Ab-initio Shell Model for Nuclear Structure

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Ab-initio Shell Model for Nuclear Structure

- **The nuclear shell model:** current status of microscopic interactions

- **Preliminary results**: *ab-initio* effective sd-shell Hamiltonian from the NCSM solution for A=18 via **Okubo-Lee-Suzuki (OLS) similarity transformation** and highlights on **Daejeon16** realistic NN potential

- **Proposed project**
  - Improvement and charge-dependence of the Daejeon16 potential;
  - Construction of valence-space interactions with Daejeon16 via OLS;
  - Construction of effective electromagnetic operators;
  - Derivation of the effective interaction of *p-sd-pf* shell model space.

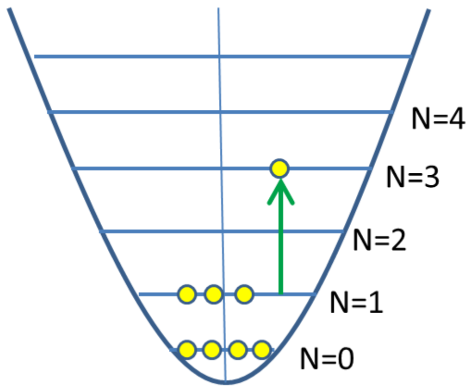
- **Conclusions and prospects**

Shell model - (full) configuration-interaction approach

$$H = T + V = (T + U) + (V - U) = H_0 + V_{res}$$

Independent particle Hamiltonian — $(T+U)$

residual interaction — $(V-U)$



$$H|\Psi_n\rangle = E_n|\Psi_n\rangle$$

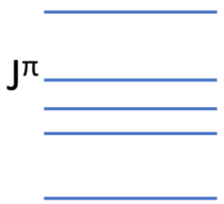
$$|\Psi_n\rangle = \sum_k c_{kn}\,|\Phi_k\rangle$$

$$H_0|\Phi_k\rangle = E_k^0|\Phi_k\rangle$$

$$\langle\Phi_k|\Phi_l\rangle = \delta_{kl}$$

$$\sum_{k=1}^{d} \langle\Phi_l|H|\Phi_k\rangle\, c_{kn} = E_n c_{ln}$$

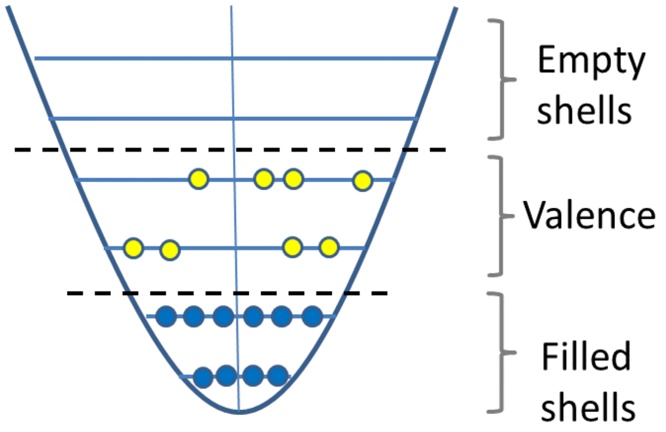
$$\begin{pmatrix} H_{11} & H_{12} & \cdots & H_{1d} \\ H_{21} & H_{22} & \cdots & H_{2d} \\ \vdots & & \ddots & \\ H_{d1} & H_{d2} & \cdots & H_{dd} \end{pmatrix}$$



Ab-initio No-Core Shell Model : sufficiently large model space so that the results for A nucleons do not depend on the basis parameters (hw and Nmax)

Conservation of symmetries of the Hamiltonian, detailed information on low-energy states and transitions

Valence-space shell model (heavier nuclei)



Full Hilbert space		Restricted model space
$H\|\Psi_p\rangle = E_p\|\Psi_p\rangle$	→	$H_{eff}\|\Psi_p^M\rangle = E_p\|\Psi_p^M\rangle$
$\langle\Psi_f\|O\|\Psi_i\rangle = O_{fi}$		$\langle\Psi_f^M\|\, O_{eff}\|\Psi_i^M\rangle = O_{fi}$

Effective operators !

$$H = \sum_\alpha \varepsilon_\alpha a_\alpha^\dagger a_\alpha + \frac{1}{4}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|V_{res}|\delta\gamma\rangle\, a_\alpha^\dagger a_\beta^\dagger\, a_\gamma\, a_\delta$$

Empirical (for ε_α)

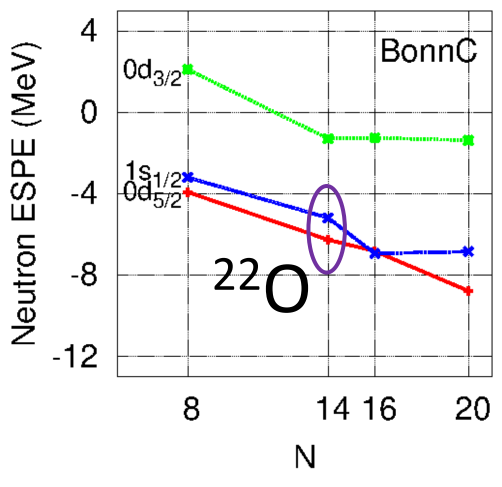
For $\langle\alpha\beta|V_{res}|\delta\gamma\rangle$: *Microscopic*, *Semi-microscopic (microscopic, constrained by the data)*, *Empirical*

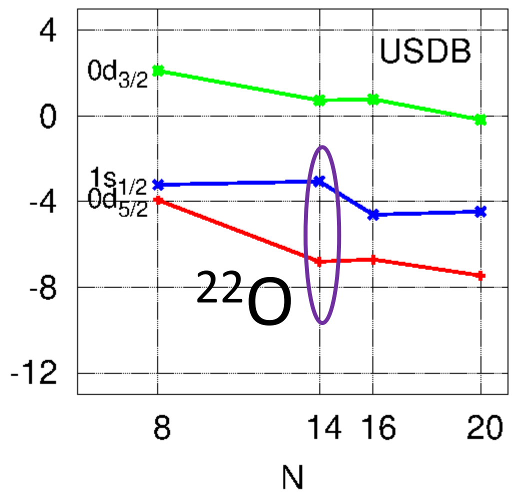
Current status :

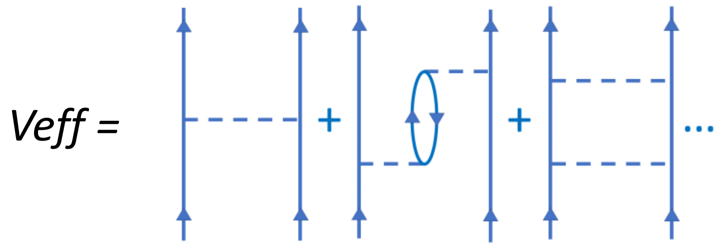
- Excellent description with empirical (phenomenological) interactions
- Microscopic interactions -> recent progress and challenges
- Importance for unexplored region of the nuclear chart (exotic nuclei) where no data exists !

Microscopic approaches to valence space interactions

Many-body perturbation theory *(G.F. Bertsch, T.T.S. Kuo, G.F. Brown, B.R.Barrett, M.Kirson, et al. - from 60's)*







If NN force is use, then poor description of the monopole term (spherical mean-field)

Missing 3N forces (inclusion requires resources !)

Non-perturbative approaches :

- **Valence-space In-Medium Similarity Renormalization Group – IMSRG** (*NN + 3N*)

  S.R. Stroberg et al, PRC93, 051301 (2016); PRL118, 032502 (2017)

- **OLS transformation applied to NCSM results**

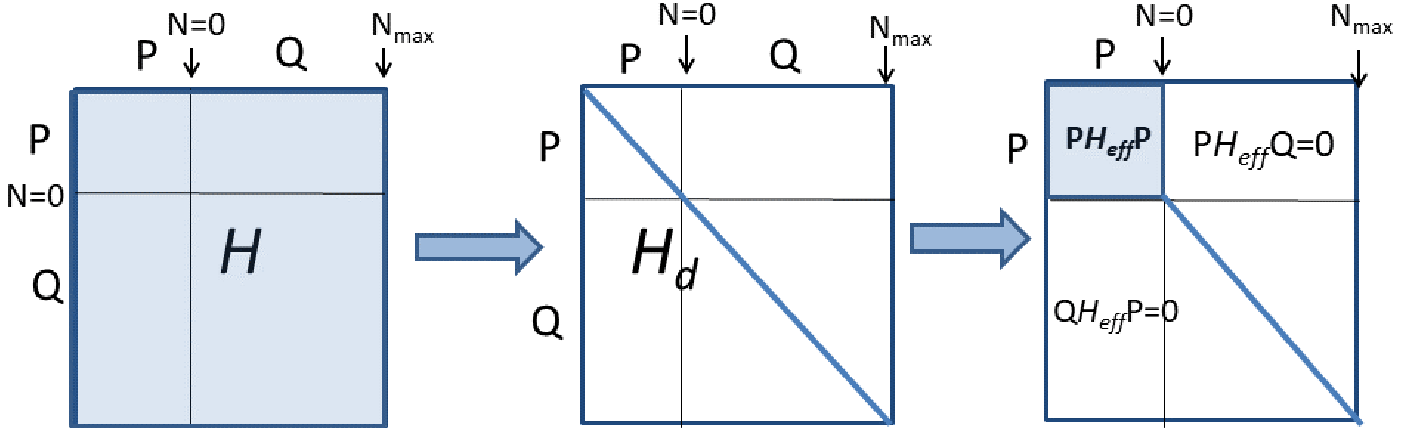
  E. Dikmen, A. Lisetskiy, B.R. Barrett, P. Maris, A.M. Shirokov, J.P. Vary, PRC91, 064301 (2015)
  N.Smirnova, B.R. Barrett, I.J. Shin, Y.Kim, A.M. Shirokov, E. Dikmen, P. Maris, J.P. Vary, PRC100, 054329 (2019)

- **Coupled-cluster theory** $(NN + 3N)$

  G.R. Jansen et al, PRC94, 011301 (2016); Z.H. Sun, T.D. Morris, G. Hagen et al, PRC98 (2018)

Ab-initio effective Hamiltonian from the NCSM

Okubo-Lee-Suzuki (OLS) similarity transformation
of the NCSM solution



$$H_d = UHU^{\dagger} \qquad H_{eff} = \frac{U_P^{\dagger}}{\sqrt{U_P U_P^{\dagger}}} H_d \frac{U_P}{\sqrt{U_P U_P^{\dagger}}}$$

FLOW

- ❑ ^{18}F from the NCSM at N_{max}
- ❑ H_{eff} for ^{18}F at N=0
- ❑ ^{16}O from the NCSM at N_{max}
  - → Core energy
- ❑ ^{17}O, ^{17}F from the NCSM at N_{max}
  - → One-body terms
- ❑ Single-particle energies ε_i

two-body matrix elements V_{ijkl}

- ❑ Use of various NN potentials:

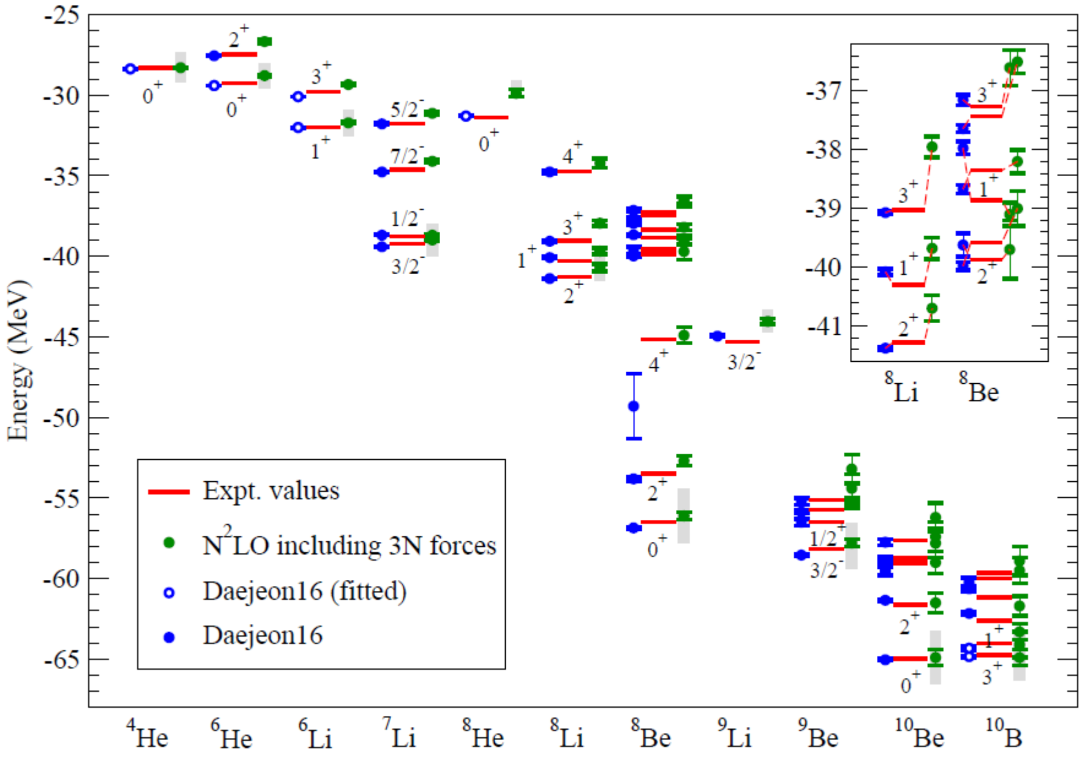
N^{3}LO, JISP16, Daejeon16, etc

S. Okubo, Prog. Theor. Phys. 12 (1954); K. Suzuki, S. Lee, Prog. Theor. Phys. 68 (1980)
E. Dikmen, A. Lisetskiy, B.R. Barrett, P. Maris, A.M. Shirokov, J.P. Vary, PRC91, 064301 (2015)
N.Smirnova, B.R. Barrett, I.J. Shin, Y.Kim, A.M. Shirokov, E. Dikmen, P. Maris, J.P. Vary, PRC100, 054329 (2019)

Modern NN potential Daejeon16

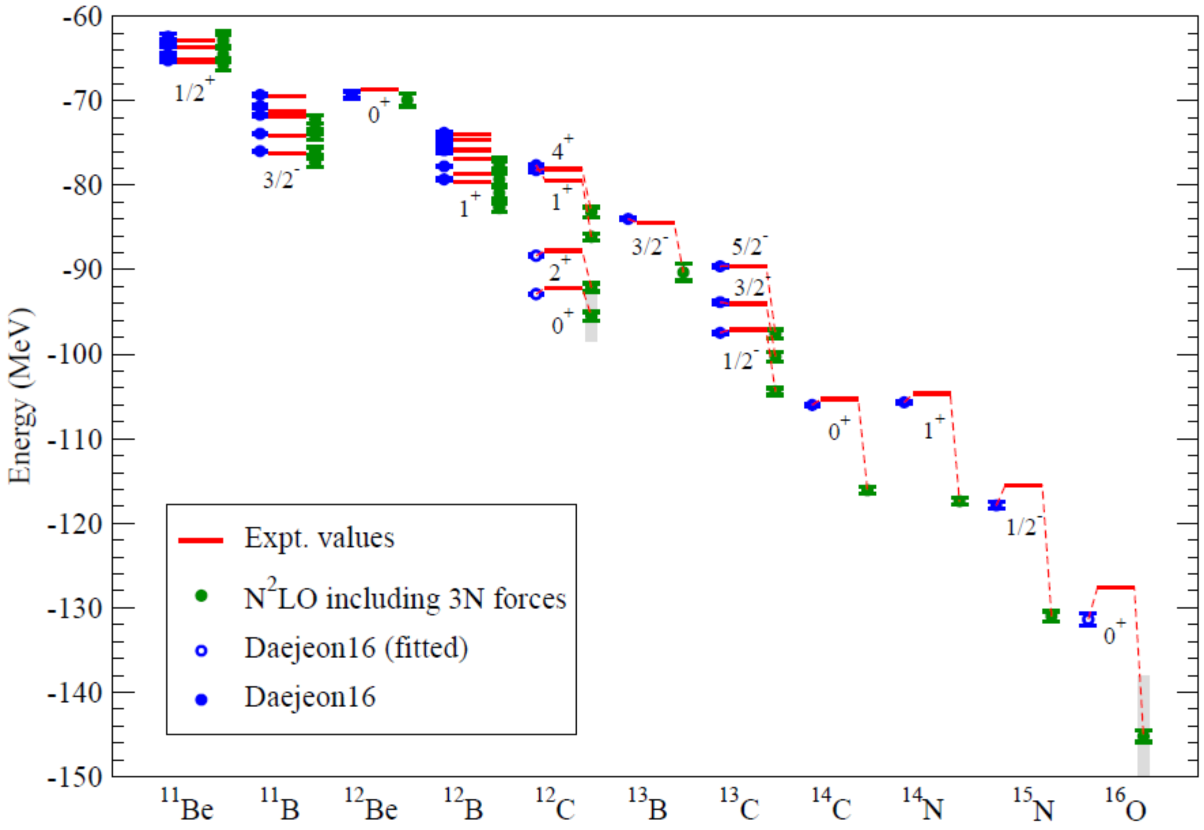
Daejeon16 is a high-precision realistic NN potential obtained from chiral N^{3}LO + SRG evolved + PETs (phase-equivalent transformations) to incorporate the effect from 3N and many-nucleons forces !

A.M. Shirokov, I.J. Shin, Y. Kim, M. Sosonkina, P. Maris, J.P. Vary, Phys. Lett. B761, 87 (2016)

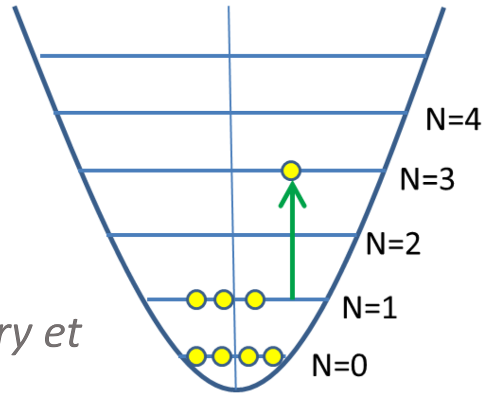


P. Maris, I.J. Shin, J.P. Vary, Proc. NTSE 2018 (Daejeon, November 2018)

I.J. Shin, Y. Kim, Tachyon II at Supercomputing Center/KISTI (KSC-2013-C3-052)

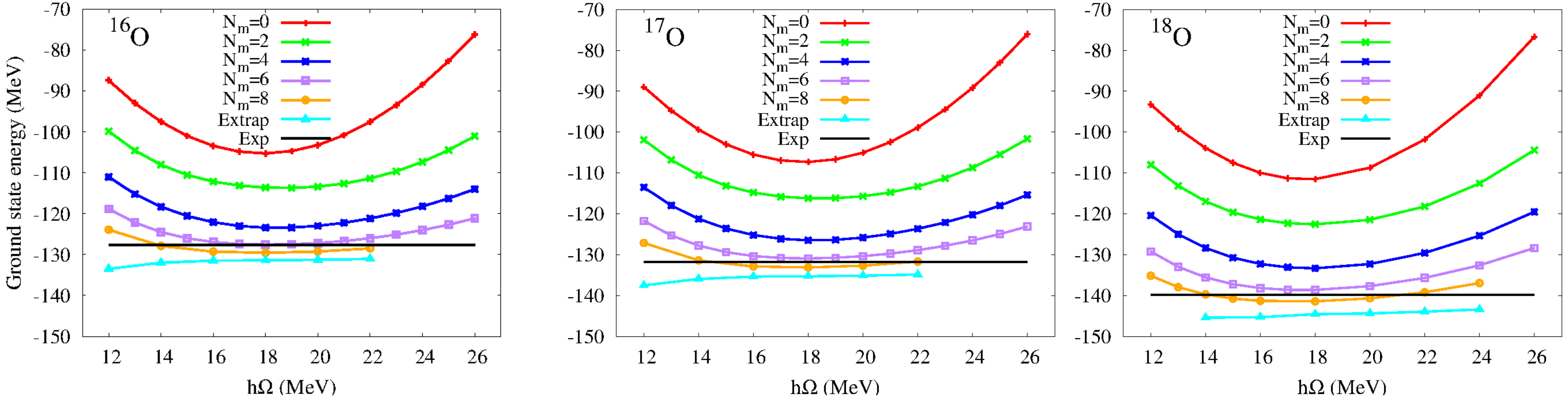


No-Core Shell Model results with Daejeon16 for sd shell nuclei



I.J. Shin, Nurion at KISTI (KSC-2020-CRE-0027).

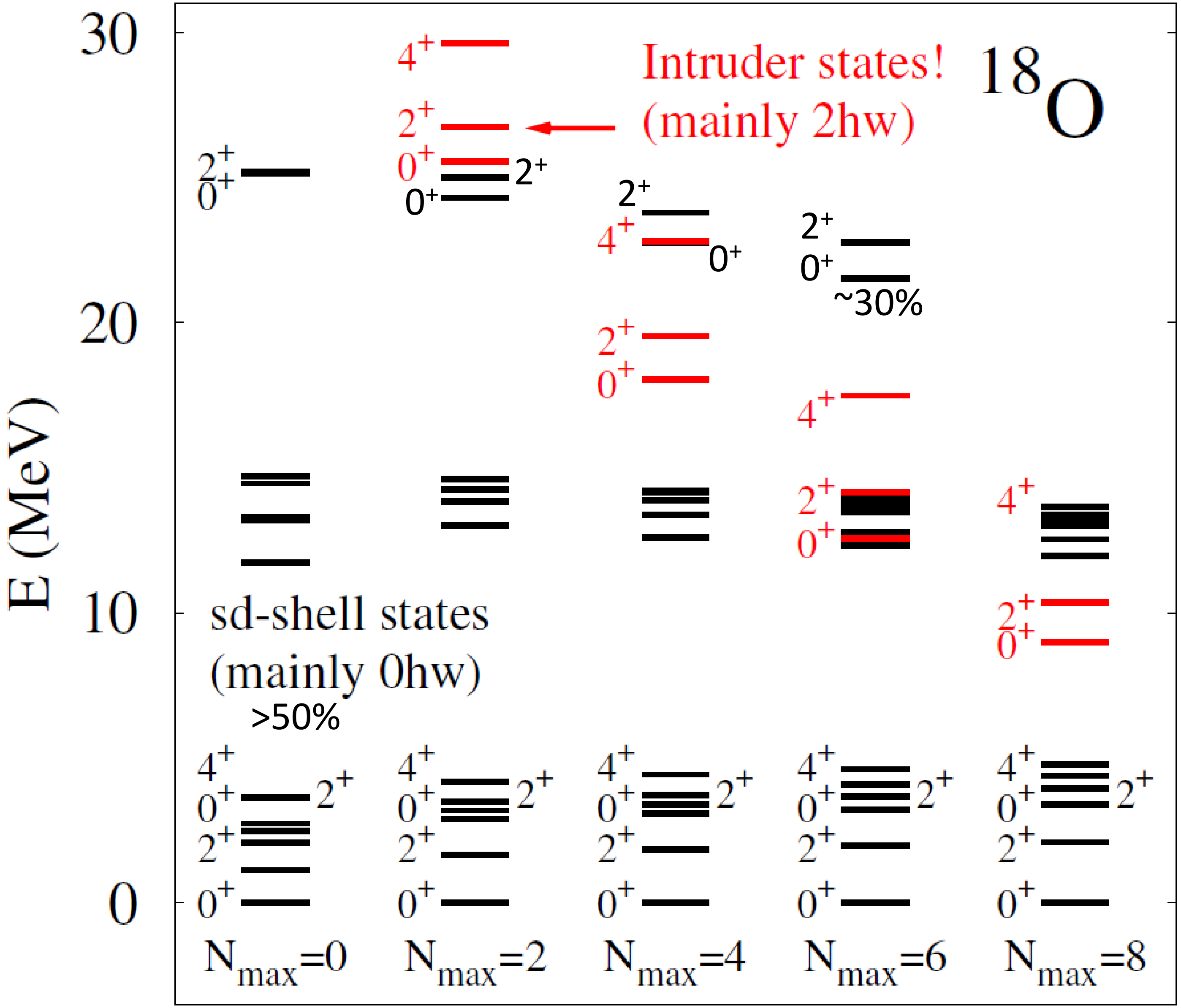
MFDn code, P. Maris, J. P. Vary et al, Iowa State University



***N. Smirnova**, B.R. Barrett, **Y. Kim, I.J. Shin**, A.M. Shirokov, E. Dikmen, P. Maris, J.P. Vary, **PRC100**, 054329 (2019)*

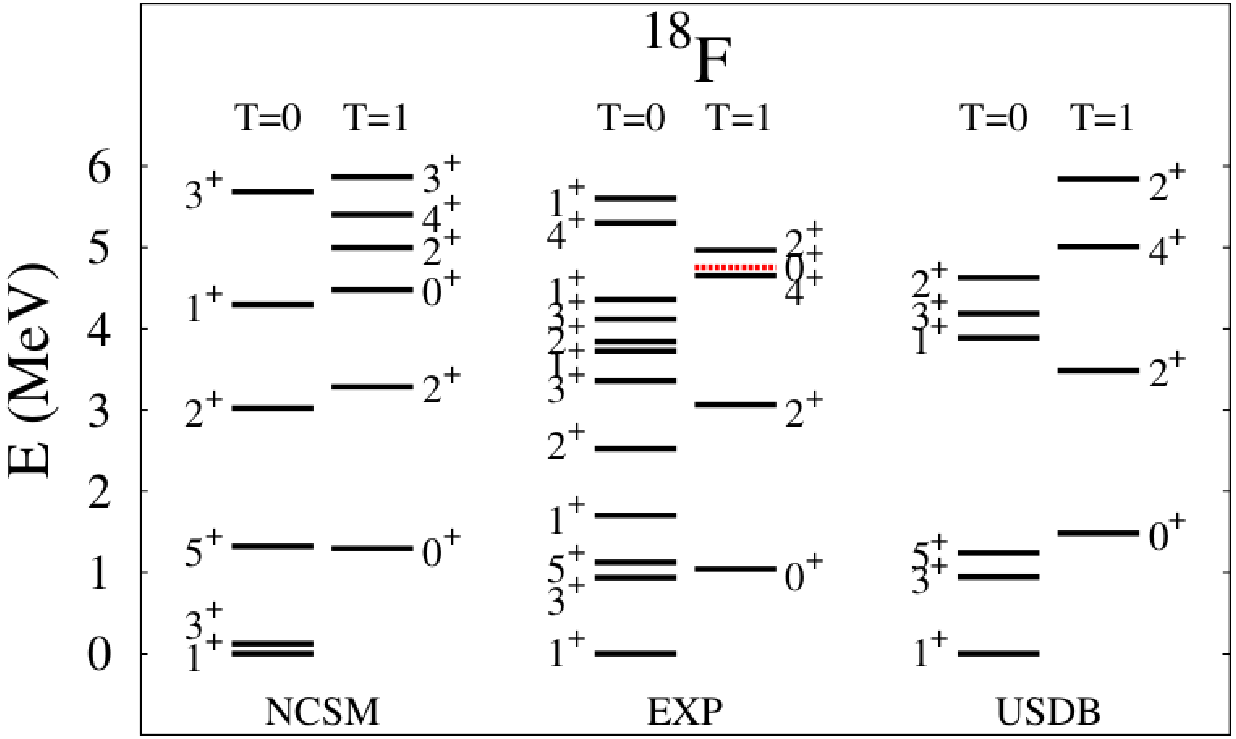
***I.J. Shin, N. Smirnova**, A.M. Shirokov, Z. Yang, B.R. Barrett, **Zh. Li, Y. Kim**, E. P. Maris, J.P. Vary, in preparation for PRC (2023)*

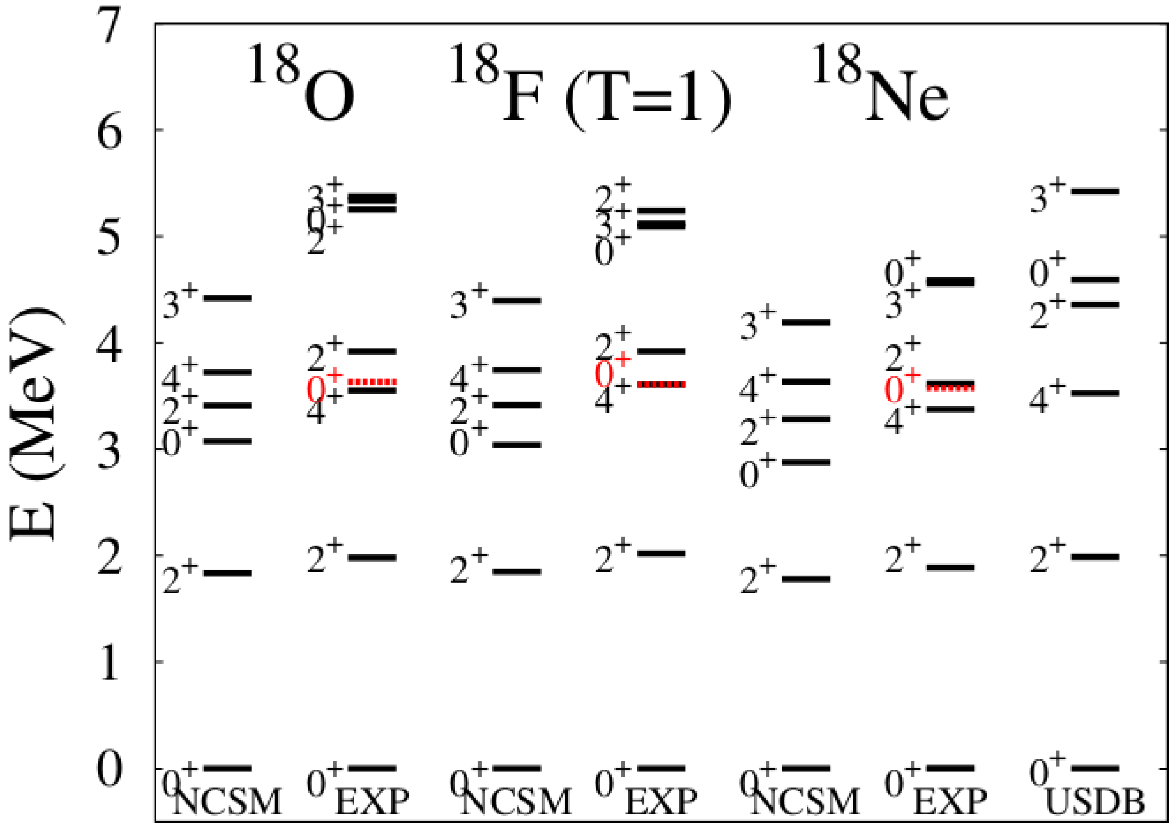
Low-energy spectrum of ^{18}O from the NCSM with Daejeon16



- The states dominated by sd-shell components are quickly converged!
- Intruder states (identified experimentally by large E2 matrix elements) are not converged yet!
- Such general structure of the spectrum is also typical for heavier sd-shell nuclei

Ab-initio effective Hamiltonian from the NCSM with Daejeon16

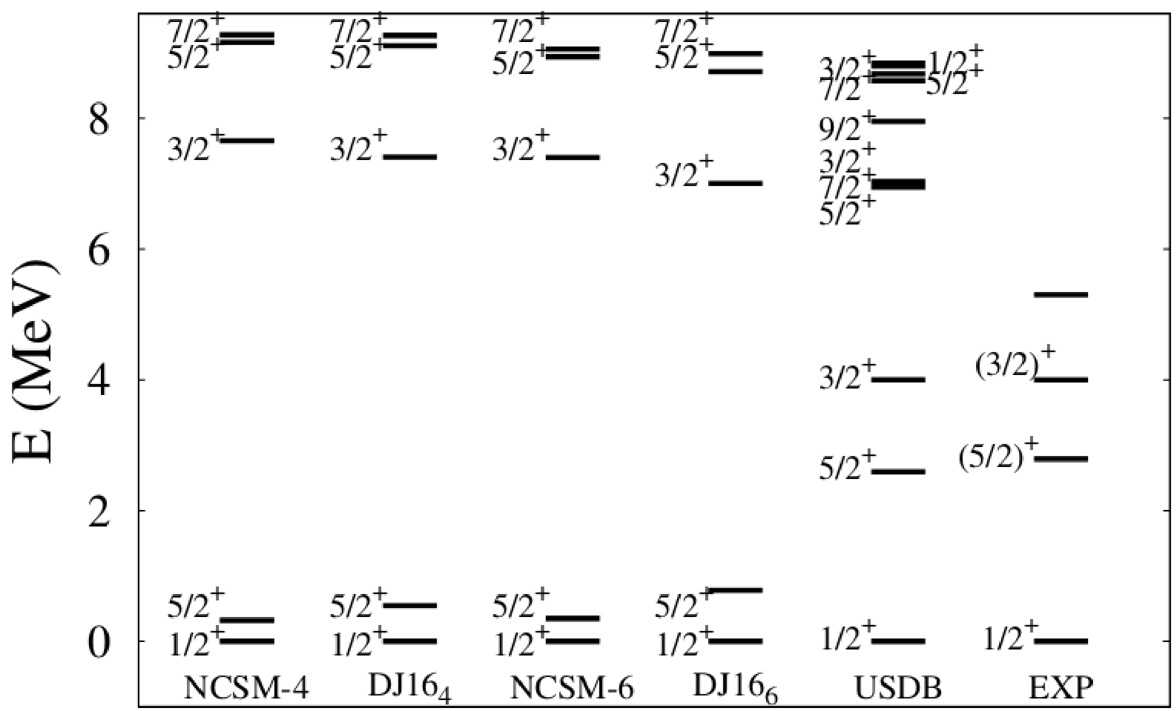




By construction, valence-space two-nucleon calculation reproduces NCSM results

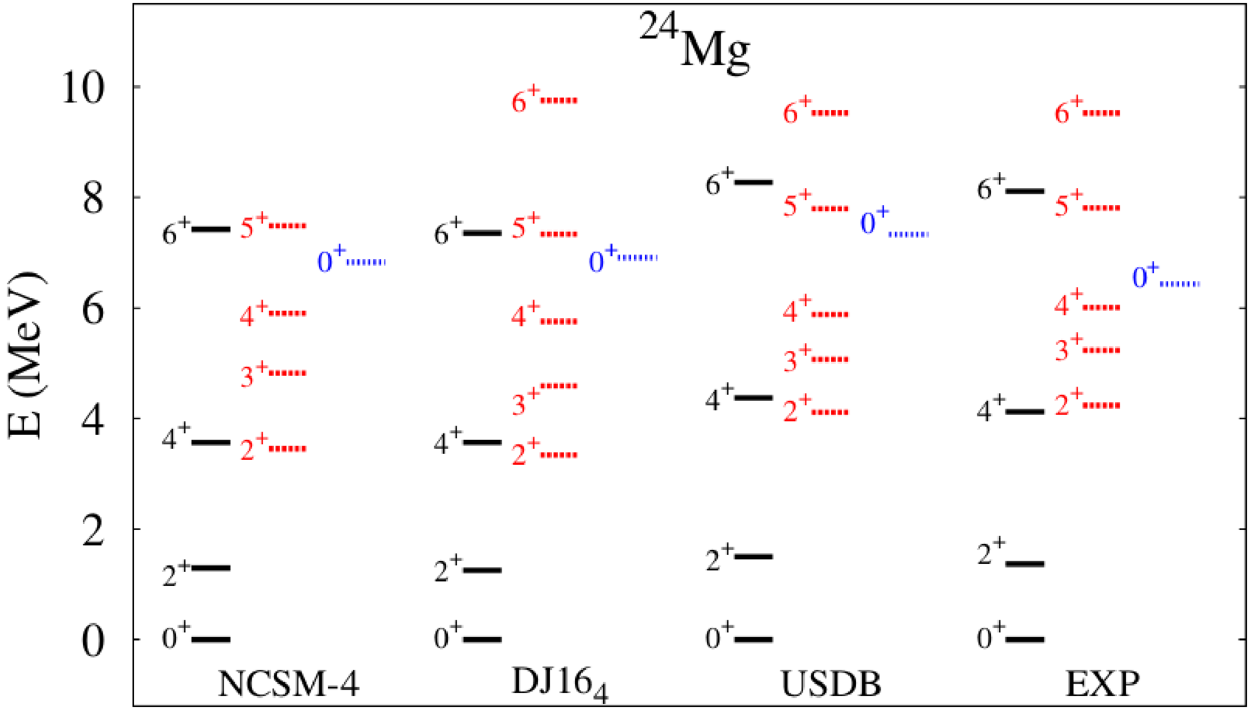
Ab-initio effective Hamiltonian from the NCSM : A>18 nuclei

^{23}O



14 states : rms error 63 keV

9 states : rms error 225 keV



Electromagnetic transition operators from the NCSM

Effective $E2$ operator in the sd shell

$$e_{n/p}(a,b)\langle b||r^2\hat{Y}_2(\hat{r})||a\rangle = \langle J_f||\hat{O}(E2)||J_i\rangle \quad (\text{from } {}^{17}\text{O}/{}^{17}F)$$

sd-shell single-particle matrix elements

from the NCSM

$$\hat{O}(E2) = \sum^{A} e_k r_k^2 \hat{Y}_2(\hat{r}_k) \quad (e_n = 0, e_p = e)$$

Bare one-body operator

State-dependent effective charges/g-factors

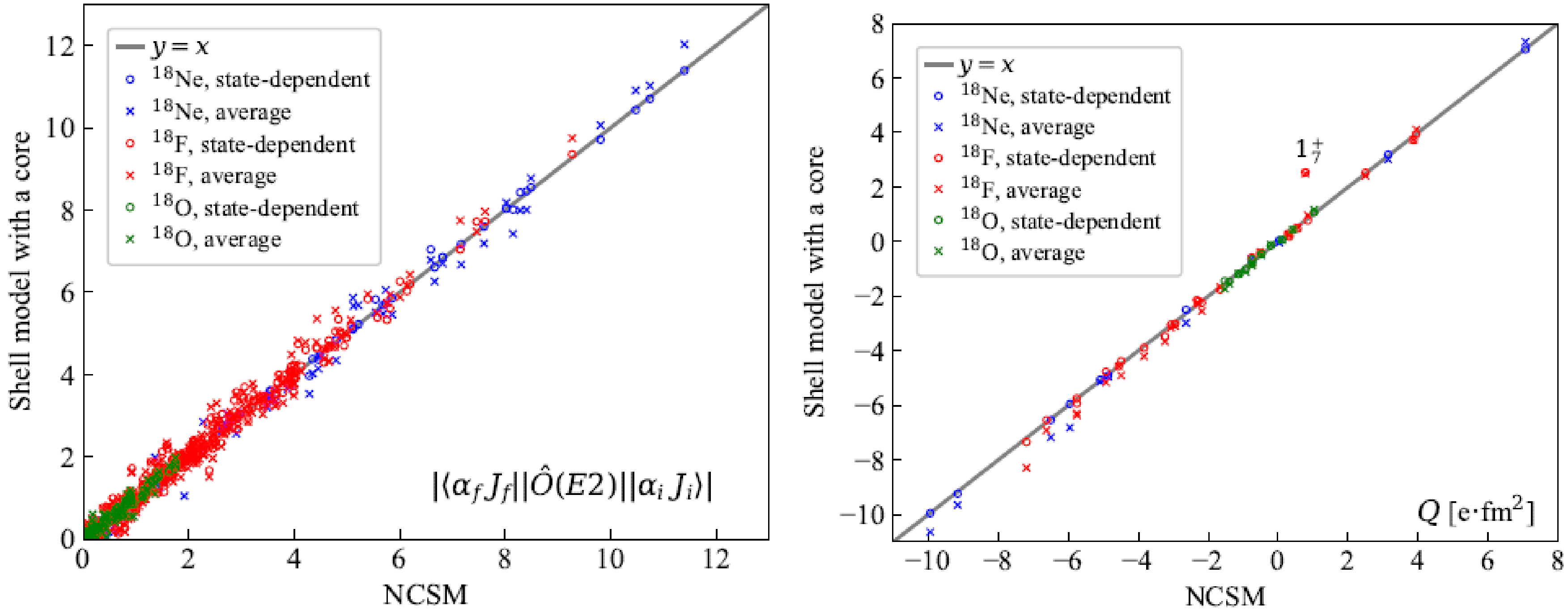
(a,b)	$e_n(a,b)$	$e_p(a,b)$	$g_n^s(a,b)$	$g_n^l(a,b)$	$g_p^s(a,b)$	$g_p^l(a,b)$
bare	0.0	1.0	-3.826	0.0	5.586	1.0
$(0d_{5/2}, 1s_{1/2})$	0.181	1.171				
$(0d_{5/2}, 0d_{3/2})$	0.281	1.236	-3.608	0.020	5.252	0.916
$(1s_{1/2}, 0d_{3/2})$	0.168	1.297				
$(0d_{5/2}, 0d_{5/2})$	0.179	1.060	-3.751	0.026	5.499	0.976
$(0d_{3/2}, 0d_{3/2})$	0.172	1.248	-3.690	0.033	5.332	0.957
$(1s_{1/2}, 1s_{1/2})$			-3.729		5.468	
	$\overline{e}_n$	$\overline{e}_p$	$\overline{g}_n^s$	$\overline{g}_n^l$	$\overline{g}_p^s$	$\overline{g}_p^l$
average	0.196	1.202	-3.695	0.026	5.388	0.950
typical	0.35	1.35	-3.826	0.0	5.586	1.0

Idem for M1 operator => Effective g-factors

Effective one-body state-dependent transition operators !

E2 operator from the NCSM : transitions and moments in A=18

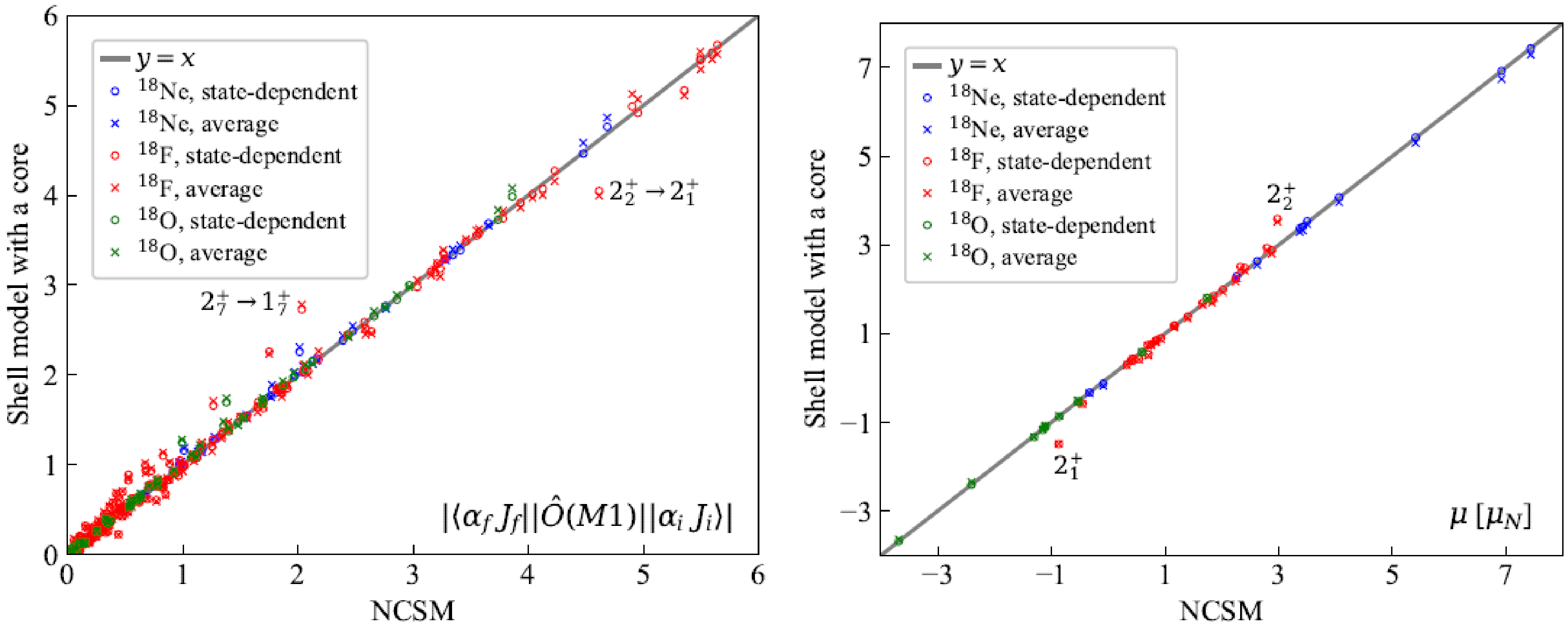
^{18}O : rms(RME) $\approx$ 0.07 e.fm^2 (66 data), rms(Q) $\approx$ 0.06 e.fm^2
^{18}F : rms(RME) $\approx$ 0.11 e.fm^2 (269 data), rms(Q)$\approx$ 0.37 e.fm^2
^{18}Ne : rms(RME)$\approx$ 0.22 e.fm^2 (66 data), rms(Q) $\approx$ 0.06 e.fm^2



Zh. Li, N. Smirnova, A.M. Shirokov, **I.J. Shin**, B.R. Barrett, P. Maris, J.P. Vary, *Effective operators for valence space calculations from the ab initio No-Core Shell Model,* Chapter in the Memorial volume devoted to Prof. A. Arima ``Symmetry, Shells, and Society''; edited by Profs. T.T.S. Kuo, K. K. Phua and T. Otsuka; World Scientific (2022).

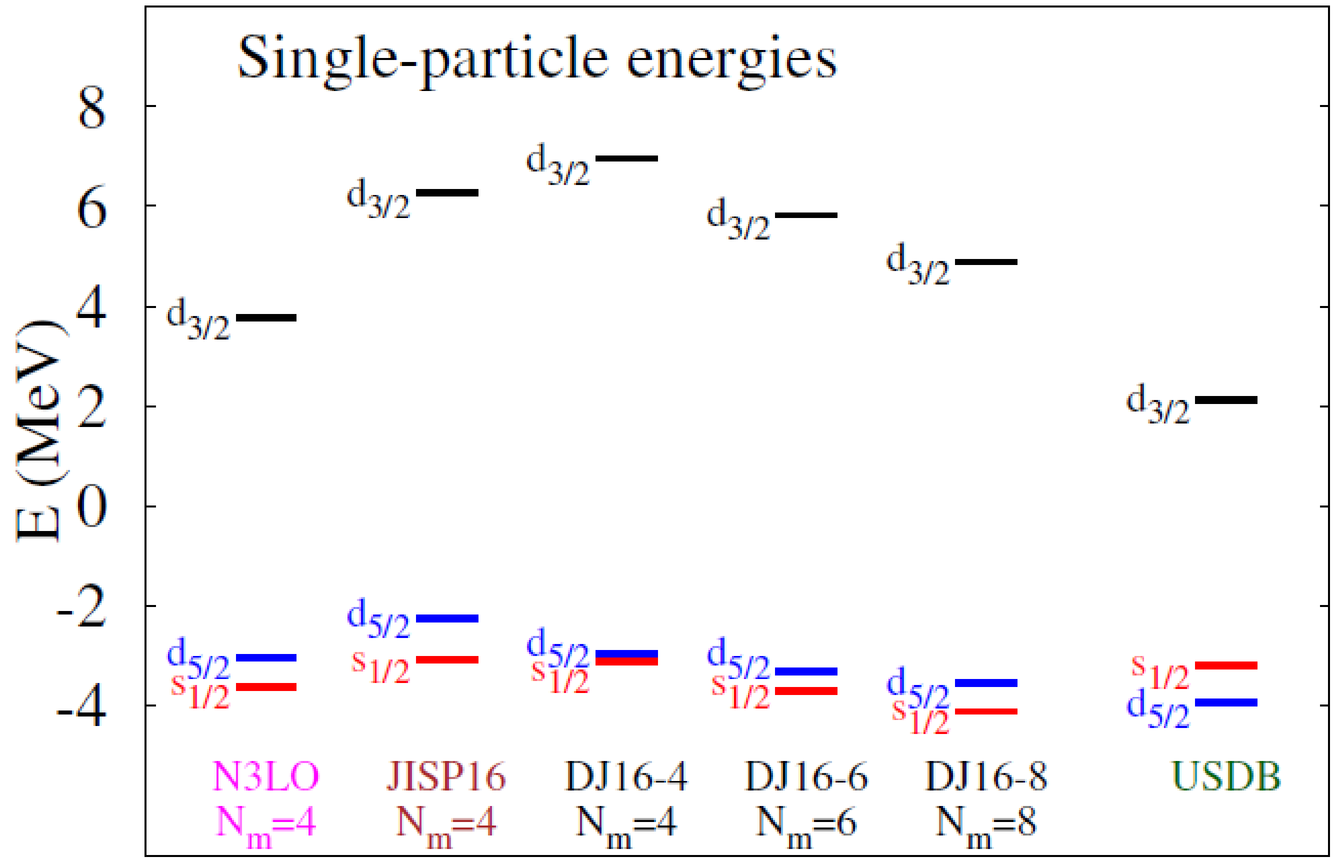
M1 operator from the NCSM : transitions and moments in A=18

^{18}O : rms(RME) $\approx$ 0.06 μ_N (43 data), rms(μ) $\approx$ 0.02 μ_N
^{18}F : rms(RME) $\approx$ 0.09 μ_N (212 data), rms(μ)$\approx$ 0.19 μ_N
^{18}Ne : rms(RME)$\approx$ 0.06 μ_N (43 data), rms(μ) $\approx$ 0.02 μ_N



Zh. Li, N. Smirnova, A.M. Shirokov, **I.J. Shin**, B.R. Barrett, P. Maris, J.P. Vary, *Effective operators for valence space calculations from the ab initio No-Core Shell Model,* Chapter in the Memorial volume devoted to Prof. A. Arima ``Symmetry, Shells, and Society''; edited by Profs. T.T.S. Kuo, K. K. Phua and T. Otsuka; World Scientific (2022).

Ab-initio effective Hamiltonian from the NCSM : Theory & Experiment



Drawbacks for all NN potentials:

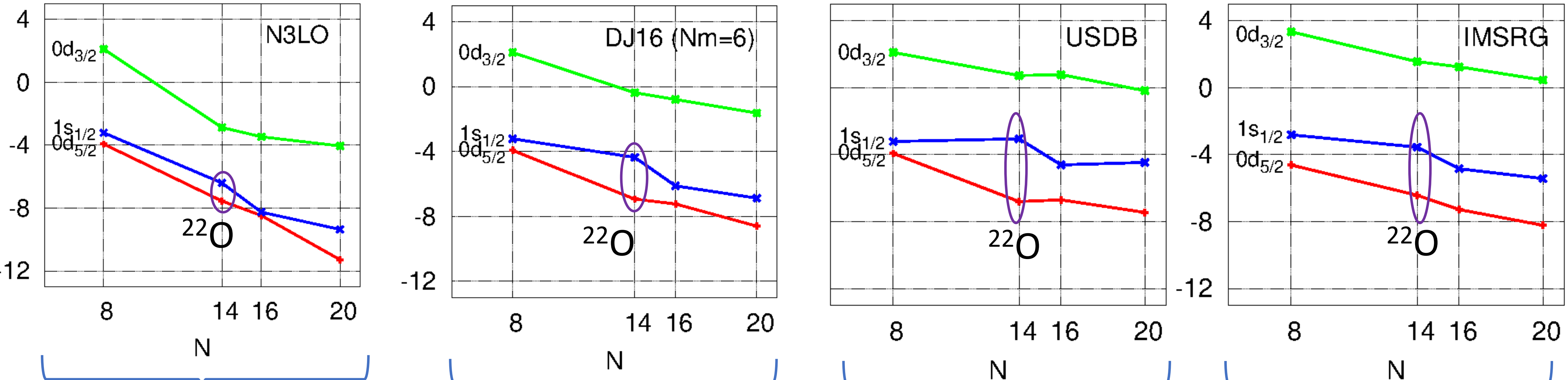
- ❑ *Inversion of s1/2 and d5/2 orbitals*
- ❑ *Too large d3/2 – d5/2 spin-orbit splitting*

We adopt USDB single-particle energies and impose an $A^{-1/3}$ mass dependence on TBMEs

N3LO : from chiral EFT by D.R.Entem, R.Machleidt, PRC68 (2003)
JISP16 : A.M. Shirokov et al, PRC70, 044005 (2004)
Daejeon16 : A.M. Shirokov et al, PLB761, 87 (2016) – based on N3LO + SRG evolved + phase-equivalently transformed

Comparison of monopole properties valence-space interactions

Neutron ESPEs in O-isotopes



From NN interaction

From Daejeon16 NN interaction

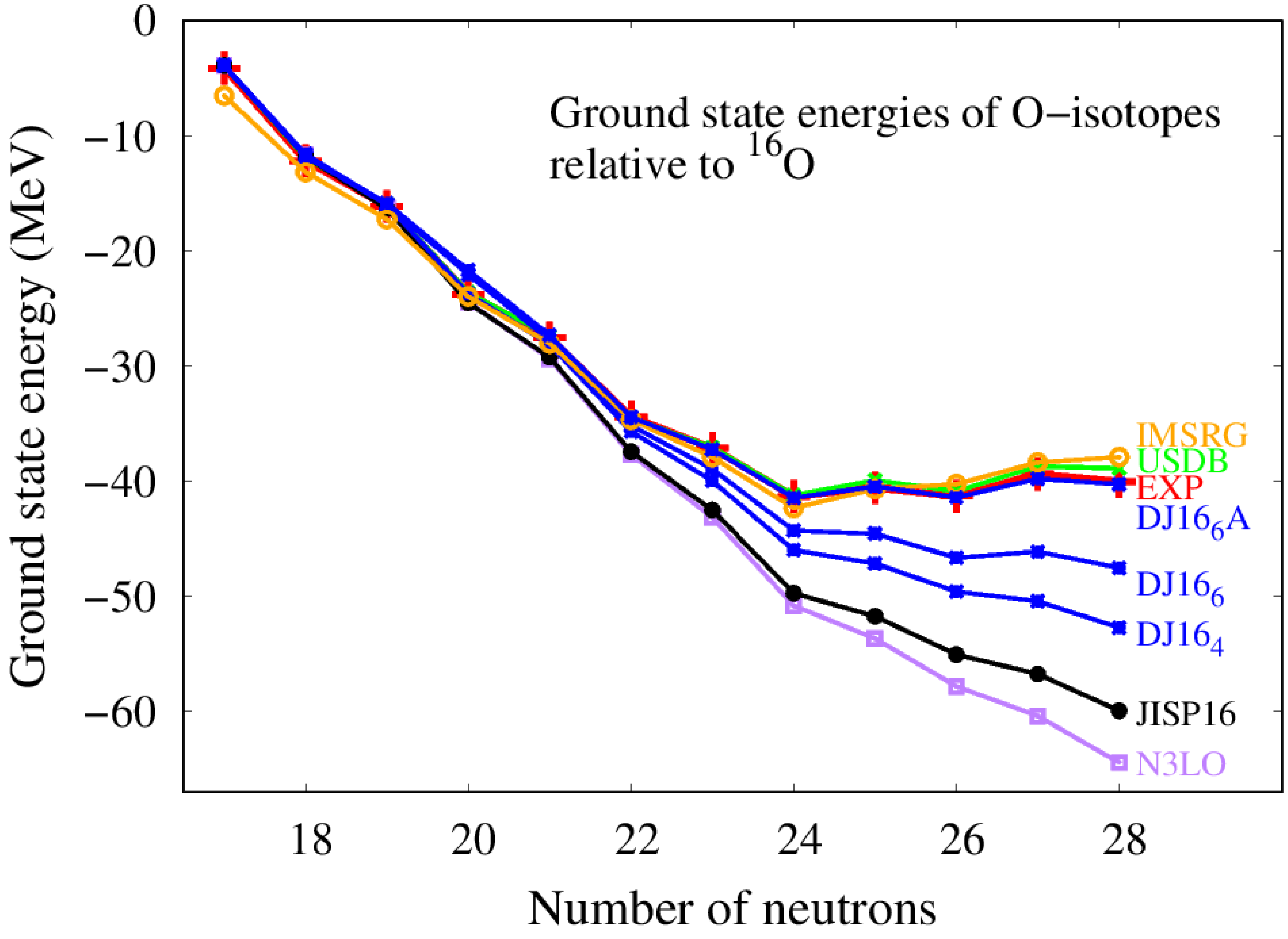
Empirical = experiment

From NN+3N interaction

Small monopole modifications to DJ16 (change of centroids by ~100-300 keV) are needed !

N. Smirnova, B.R. Barrett, Y. Kim, I.J. Shin, A.M. Shirokov, E. Dikmen, P. Maris, J.P. Vary, ***PRC100****, 054329 (2019)*
I.J. Shin, N. Smirnova, A.M. Shirokov, Z. Yang, B.R. Barrett, Zh. Li, Y. Kim, E. P. Maris, J.P. Vary, in preparation for PRC (2023)

Ab-initio effective Hamiltonian from the NCSM



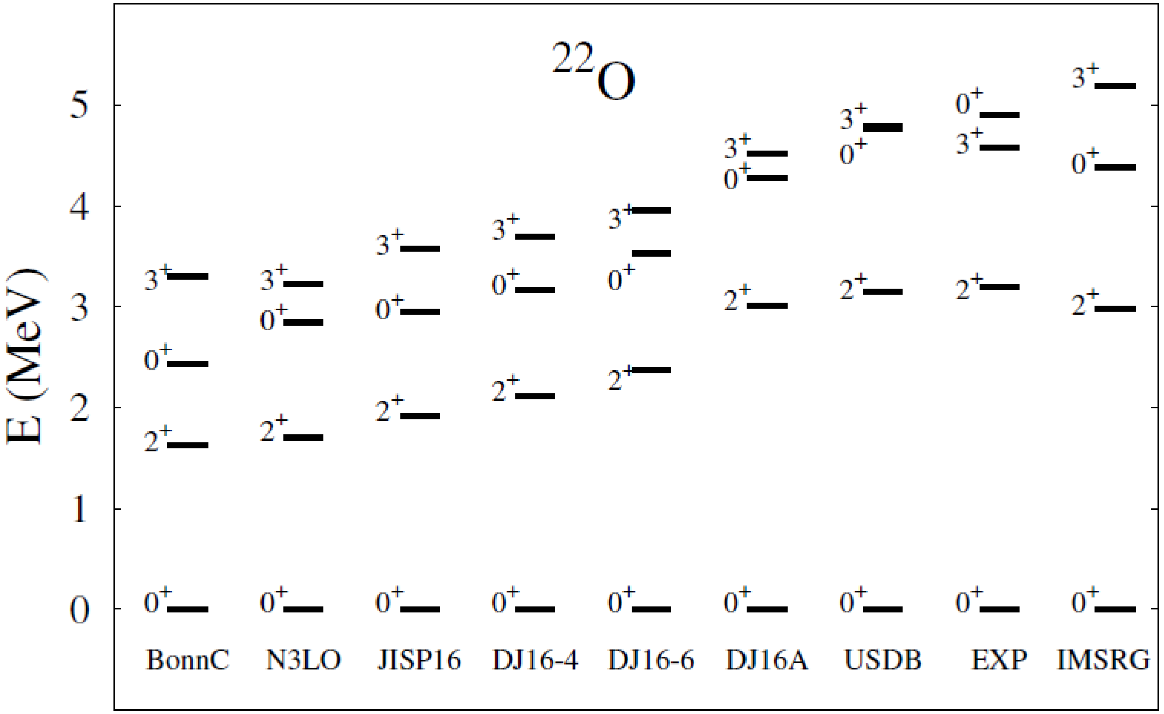
$DJ16_6$: rms = 3671 keV

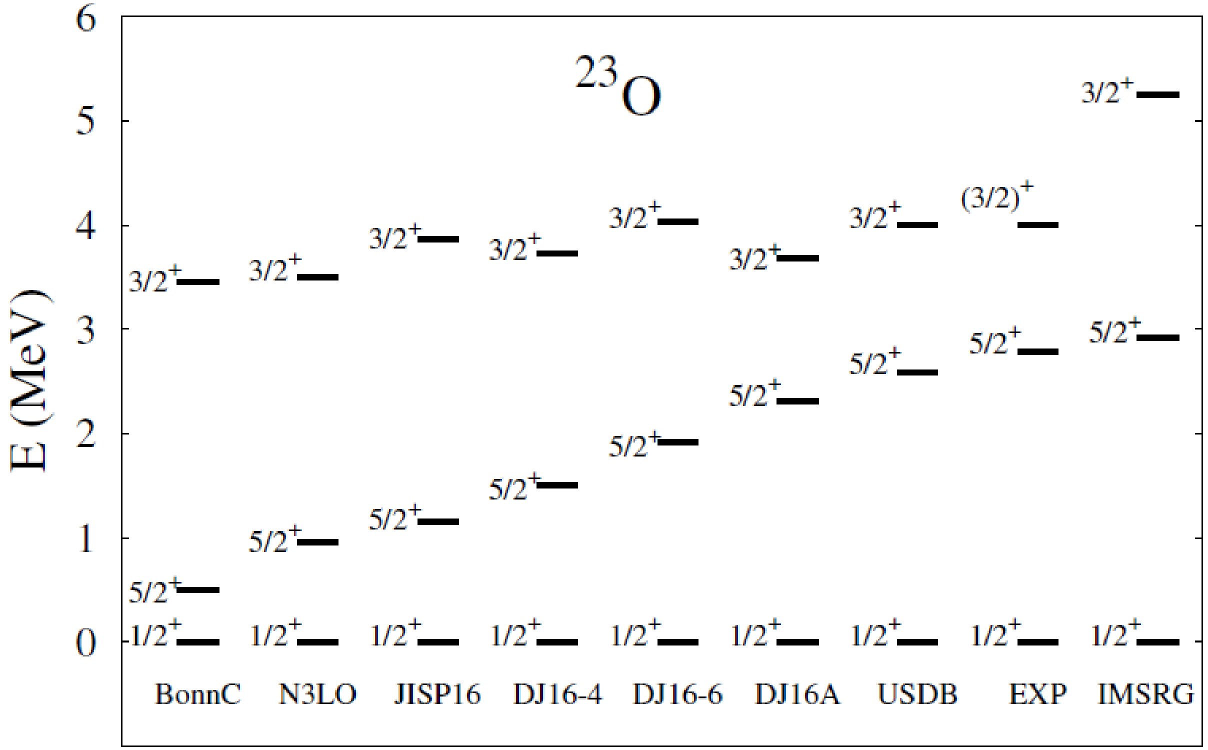
$DJ16_6A$ ($DJ16_6$ with monopole modifications): rms = 235 keV

USDB : rms =467 keV

« Improved sd shell effective interactions from Daejeon16 »
I.J. Shin, N. Smirnova, A.M. Shirokov, Z. Yang, B.R. Barrett, Zh. Li, Y. Kim, E. P. Maris, J.P. Vary, in preparation for PRC (2023)

Ab-initio effective Hamiltonian from the NCSM



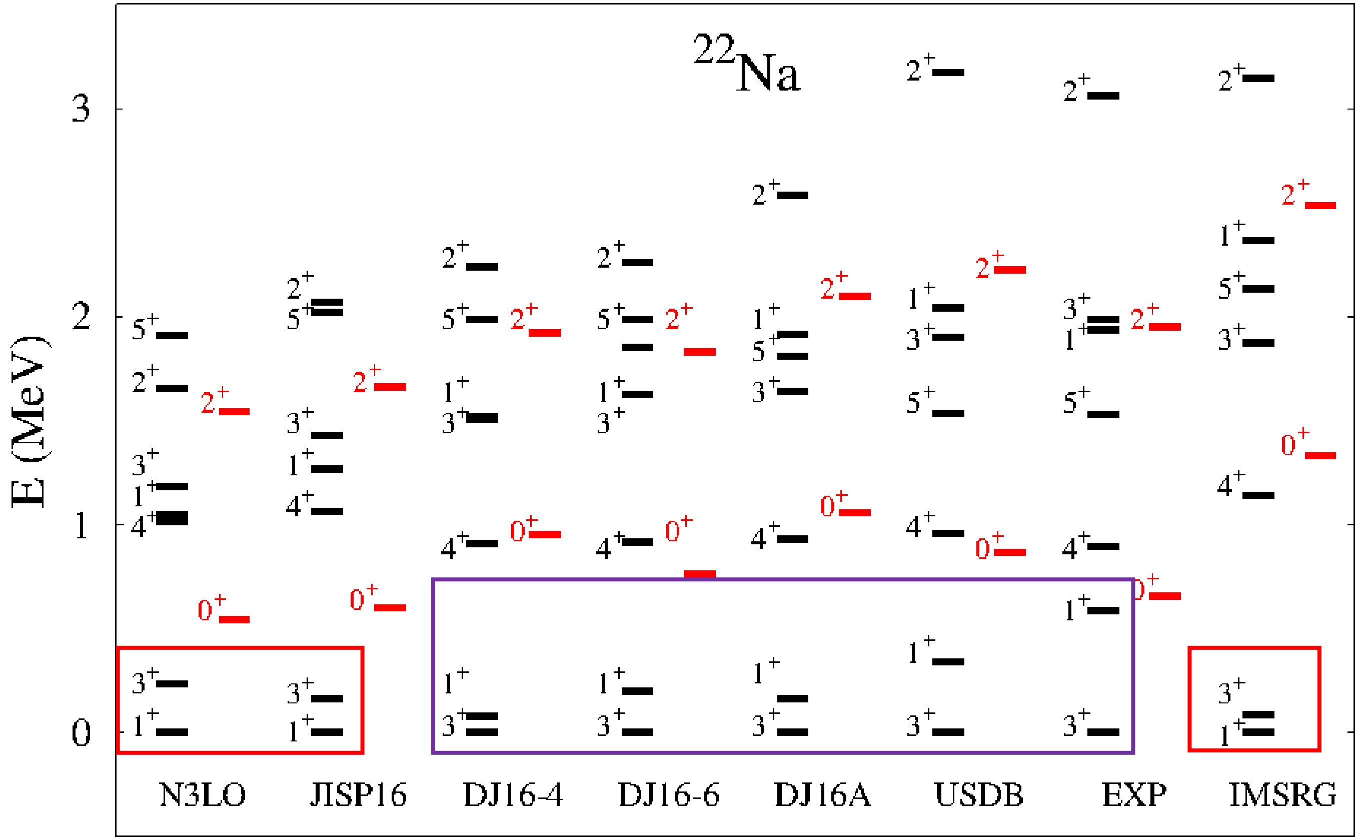


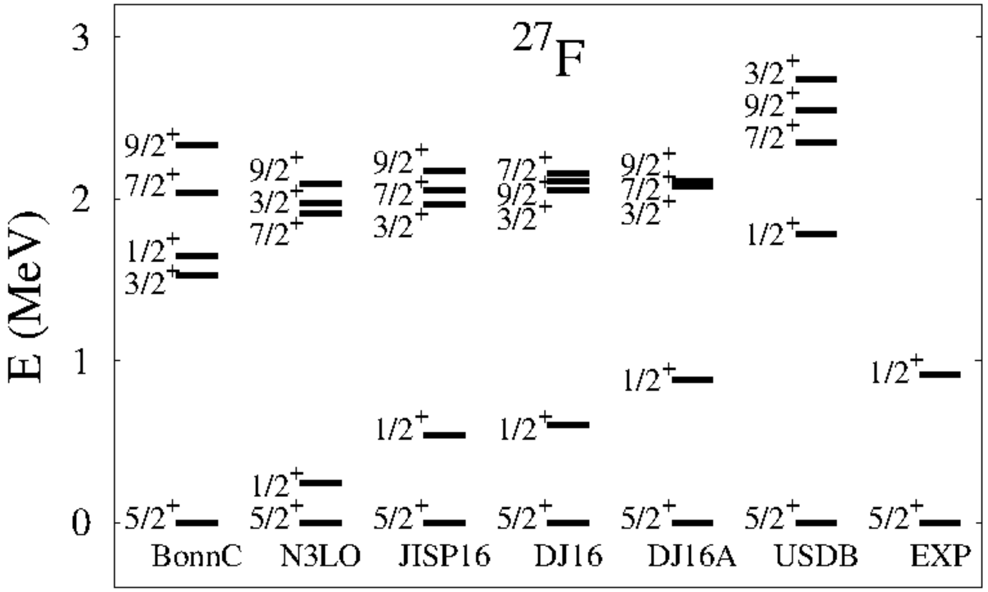
Increase of N=14 subshell gap

DJ16A is DJ16-4 with monopole modifications

Increase of N=14 subshell gap

Microscopic effective interactions





RMS (microscopic) > RMS (phenomenological)

Goals of the Present Project

- Improvement of the Daejeon16 potential (refining of Phase-Equivalent Transformations up to A=17 to get robust single-particle energies and to avoid monopole adjustments and) – work in progress

- Incorporation of the charge-dependence (pp, nn and pn channels) !

- Extension of the NCSM calculations with Daejeon16 to larger model spaces N_{max}=8 and derivation of sd shell interactions via OLS transformation

- Construction of consistent effective electromagnetic operators for newly derived valence space Hamiltonians

- Construction of effective interaction for 1hw valence-spaces (*p-sd-pf*), necessary for the description of negative parity states in the sd-shell nuclei (vital for nuclear astrophysics)

I.J. Shin, Y. Kim, Nurion at KISTI (KSC-2022-CRE-0373 and KSC-2023-CHA-0005)

N. Smirnova, Z. Li, MCIA, University of Bordeaux

Conclusions and Perspectives

- Daejeon16: high-precise NN potential which effectively includes 3N and many-nucleon forces

- Micrscopic valence-space interactions obtained via OLS transformation of the NCSM solution look encouraging.

- This work paves the way towards microscopic foundations of the nuclear shell model and links it to the *ab-initio* nuclear theory

- Importance of further developments of microscopic approaches towards precision nuclear theory for spectroscopy of exotic nuclei, fundamental interaction studies and astrophysical applications

Budget Requests

LIA specific funding requested from France		
Description	**Amount (euros)**	**Requested to: ***
Visit of N. Smirnova to Daejeon, Korea (travel costs)	1250	IN2P3
Visit of Zh. Li to Daejeon, Korea (travel costs)	1250	IN2P3
Visit of Y. Kim to Bordeaux, France (local costs)	1000	IN2P3
Visit of I.J.. Kim to Bordeaux, France (local costs)	1000	IN2P3
Total	4500	

THANK YOU FOR YOUR ATTENTION !