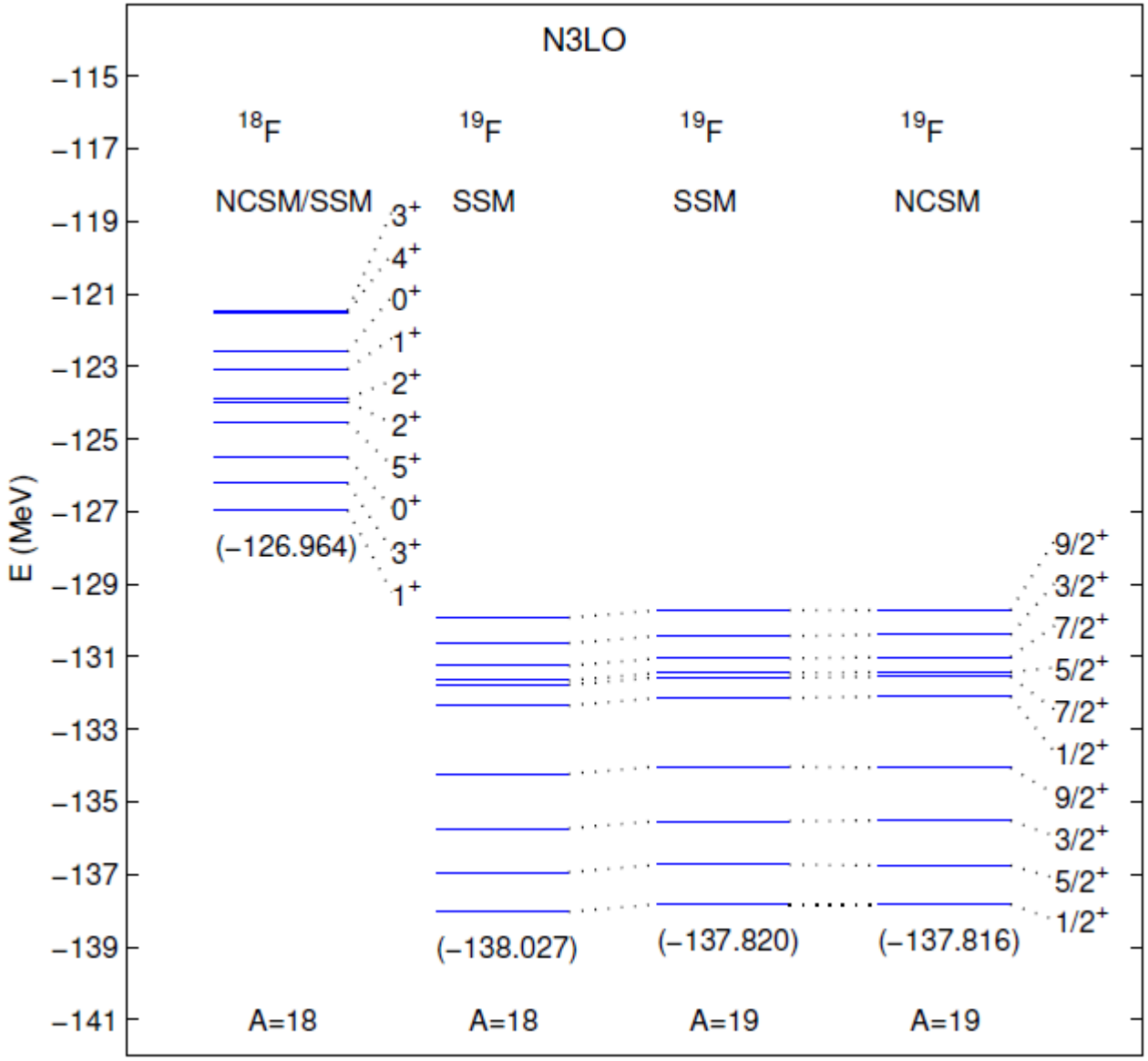
- Next, add CM harmonic-oscillator Hamiltonian

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

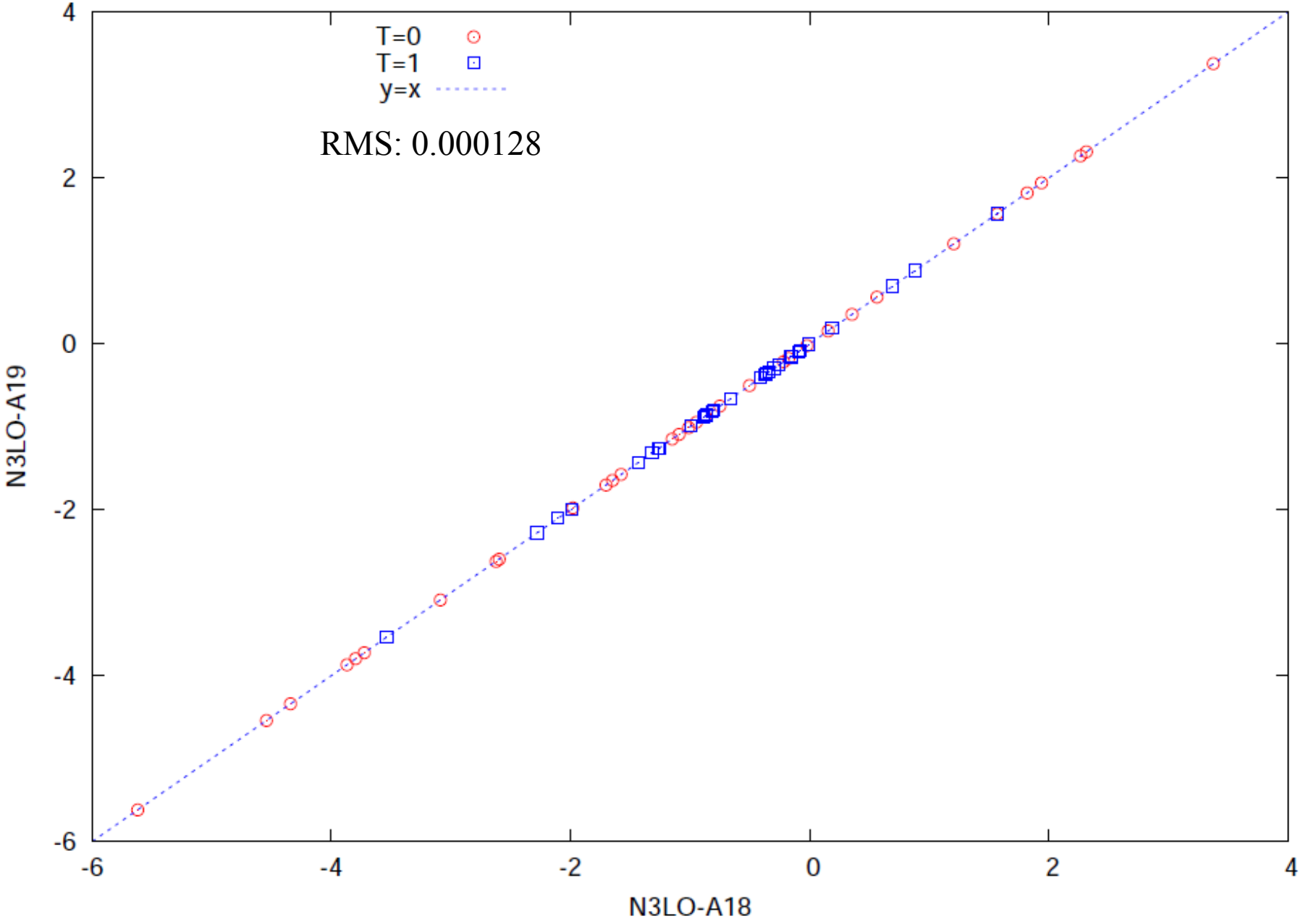
To H_A, yielding

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

Defines a basis (*i.e.* HO) for evaluating V_{ij}

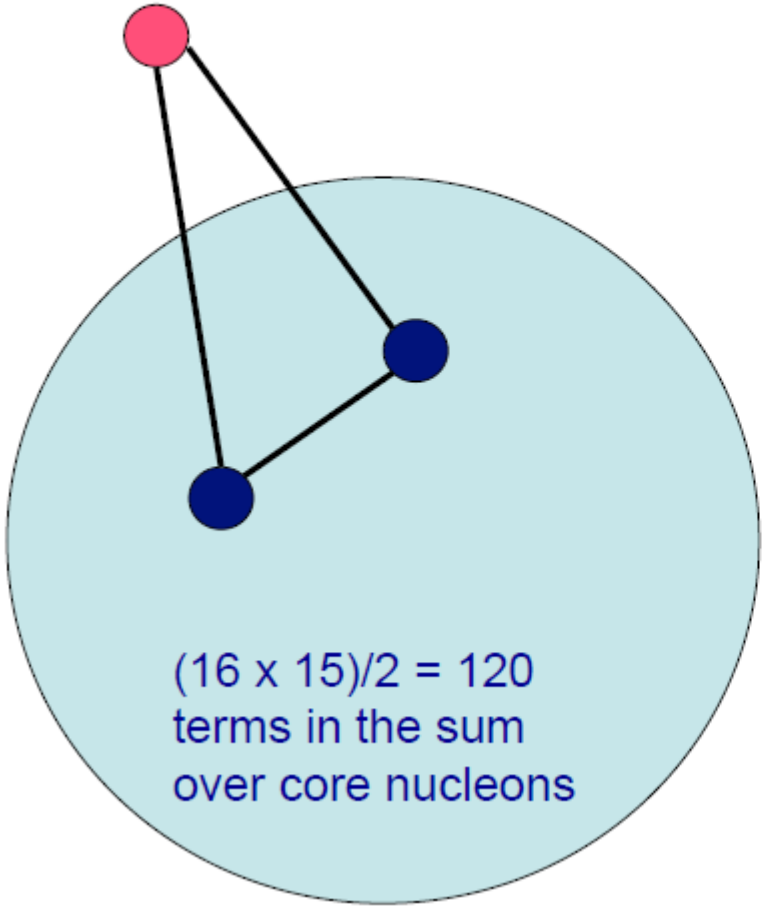

N3LO
E (MeV)
−115
−117
−119
−121
−123
−125
−127
−129
−131
−133
−135
−137
−139
−141
18F
NCSM/SSM
19F
SSM
19F
SSM
19F
NCSM
3+
4+
0+
1+
2+
2+
5+
0+
3+
1+
(−126.964)
9/2+
3/2+
7/2+
5/2+
7/2+
1/2+
9/2+
3/2+
5/2+
1/2+
(−138.027)
(−137.820)
(−137.816)
A=18
A=18
A=19
A=19

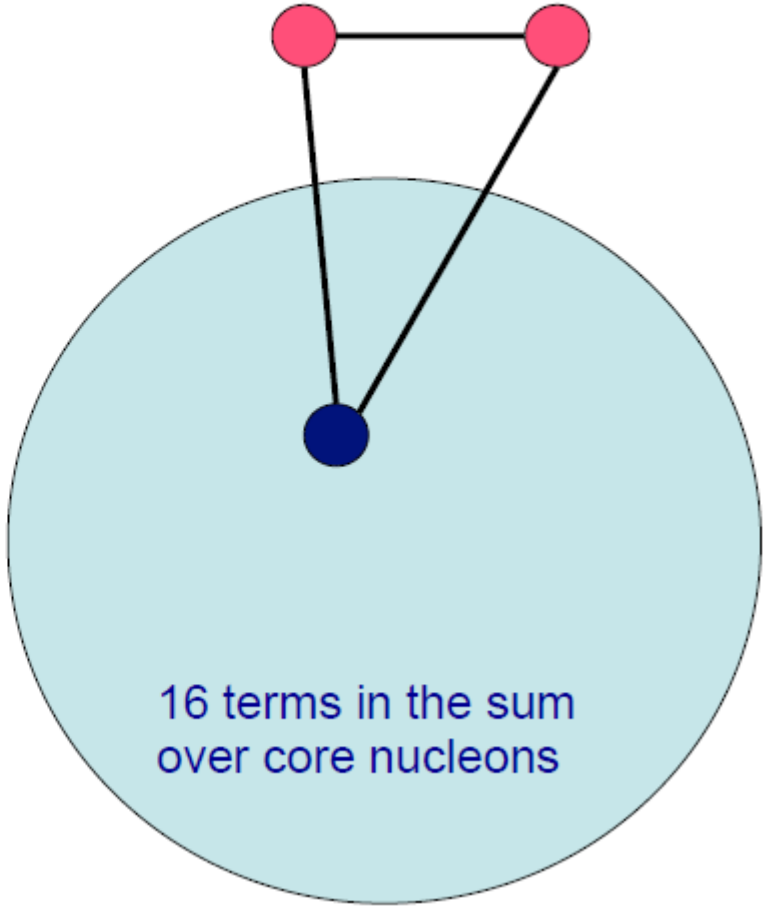
PRELIMINARY RESULT



II. Results: b) Fluorine isotopes

Effects of 3NFs on single-particle energies
vs effects of 3NFs on TBMEs





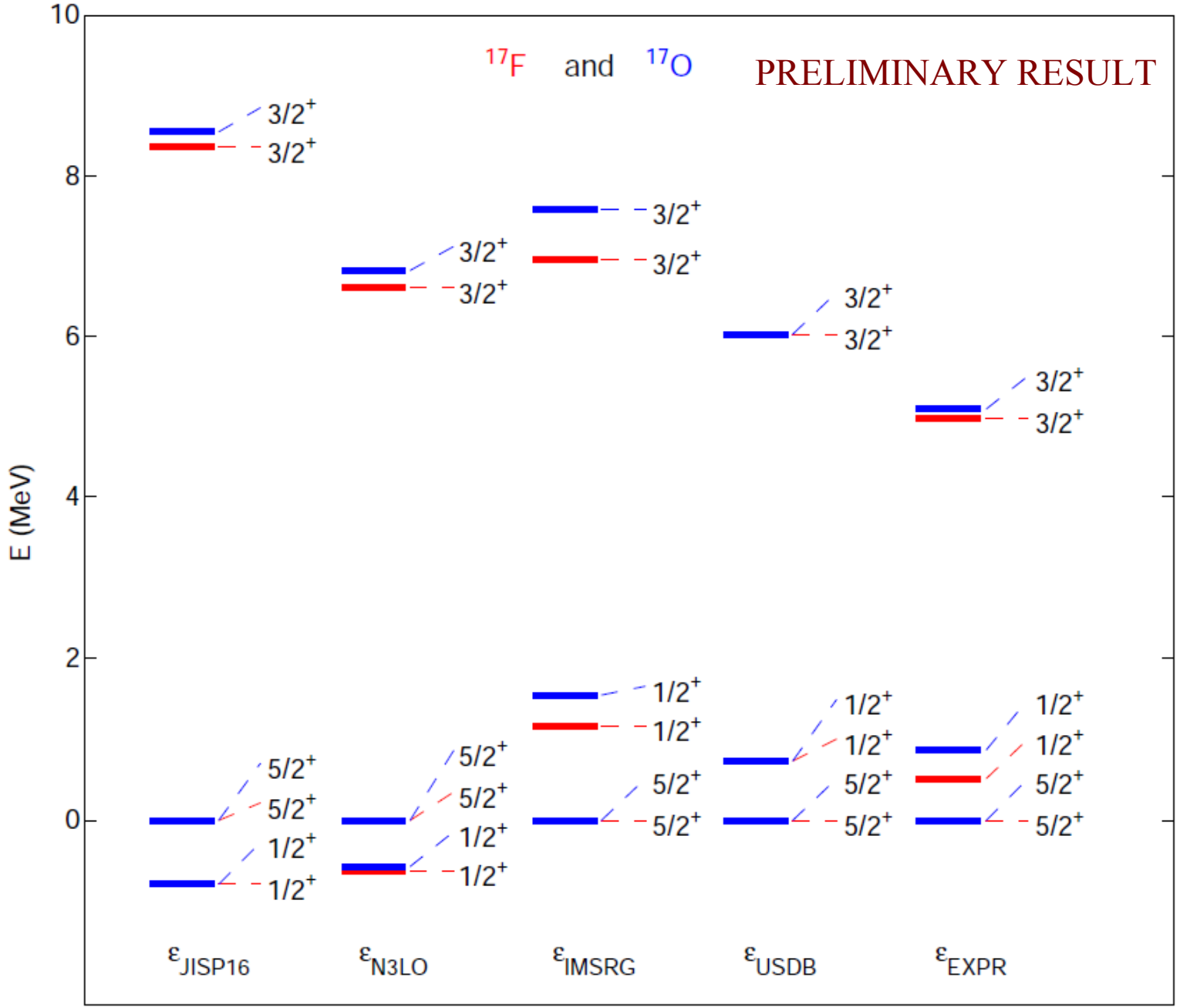
Survey of the Fluorine isotopes

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.

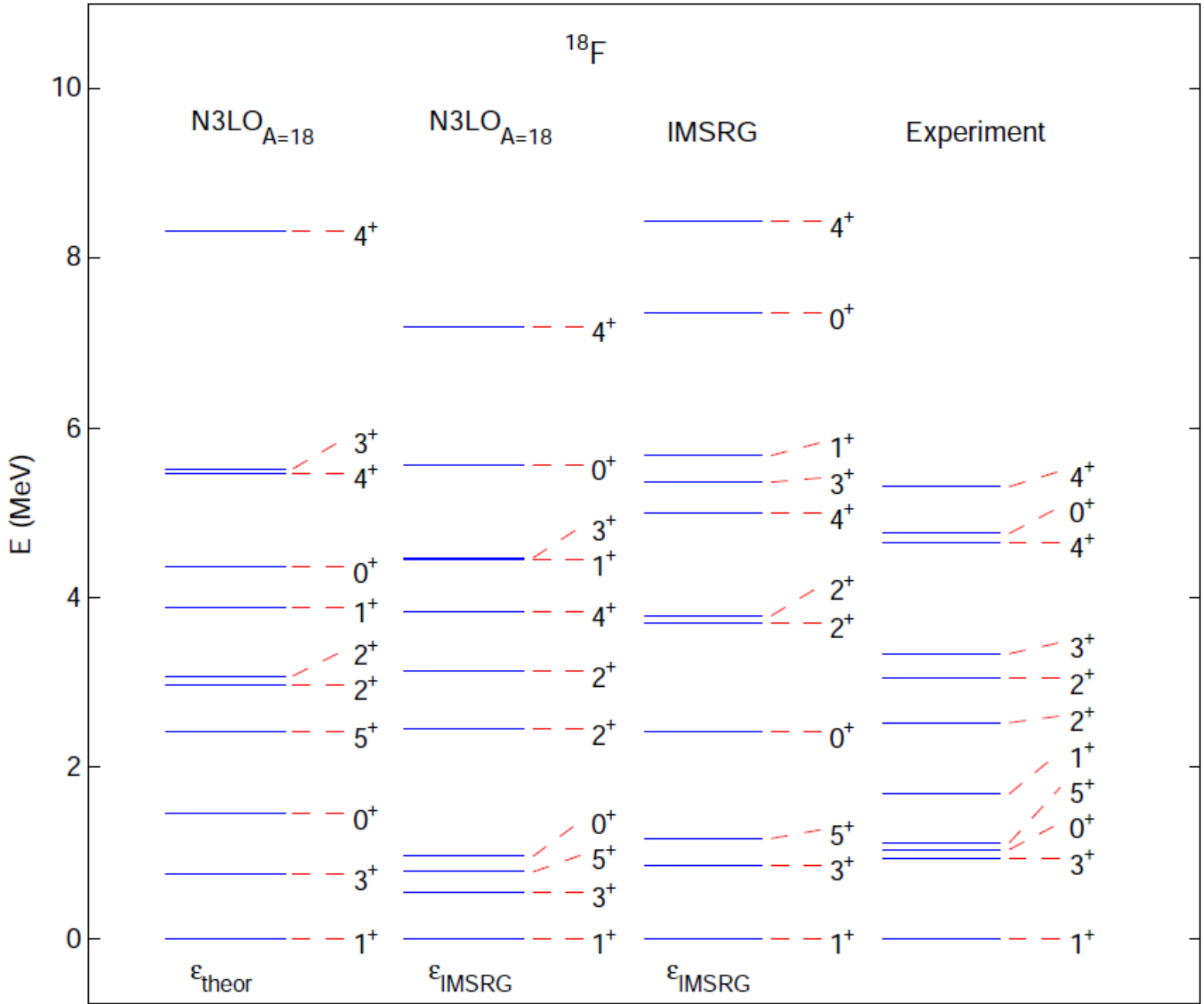
2. Approximate the effect of 3NFs by replacing our theoretical single-particle energies with the theoretical ones obtained in the IM-SRG calculations of S.R. Stroberg et al.*

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

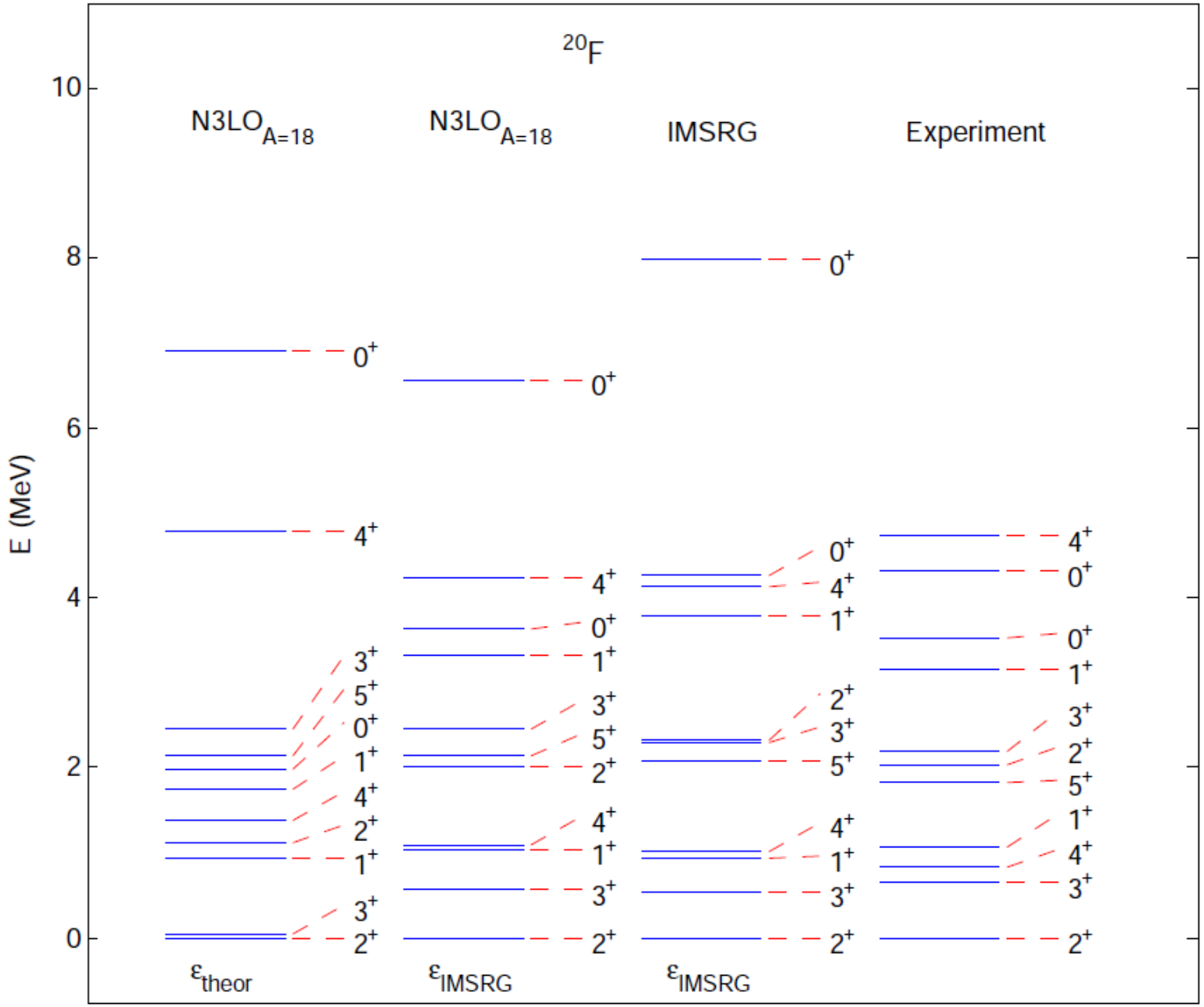
* S.R. Stroberg et al., arXiv Nucl-th 1511.02802 (2015)


^{17}F and ^{17}O
PRELIMINARY RESULT
E (MeV)
10
8
6
4
2
0
3/2+
3/2+
3/2+
3/2+
3/2+
3/2+
3/2+
3/2+
3/2+
3/2+
1/2+
1/2+
5/2+
5/2+
1/2+
1/2+
5/2+
5/2+
1/2+
1/2+
5/2+
5/2+
1/2+
1/2+
5/2+
5/2+
ε JISP16
ε N3LO
ε IMSRG
ε USDB
ε EXPR

PRELIMINARY RESULT



PRELIMINARY RESULT

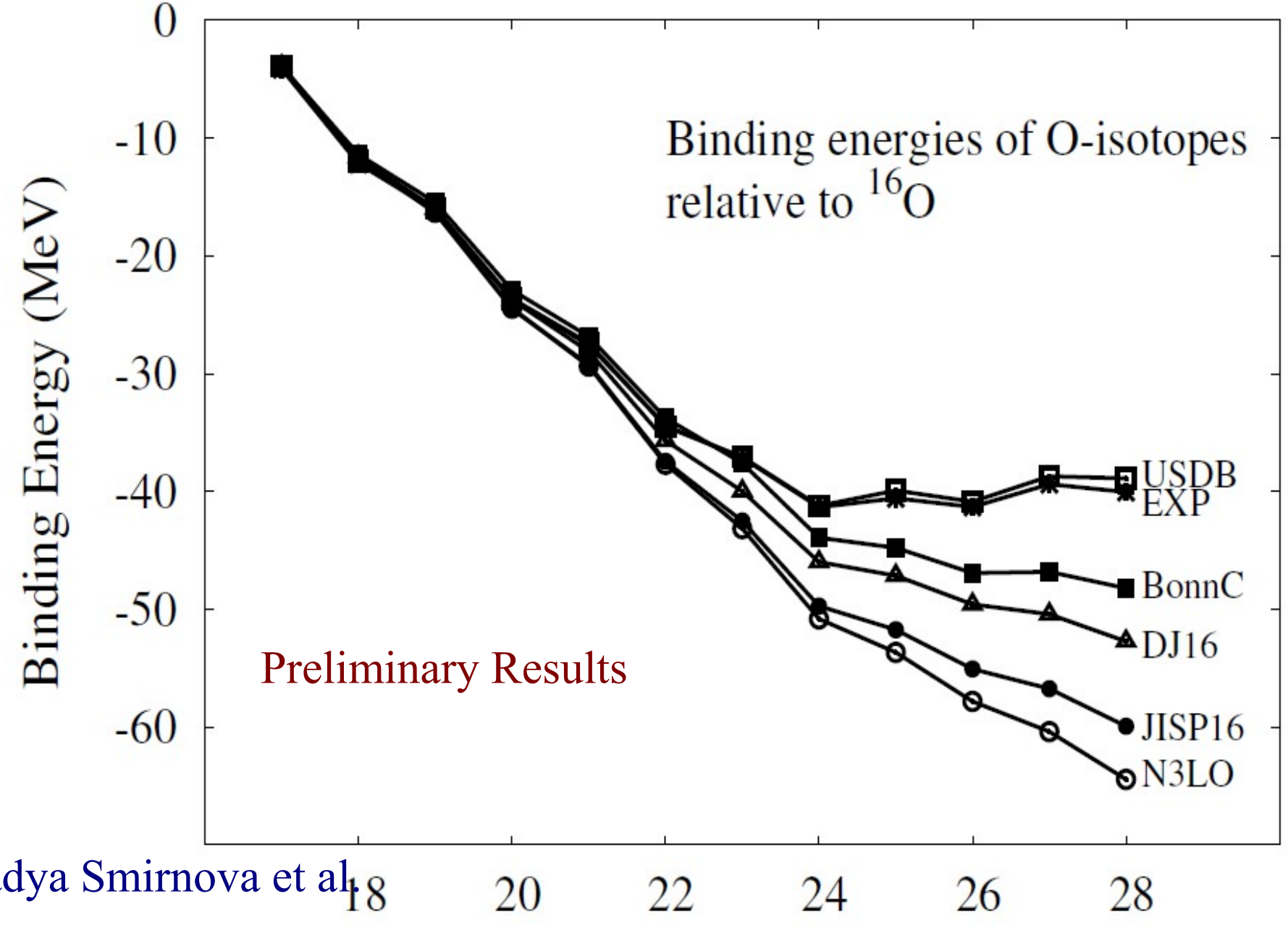


II. Results: c) Effective Interaction Comparisons:

i.) N3LO (E&M)

ii.) JISP16

iii.) DJ16



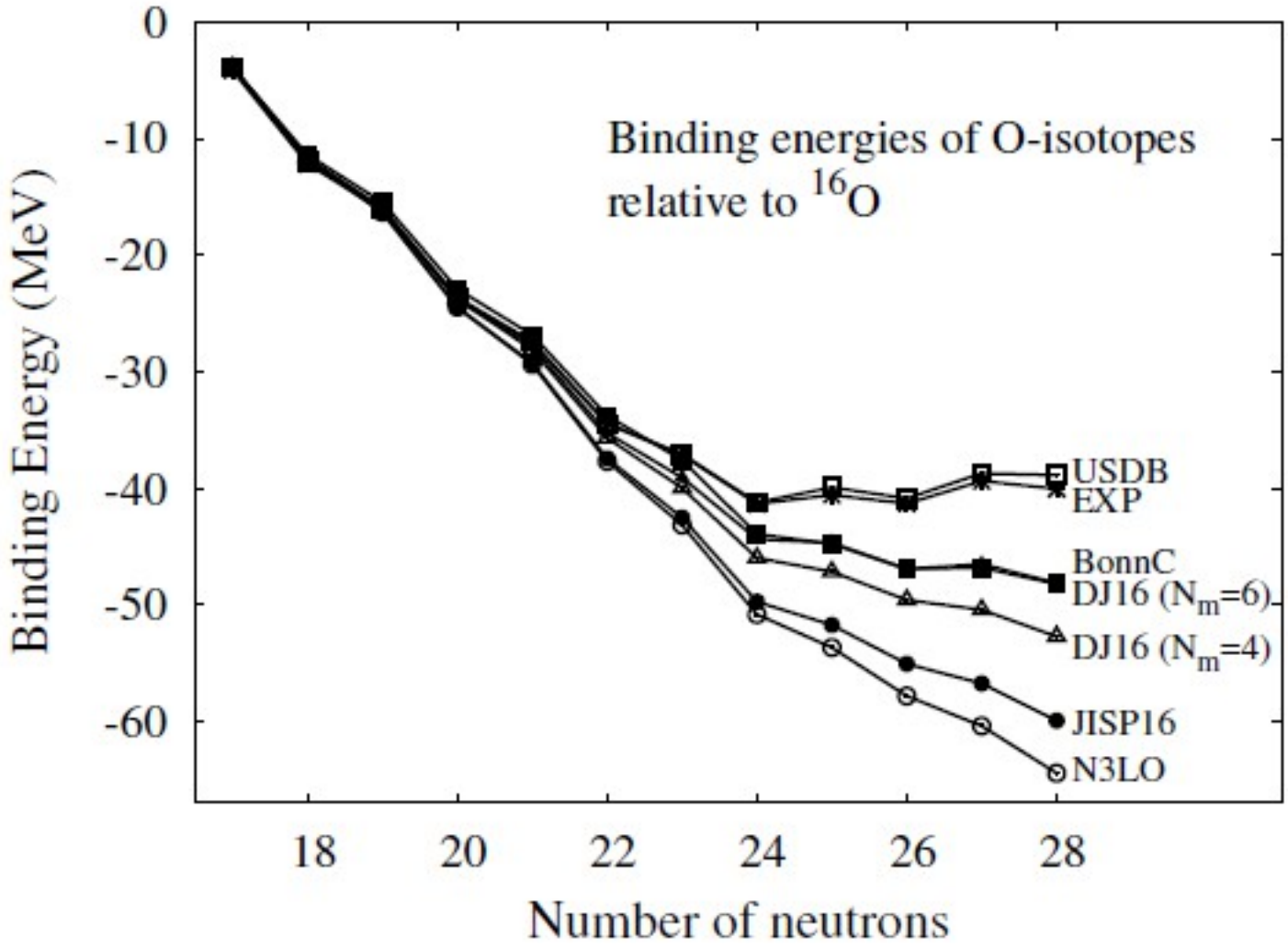
Nadya Smirnova et al.

Points of Interest

1. The Monopole Term

2. The A-Dependence

3. Handcrafted Improvements


Binding energies of O-isotopes
relative to ^{16}O
Binding Energy (MeV)
0
-10
-20
-30
-40
-50
-60
18
20
22
24
26
28
Number of neutrons
USDB
EXP
BonnC
DJ16 (N_m=6)
DJ16 (N_m=4)
JISP16
N3LO

III. SUMMARY AND OUTLOOK

1. The interactions and approaches used in this study reproduced the gross trends and features of the experimental data for the Fluorine isotopes studied so far.
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. Of the three eff. Interactions: N3LO, JISP16 and DJ16; DJ16 is the most robust and closest to USDB in structure with adjustment.

OUTLOOK: Extend our calculations to other nuclei in the sd-shell to study charge dependence. Also study the hw dependence of our results.

Effective Hamiltonian for NCSM

Solving $H^{\Omega}_{A,\,a=2}\,\Psi_{a=2} = E^{\Omega}_{A,\,a=2}\,\Psi_{a=2}$ 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: $H^{\mathrm{eff}}_{A,a} \to H_A$

Effective Hamiltonian for SSM

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;

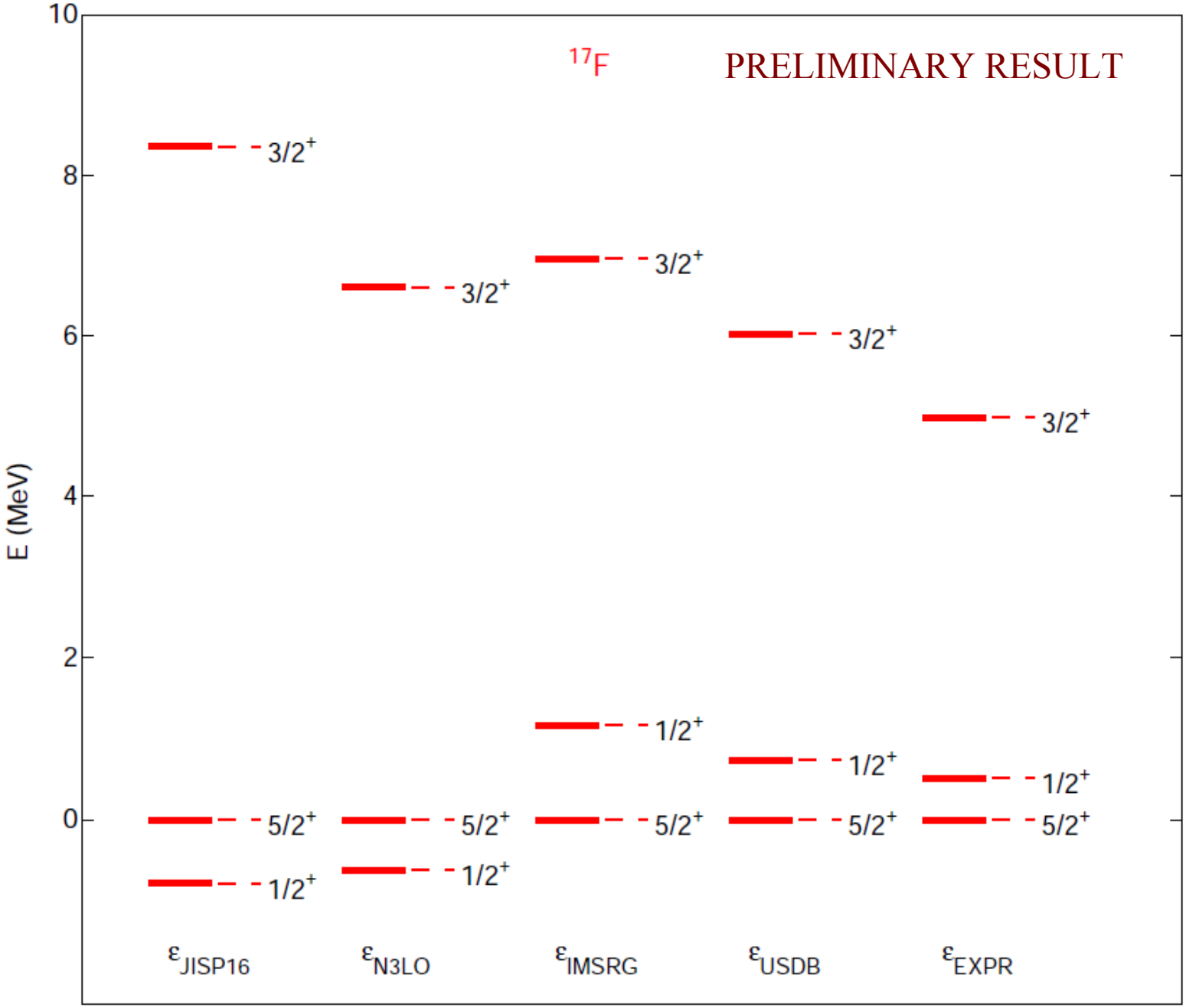
$$\mathcal{H}^{N_{1,\max},N_{\max}}_{A,a_1} = \frac{U^{A,\dagger}_{a_1,P_1}}{\sqrt{U^{A,\dagger}_{a_1,P_1}U^{A}_{a_1,P_1}}} E^{N_{\max},\Omega}_{A,a_1,P_1} \frac{U^{A}_{a_1,P_1}}{\sqrt{U^{A,\dagger}_{a_1,P_1}U^{A}_{a_1,P_1}}}$$

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;

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


^{17}F
PRELIMINARY RESULT
E (MeV)
10
8
6
4
2
0
3/2+
3/2+
3/2+
3/2+
3/2+
1/2+
1/2+
1/2+
5/2+
5/2+
5/2+
5/2+
5/2+
ε JISP16
ε N3LO
ε IMSRG
ε USDB
ε EXPR

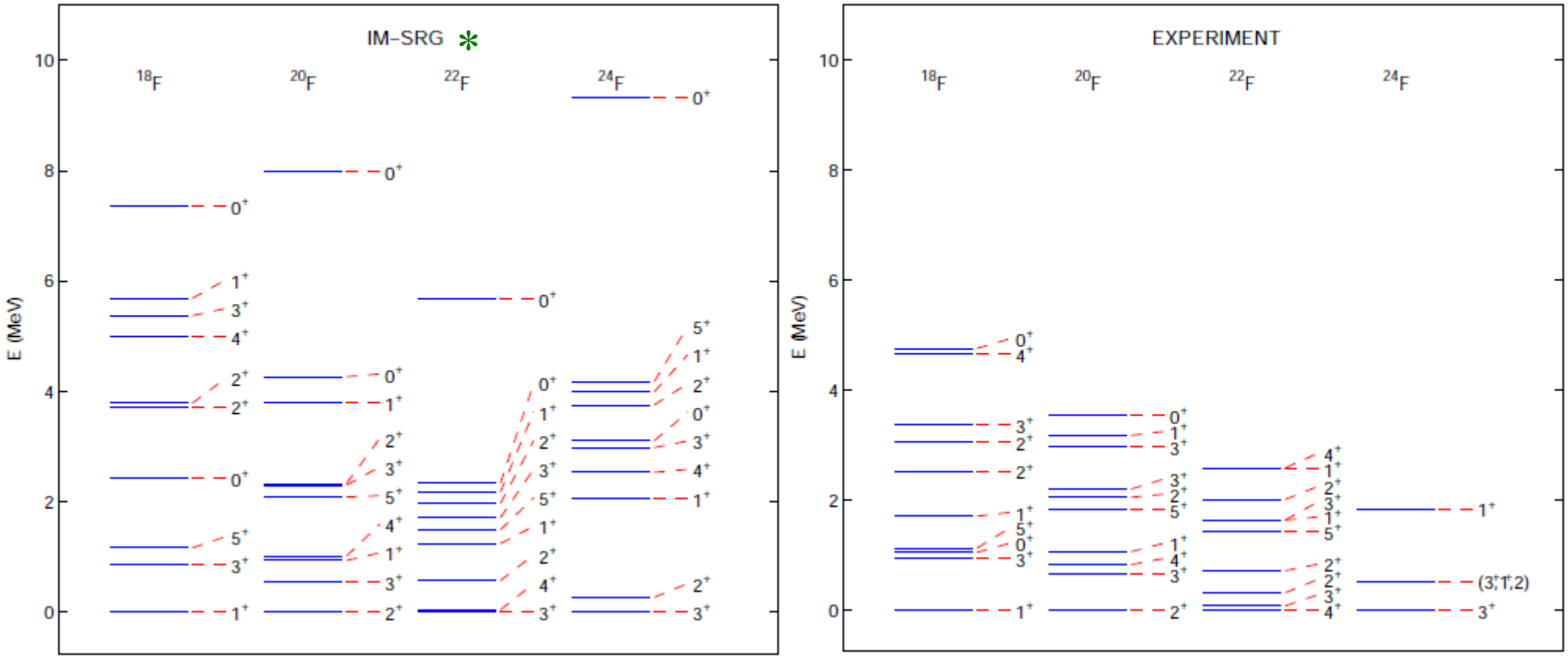
Preliminary Results

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	

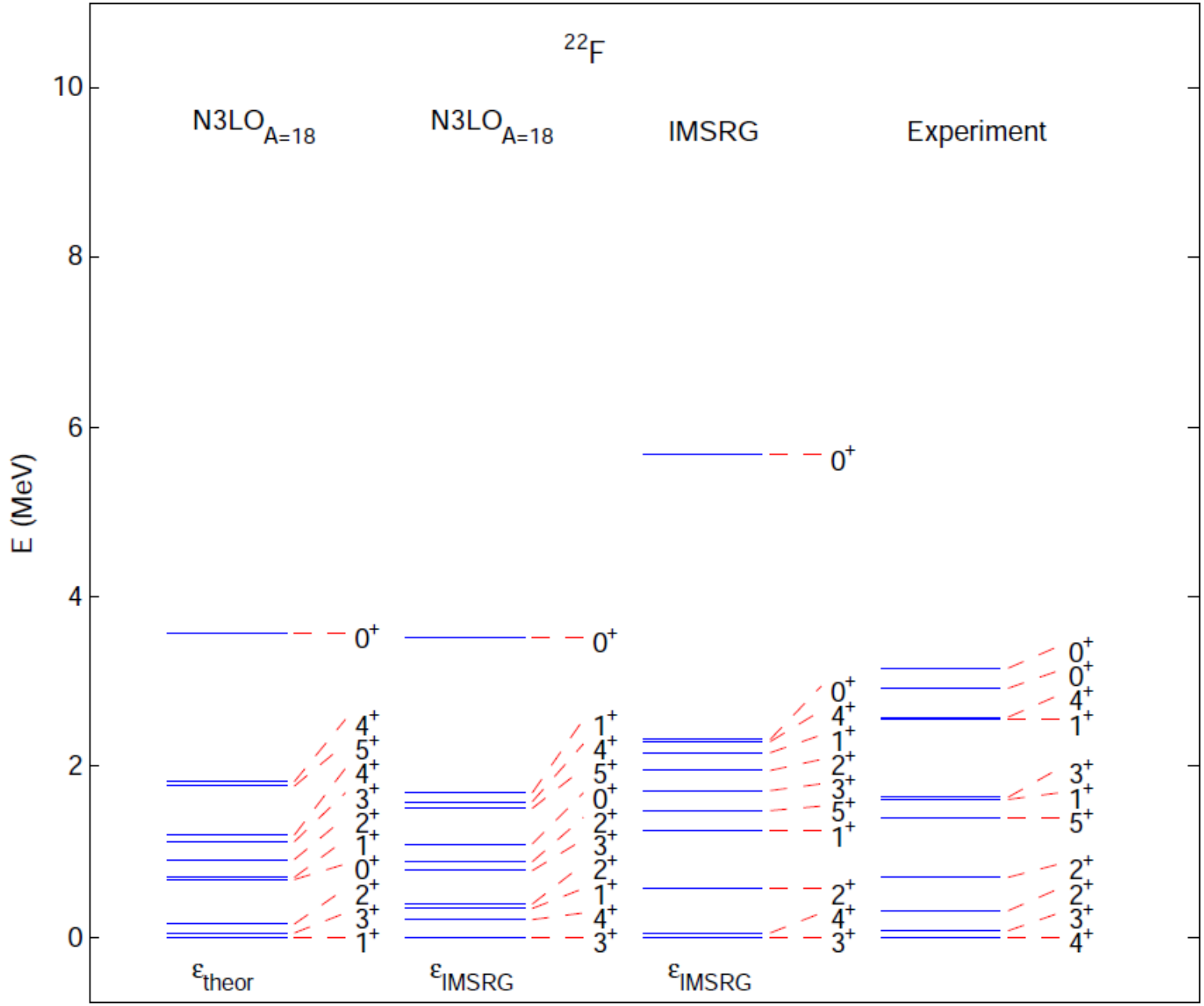
* B.A. Brown & W.A. Richter, PRC 74, 034315 (2006)

** S.R. Stroberg, et al., arXiv Nucl-th 1511.02802

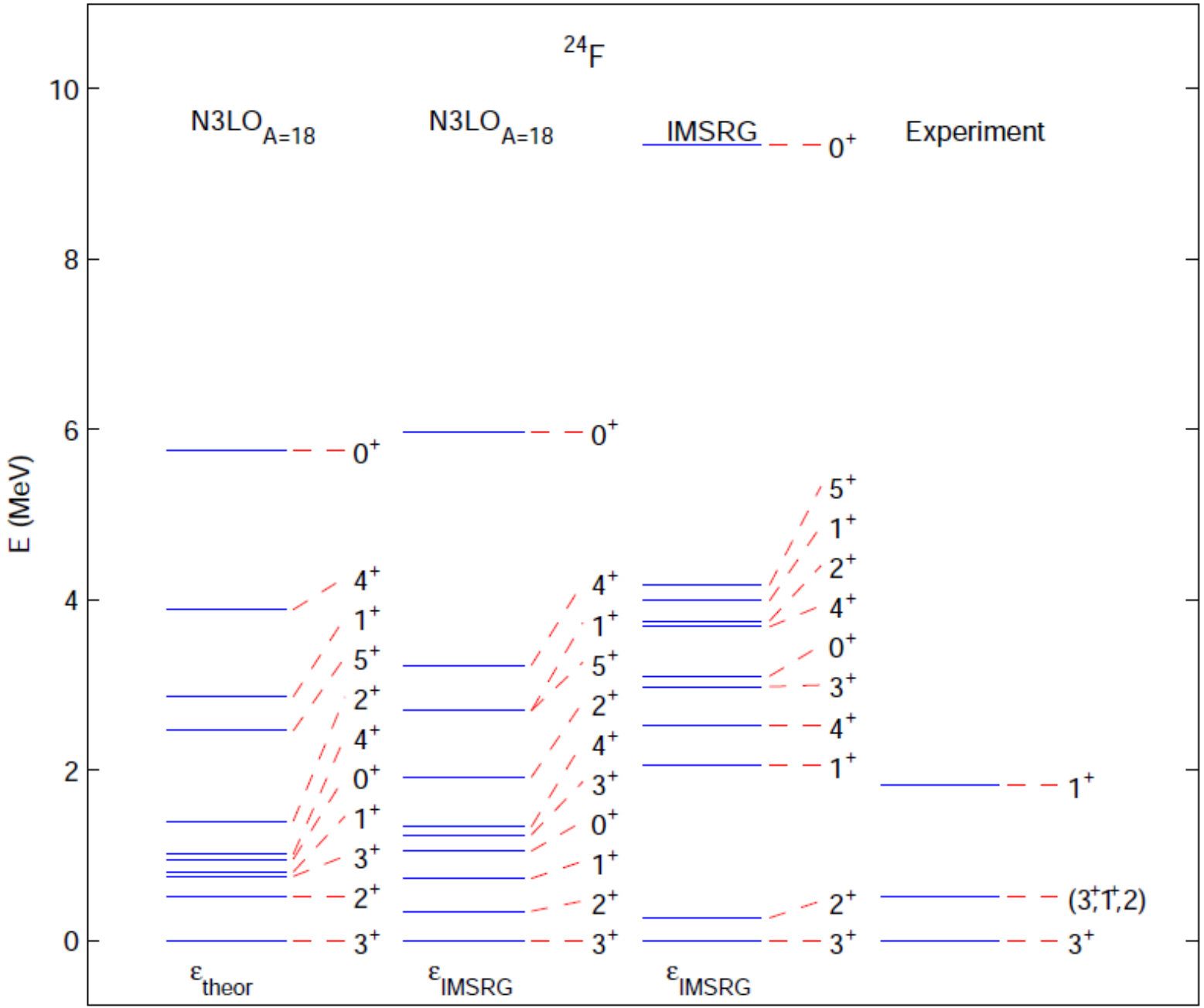


* S.R. Stroberg, et al., arXiv Nucl-th 1511.02802

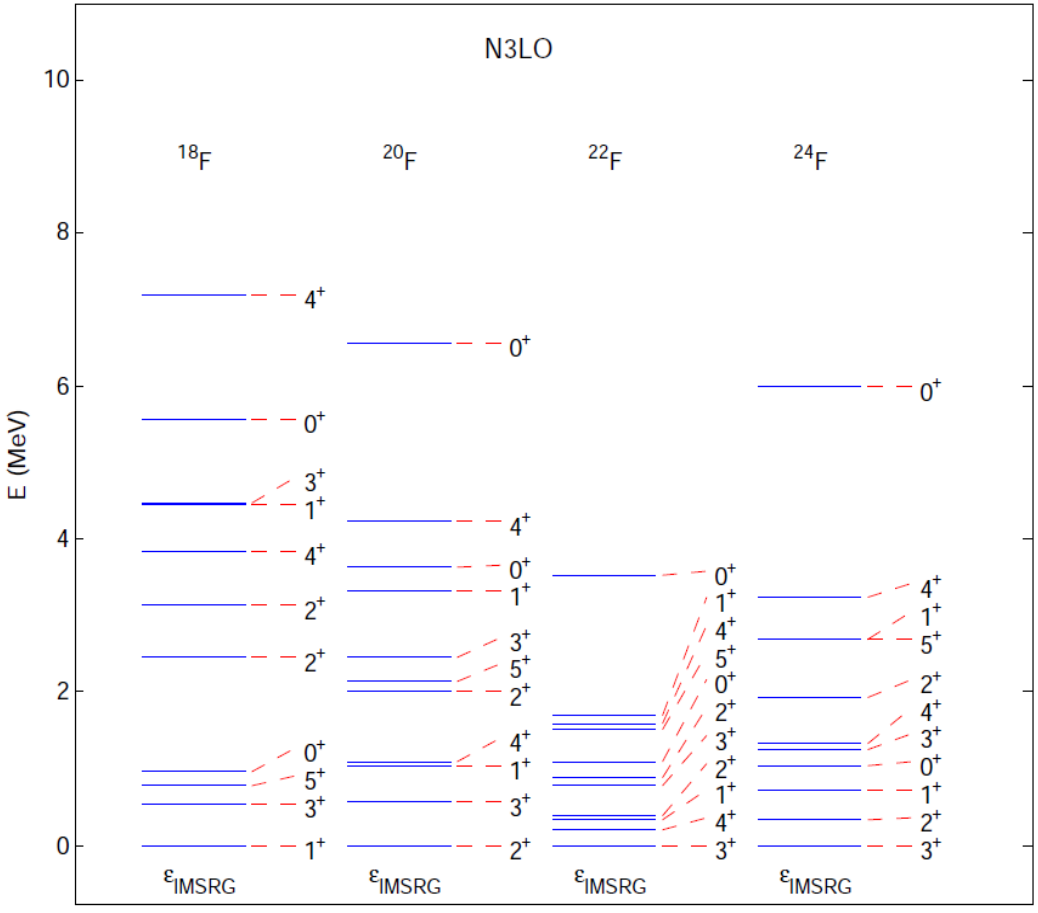
PRELIMINARY RESULT

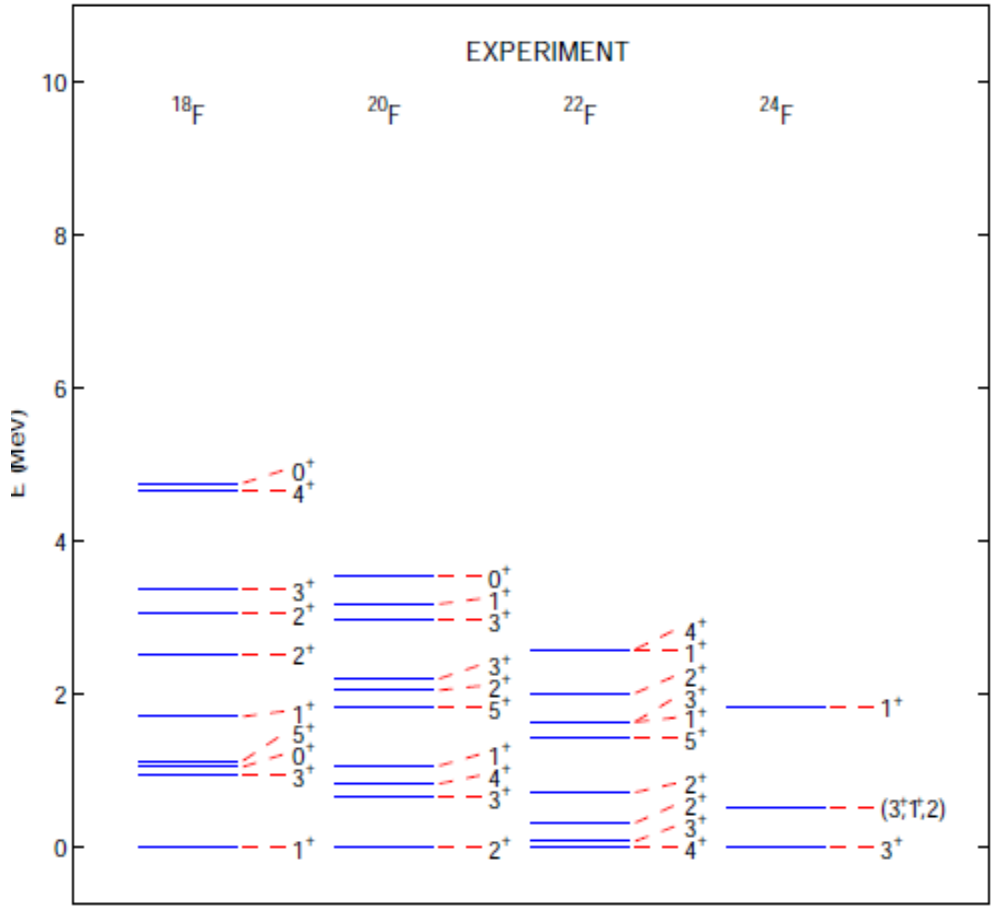


PRELIMINARY RESULT



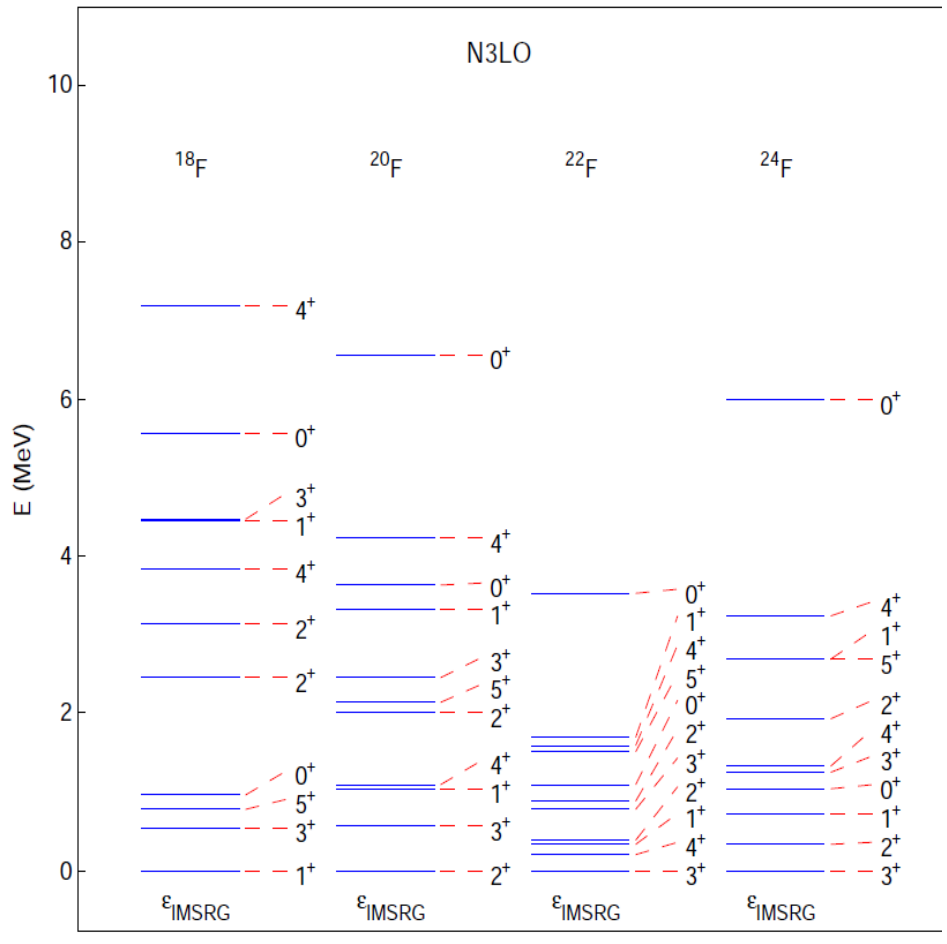
PRELIMINARY RESULTS

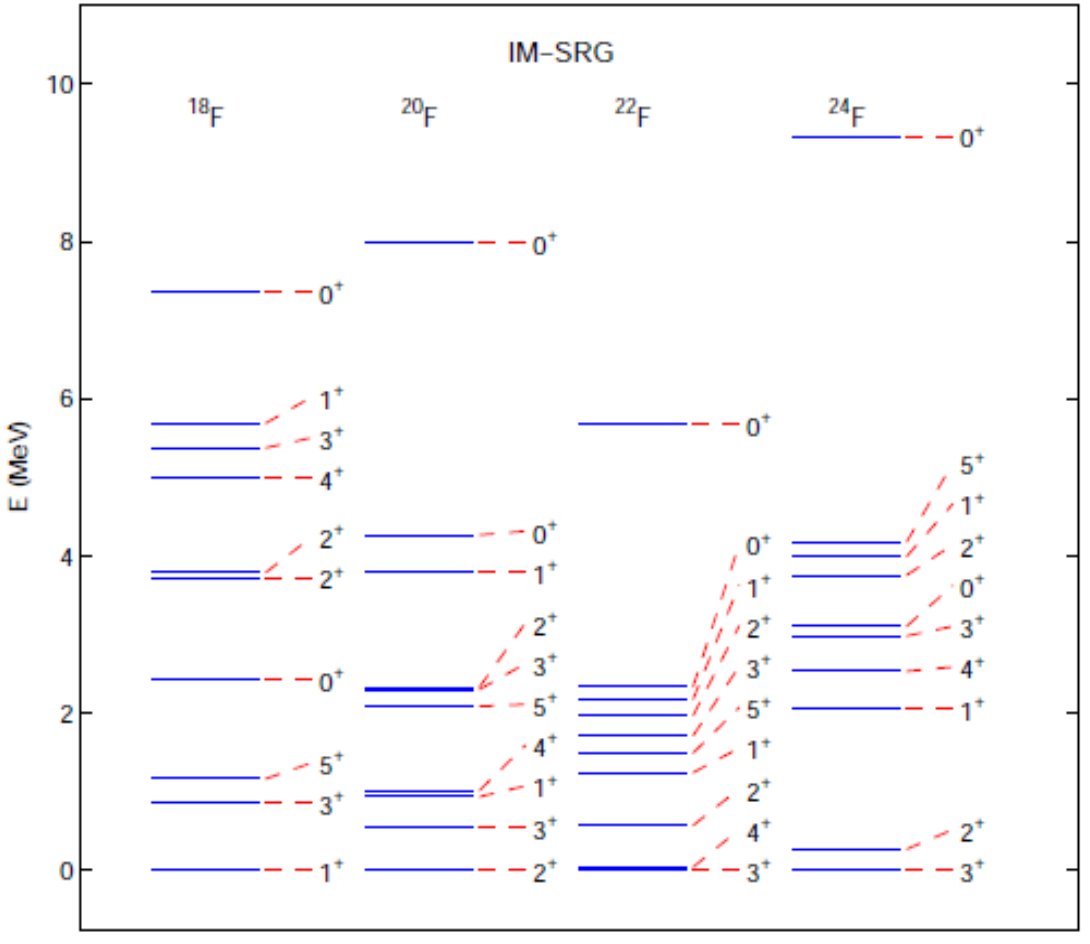




N3LO + IMSRG spe vs Experiment

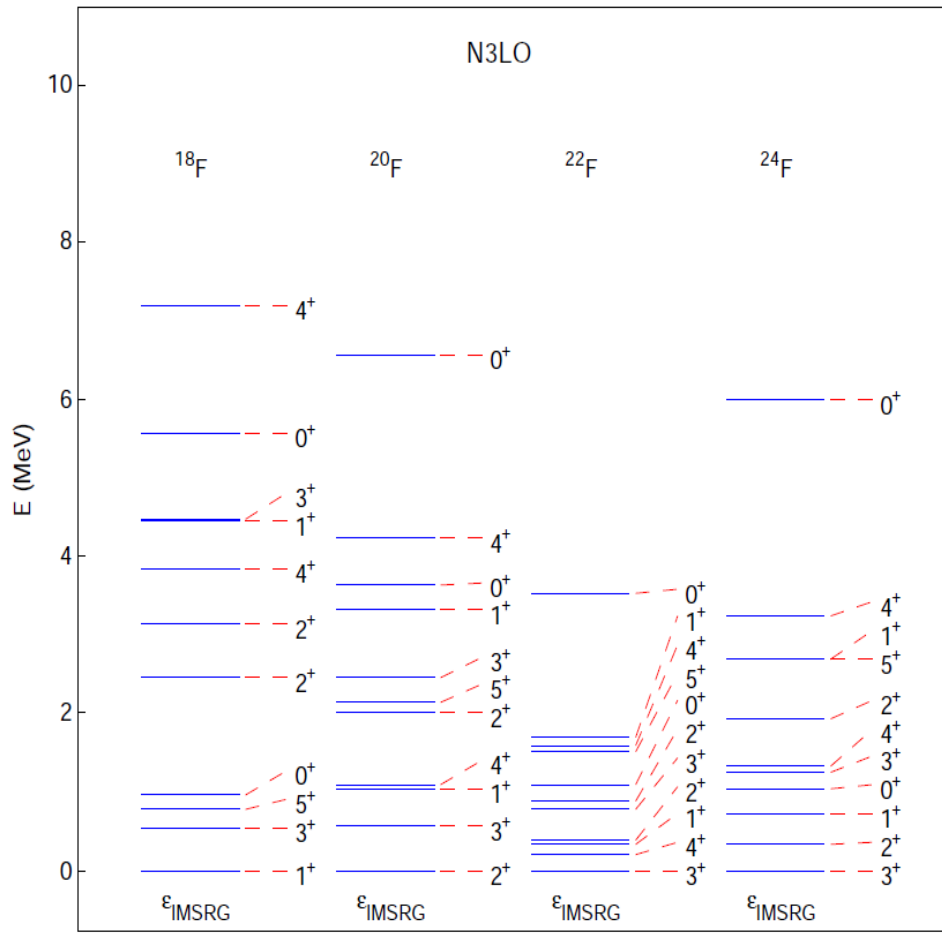
PRELIMINARY RESULTS

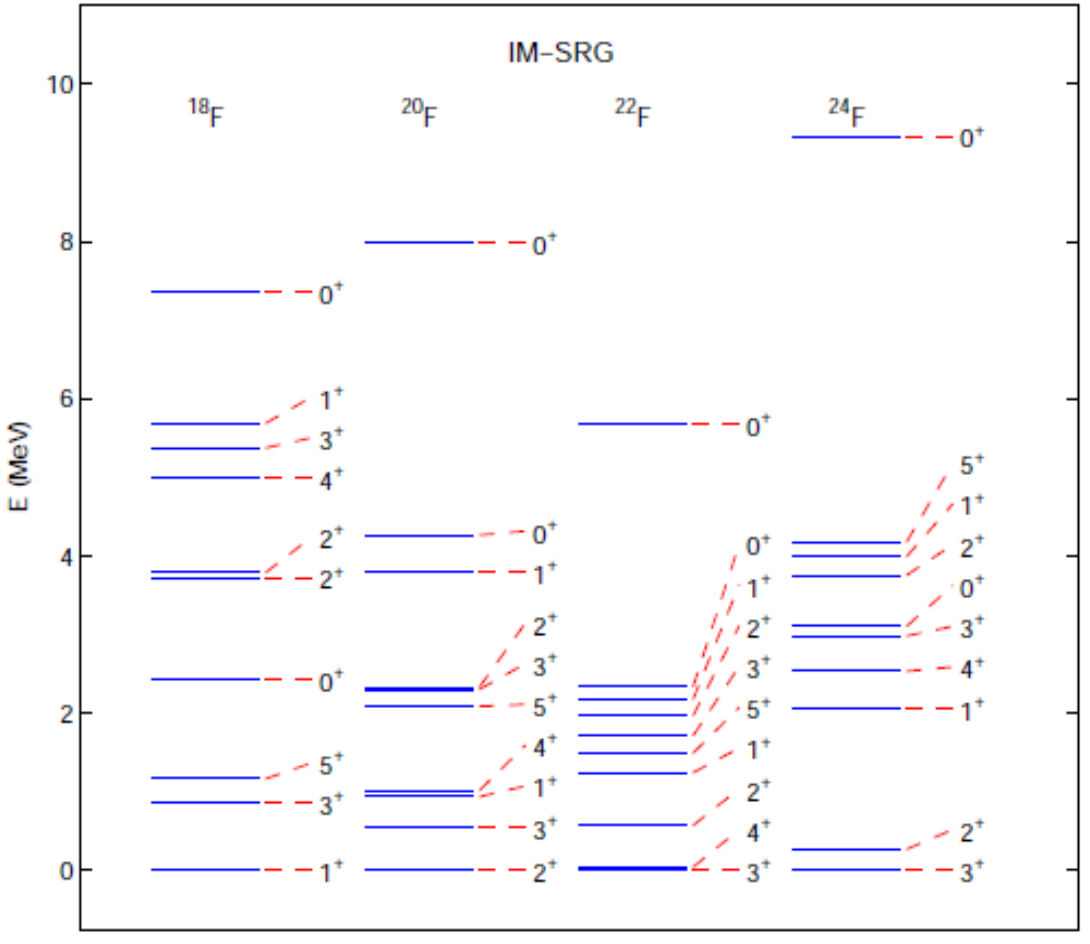




N3LO + IMSRG spe vs IM-SRG

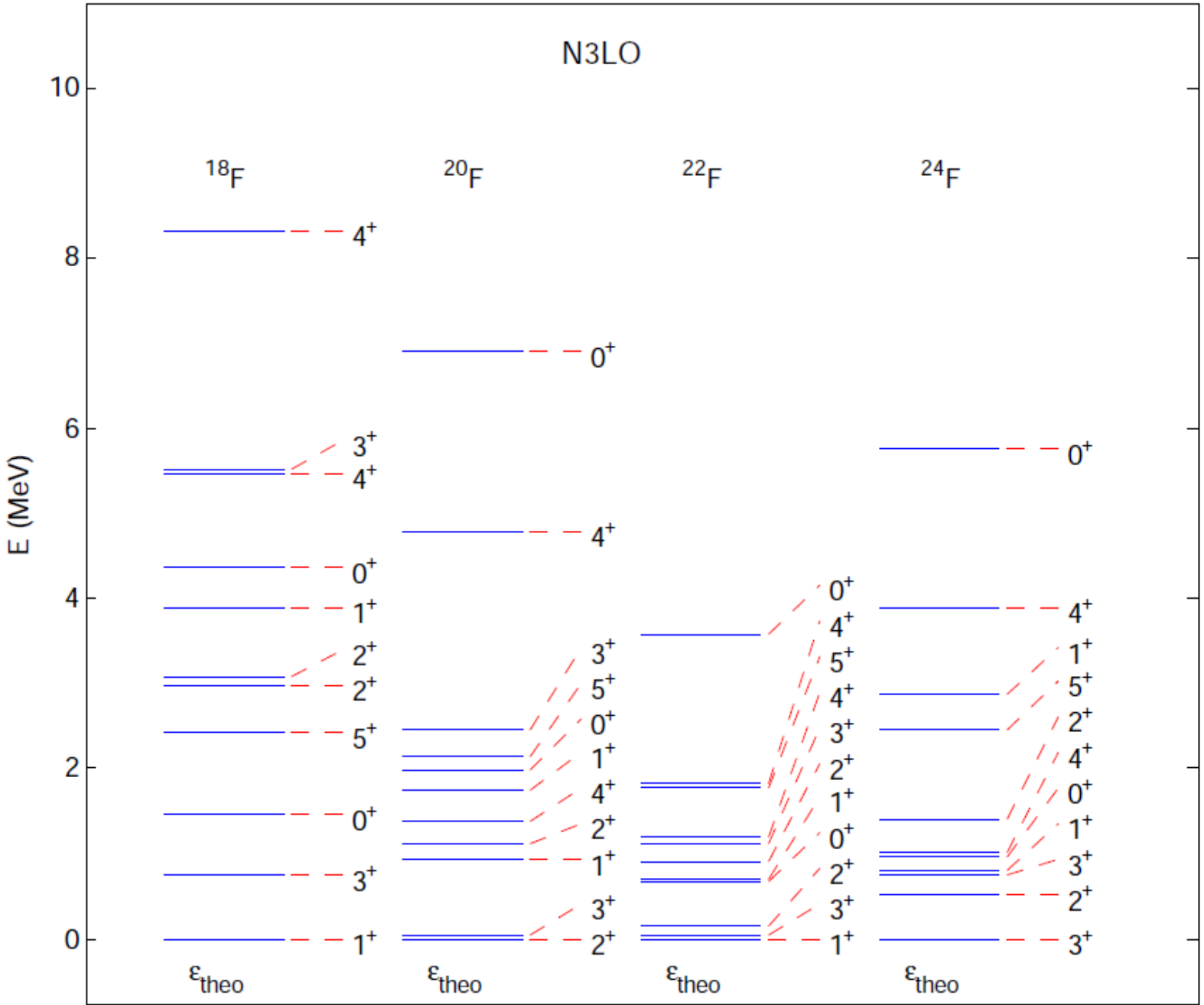
PRELIMINARY RESULTS



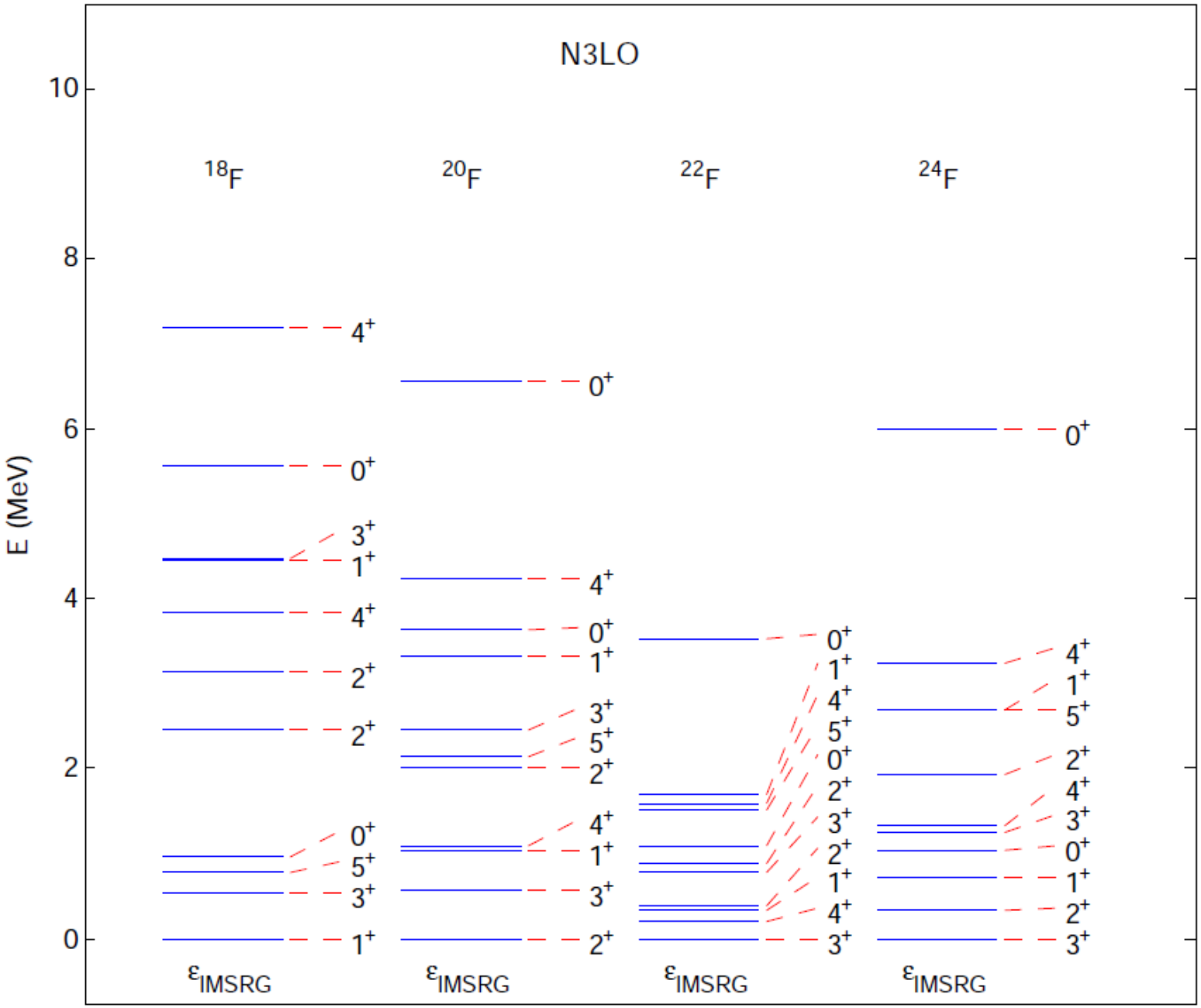


N3LO + IMSRG spe vs IM-SRG

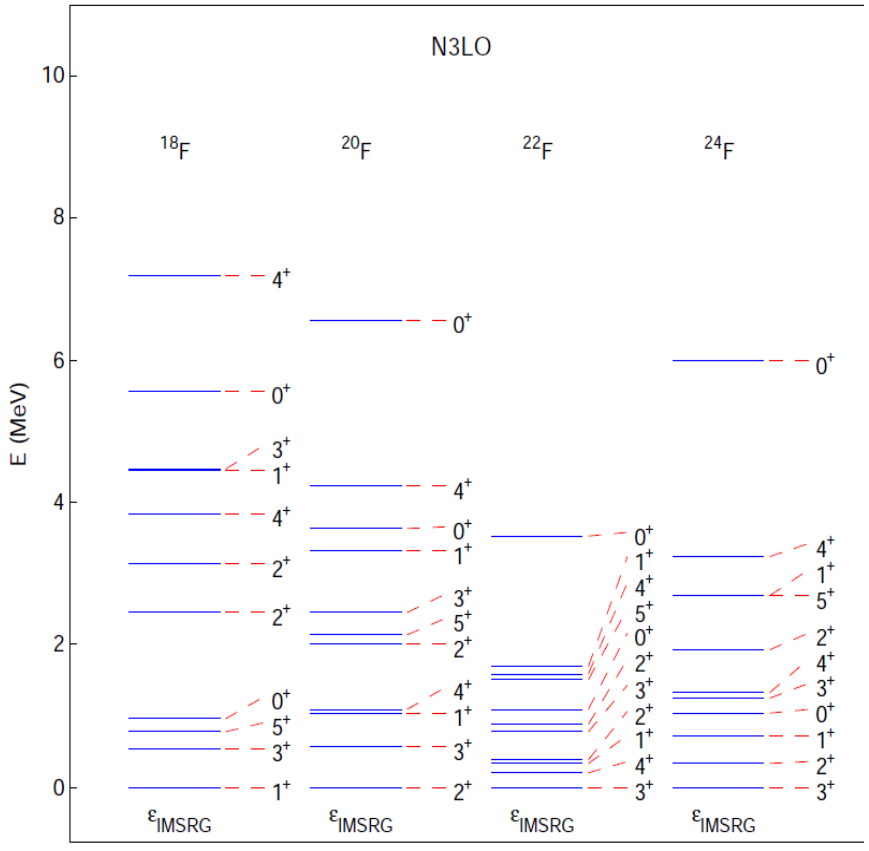
PRELIMINARY RESULT

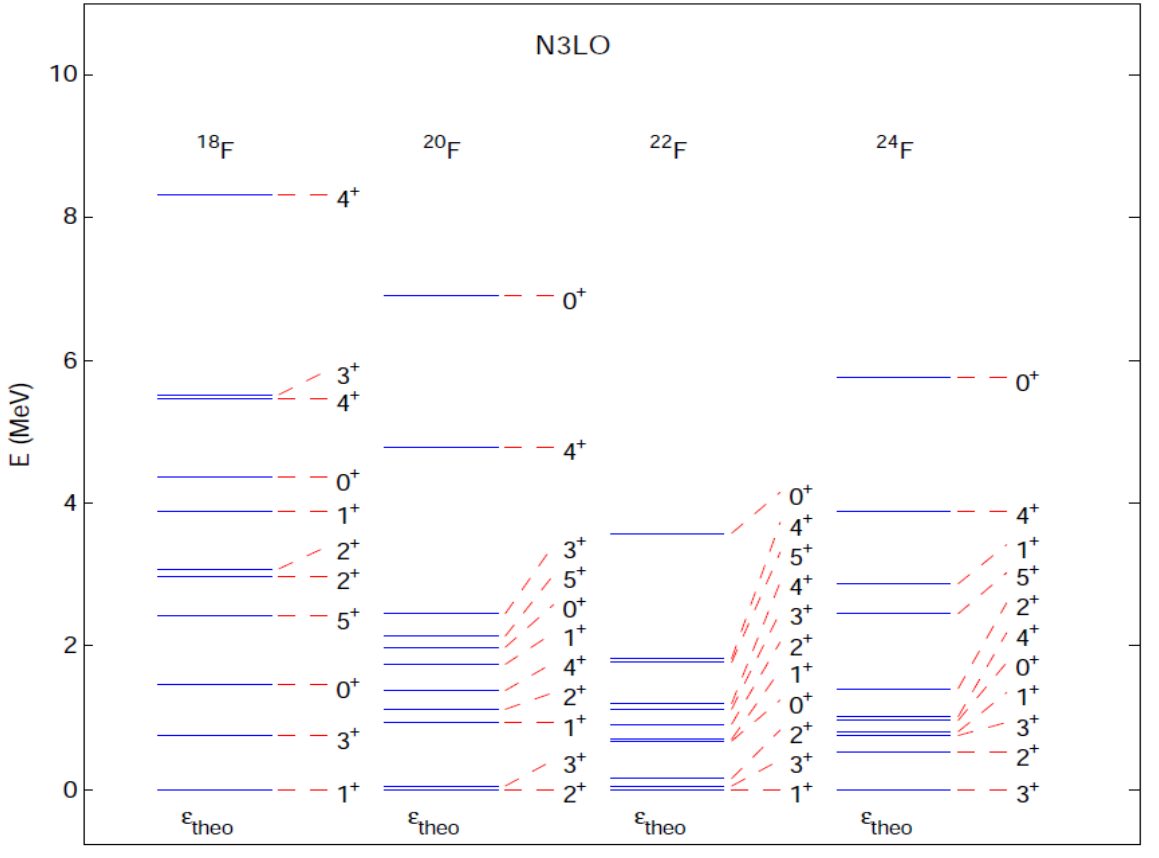


PRELIMINARY RESULT



PRELIMINARY RESULTS





N3LO + IMSRG spe vs N3LO + theoretical spe