Effective interactions and effective operators from the No-Core Shell Model

N. A. Smirnova, Zhen Li, *LP2IB, CNRS/IN2P3 – University of Bordeaux, France*
I.J.Shin, Y. Kim, *IBS, Daejeon, Republic of Korea*
A.M. Shirokov, *SINP, Moscow State University, Russia*
B.R. Barrett, *Arizona State University, USA*
J.P. Vary, P. Maris, *Iowa State University, USA*

Nuclear Tapas: the Shell Model as a Cornerstone of Nuclear Structure
Workshop in honor to scientific carrier of Prof. Alfredo Poves,
Madrid, 27 – 28 April 2023

Effective interactions and effective operators from the No-Core Shell Model

- ❑ **Introduction**

- ❑ **Formalism**: *ab-initio* effective sd-shell Hamiltonian from the NCSM solution for A=18 via Okubo-Lee-Suzuki similarity transformation

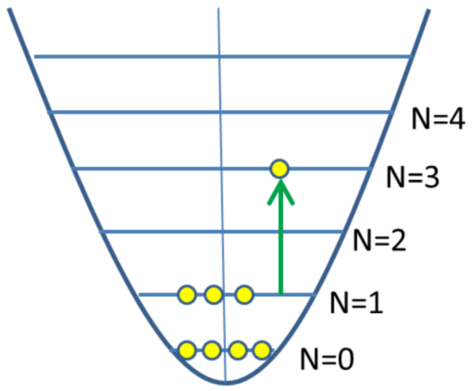
- ❑ **Theory & Theory**:
  - comparison of the NCSM solution with Daejeon16 with valence-space calculations for A>18 ;
  - construction of effective electromagnetic operators.

- ❑ **Theory & Experiment**: Analysis of TBMEs, monopole corrections and comparison with experiment and with phenomenological USDB interaction

- ❑ **Conclusions and prospects**

Shell model - (full) configuration-interaction approach

$$H = T + V = \underbrace{(T + U)}_{\text{Independent particle Hamiltonian}} + \underbrace{(V - U)}_{\text{residual interaction}} = H_0 + V_{res}$$

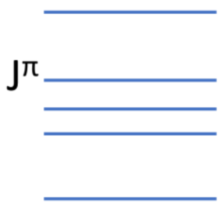


$$\boxed{H|\Psi_n\rangle = E_n|\Psi_n\rangle}$$

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

$$\boxed{H_0|\Phi_k\rangle = E_k^0|\Phi_k\rangle} \qquad \boxed{\langle\Phi_k|\Phi_l\rangle = \delta_{kl}}$$

$$\boxed{\sum_{k=1}^{d}\langle\Phi_l|H|\Phi_k\rangle\, c_{kn} = E_n c_{ln}} \Rightarrow \begin{pmatrix} H_{11} & H_{12} & \cdots & H_{1d} \\ H_{21} & H_{22} & \cdots & H_{2d} \\ \vdots & & \ddots & \\ H_{d1} & H_{d2} & \cdots & H_{dd} \end{pmatrix} \Rightarrow$$

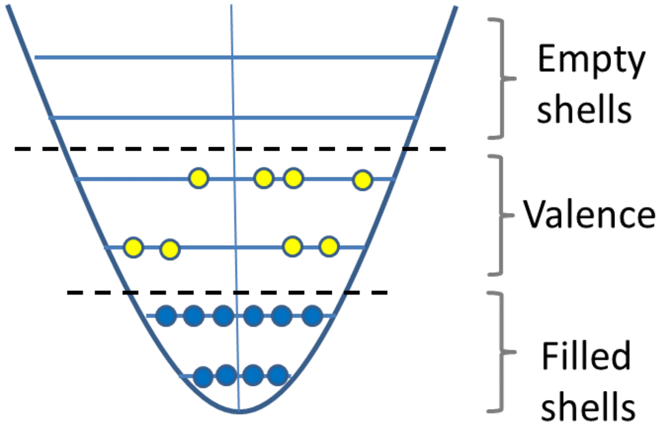


Ab-initio **No-Core Shell Model : sufficiently large model space so that the results for A nucleons do not depend on the basis parameters (hw and Nmax)**

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

Valence-space shell model for heavier nuclei

Restricted model space



Effective operators

$$\boxed{H|\Psi_n\rangle = E_n|\Psi_n\rangle} \longrightarrow \boxed{H_{eff}|\Psi_n^M\rangle = E_n|\Psi_n^M\rangle}$$

$$H = T + V = \underbrace{(T+U)}_{\text{exactly solvable}} + \underbrace{(V-U)}_{\text{residual interaction}} = H_0 + V_{res}$$

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

Empirical

Microscopic

Semi-microscopic (microscopic, constrained by the data)

Empirical

- **Current status :**
- Excellent description with empirical (phenomenological) interactions
- Microscopic interactions -> recent progress and challenges

Effective Interactions : monopole-multipole decomposition

Multipole decomposition :

$$H = \sum_\alpha \varepsilon_\alpha a_\alpha^\dagger a_\alpha + \frac{1}{4}\sum_{ijkl,\lambda} w_{ijkl,\lambda} [\, a_i^\dagger \tilde{a}_j \,]^{(\lambda)} [\, a_k^\dagger \tilde{a}_l \,]^{(\lambda)} + \cdots$$

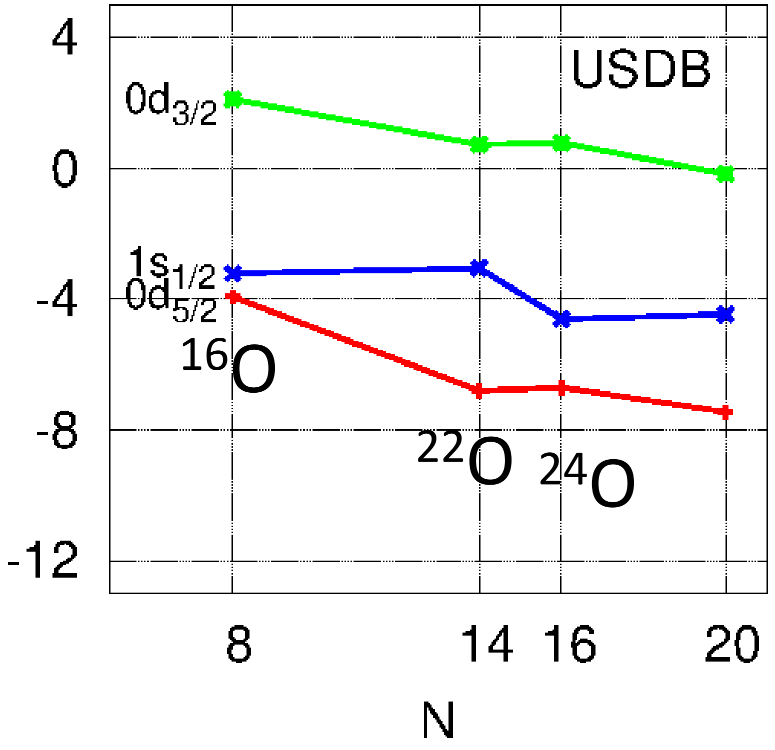
$$H = \underbrace{\sum_i \varepsilon_i n_i + \sum_{i<j} \bar{V}_{ij} \frac{n_i(n_j-\delta_{ij})}{1+\delta_{ij}}}_{\text{Monopole part (spherical mean-field)}} + \underbrace{V_{pair} + V_{quad} + \cdots}_{\text{Multipole part (correlations)}}$$

Monopole part
(spherical mean-field)

Multipole part
(correlations)

- **Important to understand the nature of nuclear excitations (competition between sphericity and deformation)**
- **Crucial to understand defects of microscopic interactions and a way towards improvements**

Neutron ESPEs in O-isotopes
(from monopole part)



USDB – universal sd interaction: W.A. Richter, B.A.Brown, PRC74 (2006)

A.Poves, A.P. Zuker, Phys. Rep. 70, 235 (1981)
A.P. Zuker & M. Dufour, arXiv.org:nucl-th/9505012; PRC54, 1641 (1996),….
E. Caurier, G. Martinez-Pinedo, F. Nowacki, A. Poves, A.P. Zuker, RMP77,427 (2005)

Microscopic approaches to valence-space interactions

$$H|\Psi_k\rangle = E_k|\Psi_k\rangle$$

$$\langle\Psi_f|O|\Psi_i\rangle = O_{fi}$$

Effective operators

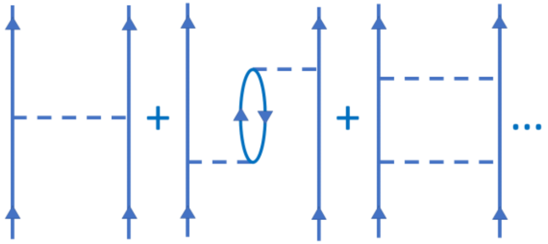
$$H_{eff}|\Psi_k^M\rangle = E_k|\Psi_k^M\rangle$$

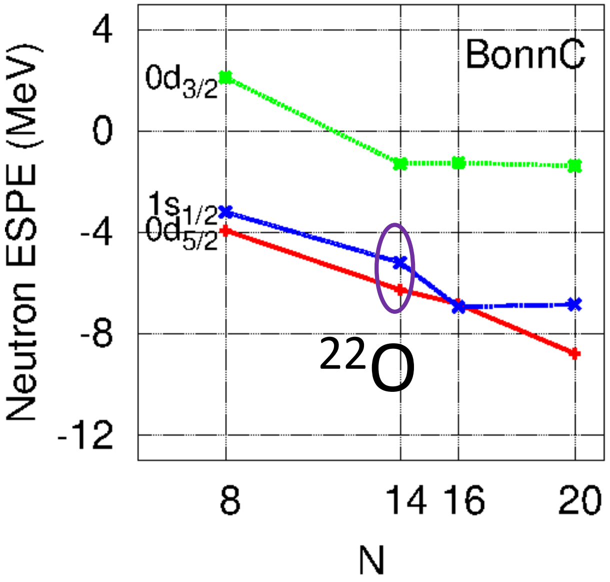
$$\langle\Psi_f^M|\,O_{eff}|\Psi_i^M\rangle = O_{fi}$$

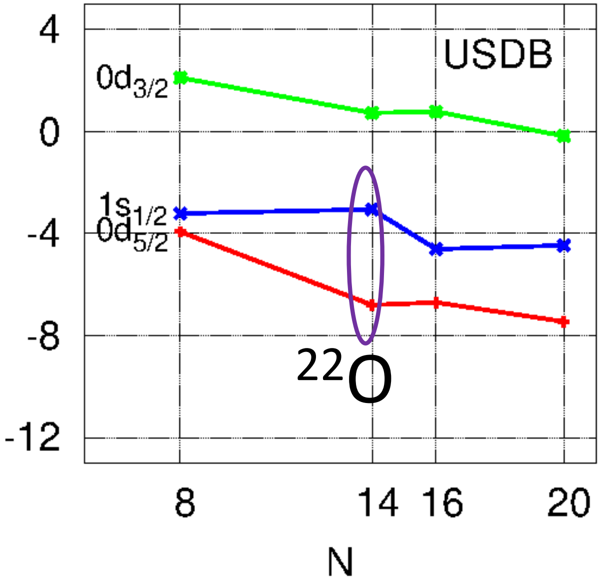
Many-body perturbation theory based on the G-matrix (NN)

G.F. Bertsch, T.T.S. Kuo, G.F. Brown, B.R. Barrett, M. Kirson, …. (from 60's)
M. Hjorth-Jensen, T.T.S. Kuo, E. Osnes, PR261, 126 (1995)

Veff =







Poor description of the monopole term (spherical mean-field) ⟵ Missing 3N forces

Conjectured : A.Poves, A.P. Zuker, PR70 (1981)
A.P. Zuker, PRL90, 042502 (2003)
Confirmed : T. Otsuka et al (2010), J. Holt et al (2012, 2014,..); L. Coraggio et al (2018 – 2020), etc.

Microscopic approaches to valence space interactions

Non-perturbative approaches :

For review see S. R. Stroberg, H. Heigert, S.K. Bogner, J.D. Holt, Ann. Rev. Nucl. Part. Science ***69,*** *307 (2019).*

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

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

  $\boxed{H(s) = U(s)H(0)U^{\dagger}(s),}$ $\boxed{dH(s)/ds = [\eta(s), H(s)]}$

- **OLS transformation applied to NCSM results**

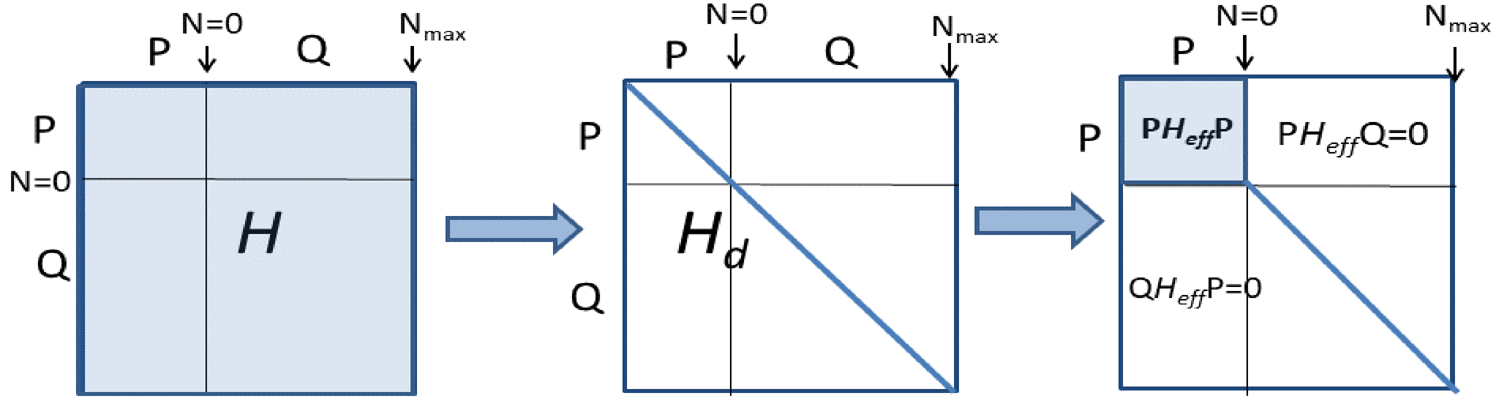
  E. Dikmen, A.F. Lisetskiy, B.R. Barrett, P. Maris, A.M. Shirokov, J.P. Vary, PRC91, 064301 (2015)
  N.Smirnova, B.R. Barrett, I.J. Shin, Y.Kim, A.M. Shirokov, E. Dikmen, P. Maris, J.P. Vary, PRC100, 054329 (2019)

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

  G.R. Jansen et al, PRC94, 011301 (2016); Z.H. Sun, T.D. Morris, G. Hagen et al, PRC98, 054320 (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

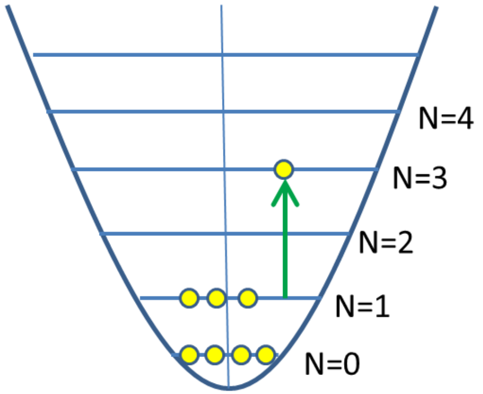
- ❑ ^{18}F from the NCSM at N_{max}
- ❑ H_{eff} for ^{18}F at N=0
- ❑ ^{16}O from the NCSM at N_{max}
  - ➡ Core energy
- ❑ ^{17}O, ^{17}F from the NCSM at N_{max}
  - ➡ One-body terms
- ❑ Single-particle energies $\boldsymbol{\varepsilon_i}$

two-body matrix elements $\boldsymbol{V_{ijkl}}$

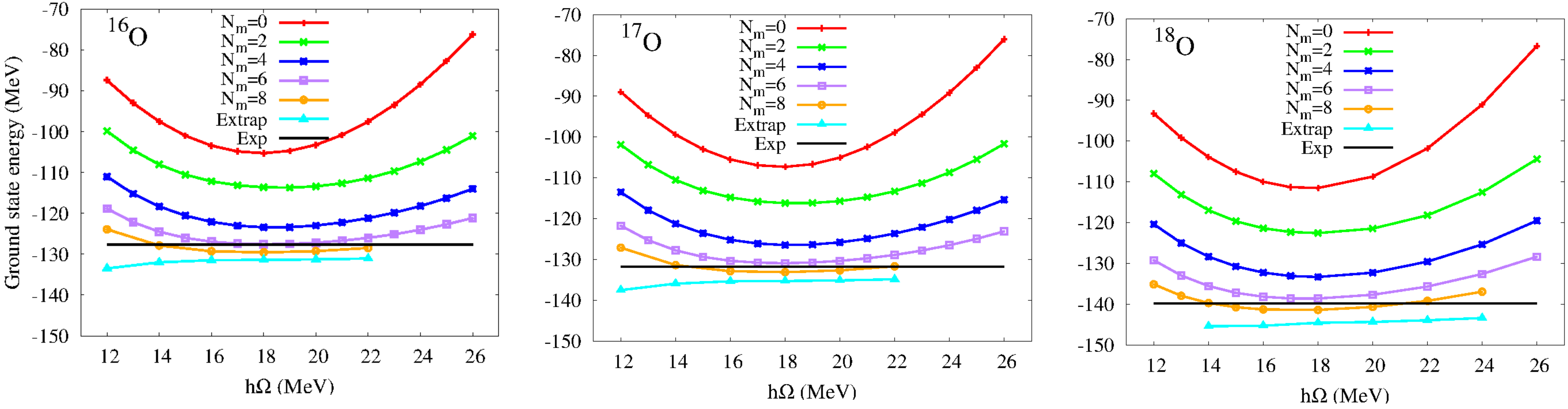
S. Okubo, Prog. Theor. Phys. 12 (1954); K. Suzuki, S. Lee, Prog. Theor. Phys. 68 (1980)
E. Dikmen, A.F. Lisetskiy, B.R. Barrett, P. Maris, A.M. Shirokov, J.P. Vary, PRC91, 064301 (2015)
J.P. Vary , R. Basili, W.Du, M. Lockner, P. Maris, S.Pal, S.Sarker PRC98, 065502 (2018)
N.Smirnova, B.R. Barrett, I.J. Shin, Y.Kim, A.M. Shirokov, E. Dikmen, P. Maris, J.P. Vary, PRC100 (2019)

No-Core Shell Model

$$H = \sum_{i<j} \frac{\left(\vec{p_i} - \vec{p_j}\right)^2}{2mA} + \sum_{i<j}^{A} V_{ij} + \left(\sum_{i<j<k}^{A} V_{ijk} \right)$$



Daejeon16 NN potential (N3LO + SRG evolved + PETs)

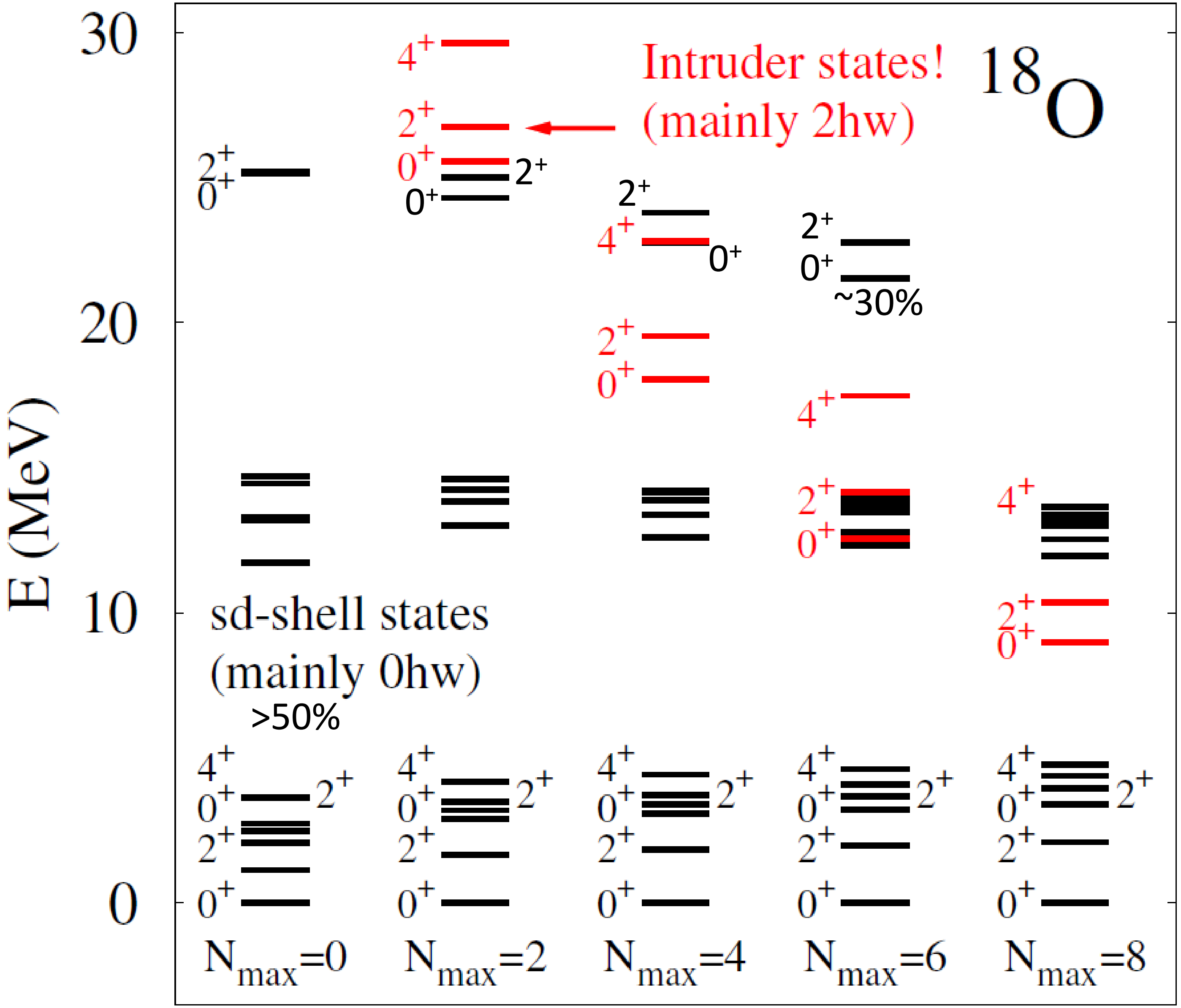


Daejeon16: *A.M. Shirokov, I.J. Shin, et al, PLB 761, 87 (2016)*

B.R. Barrett, P. Navratil, J.P. Vary, Ab initio no core shell model, ***PPNP 69****, 131 (2013).*

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

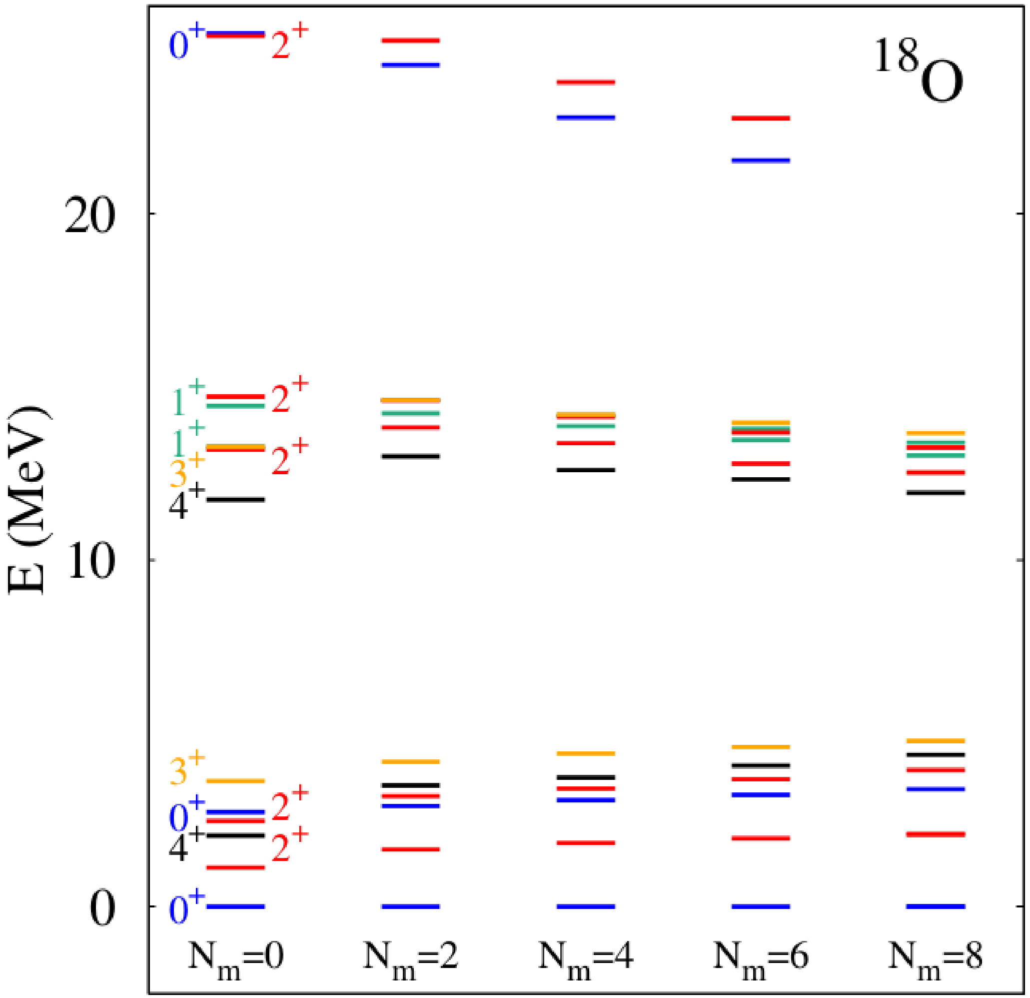
Low-energy spectrum of ^{18}O from the NCSM with Daejeon16

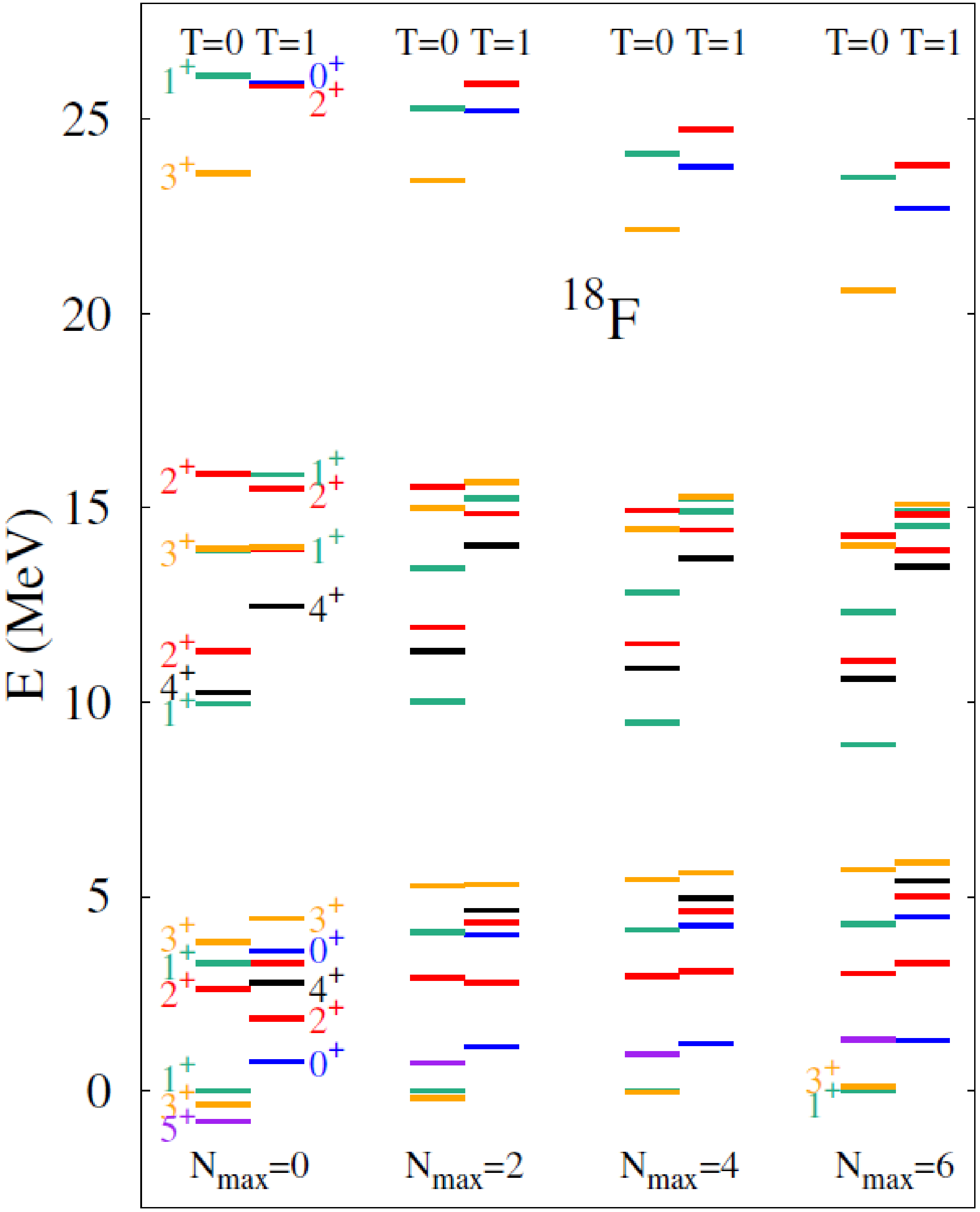


- The states dominated by sd-shell components are quickly converged!
- Intruder states (identified experimentally by large E2 matrix elements) are not converged yet!
- Such general structure of the spectrum is also typical for heavier sd-shell nuclei

Selected states for A=18

$\hbar\Omega = 14\ MeV$



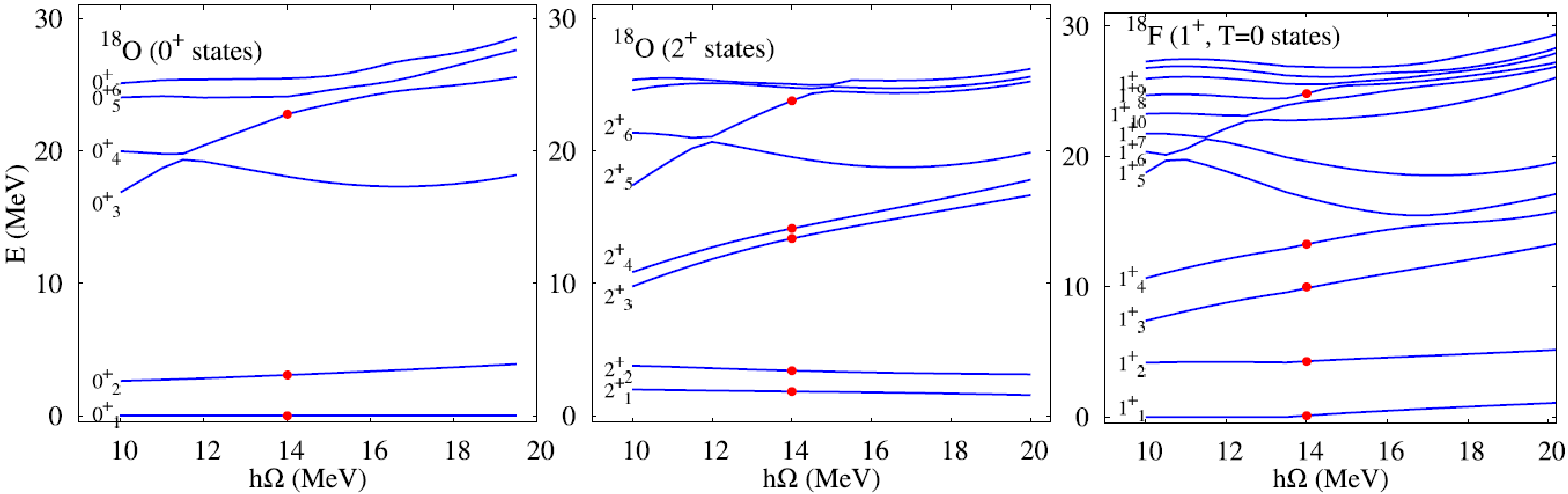


<30% of N=0 component

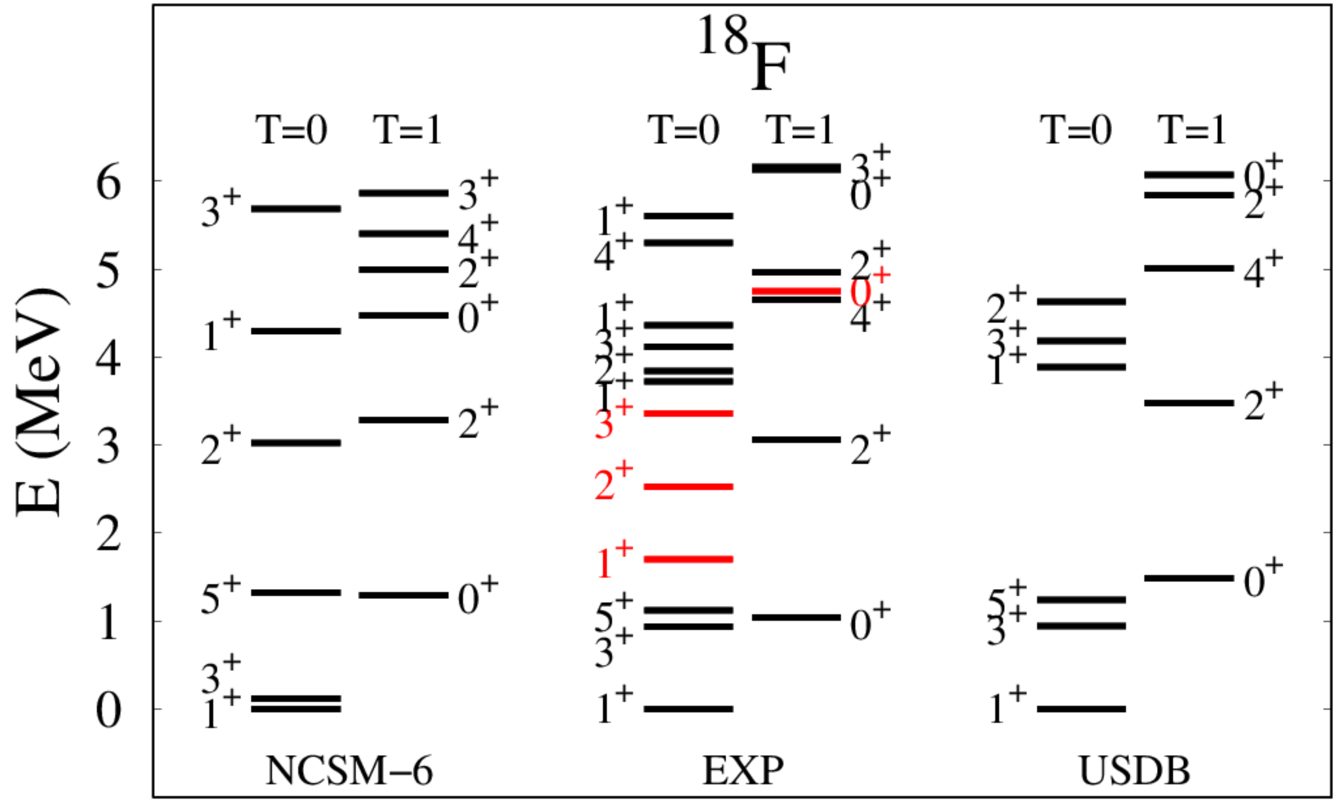
>50% of N=0 component

Excitation spectra for a given J,T and state selection for A=18 as a function of hΩ

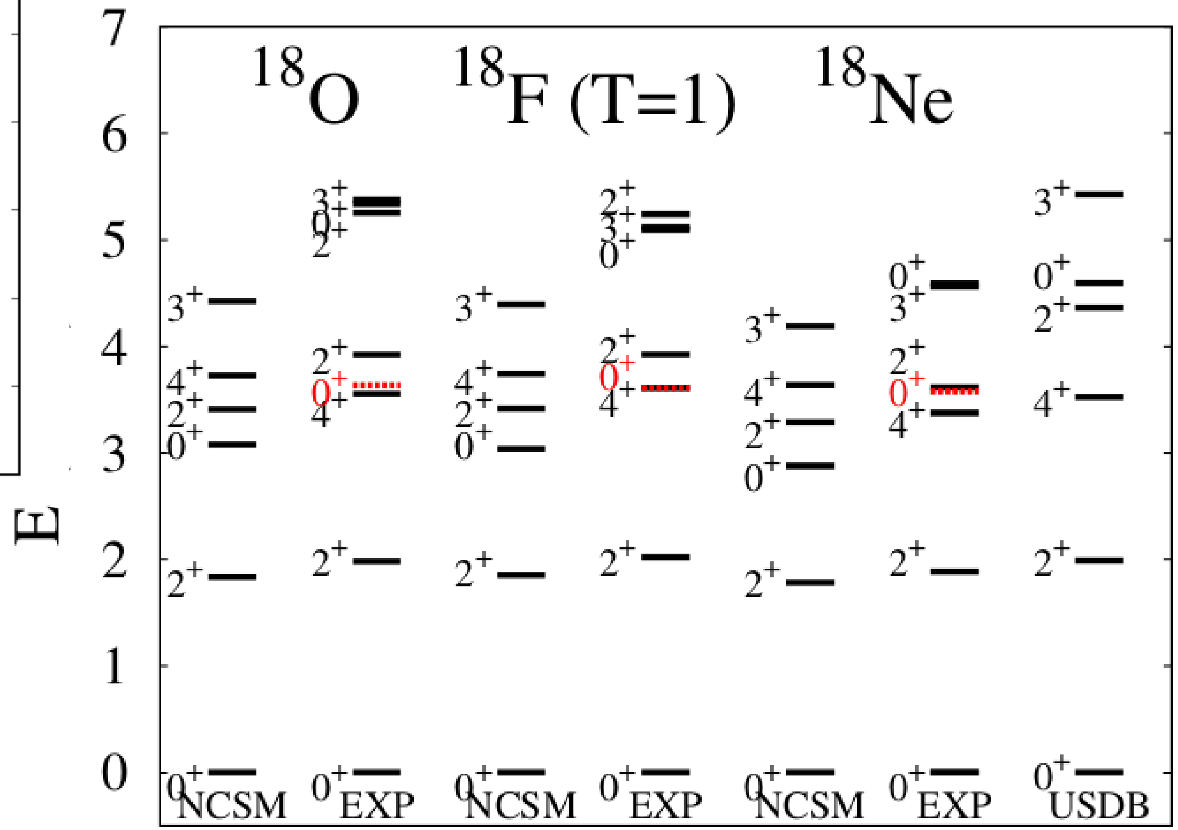
$$N_{max} = 4$$



Ab-initio effective Hamiltonian from the NCSM with Daejeon16



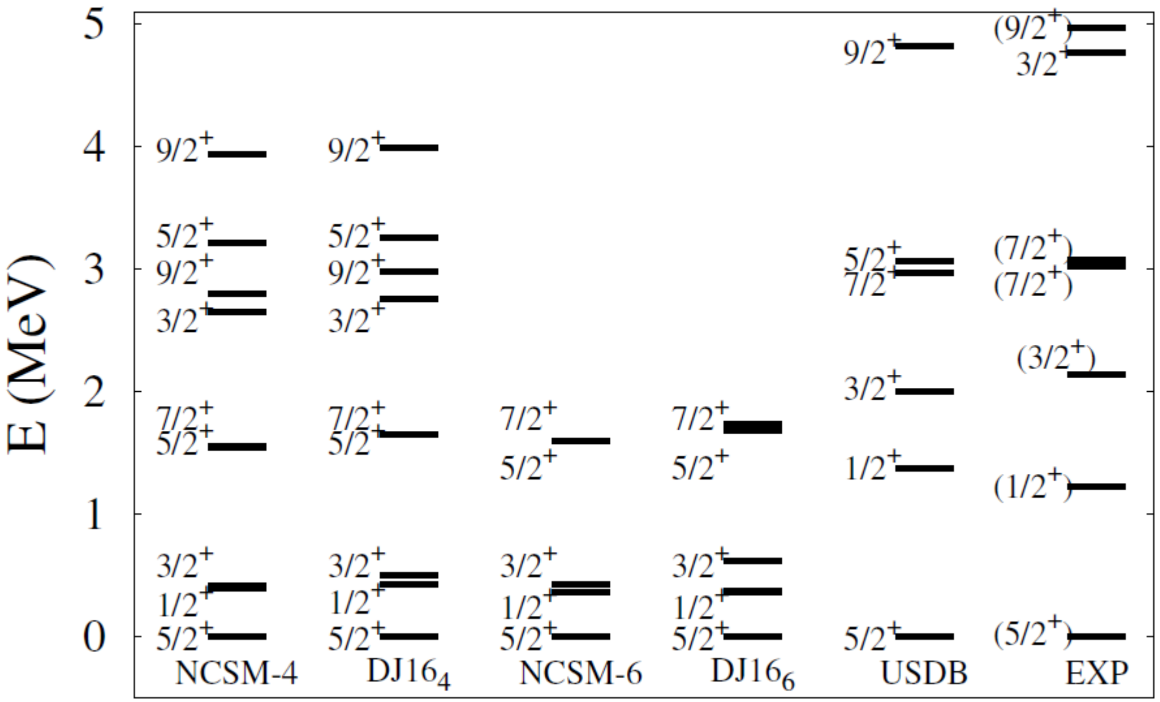
By construction, valence-space two-nucleon calculation reproduces the NCSM results



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

^{21}O

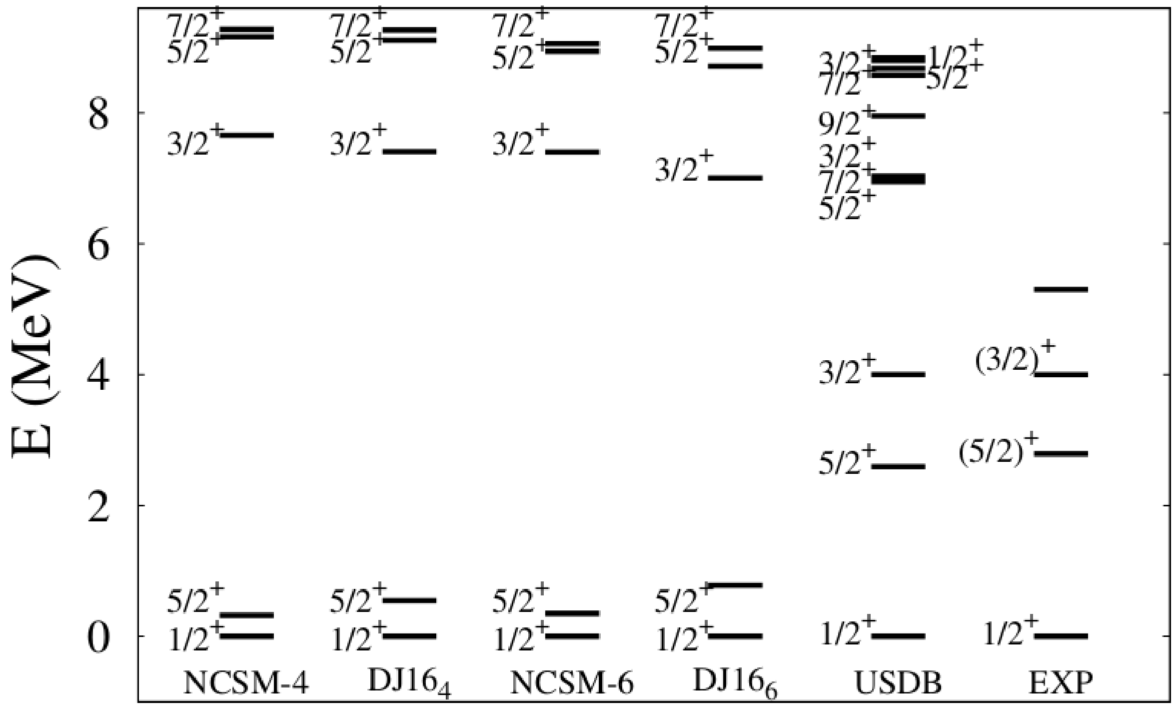
9 states : rms error 225 keV



- Valence-space TBMEs and theoretical s.p.e.'s robustly reproduce the NCSM results !

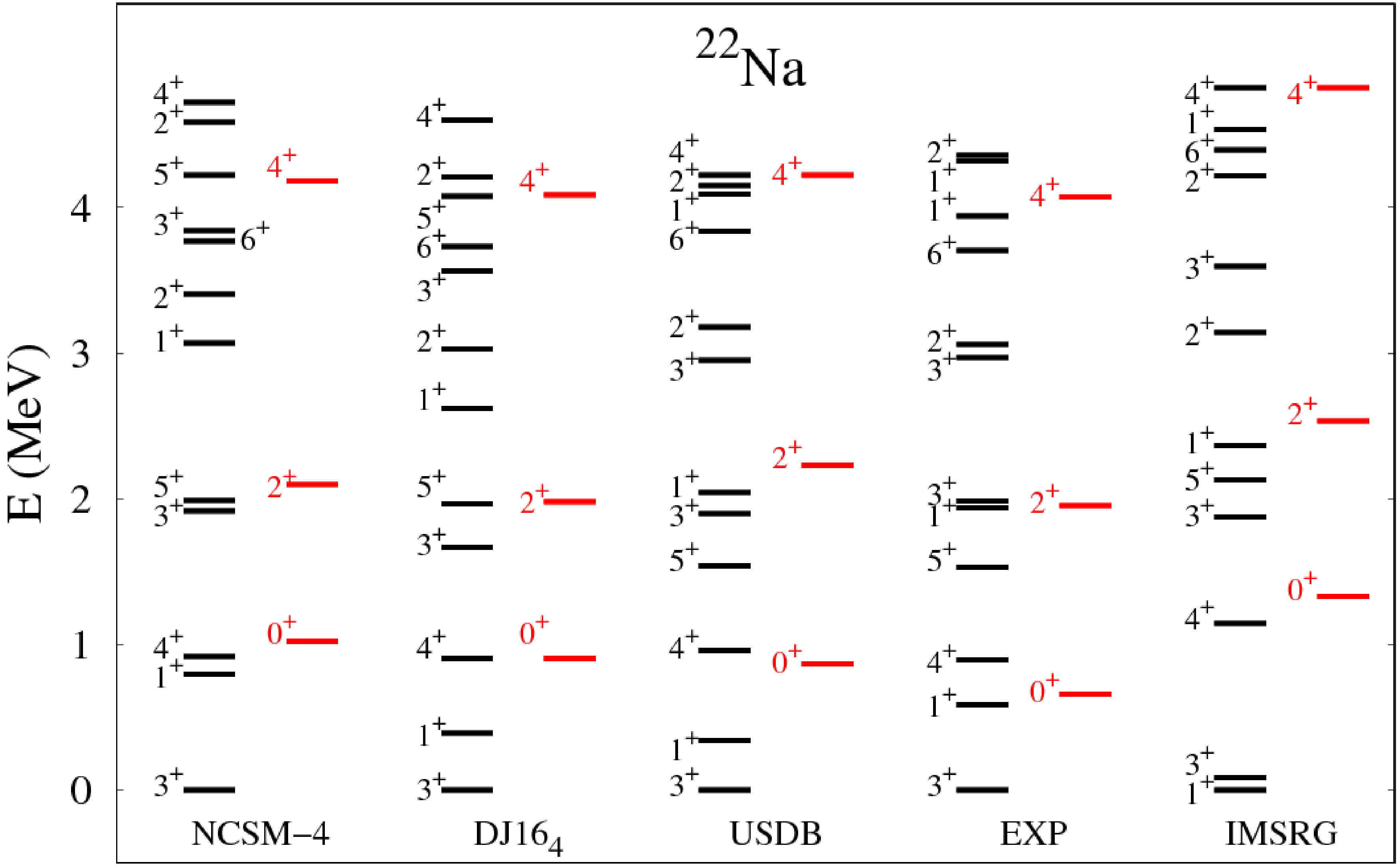
^{23}O

14 states : rms error 63 keV



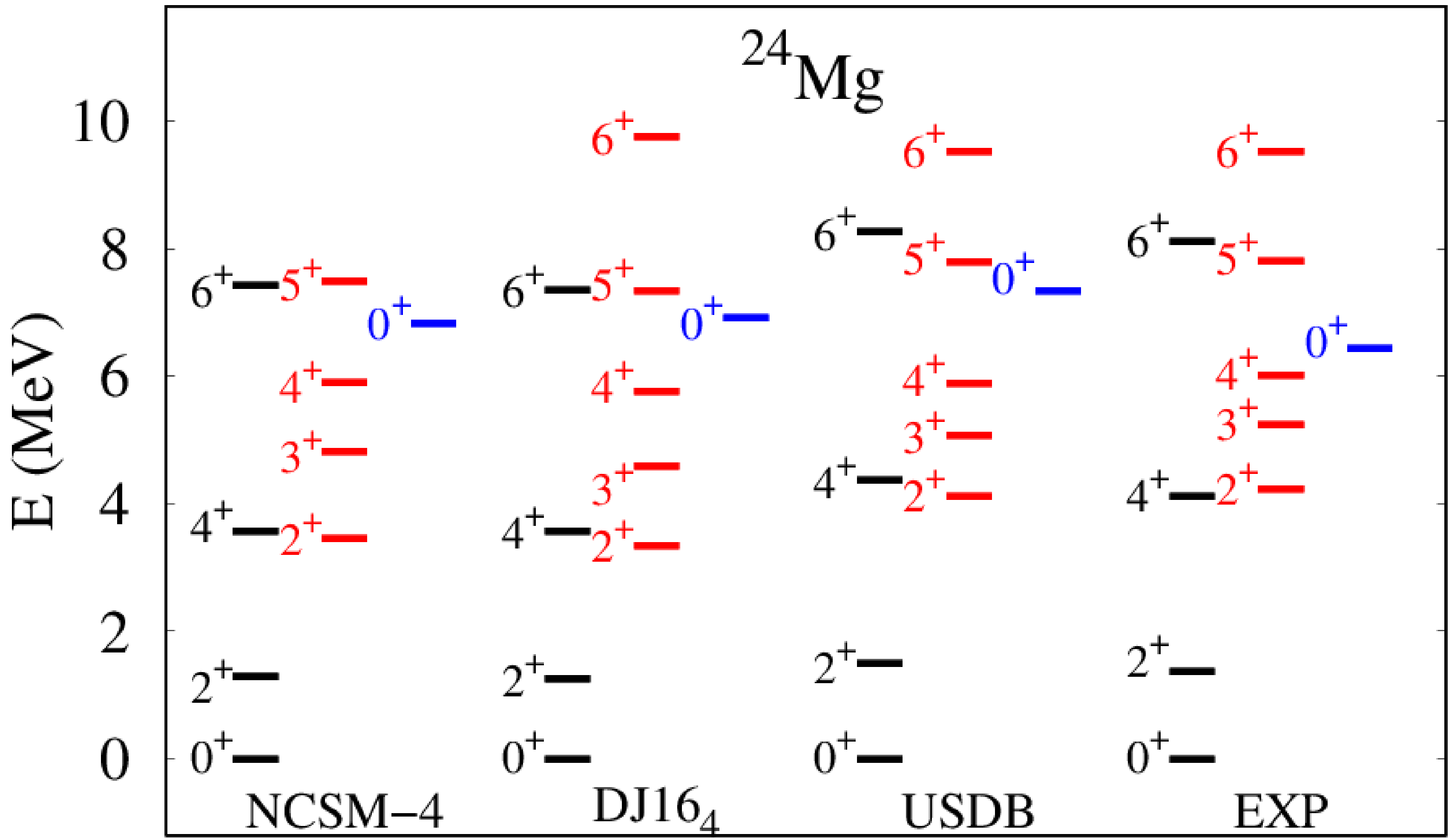
- Sometimes poor agreement with experiment …

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



14 states : rms error 220 keV

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



9 states : rms error 225 keV

Electromagnetic transition operators from the NCSM

Effective $E2$ operator in the sd shell

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

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

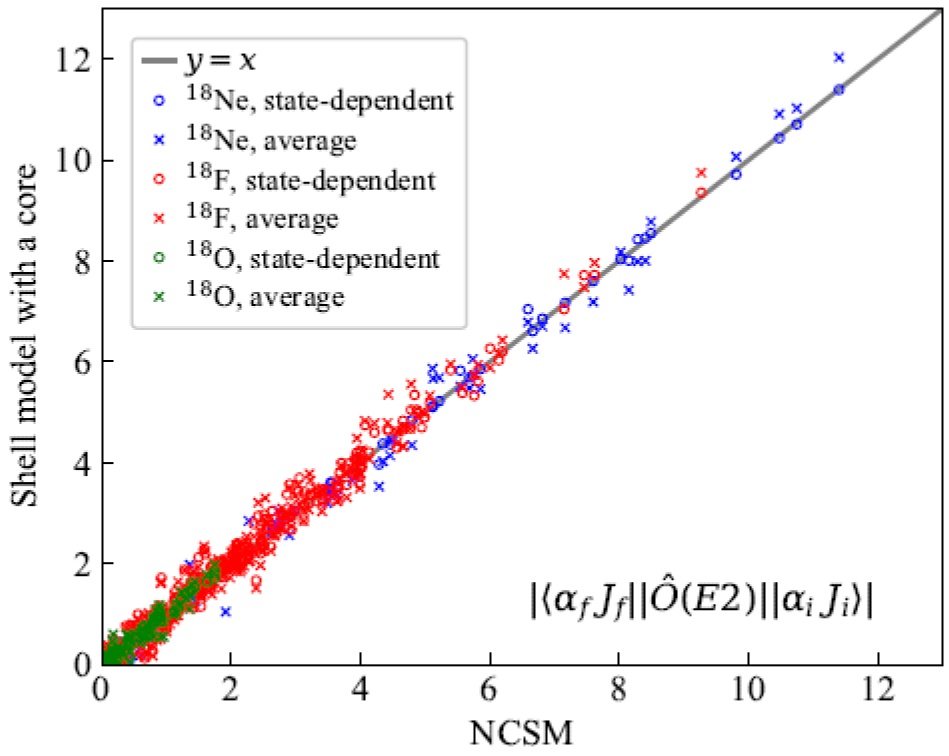
(a,b)	$e_n(a,b)$	$e_p(a,b)$	$g_n^s(a,b)$	$g_n^l(a,b)$	$g_p^s(a,b)$	$g_p^l(a,b)$
bare	0.0	1.0	-3.826	0.0	5.586	1.0
$(0d_{5/2},1s_{1/2})$	0.181	1.171				
$(0d_{5/2},0d_{3/2})$	0.281	1.236	-3.608	0.020	5.252	0.916
$(1s_{1/2},0d_{3/2})$	0.168	1.297				
$(0d_{5/2},0d_{5/2})$	0.179	1.060	-3.751	0.026	5.499	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	
	$\bar{e}_n$	$\bar{e}_p$	$\bar{g}_n^s$	$\bar{g}_n^l$	$\bar{g}_p^s$	$\bar{g}_p^l$
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

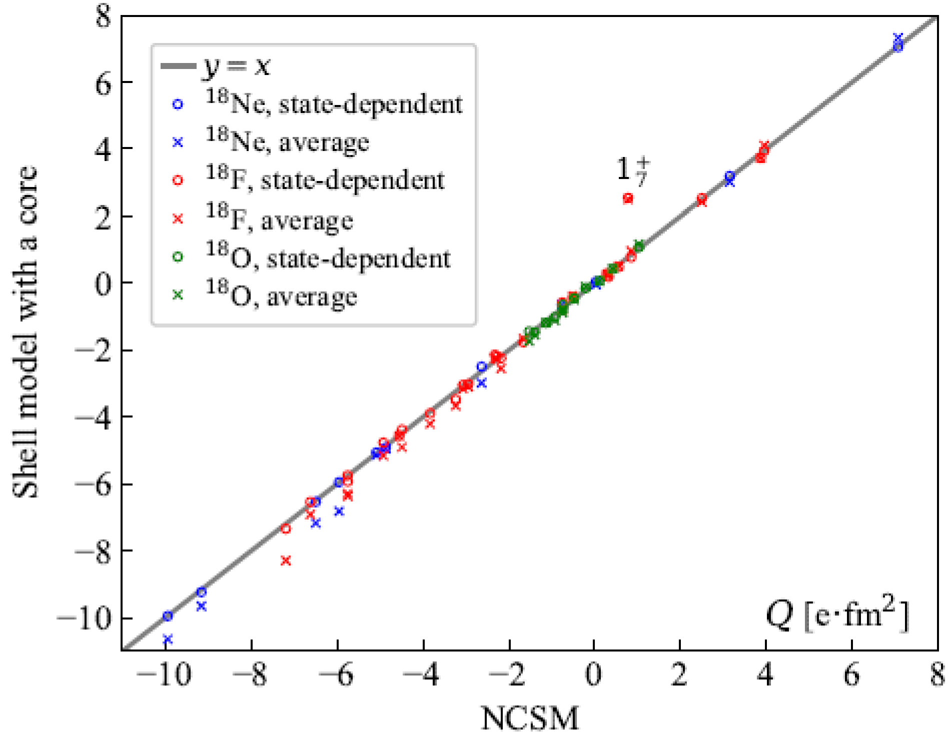
Idem for M1 operator => Effective g-factors

Effective one-body state-dependent transition operators !

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

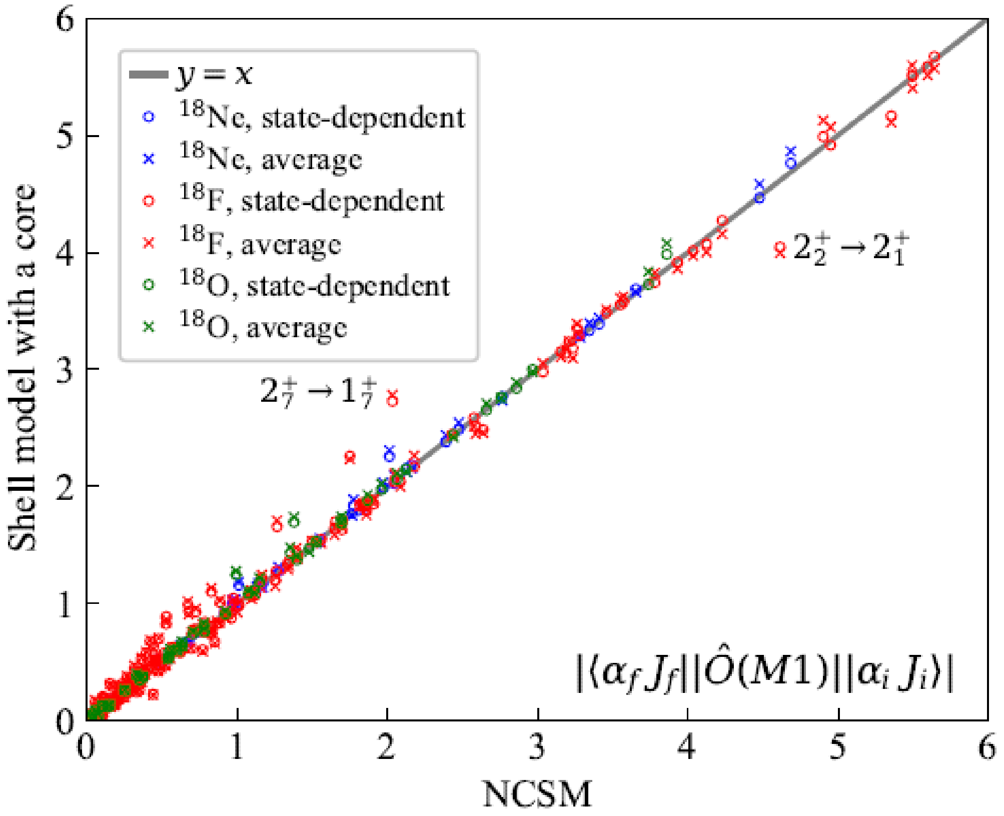
^{18}O : rms(RME) $\approx$ 0.07 e.fm^2 (66 data), rms(Q) $\approx$ 0.06 e.fm^2
^{18}F : rms(RME) $\approx$ 0.11 e.fm^2 (269 data), rms(Q)$\approx$ 0.37 e.fm^2
^{18}Ne : rms(RME)$\approx$ 0.22 e.fm^2 (66 data), rms(Q) $\approx$ 0.06 e.fm^2

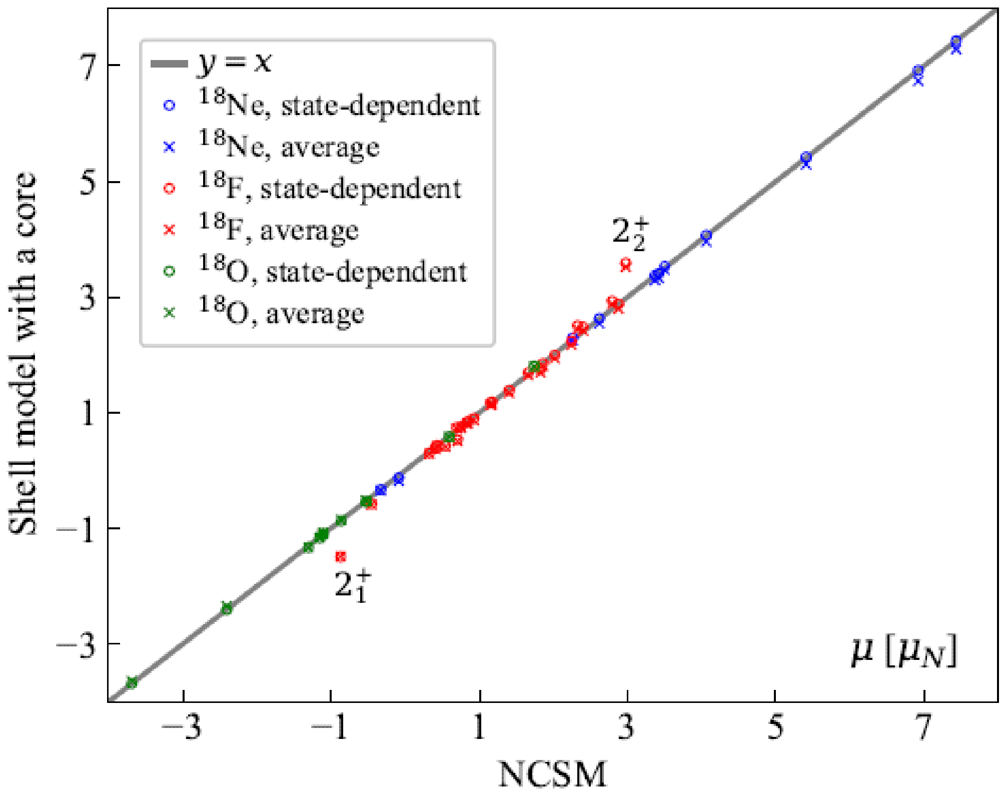




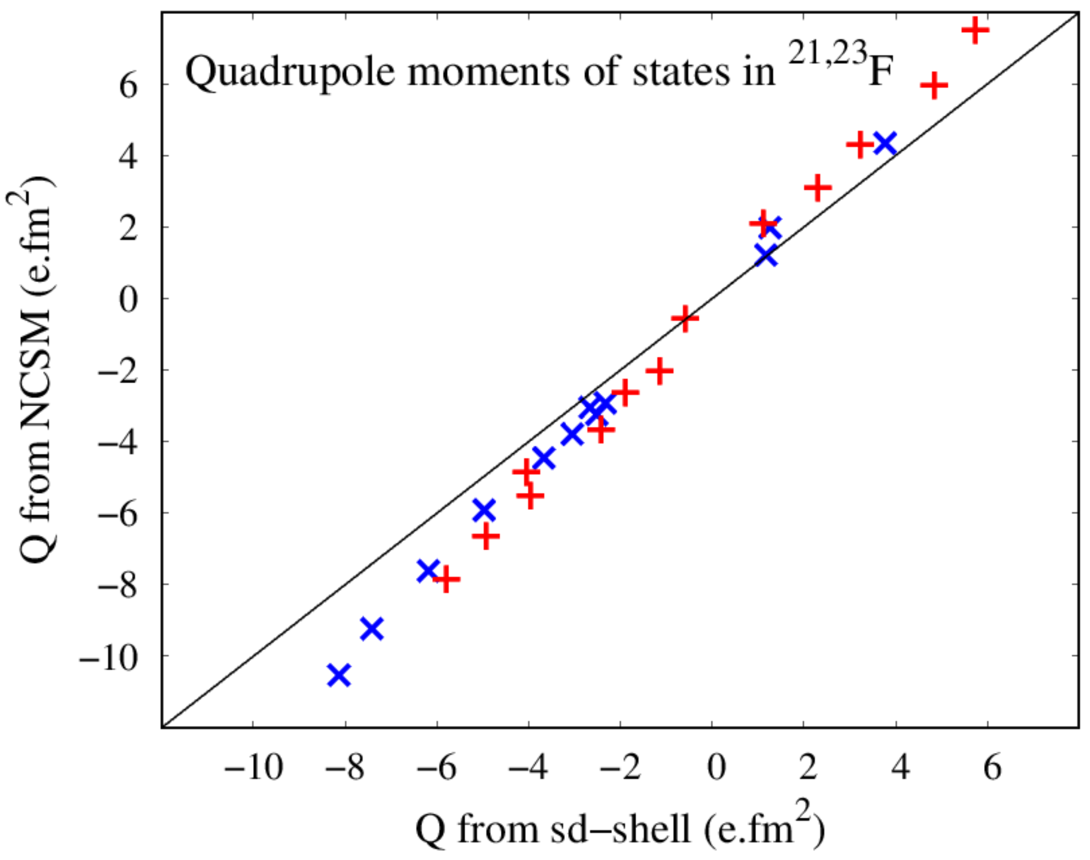
M1 operator from the NCSM : transitions and moments in A=18

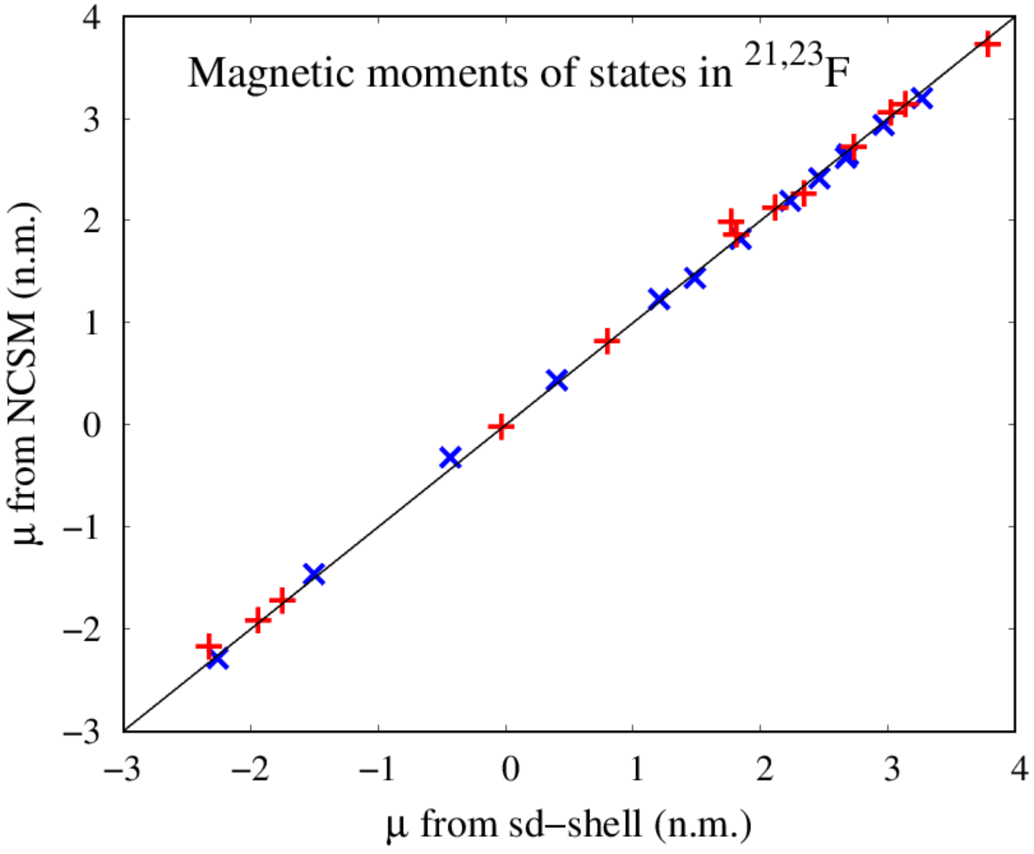
^{18}O : rms(RME) $\approx 0.06\ \mu_N$ (43 data), rms(μ) $\approx 0.02\ \mu_N$
^{18}F : rms(RME) $\approx 0.09\ \mu_N$ (212 data), rms(μ)$\approx 0.19\ \mu_N$
^{18}Ne : rms(RME)$\approx 0.06\ \mu_N$ (43 data), rms(μ) $\approx 0.02\ \mu_N$



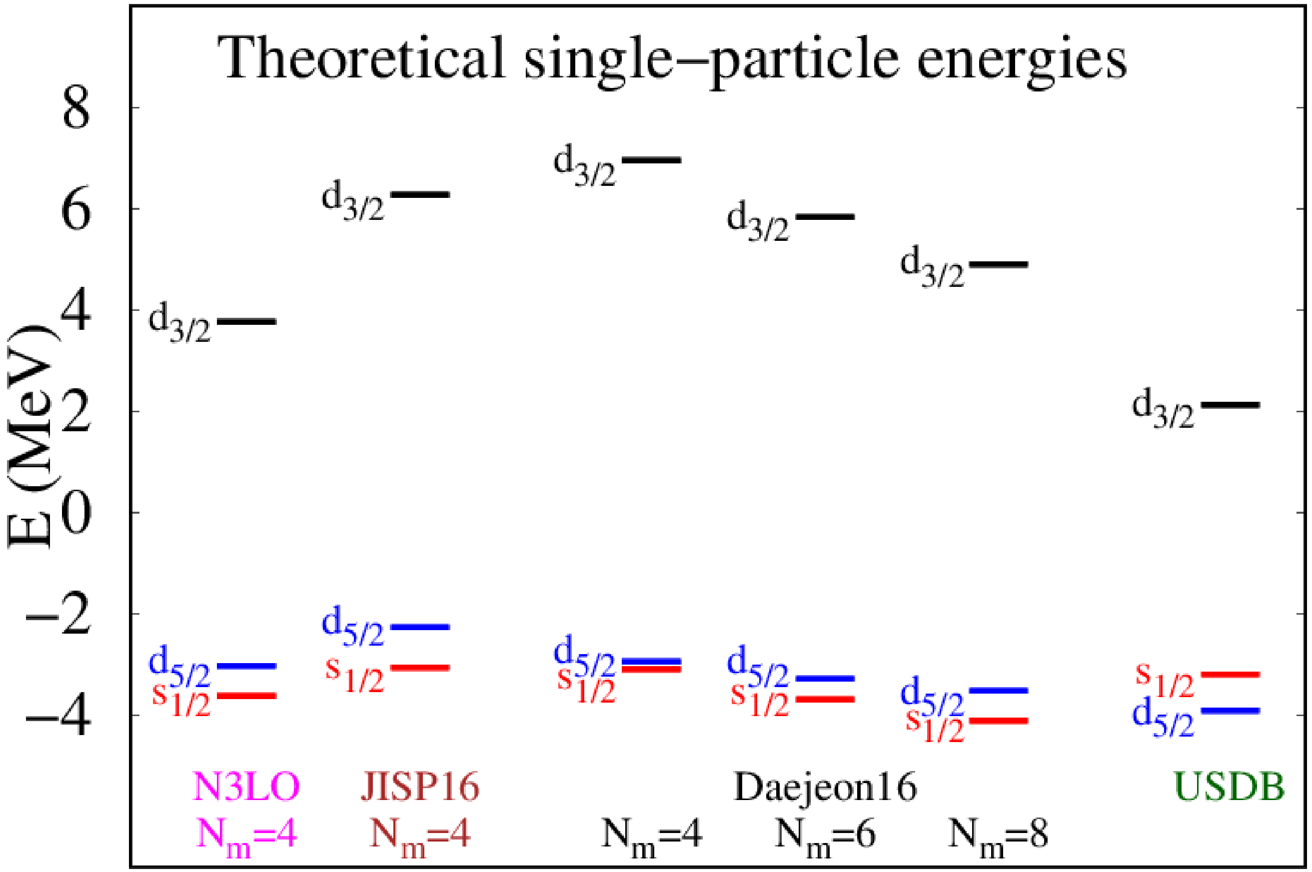


Effective E2 and M1 operators from NCSM : moments in A>18





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



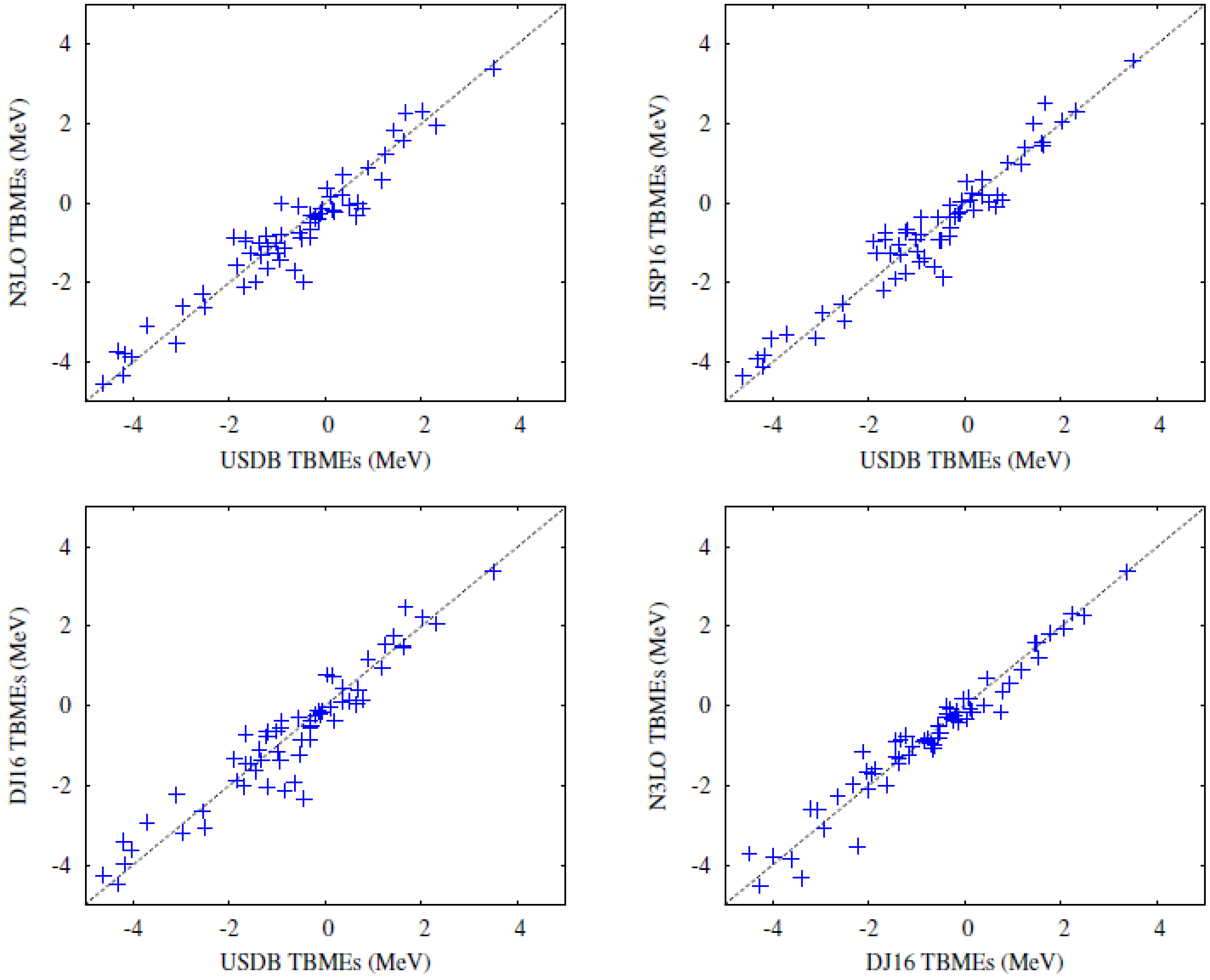
N3LO : from chiral EFT by D.R.Entem, R.Machleidt, PRC68 (2003)
JISP16 : A.M. Shirokov et al, PRC70, 044005 (2004)
Daejeon16 : A.M. Shirokov et al, PLB761, 87 (2016) – based on N3LO
+ SRG evolved + phase-equivalently transformed

Drawbacks (hw=14 MeV):

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

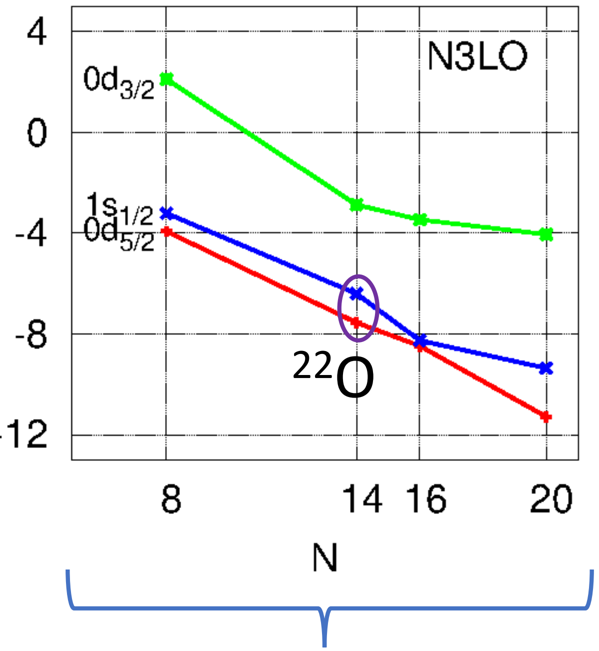
We adopt USDB single-particle energies and impose an $A^{-0.3}$ mass dependence on TBMEs

Comparison of TBMEs: microscopic & empirical (USDB)

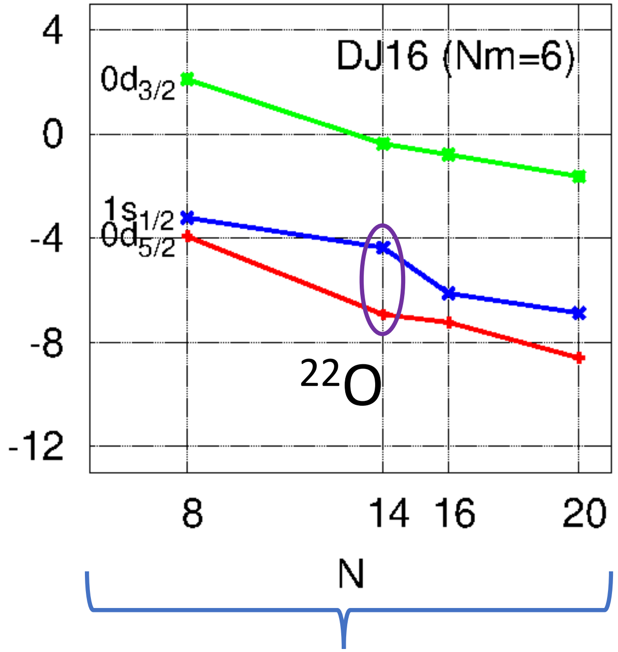


Comparison of monopole properties valence-space interactions

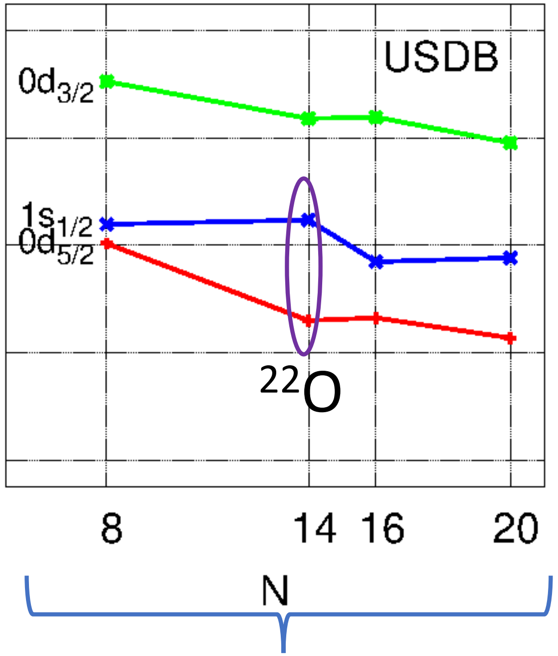
Neutron ESPEs in O-isotopes



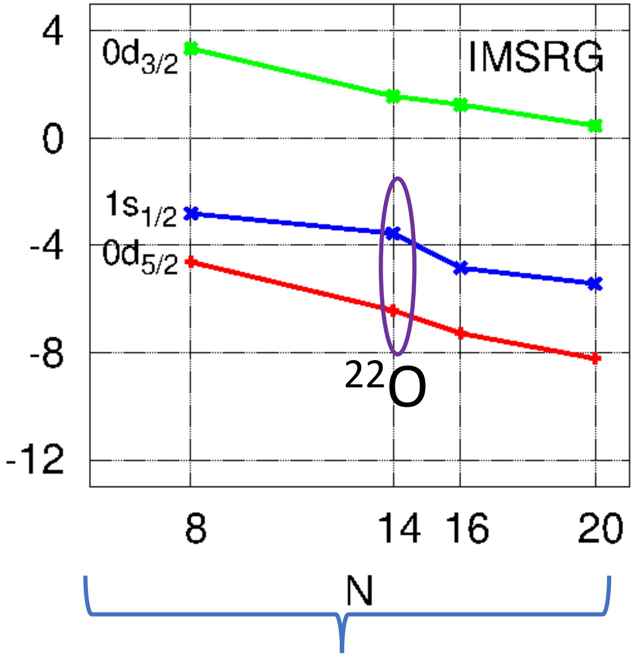
From NN interaction



From Daejeon16 NN interaction



Empirical = experiment

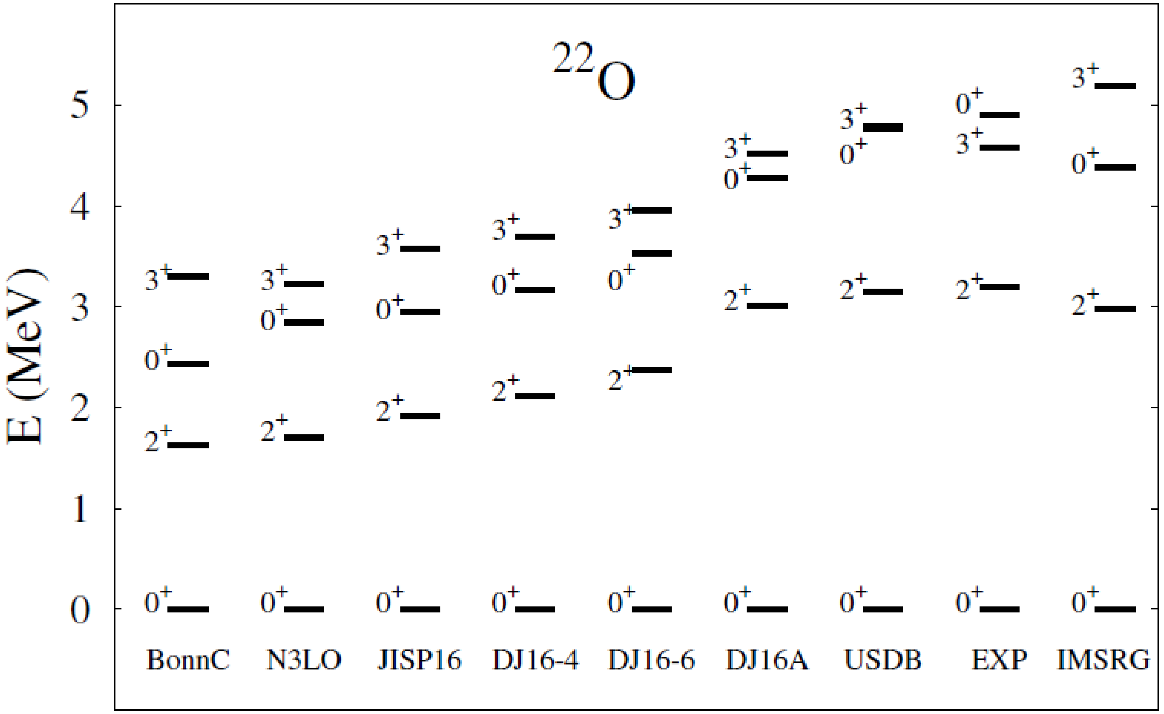


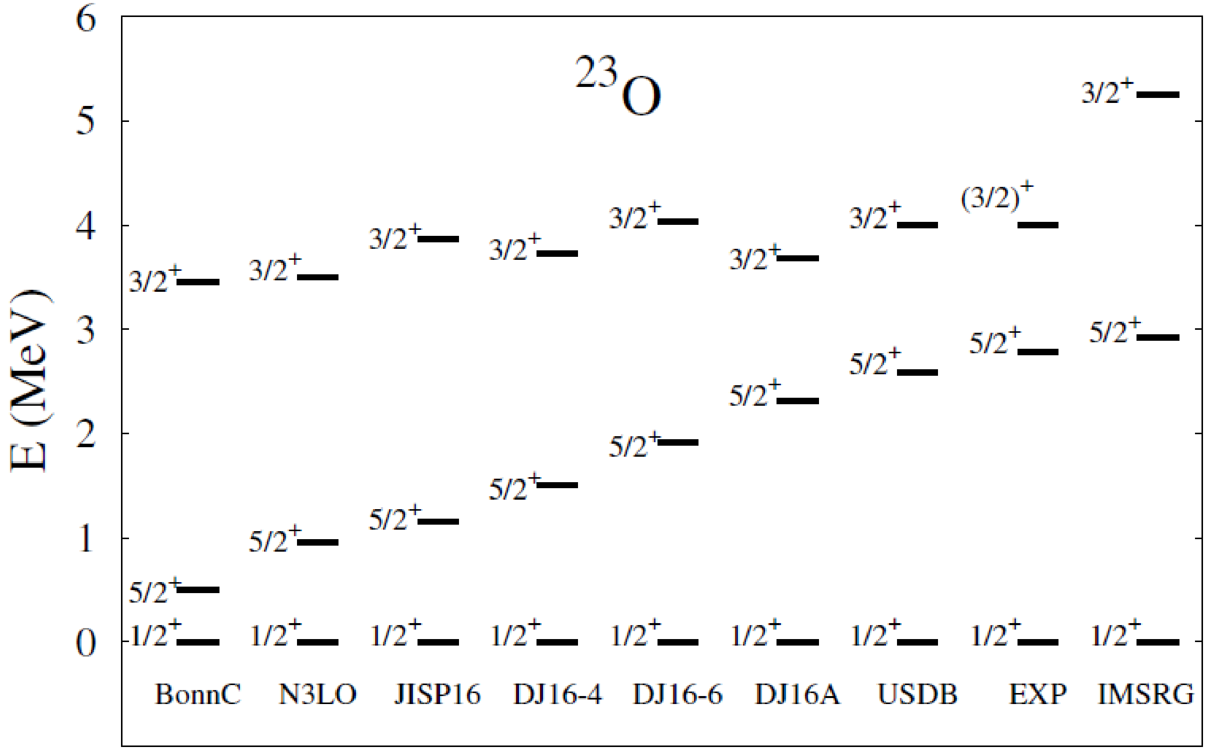
From NN+3N interaction

Small monopole modifications to DJ16 (change of centroids by ~100-300 keV) can be useful !

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

Ab-initio effective Hamiltonian from the NCSM



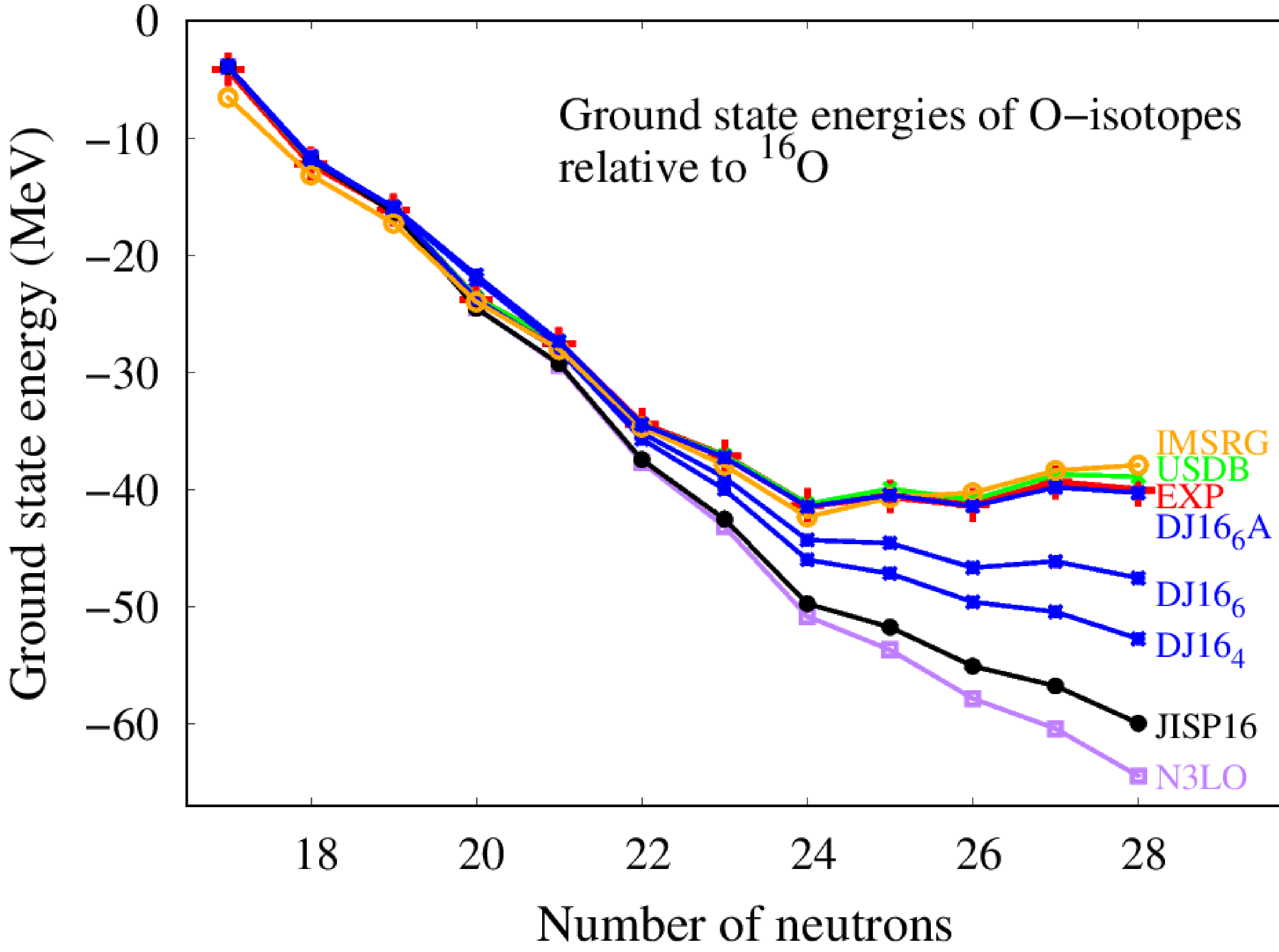


Increase of N=14 subshell gap

Increase of N=14 subshell gap

DJ16A is DJ16-4 with monopole modifications

Ab-initio effective Hamiltonian from the NCSM

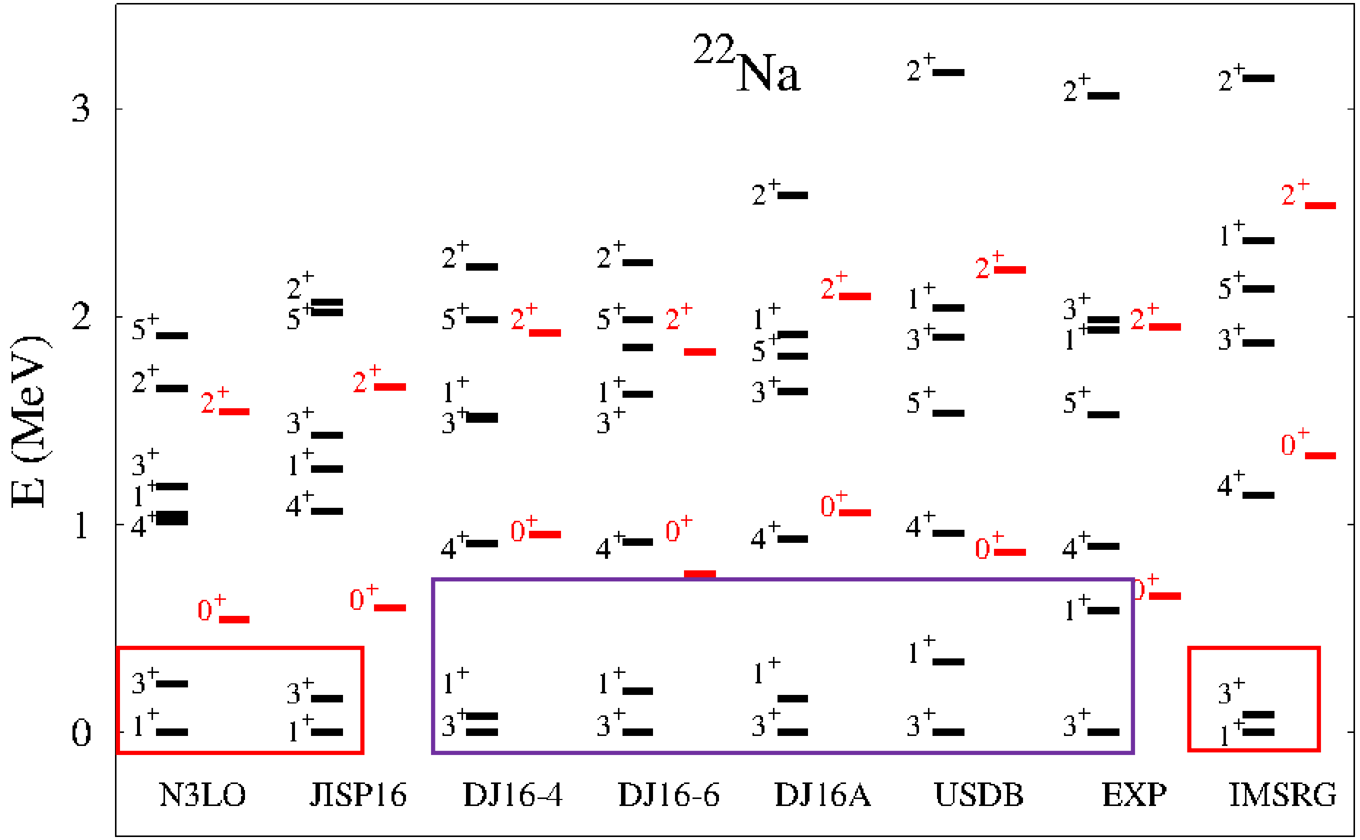


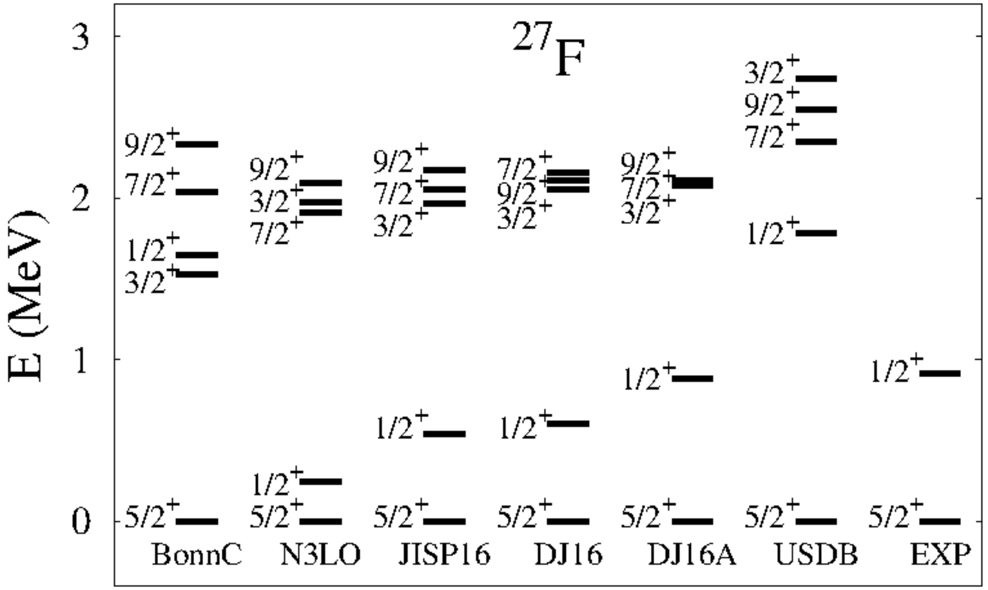
DJ16$_6$: rms = 3671 keV

DJ16$_6$A (DJ16$_6$ with monopole modifications): rms = 235 keV

USDB : rms =467 keV

Microscopic effective interactions





RMS (microscopic) > RMS (phenomenological)

For detailed nuclear spectroscopy and applications - Experimentally constrained Interactions !

Conclusions and Perspectives

- Microscopic derivation of effective valence-space interaction for the nuclear shell model is still challenging, although it rapidly progresses

- OLS transformation of the NCSM solution gives encouraging results :
  further steps are foreseen towards larger NCSM spaces and/or larger valence-spaces (*p-sd-pf*).

- Effective interaction theory -> towards microscopic foundations of the model and link 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

THANK YOU FOR YOUR ATTENTION !

MANY MORE FRUITFUL YEARS IN PHYSICS TO ALFREDO!