Fluorine isotope systematics: *ab initio* vs phenomenological analyses

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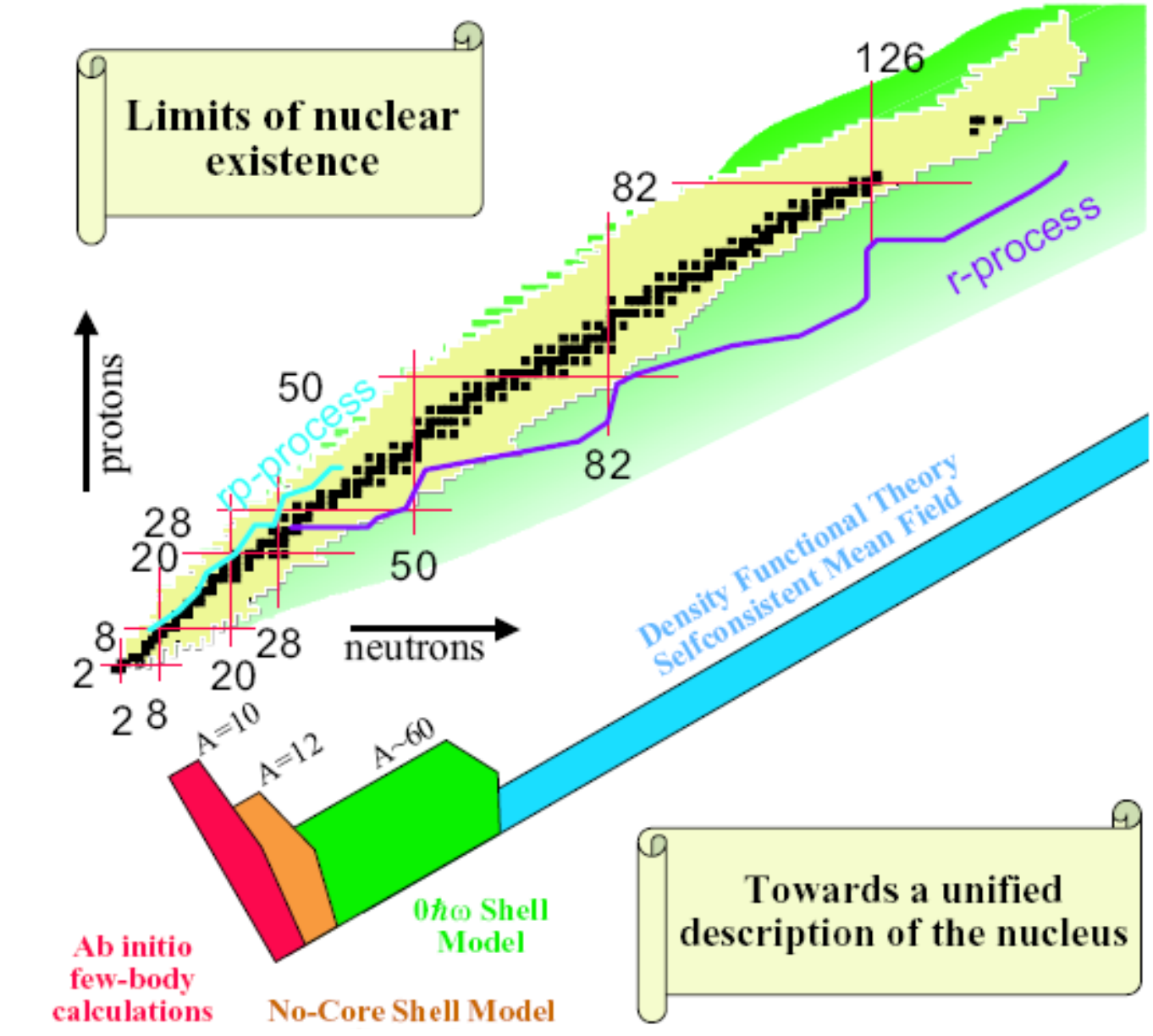
Limits of nuclear existence
126
82
82
50
50
28
20
8
2
2 8
28
20
protons
neutrons
rp-process
r-process
Density Functional Theory
Selfconsistent Mean Field
A=10
A=12
A~60
0ħω Shell Model
Towards a unified description of the nucleus
Ab initio few-body calculations
GFMC formalism
No-Core Shell Model
Coupled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

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

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)

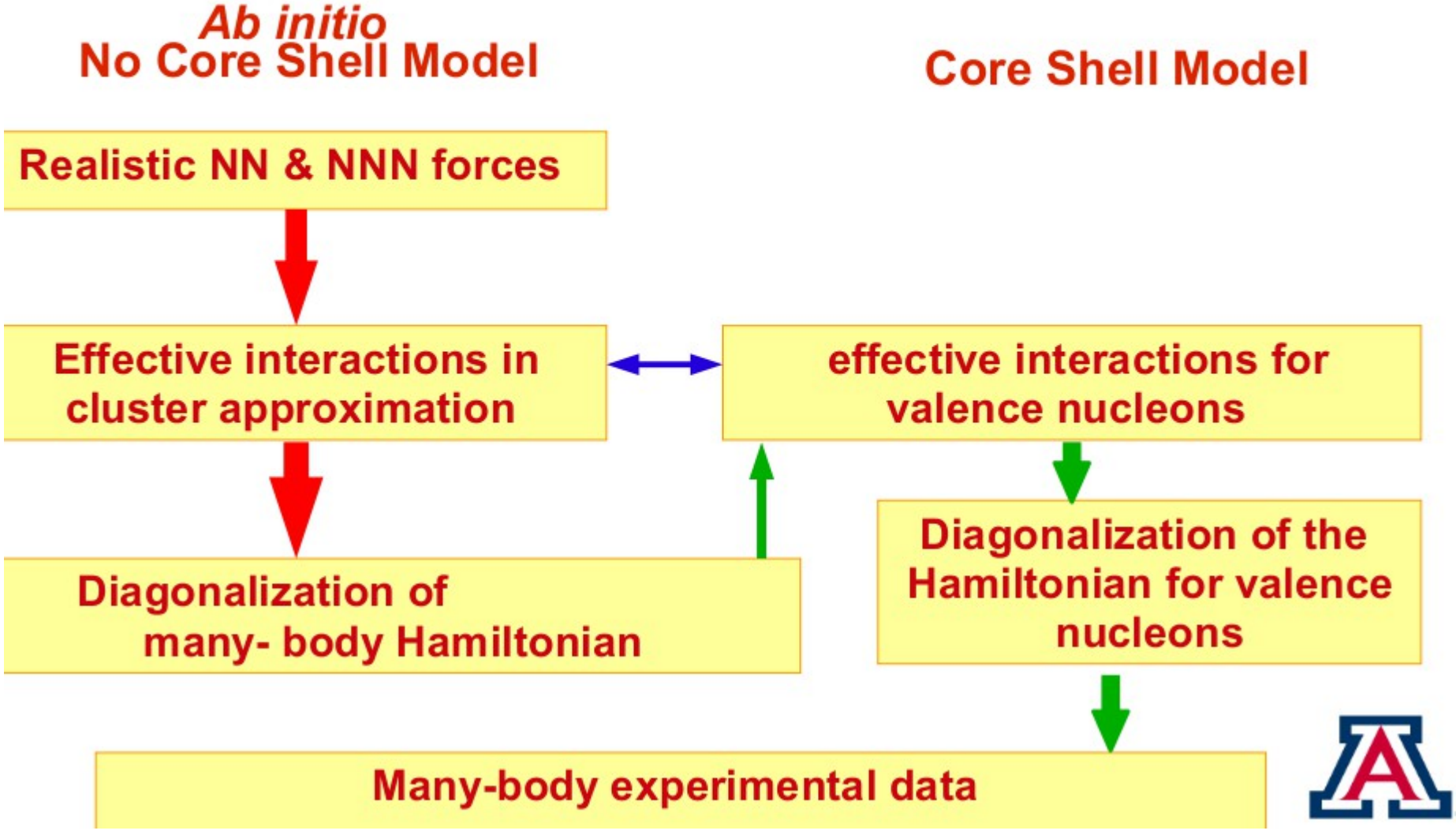
We construct effective two- and three-body Hamiltonians for the p-shell by performing $12\hbar\Omega$ *ab initio* no-core shell model (NCSM) calculations for $A = 6$ and 7 nuclei and explicitly projecting the many-body Hamiltonians onto the $0\hbar\Omega$ space. We then separate these effective Hamiltonians 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)

From few-body to many-body

Using the NCSM to calculate the shell model input



Effective interaction in a projected model space

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

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

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

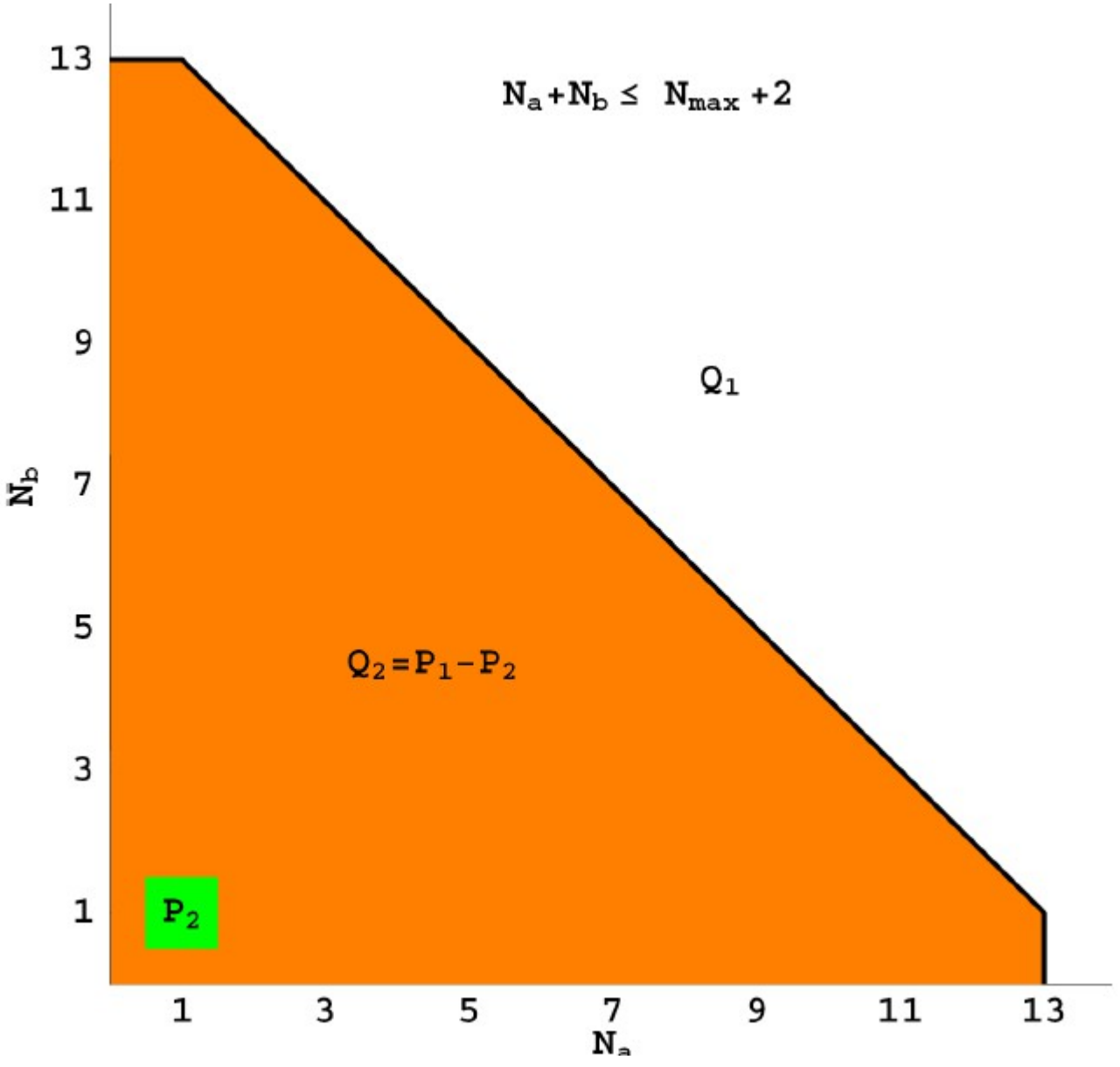
P is a projection operator from S into $\mathcal{S}$

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

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

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.


$N_a+N_b \leq N_{max}+2$
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

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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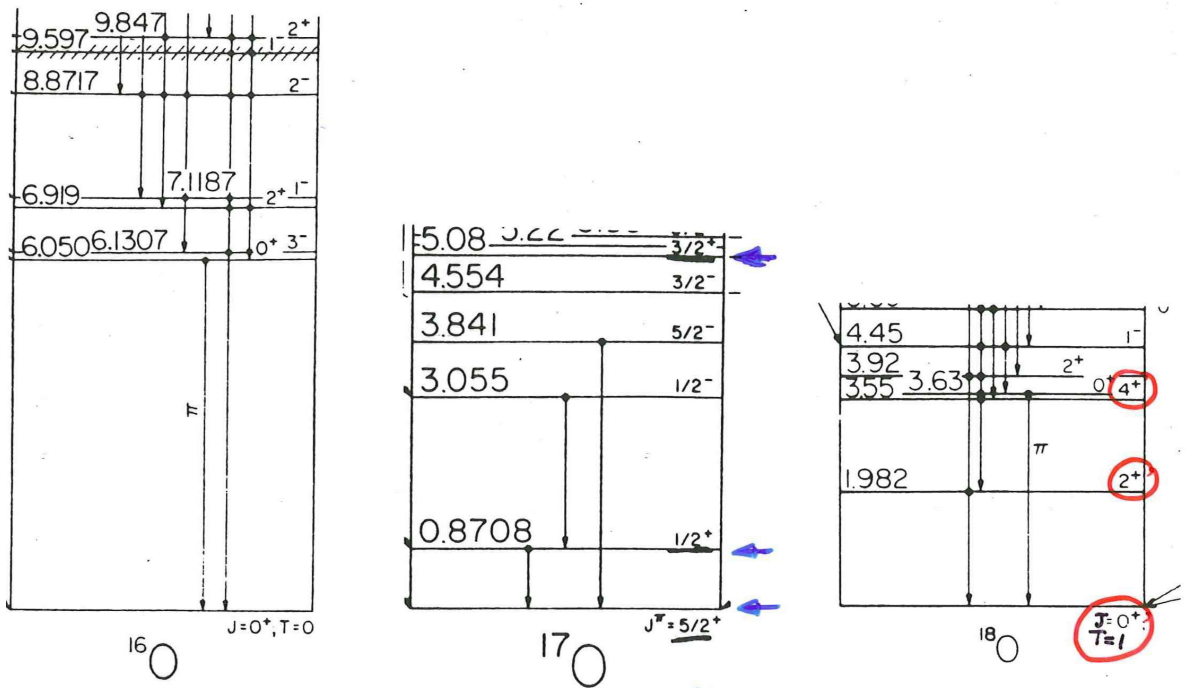
(Dated: February 3, 2015)

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

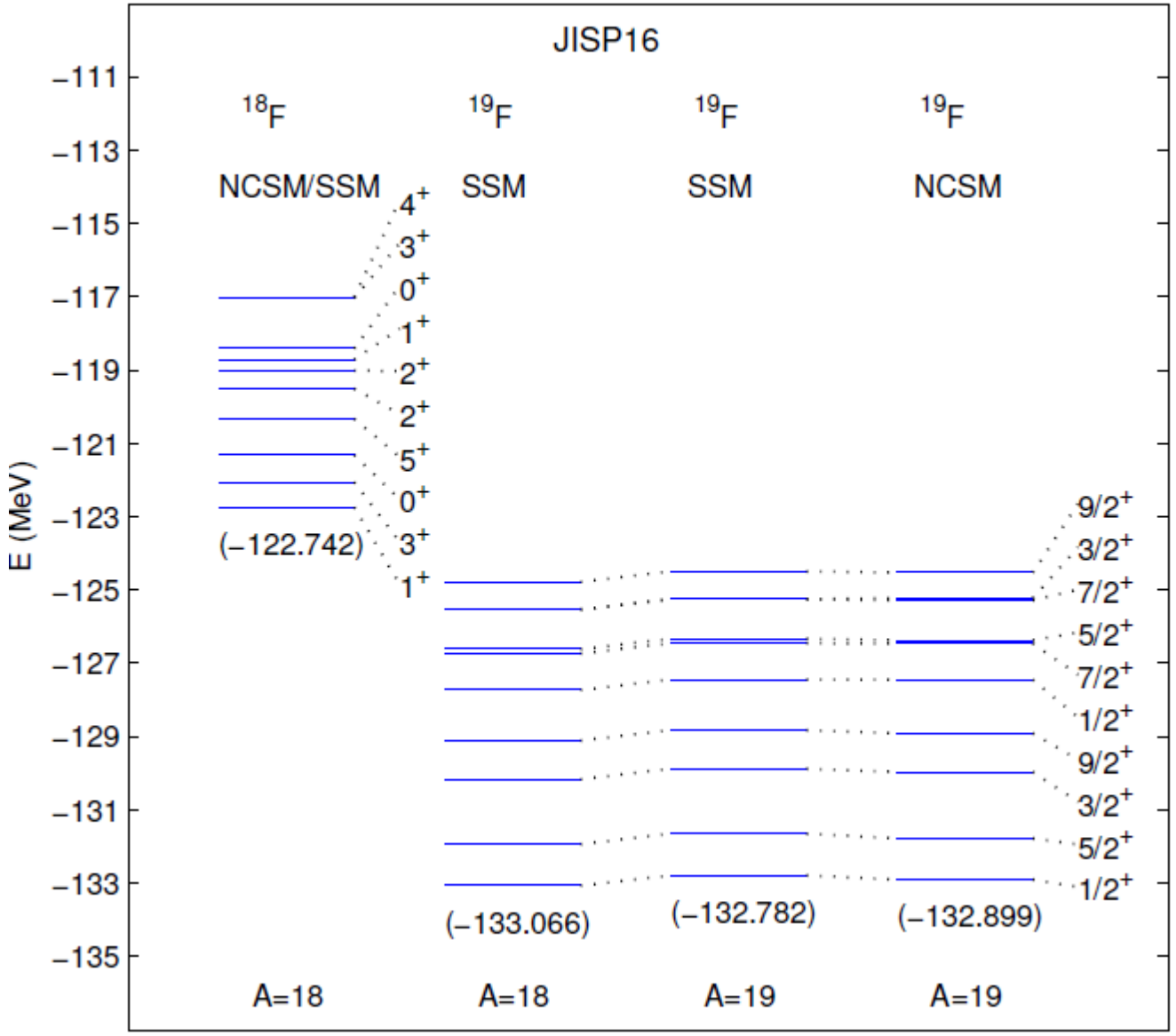
- Next, add CM harmonic-oscillator Hamiltonian

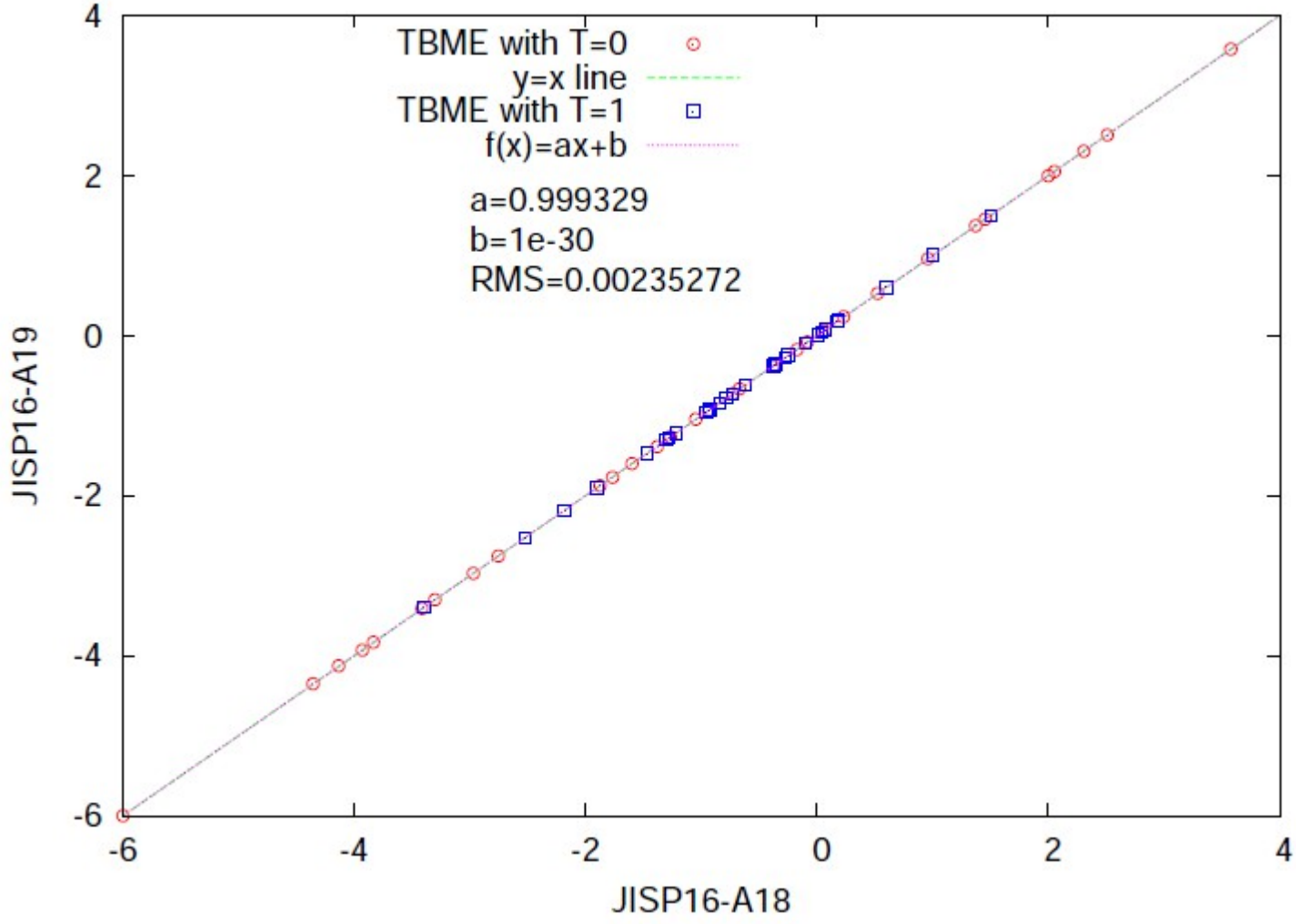
$$H_{CM}^{HO} = \frac{\vec{P}^{\,2}}{2Am} + \frac{1}{2}Am\Omega^2\vec{R}^{\,2}; \quad \vec{R} = \frac{1}{A}\sum_{i=1}^{A}\vec{r}_i\,, \quad \vec{P} = Am\dot{\vec{R}}$$

To H_A, yielding

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

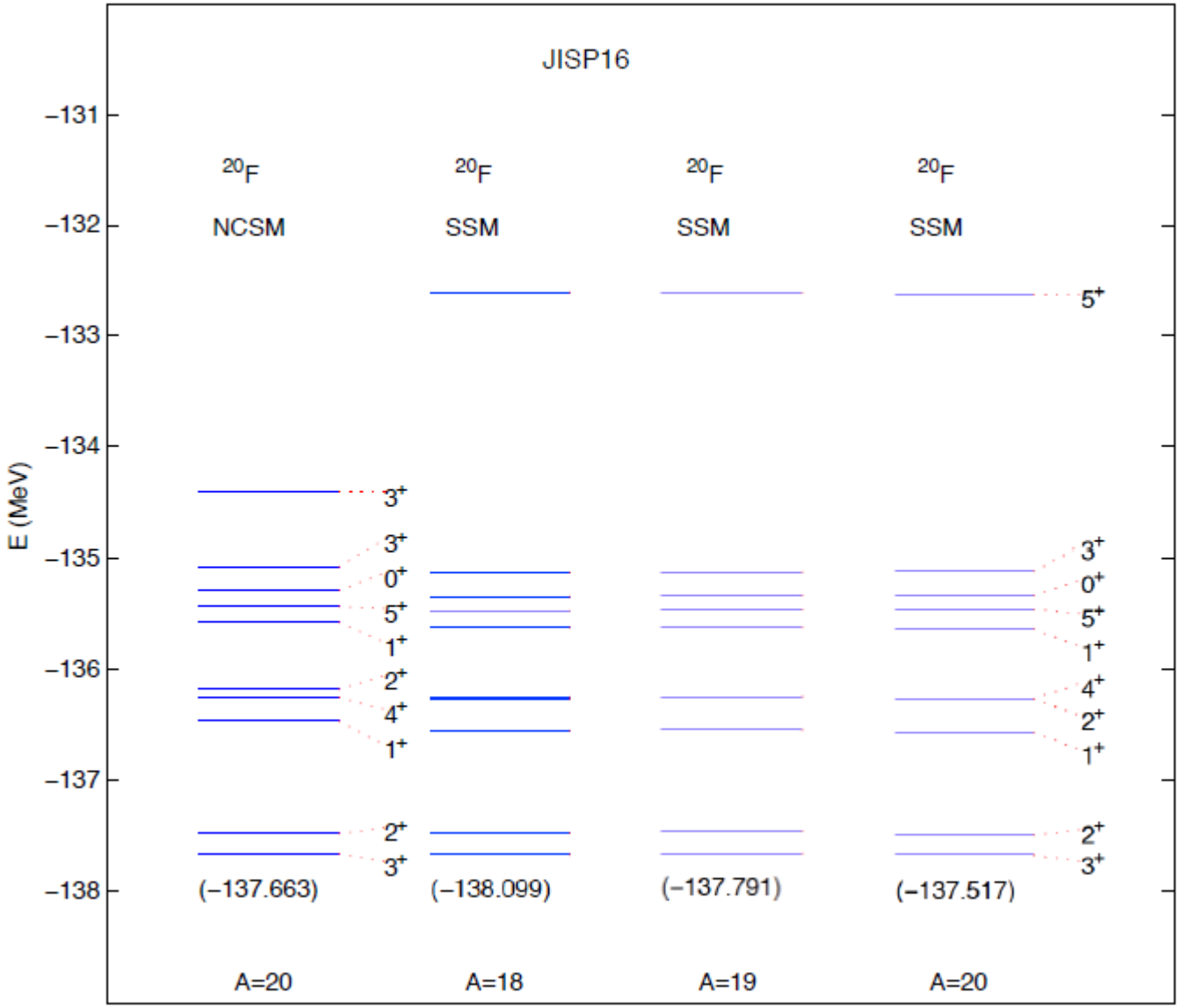
Defines a basis (*i.e.* HO) for evaluating V_{ij}


JISP16
^{18}F
^{19}F
^{19}F
^{19}F
NCSM/SSM
SSM
SSM
NCSM
E (MeV)
−111
−113
−115
−117
−119
−121
−123
−125
−127
−129
−131
−133
−135
4+
3+
0+
1+
2+
2+
5+
0+
3+
1+
(−122.742)
(−133.066)
(−132.782)
(−132.899)
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 Results

Preliminary Results



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 JISP16 NN interaction, to test how well they reproduce data trends.
2. Assume that the effects of 3NFs can be approximated by replacing the theoretical single-particle energies with the empirical ones used by Brown & Richter* for their USDB effective interaction.
3. Compare our results for 18,20,22,24 F with those obtained with the USDB effective interaction and with those obtained with the IM-SRG approach** using an EFT N3LO NN plus N2LO NNN interaction.

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

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

Preliminary Results

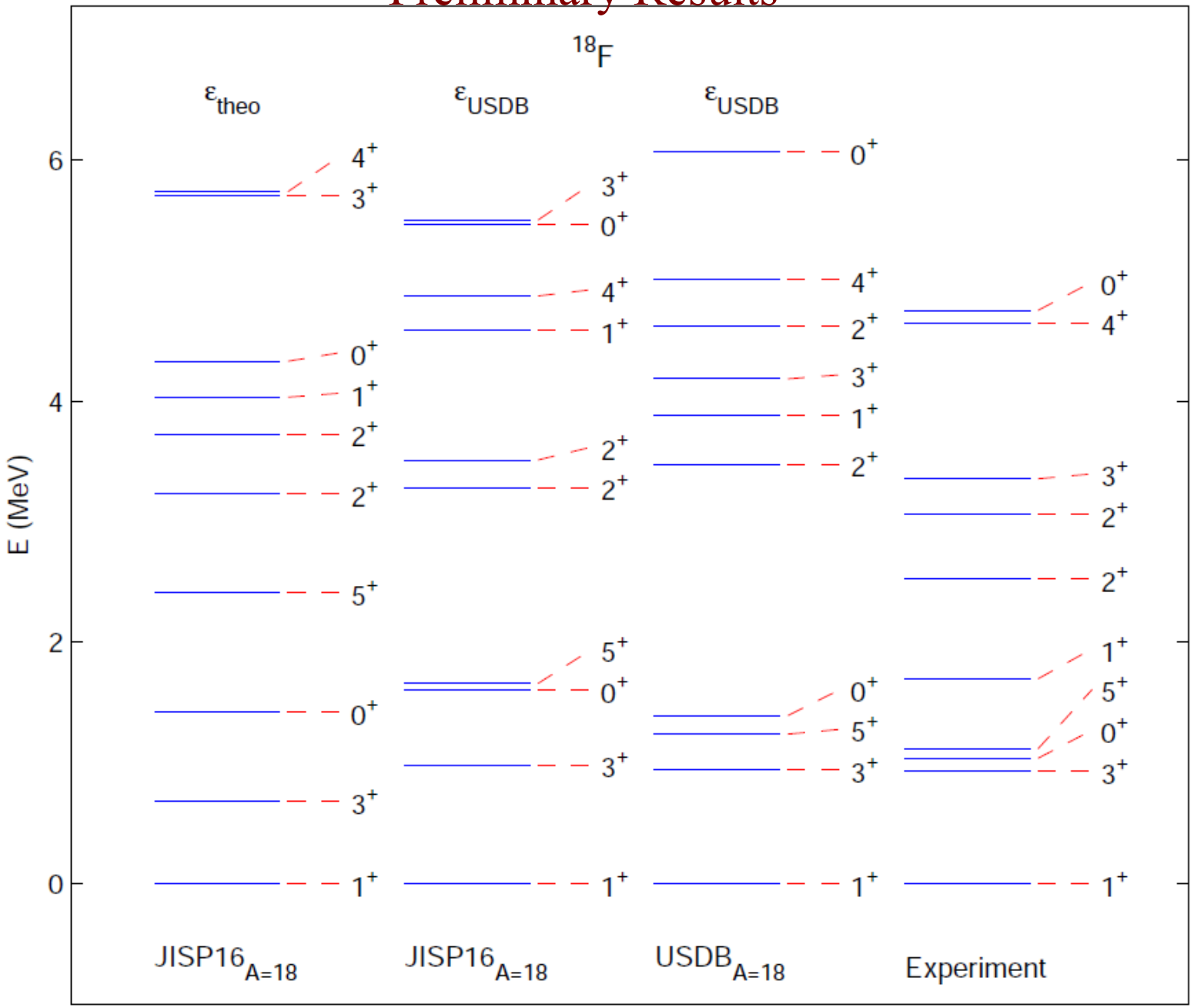
TABLE I: The single-particle energies (in MeV) used in the standard shell model calculations of F isotopes. (n) and (p) represent neutron and proton, respectively.

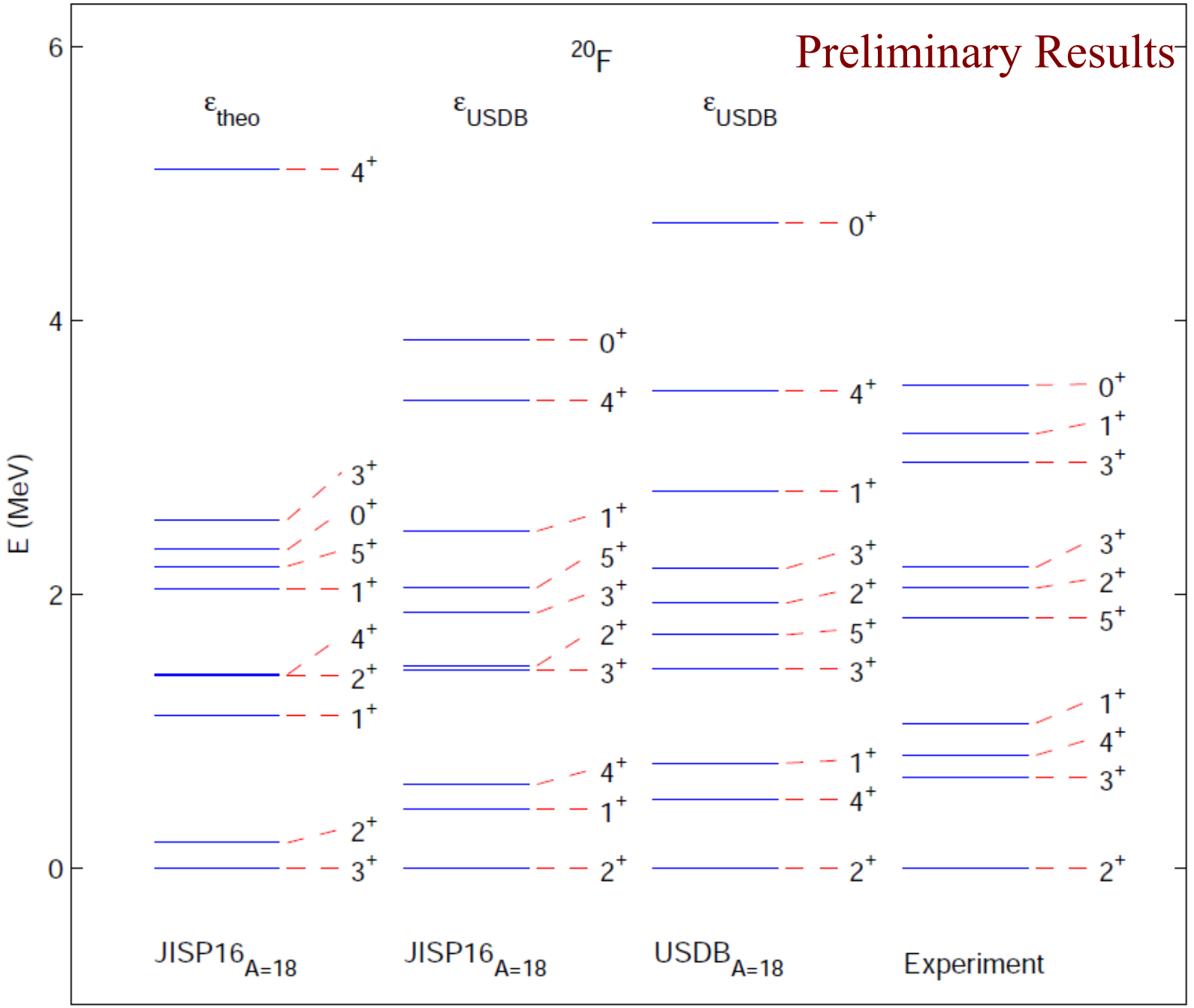
j_i	$\frac{1}{2}$	$\frac{5}{2}$	$\frac{3}{2}$	
JISP16$_{A=18}$ (^{17}O) : (n)	-3.068	-2.270	6.262	
JISP16$_{A=18}$ (^{17}F) : (p)	0.603	1.398	9.748	
USDA	-3.0612	-3.9436	1.9798	*
USDB	-3.2079	-3.9257	2.1117	*
IM-SRG (^{17}O) : (n)	-3.089	-4.643	2.940	**
IM-SRG (^{17}F) : (p)	0.255	-0.909	6.035	**

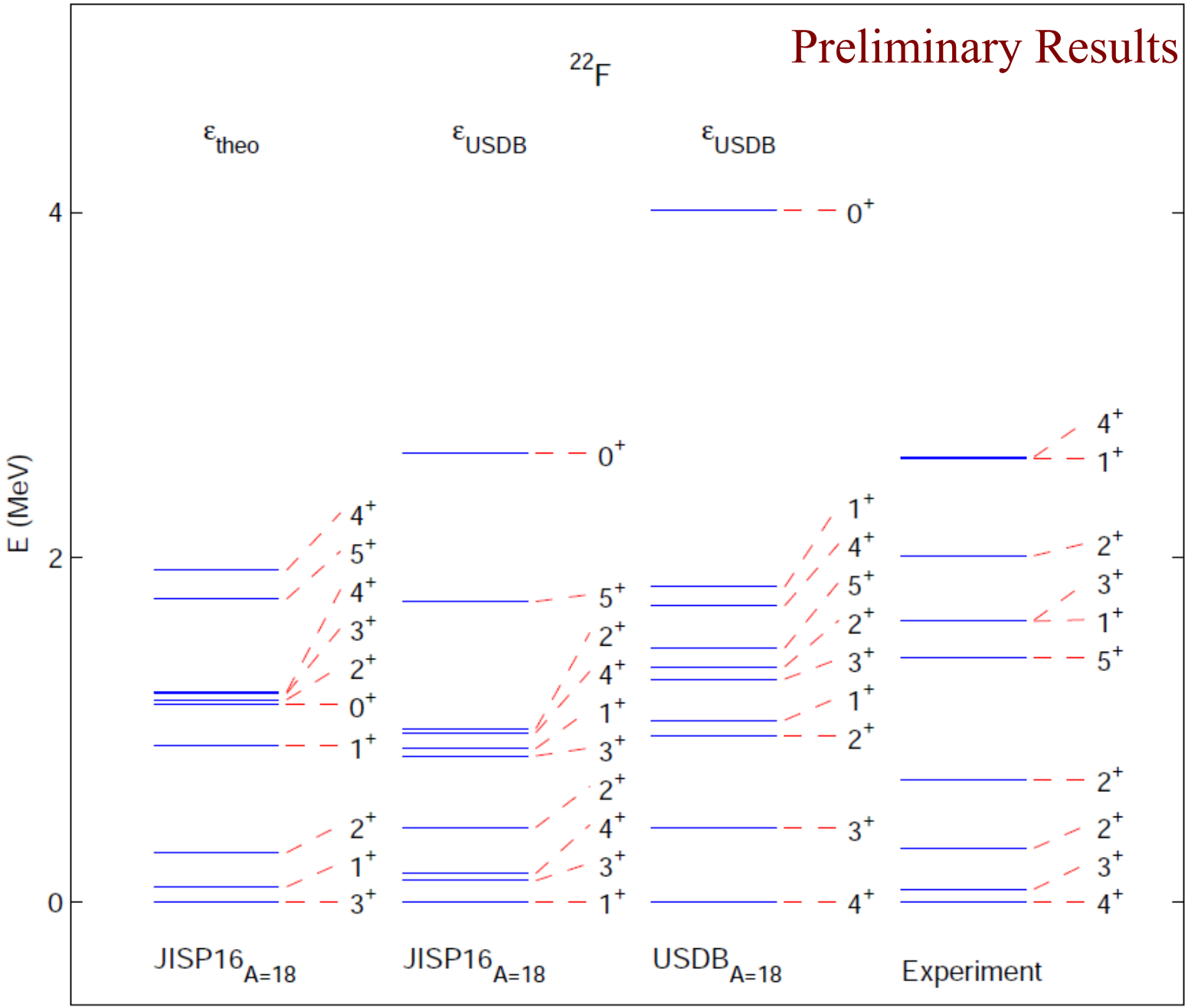
* B.A. Brown & W.A. Richter, PRC 74, 034315 (2006)

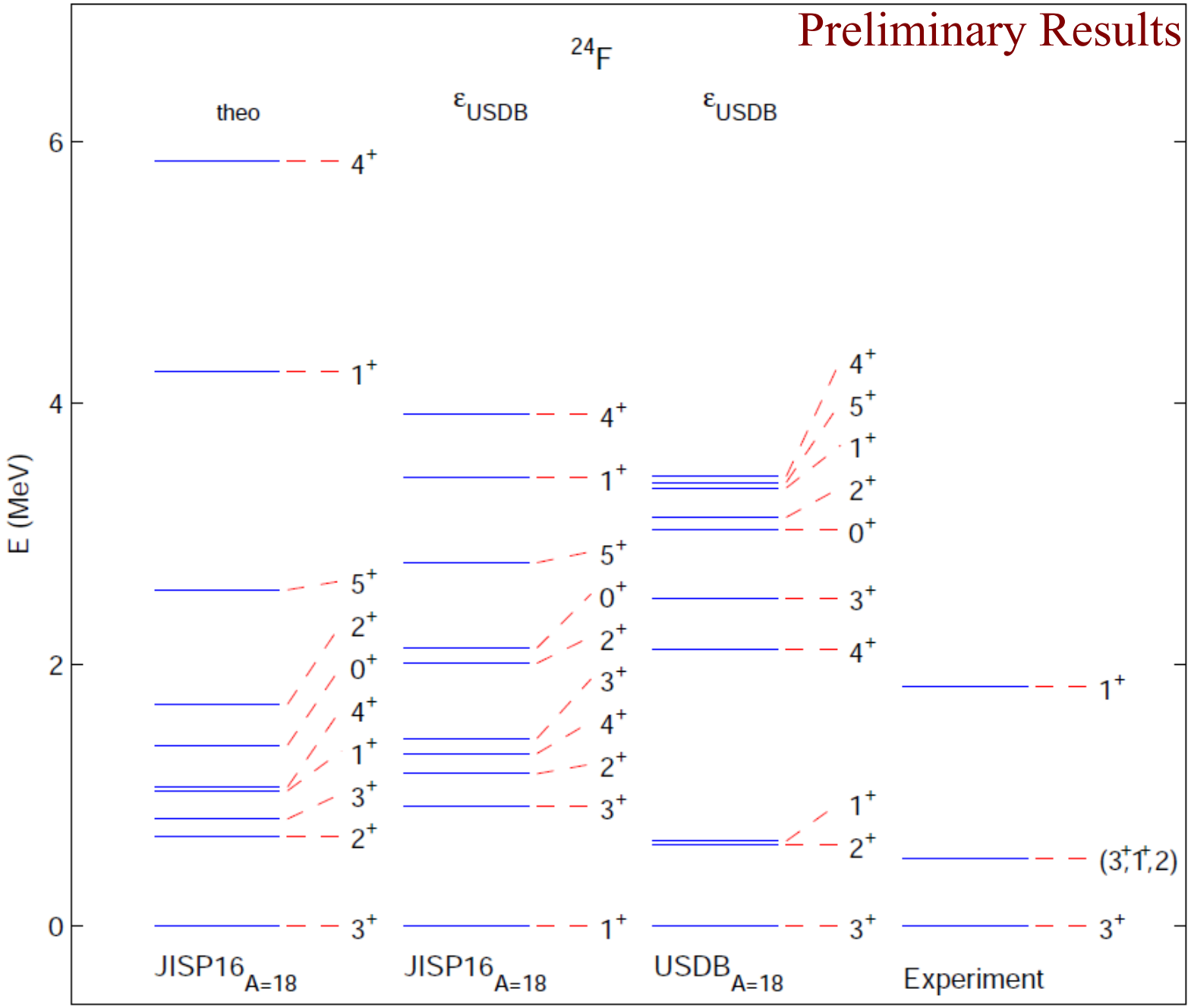
** S.R. Stroberg, et al., arXiv Nucl-th 1511.02802 (2015)

Preliminary Results

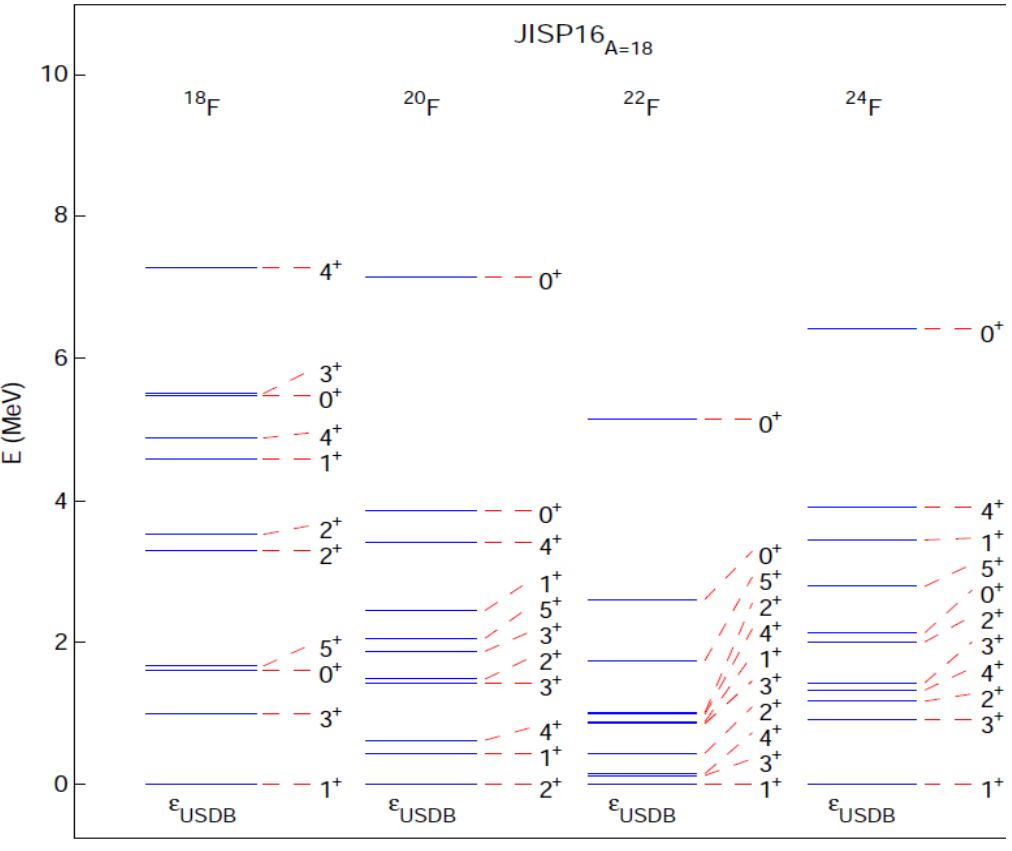


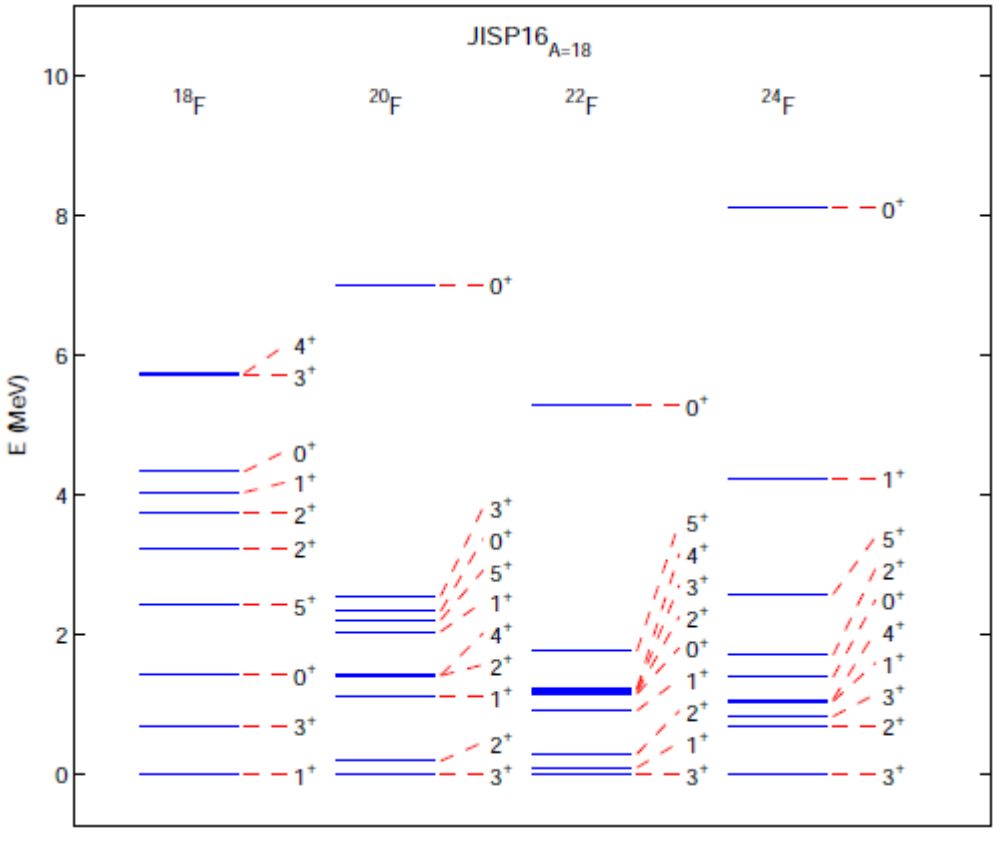

Preliminary Results
^{20}F
E (MeV)
6
4
2
0
ε_{theo}
ε_{USDB}
ε_{USDB}
4^+
3^+
0^+
5^+
1^+
4^+
2^+
1^+
2^+
3^+
0^+
4^+
1^+
5^+
3^+
2^+
3^+
4^+
1^+
2^+
0^+
4^+
1^+
3^+
2^+
5^+
3^+
1^+
4^+
2^+
0^+
1^+
3^+
3^+
2^+
5^+
1^+
4^+
3^+
2^+
JISP16$_{A=18}$
JISP16$_{A=18}$
USDB$_{A=18}$
Experiment


Preliminary Results
^{22}F
ε_{theo}
ε_{USDB}
ε_{USDB}
E (MeV)
4
2
0
0^+
4^+
5^+
4^+
3^+
2^+
0^+
1^+
2^+
1^+
3^+
0^+
5^+
2^+
4^+
1^+
3^+
2^+
4^+
3^+
1^+
1^+
4^+
5^+
2^+
3^+
1^+
2^+
3^+
4^+
4^+
1^+
2^+
3^+
1^+
5^+
2^+
2^+
3^+
4^+
JISP16$_{A=18}$
JISP16$_{A=18}$
USDB$_{A=18}$
Experiment

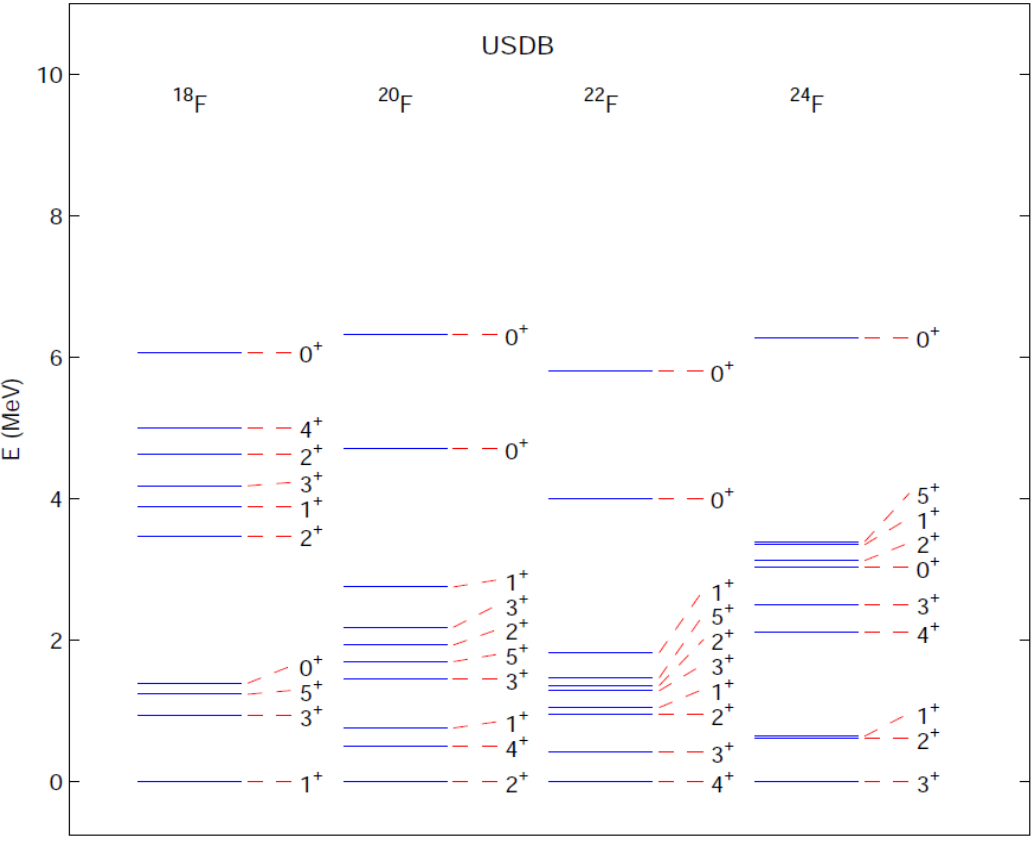

Preliminary Results
^{24}F
theo
ε_{USDB}
ε_{USDB}
E (MeV)
0
2
4
6
4^+
1^+
5^+
2^+
0^+
4^+
1^+
3^+
2^+
3^+
4^+
1^+
5^+
0^+
2^+
3^+
4^+
2^+
3^+
1^+
4^+
5^+
1^+
2^+
0^+
3^+
4^+
1^+
2^+
3^+
1^+
$(3^+,1^+,2)$
3^+
JISP16$_{A=18}$
JISP16$_{A=18}$
USDB$_{A=18}$
Experiment

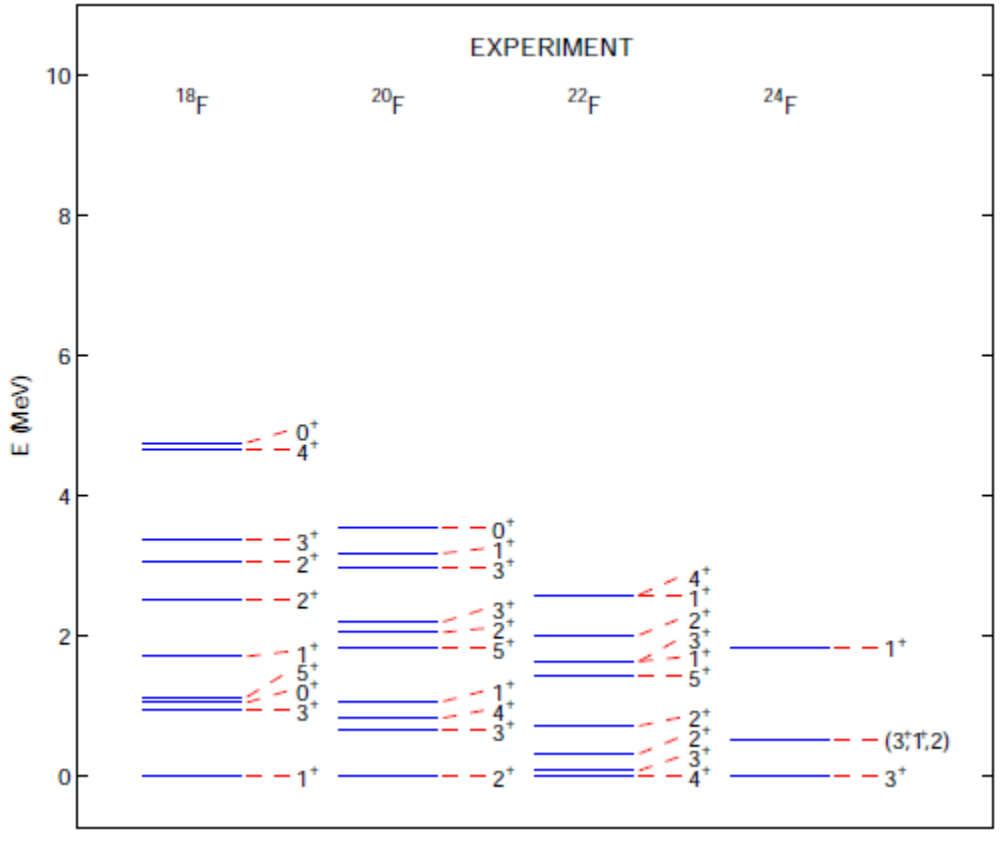
Preliminary Results





Preliminary Results





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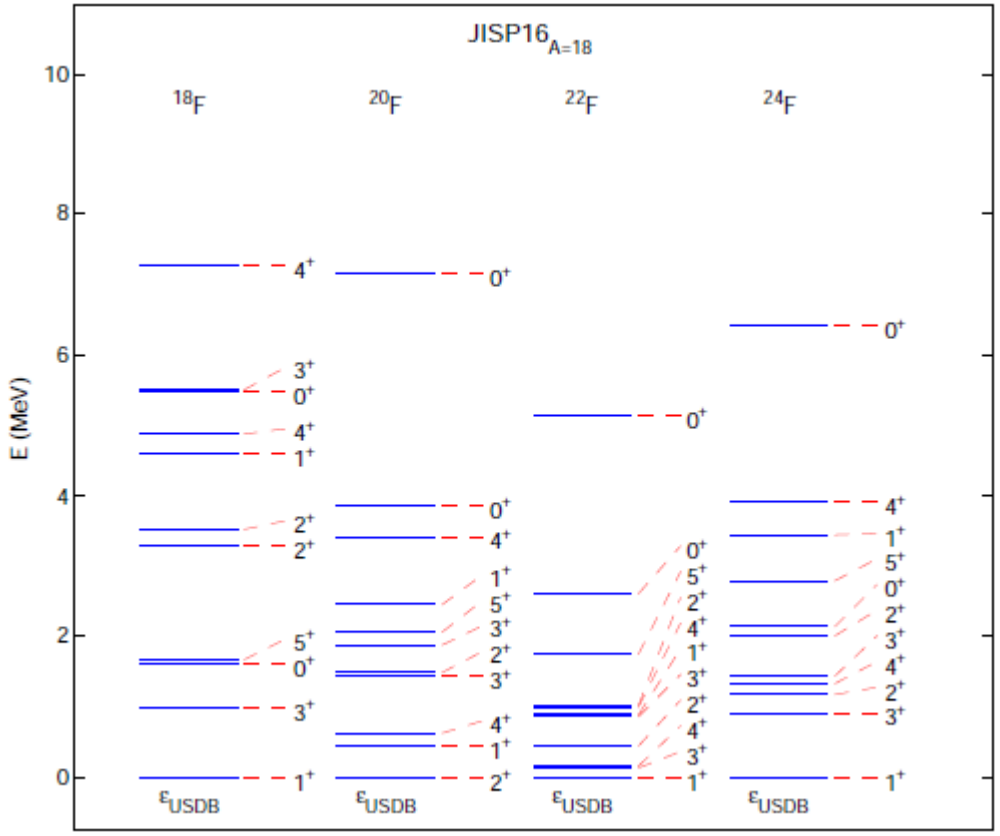

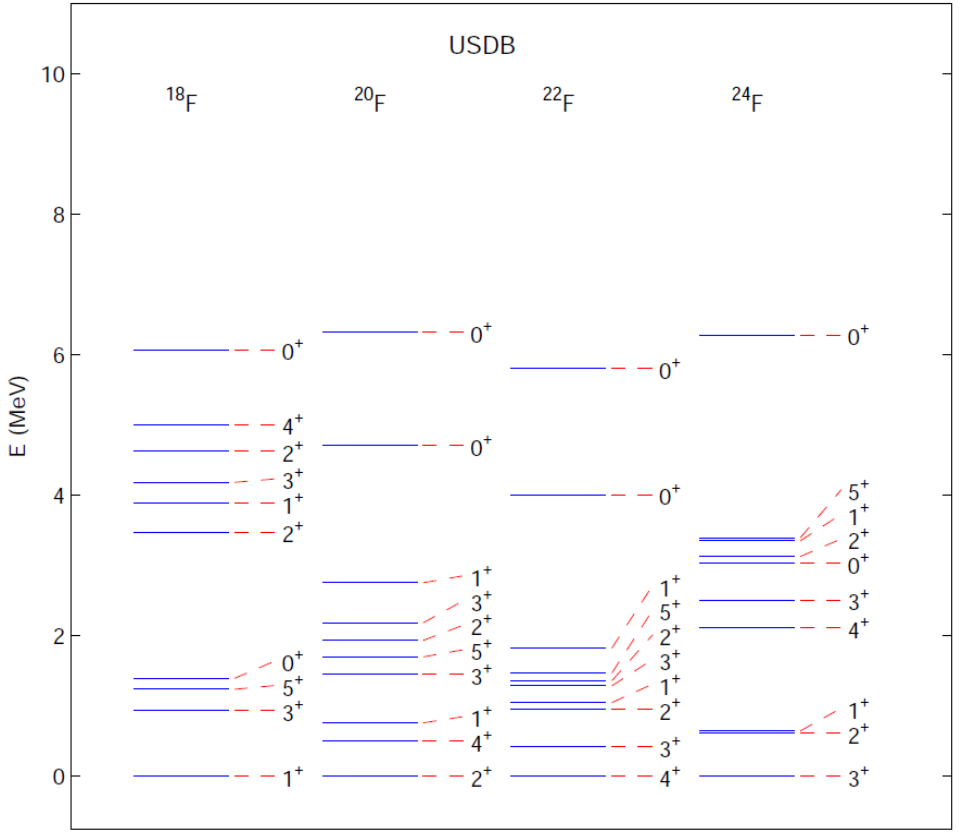

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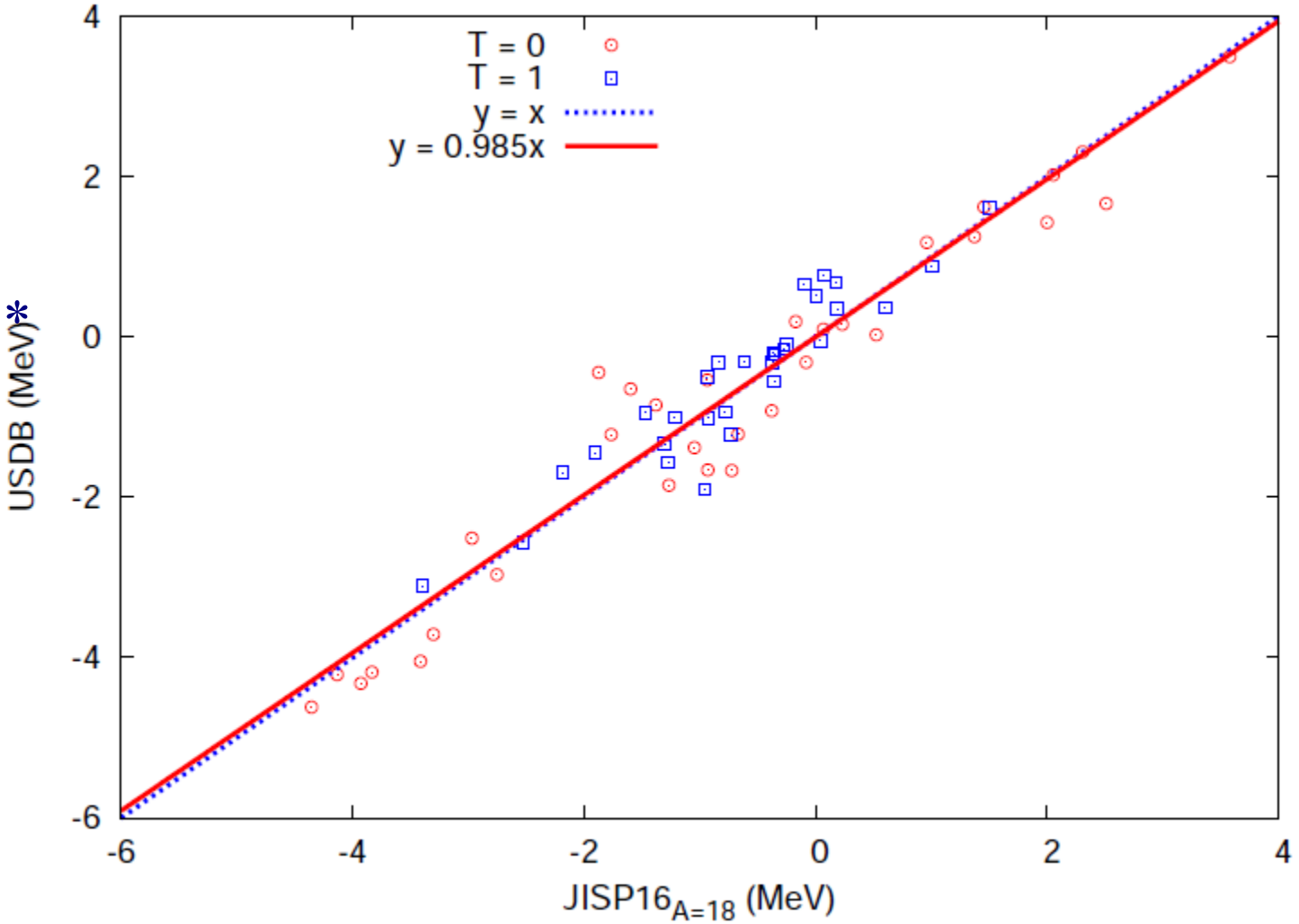
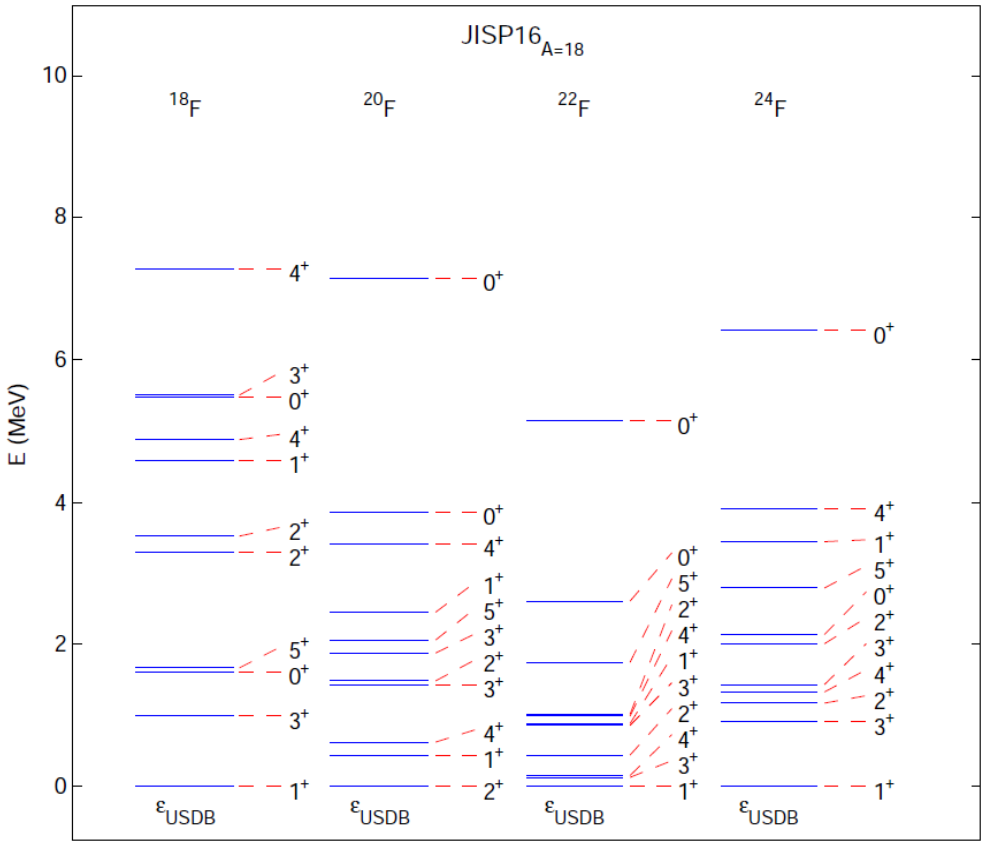
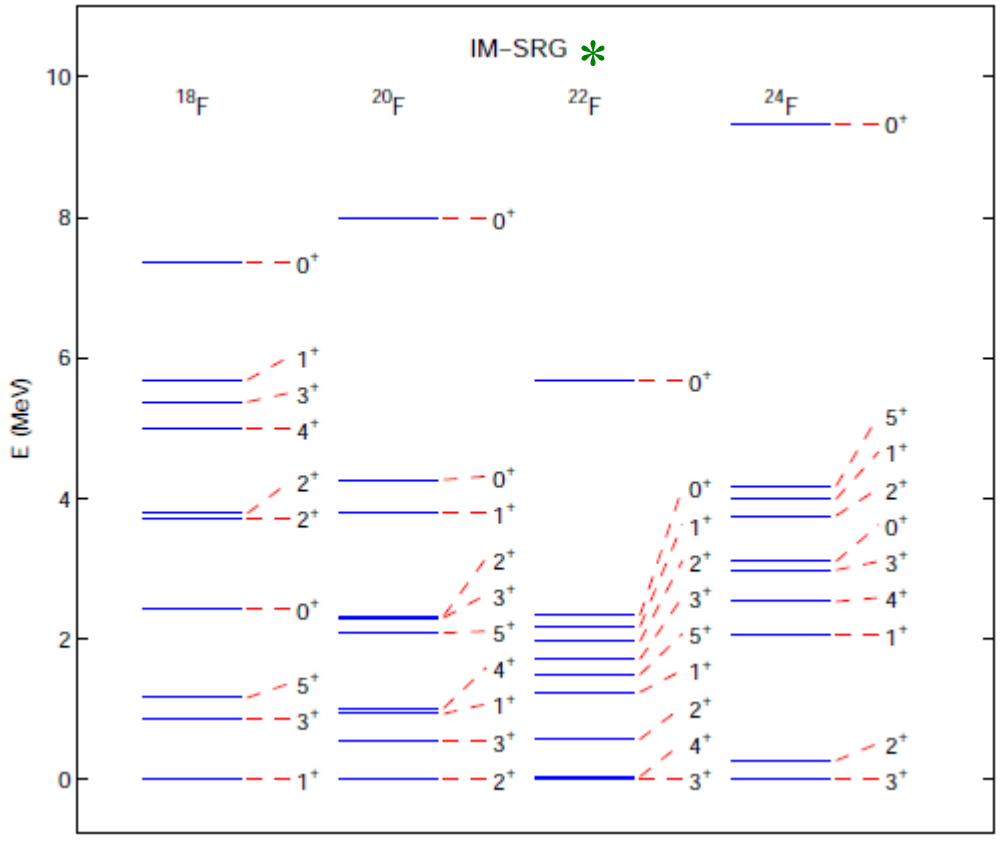


RMS deviation of 471 keV

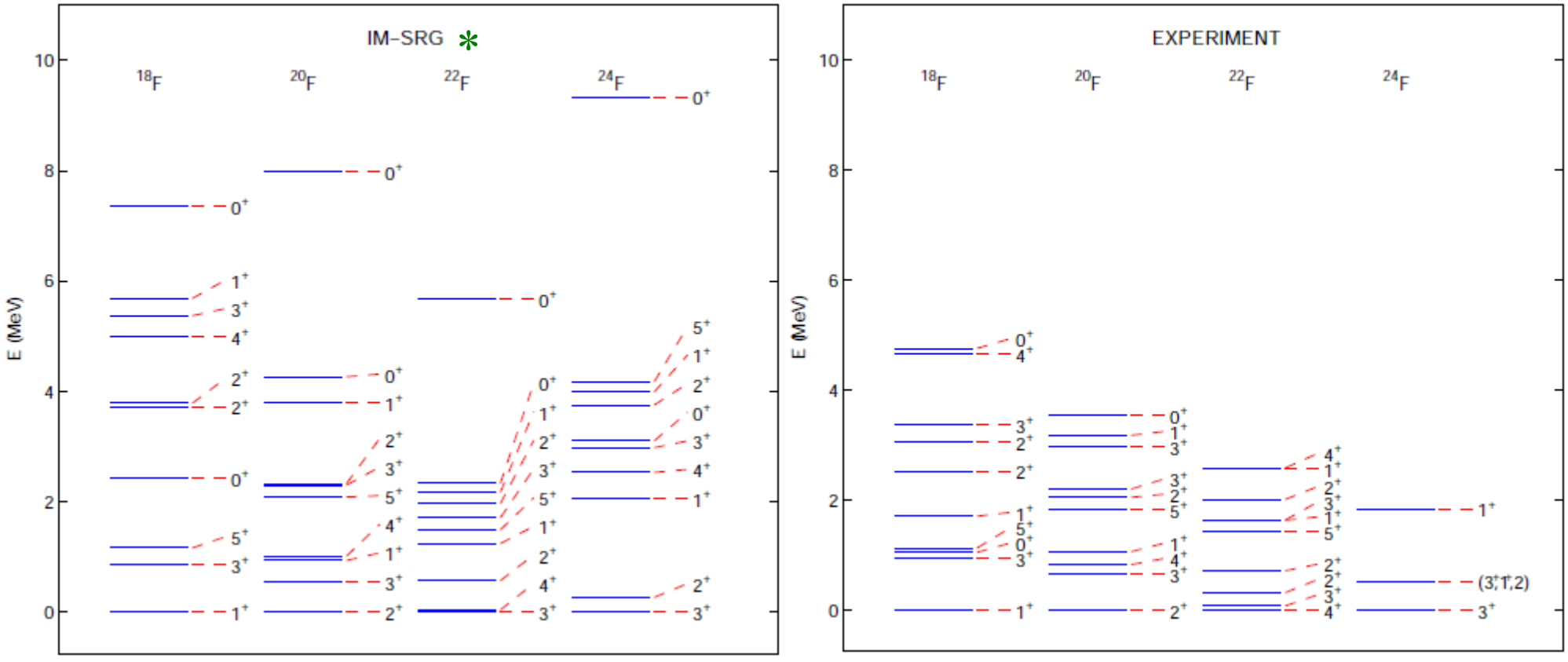
* B.A. Brown & W.A. Richter, PRC 74, 034315 (2006)

Preliminary Results



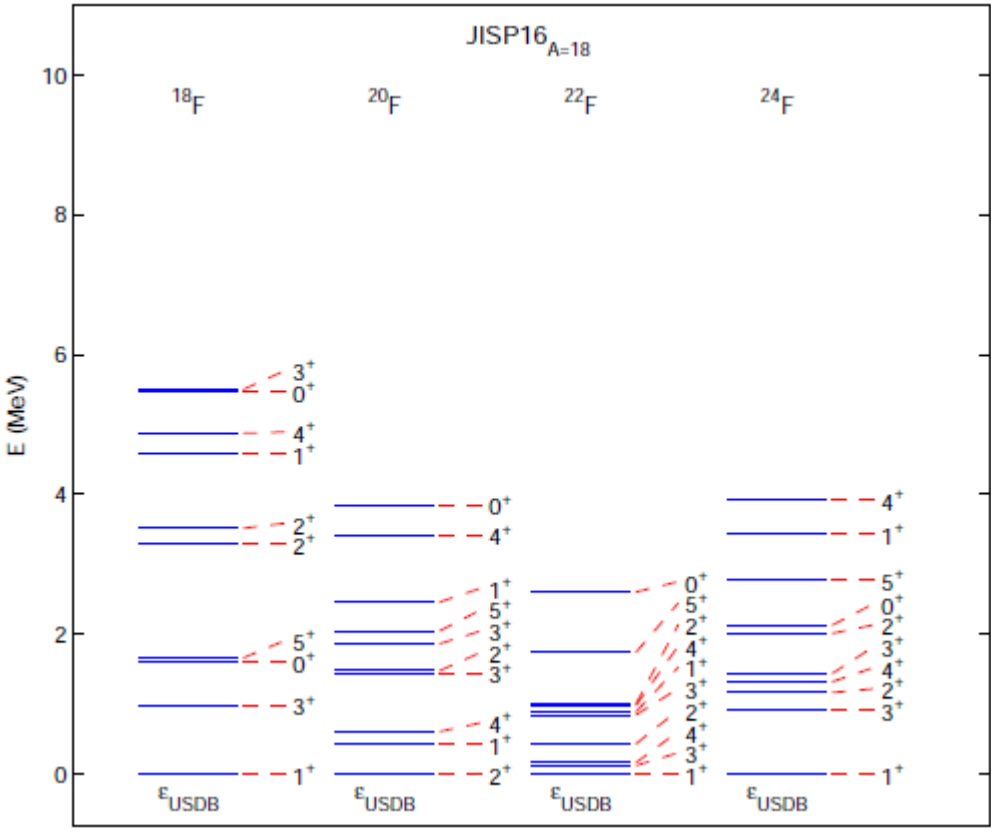


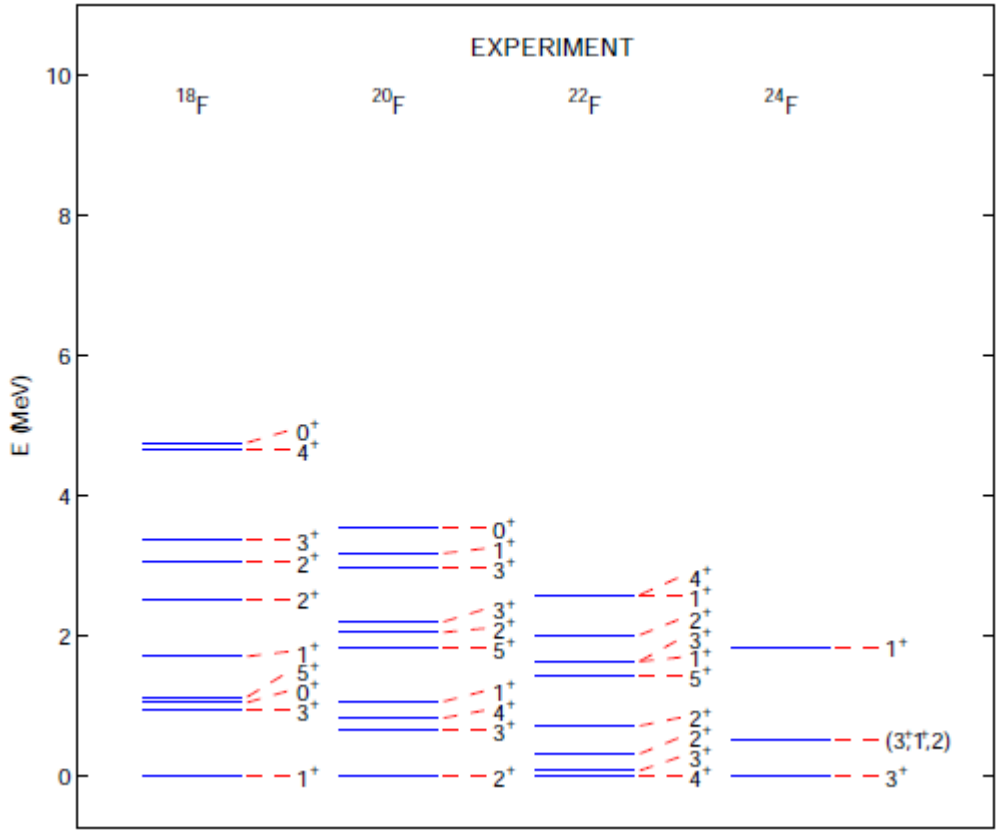
* S.R. Stroberg, et al., arXiv Nucl-th 1511.02802



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

Preliminary Results



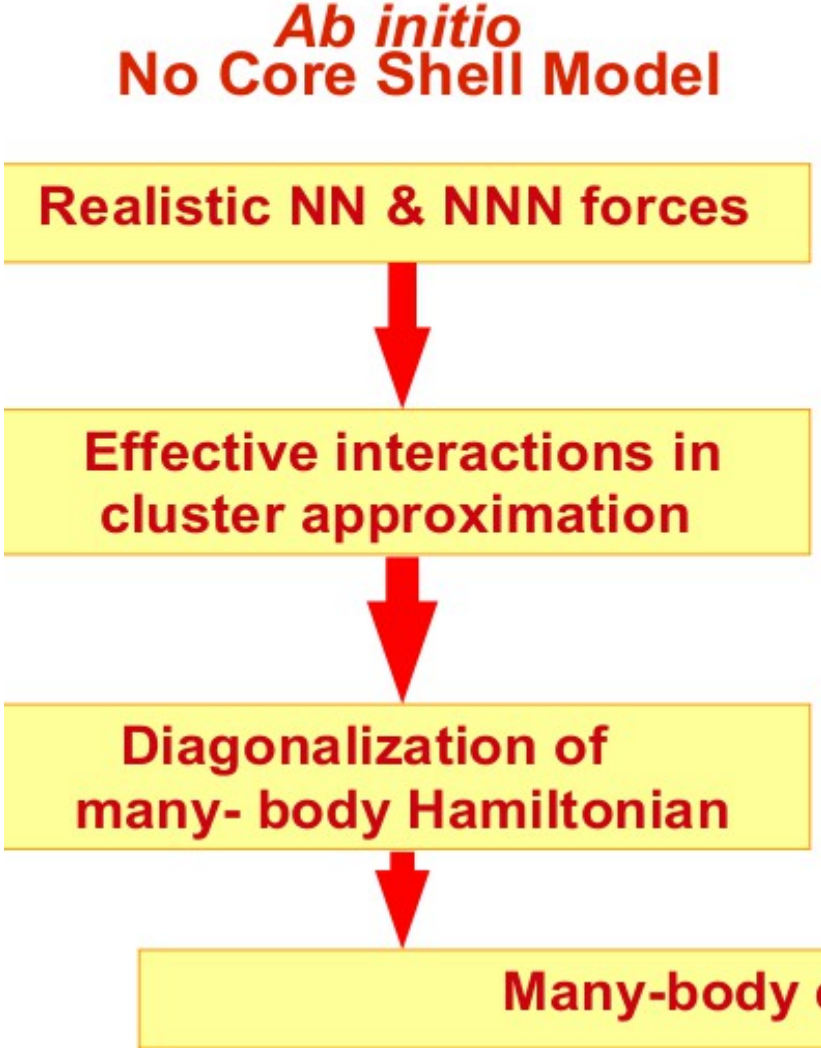


SUMMARY AND OUTLOOK

1. All three 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 the theoretical s.p. energies with the empirical ones for the USDB interaction, perhaps approximating the effects of a NNN interaction, improved, in general, 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 it is worthwhile to further improve our interactions and increase the size of the 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.

From few-body to many-body



Flow chart for a standard NCSM calculation

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

Effective Interaction

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

$$\mathcal{H} = \mathcal{H}^{(I)} + \mathcal{H}^{(A)} \quad \gtrapprox_{a < A} \quad \mathcal{H}^{(I)} + \mathcal{H}^{(a)}$$

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;

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

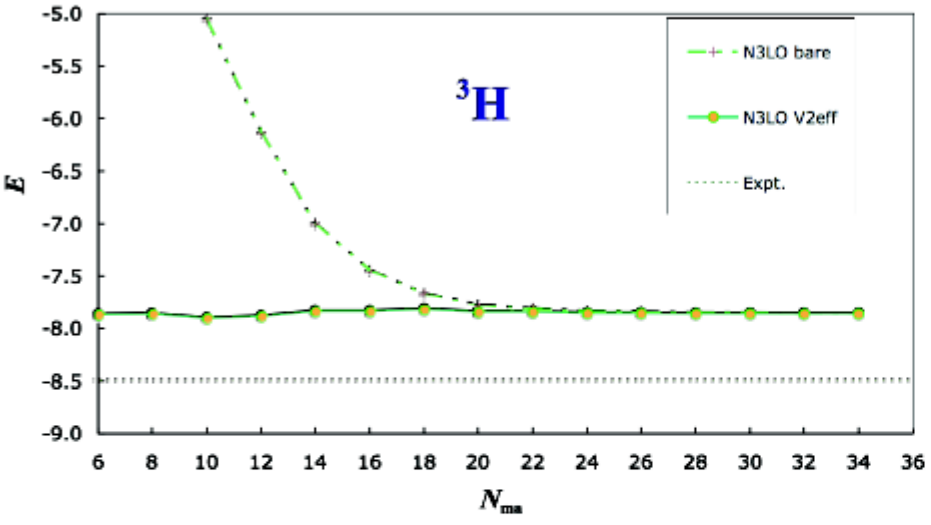
$$H^{N_{\max},\Omega,\mathrm{eff}}_{A,2} = \frac{U^{\dagger}_{2,P}}{\sqrt{U^{\dagger}_{2,P} U_{2,P}}} E^{\Omega}_{A,2,P} \frac{U_{2,P}}{\sqrt{U^{\dagger}_{2,P} U_{2,P}}}$$

Two ways of convergence:

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

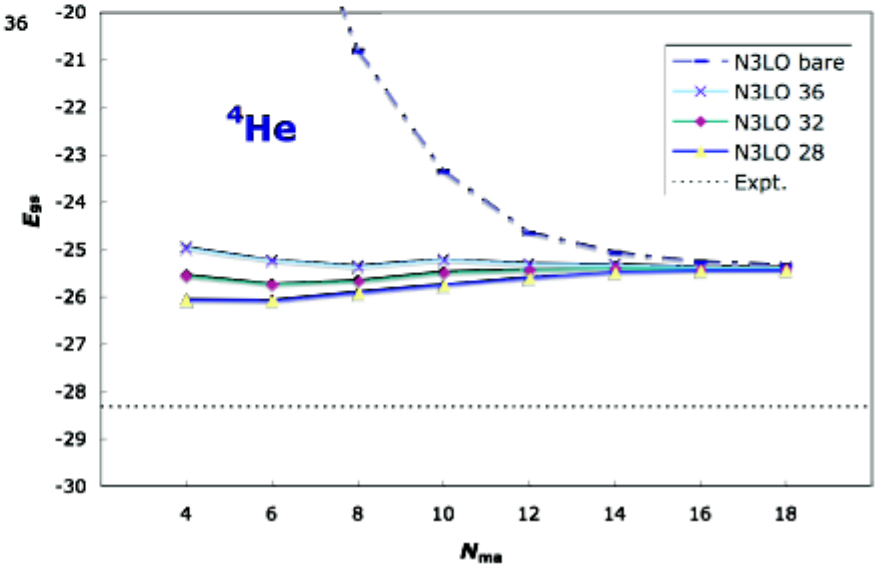
2) For $a \to A$ and fixed P: $H^{\mathrm{eff}}_{A,a} \to H_A$

- NCSM convergence test
  - Comparison to other methods



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

- Short-range correlations ⇒ effective interaction
- Medium-range correlations ⇒ 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



P. Navratil, INT Seminar, November 13, 2007, online

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;

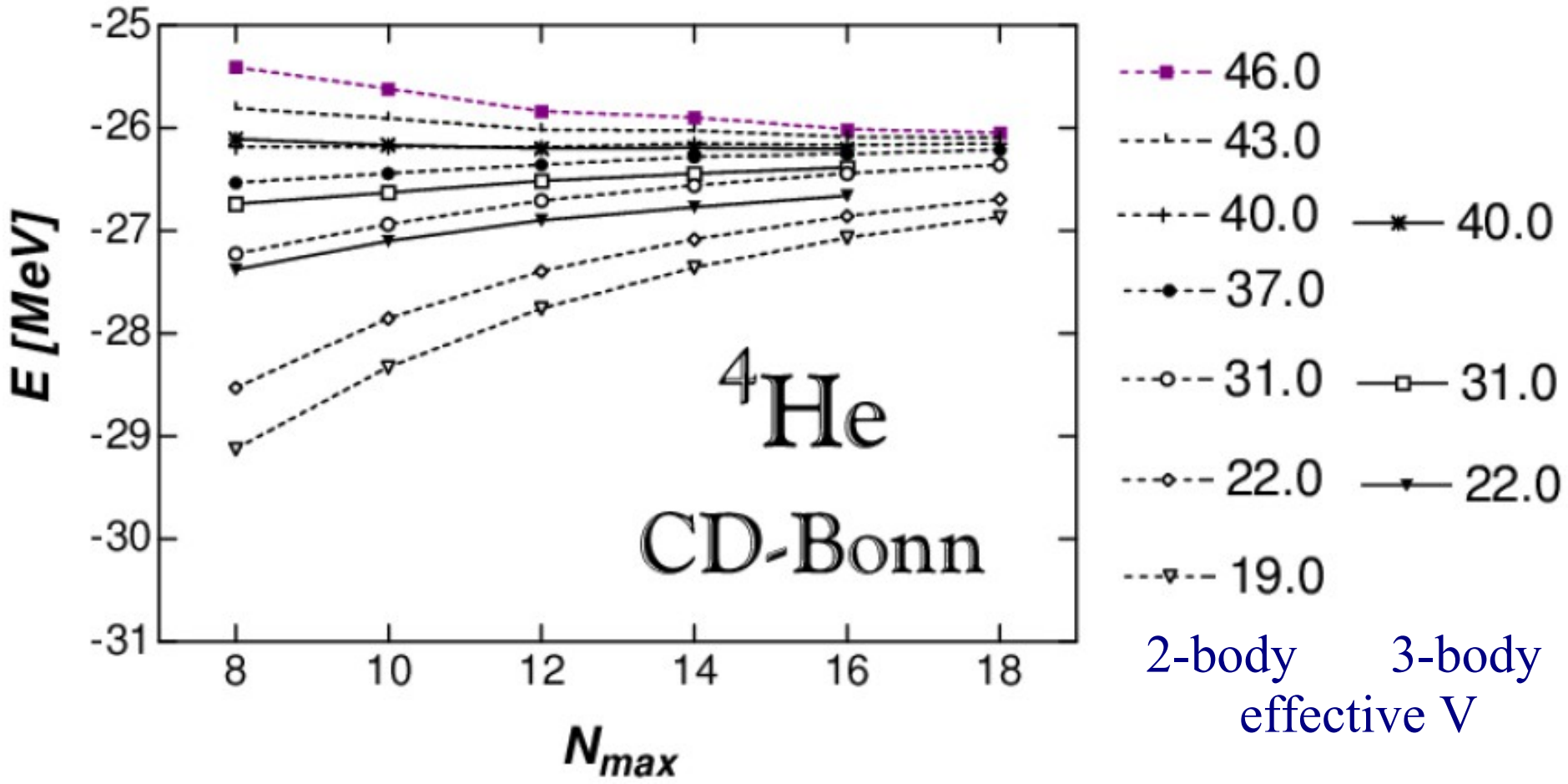
$$\mathcal{H}^{N_{1,\max},N_{\max}}_{A,a_1} = \frac{U^{A,\dagger}_{a_1,P_1}}{\sqrt{U^{A,\dagger}_{a_1,P_1}U^{A}_{a_1,P_1}}} E^{N_{\max},\Omega}_{A,a_1,P_1} \frac{U^{A}_{a_1,P_1}}{\sqrt{U^{A,\dagger}_{a_1,P_1}U^{A}_{a_1,P_1}}}$$

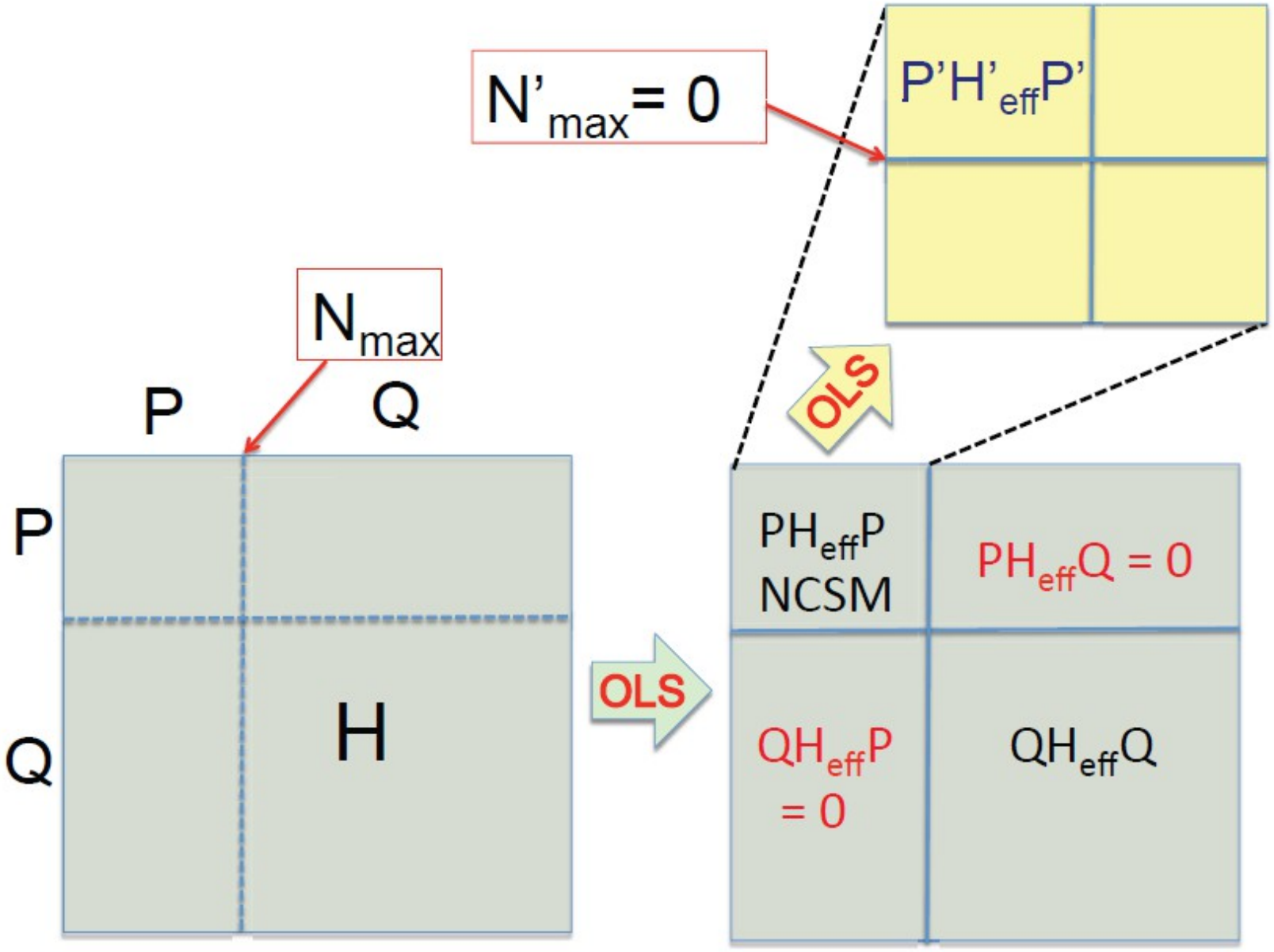
Valence Cluster Expansion

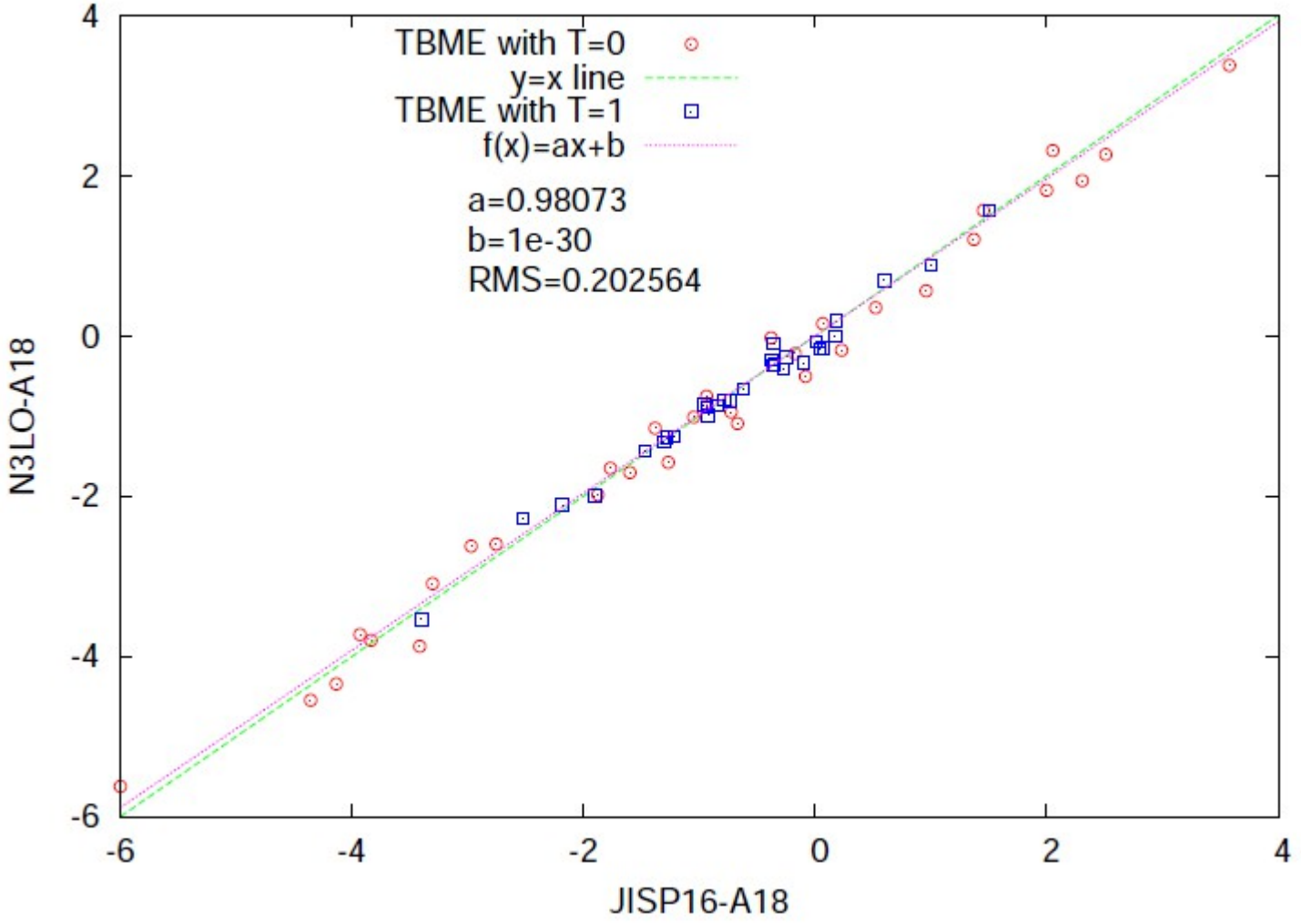
$N_{1,max}$ = 0 space (p-space) ; $a_1 = A_c + a_v$; a_1 - order of cluster;

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

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


E [MeV]
-25
-26
-27
-28
-29
-30
-31
8
10
12
14
16
18
N_{max}
^{4}He
CD-Bonn
46.0
43.0
40.0
40.0
37.0
31.0
31.0
22.0
22.0
19.0
2-body
3-body
effective V


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

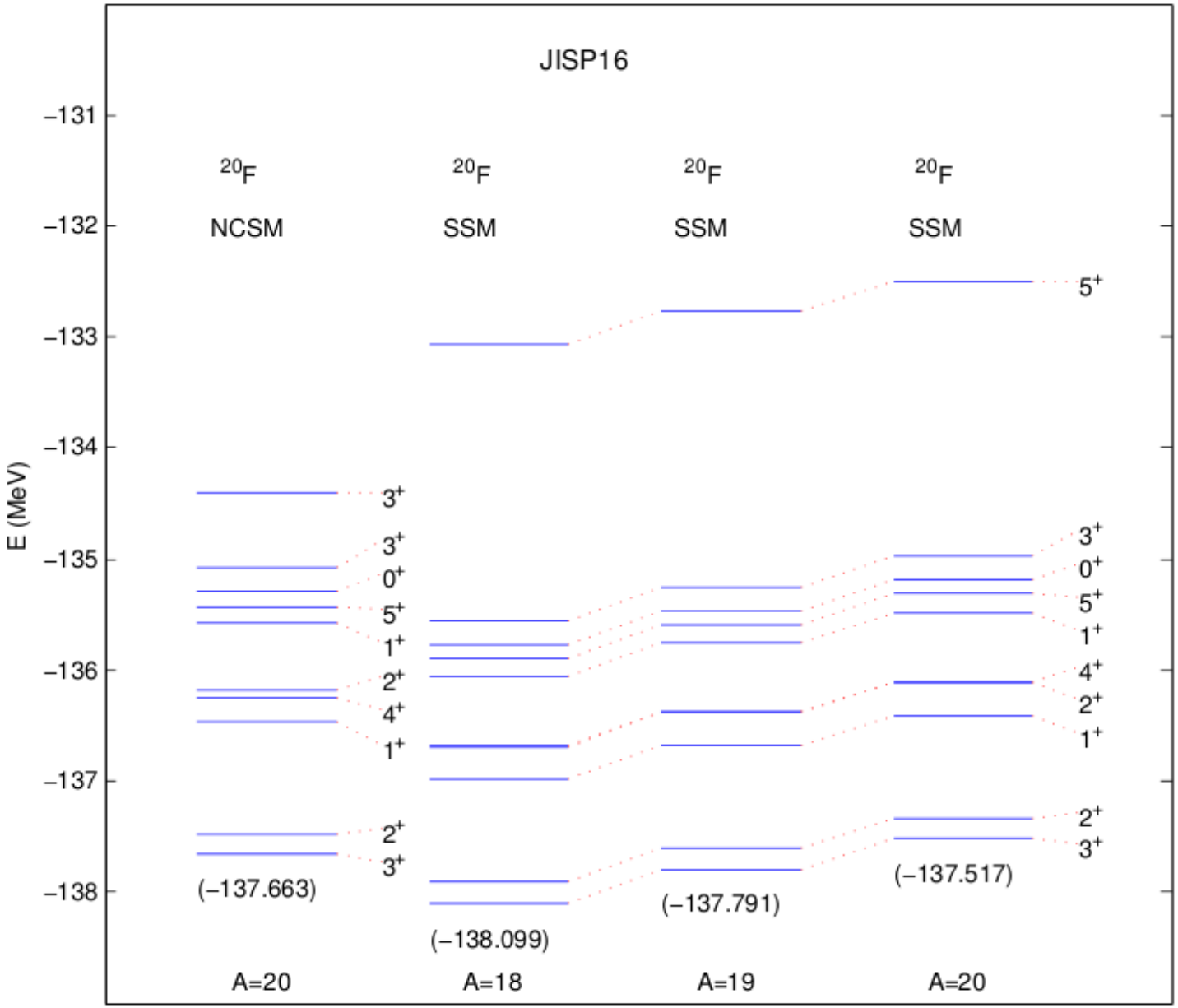


Preliminary Results

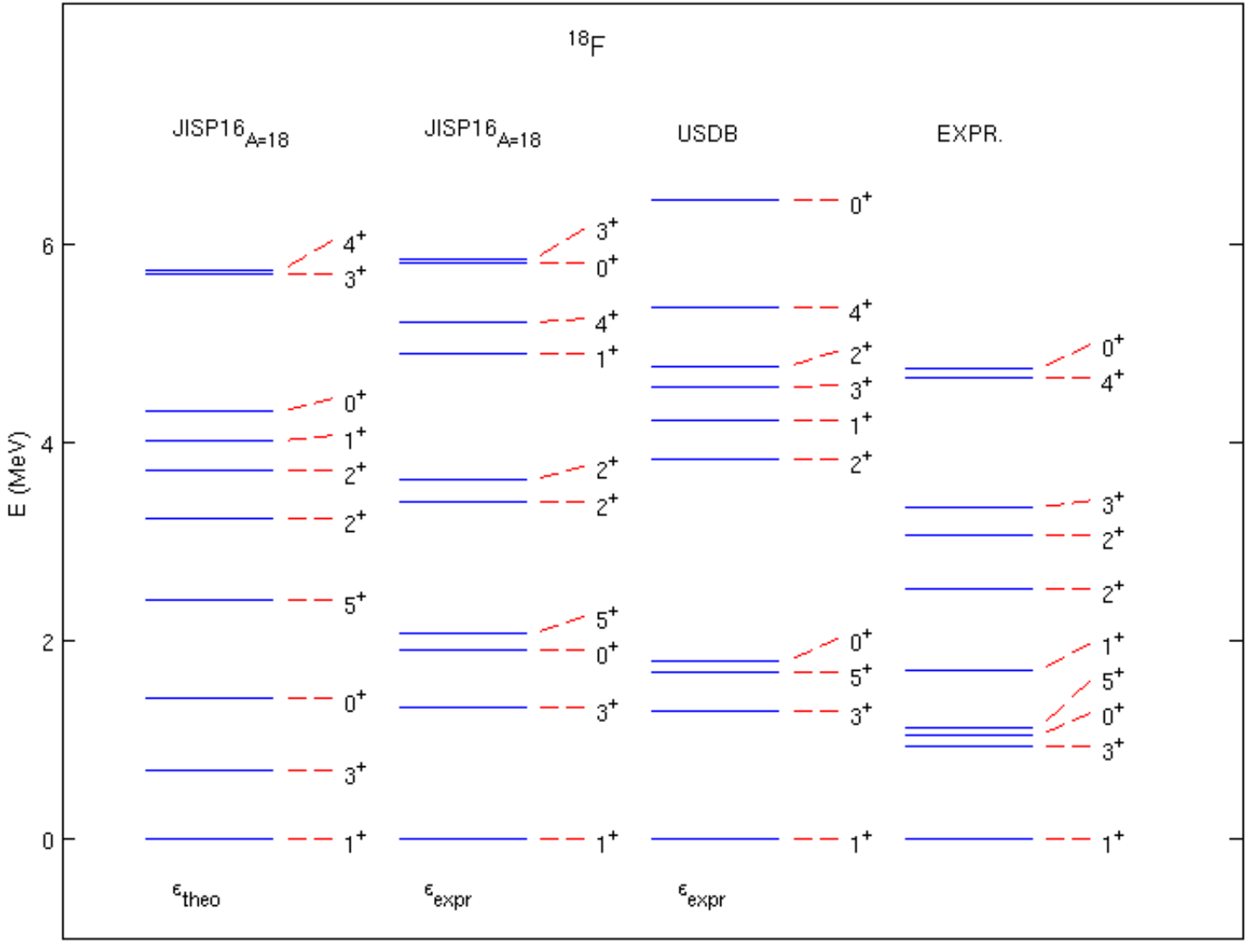
TABLE III: The NCSM energies (in MeV) of the lowest 28 states J_i^π of ^{18}F calculated in $4\hbar\Omega$ model space using JISP16 and chiral N3LO NN interactions with $\hbar\Omega = 14$ MeV.

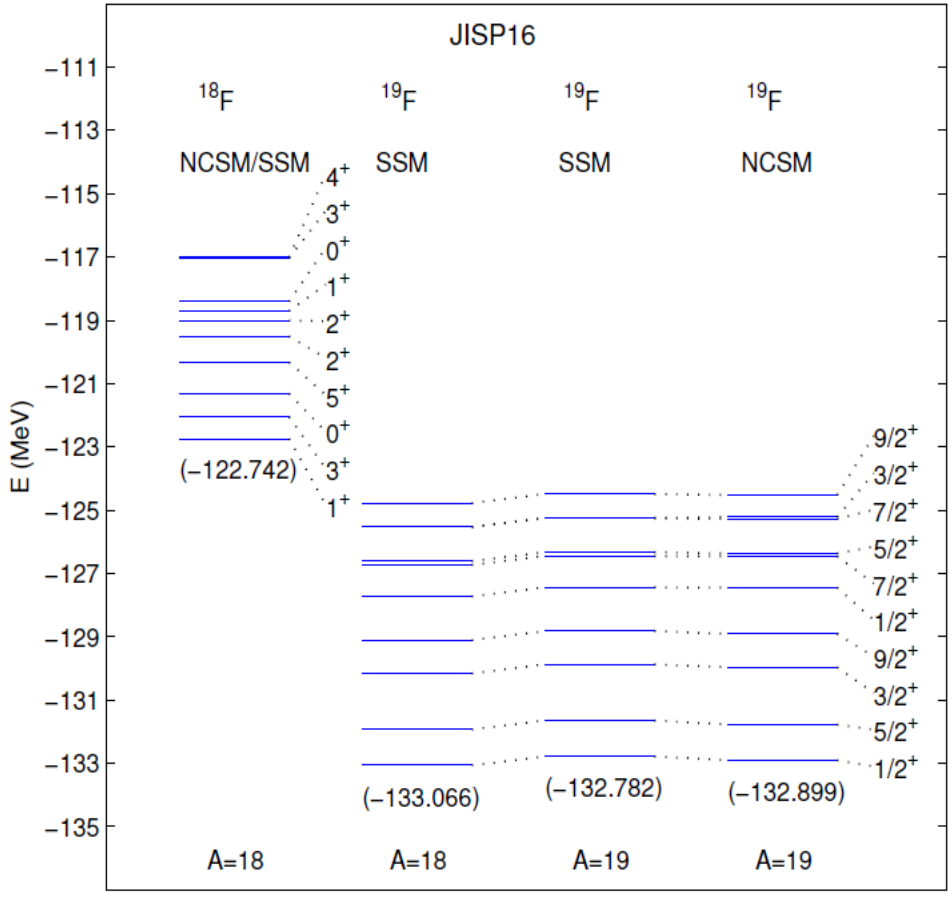
J_i^π	T	JISP16	J_i^π	T	N3LO
1_1^+	0	-122.742	1_1^+	0	-126.964
3_1^+	0	-122.055	3_1^+	0	-126.214
0_1^+	1	-121.320	0_1^+	1	-125.510
5_1^+	0	-120.329	5_1^+	0	-124.545
2_1^+	1	-119.505	2_1^+	1	-123.974
2_2^+	0	-119.011	2_2^+	0	-123.890
1_2^+	0	-118.709	1_2^+	0	-123.077
0_2^+	1	-118.410	0_2^+	1	-122.586
2_3^+	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

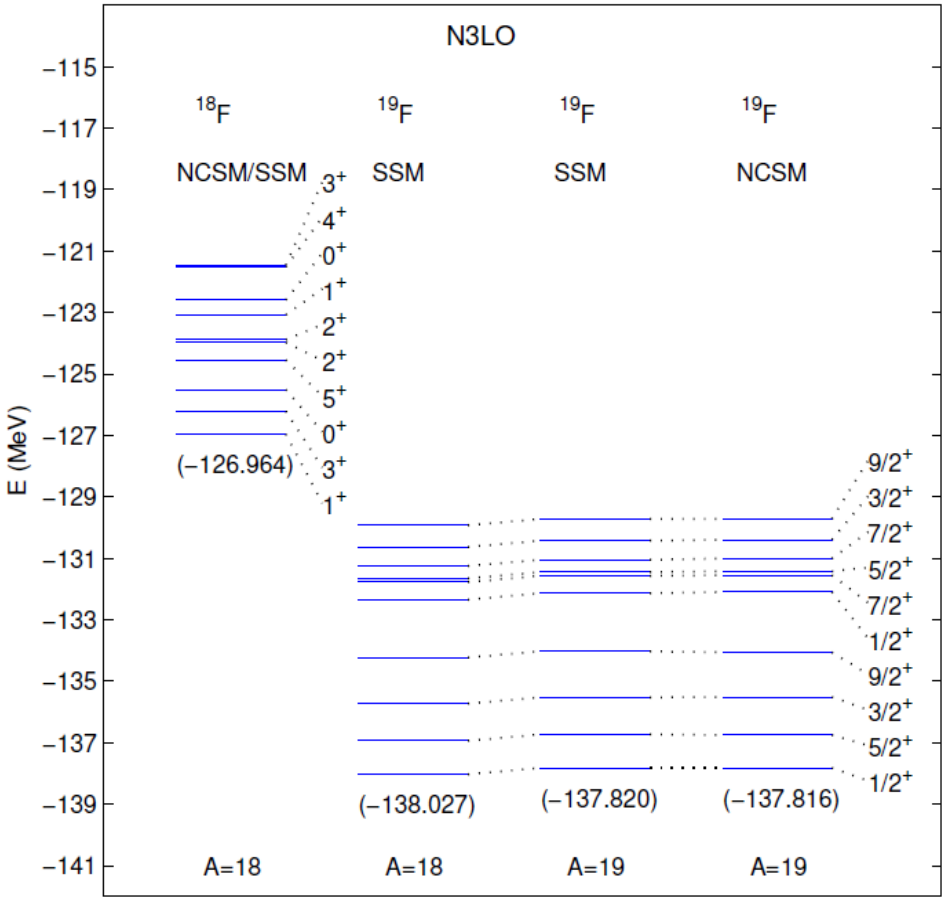
PRELIMINARY RESULTS



Preliminary Results




JISP16
E (MeV)
−111
−113
−115
−117
−119
−121
−123
−125
−127
−129
−131
−133
−135
18F
19F
19F
19F
NCSM/SSM
SSM
SSM
NCSM
4+
3+
0+
1+
2+
2+
5+
0+
3+
1+
(−122.742)
9/2+
3/2+
7/2+
5/2+
7/2+
1/2+
9/2+
3/2+
5/2+
1/2+
(−133.066)
(−132.782)
(−132.899)
A=18
A=18
A=19
A=19


N3LO
E (MeV)
−115
−117
−119
−121
−123
−125
−127
−129
−131
−133
−135
−137
−139
−141
18F
19F
19F
19F
NCSM/SSM
SSM
SSM
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