

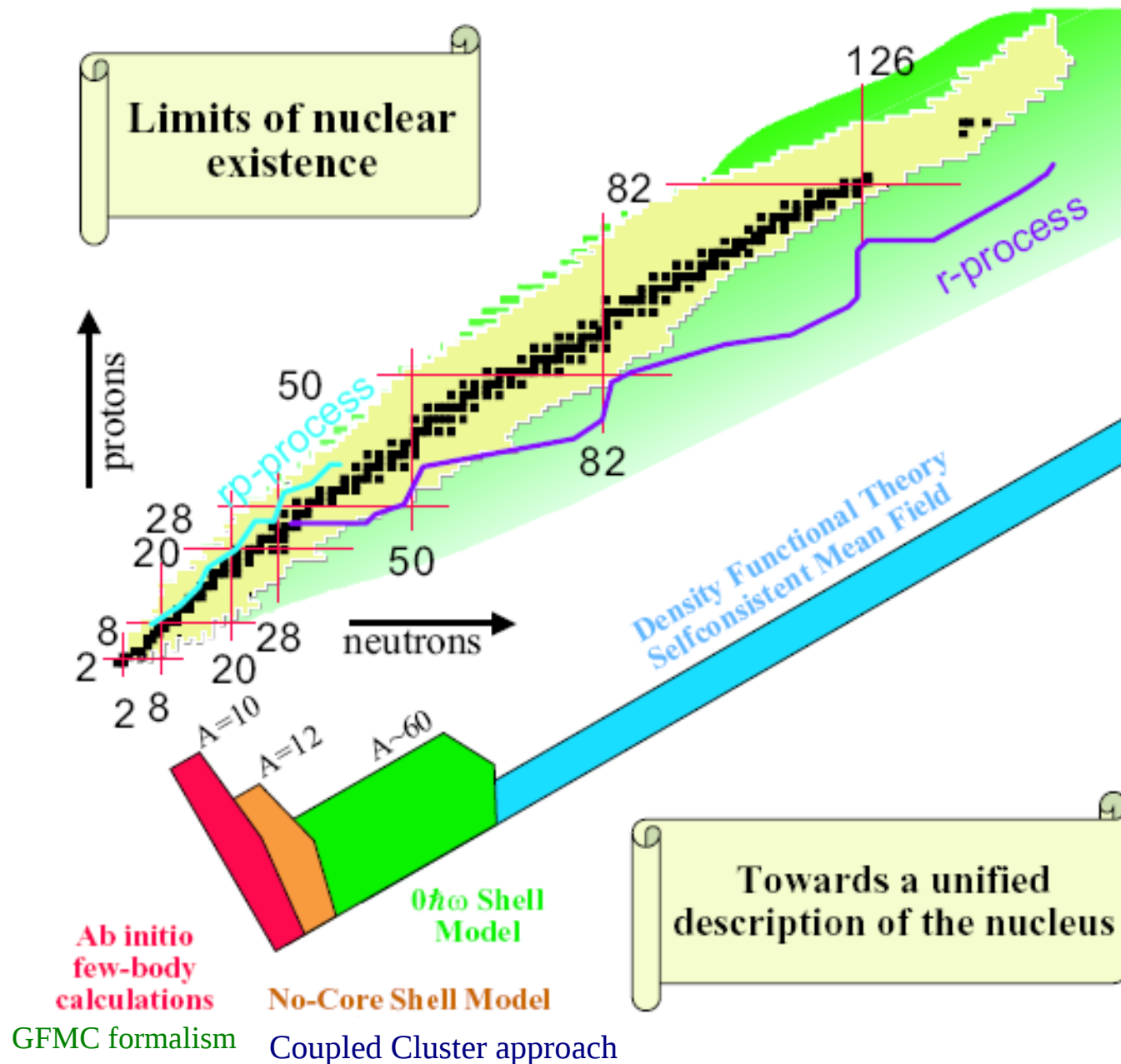
Fluorine isotope systematics: comparing *ab initio* approaches

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OUTLINE

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

II. Results:

- a.) General sd-shell
- b.) Fluorine isotopes

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

Ab initio
No Core Shell Model

Realistic NN & NNN forces

Effective interactions in
cluster approximation

Diagonalization of
many-body Hamiltonian

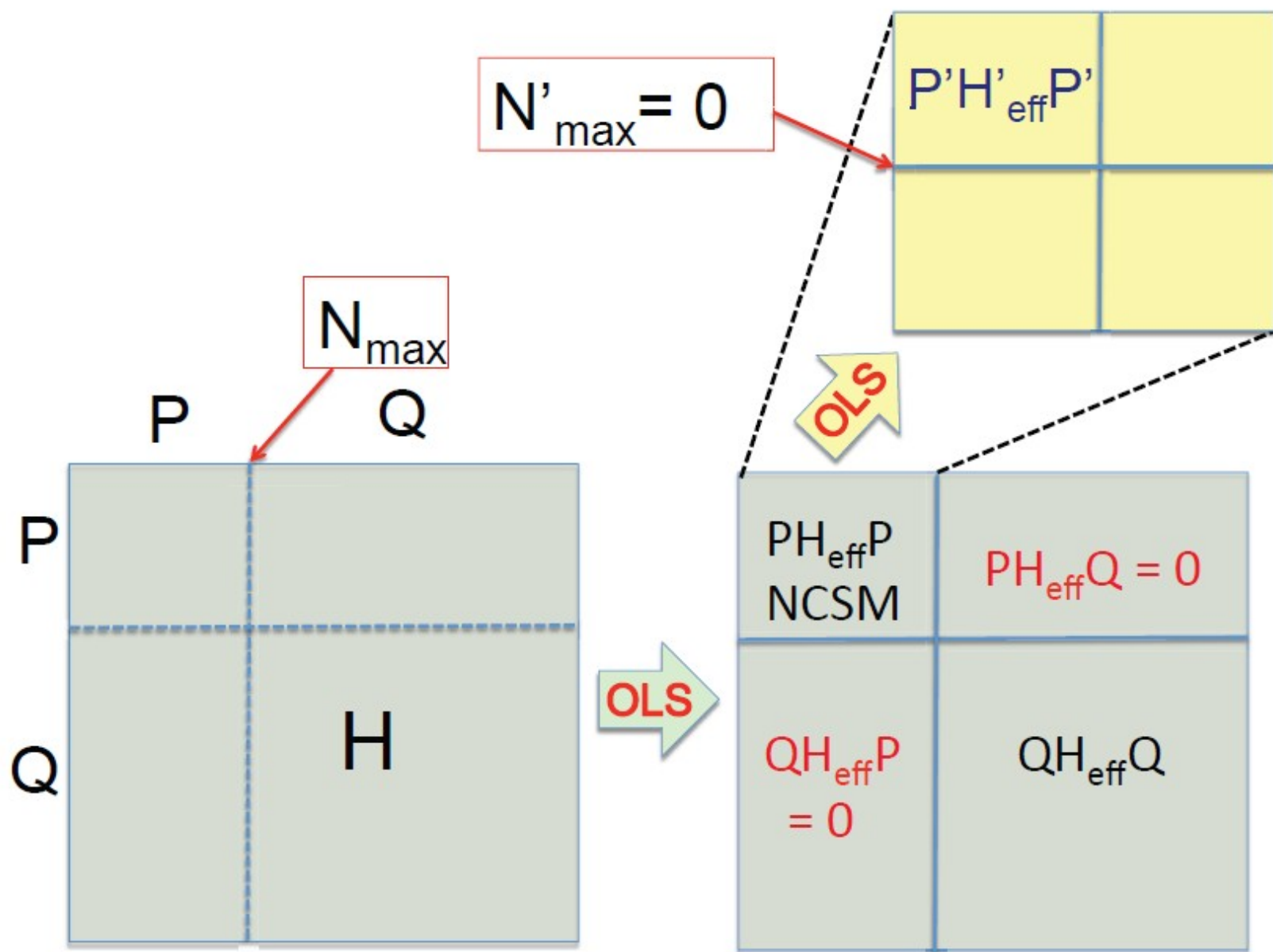
Core Shell Model

effective interactions for
valence nucleons

Diagonalization of the
Hamiltonian for valence
nucleons

Many-body experimental data





Effective interaction in a projected model space

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

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

$$\Phi_{\beta} = P\Psi_{\beta}$$

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

$$\langle \tilde{\Phi}_{\gamma} | \Phi_{\beta} \rangle = \delta_{\gamma\beta}$$

$$\mathcal{H} = \sum_{\beta \in \mathcal{S}} |\Phi_{\beta} \rangle E_{\beta} \langle \tilde{\Phi}_{\beta}|$$

Effective Hamiltonian for NCSM

Solving

$$\mathbf{H}_{A,a=2}^{\Omega} \Psi_{a=2} = \mathbf{E}_{A,a=2}^{\Omega} \Psi_{a=2}$$

in “infinite space” $2n+1 = 450$
relative coordinates

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

$$E_{A,2}^{\Omega} = U_2 H_{A,2}^{\Omega} U_2^{\dagger}$$

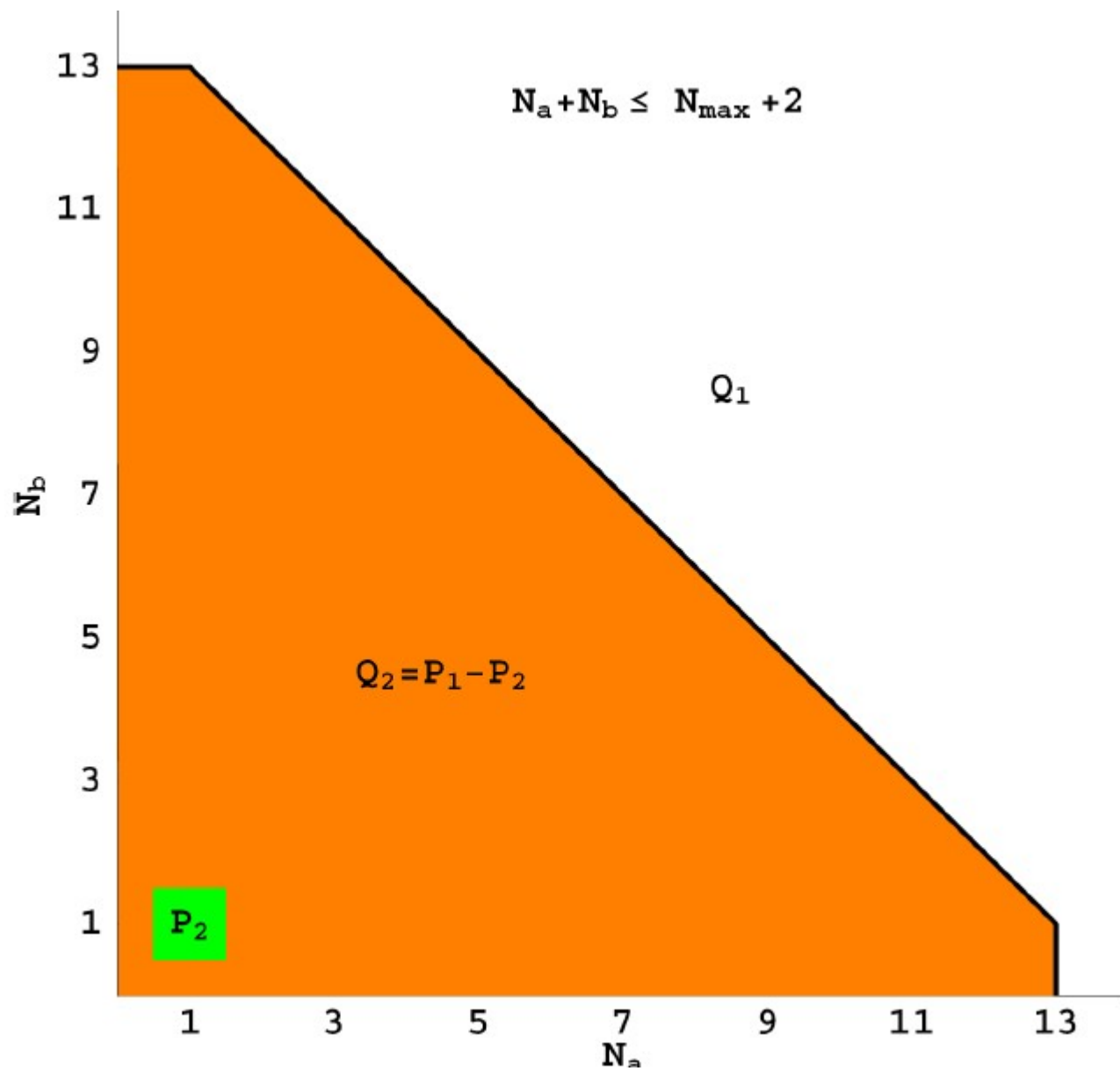
$$U_2 = \begin{pmatrix} U_{2,P} & U_{2,PQ} \\ U_{2,QP} & U_{2,Q} \end{pmatrix} \quad E_{A,2}^{\Omega} = \begin{pmatrix} E_{A,2,P}^{\Omega} & 0 \\ 0 & E_{A,2,Q}^{\Omega} \end{pmatrix}$$

$$H_{A,2}^{N_{\max}, \Omega, \text{eff}} = \frac{U_{2,P}^{\dagger}}{\sqrt{U_{2,P}^{\dagger} U_{2,P}}} E_{A,2,P}^{\Omega} \frac{U_{2,P}}{\sqrt{U_{2,P}^{\dagger} U_{2,P}}}$$

Two ways of convergence:

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

2) For $a \rightarrow A$ and fixed P : $\widetilde{H}_{A,a}^{\text{eff}} \rightarrow H_A$



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](https://doi.org/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.

Effective Hamiltonian for SSM

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

Two ways of convergence:

1) For $P \rightarrow 1$ and fixed a : $H_{A,a=2}^{\text{eff}} \rightarrow H_A$: previous slide

2) For $a_1 \rightarrow A$ and fixed P_1 : $H_{A,a_1}^{\text{eff}} \rightarrow H_A$

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

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

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;

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

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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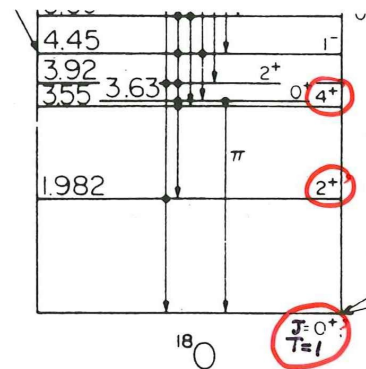
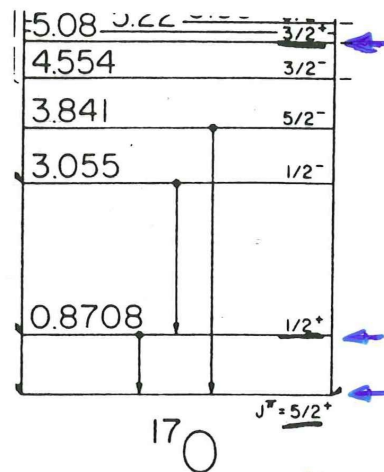
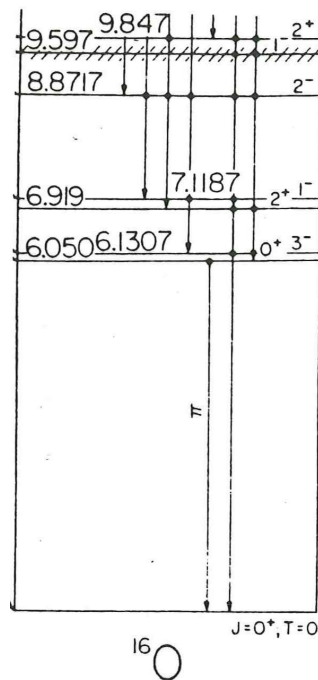
⁵*Pacific National University, 136 Tikhookeanskaya st., Khabarovsk 680035, Russia*

(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 $N_{\text{max}} = 4$, 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



$$E_{0d_{5/2}} = 0.0 \text{ MeV}$$

$$E_{1s_{1/2}} = 0.87 \text{ MeV}$$

$$E_{0d_{3/2}} = 5.08 \text{ MeV}$$

$$H^{sd}(\mathbf{P}, \mathbf{r})^{sd} = \left\{ \sum_i \epsilon_i + v_{\text{eff}}^{sd} \right\} (\mathbf{P}, \mathbf{r})^{sd}$$

$$\{H_0 + v_{\text{eff}}^{sd}\}(\mathbf{P}, \mathbf{r})^{sd} = E^{sd}(\mathbf{P}, \mathbf{r})^{sd}$$

Input: The results of $N_{\text{max}} = 4$ 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 $A = 19$.

	$A = 18$			$A = 19$		
	$E_{\text{core}} = -115.529$			$E_{\text{core}} = -115.319$		
j_i	$\frac{1}{2}$	$\frac{5}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	$\frac{5}{2}$	$\frac{3}{2}$
$\epsilon_{j_i}^n$	-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 $A = 19$.

	$A = 18$			$A = 19$		
	$E_{\text{core}} = -118.469$			$E_{\text{core}} = -118.306$		
j_i	$\frac{1}{2}$	$\frac{5}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	$\frac{5}{2}$	$\frac{3}{2}$
$\epsilon_{j_i}^n$	-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

$A = 18$

Coupled Cluster, E_{core} : -130.462
Idaho NN N3LO + 3N N2LO

$A = 19$

-130.056 from G.R. Jansen
et al. PRL 113,
142502 (2014)

IM-SRG, E_{core} : -130.132
Idaho NN N3LO + 3N N2LO

-129.637 from H. Hergert
private comm.

No-Core Shell-Model Approach

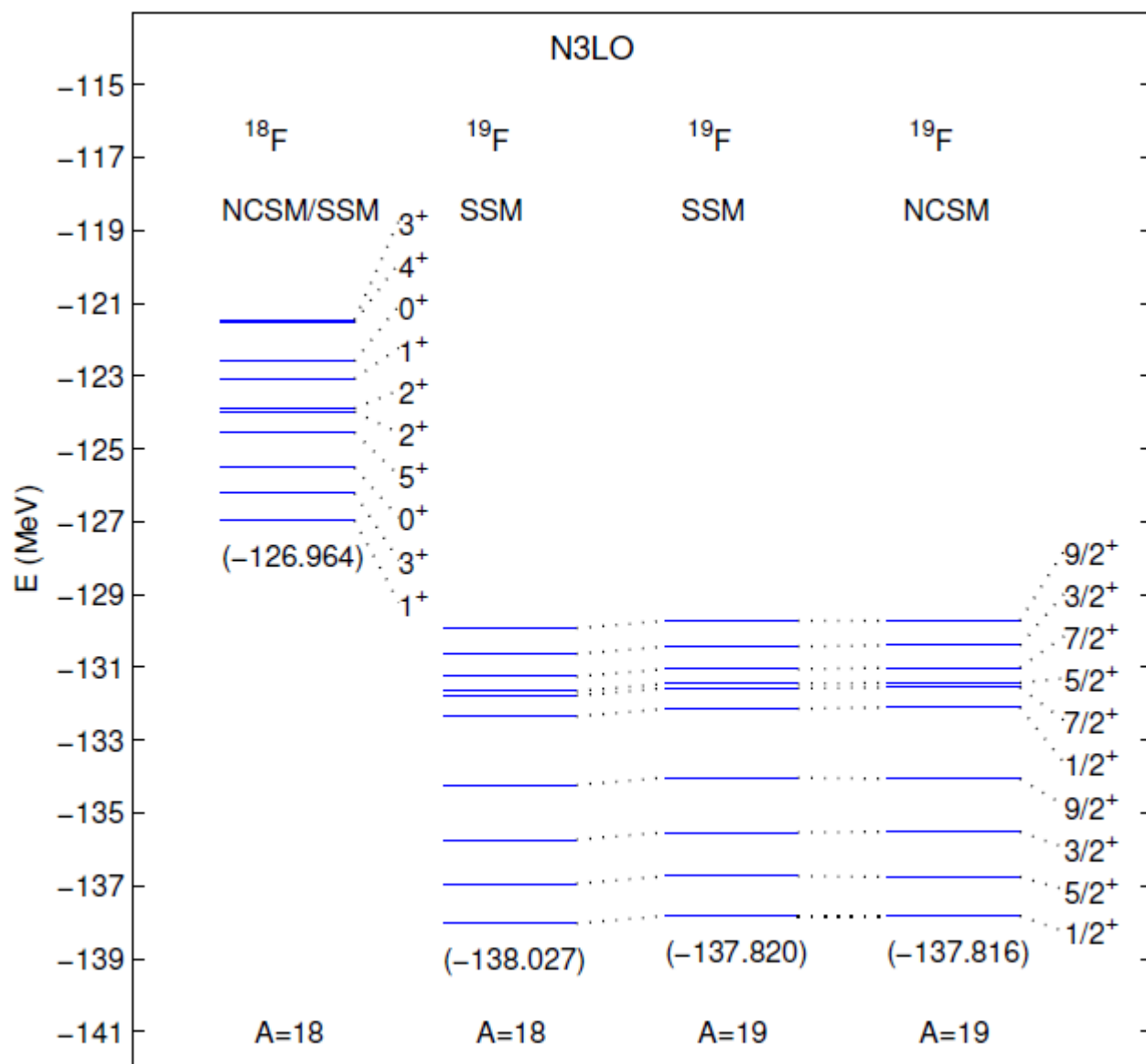
- Next, add CM harmonic-oscillator Hamiltonian

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

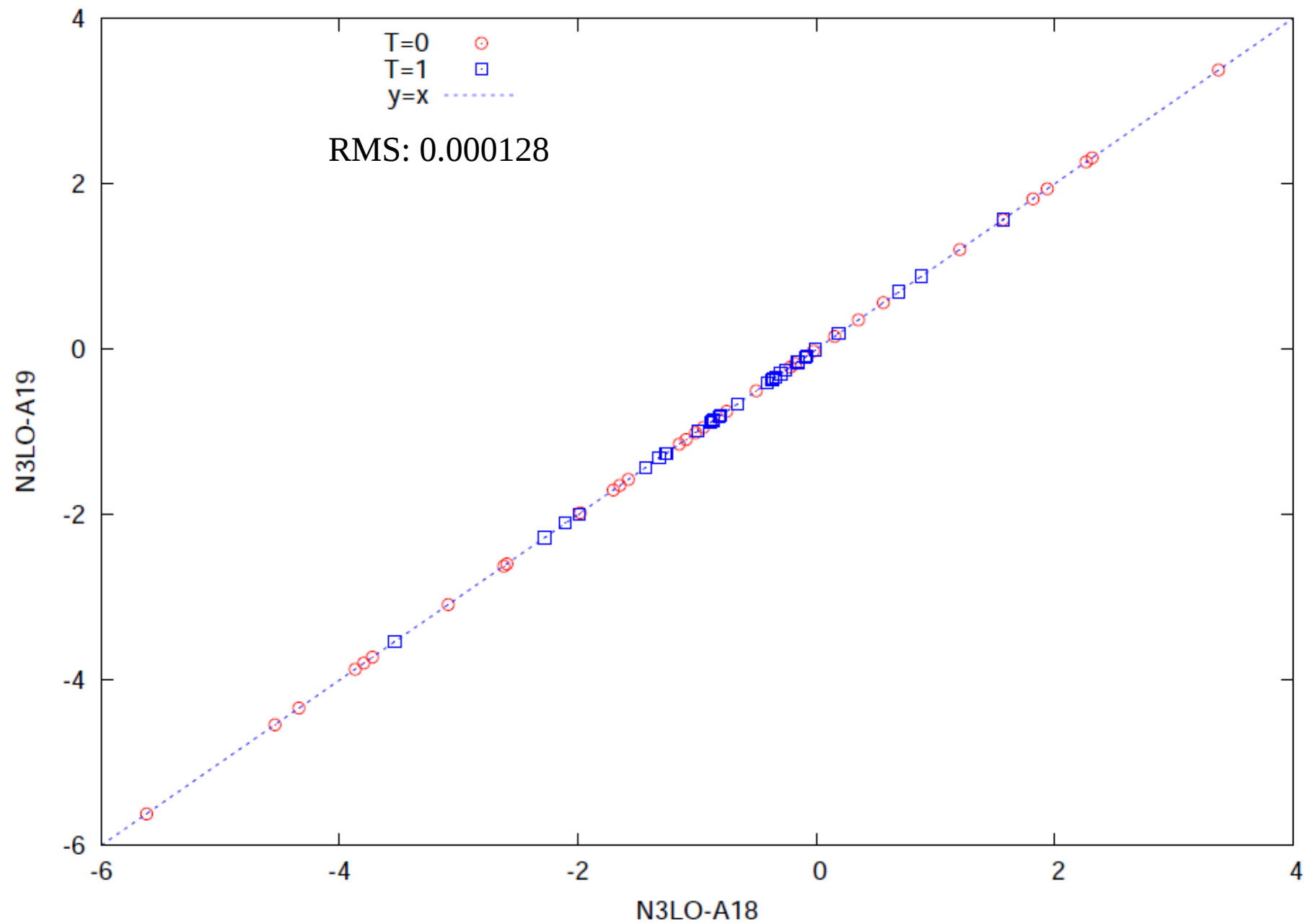
To H_A , yielding

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

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



PRELIMINARY RESULT



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 $^{18,20,22,24}\text{F}$ 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)

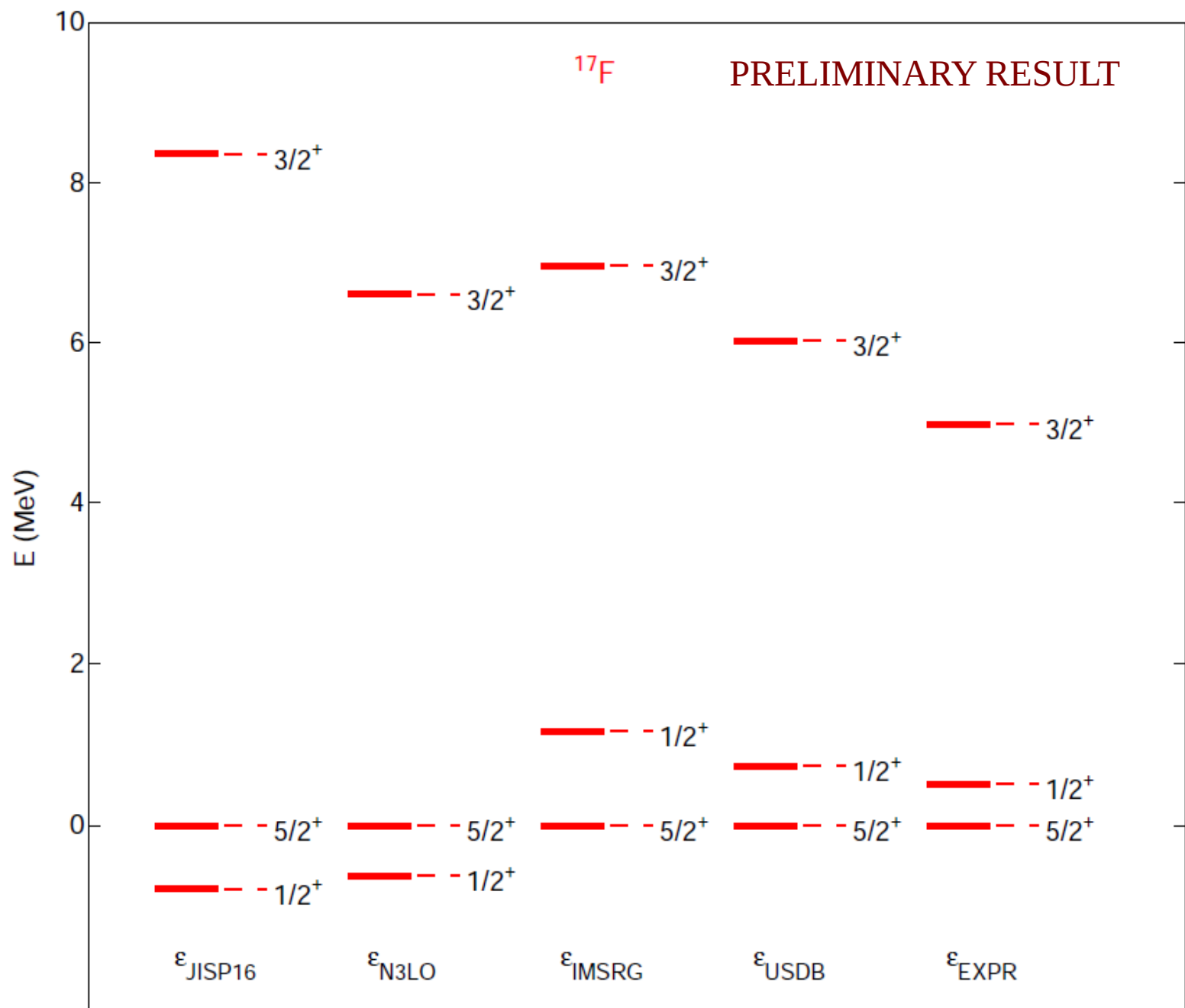
Preliminary Results

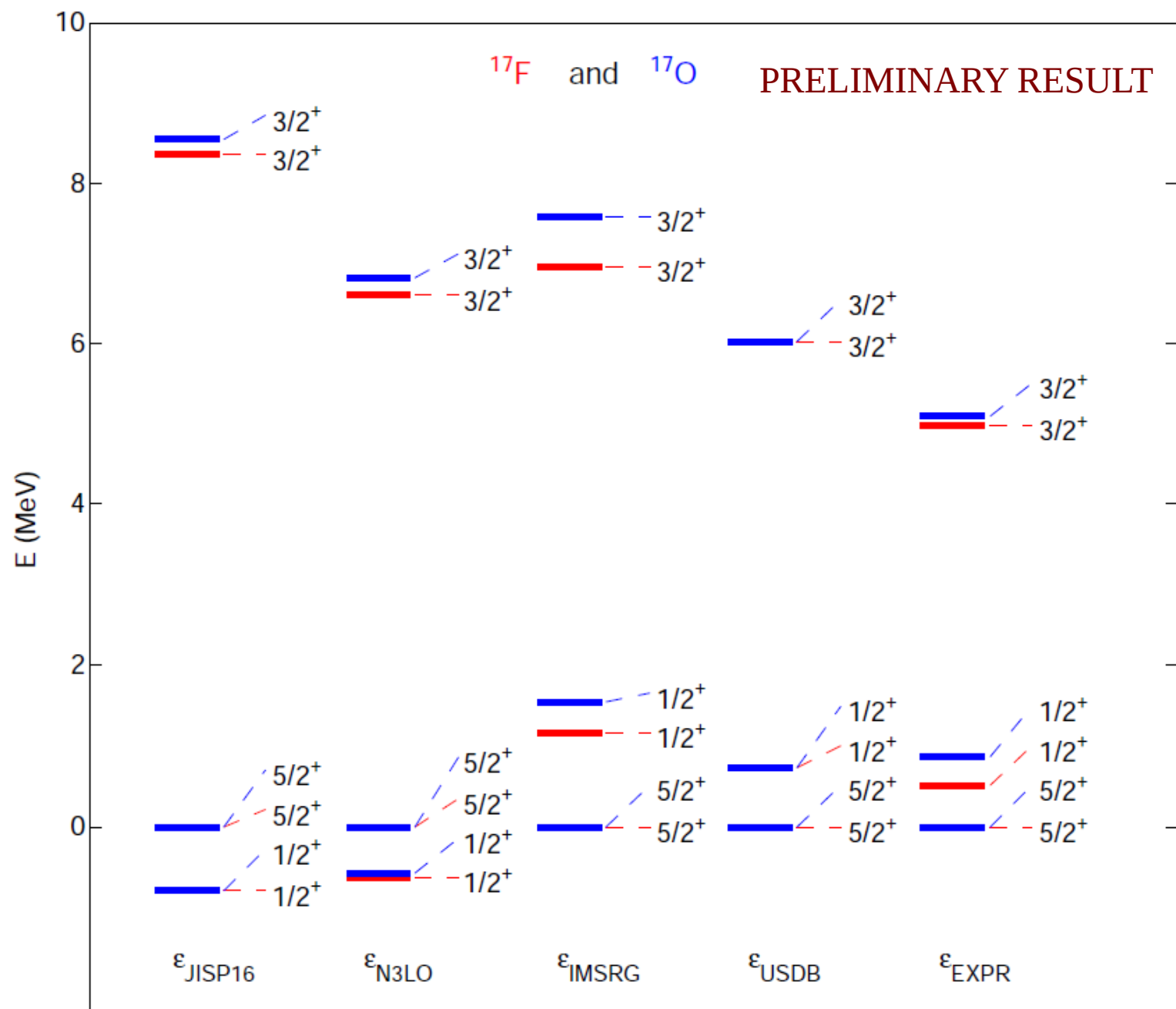
TABLE I: The single-particle energies (in MeV) used in the standard shell model calculations of F isotopes. (n) and (p) represent neutron and proton, respectively.

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	

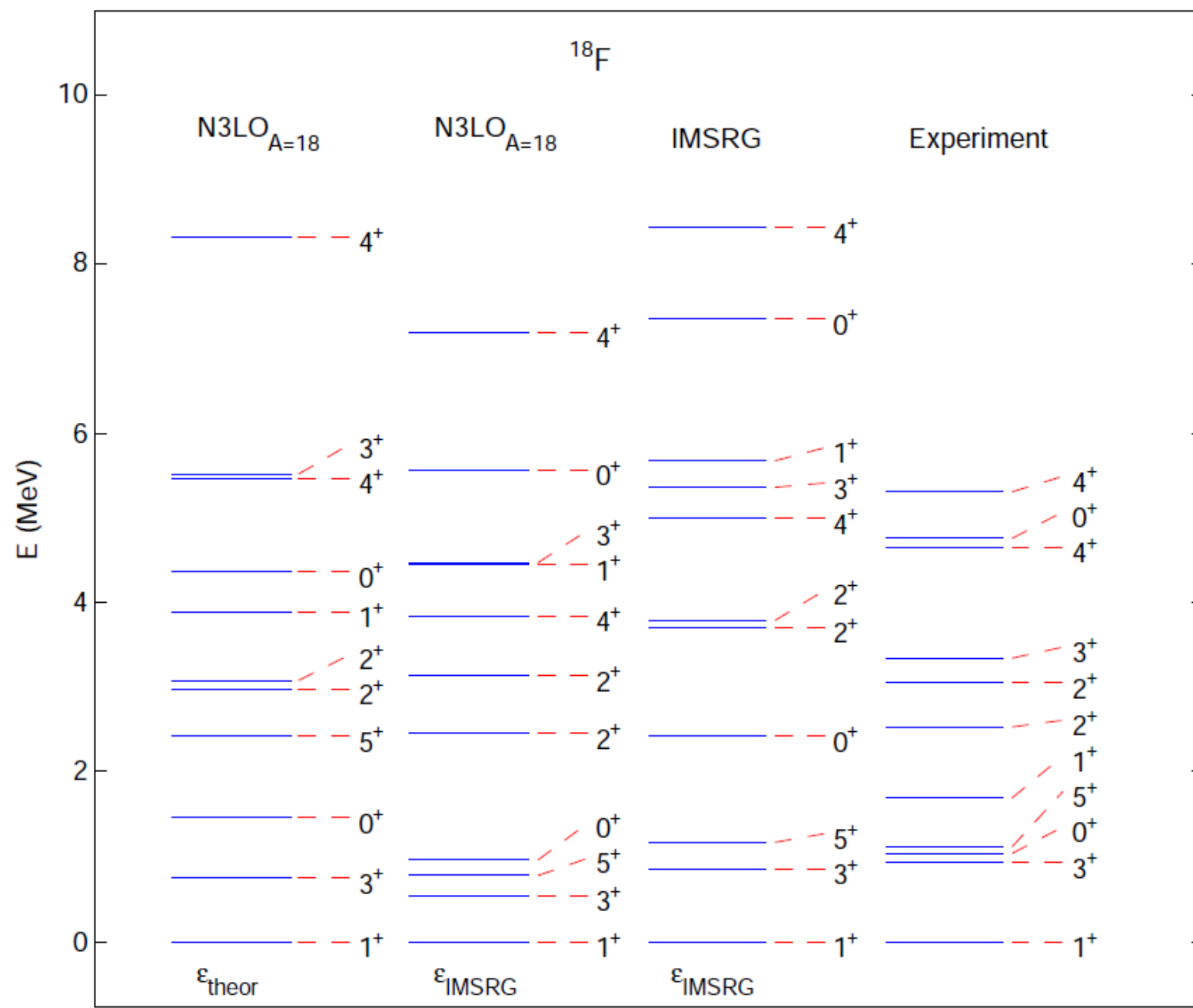
* B.A. Brown & W.A. Richter, PRC 74, 034315 (2006)

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

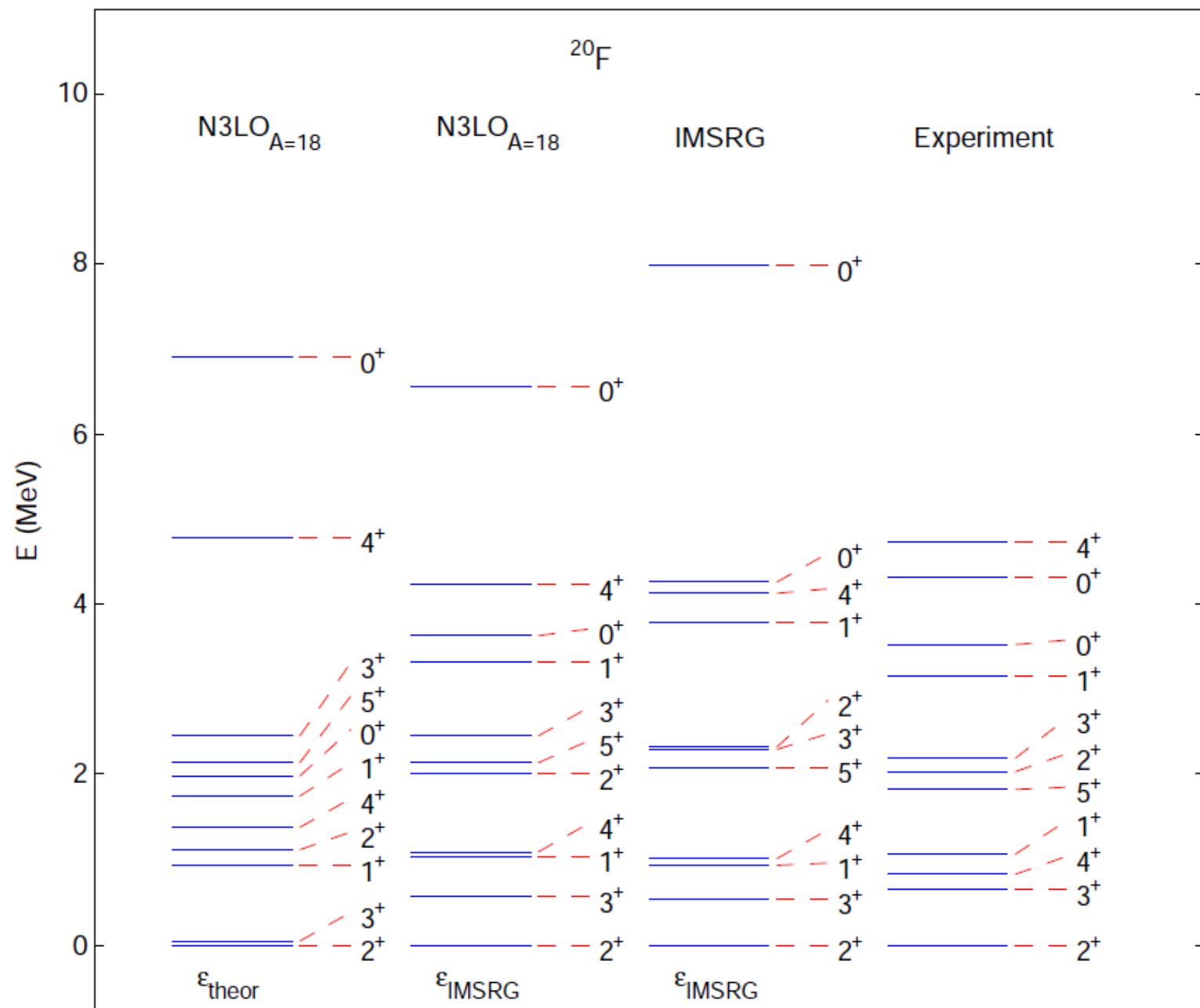




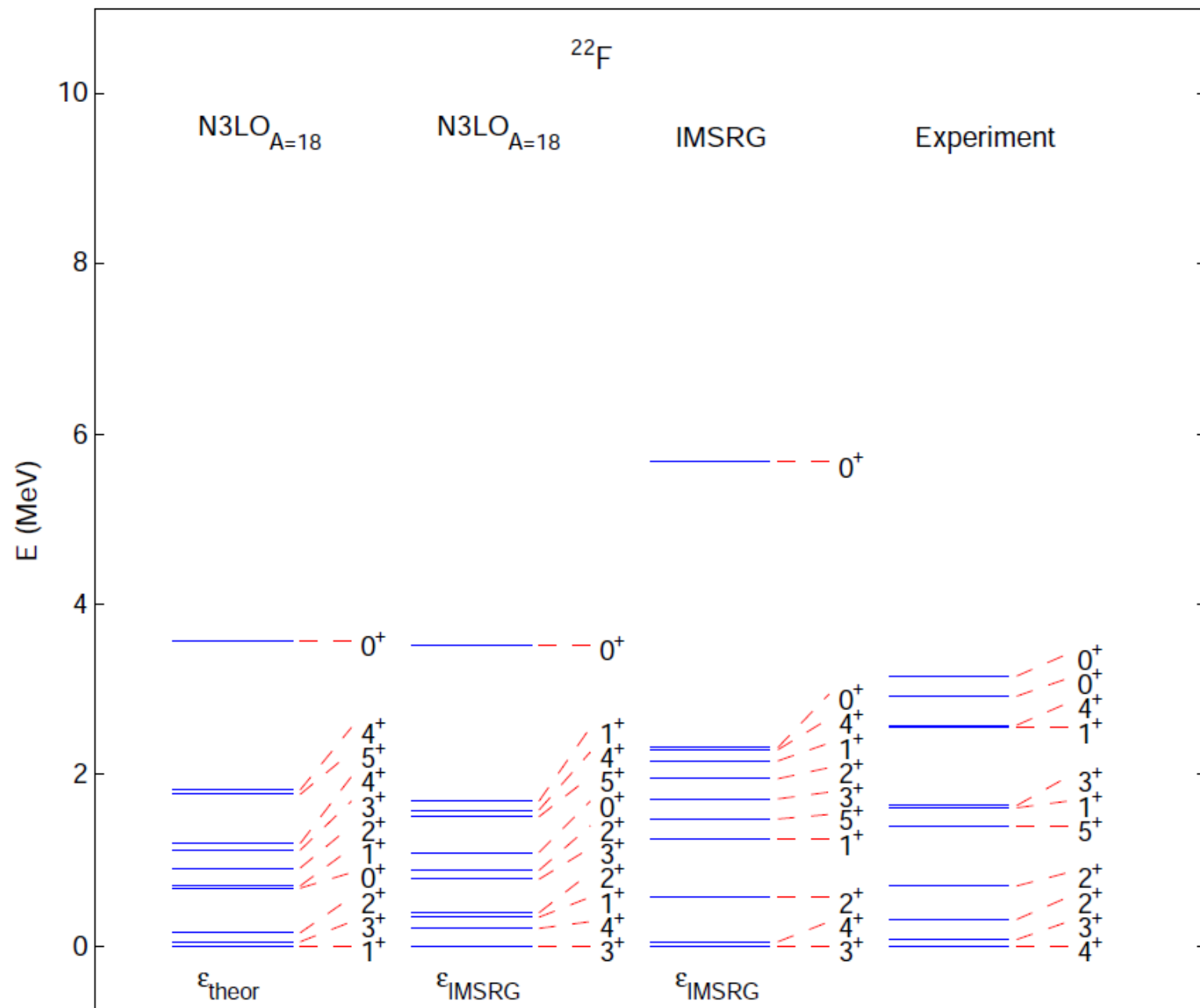
PRELIMINARY RESULT



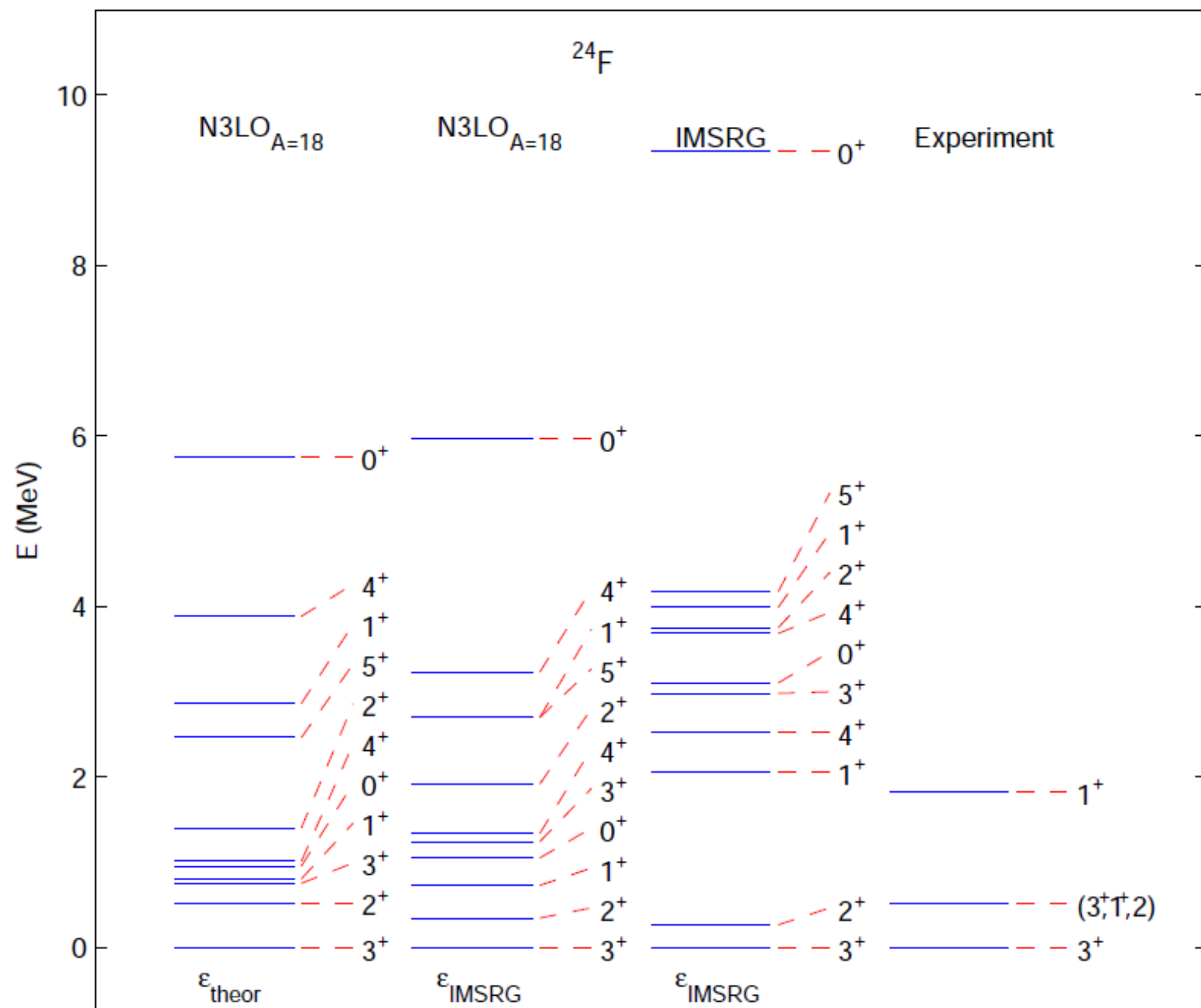
PRELIMINARY RESULT



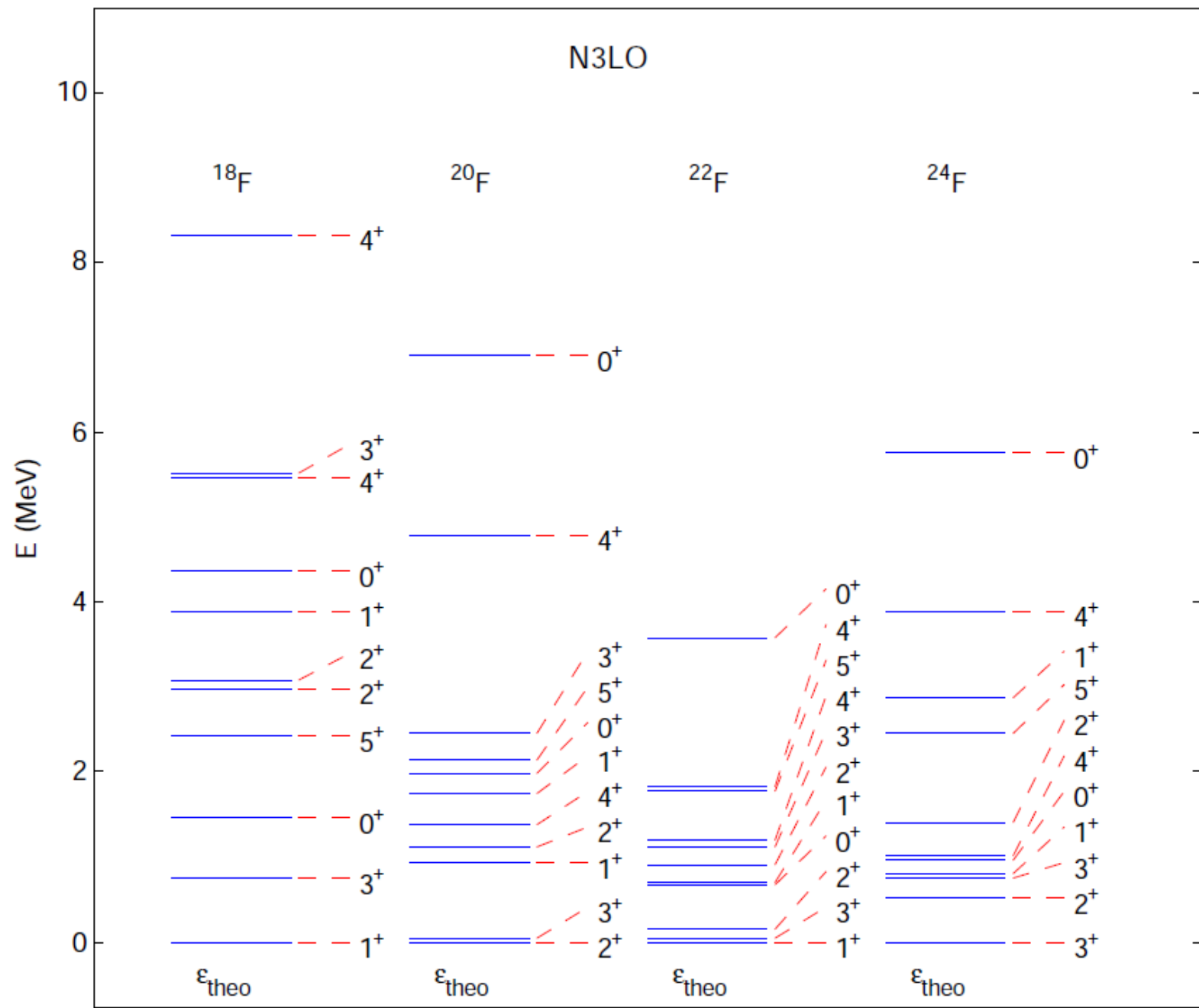
PRELIMINARY RESULT



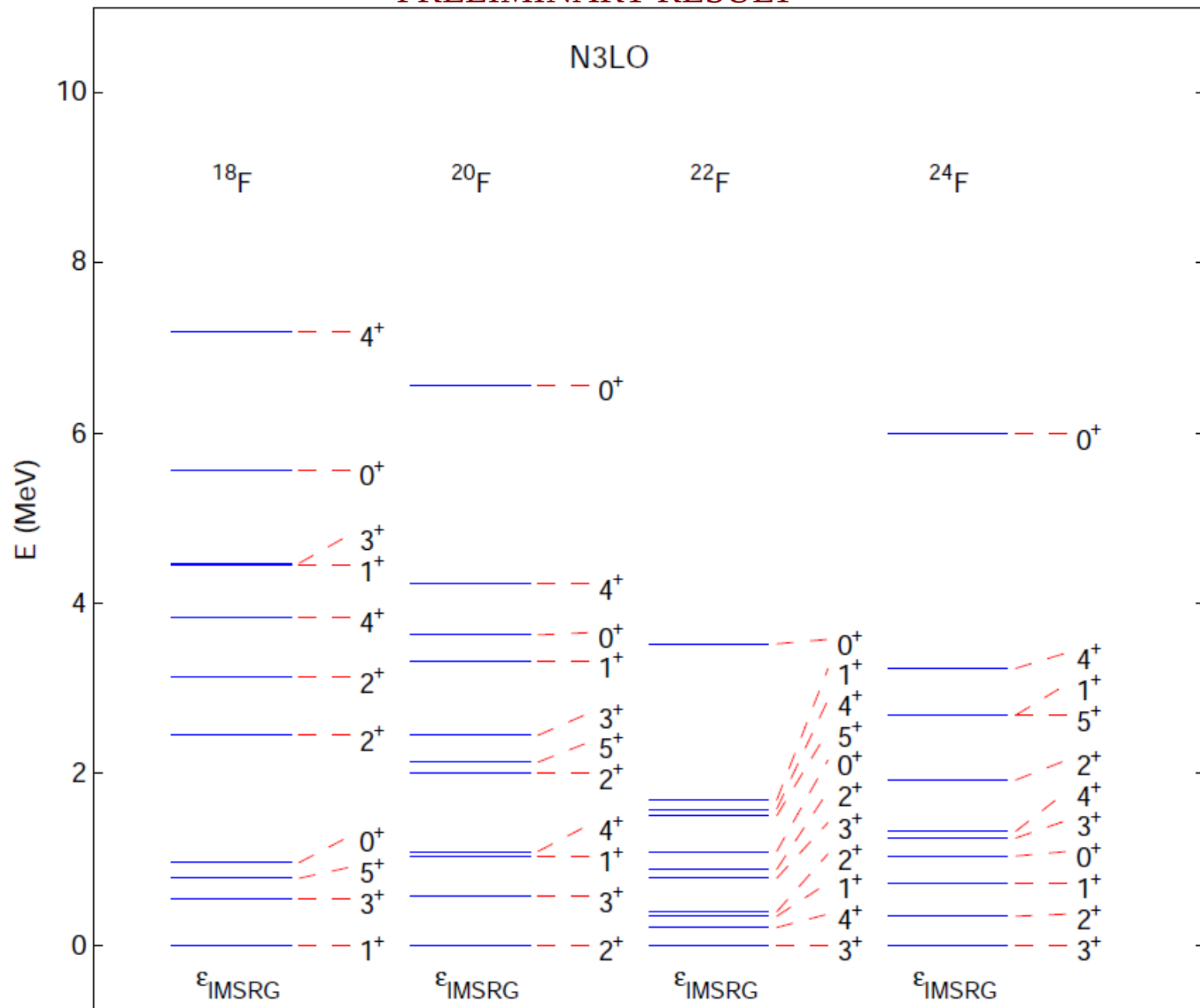
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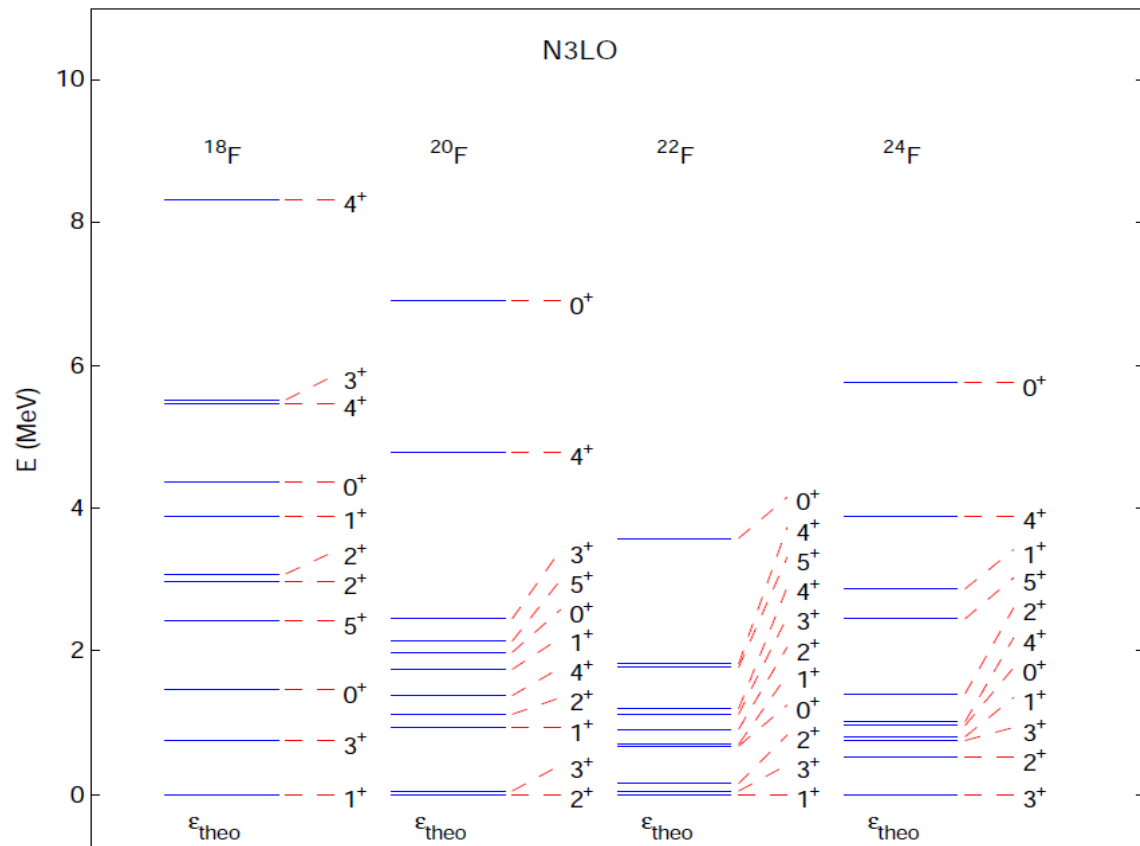
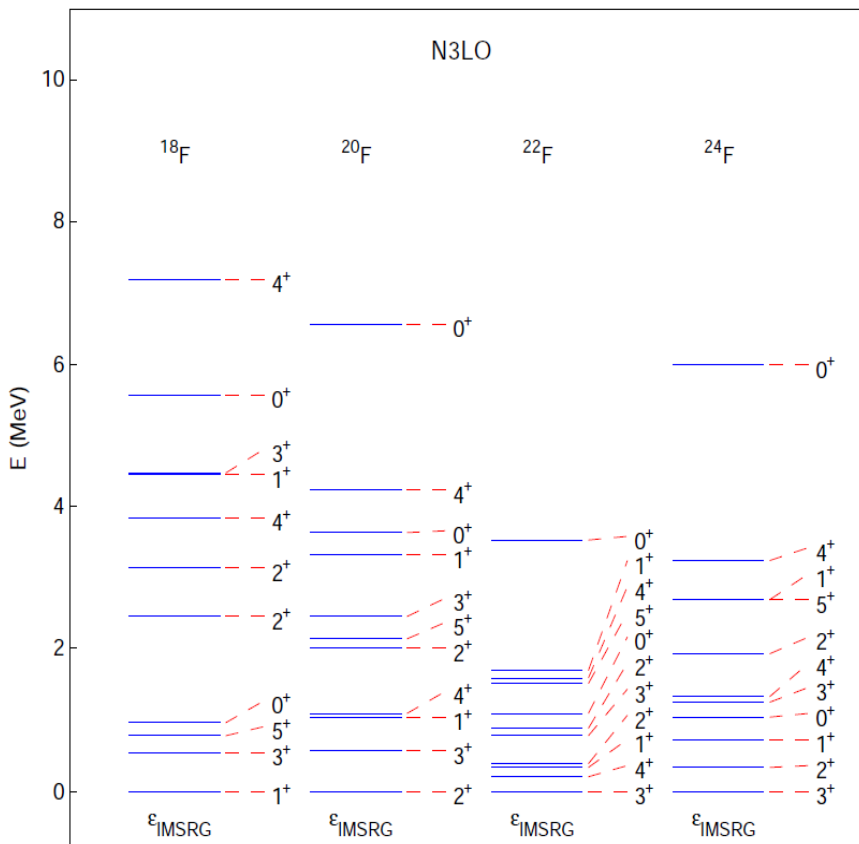
PRELIMINARY RESULT



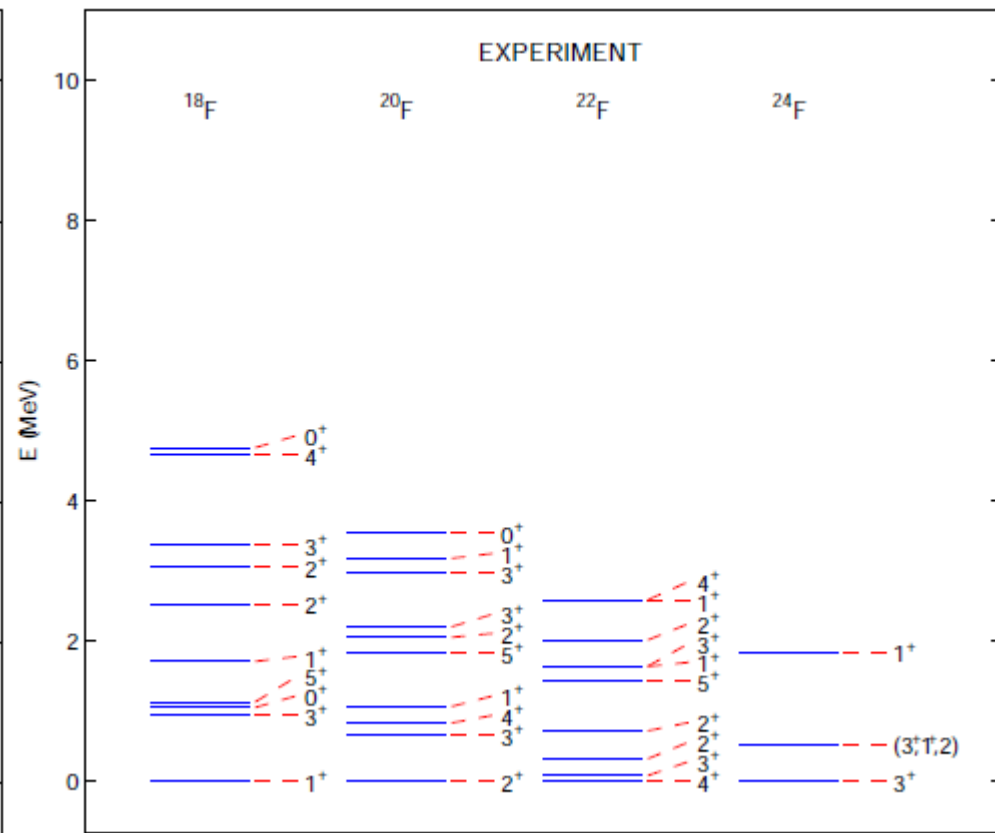
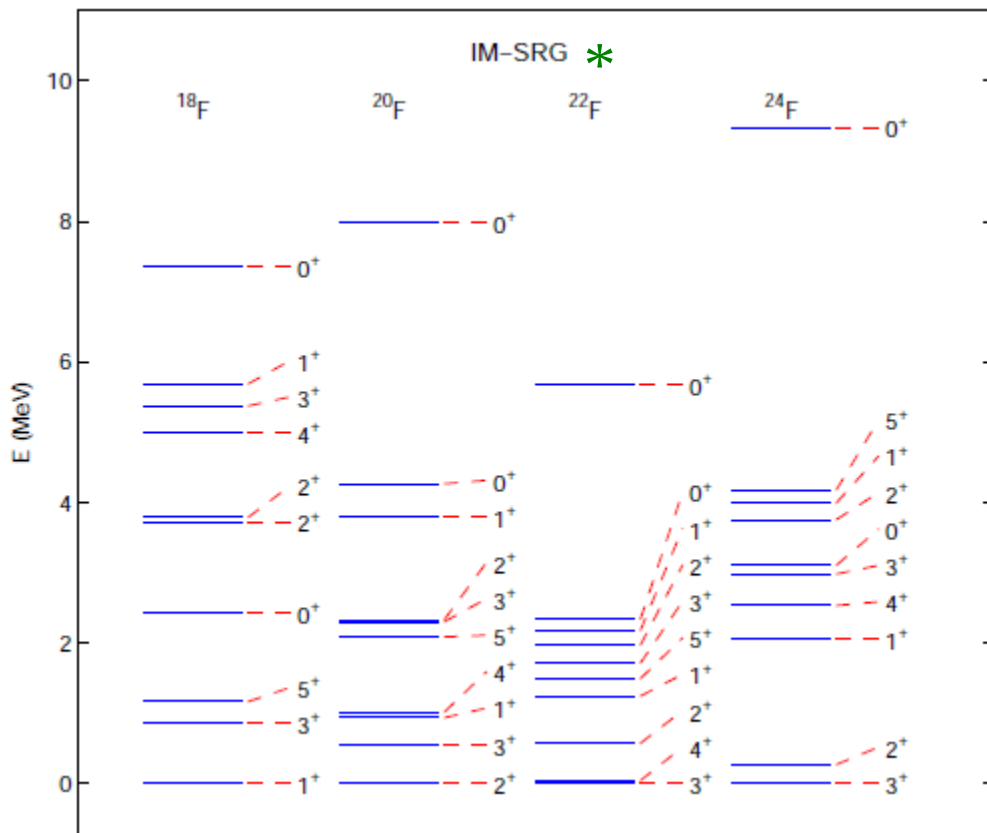
PRELIMINARY RESULT



PRELIMINARY RESULTS

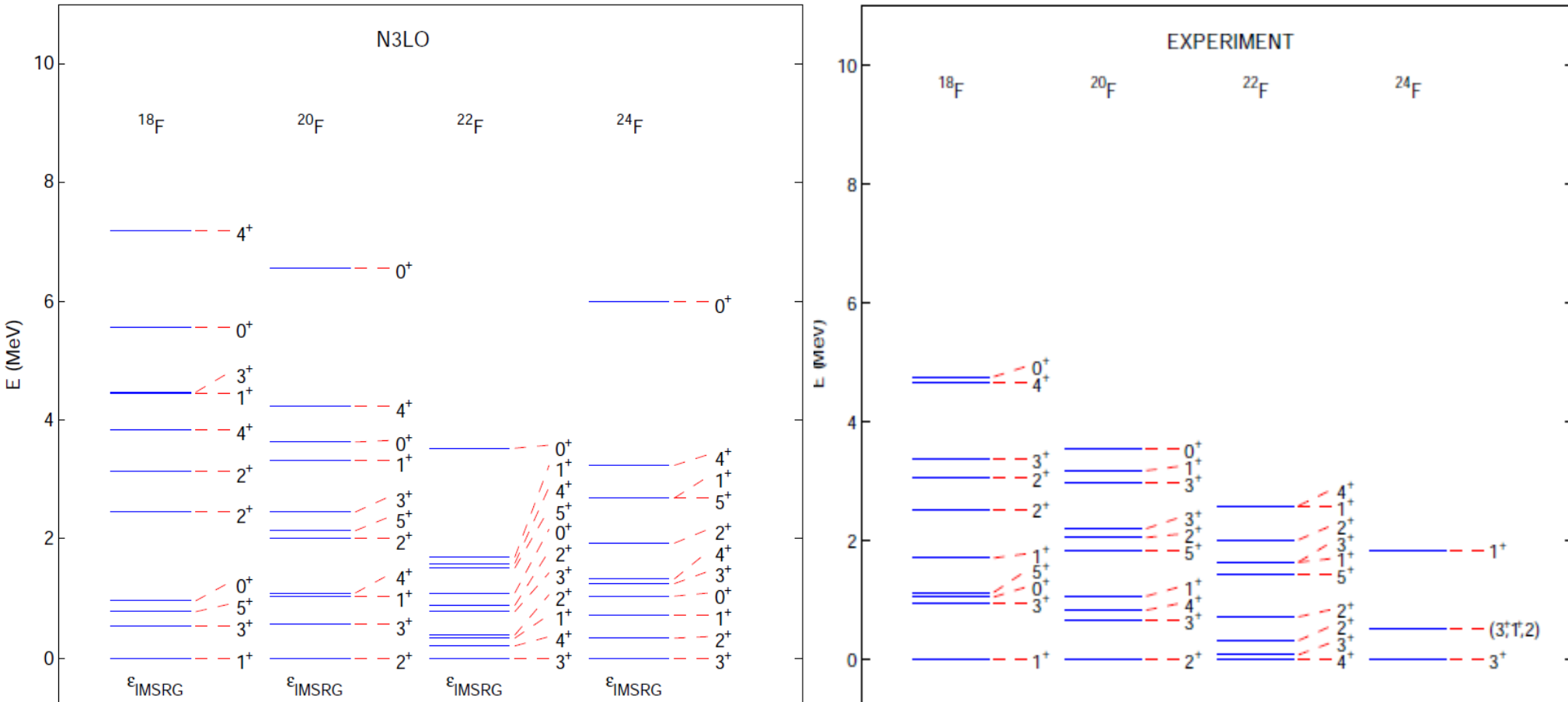


N3LO + IMSRG spe vs N3LO + theoretical spe



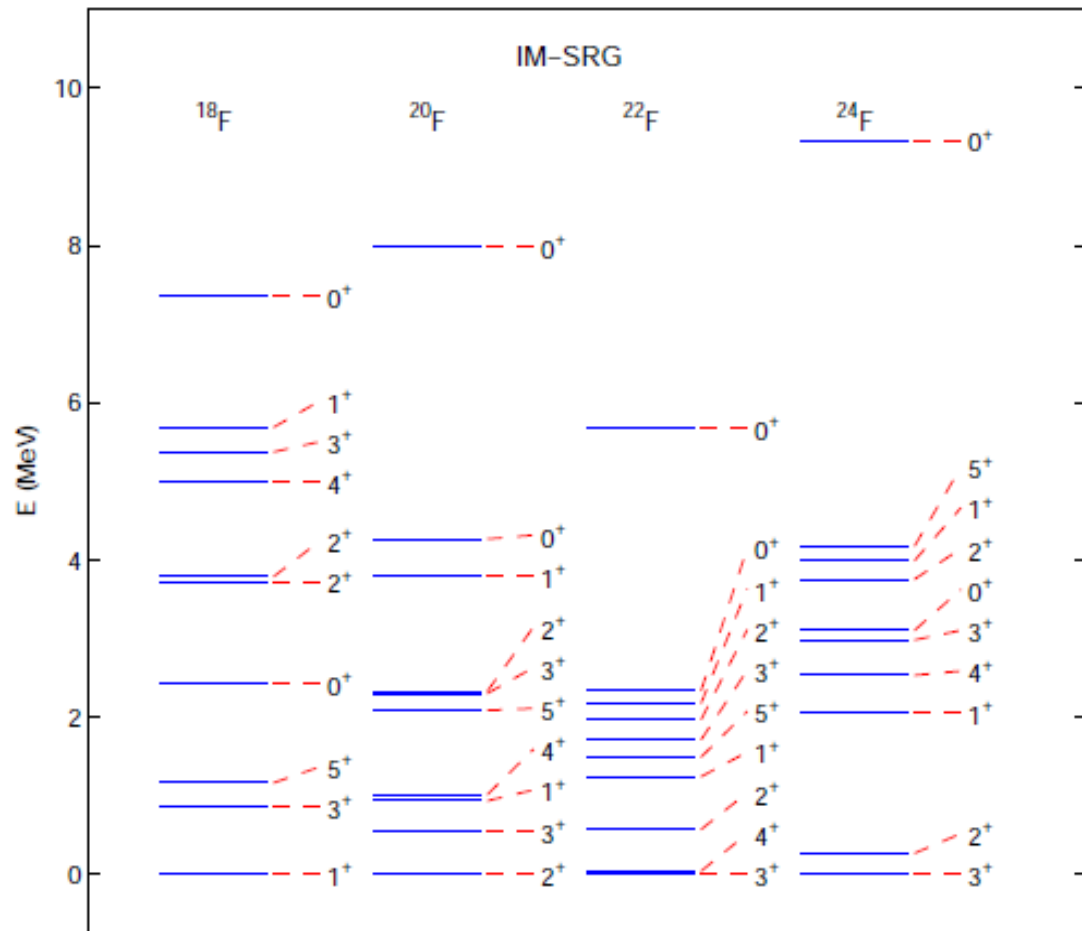
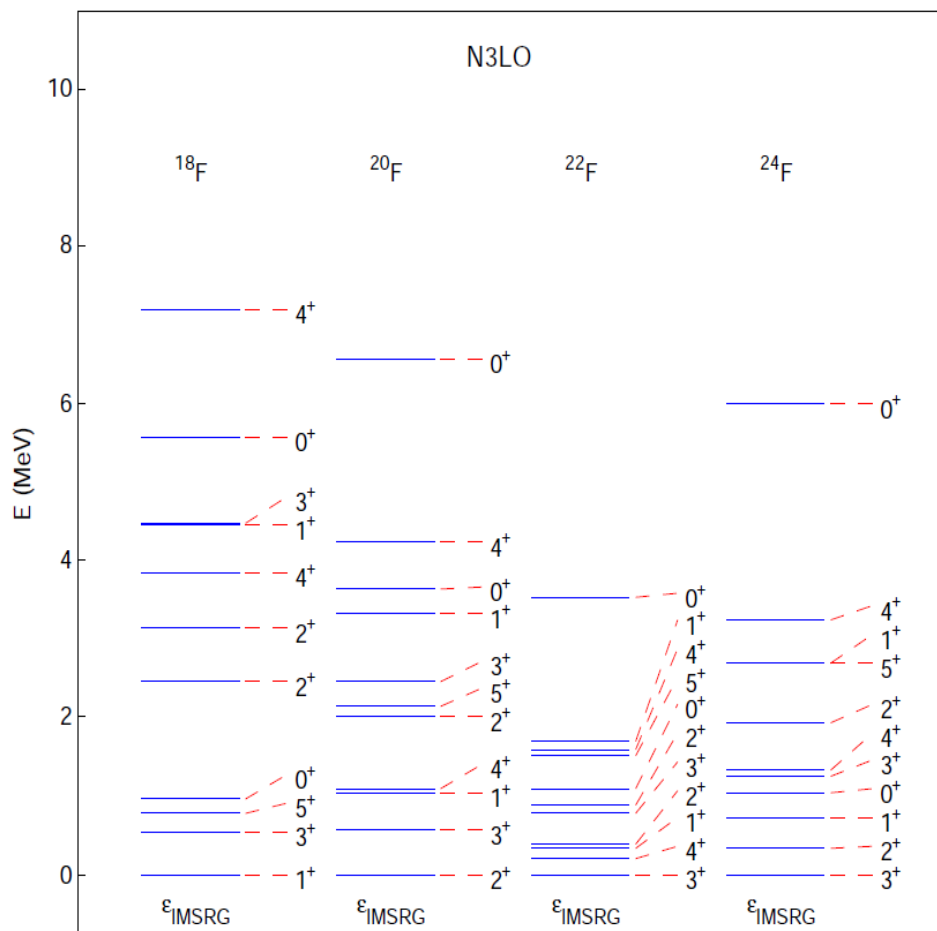
* S.R. Stroberg, et al., arXiv Nucl-th 1511.02802

PRELIMINARY RESULTS



N3LO + IMSRG spe vs Experiment

PRELIMINARY RESULTS

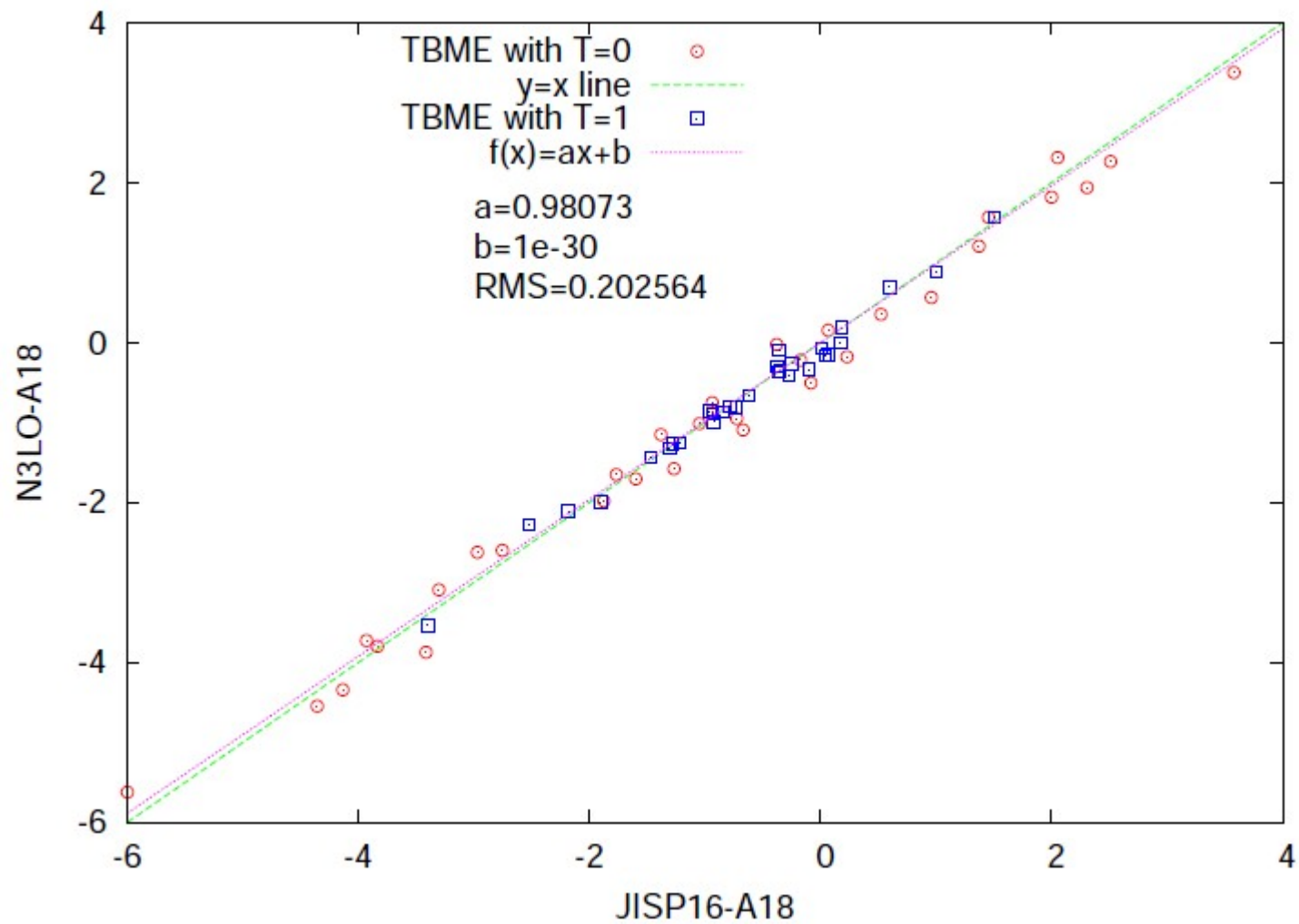


N3LO + IMSRG spe vs IM-SRG

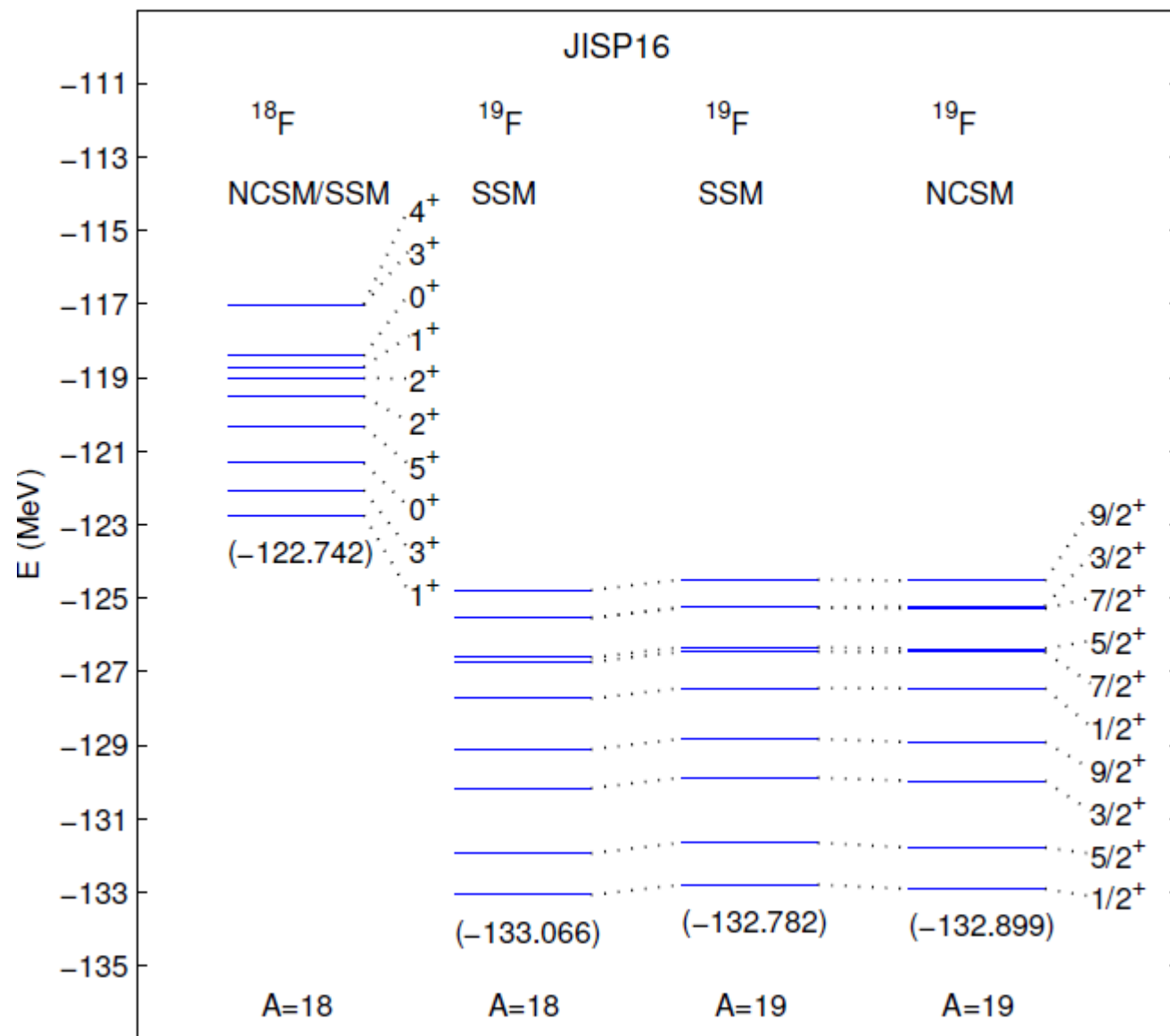
SUMMARY AND OUTLOOK

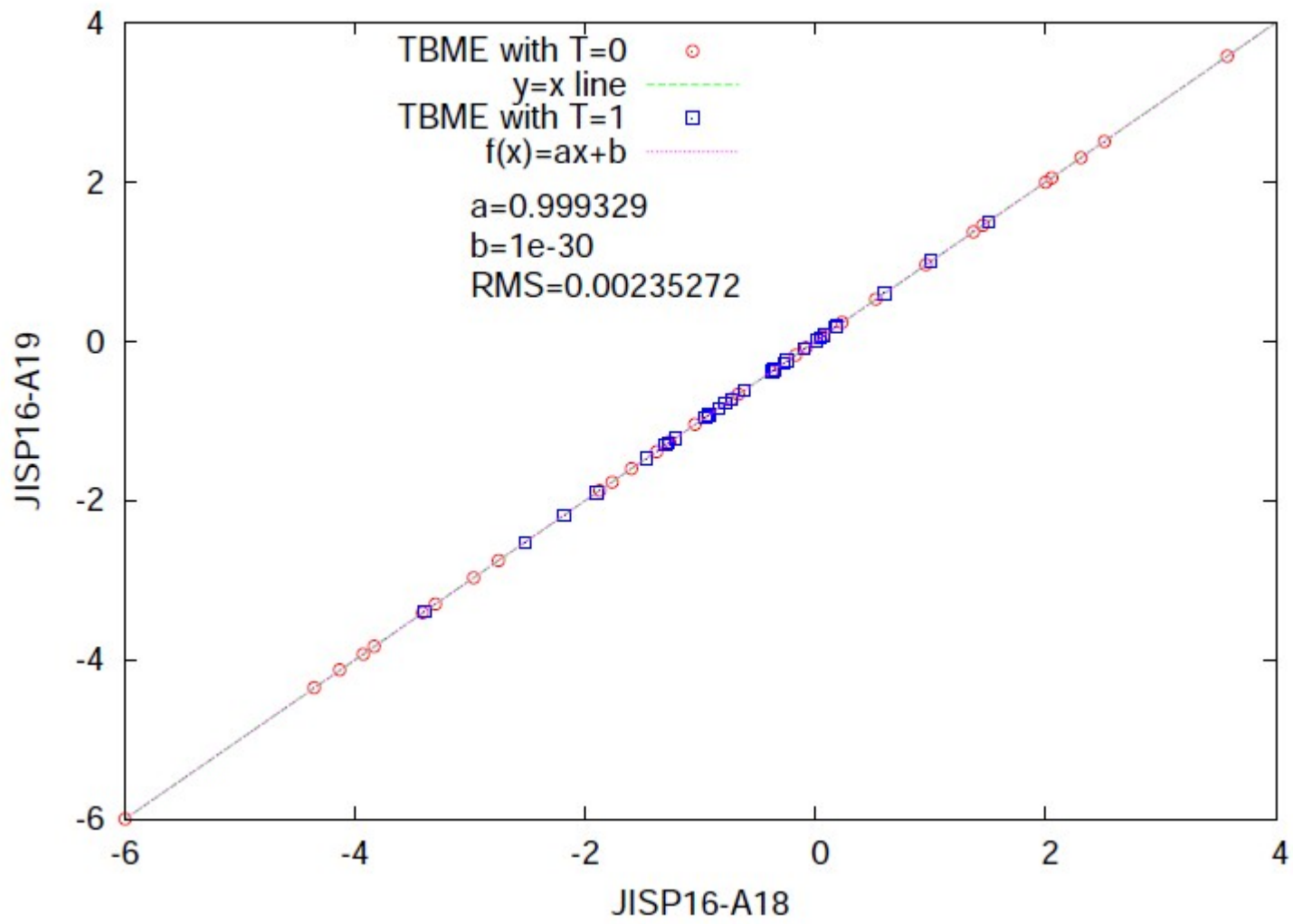
1. The interactions and approaches used in this study reproduced the gross trends and features of the experimental data for the 18,20,22,24 F isotopes.
2. Replacing our theoretical s.p. energies with those obtained in the IM-SRG calculations of Stroberg et al. to approximate the effects of a NNN interaction, 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.



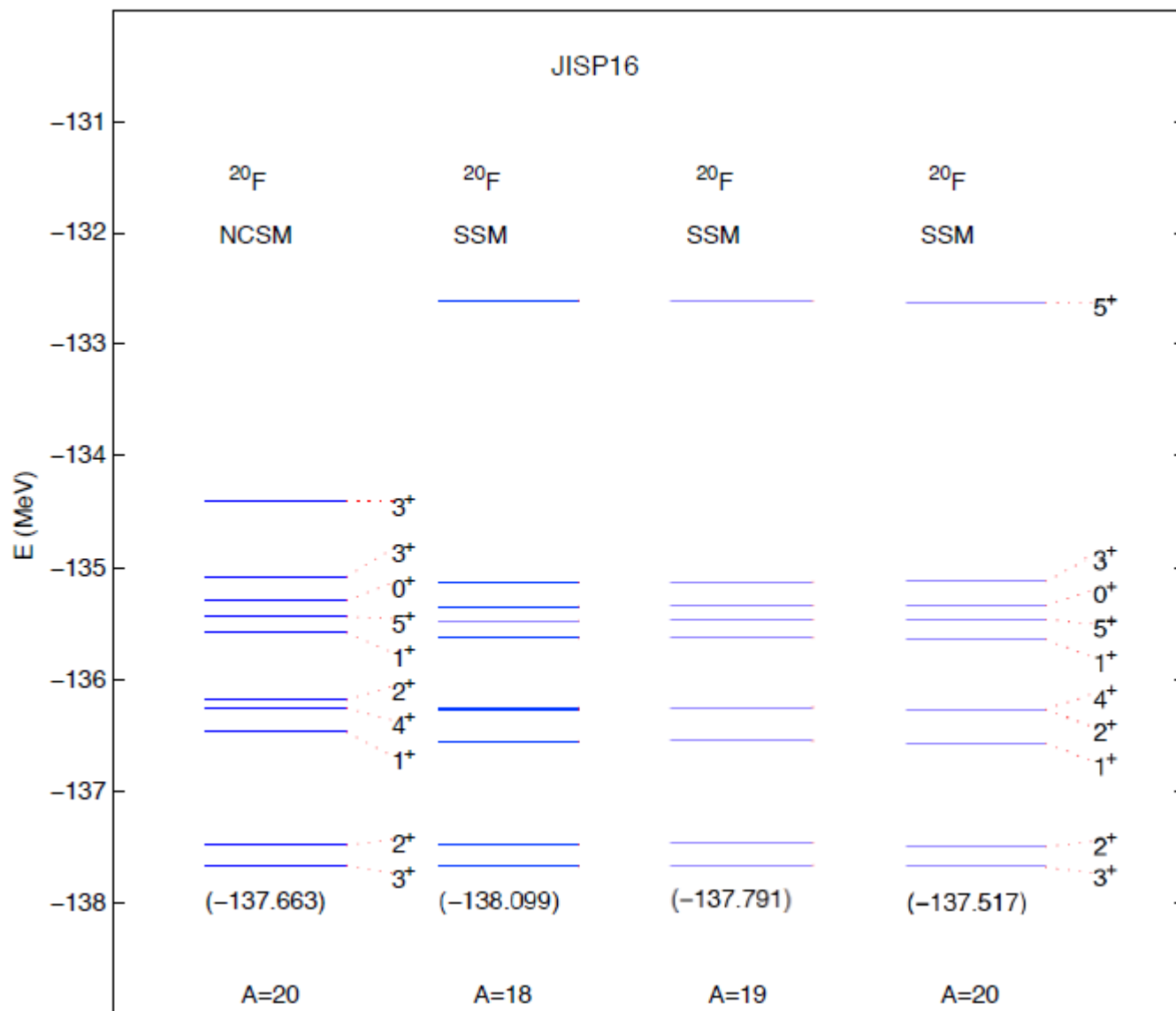
Preliminary Results



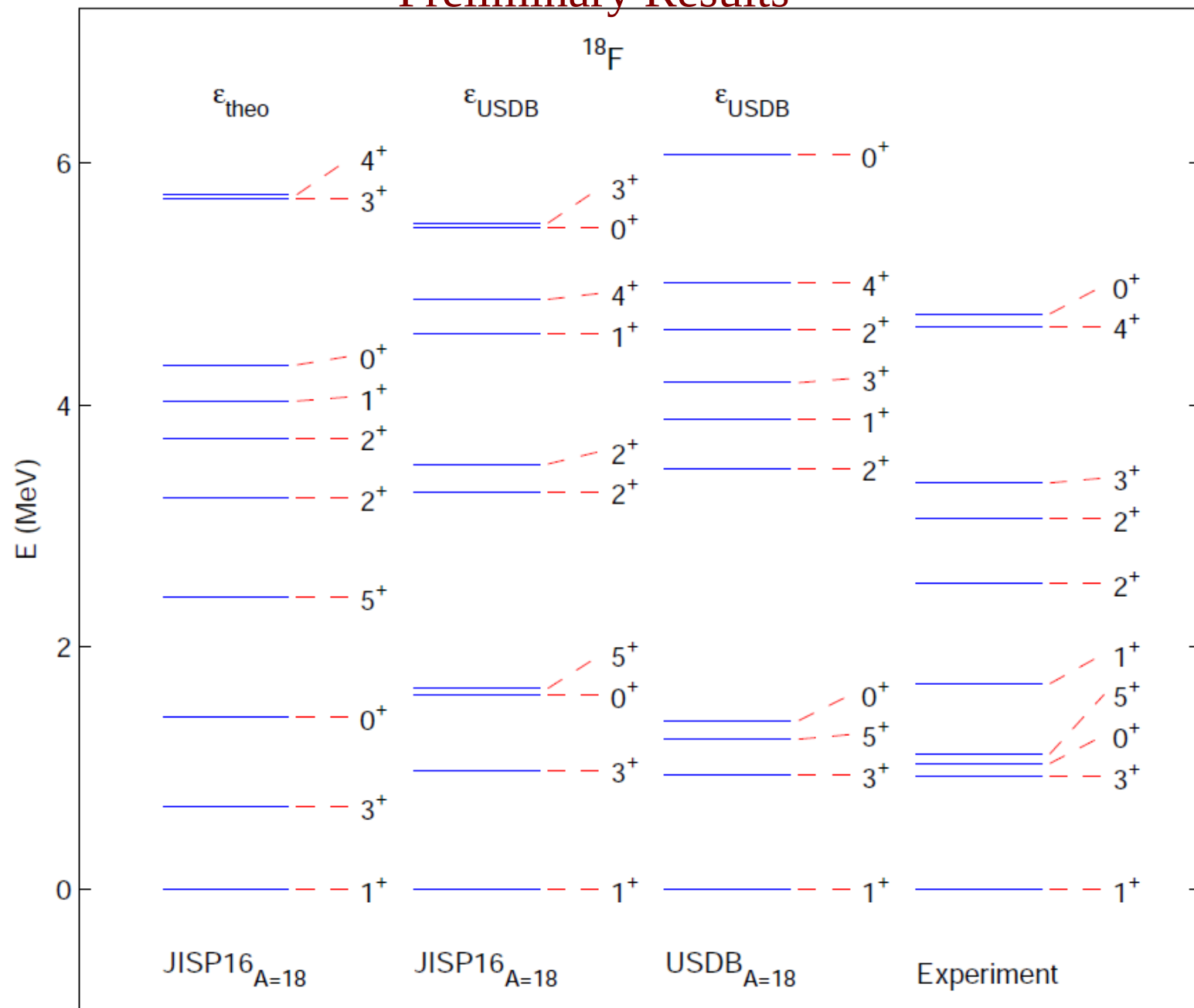


Preliminary Results

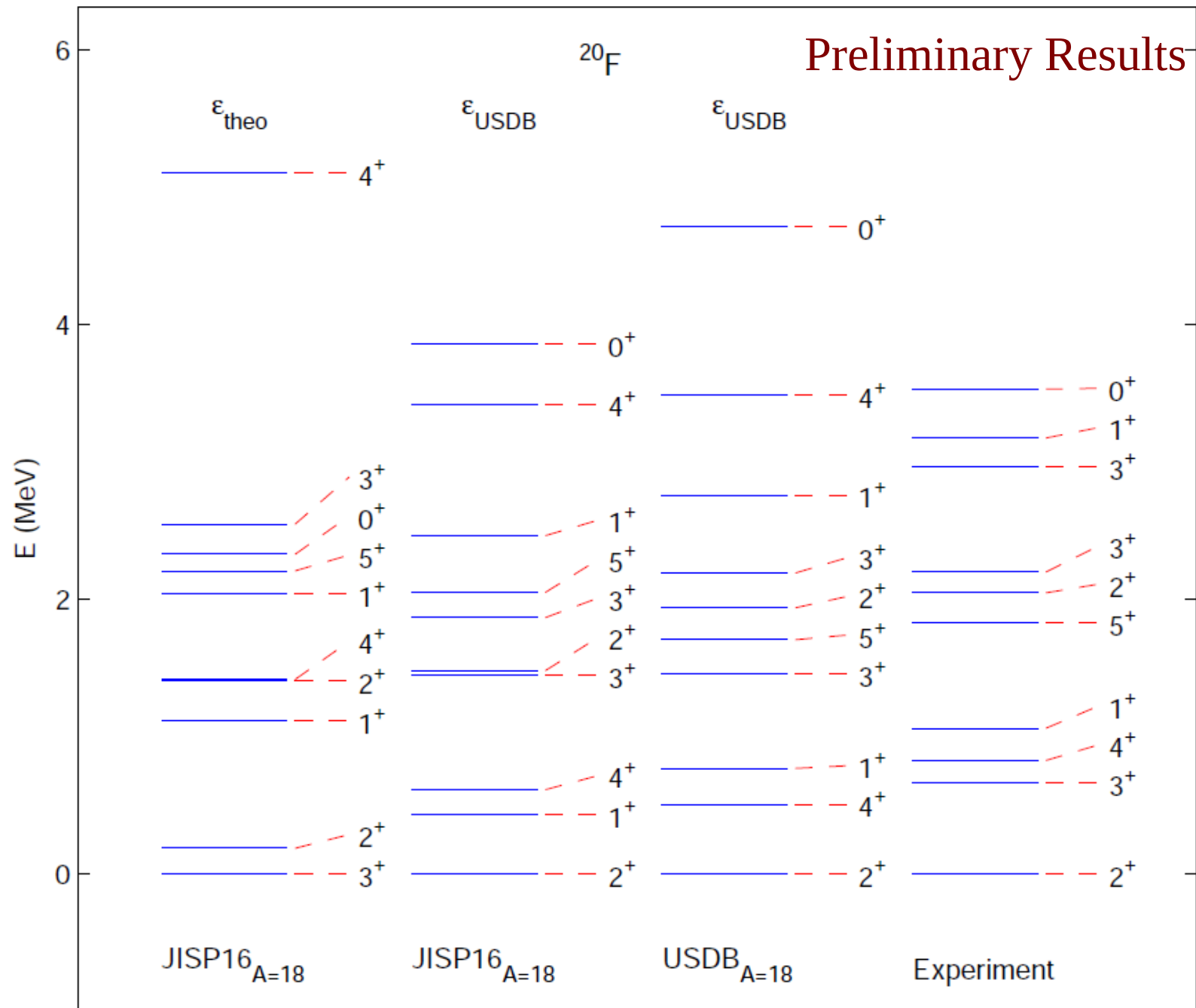
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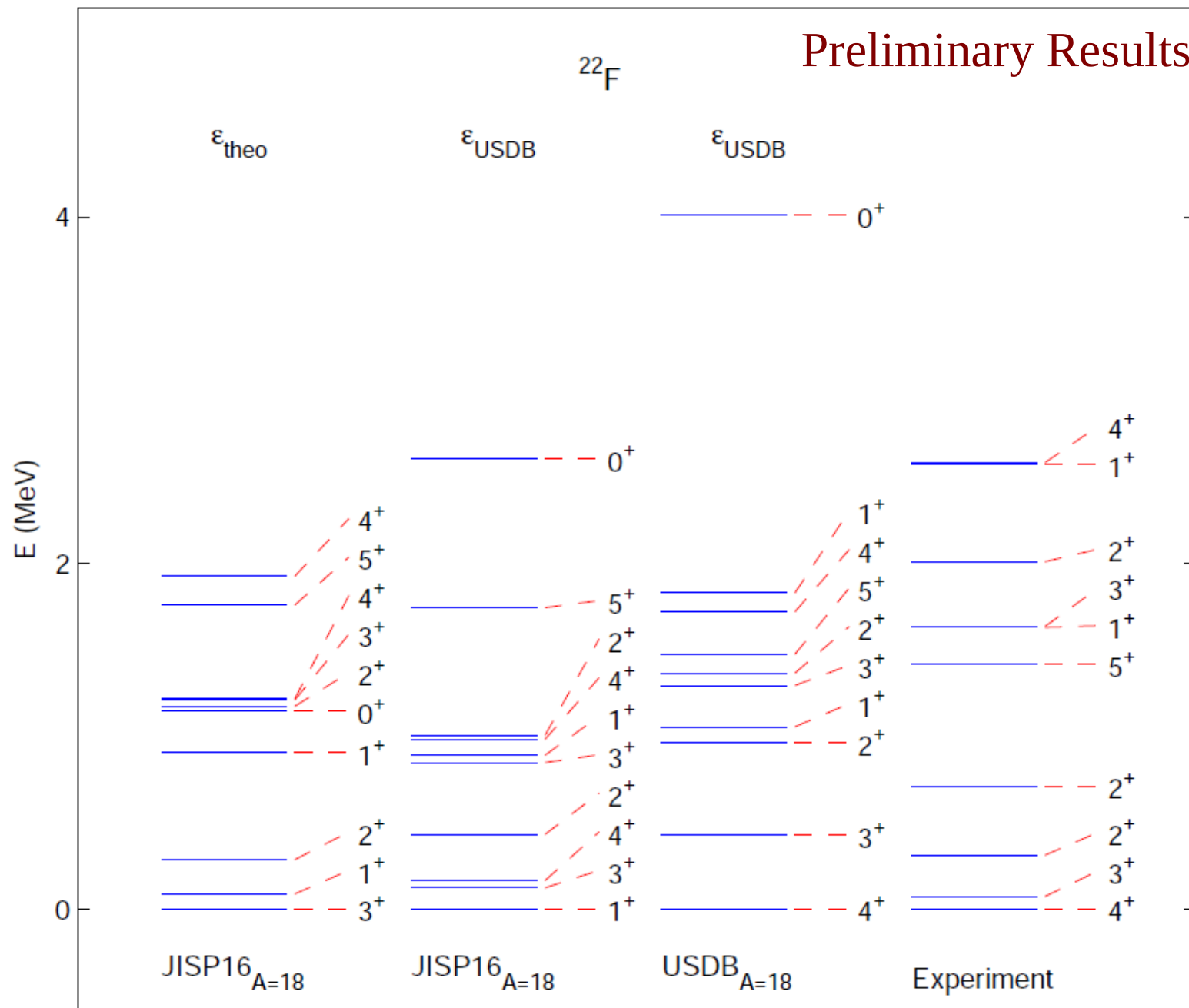
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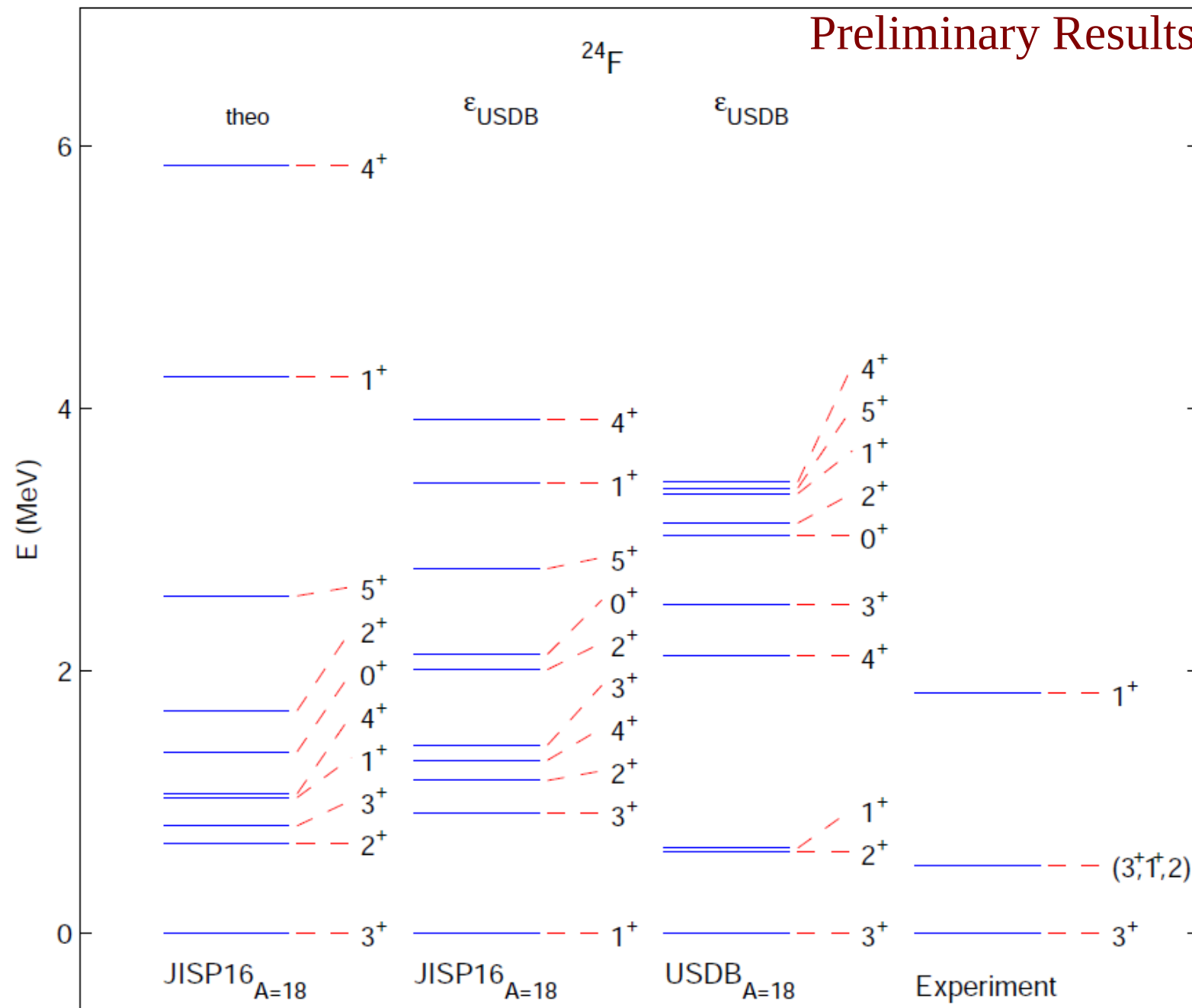
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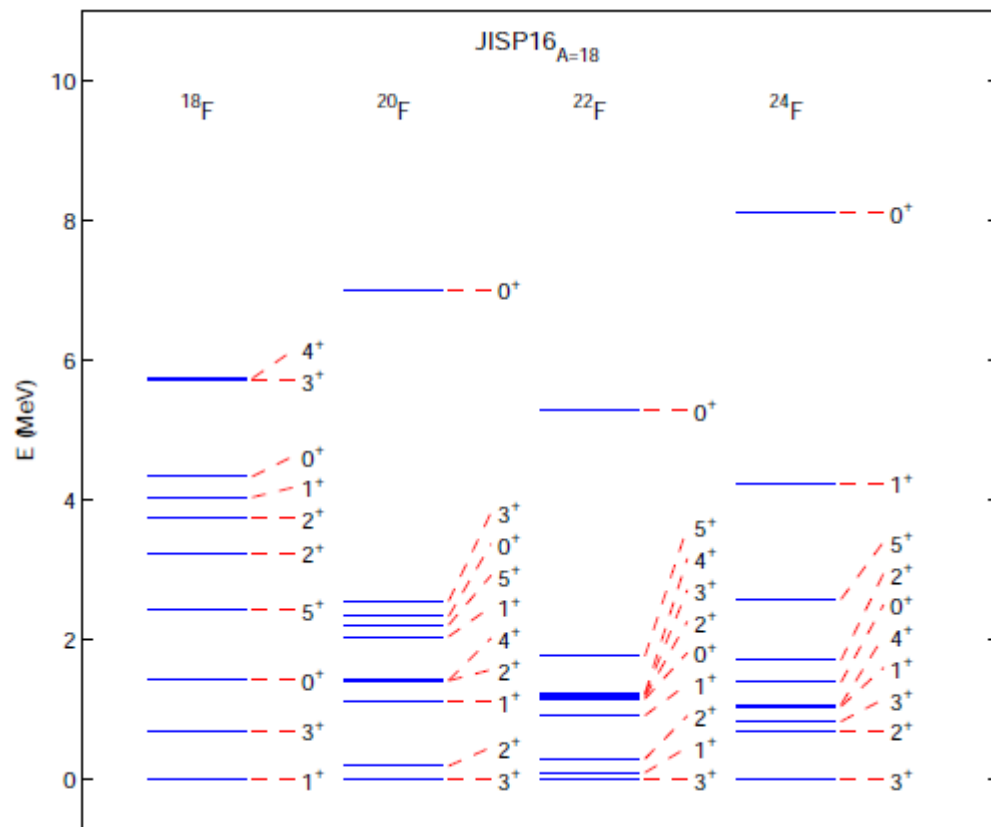
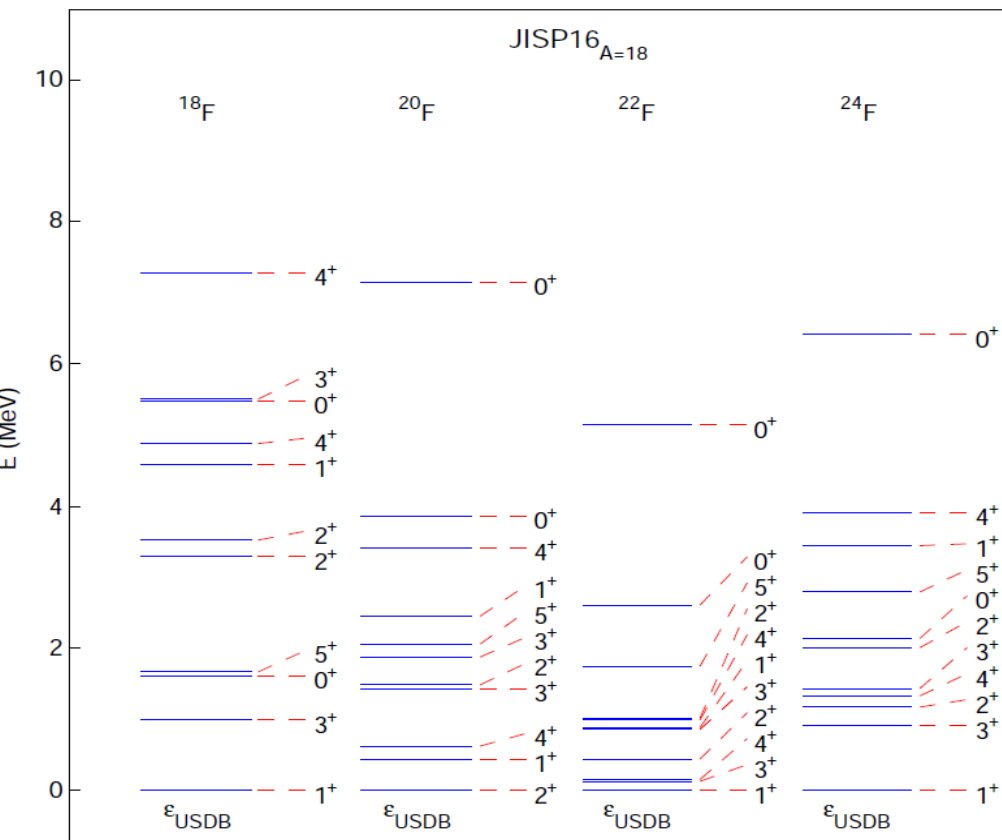
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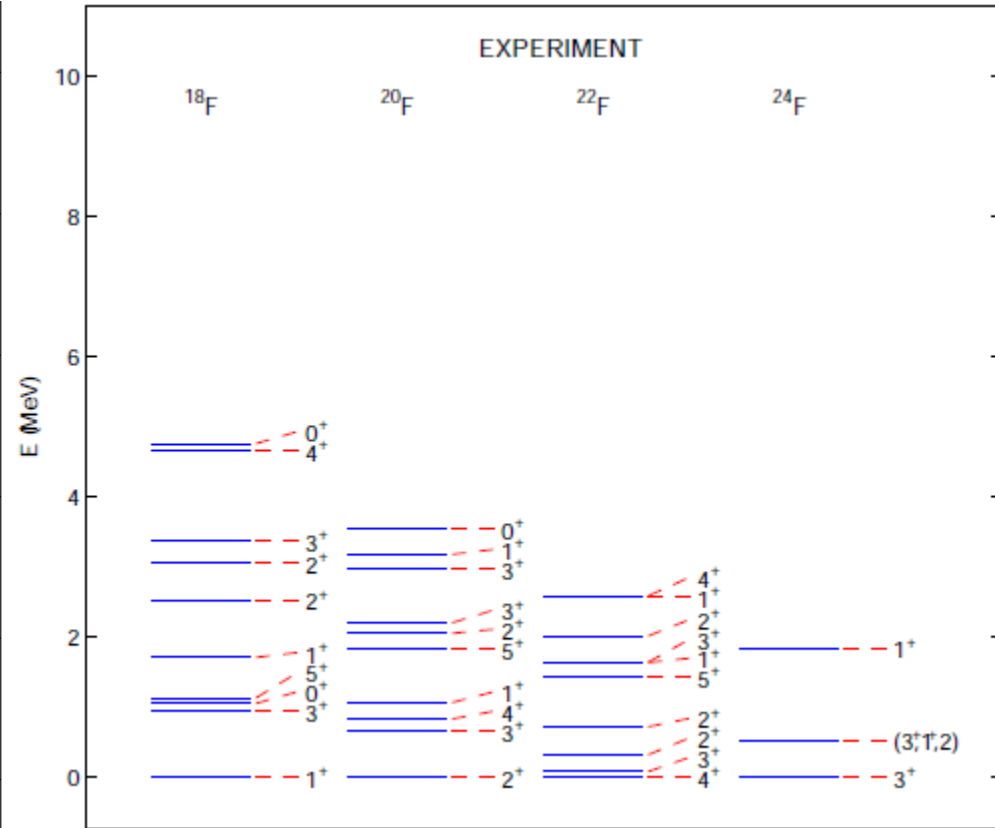
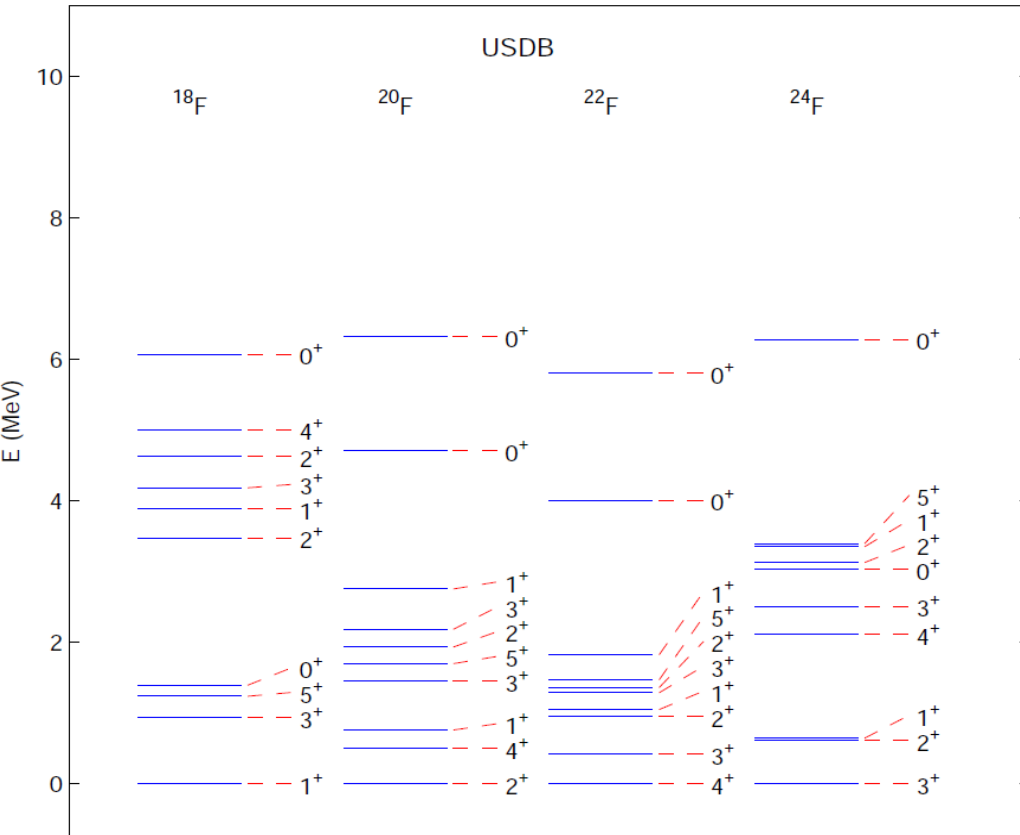
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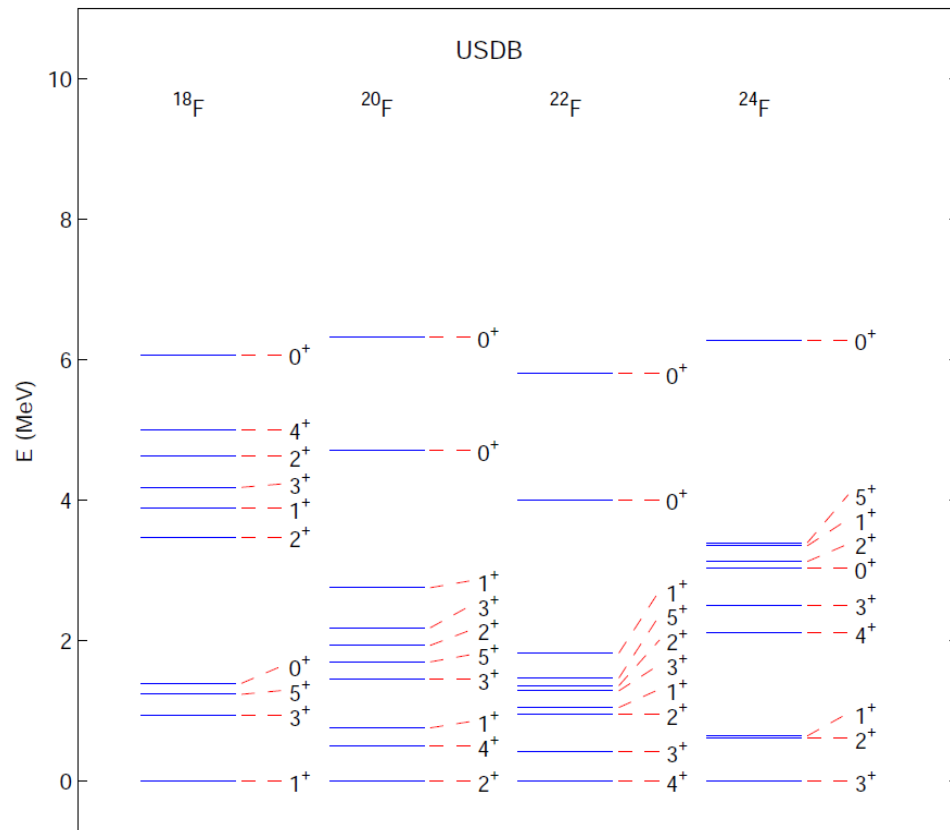
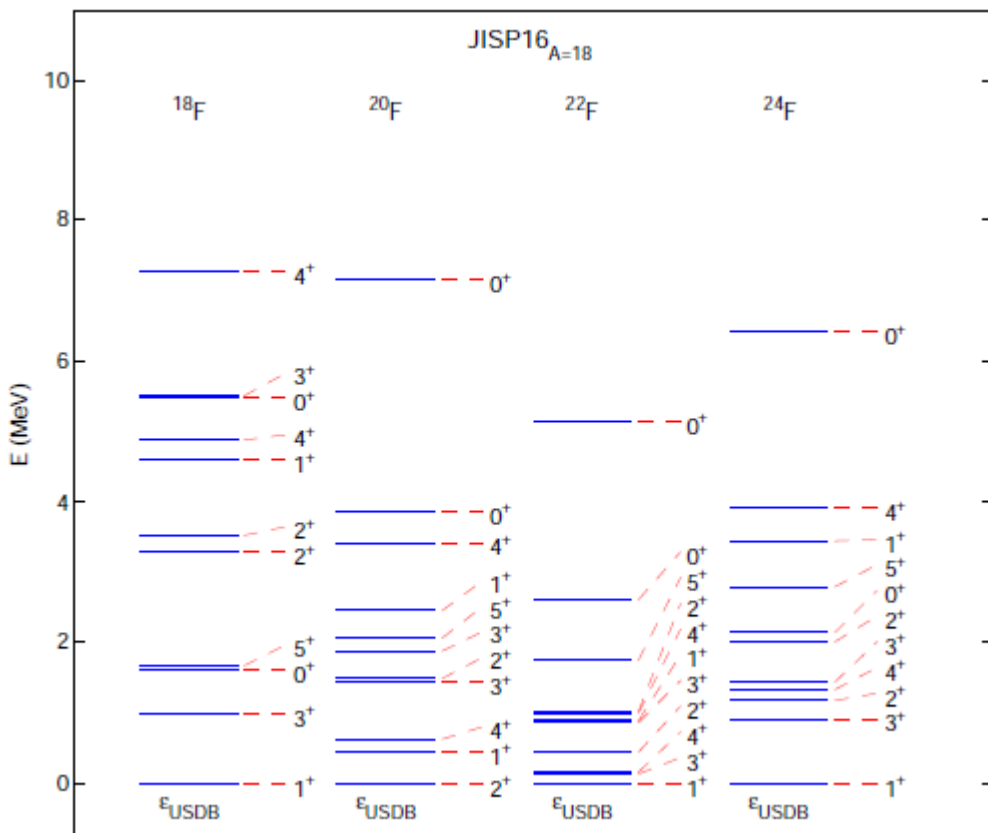
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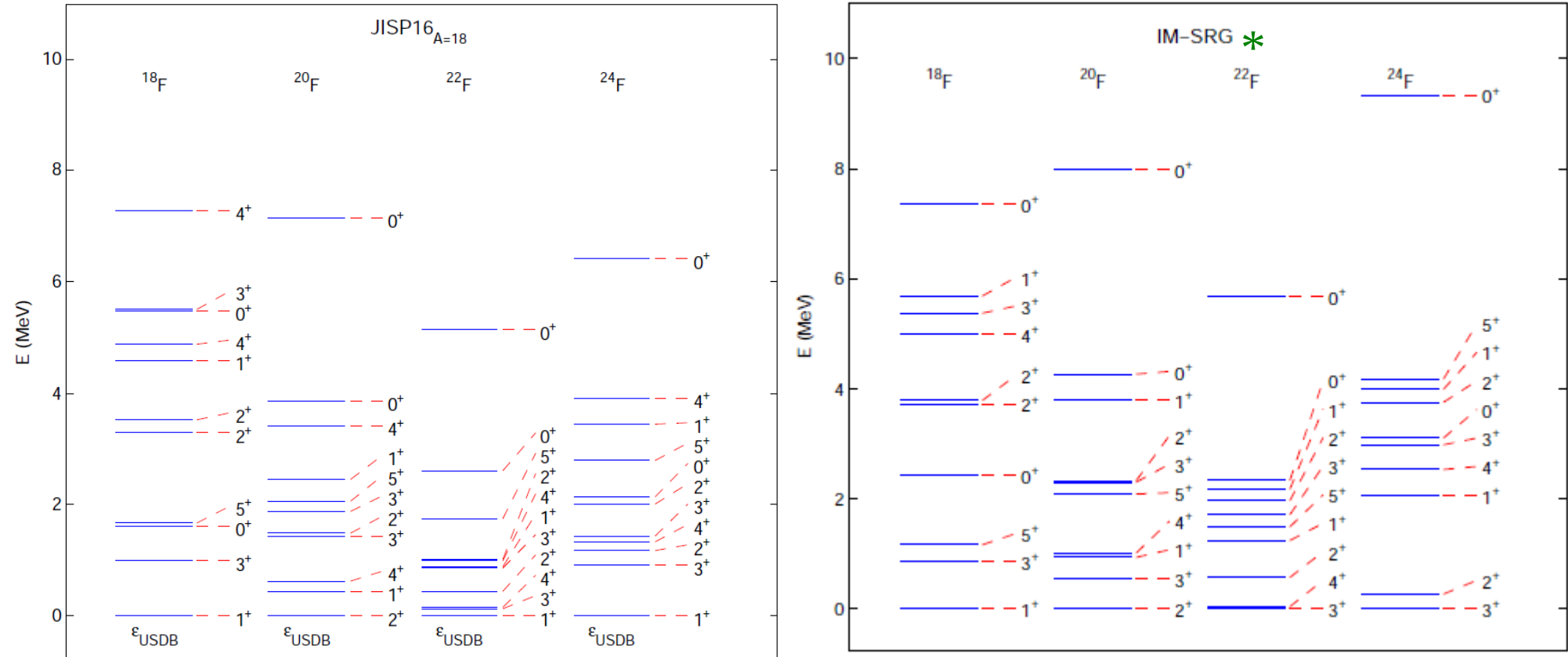
Preliminary Results



Preliminary Results

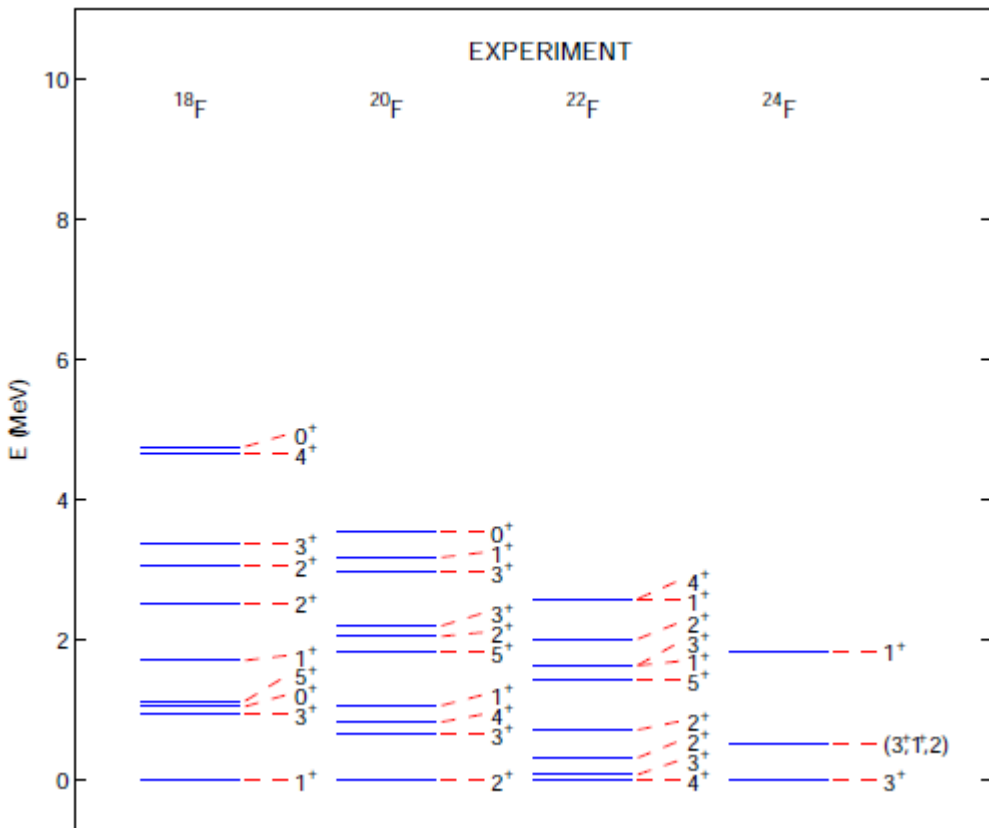
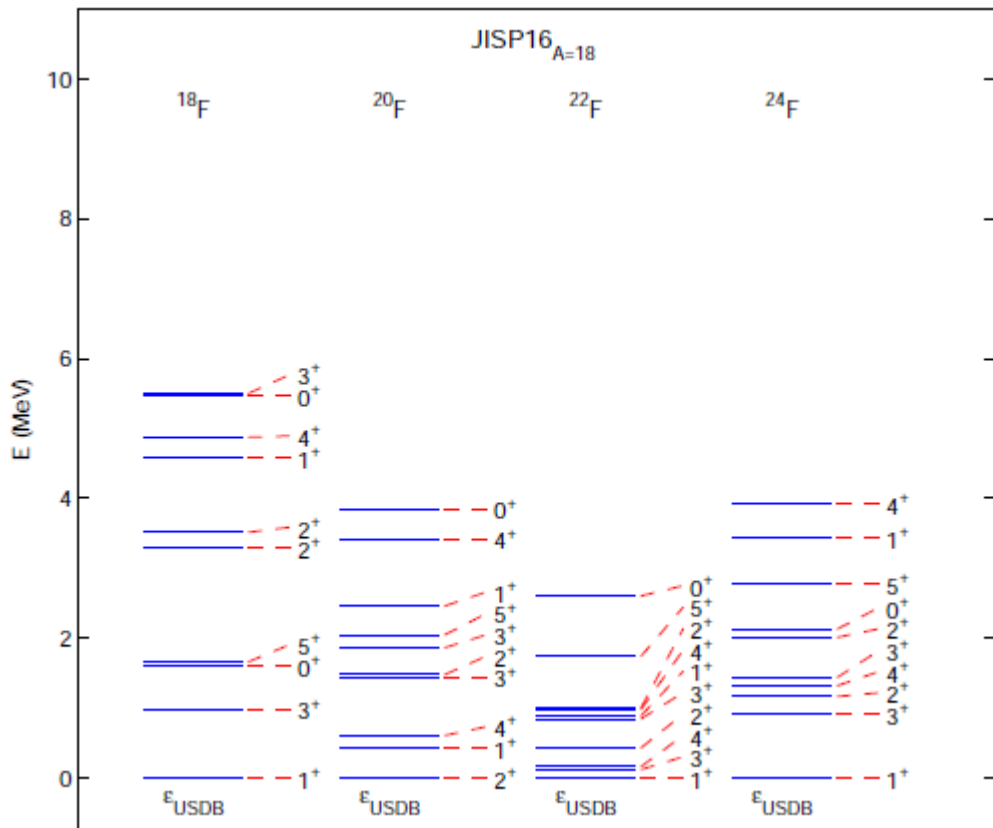


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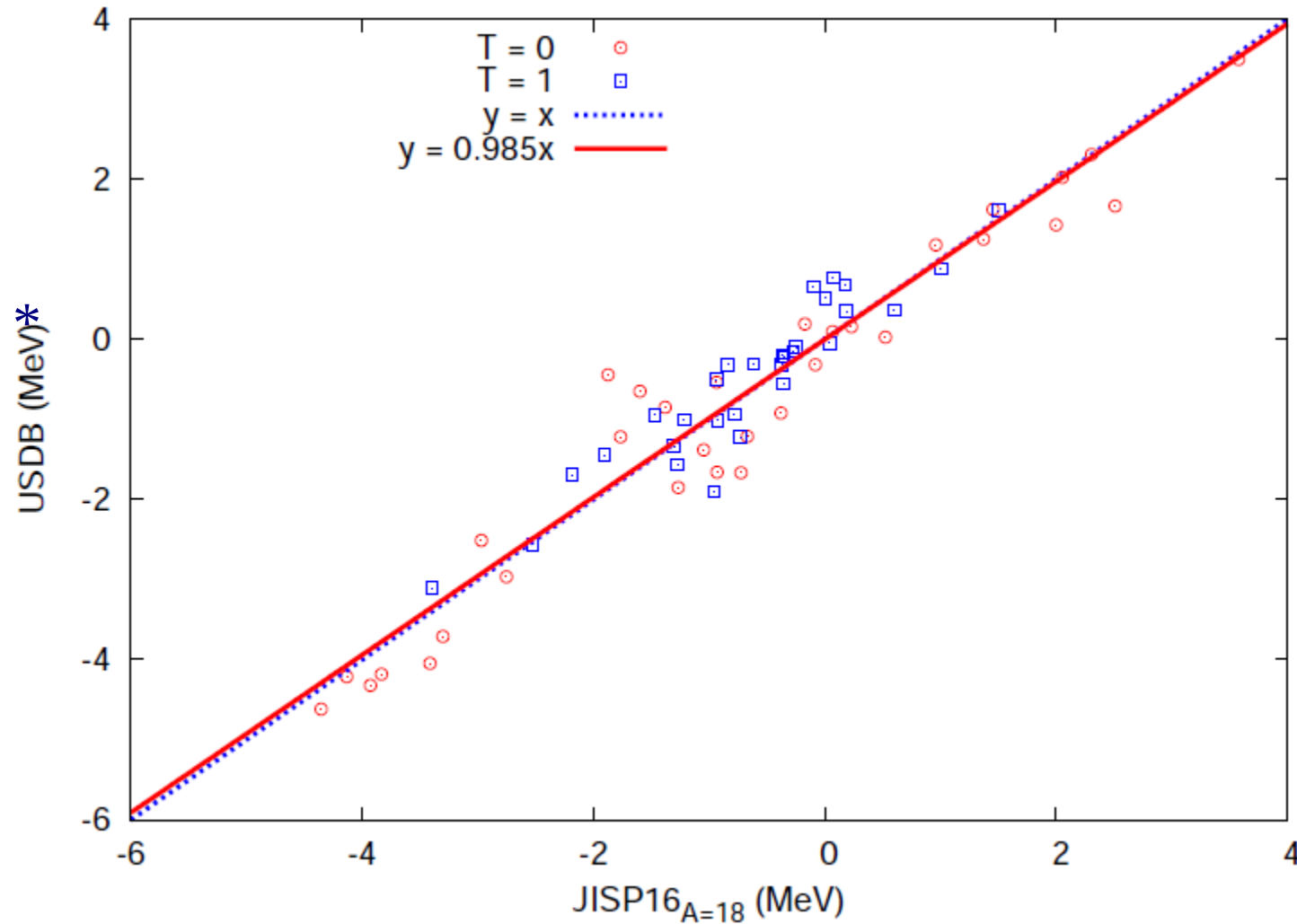


* S.R. Stroberg, et al., arXiv Nucl-th 1511.02802

Preliminary Results



Preliminary Results



RMS deviation of 471 keV

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

Towards a unified description of the nucleus

The goal of nuclear structure theory:

exact treatment of nuclei based on NN, NNN,... interactions

⇒ need to build a bridge between:

ab initio few-body & light nuclei calculations: $A \lesssim 24$

$0\hbar\Omega$ Shell Model calculations: $16 \leq A \leq 60$

Density Functional Theory calculations: $A \geq 60$

From few-body to many-body

Ab initio
No Core Shell Model

Flow chart for a standard
NCSM calculation

Realistic NN & NNN forces



**Effective interactions in
cluster approximation**



**Diagonalization of
many- body Hamiltonian**



Many-body experimental data

No Core Shell Model

“*Ab Initio*” approach to microscopic nuclear structure calculations, in which all A nucleons are treated as being active.

Want to solve the A-body Schrödinger equation

$$H_A \Psi^A = E_A \Psi^A$$

R P. Navrátil, J.P. Vary, B.R.B., PRC 62, 054311 (2000)
BRB, P. Navratil, J.P. Vary, Prog.Part.Nucl.Phys. 69, 131 (2013).
P. Navratil, et al., J. Phys. G: Nucl. Part. Phys. 36, 083101
(2009)

No-Core Shell-Model Approach

- Start with the purely intrinsic Hamiltonian

$$H_A = T_{rel} + \mathcal{V} = \frac{1}{A} \sum_{i < j=1}^A \frac{(\vec{p}_i - \vec{p}_j)^2}{2m} + \sum_{i < j=1}^A V_{NN} \left(+ \sum_{i < j < k}^A V_{ijk}^{3b} \right)$$

Note: There are no phenomenological s.p. energies!

Can use any
NN potentials

Coordinate space: Argonne V8', AV18
Nijmegen I, II

Momentum space: CD Bonn, EFT Idaho

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

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

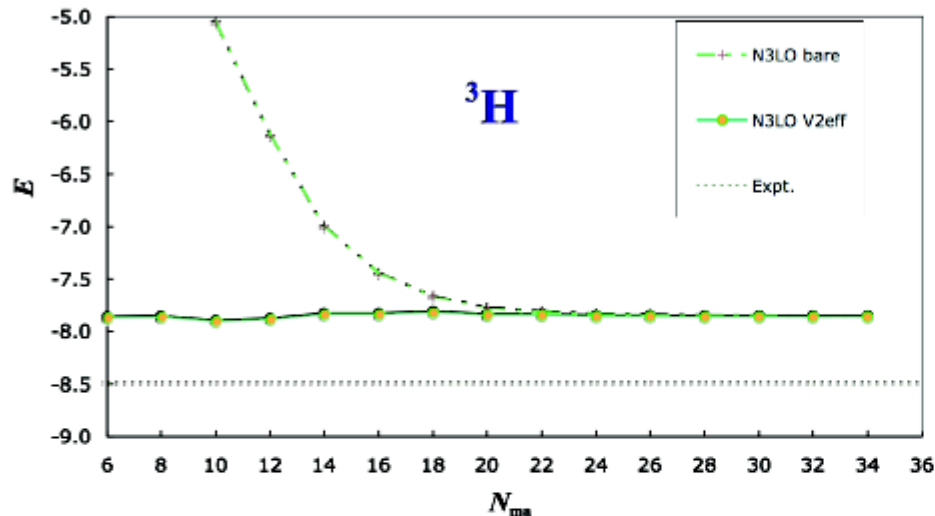
Defines a basis (i.e. **HO**) for evaluating V_{ij}

Effective Interaction

- Must truncate to a **finite** model space $V_{ij} \dashrightarrow V_{ij}^{\text{effective}}$
- In general, V_{ij}^{eff} is an **A**-body interaction
- We want to make an **a**-body cluster approximation

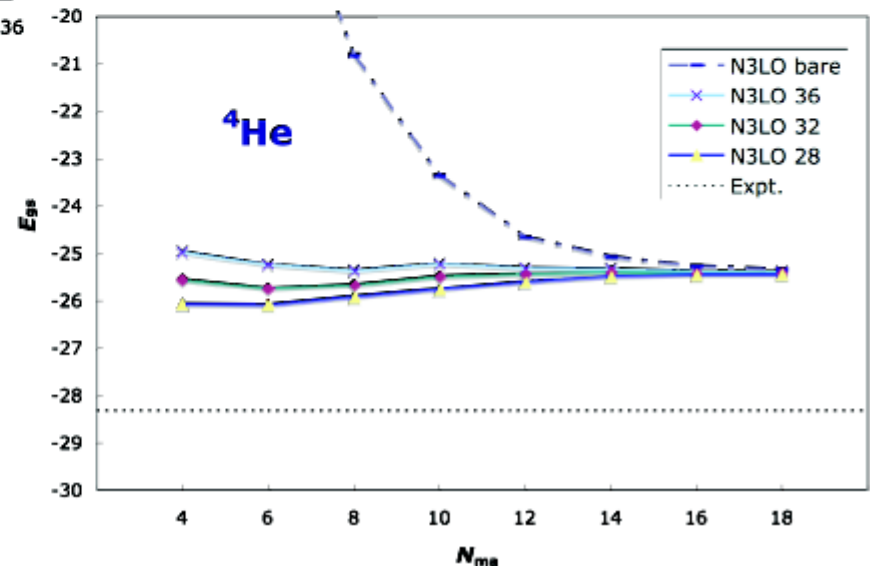
$$\mathcal{H} = \mathcal{H}^{(I)} + \mathcal{H}^{(A)} \underset{a < A}{\approx} \mathcal{H}^{(I)} + \mathcal{H}^{(a)}$$

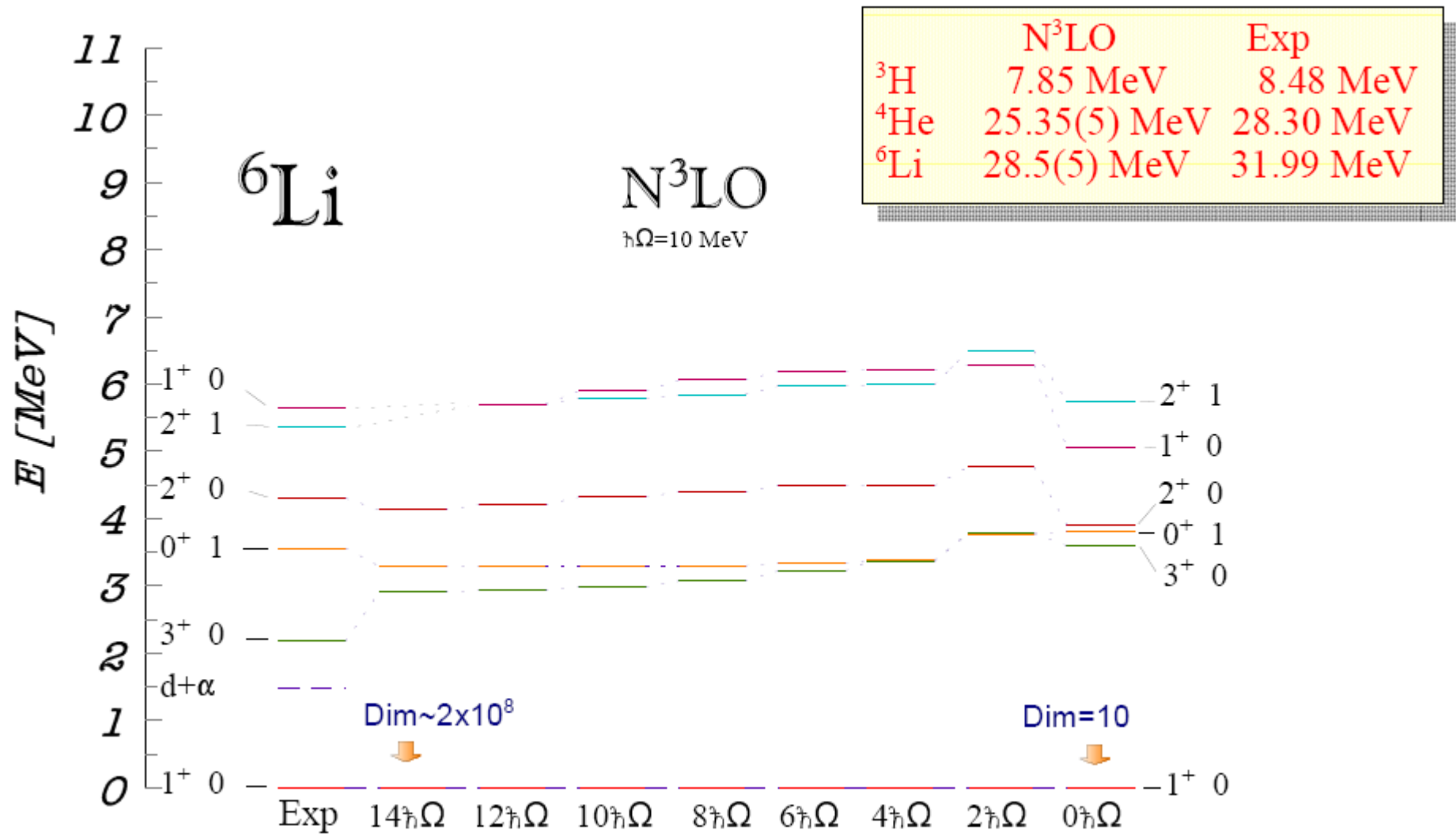
- NCSM convergence test
- Comparison to other methods



N ³ LO NN	NCSM	FY	HH
${}^3\text{H}$	7.852(5)	7.854	7.854
${}^4\text{He}$	25.39(1)	25.37	25.38

- Short-range correlations \Rightarrow effective interaction
- Medium-range correlations \Rightarrow multi- $\hbar\Omega$ model space
- Dependence on
 - size of the model space (N_{max})
 - HO frequency ($\hbar\Omega$)
- Not a variational calculation
- Convergence OK
- NN interaction insufficient to reproduce experiment





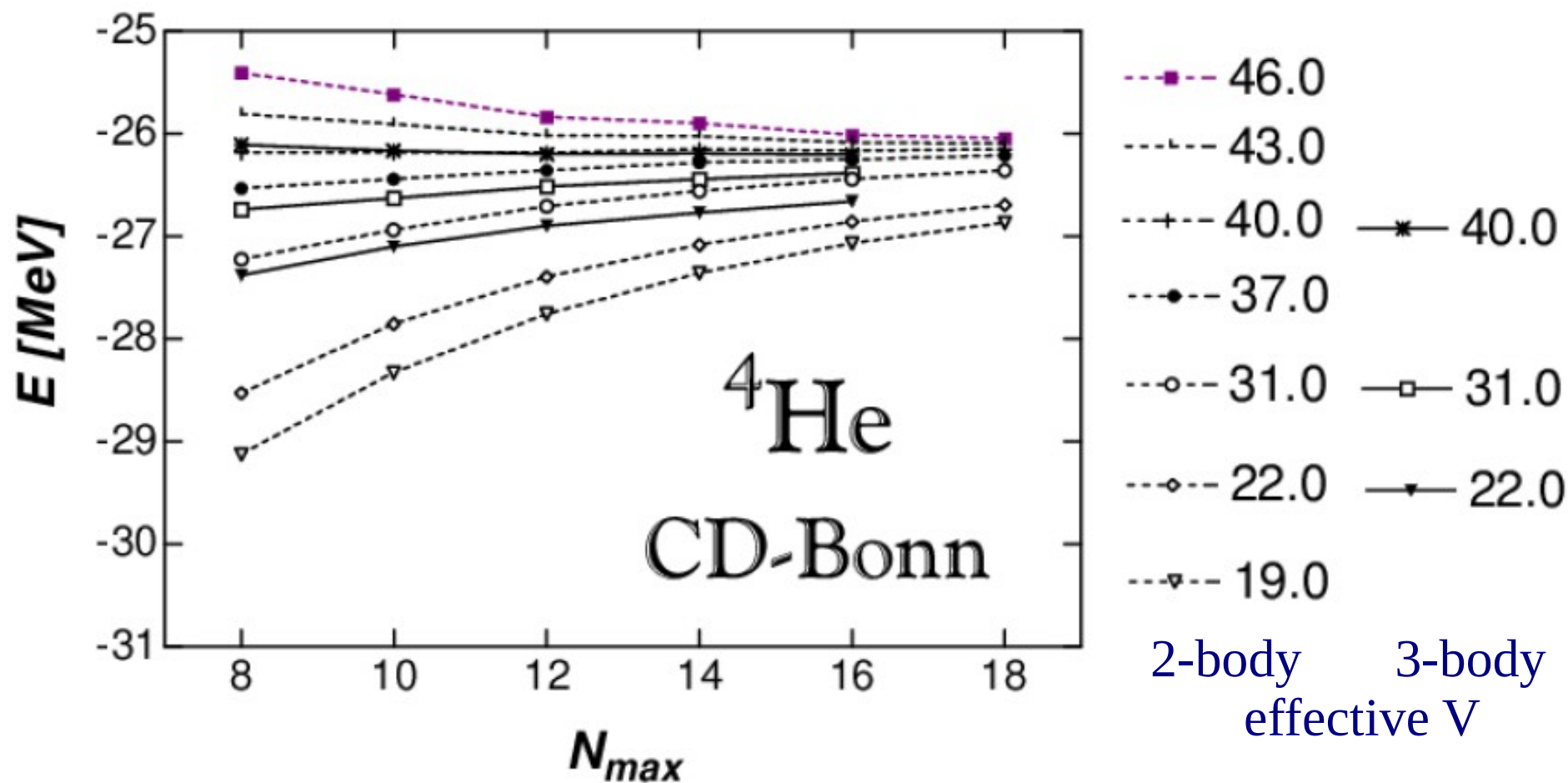
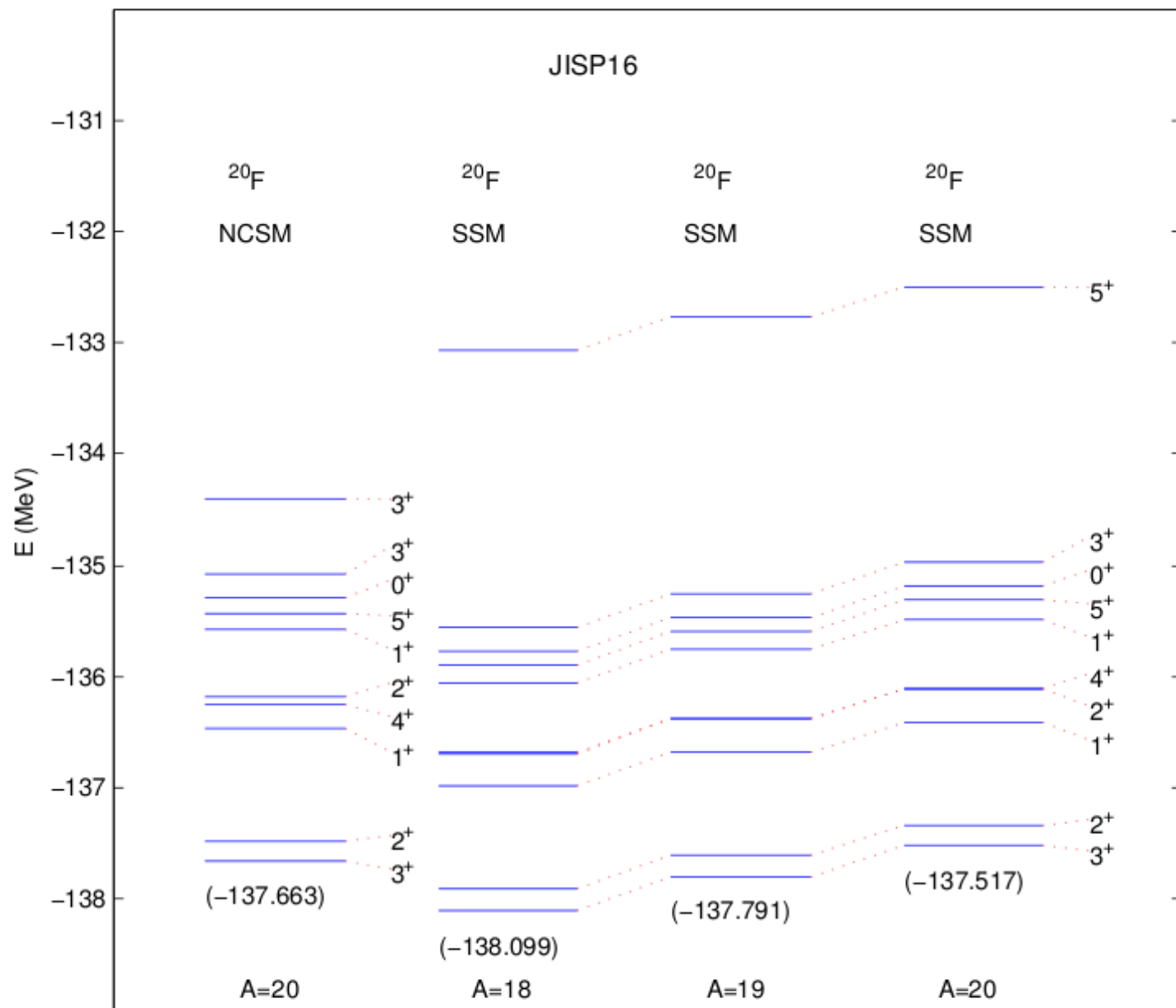


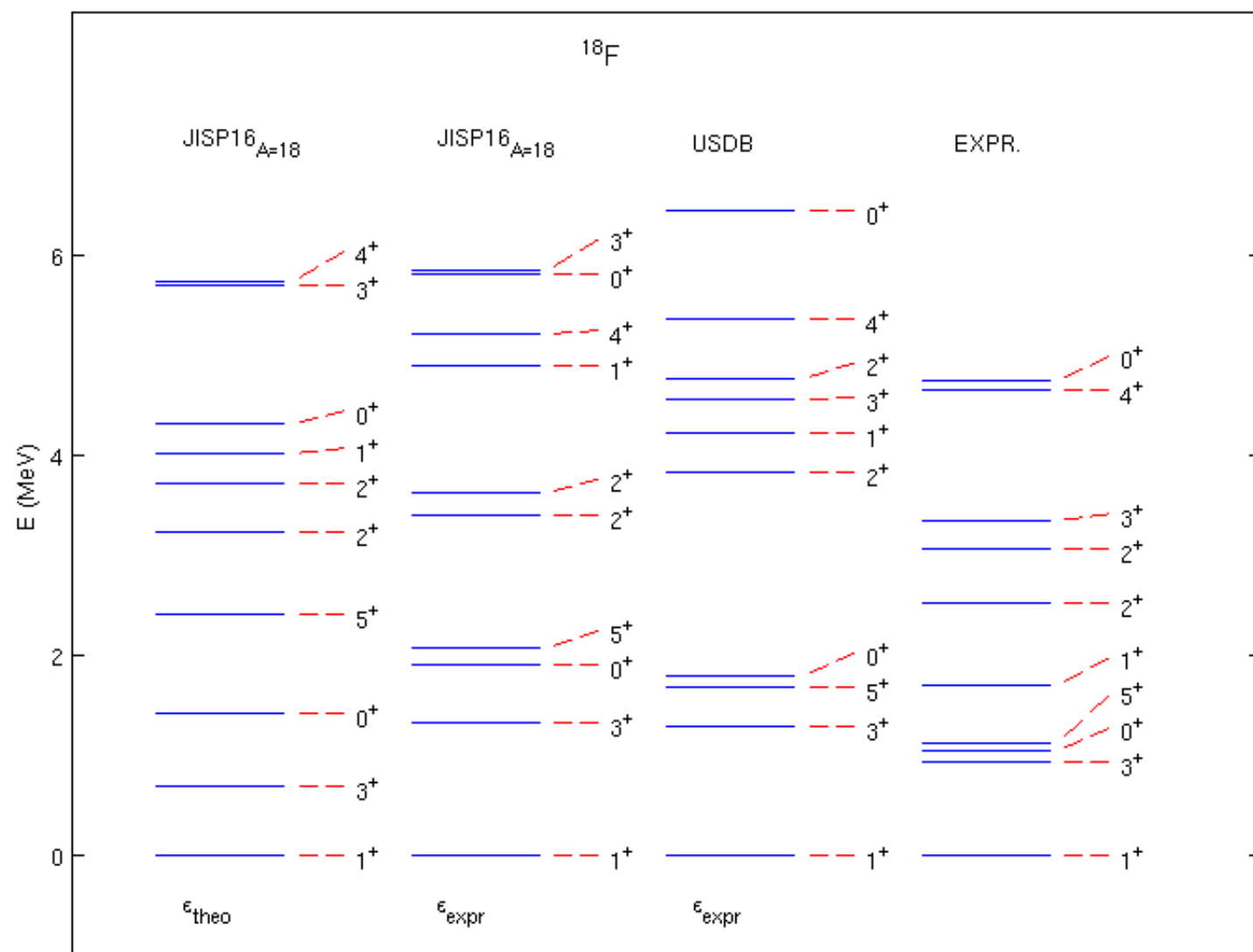
TABLE III: The NCSM energies (in MeV) of the lowest 28 states J_i^π of ^{18}F calculated in $4\hbar\Omega$ model space using JISP16 and chiral N3LO NN interactions with $\hbar\Omega = 14$ MeV.

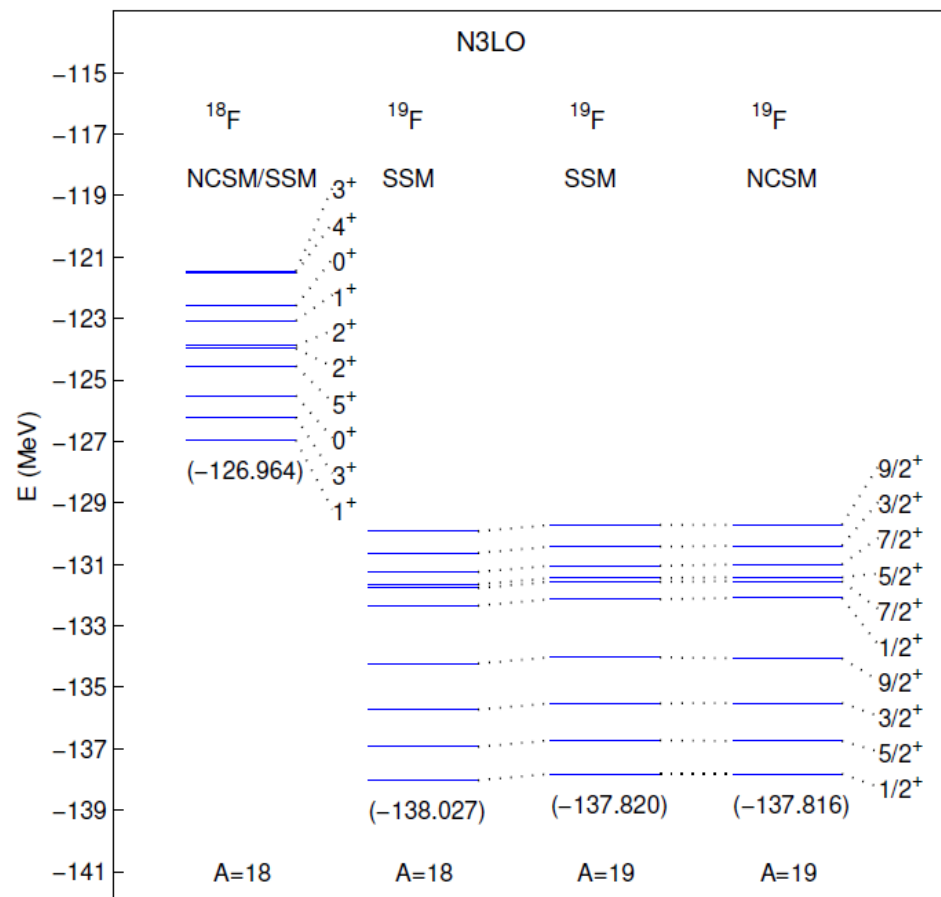
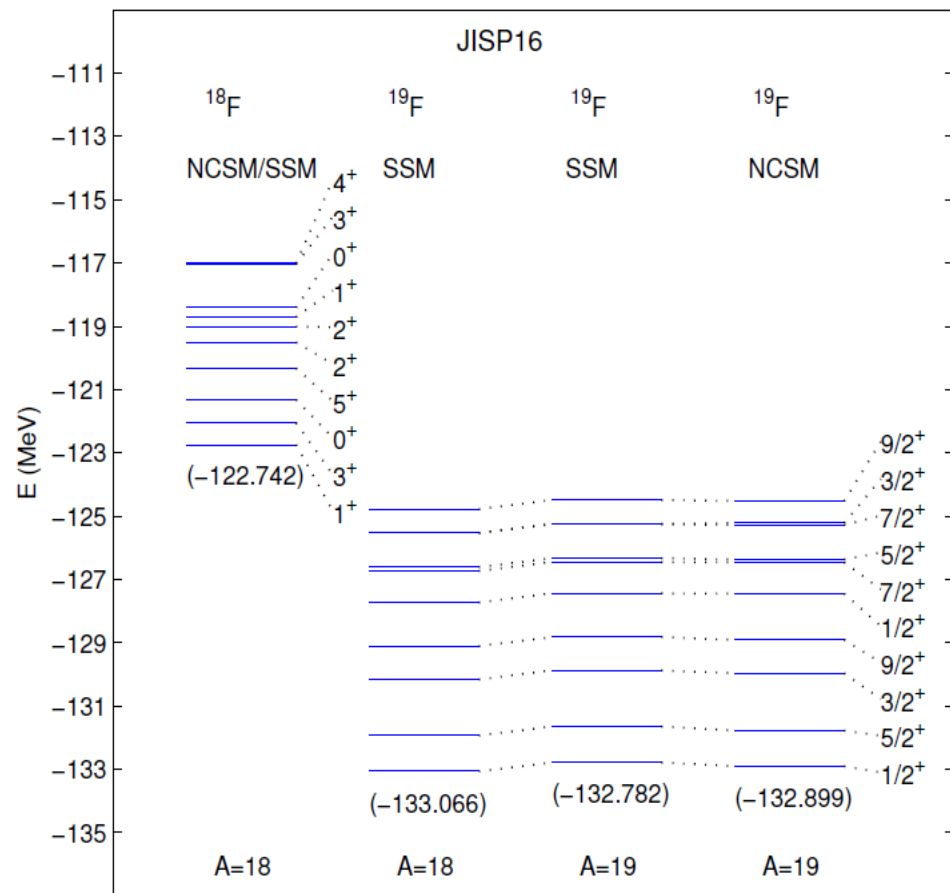
J_i^π	T	JISP16	J_i^π	T	N3LO
1_1^+	0	-122.742	1_1^+	0	-126.964
3_1^+	0	-122.055	3_1^+	0	-126.214
0_1^+	1	-121.320	0_1^+	1	-125.510
5_1^+	0	-120.329	5_1^+	0	-124.545
2_1^+	1	-119.505	2_1^+	1	-123.974
2_2^+	0	-119.011	2_2^+	0	-123.890
1_2^+	0	-118.709	1_2^+	0	-123.077
0_2^+	1	-118.410	0_2^+	1	-122.586
2_3^+	1	-117.211	2_3^+	1	-121.588
3_2^+	1	-117.035	4_1^+	1	-121.512
4_1^+	1	-117.004	3_2^+	1	-121.450
3_3^+	0	-116.765	3_3^+	0	-121.376
1_3^+	0	-113.565	1_3^+	0	-119.658
4_2^+	0	-112.314	4_2^+	0	-118.656
2_4^+	0	-111.899	2_4^+	0	-117.950
1_4^+	0	-110.357	1_4^+	0	-116.106
4_3^+	1	-109.625	4_3^+	1	-115.785
2_5^+	1	-109.292	2_5^+	1	-115.407
1_5^+	1	-108.752	3_4^+	0	-115.309
3_4^+	0	-108.706	1_5^+	1	-114.870
2_6^+	0	-108.485	2_6^+	0	-114.787
1_6^+	1	-108.055	1_6^+	1	-114.392
2_7^+	1	-108.041	3_5^+	1	-114.258
3_5^+	1	-107.874	2_7^+	1	-114.176
3_6^+	0	-101.528	3_6^+	0	-109.316
1_7^+	0	-99.946	1_7^+	0	-107.798
0_3^+	1	-99.848	2_8^+	1	-107.473
2_8^+	1	-99.607	0_3^+	1	-107.436

PRELIMINARY RESULTS



Preliminary Results





Two-body VCE for ${}^6\text{Li}$

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

Need NCSM results
in N_{\max} space for

${}^4\text{He}$

${}^5\text{He}$ ${}^5\text{Li}$

${}^6\text{He}$ ${}^6\text{Li}$ ${}^6\text{Be}$

With effective interaction for $A=6$!!!

$$H_{A=6,2}^{N_{\max}, \Omega, \text{eff}}$$

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

${}^4\text{He}$

${}^5\text{He}$ ${}^5\text{Li}$

${}^6\text{He}$ ${}^6\text{Li}$ ${}^6\text{Be}$

${}^7\text{He}$ ${}^7\text{Li}$ ${}^7\text{B}$ ${}^7\text{Be}$

With effective interaction for A !!!

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




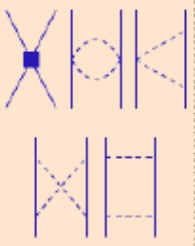


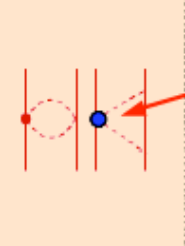
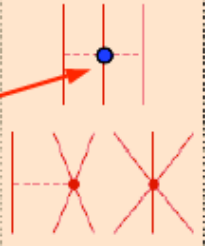


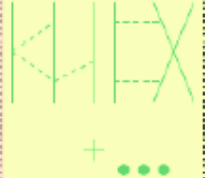

Construct 3-body interaction in terms of 3-body matrix elements: **Yes**

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



Chiral effective field theory (EFT) for nuclear forces

Separation of scales: low momenta $\frac{1}{\lambda} = Q \ll \Lambda_b$ breakdown scale Λ_b

	NN	3N	4N
LO $\mathcal{O}\left(\frac{Q^0}{\Lambda^0}\right)$			
NLO $\mathcal{O}\left(\frac{Q^2}{\Lambda^2}\right)$			
N ² LO $\mathcal{O}\left(\frac{Q^3}{\Lambda^3}\right)$			
N ³ LO $\mathcal{O}\left(\frac{Q^4}{\Lambda^4}\right)$			

explains pheno hierarchy:

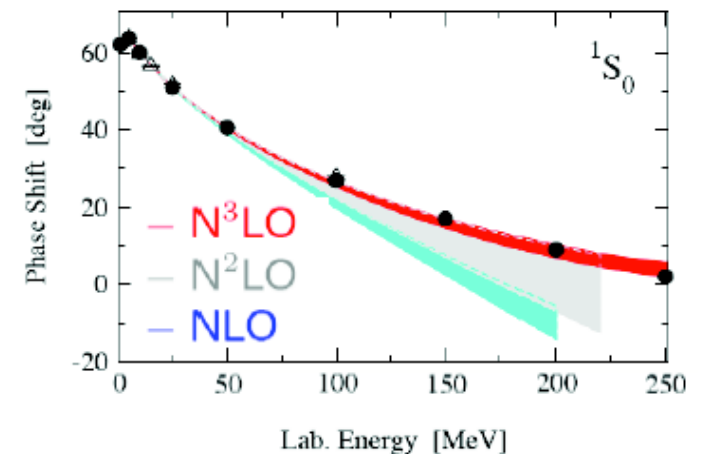
NN > 3N > 4N > ...

NN-3N, πN , $\pi\pi$, electro-weak, ...

consistency

3N, 4N: 2 new couplings to N³LO!

theoretical error estimates



Weinberg, van Kolck, Kaplan, Savage, Wise, Epelbaum, Meissner, Nogga, Machleidt, ... A. Schwenk