2025 Joint workshop of FKPPN and TYL/FJPPN

Ab-initio Shell Model for Nuclear Structure

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A new project between Japan and Korea

“IBS&RIKEN TOP-Tier Platform in Extreme Rare Isotope Science”

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국제공동연구센터 구축 및 운영

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차별화된 도전적 연구과제 추진

Creating an International Collaborative Research Center

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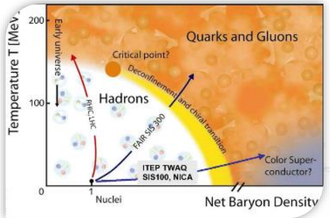
It would be great to have a similar program for FKPPN!!!

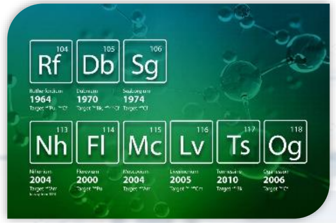
Accelerator complex
ISOL + In-Flight Fragmentation

Origin of Matter

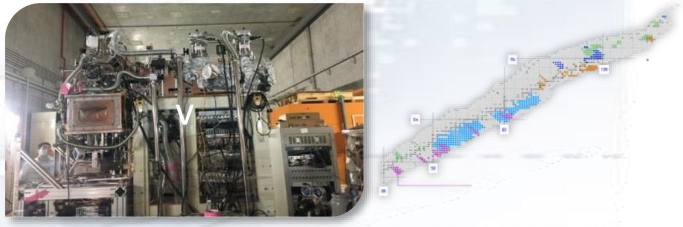
Nuclear Astrophysics



Nuclear Matter

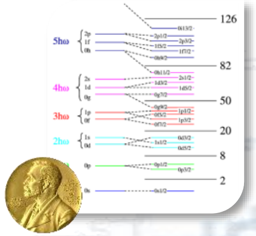


Super Heavy Element Search

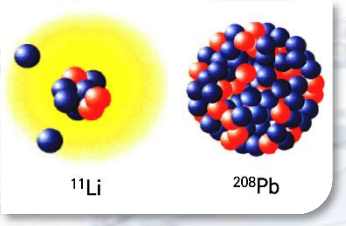


High-Precision Mass Measurement

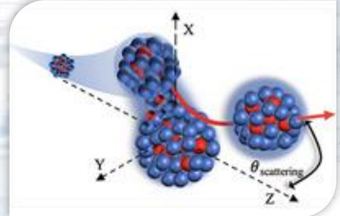
Properties of Exotic Nuclei



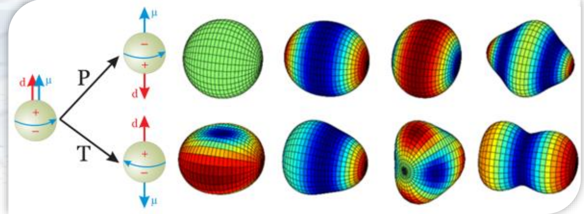
Magic Number



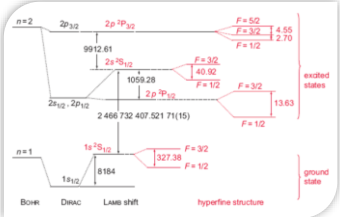
Nuclear Structure



Nuclear Reaction

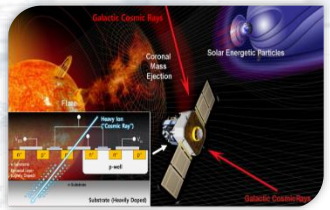


Electric Dipole Moment and Symmetry

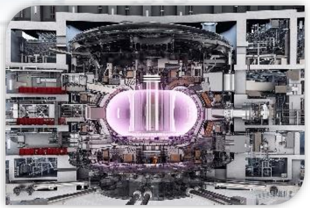


Hyperfine Structure

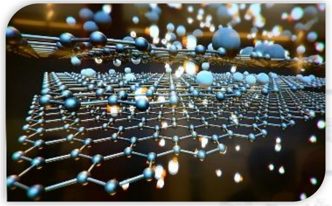
Applied Science



Aerospace

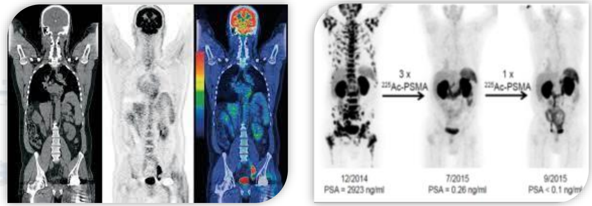


Neutron Science



Material Science

Radiation Breeding



Cancer Diagnosis & Treatment

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

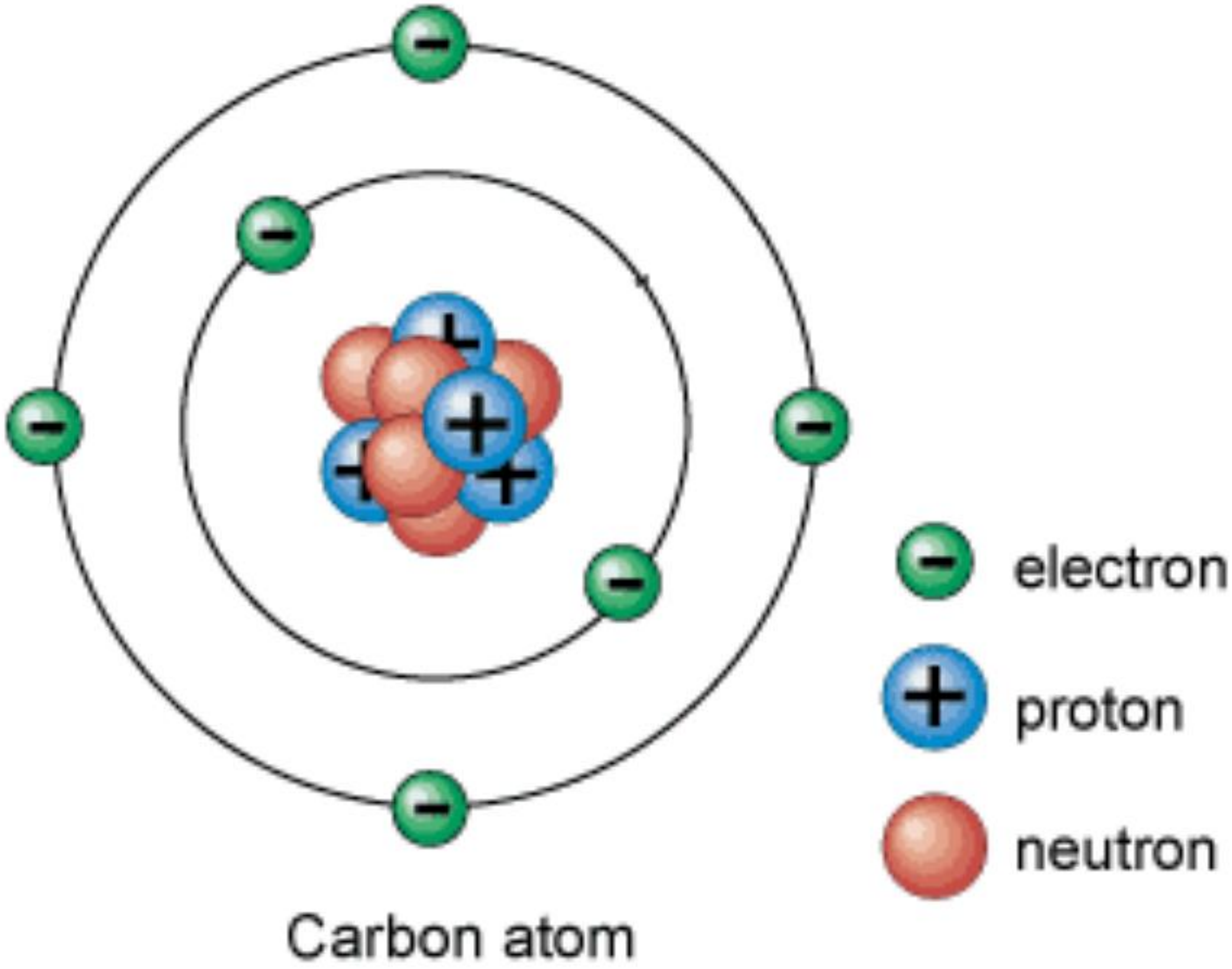
❑ **Proposed project**

- 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**

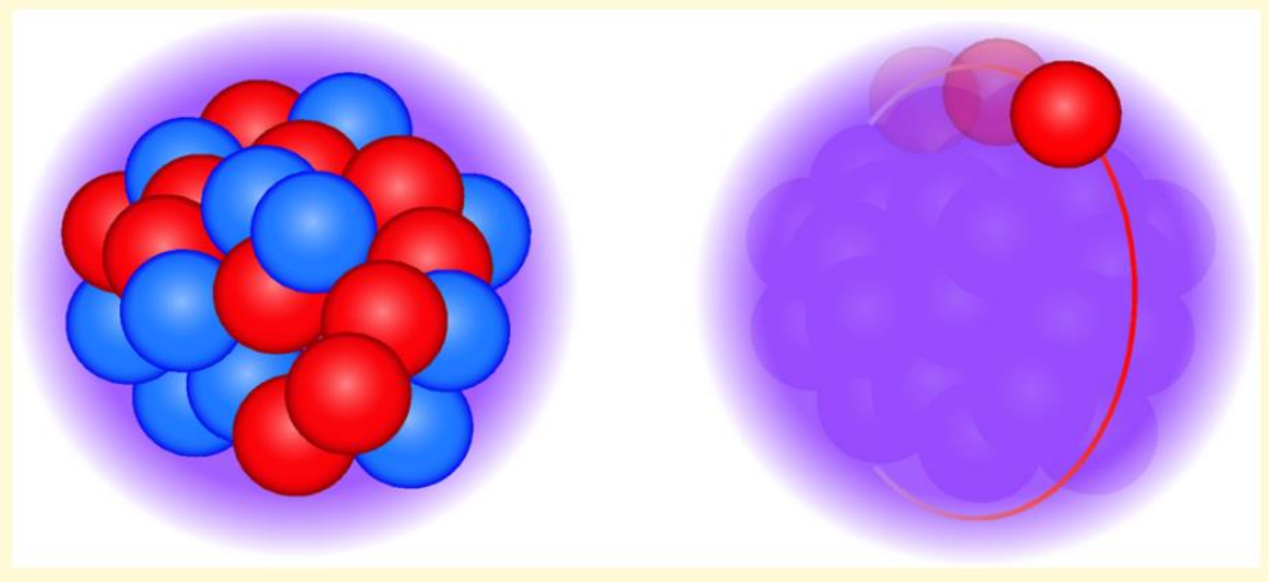
Most slides are from Nadezda A. Smirnova

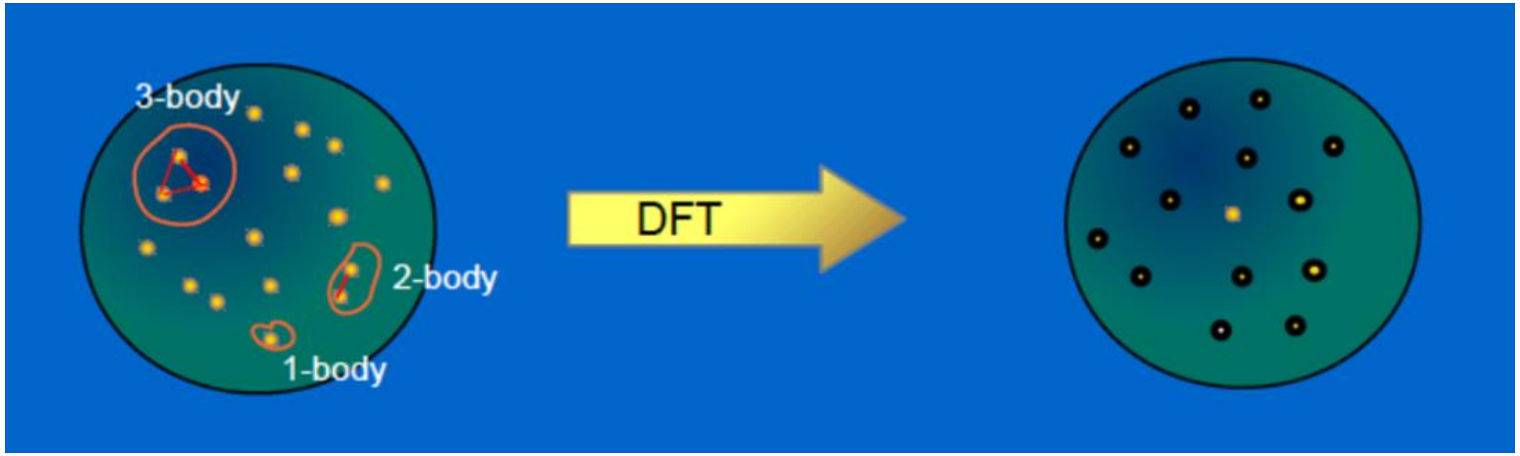
Shell model



Clusters of levels → shell structure

Mean field





Nuclear shell model

Ingredients:

- *Mean-field potential.*
- *Residual interaction between (some of) the nucleons.*

Difficulties:

- *Nucleonic interactions from QCD (EFT).*
- *Large-matrix diagonalization.*

Issues of current interest:

- *Changing shell structure and three-body forces in exotic nuclei.*
- *Continuum effects (nucleus = open quantum system).*

Nuclear shell model

Many-body quantum mechanical problem:

$$\hat{H} = \sum_{k=1}^{A} \frac{p_k^2}{2m_k} + \sum_{k<l}^{A} \hat{V}_2\left(\boldsymbol{r}_k, \boldsymbol{r}_l\right)$$

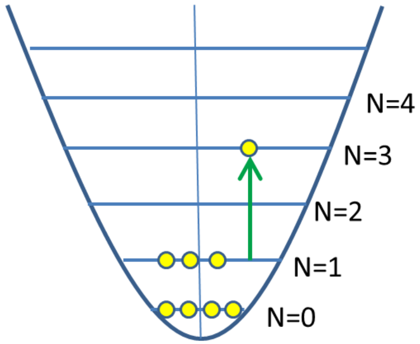
$$= \underbrace{\sum_{k=1}^{A} \left[\frac{p_k^2}{2m_k} + \hat{V}\left(\boldsymbol{r}_k\right) \right]}_{\text{mean field}} + \underbrace{\left[\sum_{k<l}^{A} \hat{V}_2\left(\boldsymbol{r}_k, \boldsymbol{r}_l\right) - \sum_{k=1}^{A} \hat{V}\left(\boldsymbol{r}_k\right) \right]}_{\text{residual interaction}}$$

Independent-particle assumption. Choose *V* and neglect residual interaction:

$$\hat{H} \approx \hat{H}_{\mathrm{IP}} = \sum_{k=1}^{A} \left[\frac{p_k^2}{2m_k} + \hat{V}\left(\boldsymbol{r}_k\right) \right]$$

Shell model - (full) configuration-interaction approach

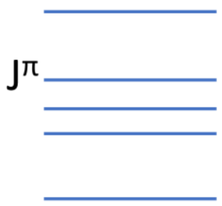
$$H = T + V = \underbrace{(T + U)}_{\text{Independent particle Hamiltonian}} + \underbrace{(V - U)}_{\text{residual interaction}} = H_0 + V_{res}$$



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

$$\boxed{|\Psi_n\rangle = \sum_k c_{kn}\,|\Phi_k\rangle} \qquad \boxed{H_0|\Phi_k\rangle = E_k^0|\Phi_k\rangle} \qquad \boxed{\langle\Phi_k|\Phi_l\rangle = \delta_{kl}}$$

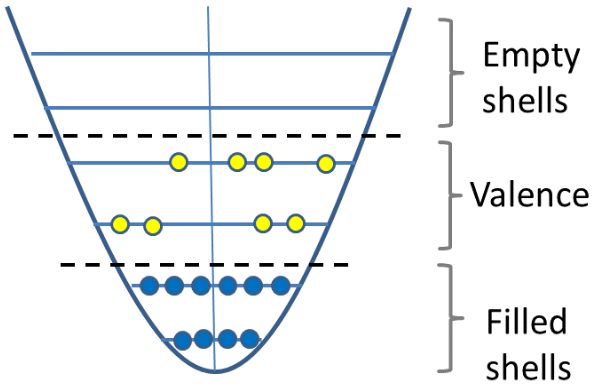
$$\boxed{\sum_{k=1}^{d}\langle\Phi_l|H|\Phi_k\rangle\, c_{kn} = E_n c_{ln}} \Rightarrow \begin{pmatrix} H_{11} & H_{12} & \cdots & H_{1d} \\ H_{21} & H_{22} & \cdots & H_{2d} \\ \vdots & & \ddots & \\ H_{d1} & H_{d2} & \cdots & H_{dd} \end{pmatrix} \Rightarrow$$



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 (heavier nuclei)



Full Hilbert space

$$\boxed{H|\Psi_p\rangle = E_p|\Psi_p\rangle}$$

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

$$\Rightarrow$$

Restricted model space

$$\boxed{H_{eff}|\Psi_p^M\rangle = E_p|\Psi_p^M\rangle}$$

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

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

Microscopic

Semi-microscopic (microscopic, constrained by the data)

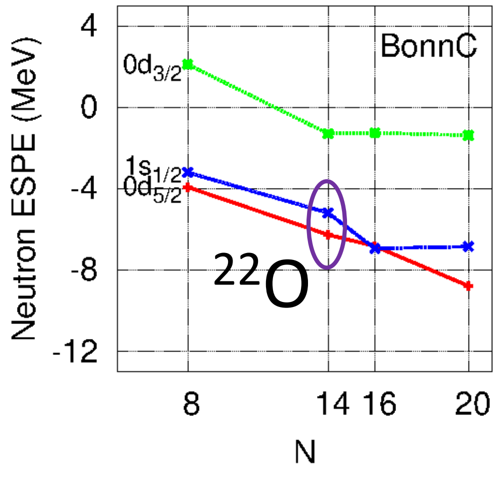
Empirical

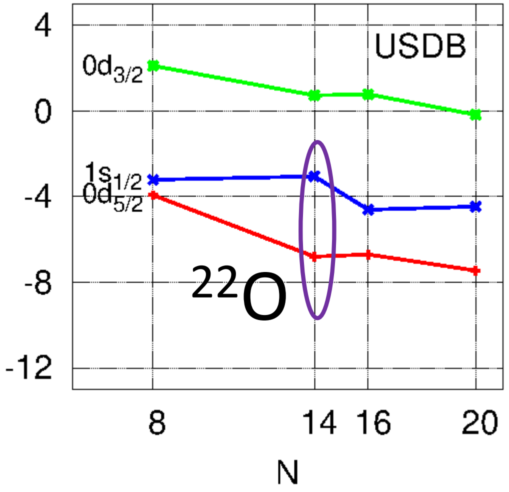
Current status :

- 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 !

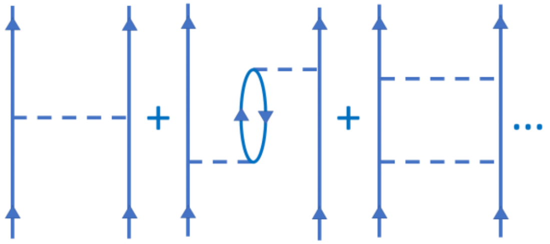
Microscopic approaches to valence space interactions

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





Veff =



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**

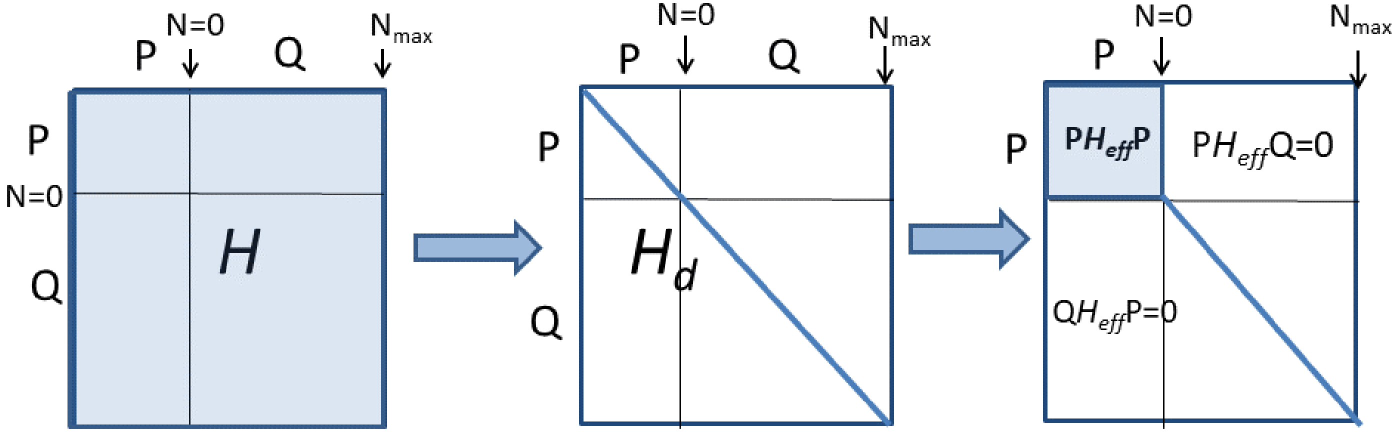
  E. Dikmen, A. Lisetskiy, B.R. Barrett, P. Maris, A.M. Shirokov, J.P. Vary, PRC91, 064301 (2015)
  N.Smirnova, B.R. Barrett, I.J. Shin, Y.Kim, A.M. Shirokov, E. Dikmen, P. Maris, J.P. Vary, PRC100, 054329 (2019)

- **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



$$H_d = UHU^{\dagger}$$

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

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

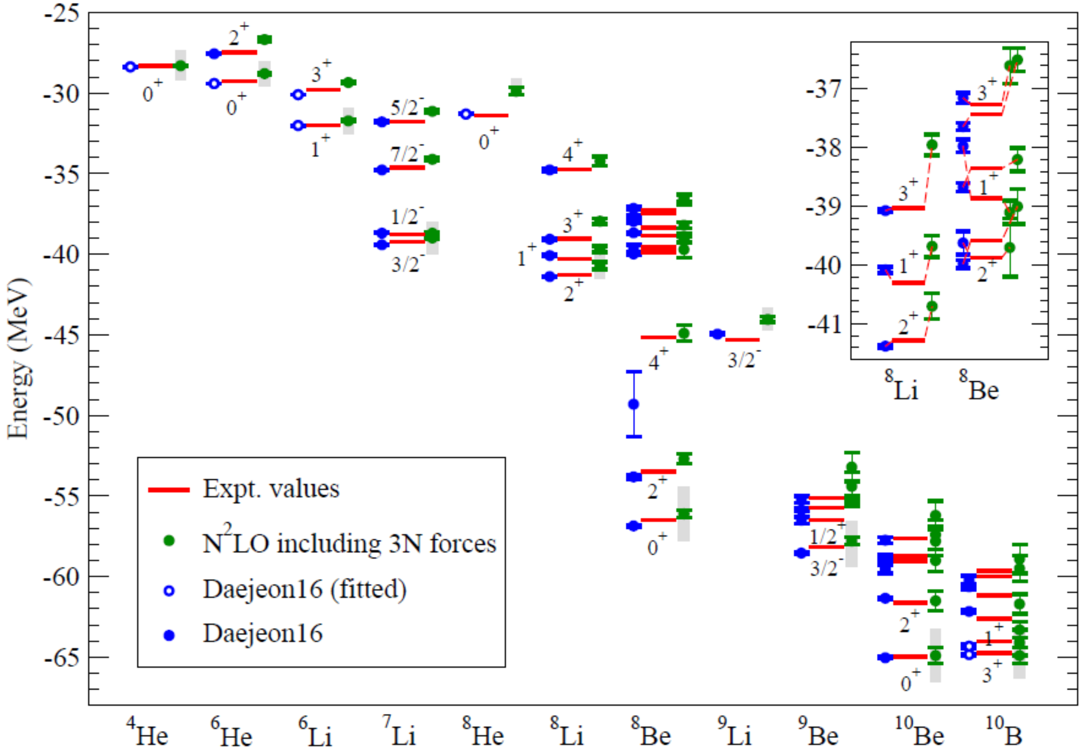
S. Okubo, Prog. Theor. Phys. 12 (1954); K. Suzuki, S. Lee, Prog. Theor. Phys. 68 (1980)
E. Dikmen, A. Lisetskiy, B.R. Barrett, P. Maris, A.M. Shirokov, J.P. Vary, PRC91, 064301 (2015)
N.Smirnova, B.R. Barrett, I.J. Shin, Y.Kim, A.M. Shirokov, E. Dikmen, P. Maris, J.P. Vary, PRC100, 054329 (2019)

Modern NN potential Daejeon16

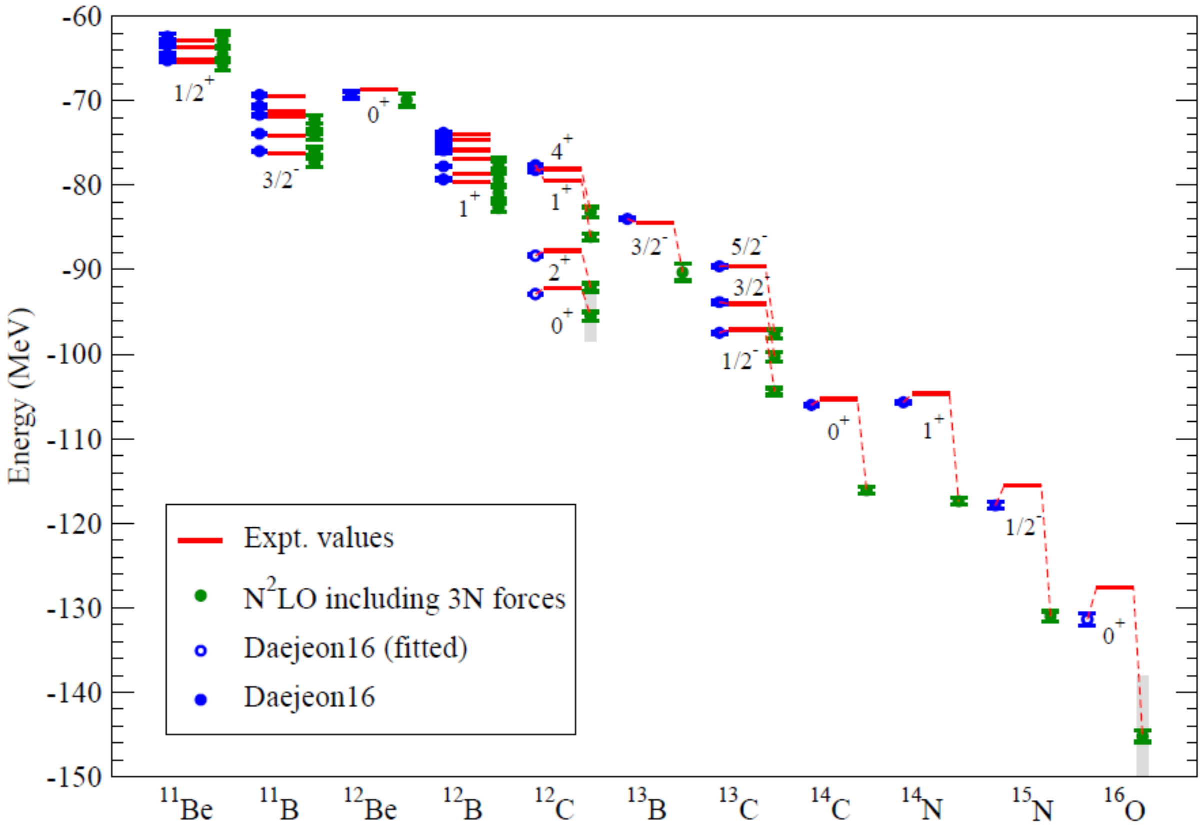
Daejeon16 is a high-precision realistic NN potential obtained from chiral N^3LO + SRG evolved + PETs (phase-equivalent transformations) to incorporate the effect from 3N and many-nucleons forces !

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

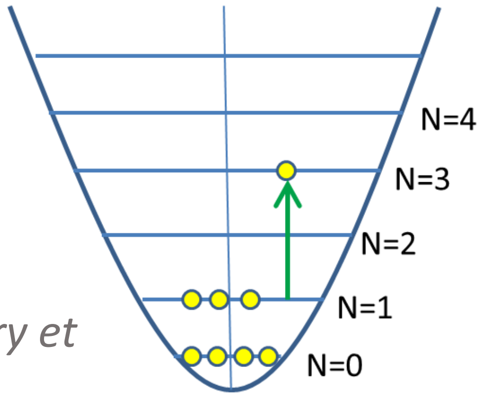
I.J. Shin, Y. Kim, Tachyon II at Supercomputing Center/KISTI (KSC-2013-C3-052)



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

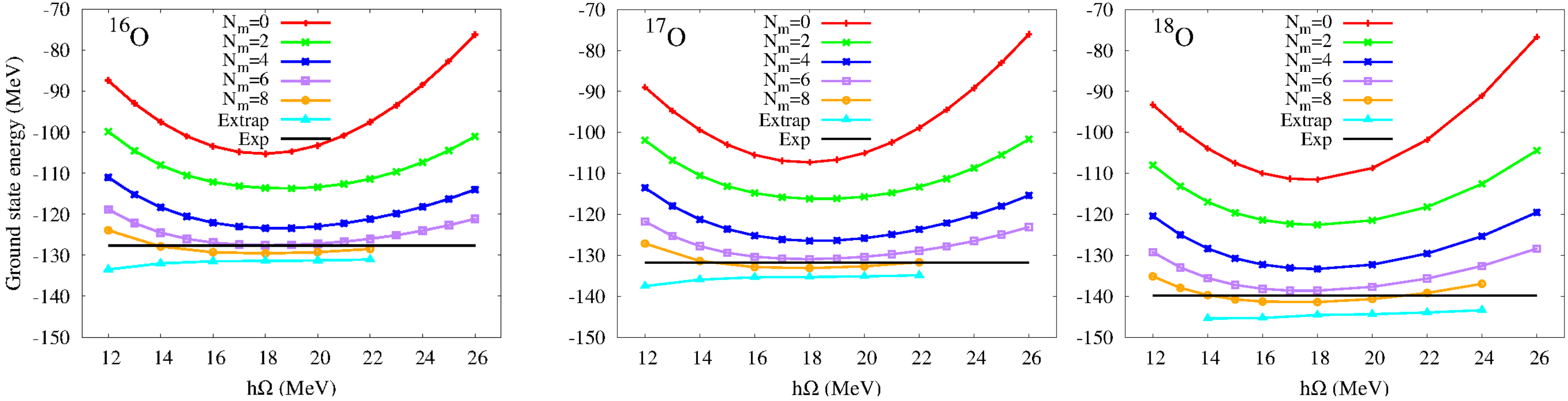


No-Core Shell Model results with Daejeon16 for sd shell nuclei



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

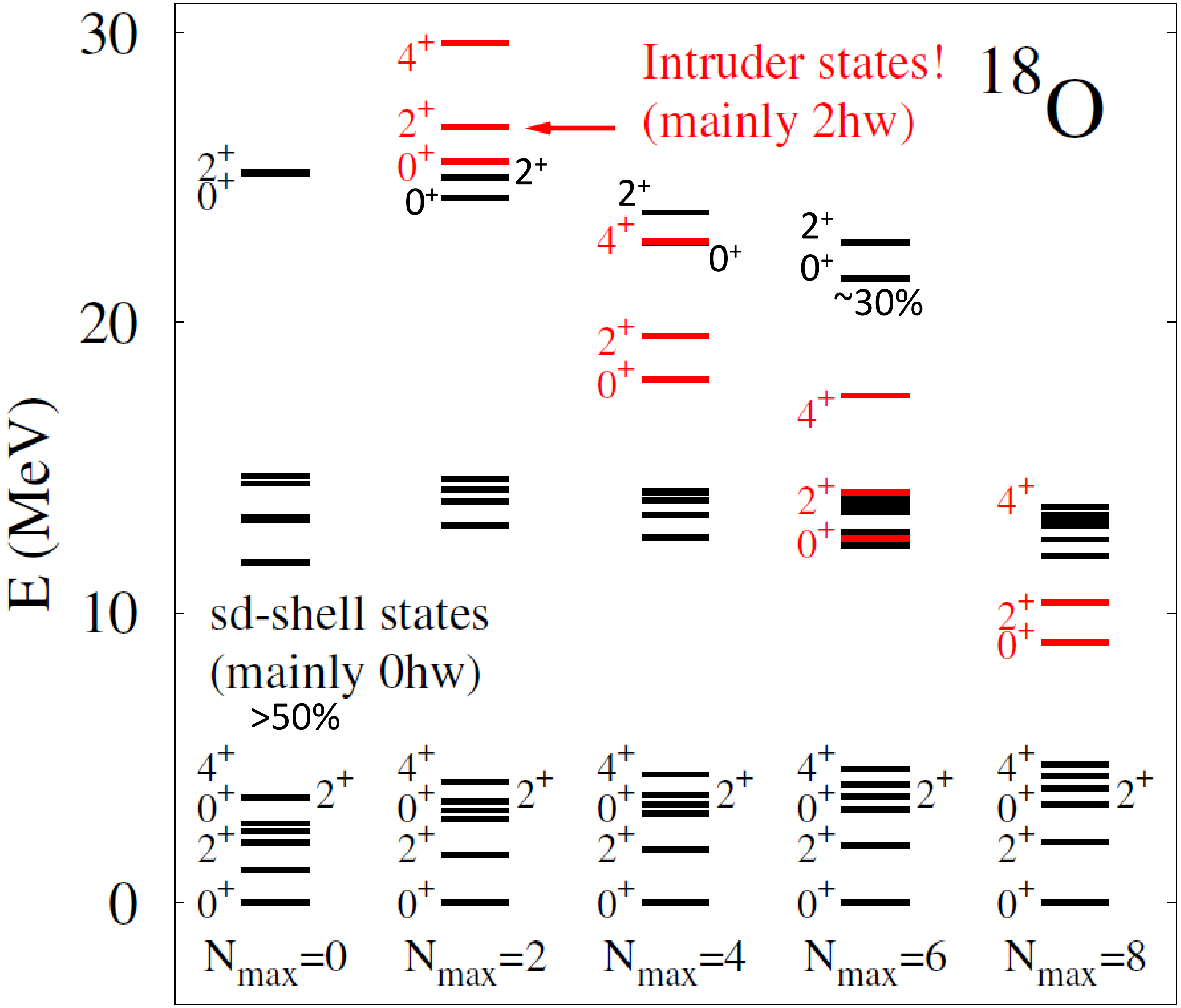
MFDn code, P. Maris, J. P. Vary et al, Iowa State University



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

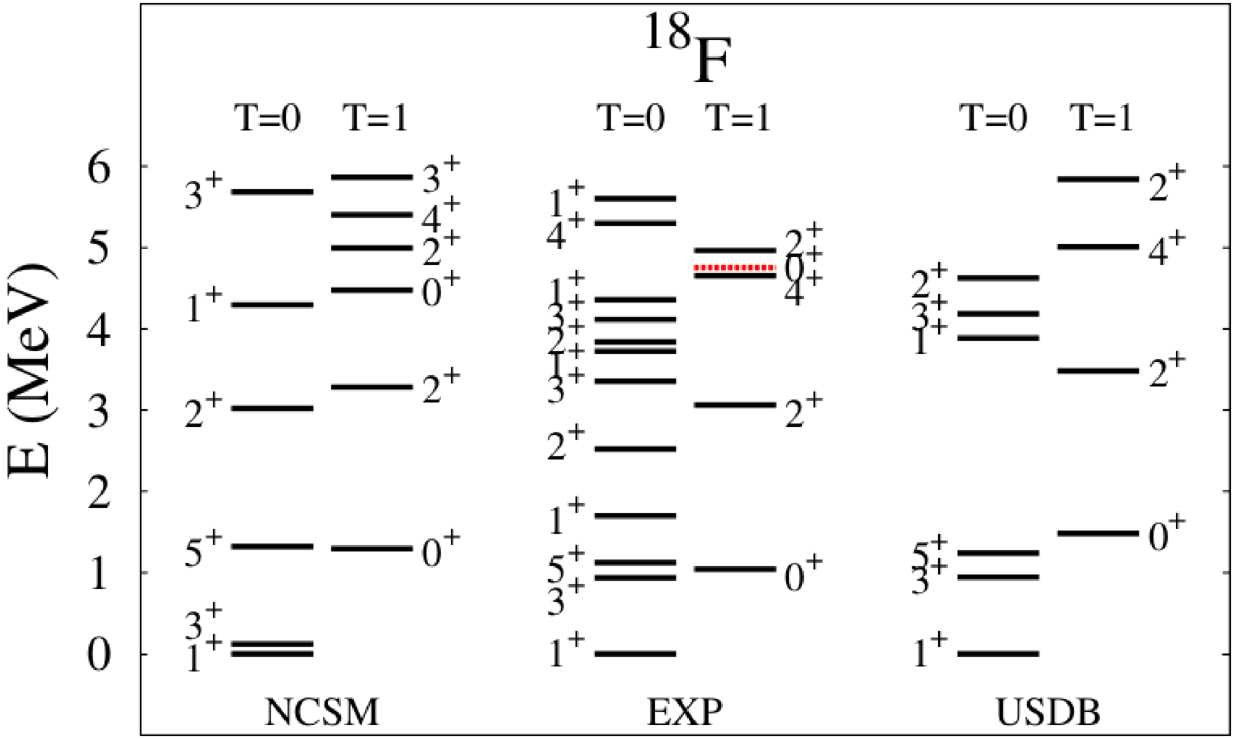
***I.J. Shin, N. Smirnova**, A.M. Shirokov, Z. Yang, B.R. Barrett, **Zh. Li, Y. Kim**, E. P. Maris, J.P. Vary*: PRC110, 034306 (2024)

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

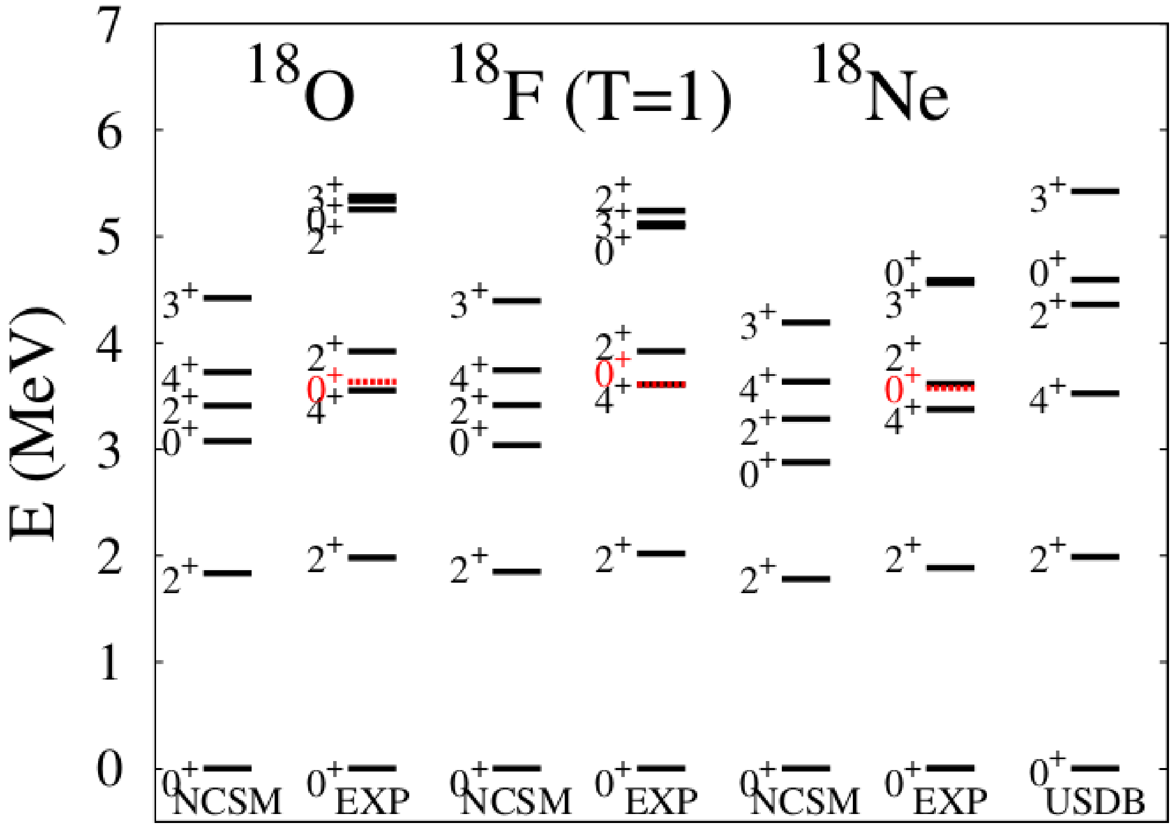


- The states dominated by sd-shell components are quickly converged!
- Intruder states (identified experimentally by large E2 matrix elements) are not converged yet!
- Such general structure of the spectrum is also typical for heavier sd-shell nuclei

Ab-initio effective Hamiltonian from the NCSM with Daejeon16

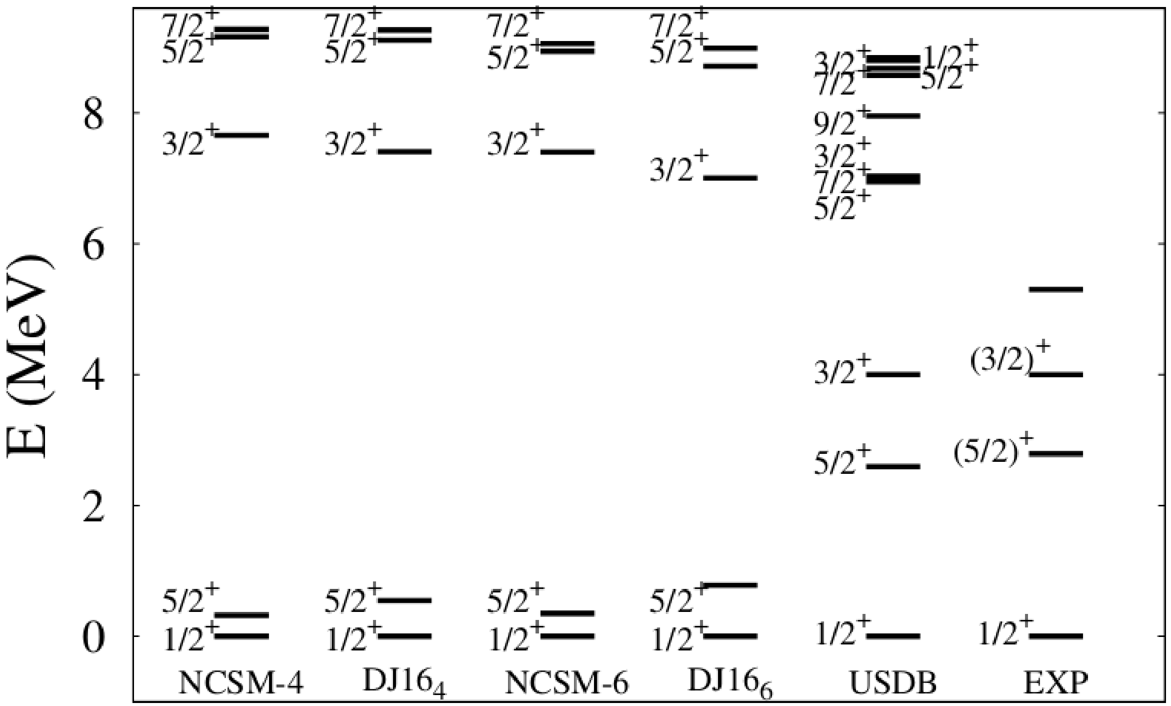


By construction, valence-space two-nucleon calculation reproduces NCSM results



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

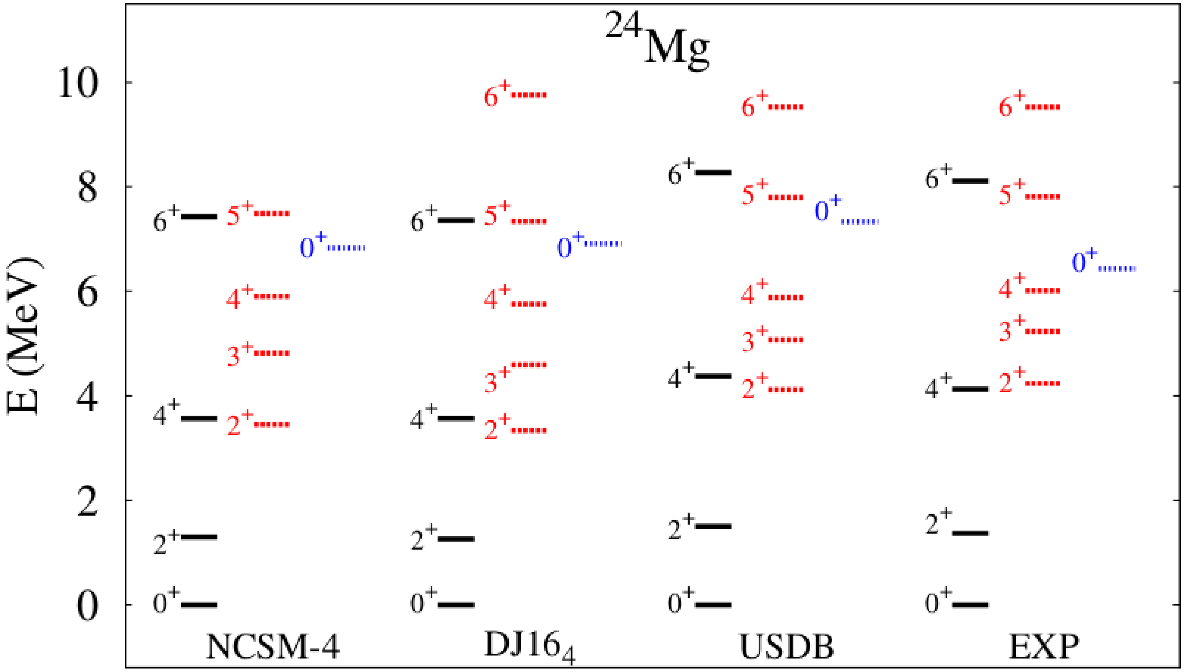
^{23}O



14 states : rms error 63 keV

- ➢ NCSM calculations are doable at Nmax=4 for the whole sd-shell !

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

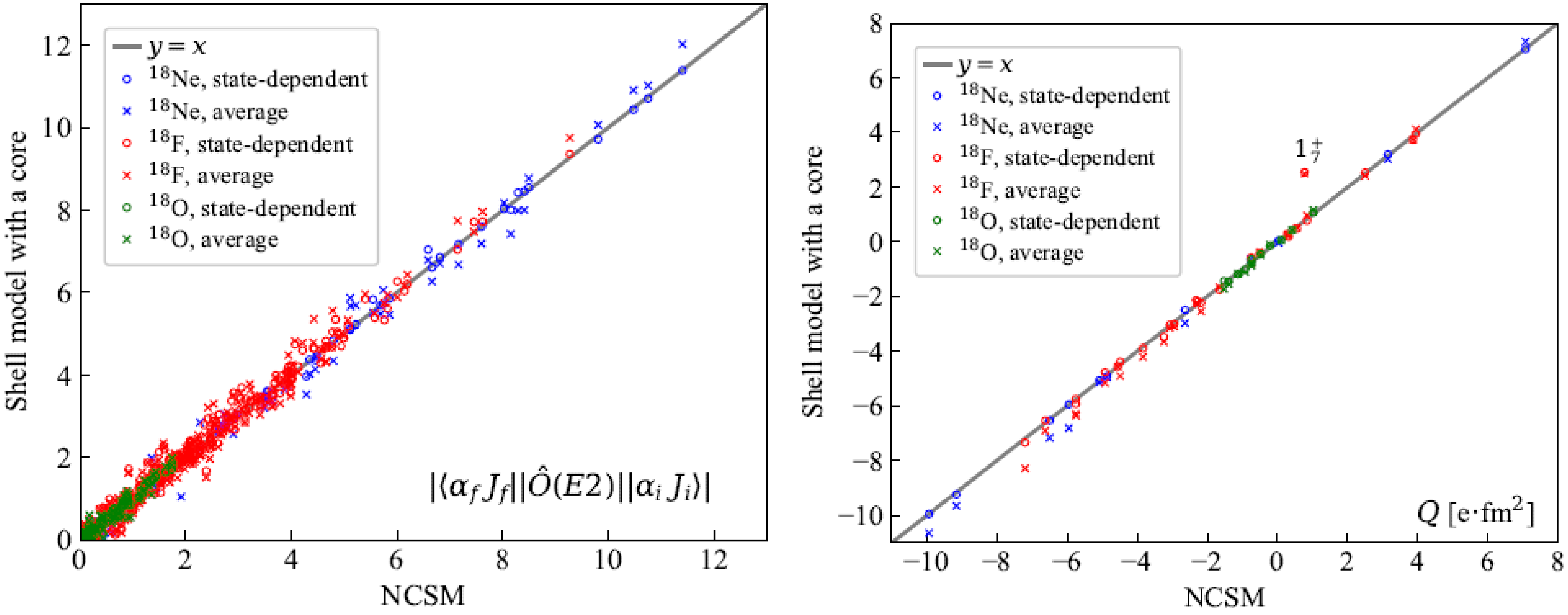
(a,b)	$e_n(a,b)$	$e_p(a,b)$	$g_n^s(a,b)$	$g_n^l(a,b)$	$g_p^s(a,b)$	$g_p^l(a,b)$
bare	0.0	1.0	-3.826	0.0	5.586	1.0
$(0d_{5/2},1s_{1/2})$	0.181	1.171				
$(0d_{5/2},0d_{3/2})$	0.281	1.236	-3.608	0.020	5.252	0.916
$(1s_{1/2},0d_{3/2})$	0.168	1.297				
$(0d_{5/2},0d_{5/2})$	0.179	1.060	-3.751	0.026	5.499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

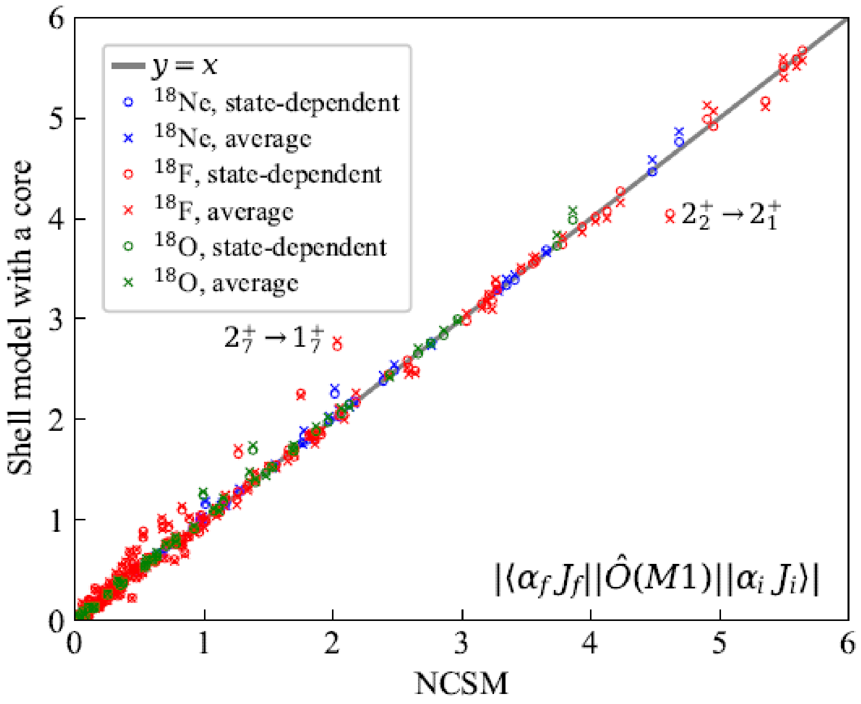
^{18}O : rms(RME) $\approx$ 0.07 e.fm^2 (66 data), rms(Q) $\approx$ 0.06 e.fm^2
^{18}F : rms(RME) $\approx$ 0.11 e.fm^2 (269 data), rms(Q)$\approx$ 0.37 e.fm^2
^{18}Ne : rms(RME)$\approx$ 0.22 e.fm^2 (66 data), rms(Q) $\approx$ 0.06 e.fm^2

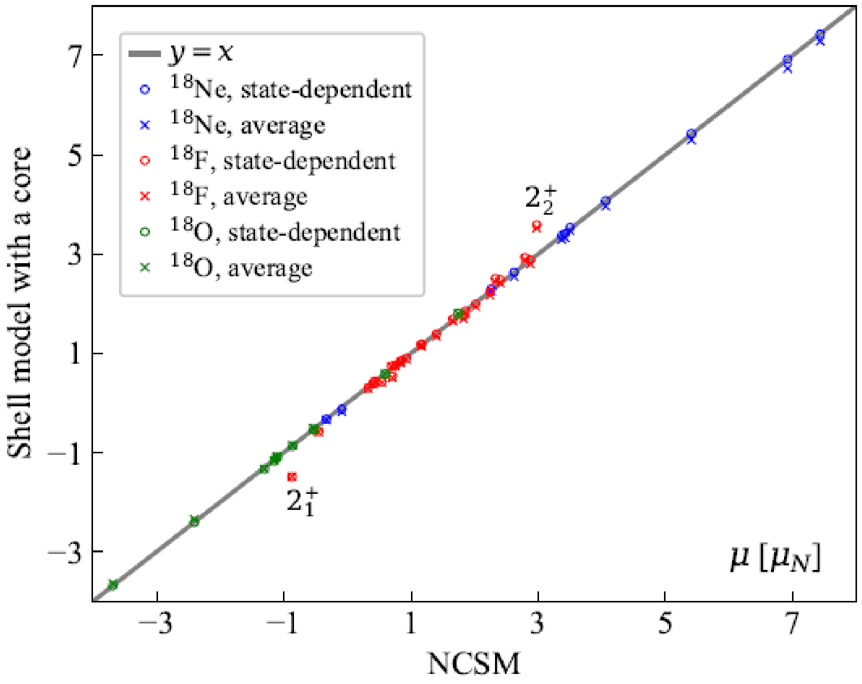


Zh. Li, N. Smirnova, A.M. Shirokov, **I.J. Shin**, B.R. Barrett, P. Maris, J.P. Vary, *Effective operators for valence space calculations from the ab initio No-Core Shell Model,* Chapter in the Memorial volume devoted to Prof. A. Arima ``Symmetry, Shells, and Society''; edited by Profs. K. K. Phua, T. Otsuka and J.P. Vary; World Scientific (2024).

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

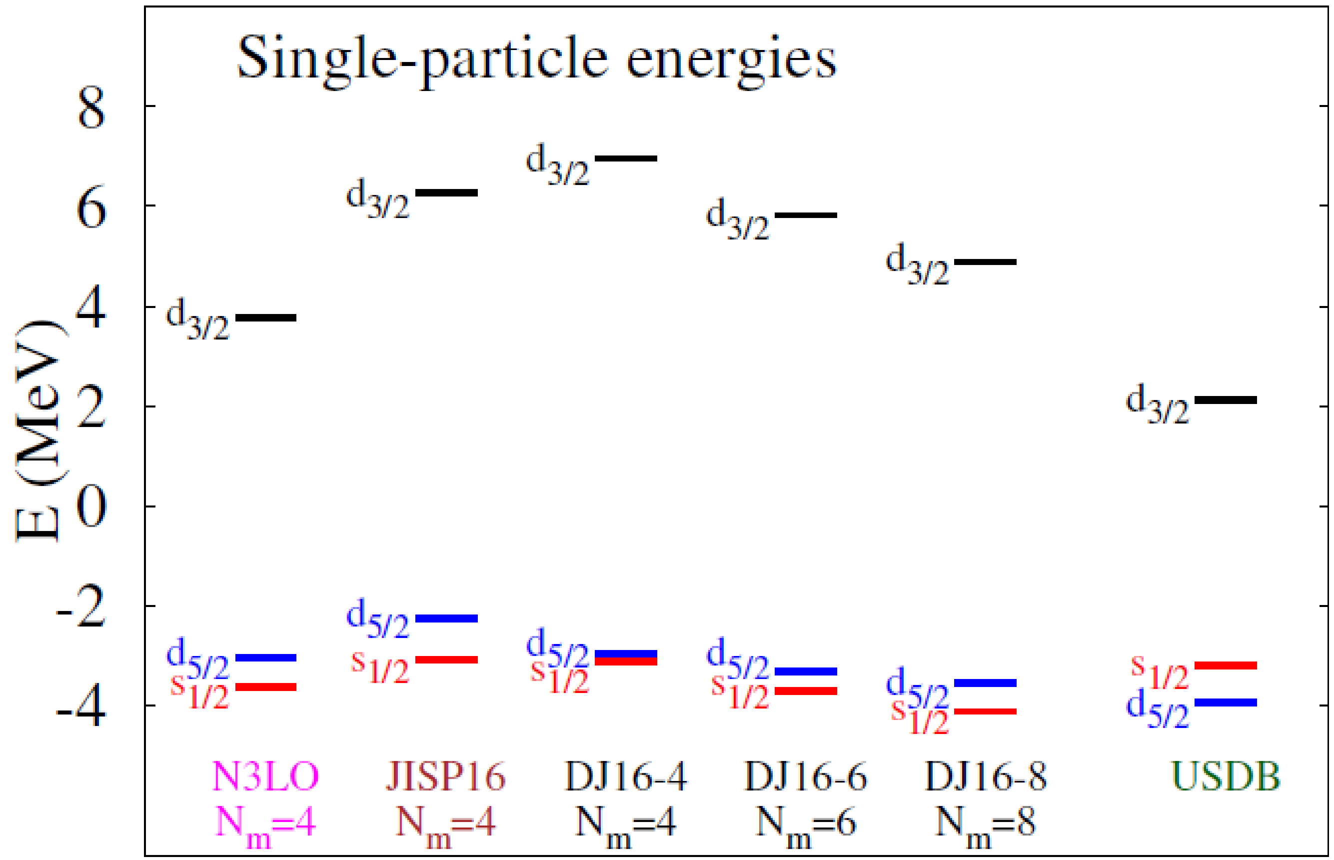
^{18}O : rms(RME) $\approx 0.06\ \mu_N$ (43 data), rms(μ) $\approx 0.02\ \mu_N$
^{18}F : rms(RME) $\approx 0.09\ \mu_N$ (212 data), rms(μ)$\approx 0.19\ \mu_N$
^{18}Ne : rms(RME)$\approx 0.06\ \mu_N$ (43 data), rms(μ) $\approx 0.02\ \mu_N$





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. K. K. Phua, T. Otsuka and J.P. Vary; World Scientific (2024).

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



Drawbacks for all NN potentials:

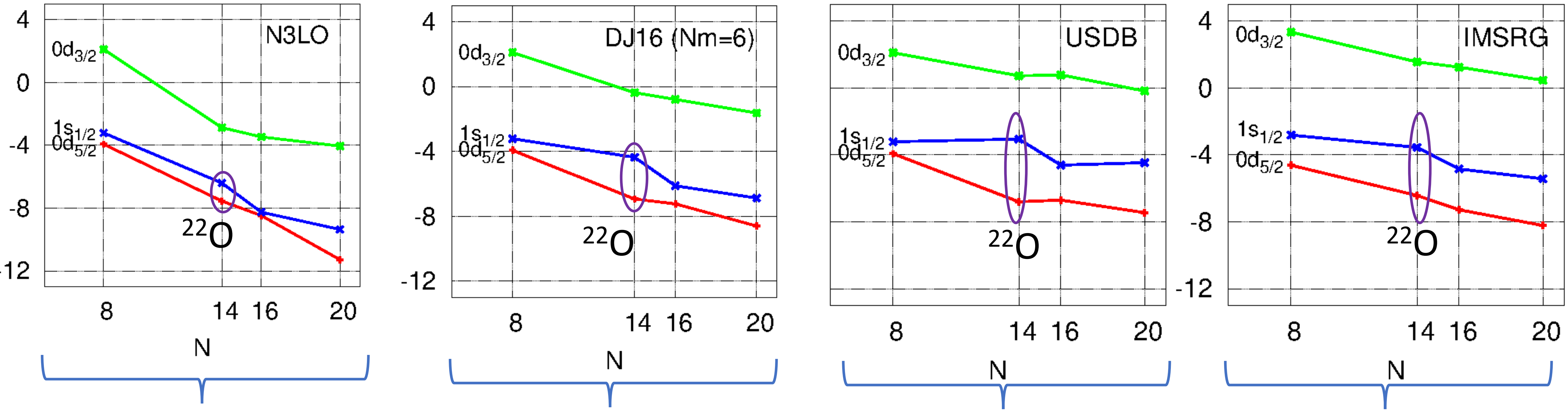
- ☐ *Inversion of s1/2 and d5/2 orbitals*
- ☐ *Too large d3/2 – d5/2 spin-orbit splitting*

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

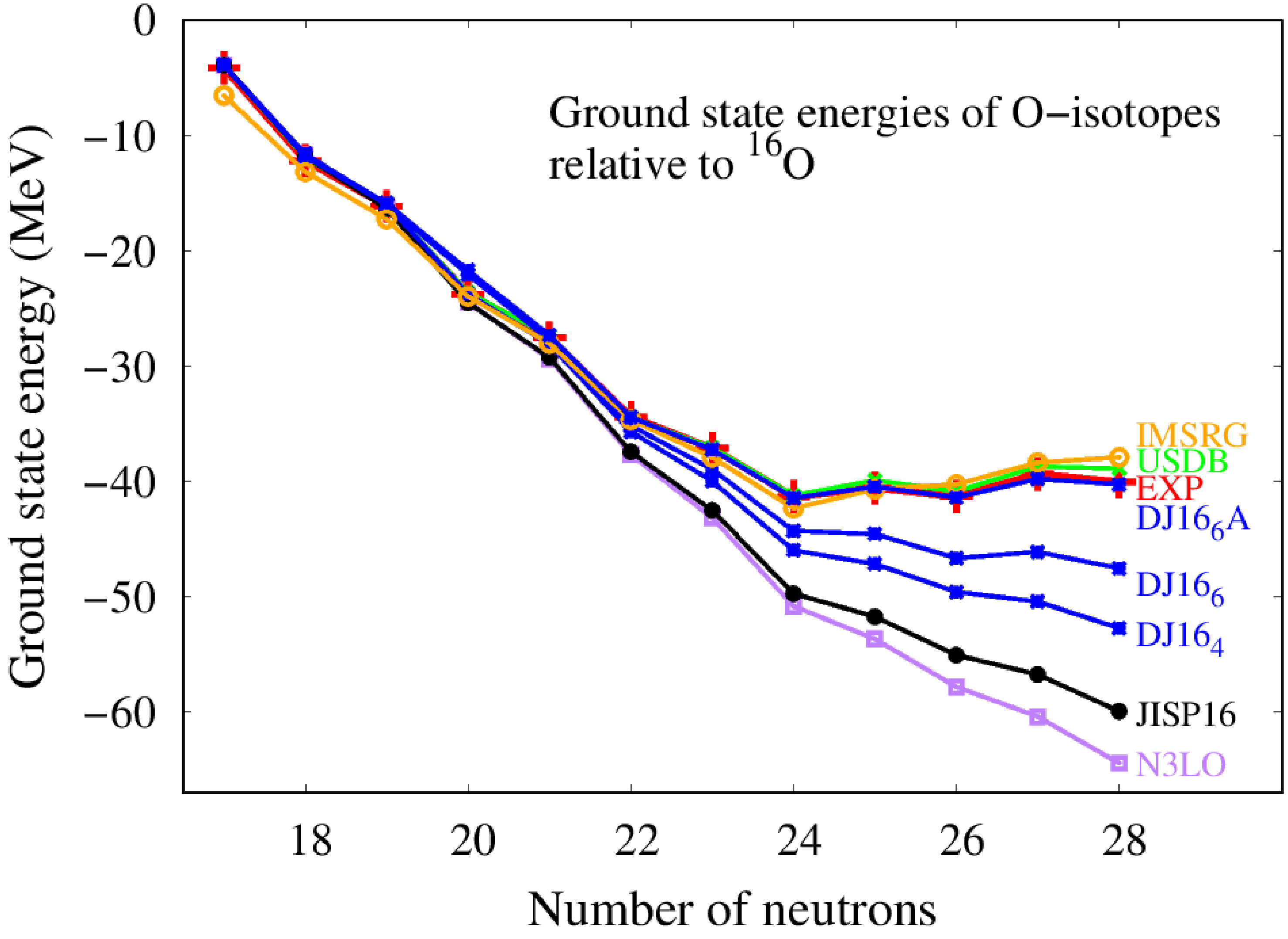
Empirical = experiment

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, P. Maris, J.P. Vary, ***PRC110****, 034306 (2024)*

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

« Improving sd-shell effective interactions from Daejeon16 »

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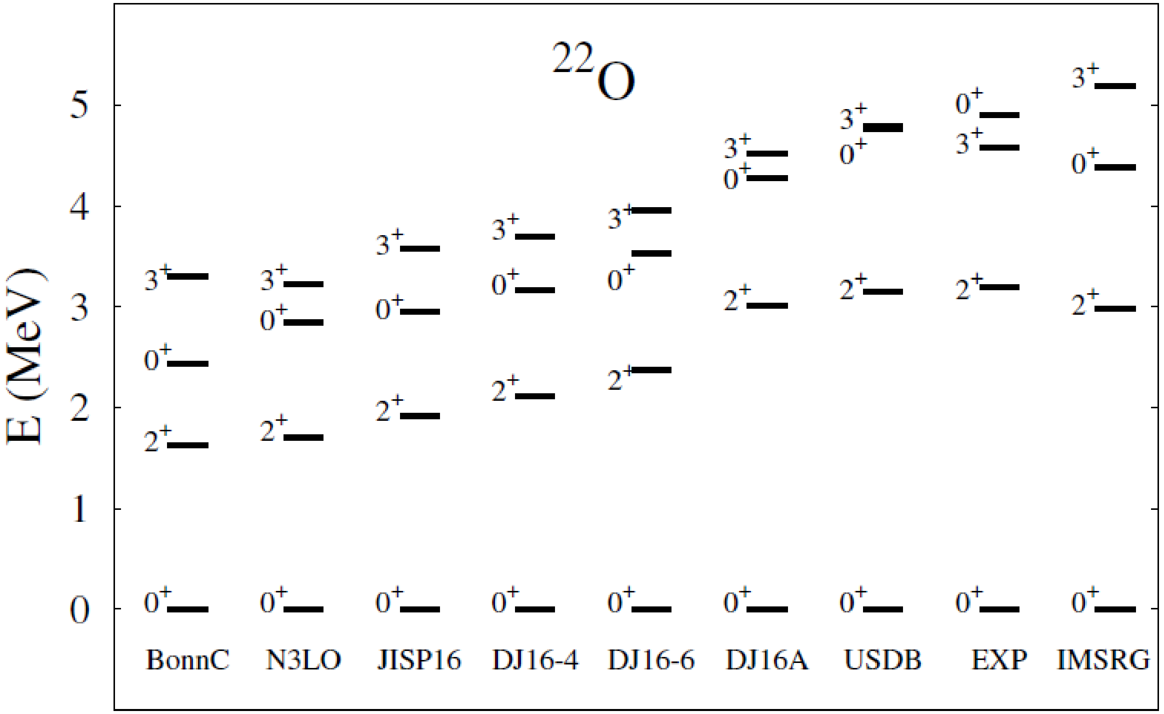
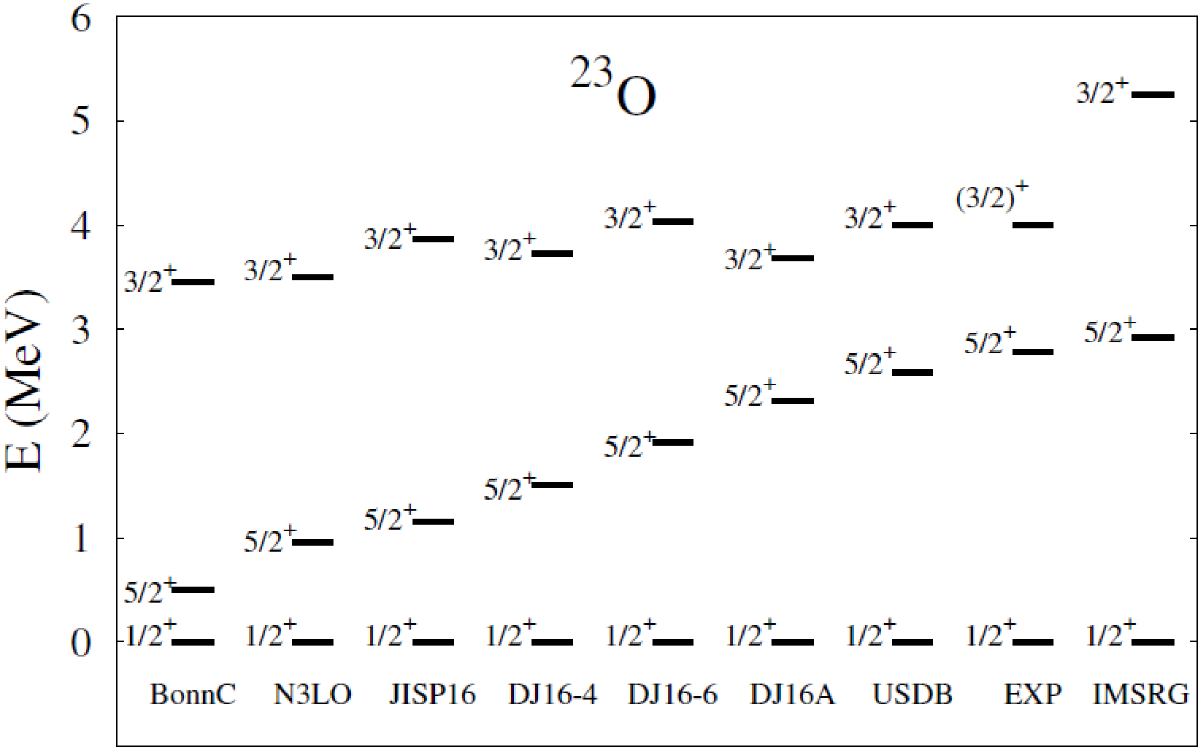
Ab-initio effective Hamiltonian from the NCSM



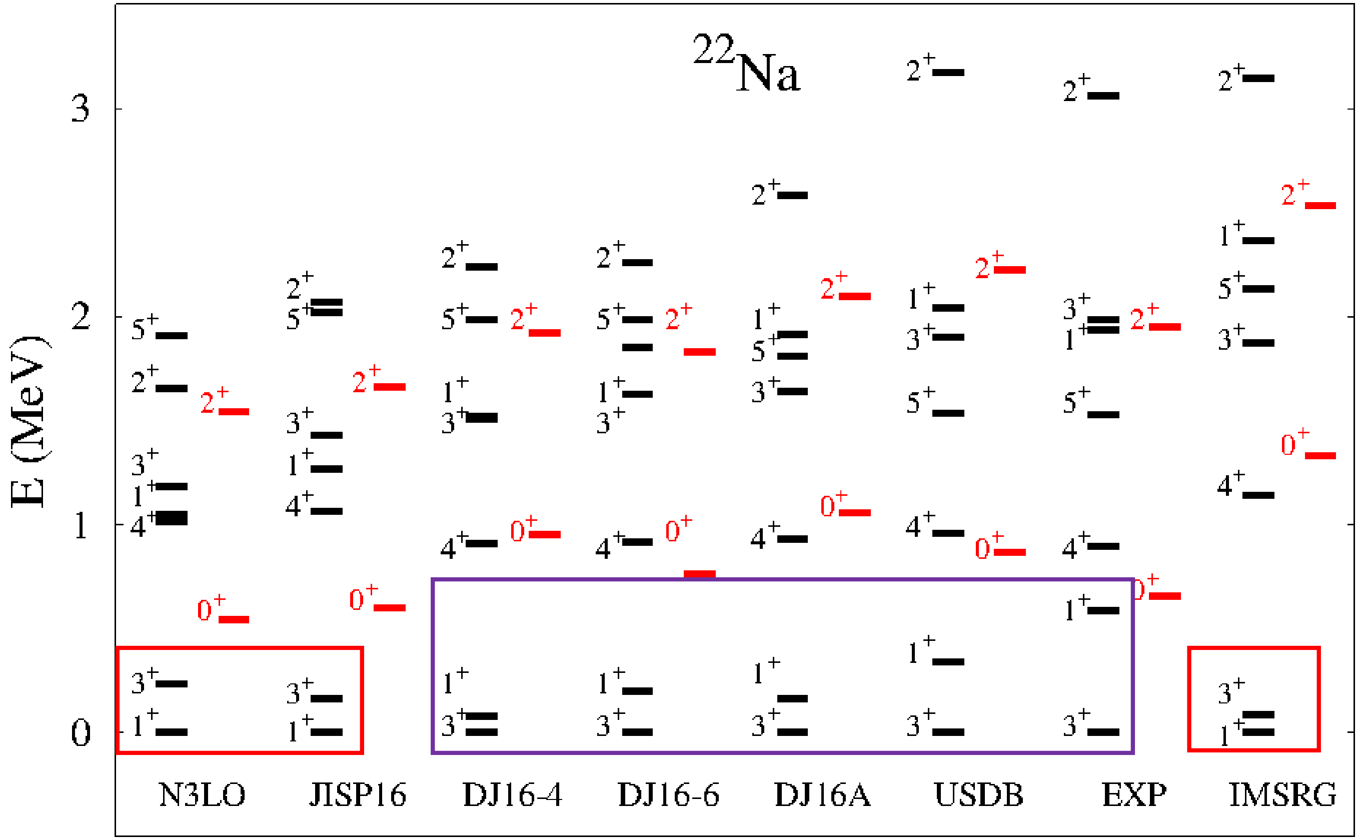


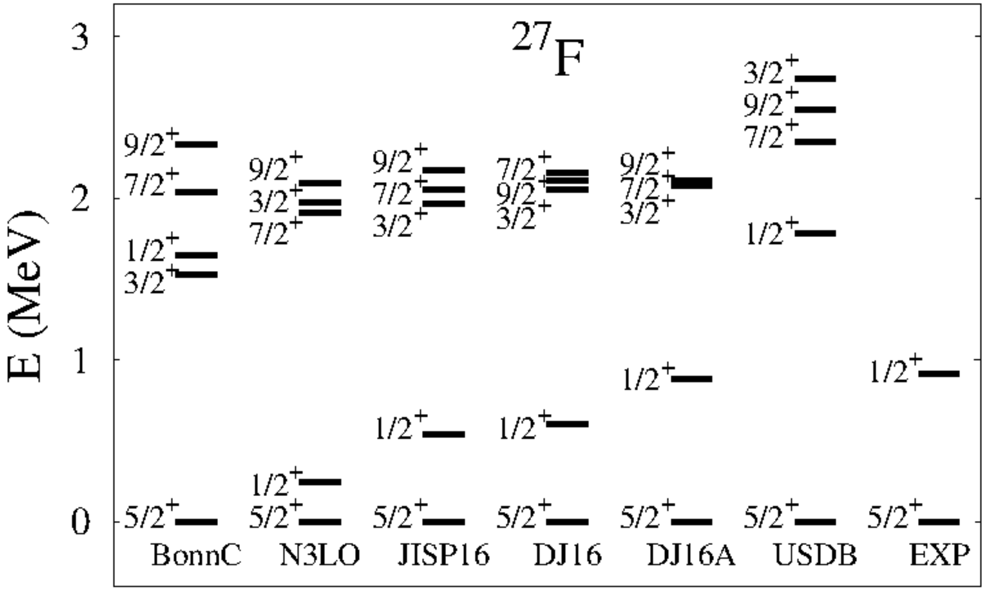
Increase of N=14 subshell gap

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) !

- 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, A. Rivero, MCIA, University of Bordeaux

Conclusions and Perspectives

- ❑ Daejeon16: high-precise NN potential which effectively includes 3N and many-nucleon forces. Still we aim at further improvements for A>16 nuclei !
- ❑ Microscopic sd-shell interactions obtained via OLS transformation of the NCSM solution look encouraging: the effect of 3N forces is significantly reduced. Objective: psdpf model space to describe negative parity states in sd shell nuclei, important for astrophysics
- ❑ First study of electromagnetic operators for nuclei beyon A=18 is in progress
- ❑ 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

- A Short-term visit of French team members to Daejeon and
- A Short-term visit of the Korean team members to Bordeaux.

THANK YOU FOR YOUR ATTENTION !