中国科学院近代物理研究所
Institute of Modern Physics, Chinese Academy of Sciences

Quadrupole dynamics of carbon isotopes and ^{10}Be

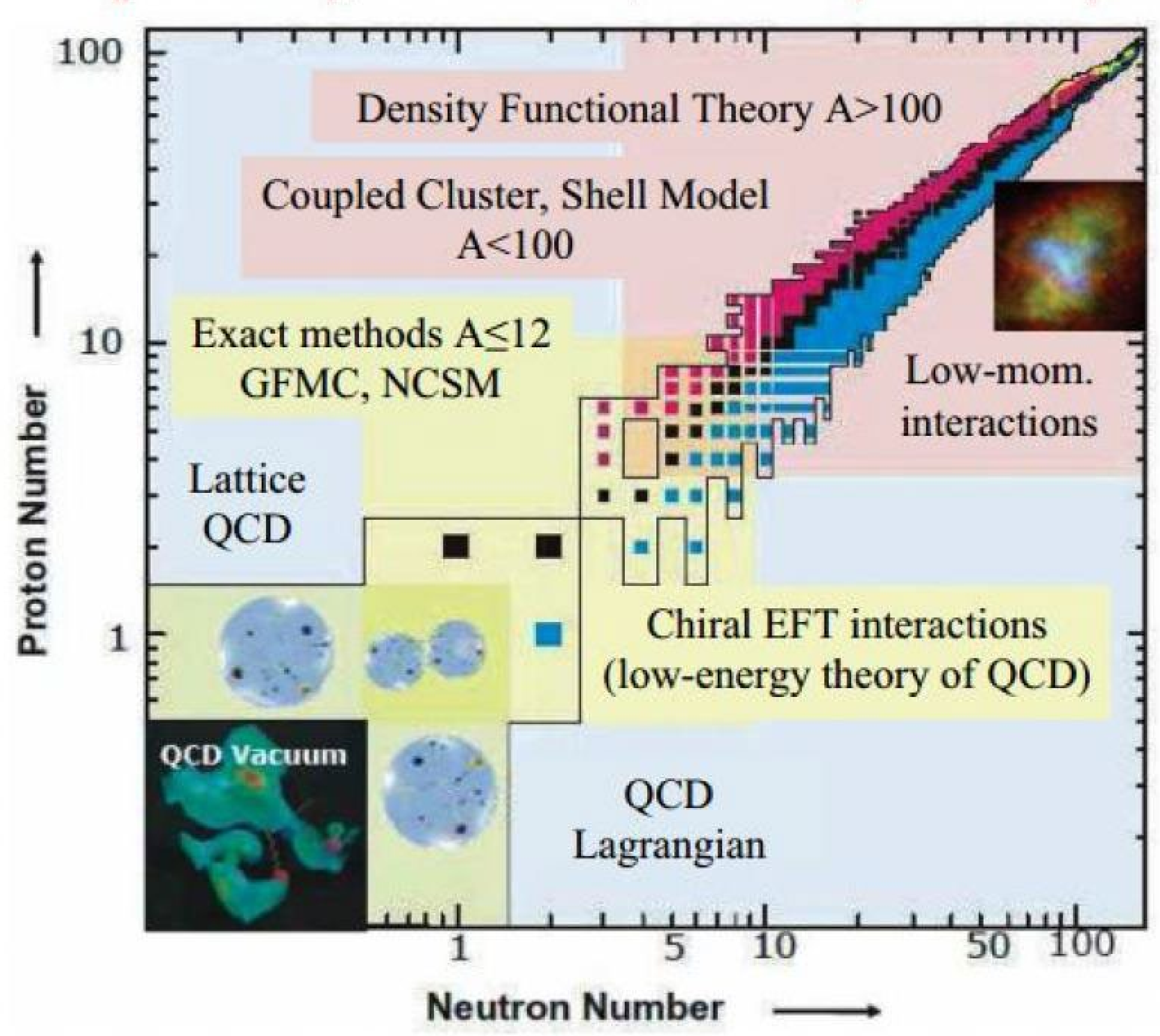
He Li （李贺）

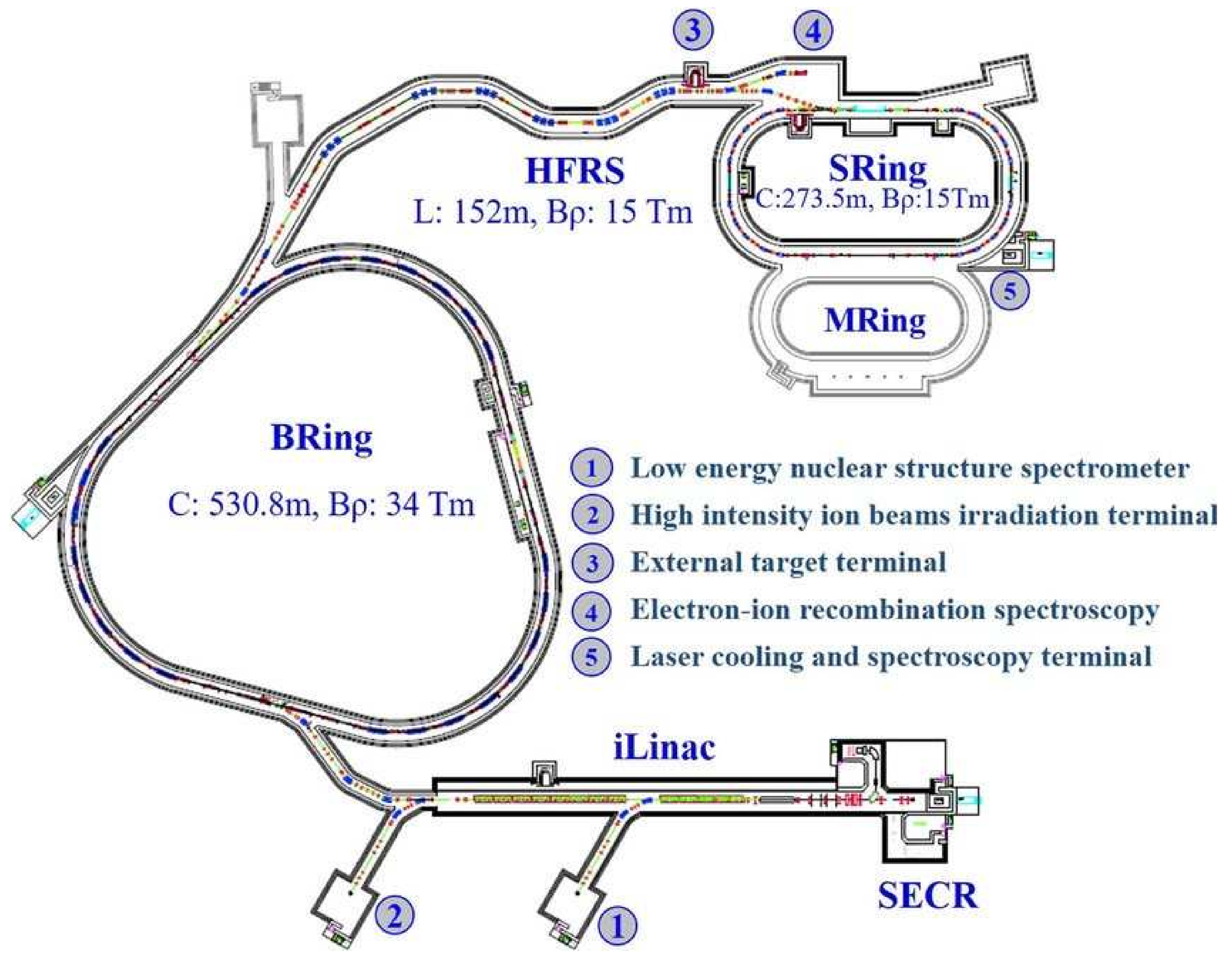
Collaborators: **Andry M. Shirokov**
James P. Vary
Xingbo Zhao（赵行波）
HOOI JIN ONG （王惠仁）
Peng Yin（尹鹏)

May 26, 2025

Outline

- ➢ Electric quadrupole ($E2$) observables in nuclei
- ➢ No-core shell model (NCSM) method
- ➢ MFDn code
- ➢ Daejeon16 and JISP16 interaction
- ➢ Sugon high-performance computer
- ➢ NCSM results and extrapolations
- ➢ Ratios of electric quadrupole ($E2$) observables
- ➢ Next plan and Conclusions





Electric quadrupole ($E2$) observables in nuclei

- **Electric quadrupole ($E2$) observables, such as electric quadrupole moments and $E2$ transition strengths reveal nuclear deformation and collective structure**

$$Q_{\lambda\mu} = \zeta^{(\mathrm{E}\lambda)} \sum_{j=1}^{A} e(j) r_j^{\lambda} Y_{\lambda\mu}(\Omega_j) \ ,$$

$$B(\sigma\lambda\,;\,\xi_i J_i \to \xi_f J_f) \equiv \frac{1}{2J_i+1} \left| (\xi_f\, J_f \| \boldsymbol{\mathcal{M}}_{\sigma\lambda} \| \xi_i\, J_i) \right|^2 .$$

$$eQ \equiv \zeta \sqrt{\frac{16\pi}{5}} \mathcal{M}(\mathrm{E2}) = \zeta \sqrt{\frac{16\pi}{5}} \sqrt{\frac{J(2J-1)}{(J+1)(2J+1)(2J+3)}} (\xi\, J \| \boldsymbol{Q}_2 \| \xi\, J)$$

- **To probe the proton-neutron asymmetric aspects of the nuclear deformation, both proton and neutron quadrupole observables are needed**

- **it is very difficult to obtain *ab initio* NCSM calculations for $E2$ observables, due to $E2$ observables are sensitive to the large-distance tails of the nuclear wave function, extrapolation method of NCSM $E2$ results is necessary**

J. Suhonen, From nucleon to nucleus(2006)

Introduction of NCSM

❖ No-Core Shell Model Method

- Given a Hamiltonian operator

$$\hat{H} = \sum_{i<j}\frac{(\vec{p}_i-\vec{p}_j)}{2mA} + \sum_{i<j}^{A} V_{ij} + \sum_{i<j<k} V_{ijk} + \cdots$$

- Solve the eigenvalue problem for wavefunction of A nucleons

$$\hat{H}\Psi_{\alpha_1\cdots\alpha_A} = \mathrm{E}\Psi_{\alpha_1\cdots\alpha_A}$$

- Expand wavefunction in basis states $|\psi\rangle = \sum \hat{a}_j \; |\phi_i\rangle$
- Express Hamiltonian in basis $\langle\phi_j|\hat{H}|\phi_i\rangle = H_{ij}$
- Diagonalize Hamiltonian matrix H_{ij}
- No-Core: All A nucleons are treated the same
- Complete basis ---- exact result
- In practice
  1. truncate basis
  2. study behavior of observables as function of truncation
- Computational challenge
  1. construct large ($10^{10} \times 10^{10}$) sparse symmetric matrix H_{ij}
  2. obtain lowest eigenvalues & eigenvectors corresponding to low-lying spectrum and eigenstates

P. Maris, NCSM_NICC_YTT(2021)
Barrett et al., Progress in Particle and Nuclear Physics (2013)

Introduction of NCSM

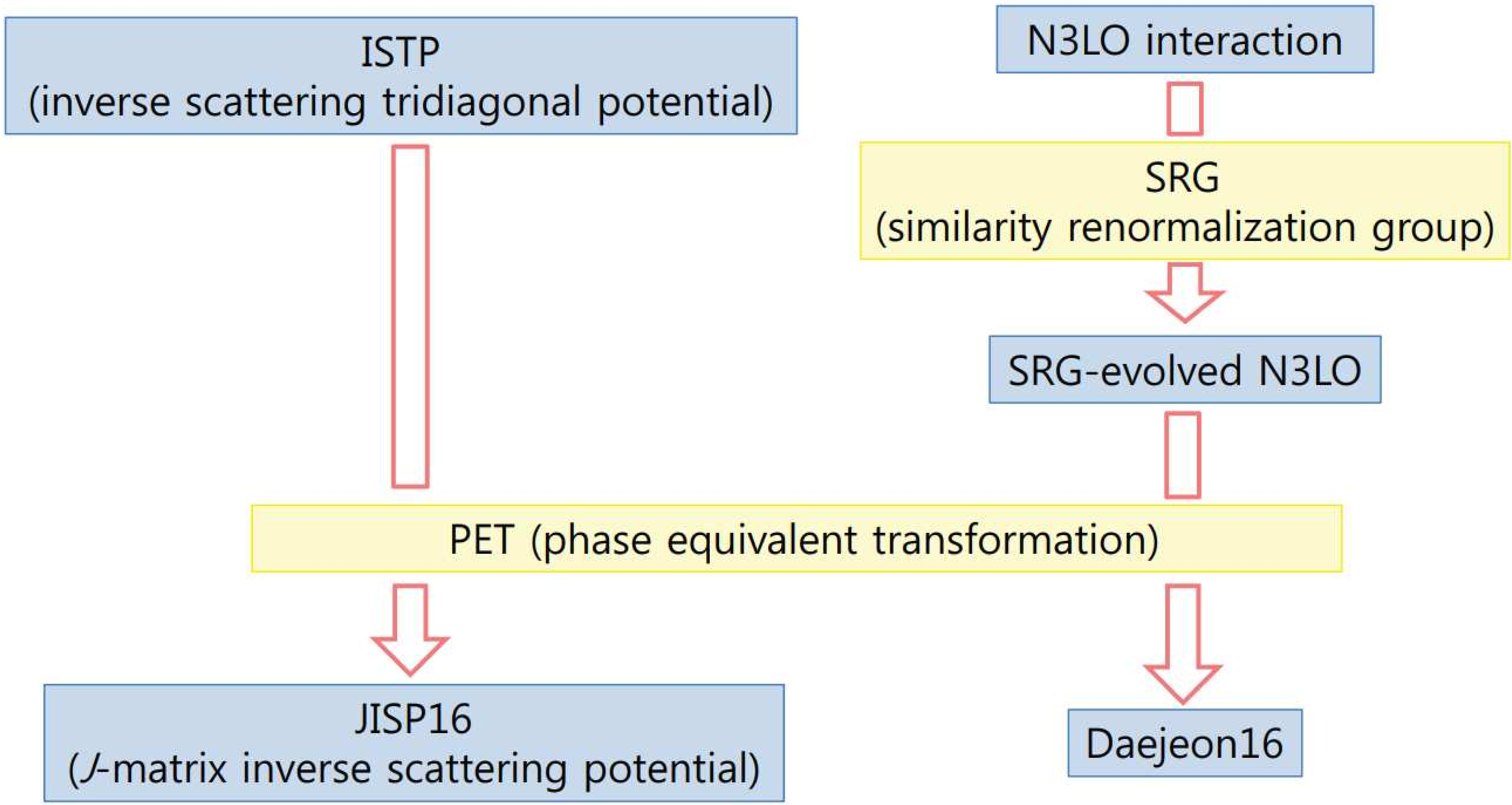
- ❖ MFDn (Many Fermion Dynamics for Nuclear Structure) code

  - Calculate the approximate low-lying spectrum (eigenvalues) and corresponding wavefunctions ψ (eigenvectors) of a (Z + N) = A-body system of Z protons and N neutrons using 2-body (and optional 3-body) interactions in a finite basis in configuration space (sparse matrix)
  - Evaluate for the requested number of states (eigenvalues)
    1. orbital occupation probabilities
    2. One-Body Density Matrix Elements (OBDMEs)
    3. expectation values of total spin J^2 and isospin T^2
       (for T^2 assuming proton and neutron radial wavefunctions are the same)
    4. expectation values for arbitrary scalar 2-body operators
    5. for Harmonic Oscillator (HO) basis
       static: quadrupole moments, M > 0: magnetic moments, r^2 …
       transitions: M1, E2, and GT(assuming isospin symmetry)

P. Maris, NCSM_NICC_YTT(2021)

Daejeon16 and JISP16 interaction

- **Daejeon16 (Daejeon, the name of a city in South Korea, where the main developments took place. PET tuned up to ^{16}O)**
  JISP16, (J-matrix inverse scattering potential, PET tuned up to ^{16}O)



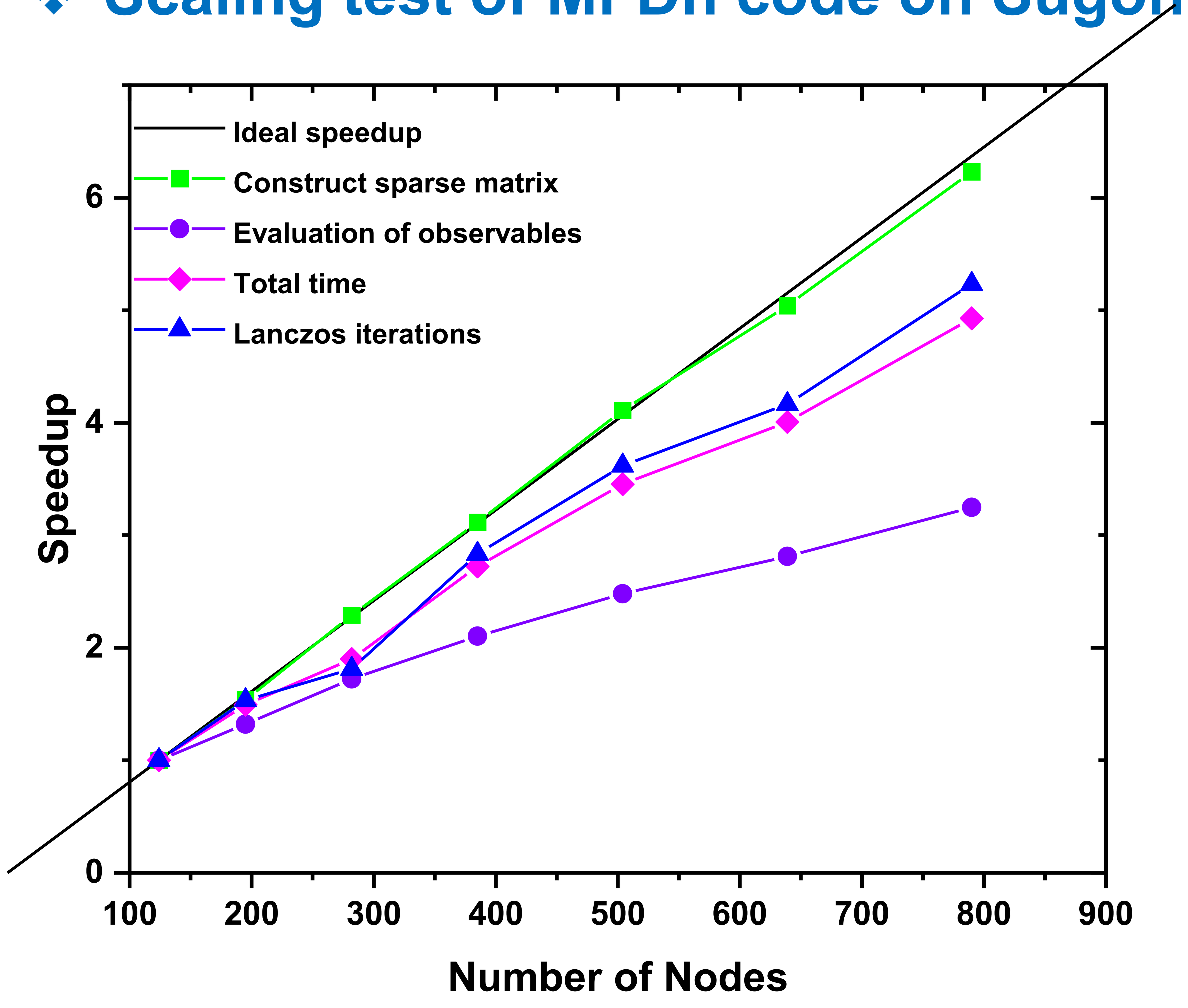
Kim et al., arXiv:1910.04367 (2019)
Shirokov et al., Physics Letters B (2016)

Sugon high performance computer

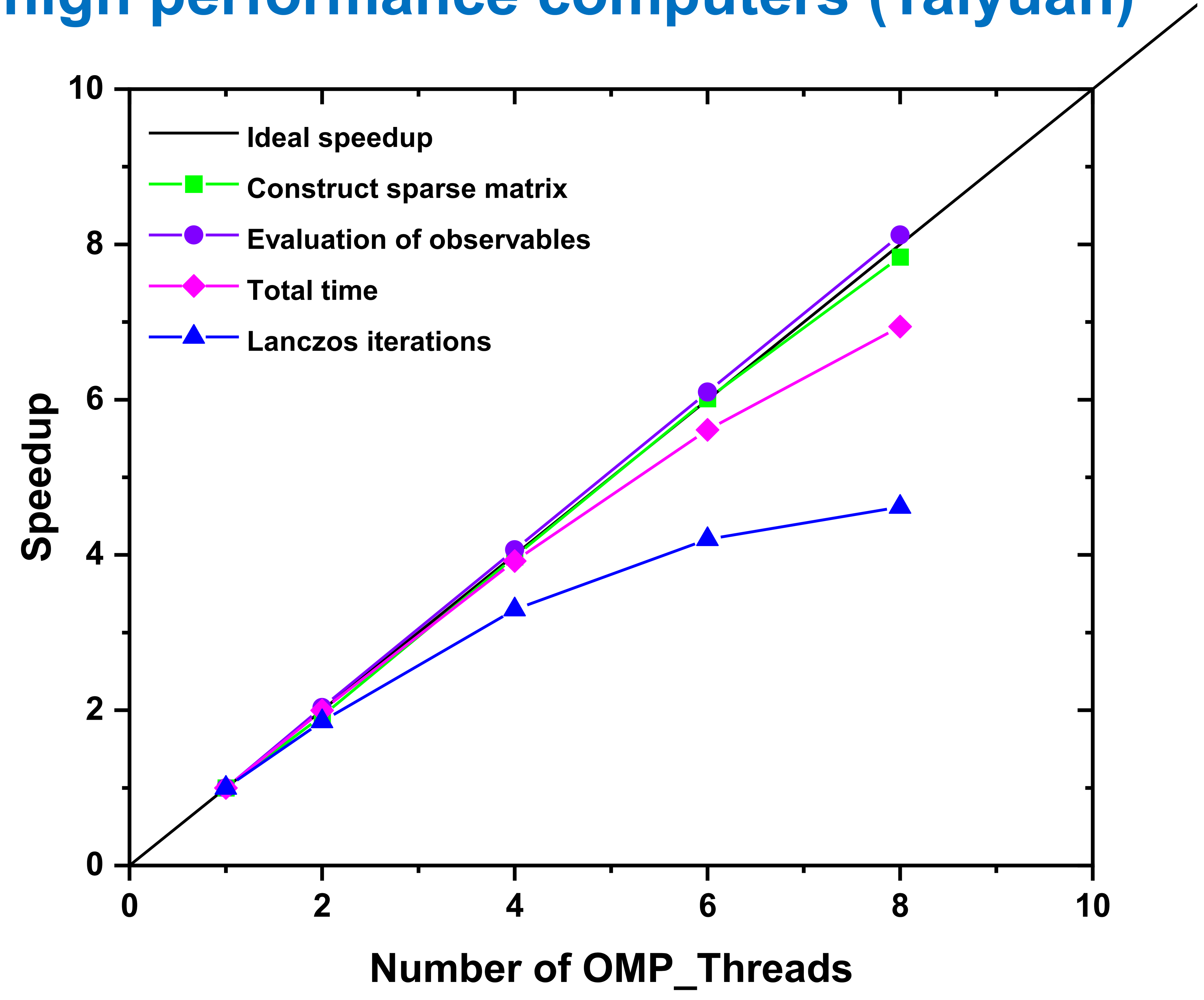
中科曙光 Sugon

- **Hygon CPU node: 32 cores, 128Gb memory**
- **Kunshan center: more than 10,000 nodes**
- **Taiyuan center: ~ 7000 nodes**
- **Xian center: ~ 2000 nodes (64 cores, 256 Gb/node)**

❖ **Scaling test of MFDn code on Sugon high performance computers (Taiyuan)**



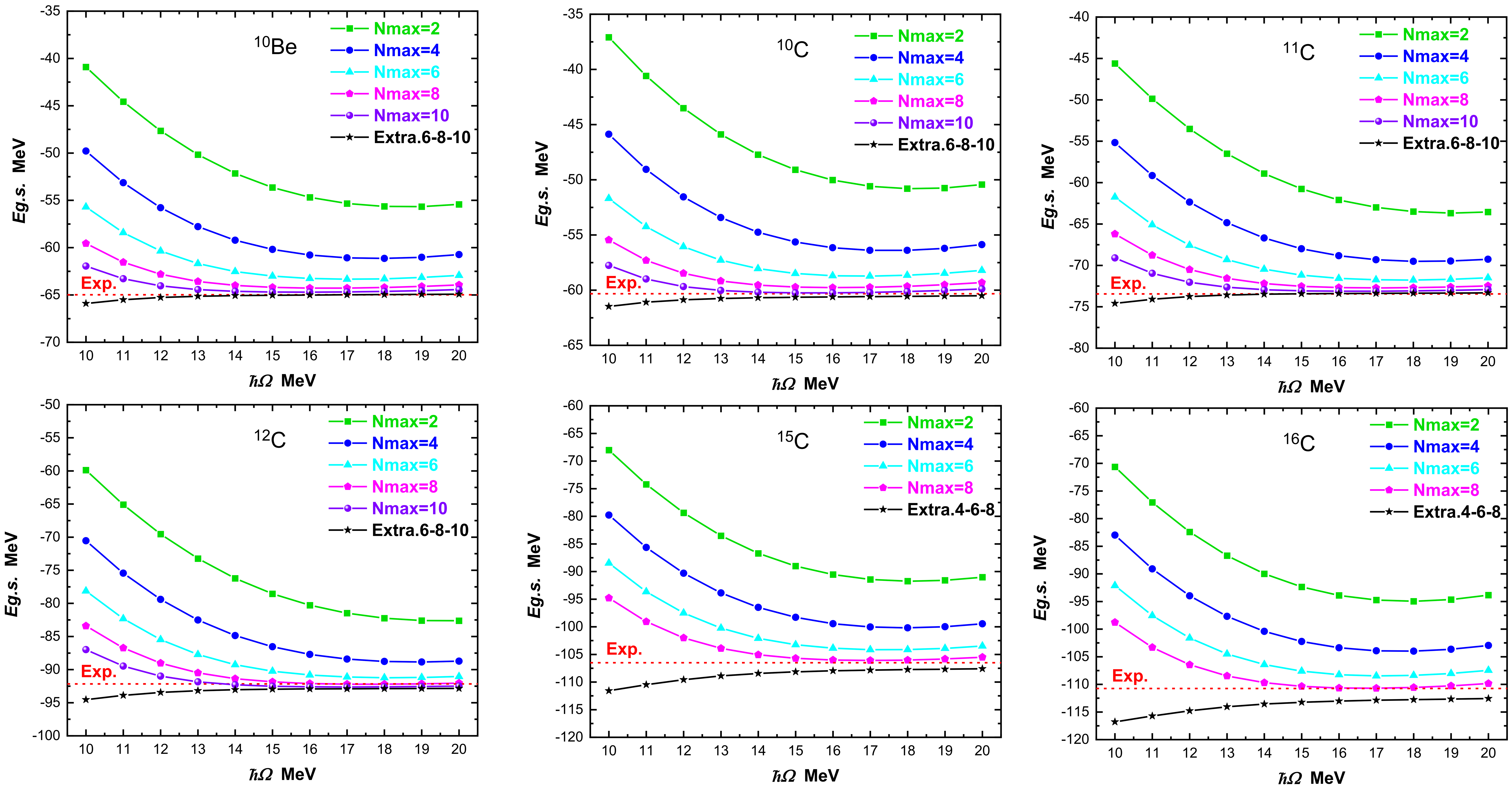
OMP_Threads=4, number of nodes up to 790



Number of nodes =790, OMP_Threads up to 8

NCSM results

❖ Ground state energy from Daejeon16



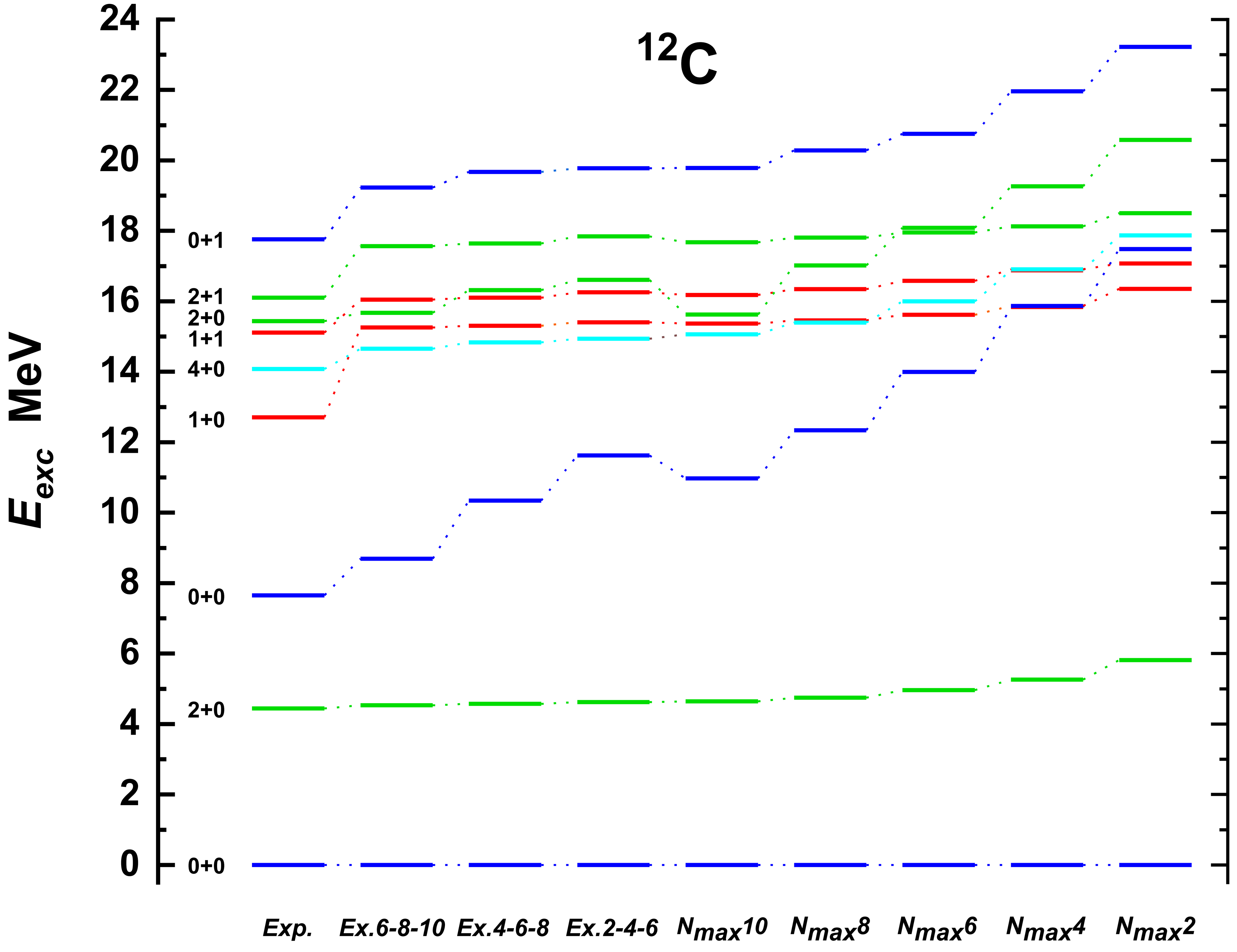
NCSM+Daejeon16 has good performance on the calculations of binding energies

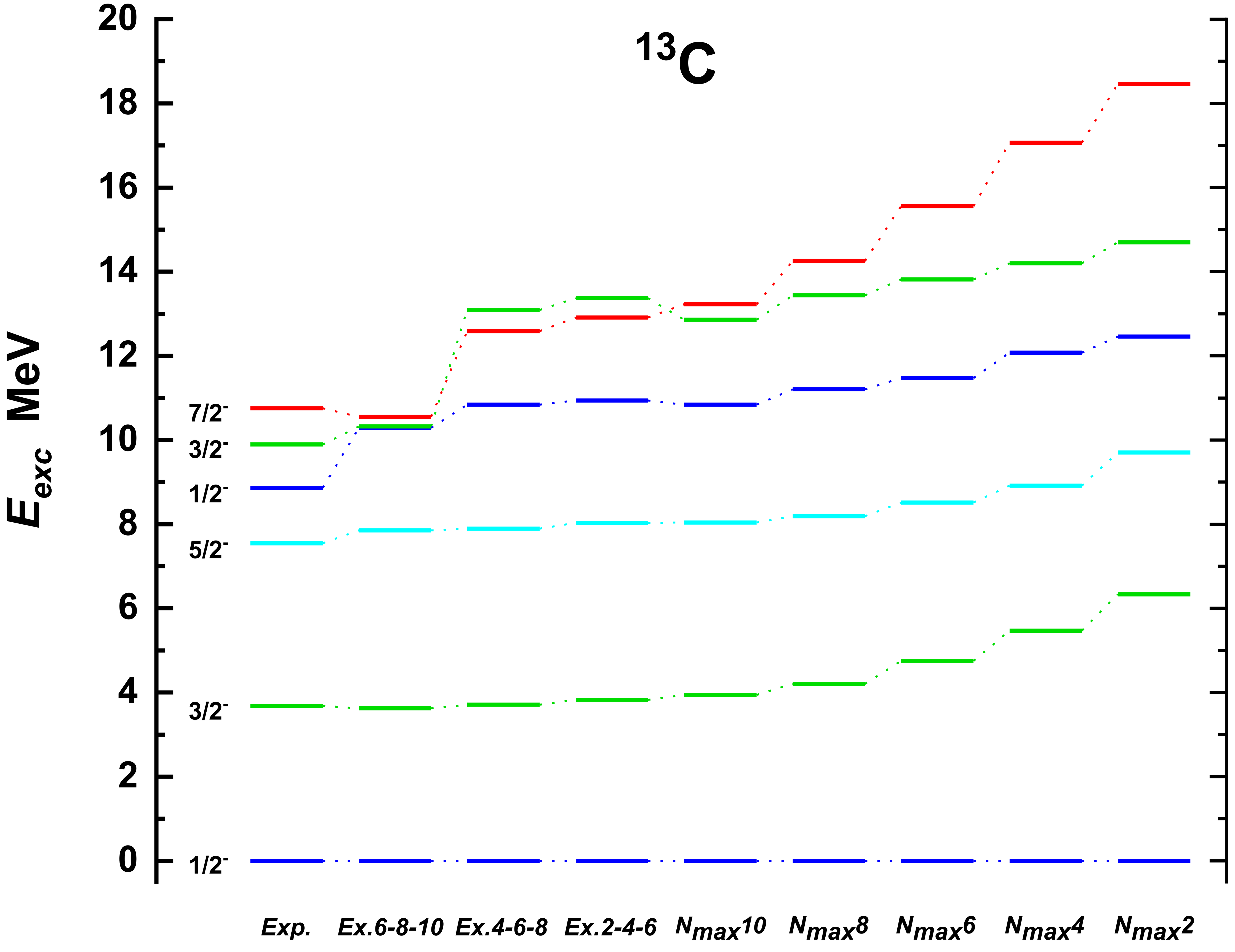
We use a simple 3-point exponential extrapolation from the reference paper

$$E^{\hbar\omega}(N_{\max}) = E^{\hbar\omega}_{\infty} + a\, e^{(-b\, N_{\max})}$$

P. Maris et al., Phys. Rev. C (2021)

❖ **Energy spectra from Daejeon16 (fixed hw = 17 MeV)**





The low-lying spectra of ^{12}C & ^{13}C from Daejeon16 have good agreement with experimental data

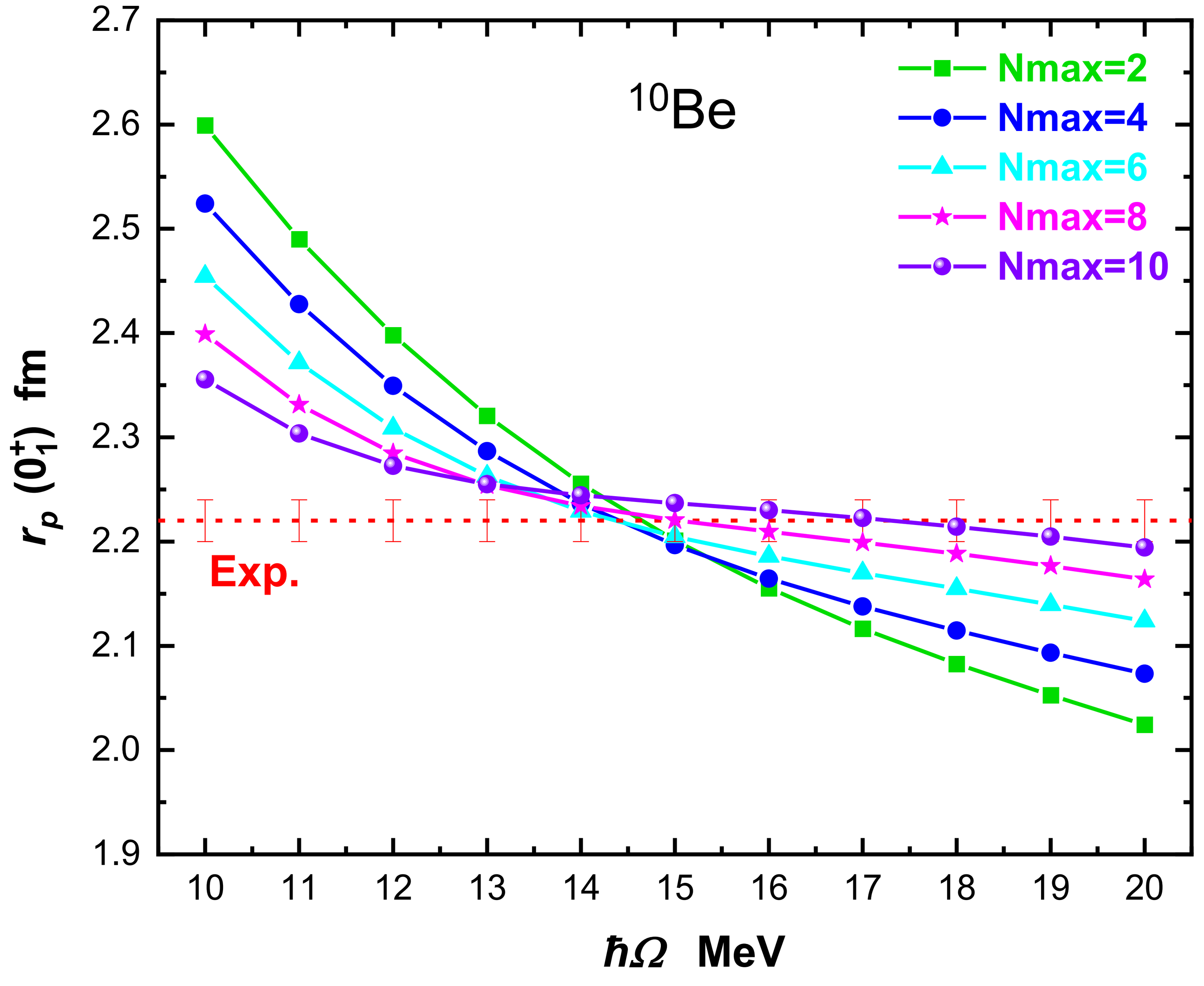
We use a simple 3-point exponential extrapolation from the reference paper

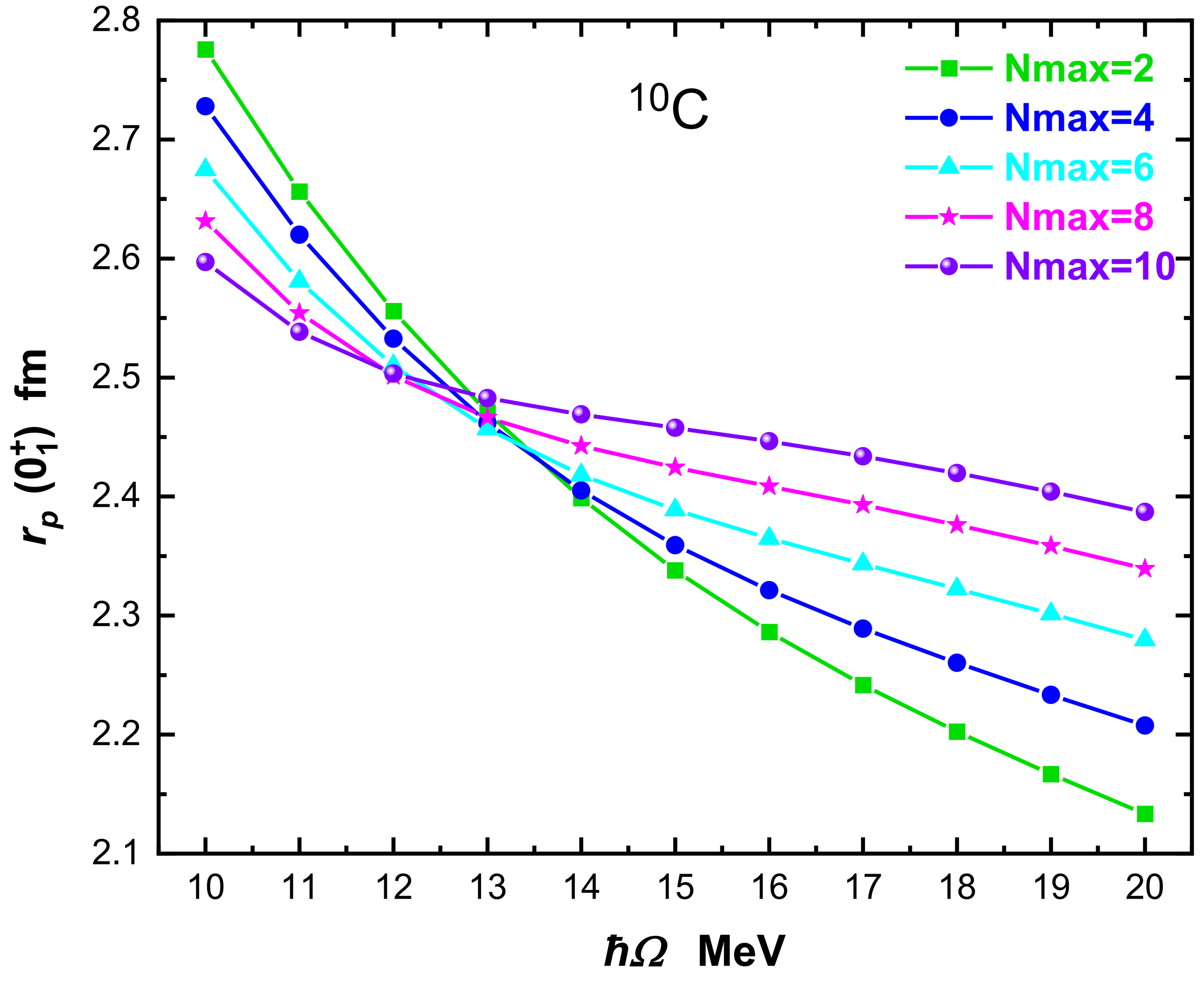
$$E^{\hbar\omega}(N_{\max}) = E^{\hbar\omega}_{\infty} + a\,\mathrm{e}^{(-b\,N_{\max})}$$

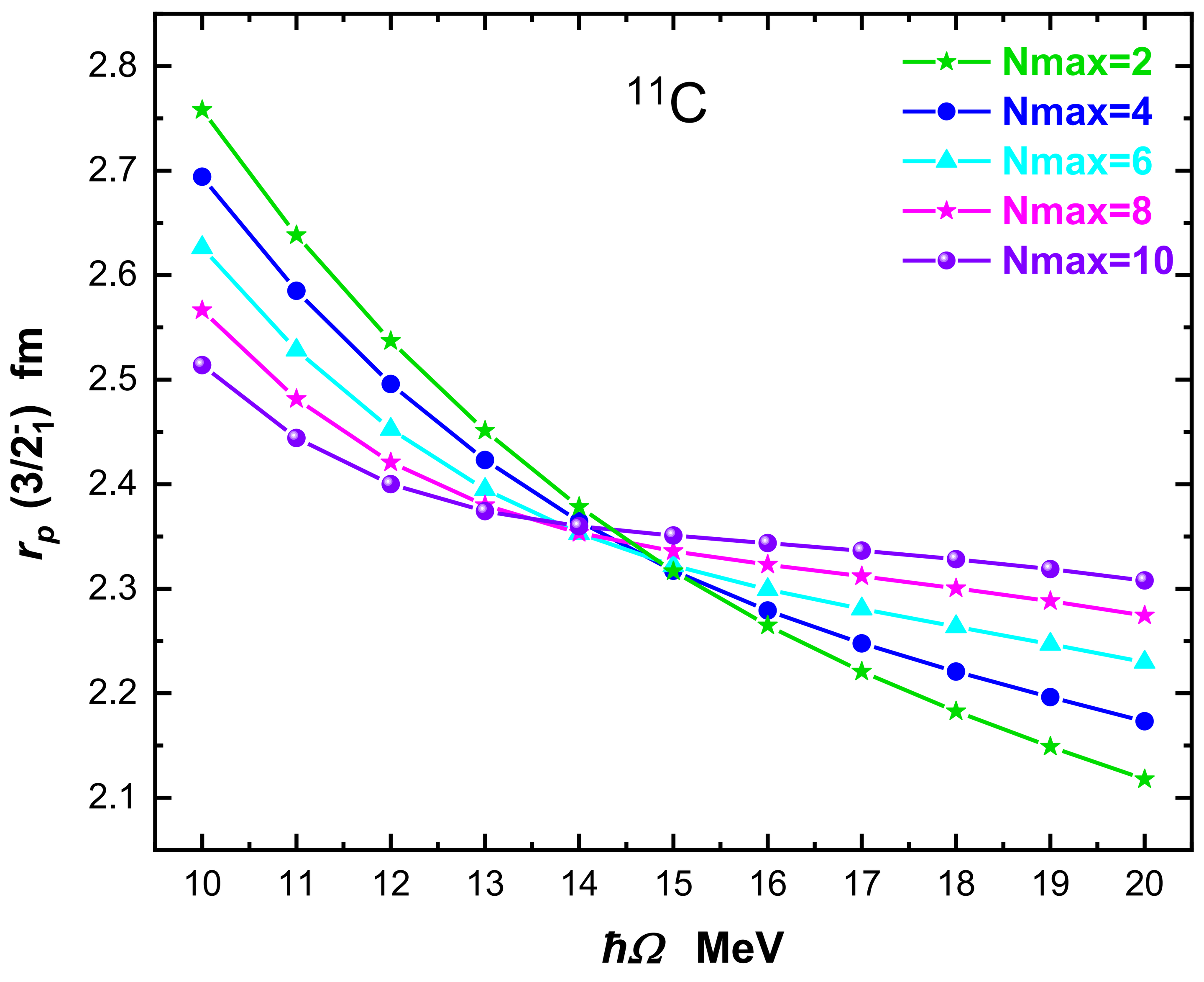
P. Maris et al., Phys. Rev. C (2021)

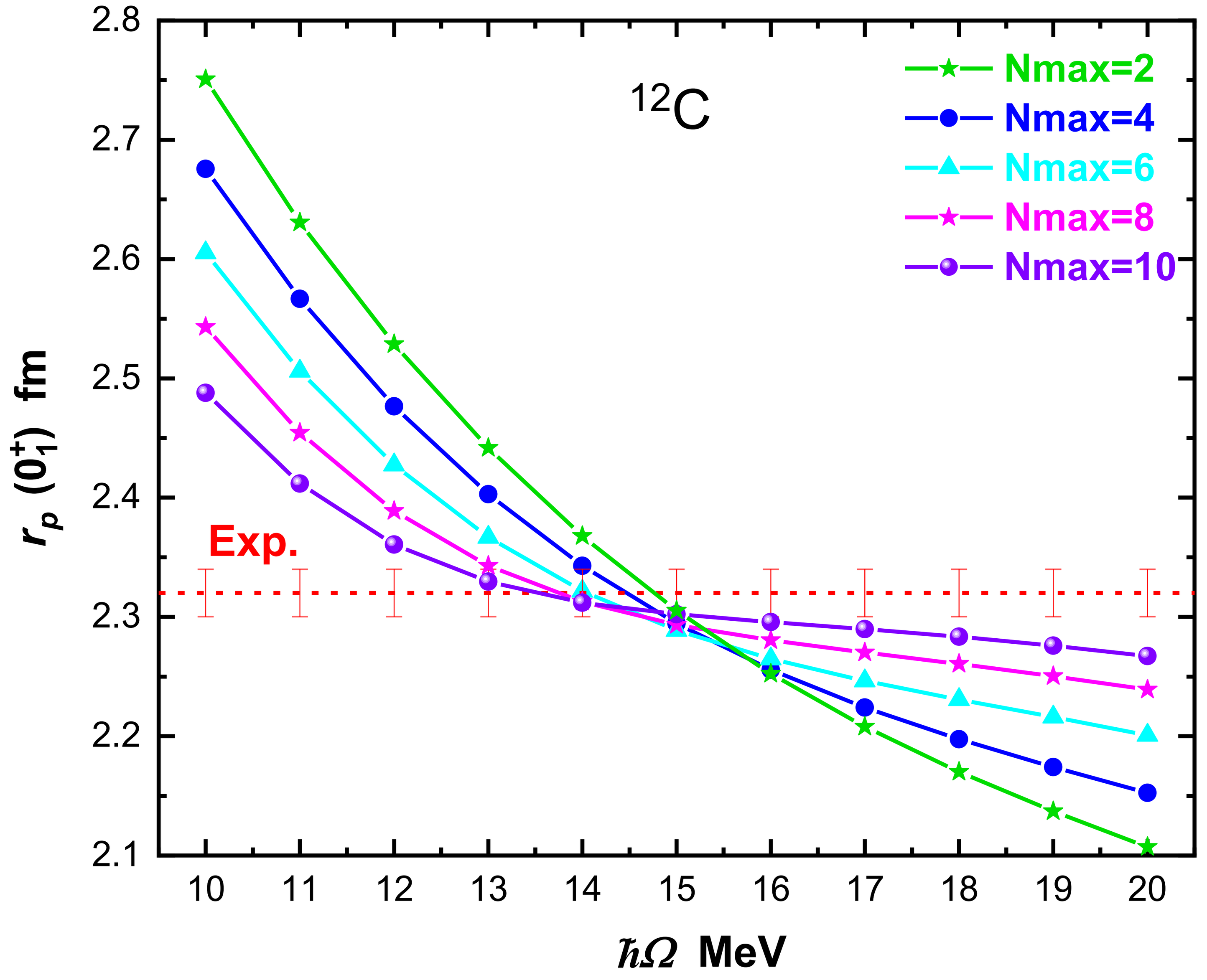
NCSM results

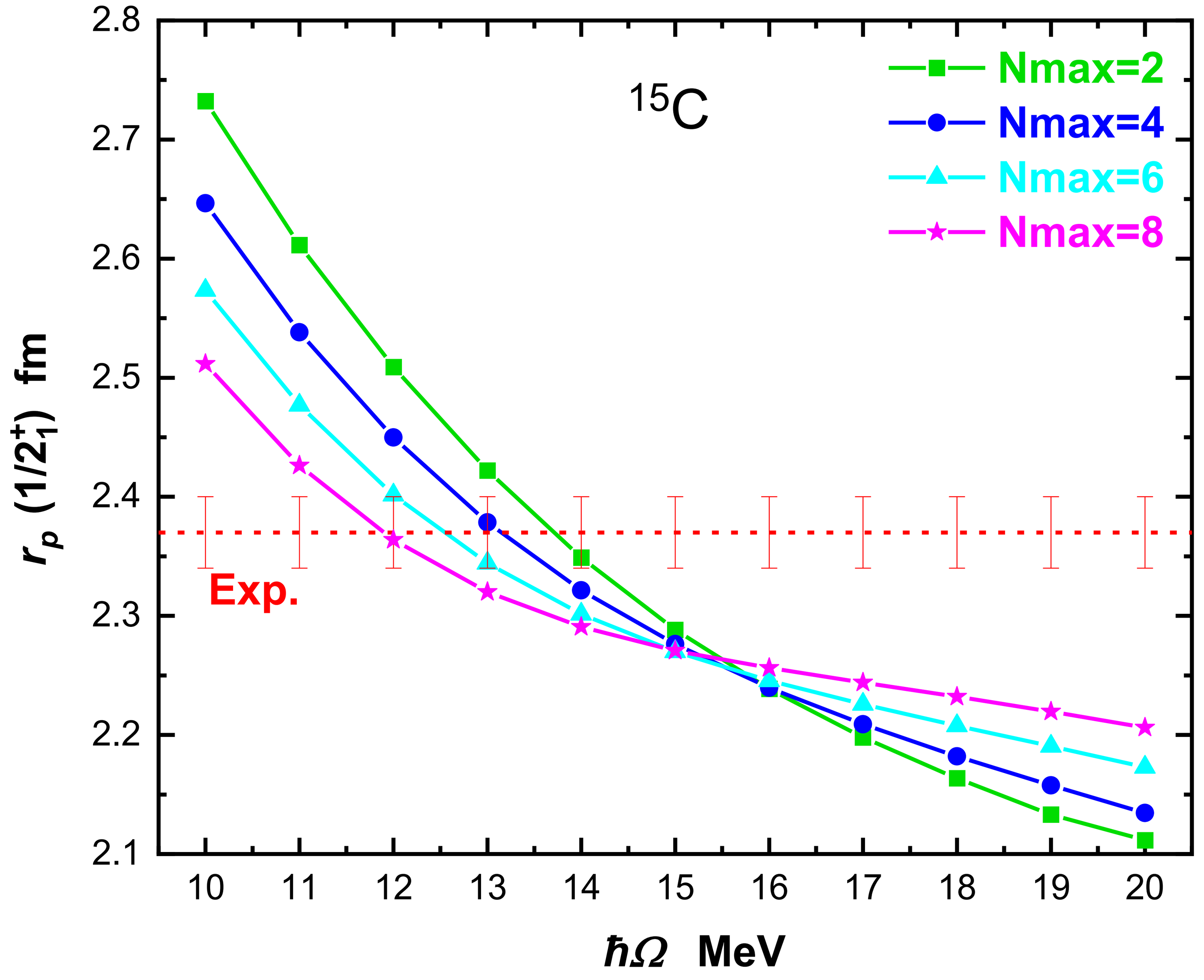
❖ **Point proton radii of ground state from Daejeon16**

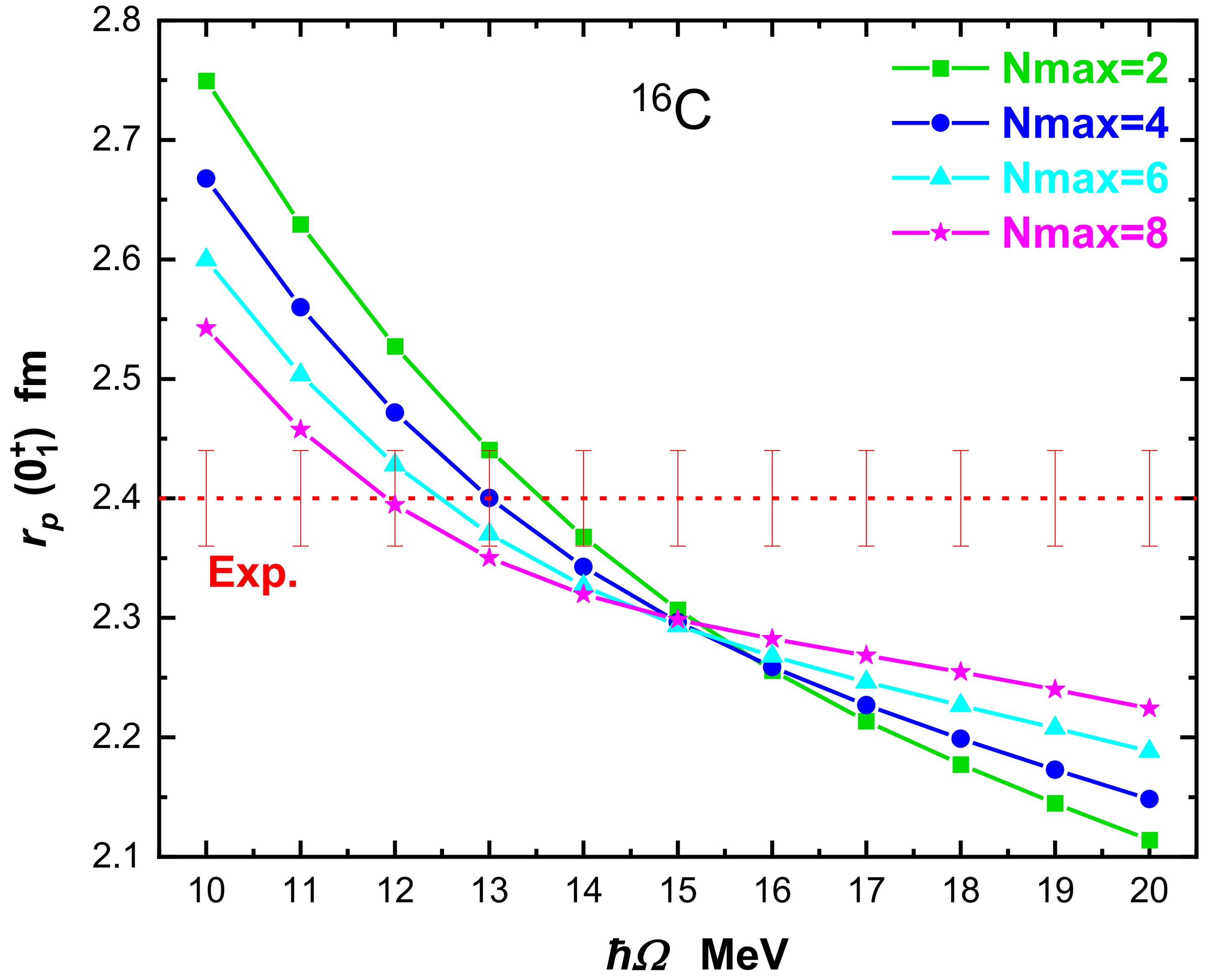






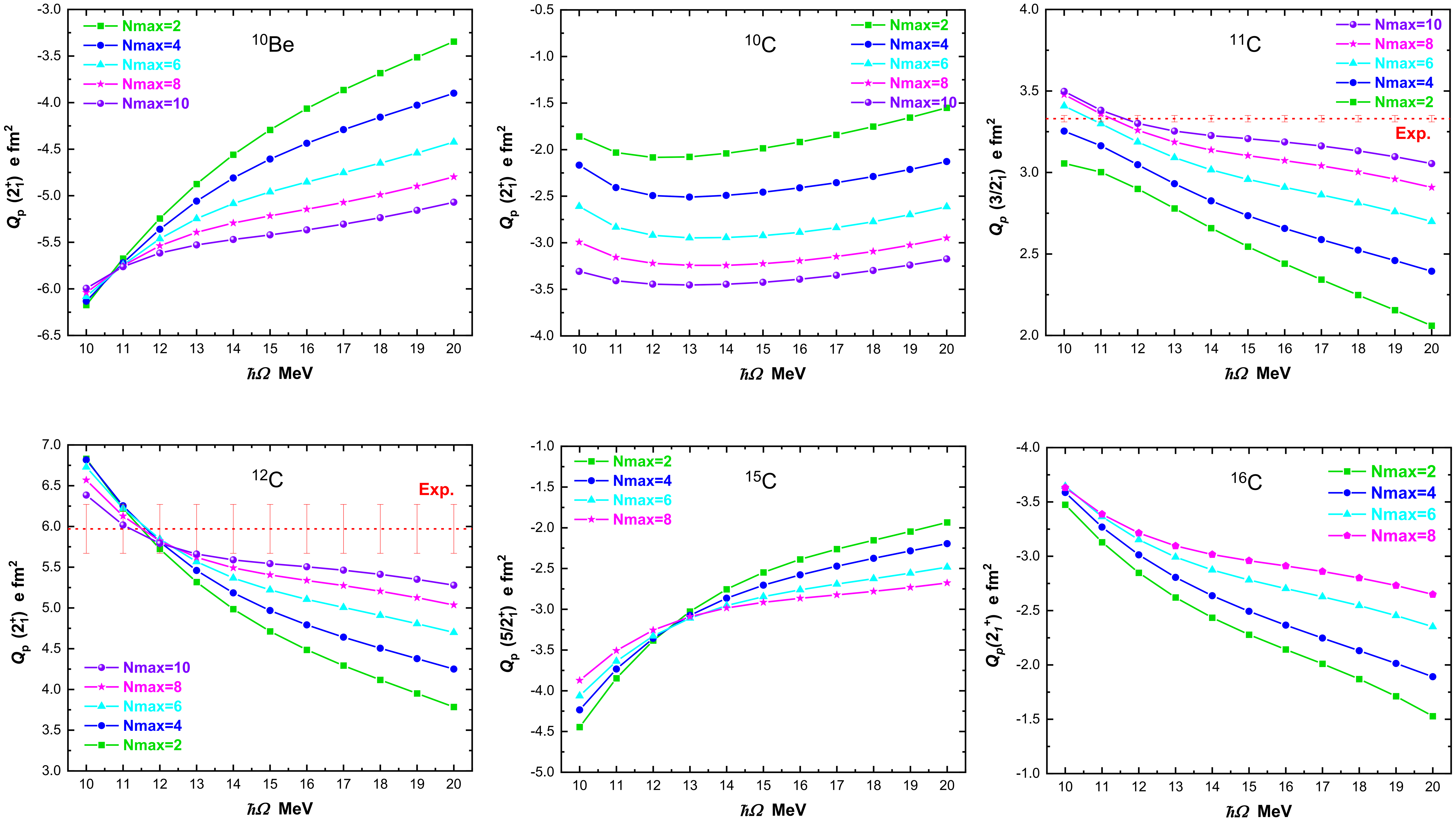






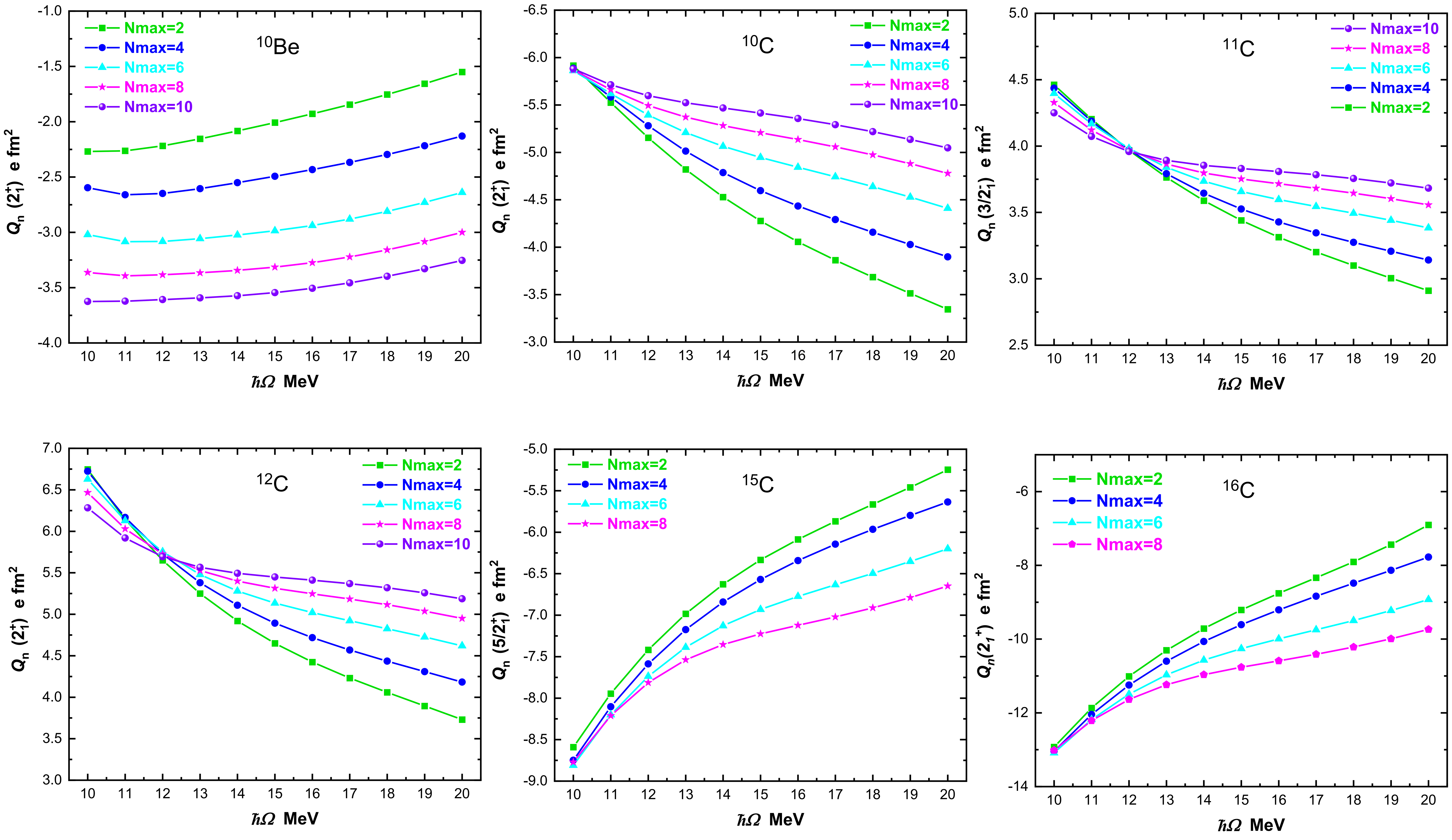
NCSM results

❖ **Proton $E2$ moments from Daejeon16**



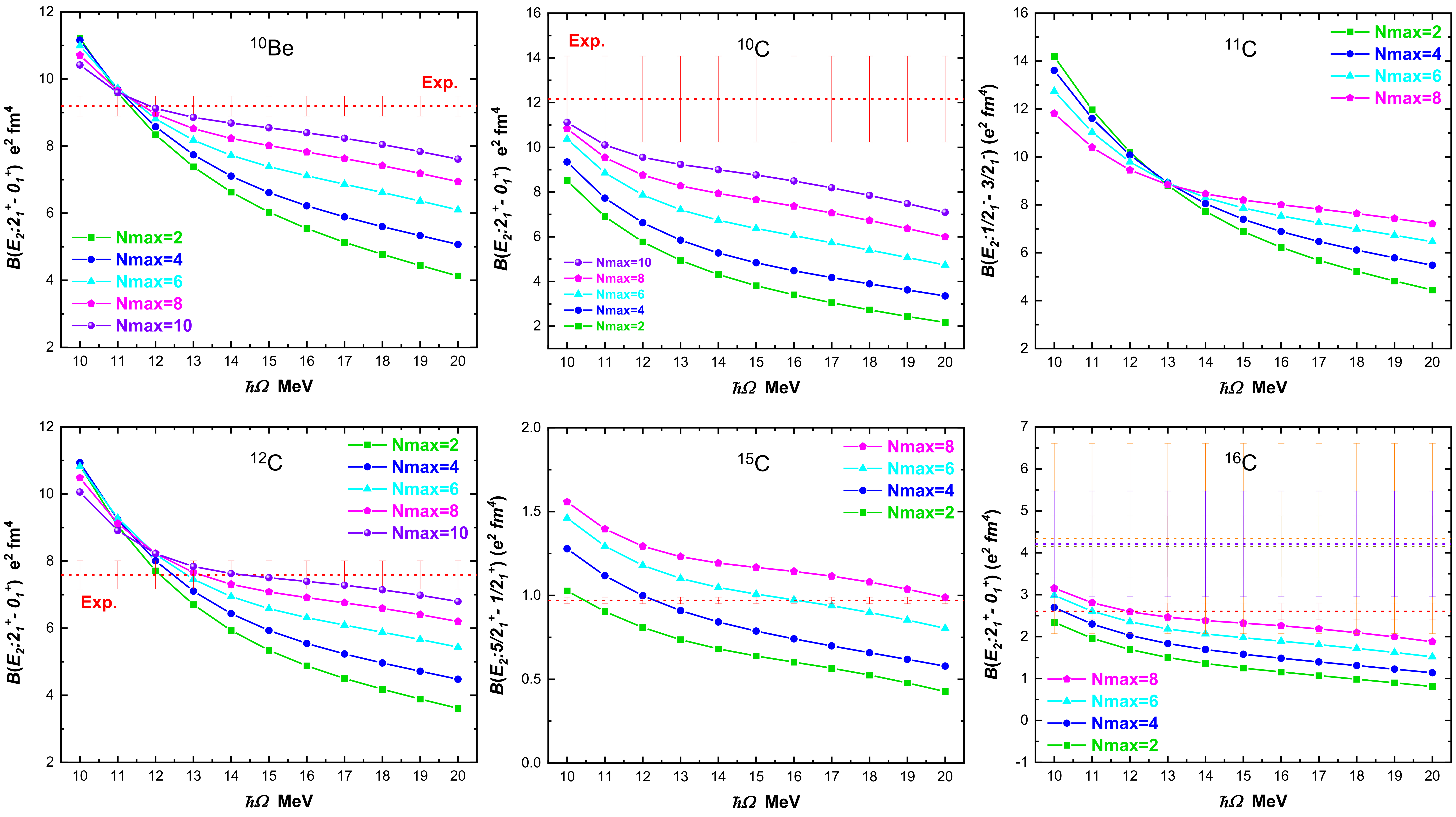
NCSM results

❖ **Neutron $E2$ moments from Daejeon16**



NCSM results

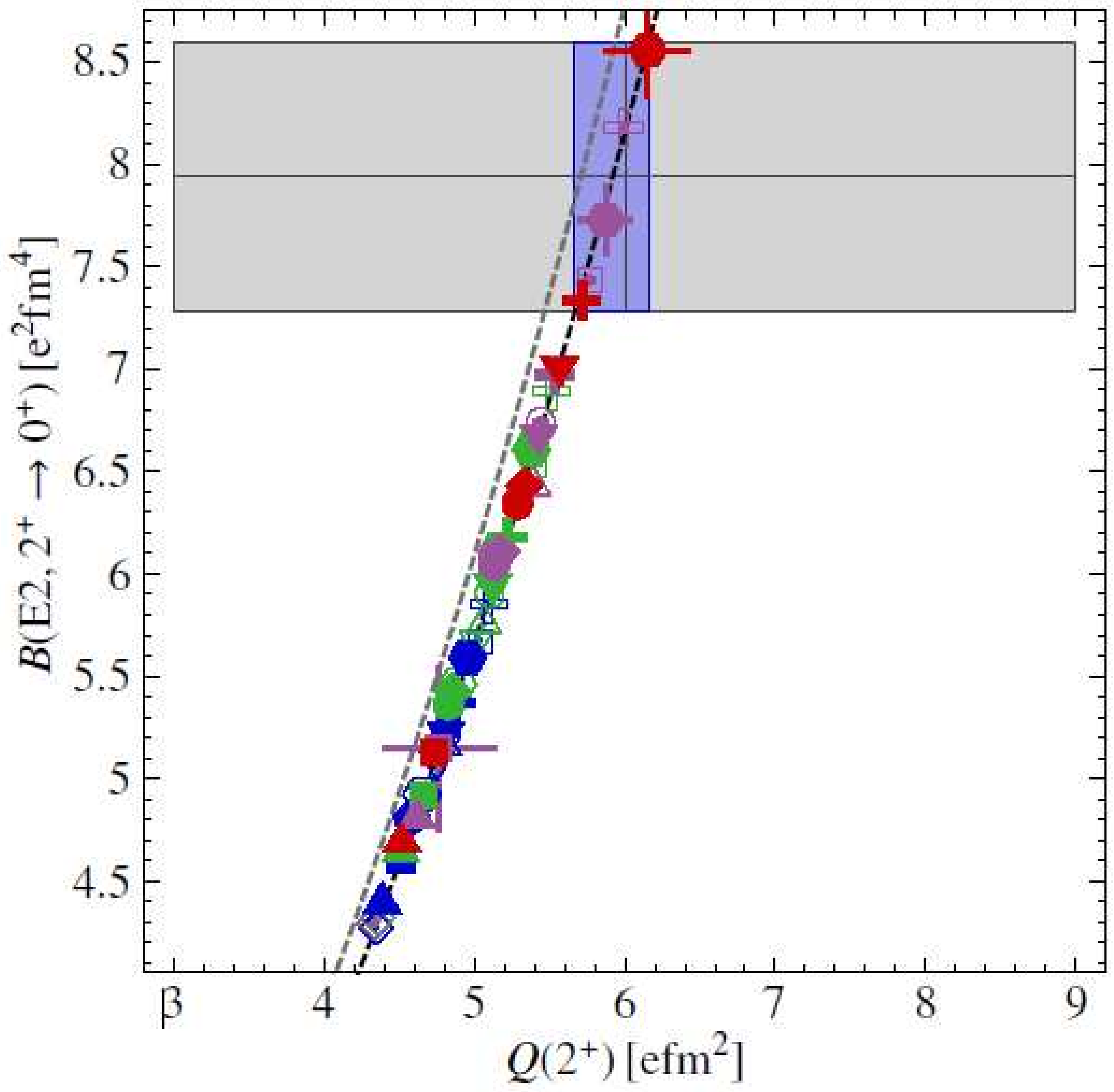
❖ $B(E2)$ from Daejeon16

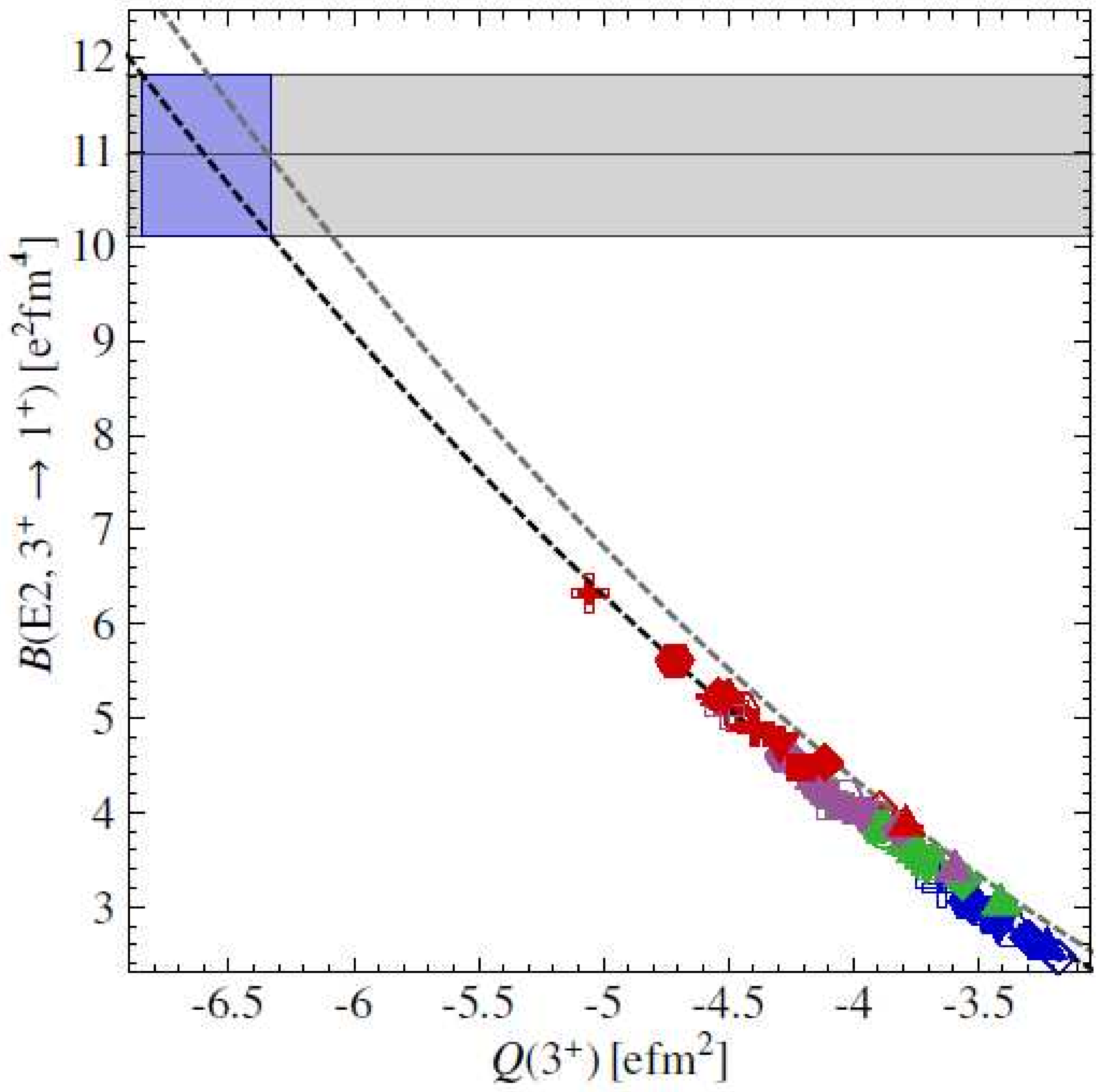


Ratios of $E2$ observables

❖ **Challenges for $E2$ observables calculation by NCSM**

1. **Slow convergence**
2. **Limit with current computer recourses**

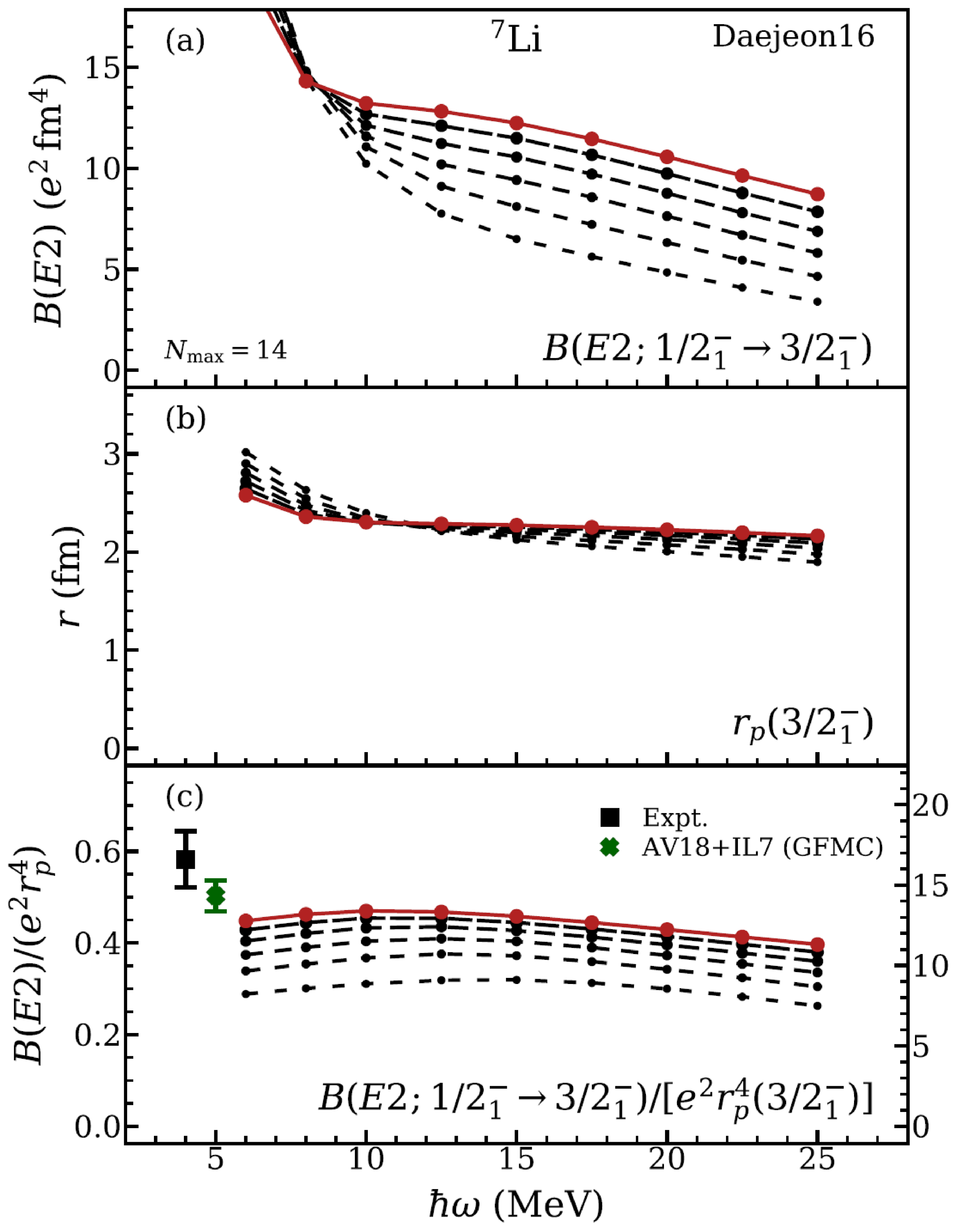


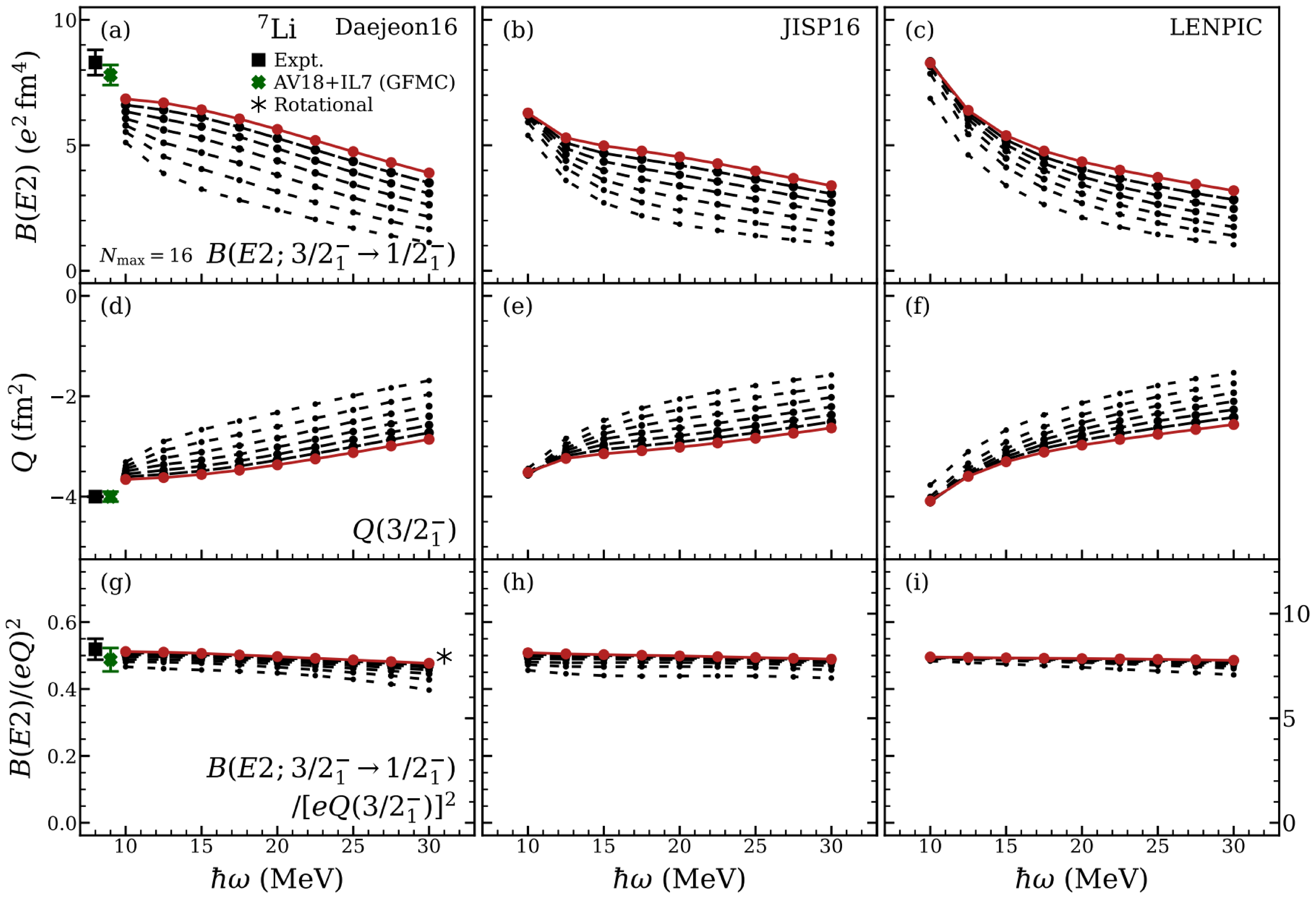


$B(E2)$: ^{12}C $(2_1^+ \to 0_1^+)$ and ^{6}Li $(3_1^+ \to 1_1^+)$, Q_p: ^{12}C (2_1^+) and ^{6}Li (3_1^+), obtained from chiral NN (empty) and $3N$ (solid) interaction by NCSM

A. Calci et al., Phys. Rev. C (2016)

Ratios of $E2$ observables





$$Q_{\lambda\mu} = \zeta^{(\mathrm{E}\lambda)} \sum_{j=1}^{A} e(j) r_j^{\lambda} Y_{\lambda\mu}(\Omega_j) \ ,$$

$$B(E2; J_i \to J_f) \propto |\langle J_f \| \textstyle\sum_{i\in p} e r_i^2 Y_2(\hat{r}_i) \| J_i \rangle|^2$$

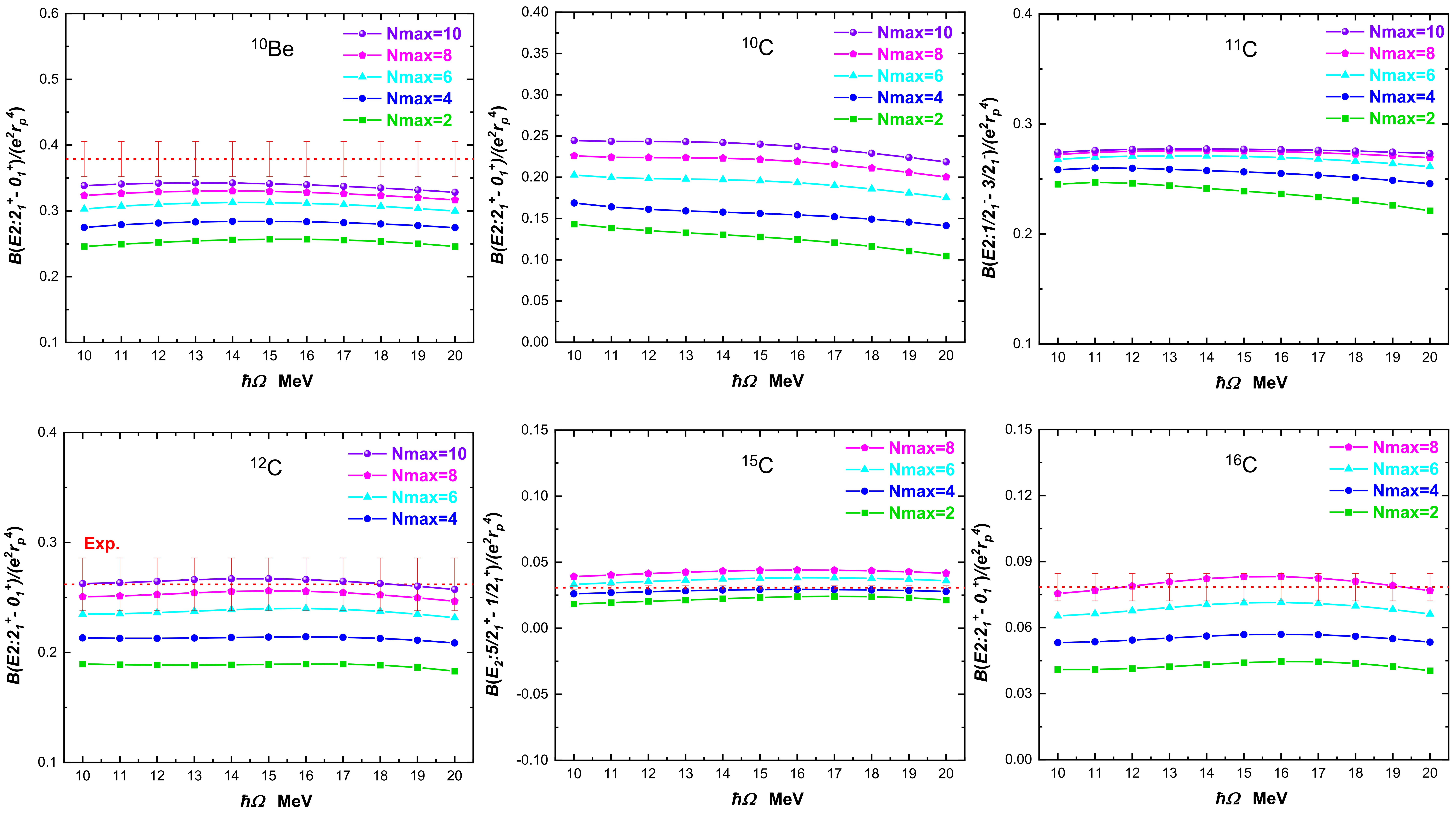
$$B(E2; J_i \to J_f) \propto |\langle J_f \| Q_2 \| J_i \rangle|^2$$

$$eQ(J) \propto \langle J \| Q_2 \| J \rangle.$$

M. Caprio et al., Phys. Rev. C (2021)
M. Caprio et al., Phys. Rev. C (2022)

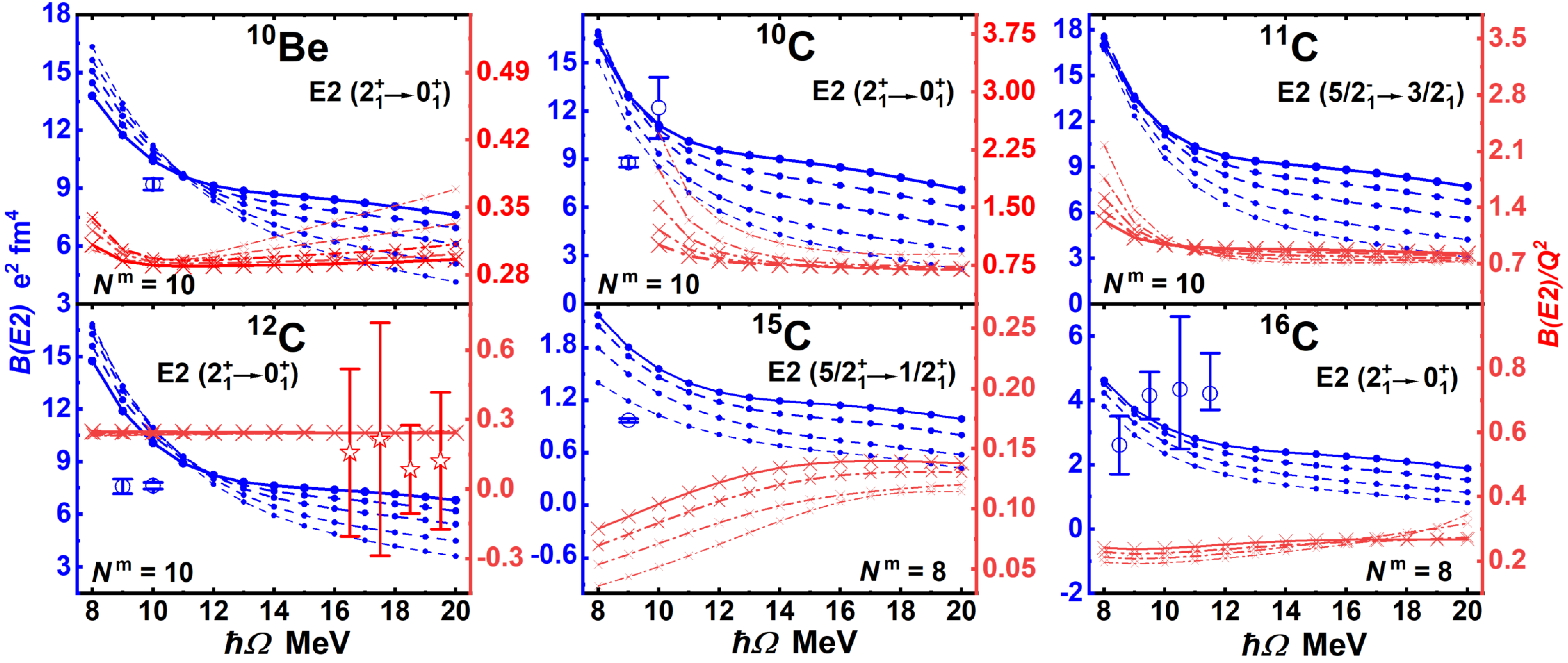
Ratios of $E2$ observables

❖ $B(E2)/r_p^4$ from Daejeon16



Ratios of $E2$ observables

❖ $B(E2)/Q_p^2$ from Daejeon16

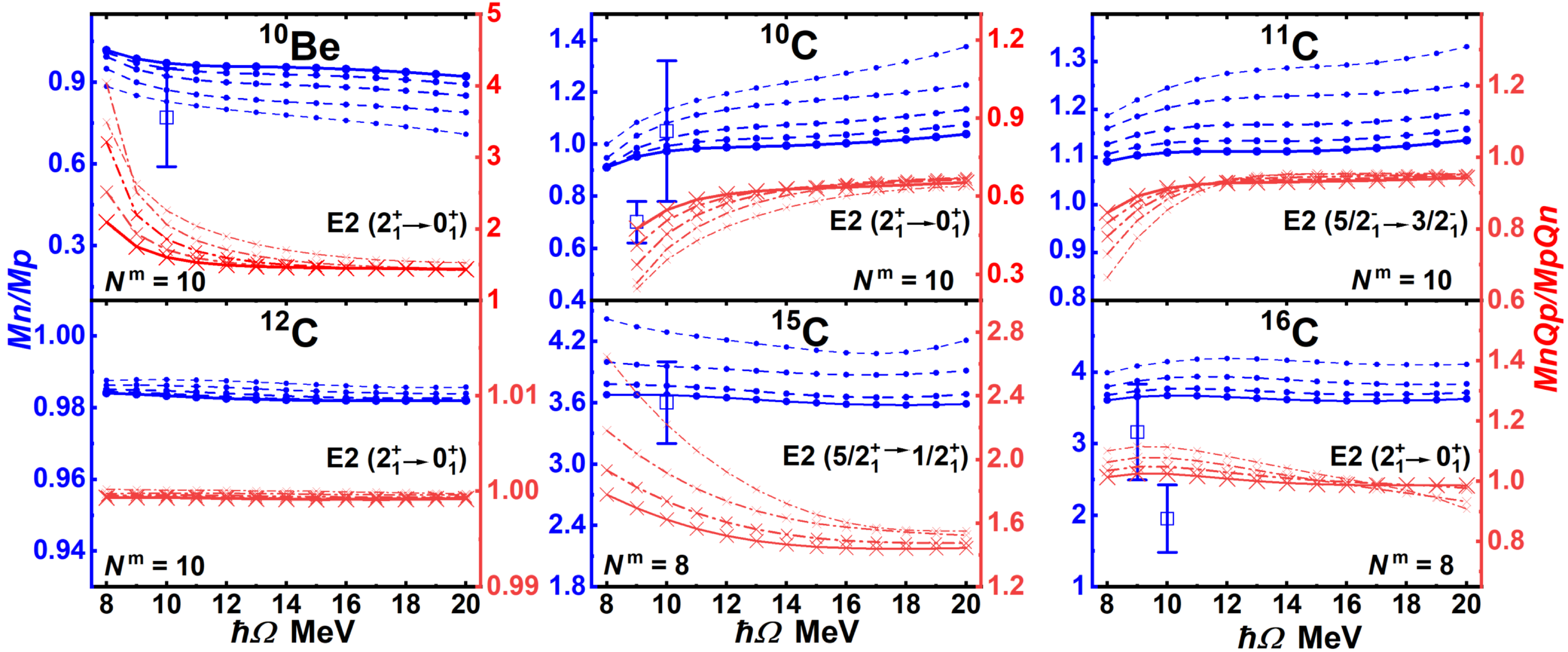


- ➢ The results of $B(E2)$ show a convergence trend as the calculation model space increases, but no convergence results are obtained
- ➢ Compared with $B(E2)$, $B(E2)/Q_p^2$ shows better convergence and is very close to the current experimental values

H. Li et al., Phys. Rev. C (2024)

Ratios of $E2$ observables

❖ M_n/M_p and M_nQ_p/M_pQ_n from Daejeon16



- Compared with $B\,(E2)$, M_n/M_p exhibits better convergence, and the approximate convergence value is very close to the experimental value
- M_nQ_p/M_pQ_n can be used for theoretical predictions of Q_n

H. Li et al., Phys. Rev. C (2024)

Ratios of $E2$ observables

❖ Predicted and experimental $E2$ observables

$E2$ transitions	$B(E2)$ (e^2 fm^4)		M_n/M_p			M_nQ_p/M_pQ_n
	Exp	Thy$_{cr}$	Exp	Thy	Previous-Thy	Thy
^{10}Be($2_1^+ \to 0_1^+$)	9.2(3) McCutchan 等 (2012)	9.48(2)	1.1(1) Iwasaki 等 (2000)	0.96(4)	0.62(SM-MK) Iwasaki 等 (2000)	1.45(27)
					0.88(AMD) Kanada-En'yo 等 (2020)	
^{10}C($2_1^+ \to 0_1^+$)	8.8(3) McCutchan 等 (2012)	12.7(8)	0.70(8) Jouanne 等 (2005)	0.98(5)	1.29(SM-MK) Sagawa 等 (2004)	0.62(15)
	12.2(19) Fisher 等 (1968)		1.05(27) Furuno 等 (2019)		1.11(AMD) Jouanne 等 (2005)	
					1.3(AMD) Kanada-En'yo (2011)	
^{11}C($\frac{5}{2}{}_1^- \to \frac{3}{2}{}_1^-$)		12(1)		1.09(5)	1.19(AMD) Jouanne 等 (2005)	0.93(4)
^{12}C($2_1^+ \to 0_1^+$)	7.63(19) D'Alessio 等 (2020)	8.08(4)		0.982(2)	1(SM-MK) Sagawa 等 (2004)	0.9992(3)
	7.94(66) Pritychenko 等 (2016)					
^{15}C($\frac{5}{2}{}_1^+ \to \frac{1}{2}{}_1^+$)	0.97(2) Chen 等 (2022)		3.6(4) Chen 等 (2022)	3.6(2)		1.44(29)
^{16}C($2_1^+ \to 0_1^+$)	2.6(9) Ong 等 (2008)		3.17(67) Ong 等 (2008)	3.6(2)	**2.54(IM-SRG)** Jiang 等 (2020)	0.99(6)
	4.15(73) Wiedeking 等 (2008)		2.4 Wiedeking 等 (2008)		6.07(SM-MK) Sagawa 等 (2004)	
	$4.34^{+2.27}_{-1.85}$ Jiang 等 (2020)		1.95(47) Jiang 等 (2020)		2.11(SM-MK) Yuan 等 (2012a)	
	$4.21^{+1.26}_{-0.50}$ Petri 等 (2012)				2.47(SM-WBT) Yuan 等 (2012a)	
					2.48(SM-YSOX) Yuan 等 (2012b)	
					3.0(SM-F) Fortune (2016)	
					4.19(AMD) Kanada-En'yo (2011)	

$B(E2)$ from others *ab initio* calculations ^{10}Be -- GFMC: 8.8(4), NCMCSM: 9.29; ^{10}C -- GFMC: 15.3(1.4), NCMCSM: 9.30 ; ^{12}C-- NCMCSM: 7.65, IMNCSM: 8.68(79)

H. Li, Ph. D. thesis (2024)

Ratios of $E2$ observables

❖ **Predicted and experimental $E2$ observables**

$E2$ transitions	Q_p (e fm^2)				Q_n (fm^2)		
	Exp	Thy+Exp	Thy1	Thy$_{cr}$	Thy+Exp	Thy1	Thy$_{cr}$
^{10}Be($2_1^+ \to 0_1^+$)		-5.64(4)	-5.73(3)	-5.81(2)	-4.3(2)	-3.8(2)	
^{10}C($2_1^+ \to 0_1^+$)		-3.43(9)	-4.1(2)		-5.8(4)	-6.4(2)	-5.9(2)
		-3.9(2)			-4.4(3)		
^{11}C($\frac{5}{2}{}_1^- \to \frac{3}{2}{}_1^-$)	3.33(2) Stone (2016)		3.6(2)		3.9(1)	4.2(3)	3.93(2)
^{12}C($2_1^+ \to 0_1^+$)	5.97(30) D'Alessio 等 (2020)	5.59(4)	5.76(5)	5.7(2)	5.9(7)	5.66(5)	5.6(2)
	6(3) Vermeer 等 (1983)	5.71(9)			5.9(5)		
	5.3(44) Kumar Raju 等 (2018)				5.2(8)		
	9.5(18) Saiz-Lomas 等 (2023)				9.3(2)		
^{15}C($\frac{5}{2}{}_1^+ \to \frac{1}{2}{}_1^+$)		-2.7(3)		-3.11(6)	-6.7(3)		-8.3(5)
^{16}C($2_1^+ \to 0_1^+$)		-3.12(9)		-3.5(8)	-10(2)		-12.4(5)
		-3.9(2)			-9.5(3)		
		-4.0(5)			-5.4(3)		
		-4.0(3)					

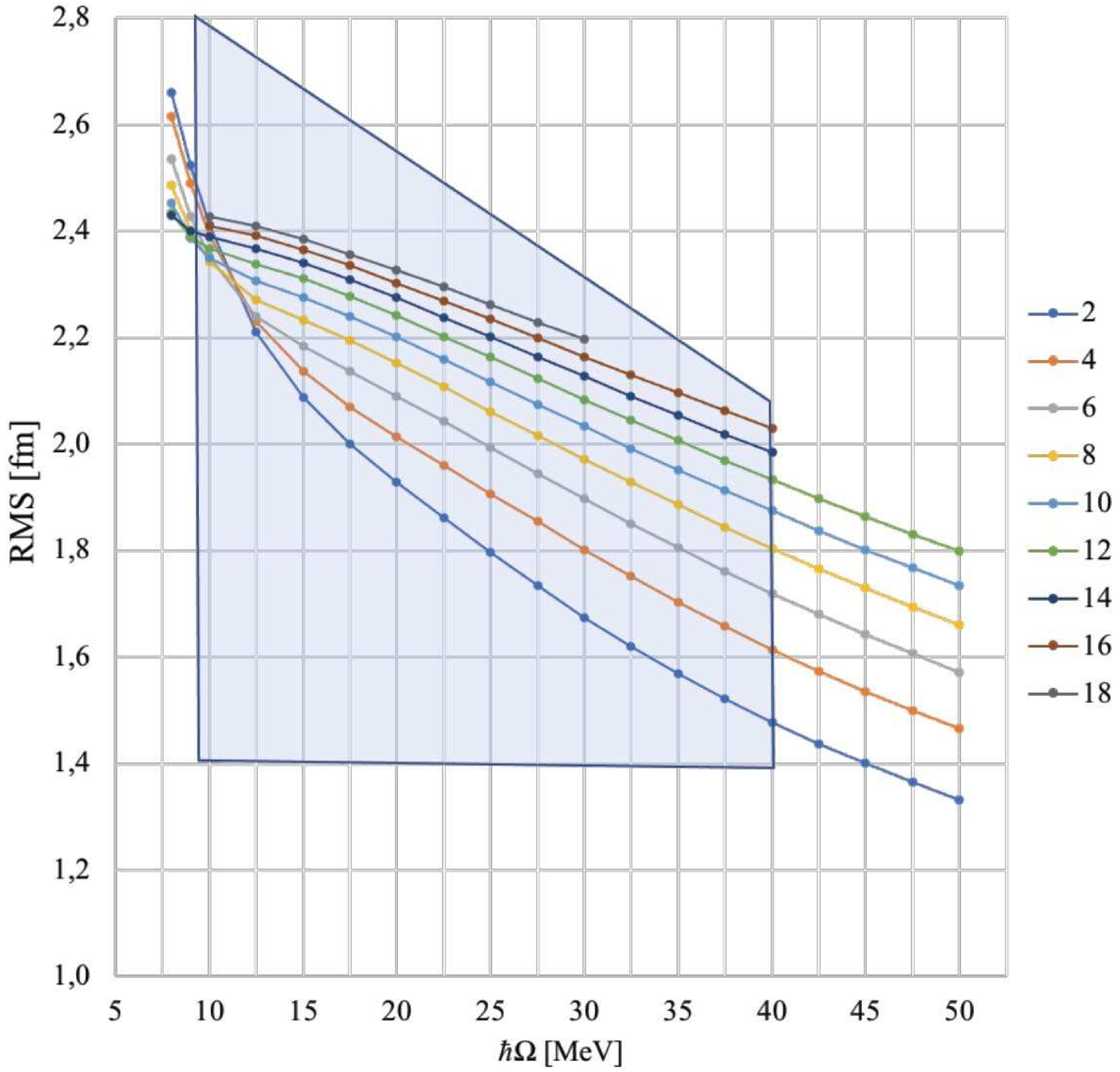
H. Li, Ph. D. thesis (2024)

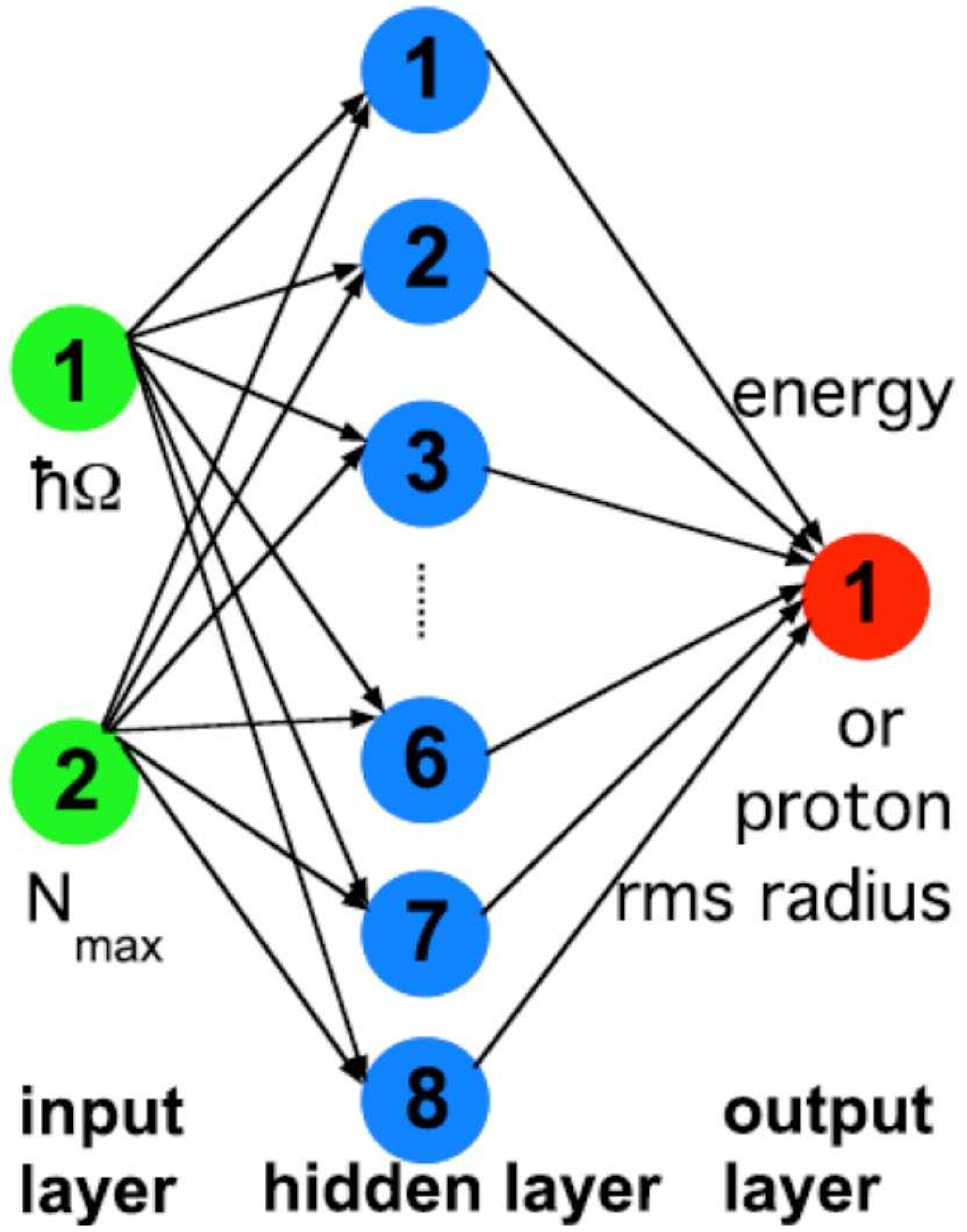
Next plan

❖ **Extrapolation of NCSM $E2$ results using machine learning and artificial neural networks**

Results:

^{6}Li, Daejeon16,
rms proton point radii
r_{exp} = 2.38(3) fm





N_{max}	exp. extrap. PRC79(2009) $E_{gs}(\Delta E)$	ANN PRC99(2019) $E_{gs}(\Delta E)$	Our results $E_{gs}(\Delta E)$
10	2.339(111)	2.481(37)	2.317(72)
12	2.360(114)	2.517(27)	2.327(135)
14	2.376(107)	2.530(49)	2.332(128)
16	2.390(95)	2.546(23)	2.411(100)
18	2.427(82)	2.518(19)	2.545(62)

A. Mazur, NTSE-2023

Conclusions

- Ground state energies and spectra of stable p-shell nuclei from Daejeon16 in good agreement with experiment.

- $E2$ observables are slowly convergent in NCSM, while the ratios of $E2$ observables show good convergence. The predictions of $E2$ observables from ratios are reasonable.

감사합니다!