Ab initio Nuclear Structure with Deep Learning: Bridging Light Nuclei and Nuclear Matter

Pengwei Zhao 赵鹏巍

Peking University

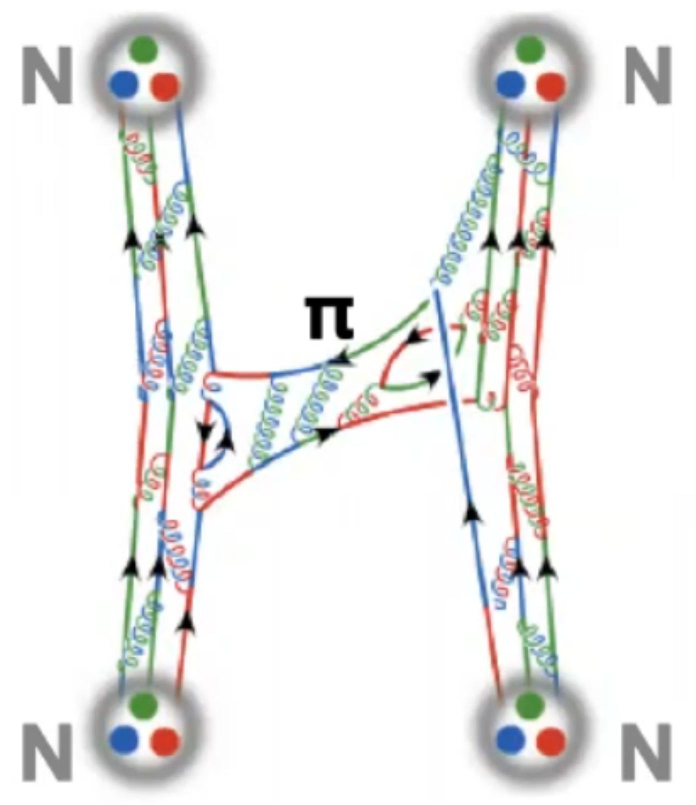
Outline

- Nuclear *ab initio* calculations
- Artificial neural networks for nuclear many-body wave functions
- Deep learning for nuclear *ab initio* calculations
- Summary

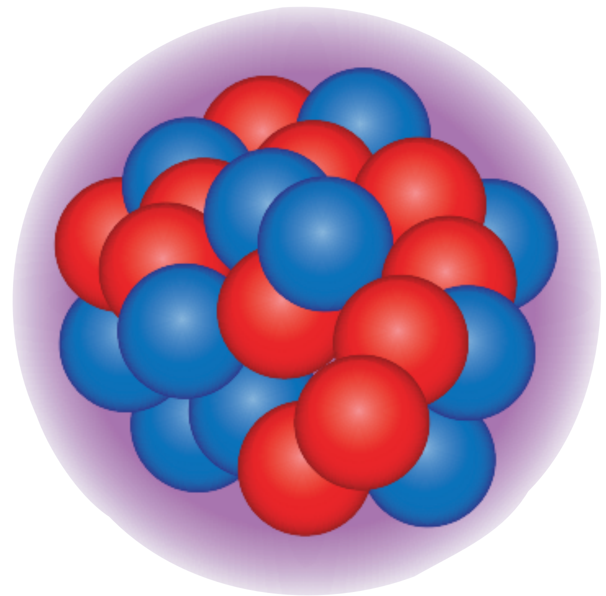
The goal of *ab initio* nuclear theory

Understand nuclear properties from a unified theoretical view rooted in the forces among nucleons.

- **Fix the nuclear force by scattering data**
  - Phenomenological, meson-exchange models
  - Effective field theories (EFTs)



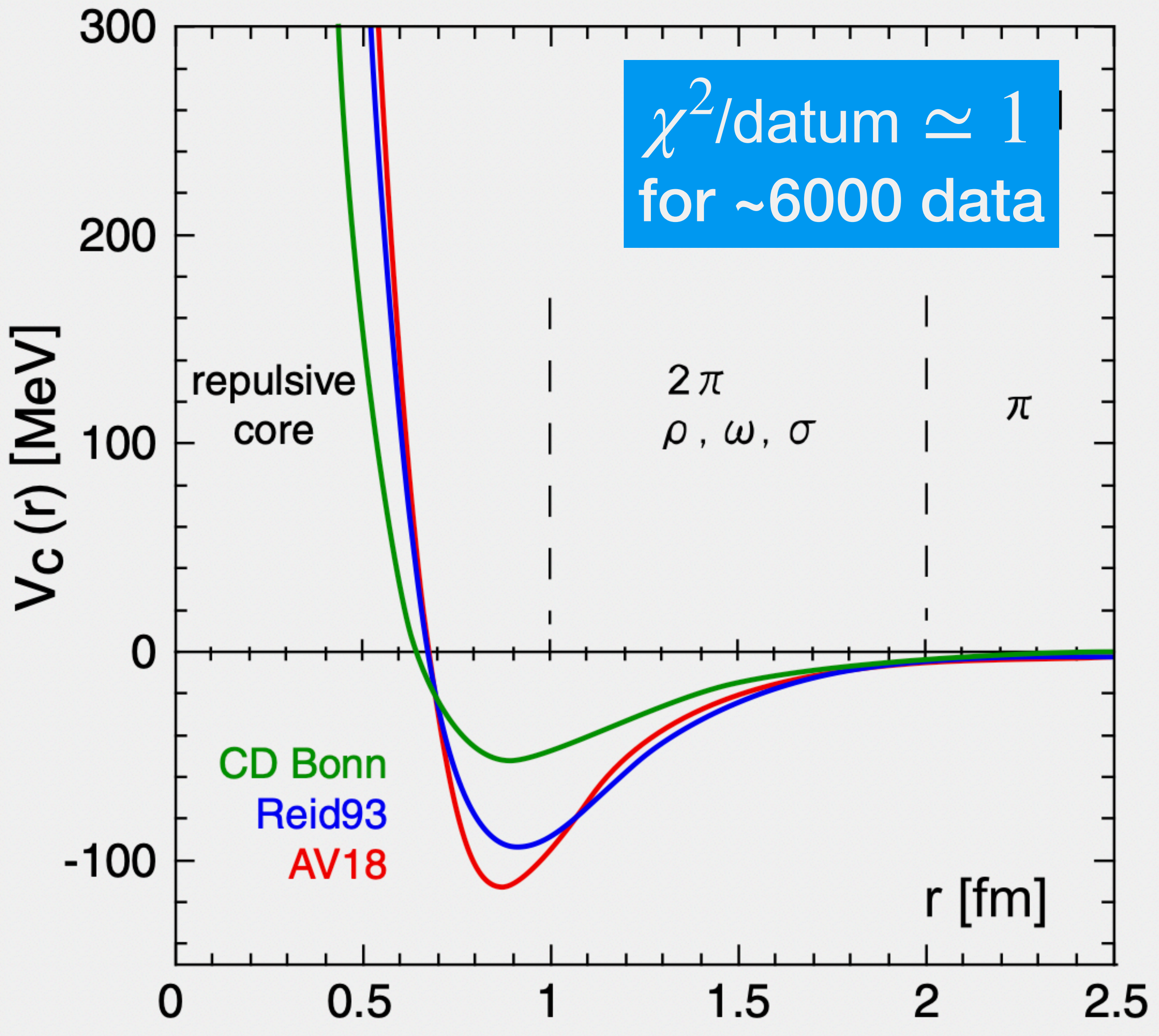
- **Solve the nuclear many-body problem**
  - Nuclear bulk properties: masses, radii, …
  - Nuclear spectra: energy levels, transitions, …
  - Nucleonic matter equation of state: neutron stars, …
  - New physics: $0\nu\beta\beta$, electric dipole moments, …
  - …



Ab initio calculations with *NN* forces

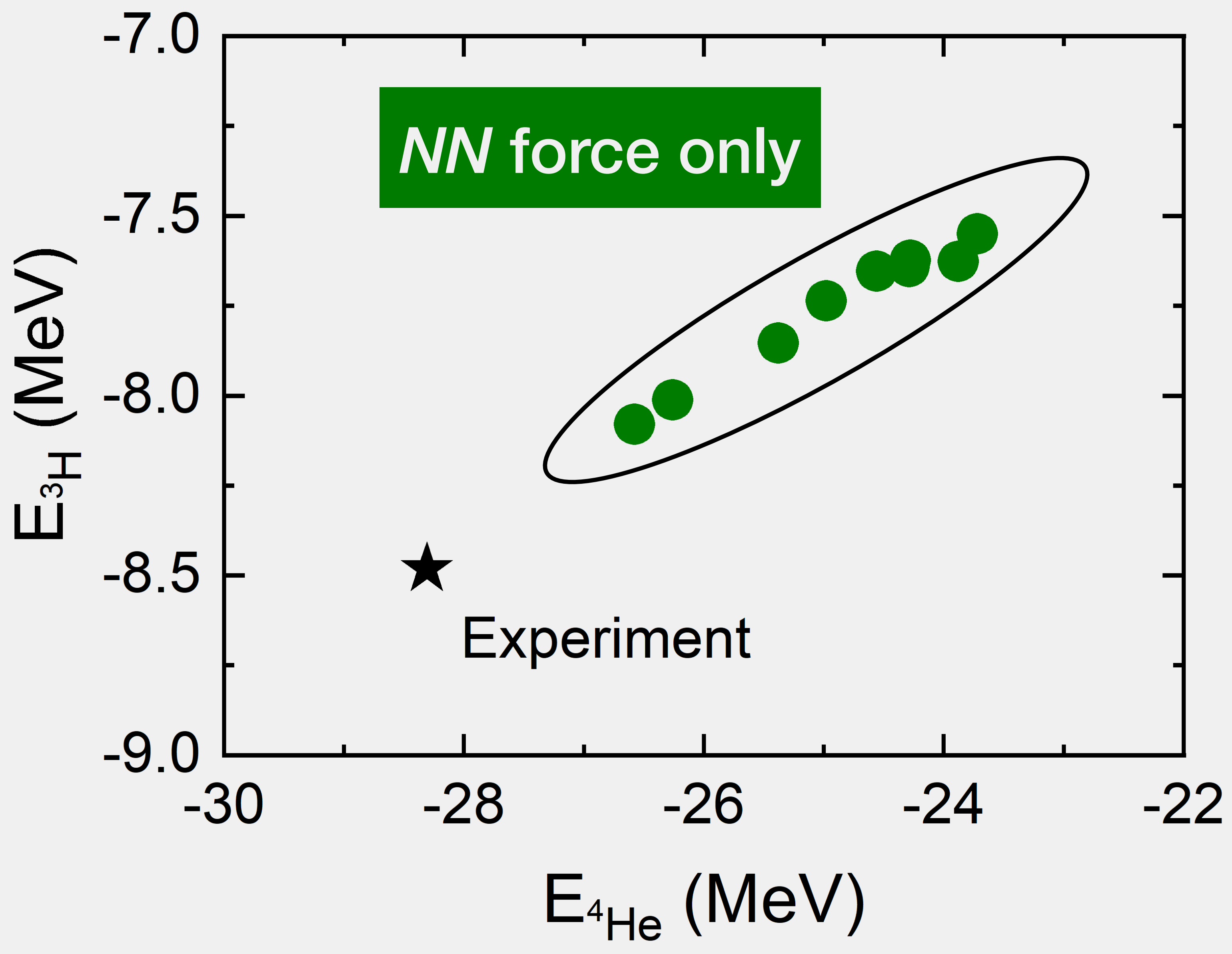
Many two-nucleon (NN) interactions, applied to nonrelativistic *ab initio* calculations, provide **insufficient binding** for light nuclei.

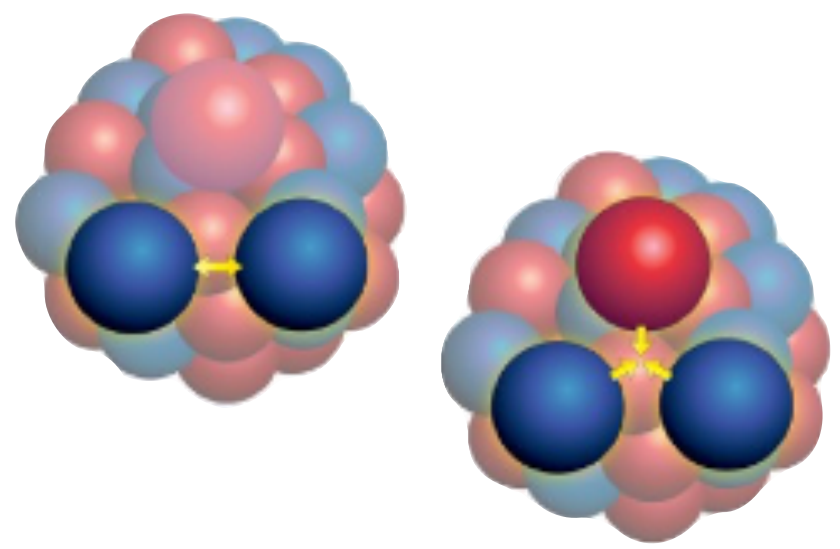
NN forces



Taken from Ishii et al., PRL 99, 022001 (2007)

^{3}H and ^{4}He



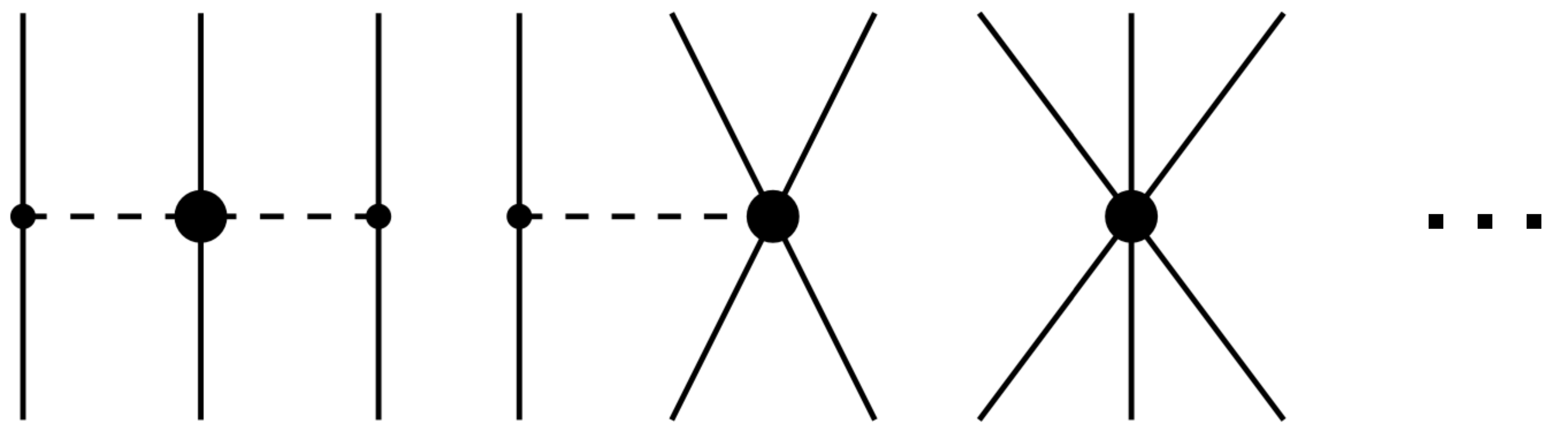


3N forces needed !

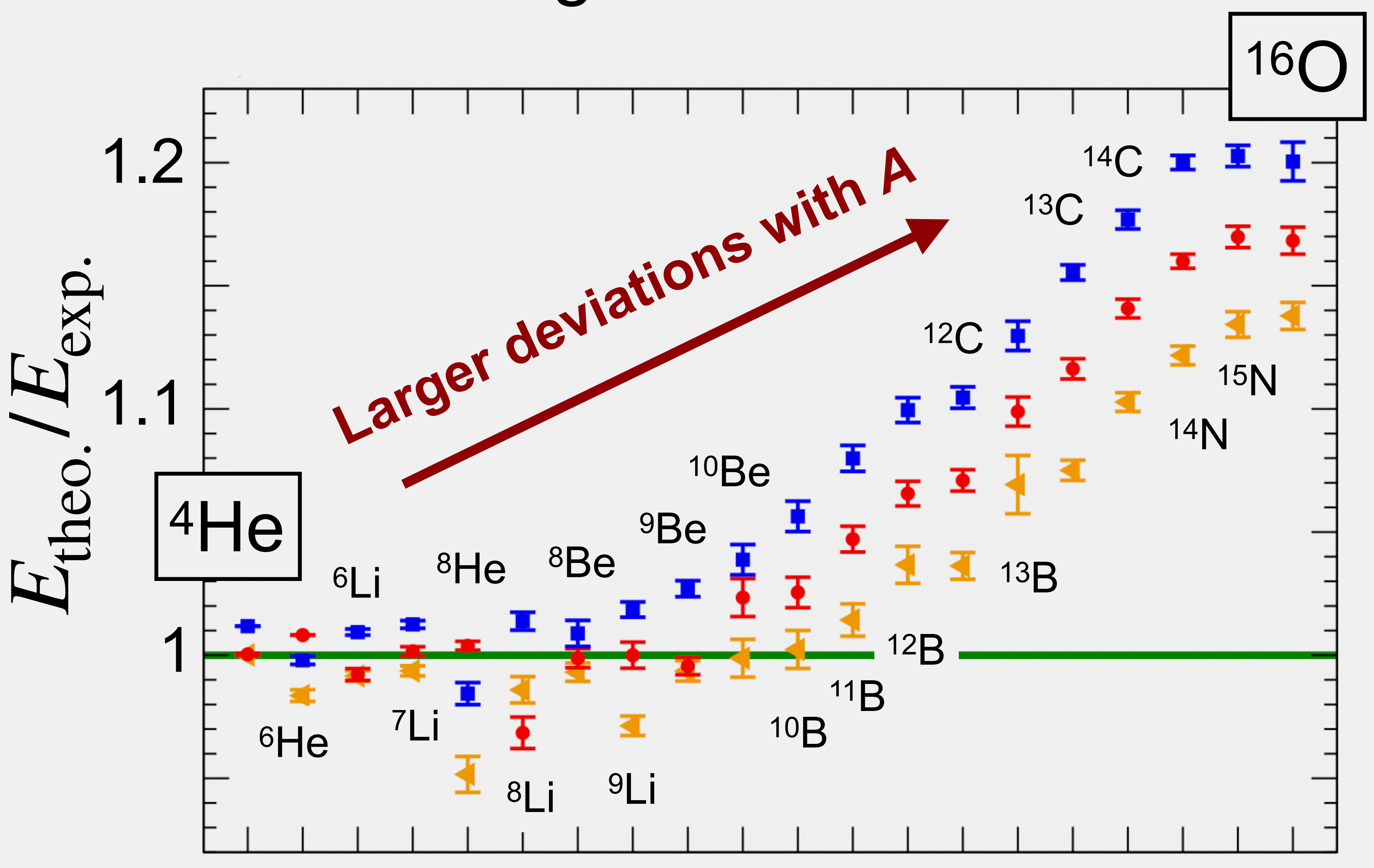
Ab initio calculations with *NN*+3*N* forces

◉ **3*N*-force models fitting to**

- A = 3 binding energy / beta decay
- pd/nd scattering
- …

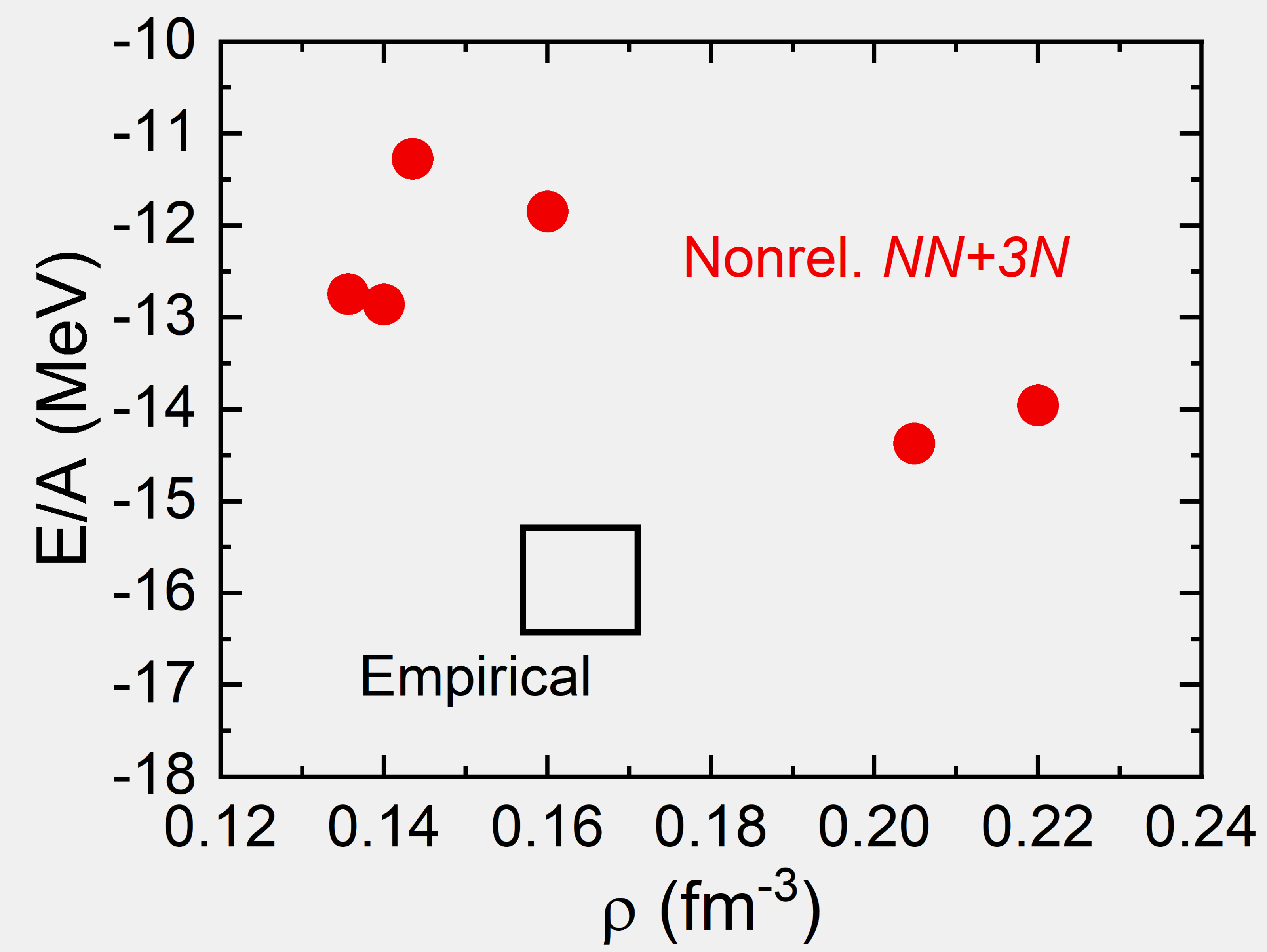


Light nuclei



Lonardoni et al., PRL 120, 122502 (2018)
LENPIC Collaboration, PRC 103, 054001 (2021)

Nuclear matter



Drischler et al., PRL 122, 042501(2019)
Akmal et al., PRC 58, 1804 (1998); Sammarruca et al., PRC 91, 054311 (2015)
Lonardoni et al., Phys. Rev. Research 2, 022033(R) (2022)

Possible solutions …

Accurate *ab initio* explanations of medium-mass nuclei ?

- **Including many-body forces** **(*4N*-, *5N*-, …, density-dependent)**
  - fit to medium-mass and heavy nuclei
  - density functional theory

tractable & non-ab initio.

- **Adjust *3N* and/or *2N* forces to medium-mass nuclei**
  - may sacrifice the accuracy for free-space scattering data
  - possible inconsistent *3N*/*2N* forces

controversial.

- **Improving nuclear forces by going for higher order**
  - N4LO inducing new operator structures of *3N* forces
  - but **complicated** …

intractable & ab initio.

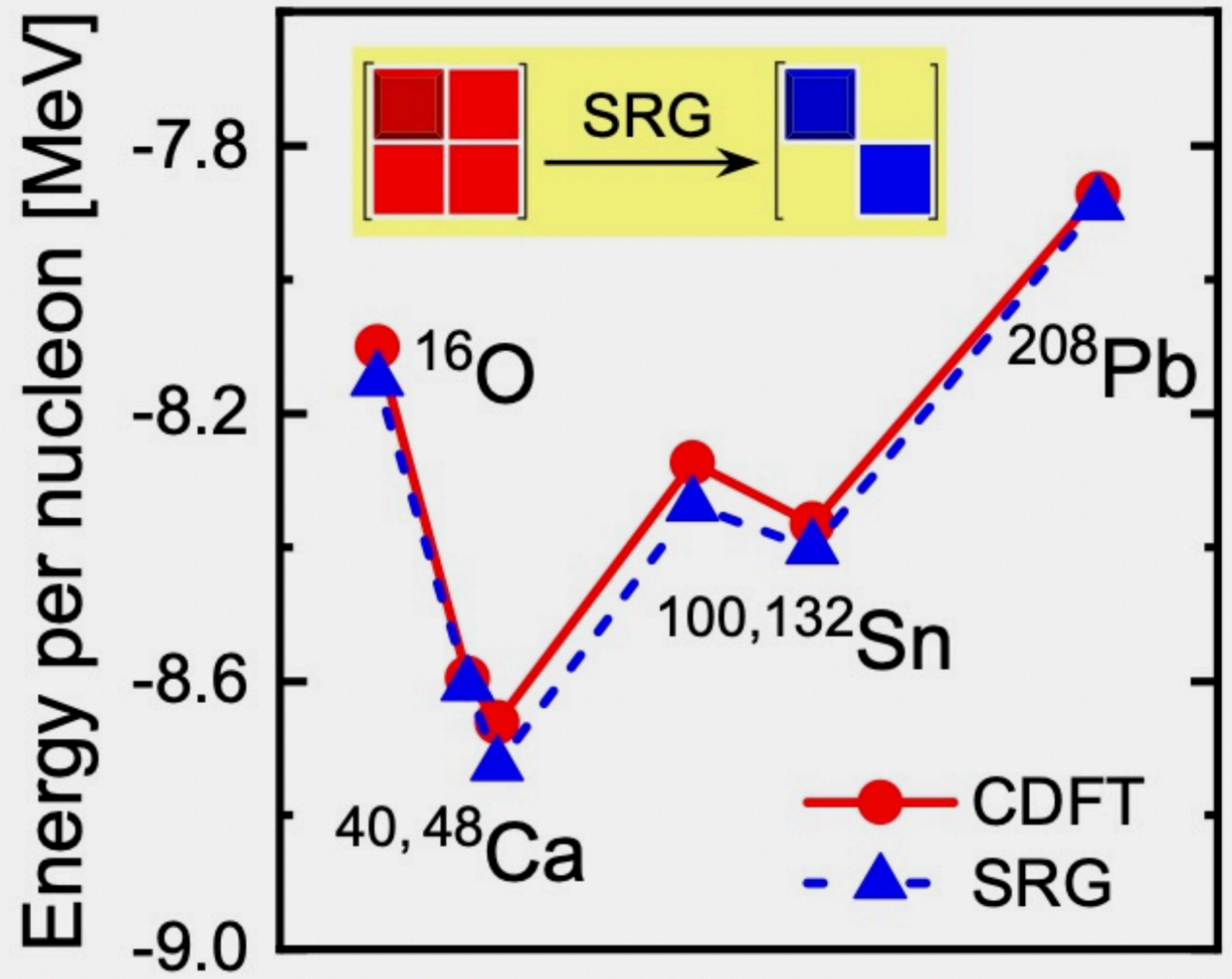
Our strategy: going for a relativistic *ab initio* framework

Relativistic effects

The relativity brings high-order effects …

Bridge the Rel. and Nonrel. DFTs

$$\underbrace{4\pi r^2\rho_v(r)}_{\text{Rel.}} = \underbrace{\rho_0 + \frac{d}{dr}\left[\frac{1}{4\tilde{M}^2}\frac{\kappa}{r}\rho_0\right] + \frac{d^2}{dr^2}\left[\frac{1}{8\tilde{M}^2}\rho_0\right] + O(\tilde{M}^{-3})}_{\text{Nonrel. (including high-order terms …)}}$$

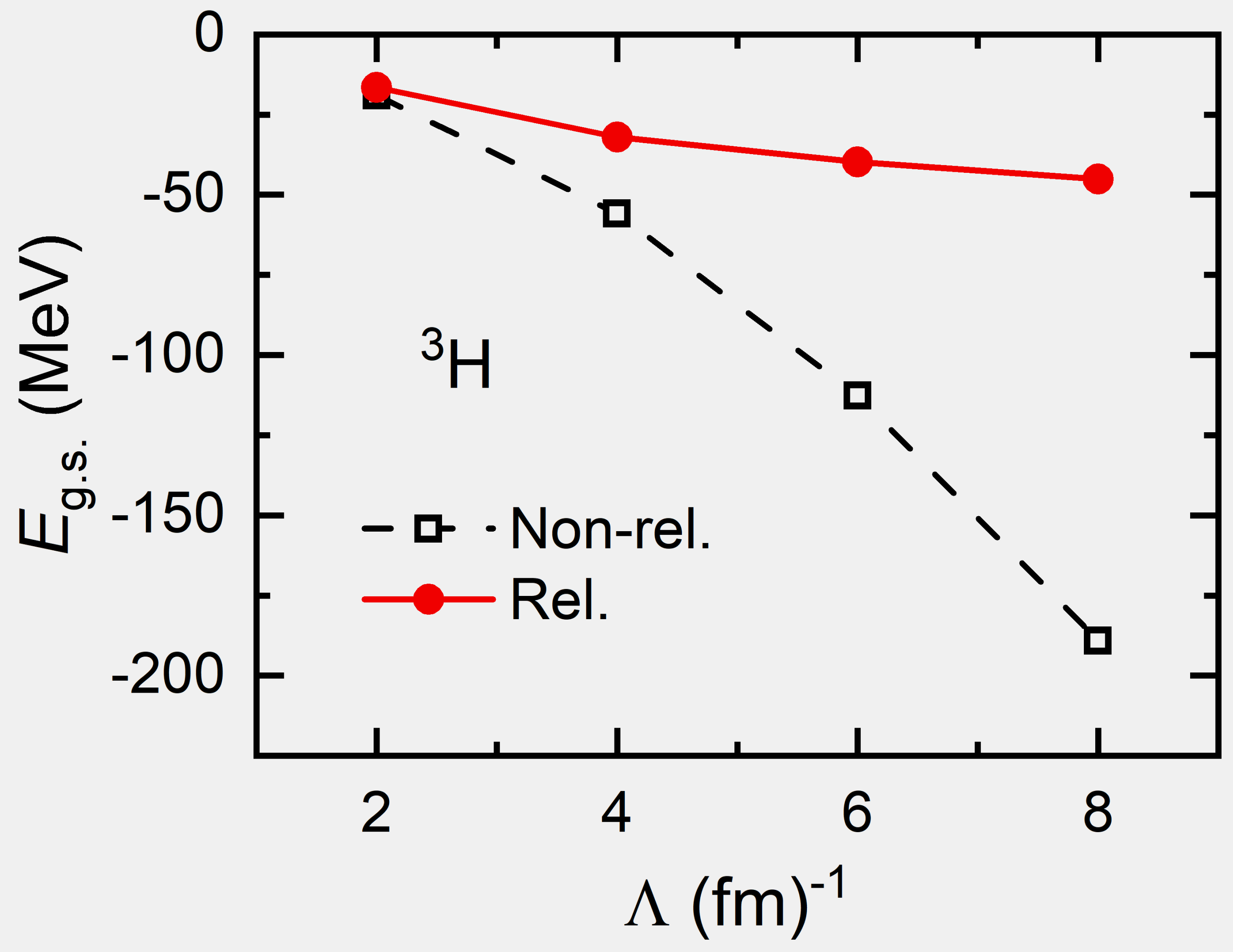


Ren and PWZ, PRC 102, 021301(R) (2020)
Editors' Suggestion

Rel. and Nonrel. VMC with LO forces

$$\left[\sum_{i=1}^{A} K_i + \sum_{i<} v(\boldsymbol{r}_{ij})\Big(\underbrace{1}_{\text{Nonrel}} + \underbrace{v_t(\boldsymbol{r}_{ij}, \hat{\boldsymbol{p}}_{ij}^2) + v_b(\boldsymbol{r}_{ij}, \hat{\boldsymbol{P}}_{ij}^2)}_{\text{Rel. corrections}}\Big)\right]\Psi(\boldsymbol{R}) = E\Psi(\boldsymbol{R})$$

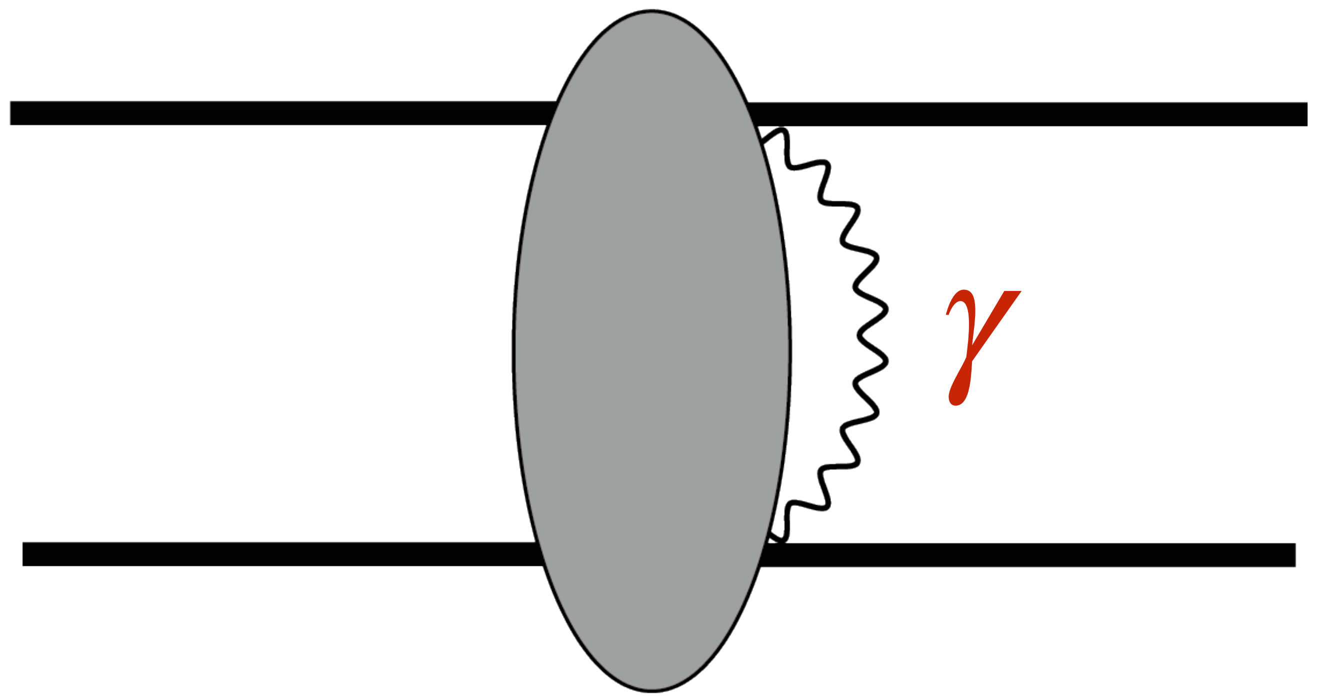
Thomas collapse avoided !



Yang and PWZ, PLB 835, 137587 (2022)

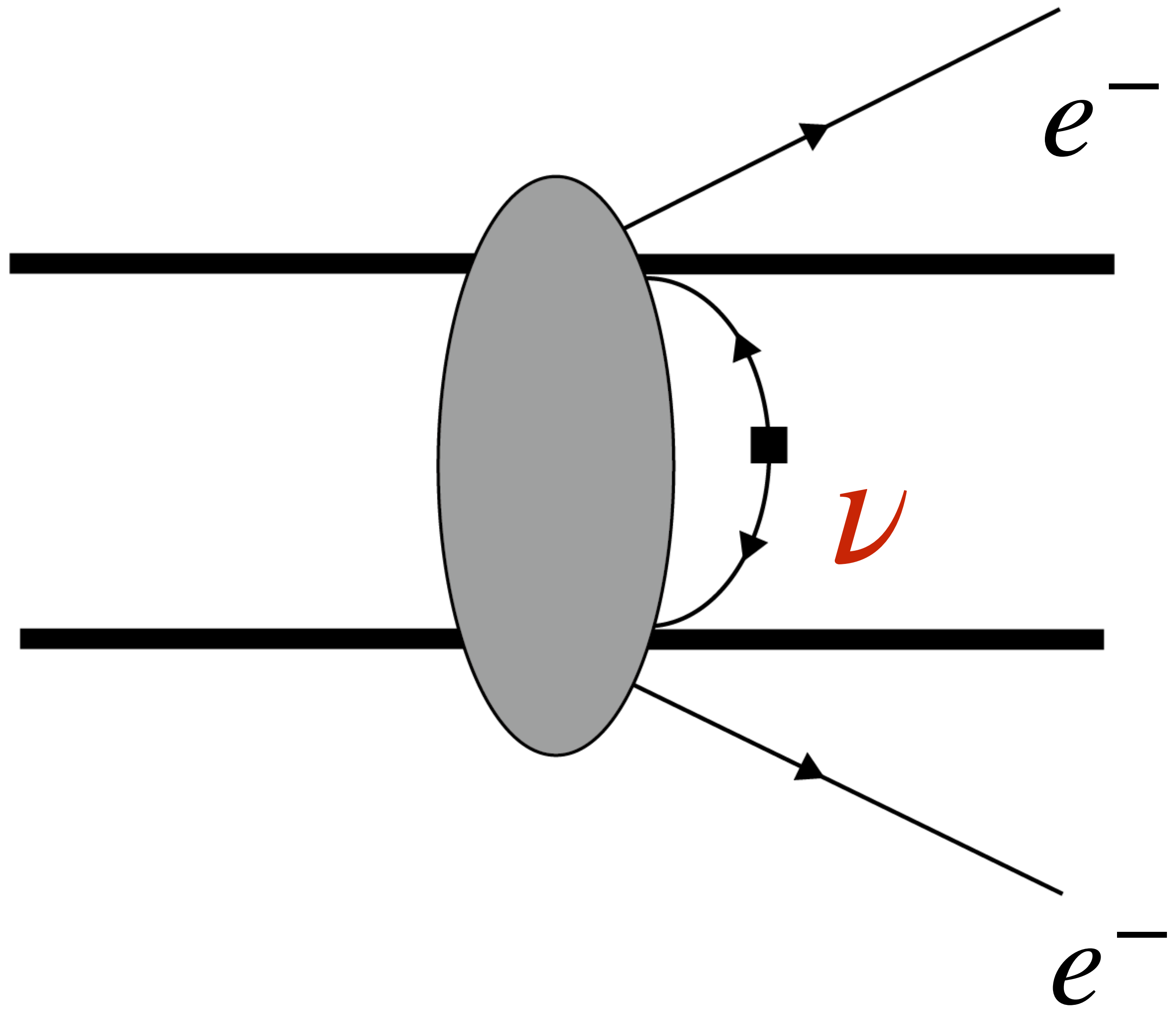
CSB and CIB of NN scattering

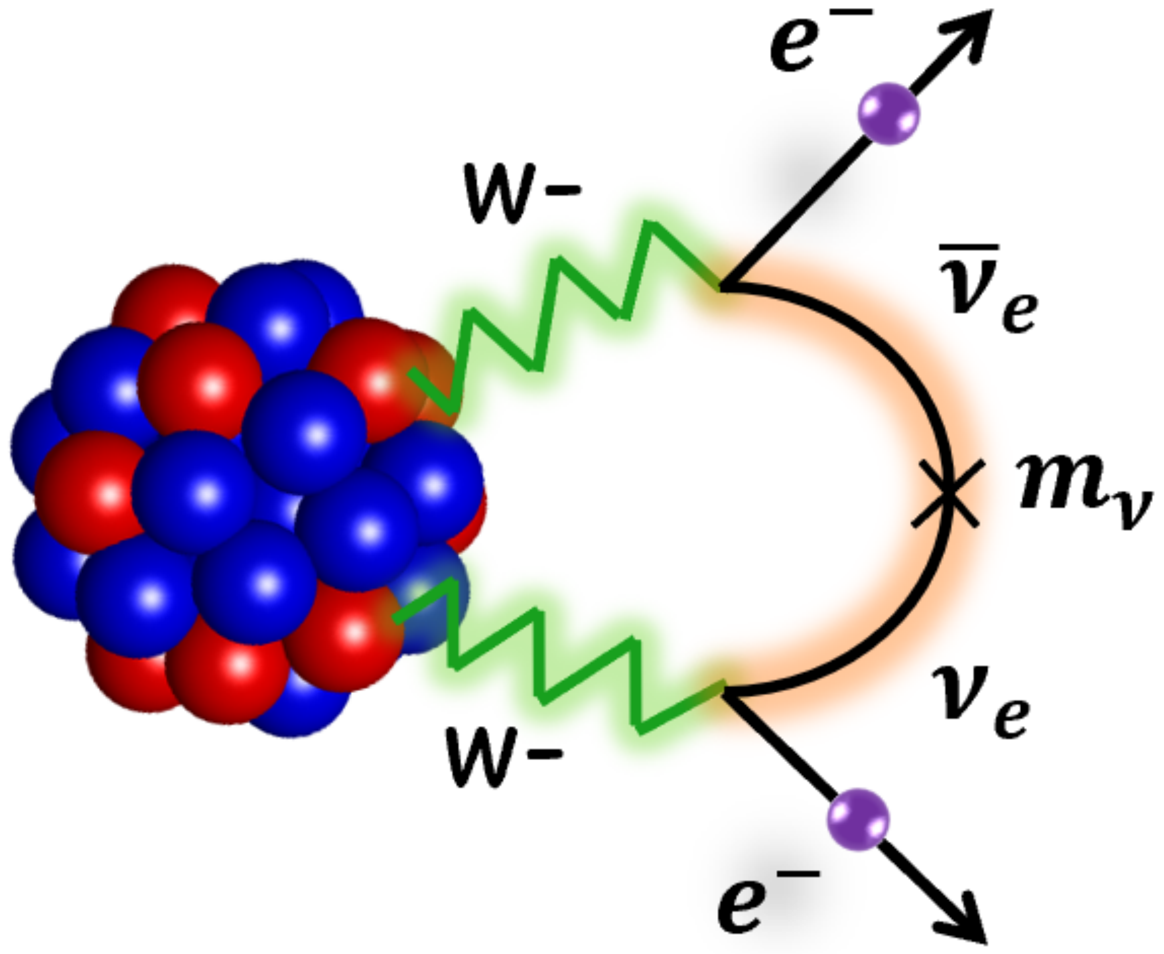
$NN \to NN$



$a_{nn} \neq a_{pp} \neq a_{np}$

$nn \to ppee$

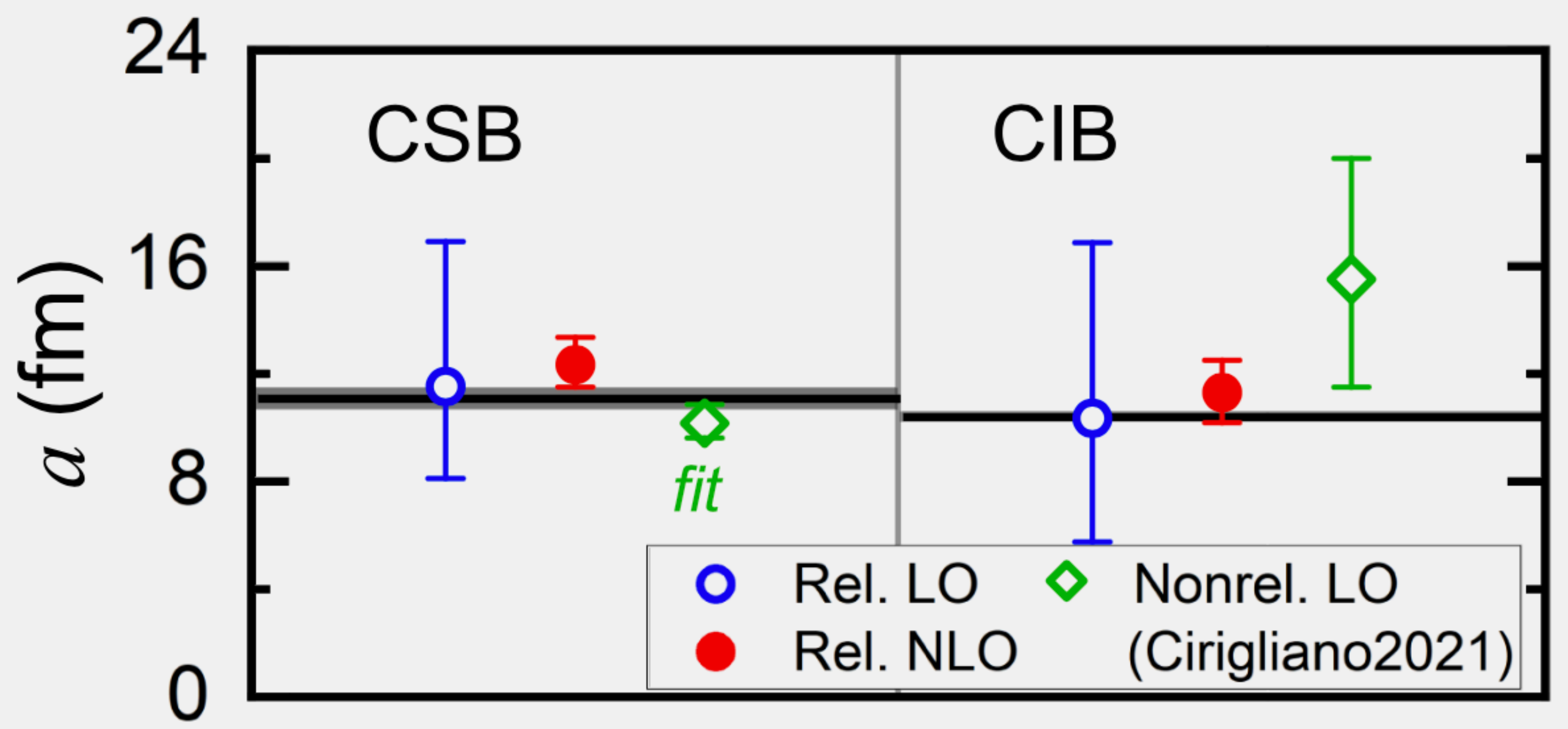




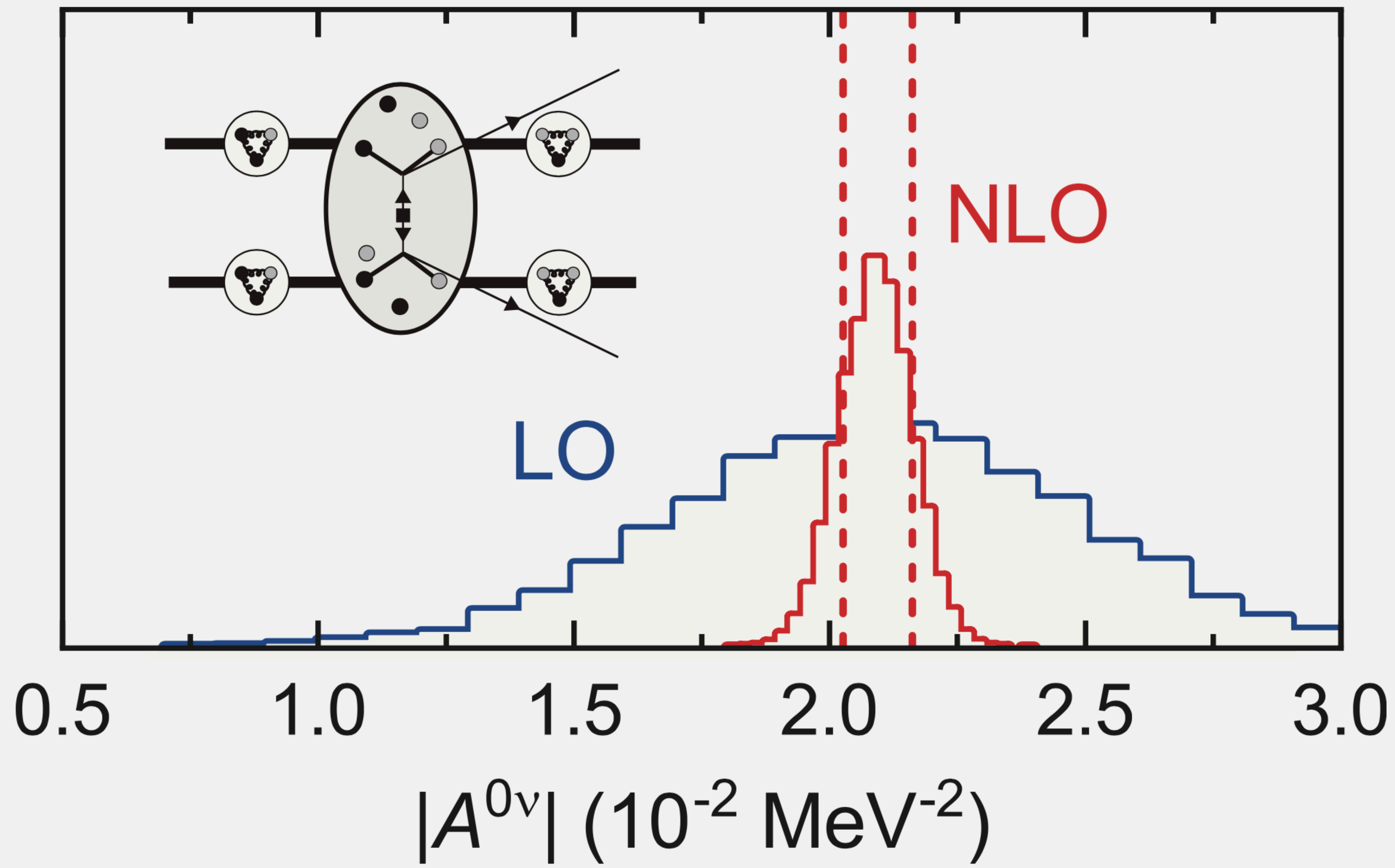
Cirigliano, Dekens, de Vries, Hoferichter, and Mereghetti, PRL 126, 172002 (2021)

Relativistic EFT: from NN scattering to $0\nu\beta\beta$

the most precise amplitude of two-neutron neutrinoless $\beta\beta$ decay to date



$$a_{\mathrm{CSB}} = a_{pp} - a_{nn} \qquad a_{\mathrm{CIB}} = \frac{a_{nn} + a_{pp}}{2} - a_{np}$$

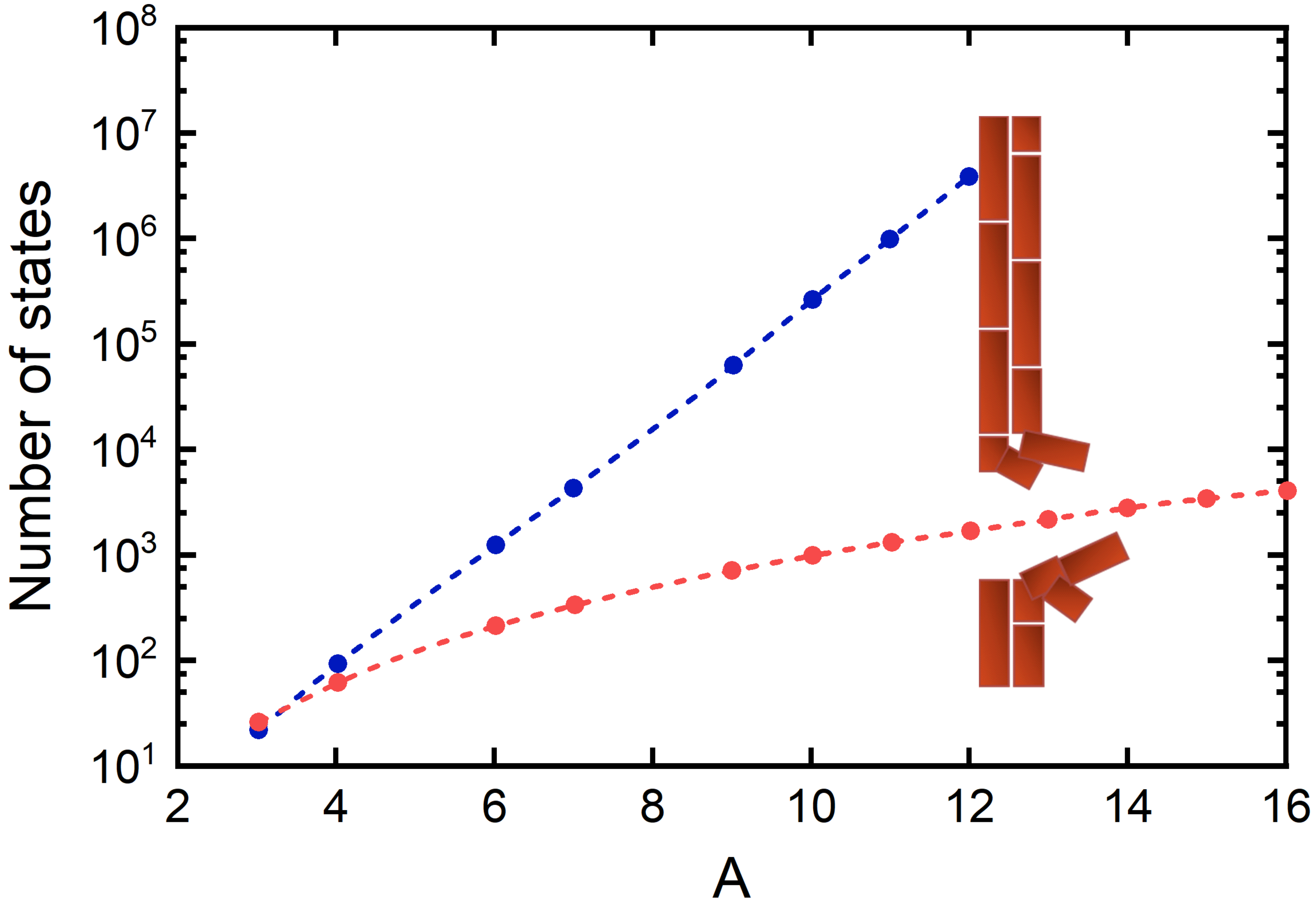


Yang and **PWZ***, PRL 134, 242502 (2025)

Challenges of nuclear many-body calculations

Curse of dimensionality: exponential increase of dimensions in spin-isospin space.

Carlson et al., Rev. Mod. Phys. 87, 1067 (2015)



Devising a polynomial scaling and accurate trial wave function ?

Artificial Neural Networks

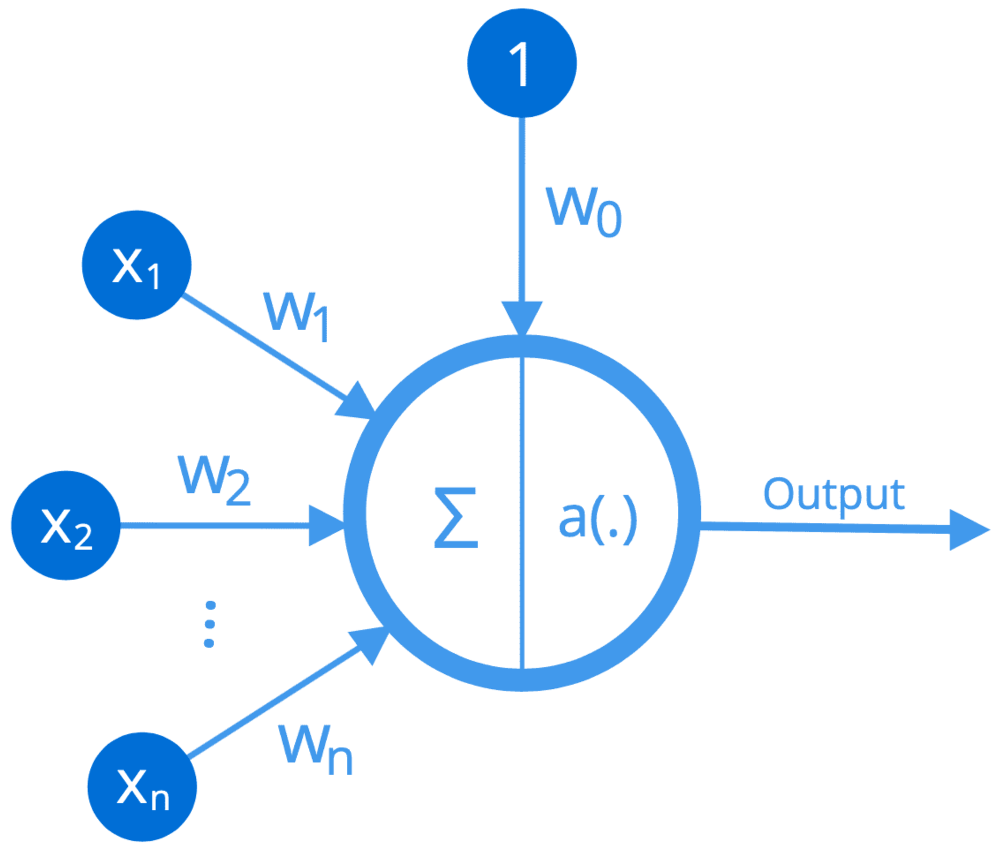
- ★ a model inspired by the human brain's neural structure.
- ★ a nested sequence of linear and non-linear functions with variable parameters.
- ★ approximate any continuous functional relationship between inputs and outputs.

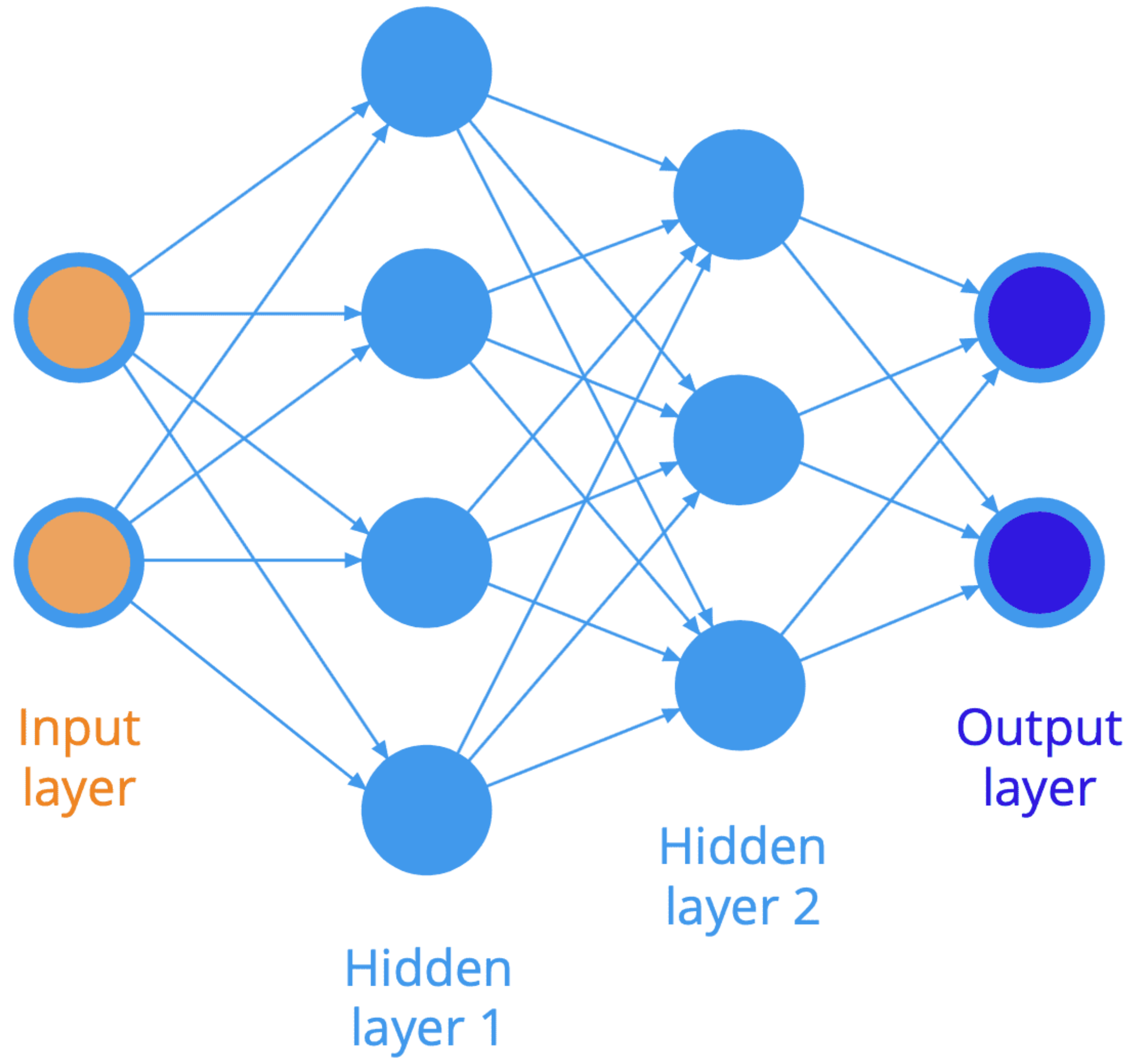
Universal Approximation Theorem: **existence / limit theorem**

A single-hidden-layer neural network can approximate any continuous function.

George Cybenko (1989); Kurt Hornik (1991)

$$\text{output} = a(z) = a\left(\left(\sum_{i=1}^{n} x_i \times w_i\right) + b\right)$$





ANN for quantum many-body problems

Carleo and Troyer, Science, **355**, 602 (2017)

RESEARCH

RESEARCH ARTICLE

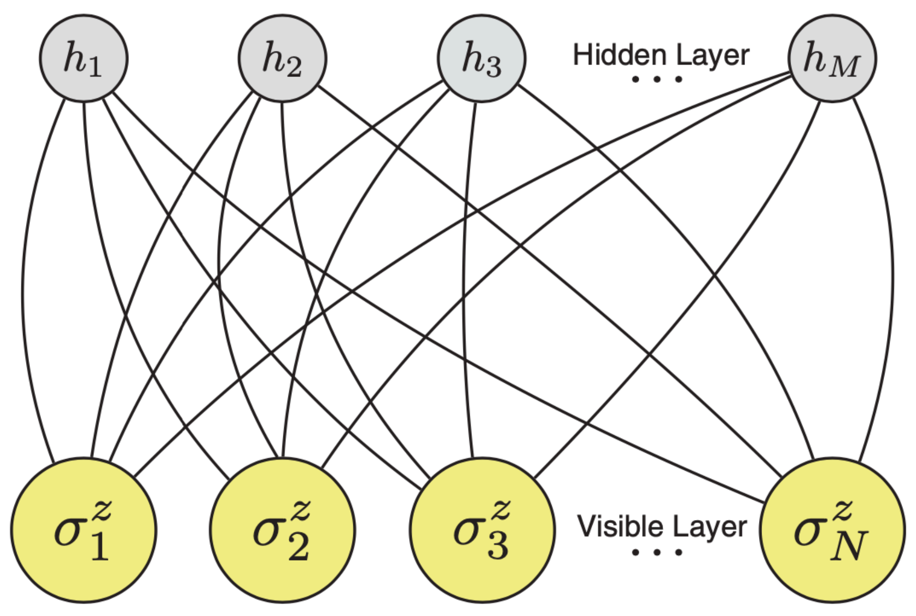
MANY-BODY PHYSICS

Solving the quantum many-body problem with artificial neural networks

Giuseppe Carleo[1*] and Matthias Troyer[1,2]

The challenge posed by the many-body problem in quantum physics originates from the difficulty of describing the nontrivial correlations encoded in the exponential complexity of the many-body wave function. Here we demonstrate that systematic machine learning of the wave function can reduce this complexity to a tractable computational form for some notable cases of physical interest. We introduce a variational representation of quantum states based on artificial neural networks with a variable number of hidden neurons. A reinforcement-learning scheme we demonstrate is capable of both finding the ground state and describing the unitary time evolution of complex interacting quantum systems. Our approach achieves high accuracy in describing prototypical interacting spins models in one and two dimensions.

$$\Psi_M(\mathcal{S};\mathcal{W}) = \sum_{\{h_i\}} e^{\sum_j a_j\sigma_j^z + \sum_i b_i h_i + \sum_{ij} W_{ij} h_i \sigma_j^z}$$



Electron systems:

FermiNet PauliNet

Hermann et al., Nat. Chem. 12, 891 (2020)

Pfau et al., PRR 2, 033429 (2020)

Nuclear systems:

- ✓ **Complicated nuclear forces**

  tensor, spin-orbit, many-body forces, …

- ✓ **More degrees of freedom**

  spatial, spin, isospin, …

- ✓ **Strongly correlated systems**

  short-range correlations, clustering, …

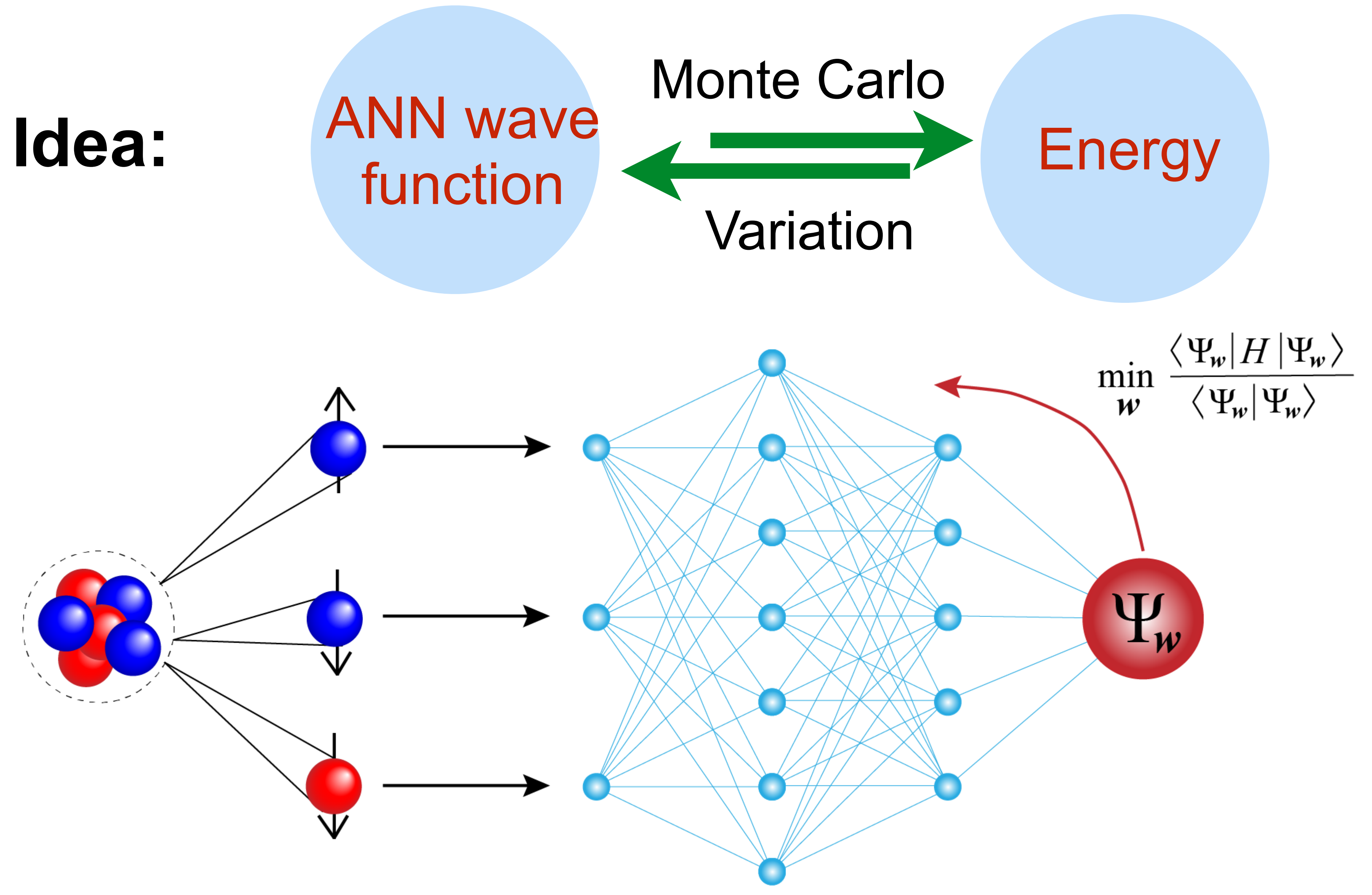
- ✓ **Self-bound systems**

  translational invariance, …

- ✓ ……

ANN for the nuclear many-body problem

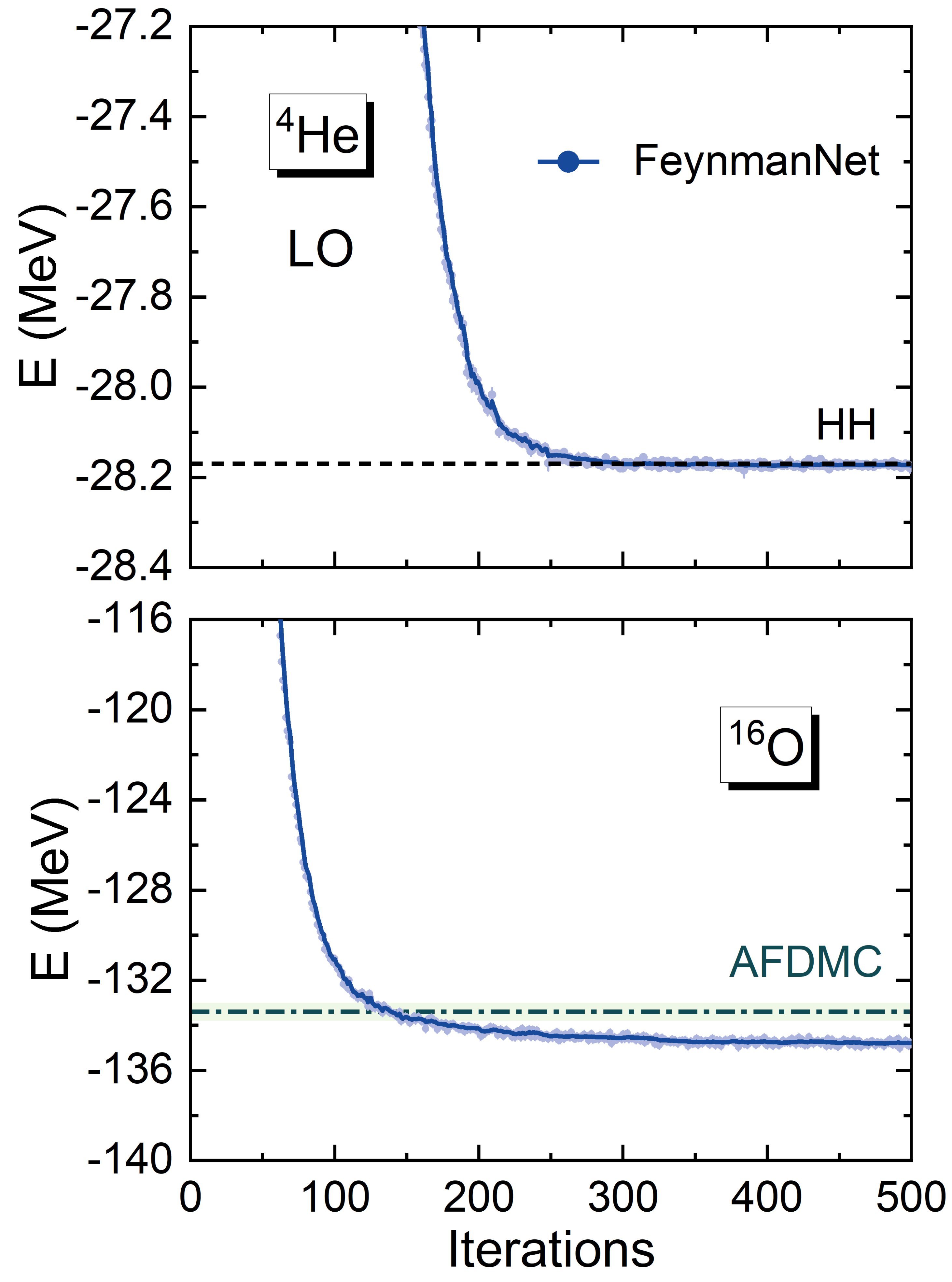
FeynmanNet: Variational Monte Carlo + Deep Neural–Networks



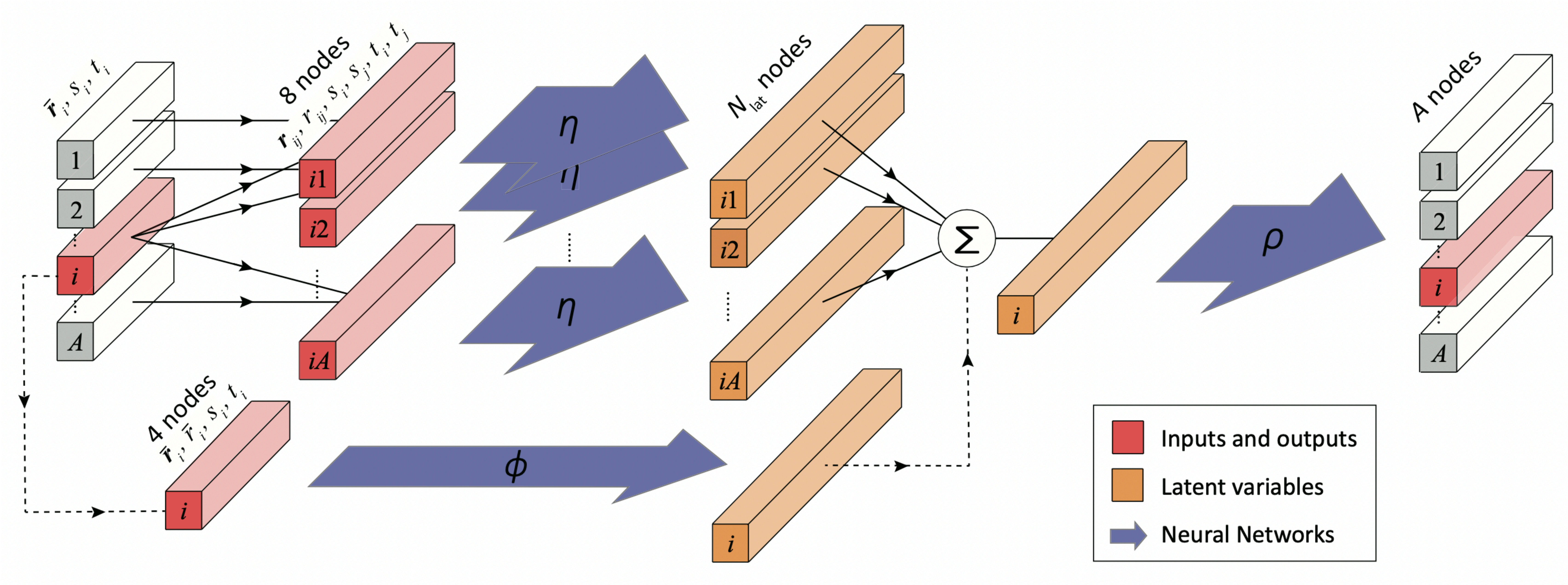
Polynomial scaling!

Yang and **PWZ***, PLB 835, 137587 (2022)

Yang and **PWZ***, PRC 107, 034320 (2023)



Architecture



Fermion Antisymmetry Encoded!

$$\Psi^{(\alpha)}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_A) = e^{\mathcal{U}^{(\alpha)}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_A)} \sum_n w_n \det \boldsymbol{\Phi}^{(\alpha,n)}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_A), \quad \alpha = \mathrm{R}, \mathrm{I}.$$

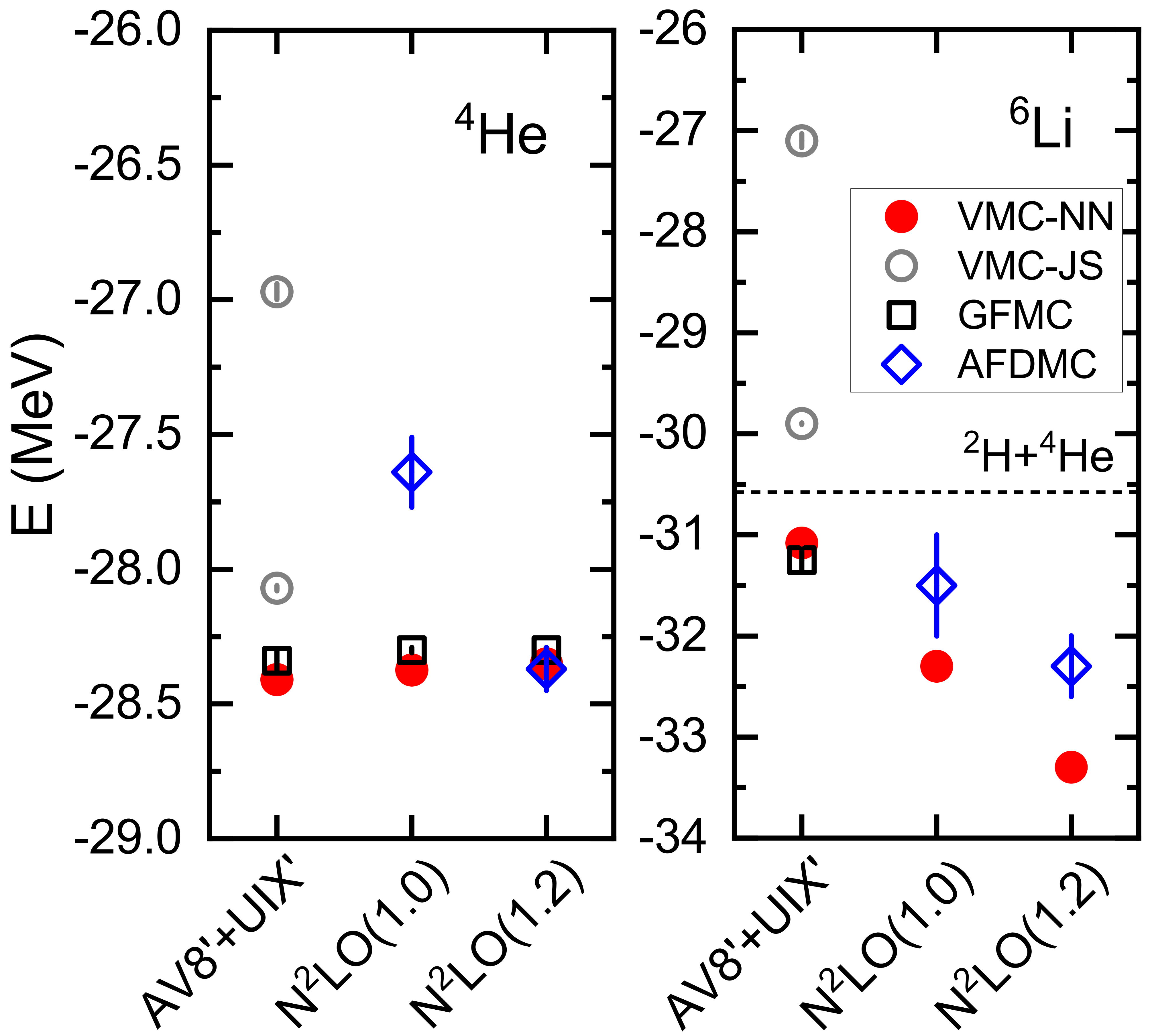
Complexed valued network!

$$[\boldsymbol{\Phi}^{(\alpha,n)}]_{i\mu} = \mathbf{f}^{(\alpha,n)}_{i\mu}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_A)\varphi_\mu(\boldsymbol{x}_i)$$

Yang and **PWZ***, PRC 107, 034320 (2023)

Backflow transformation !

FeynmanNet: accuracy with polynomial scaling

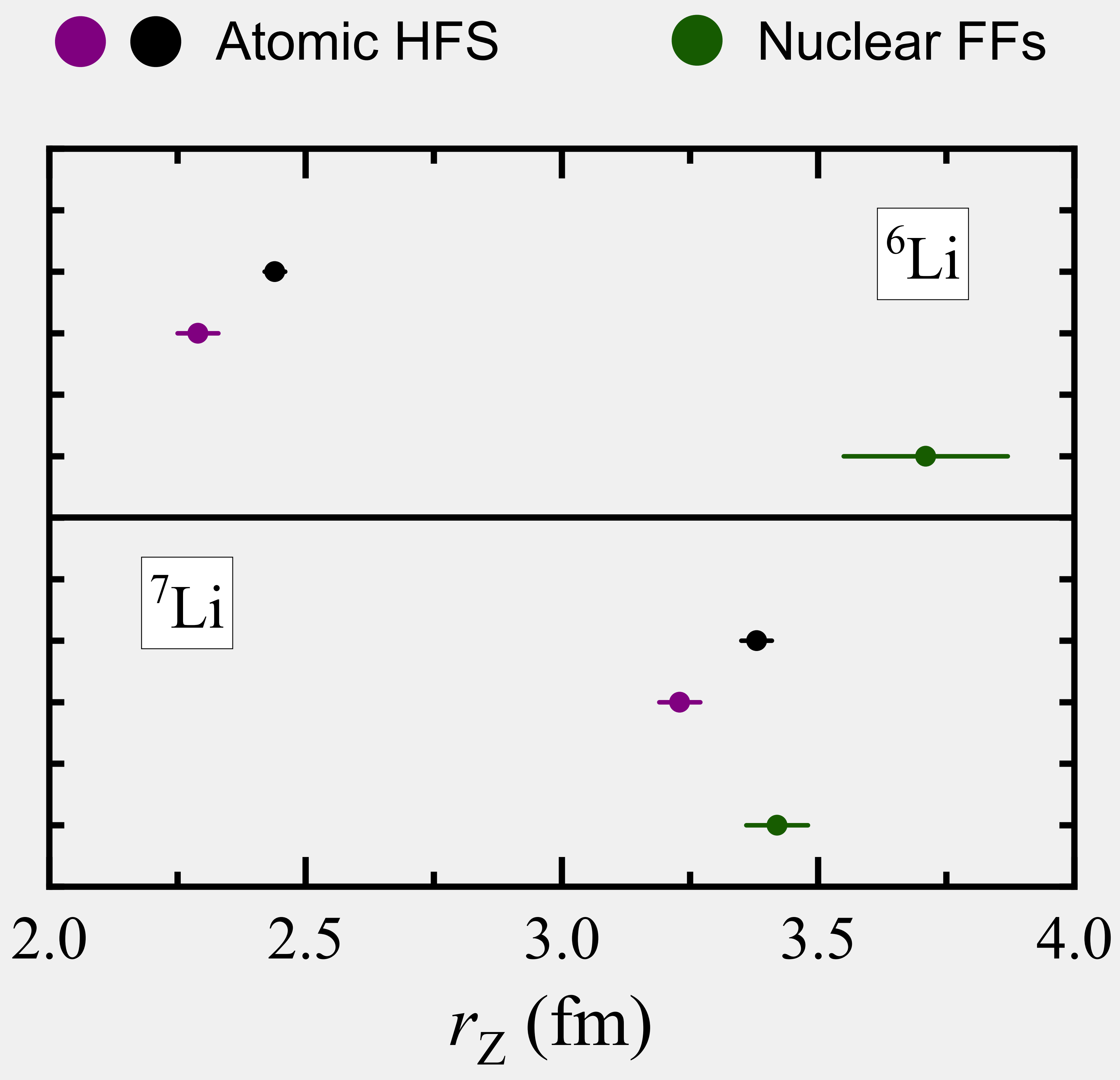


Yang, Epelbaum, Ji, **PWZ***, submitted

- ✓ **No fermion sign problem**
- ✓ **No need to soften nuclear forces**
- ✓ **Polynomial computational complexity**
- ✓ **Explicit many-body wave function**
- ✓ **…**

$$r_Z = \int d^3r\, d^3r' \rho_E(\boldsymbol{r})\rho_M(\boldsymbol{r}')|\boldsymbol{r}' - \boldsymbol{r}|.$$

The puzzle of Lithium Zemach radii



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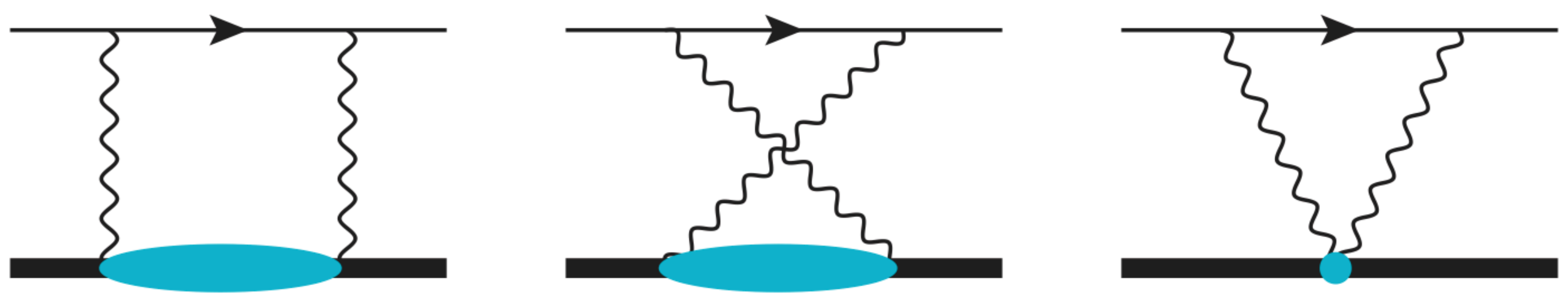


$$\delta r_{\text{pol}}(\bar{\omega}) = -\frac{1}{\mu Z} \sum_{i=1}^{A} \langle 0 | \mu_i \delta r_i(\bar{\omega}) \sigma_{zi} | 0 \rangle$$

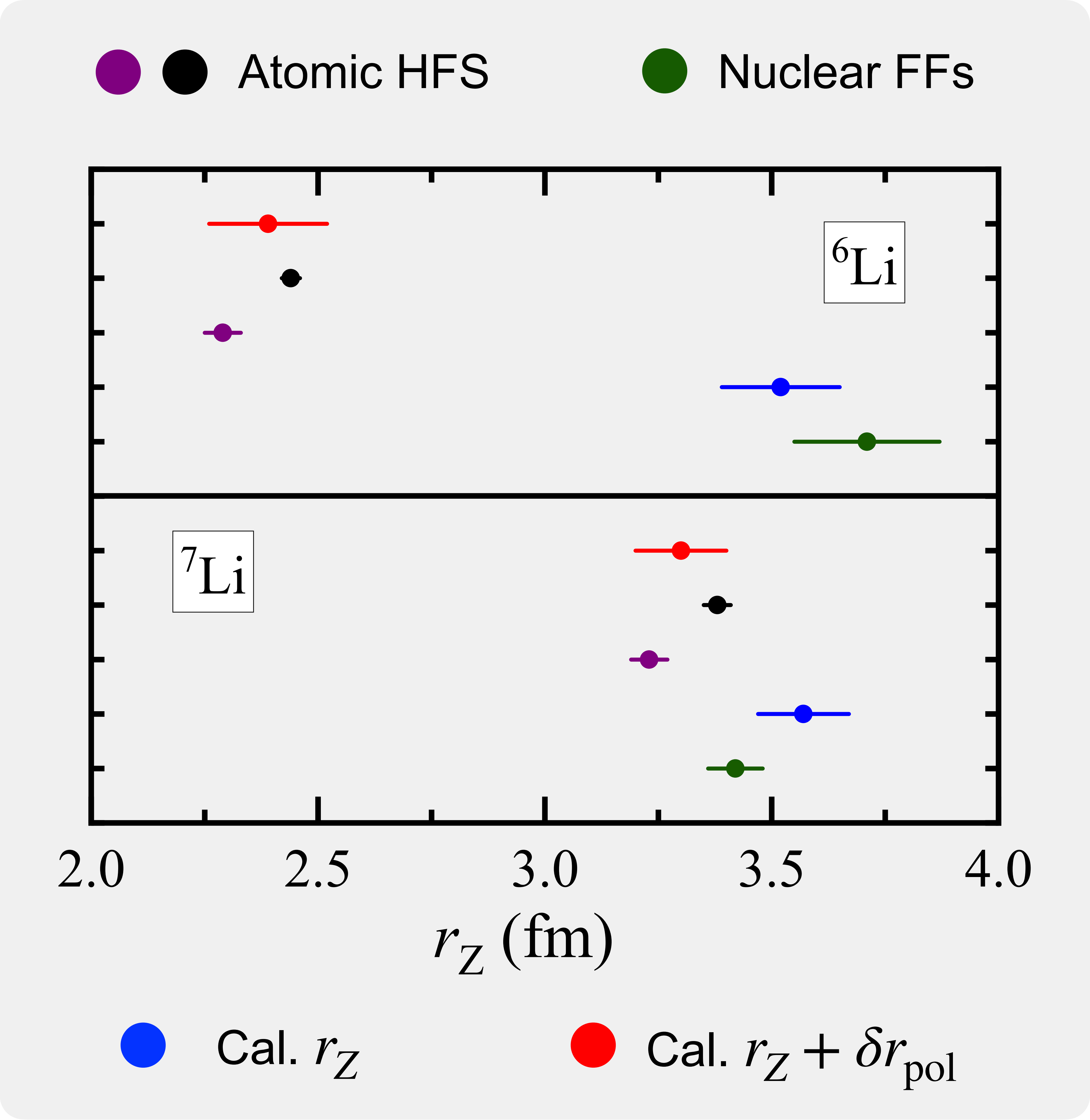
$$\simeq \begin{cases} -\dfrac{1}{Z} \dfrac{\mu_p}{\mu_p + \mu_n} \delta r_p(\bar{\omega}) & \text{odd-odd} \\ -\dfrac{1}{Z} \delta r_p(\bar{\omega}) & \text{odd-even} \\ 0 & \text{even-odd} \end{cases}$$

$\mu_p = 2.793\mu_N \quad \mu_n = -1.913\mu_N$

Nuclear polarizability: the dominant source for solving the puzzle

Yang, Epelbaum, Ji, **PWZ**, submitted

The puzzle of Lithium Zemach radii



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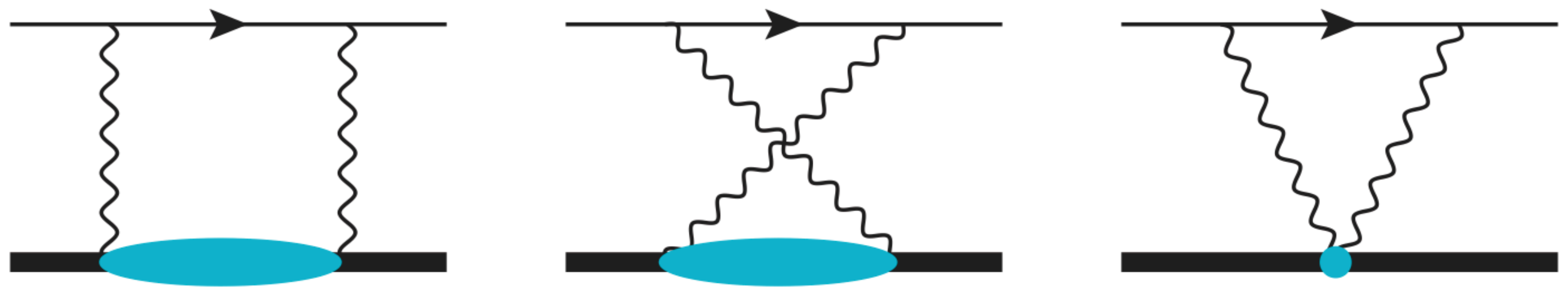

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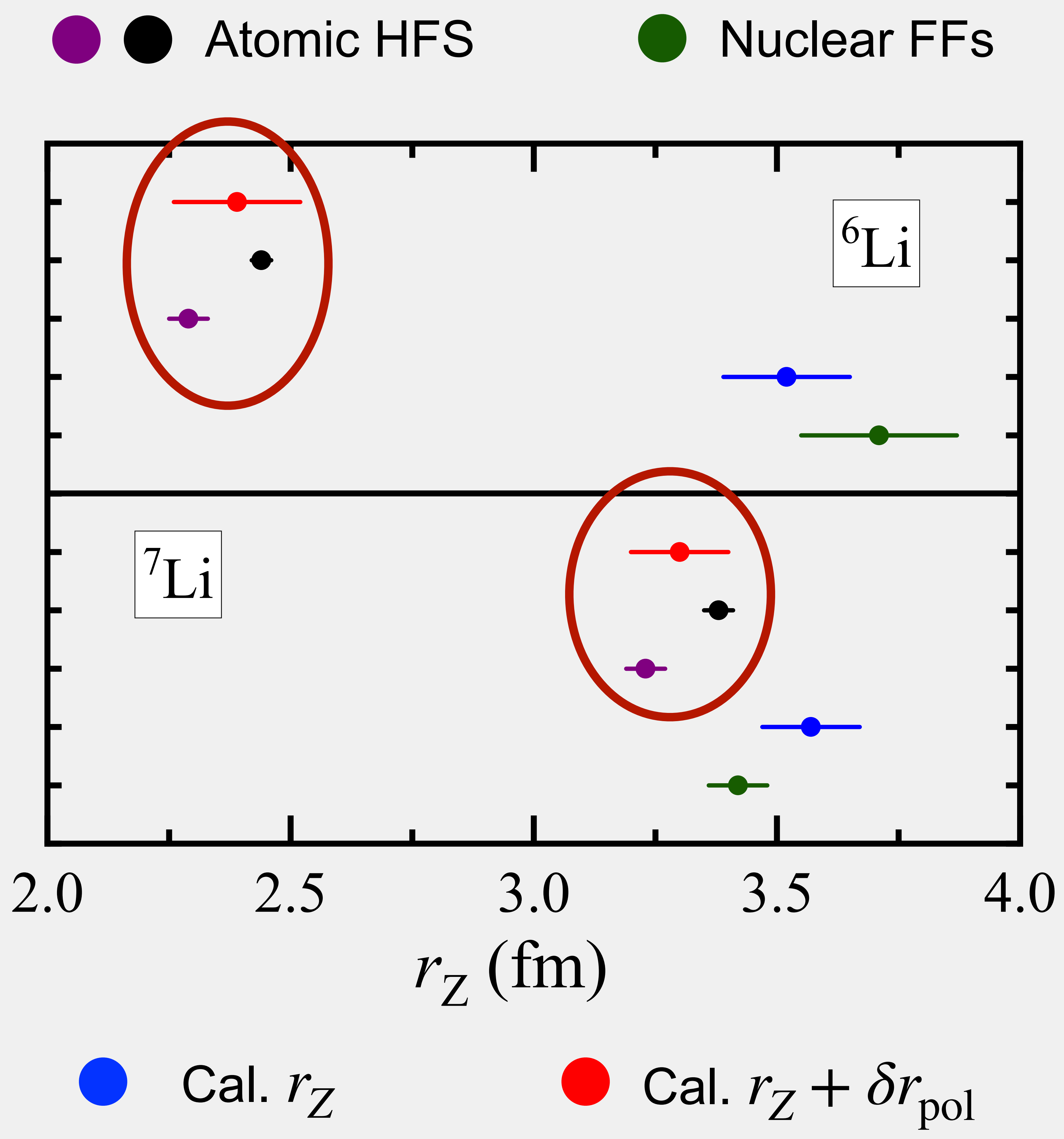

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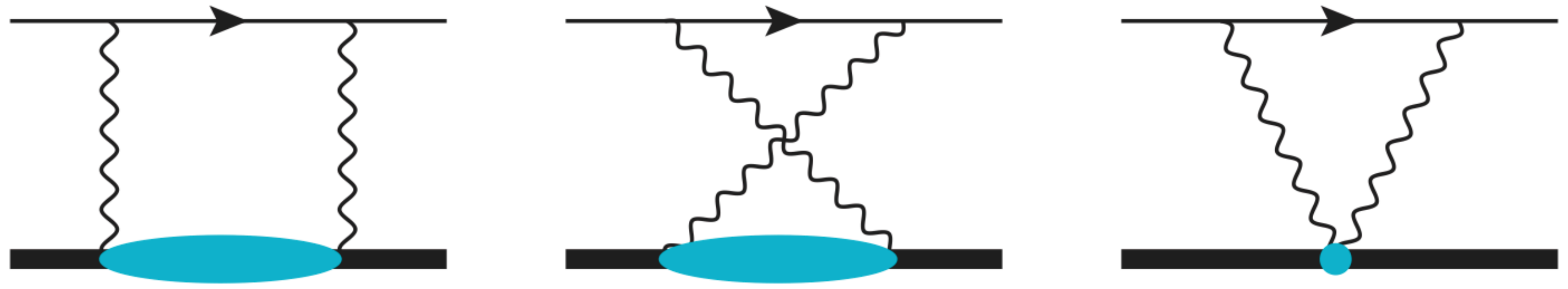

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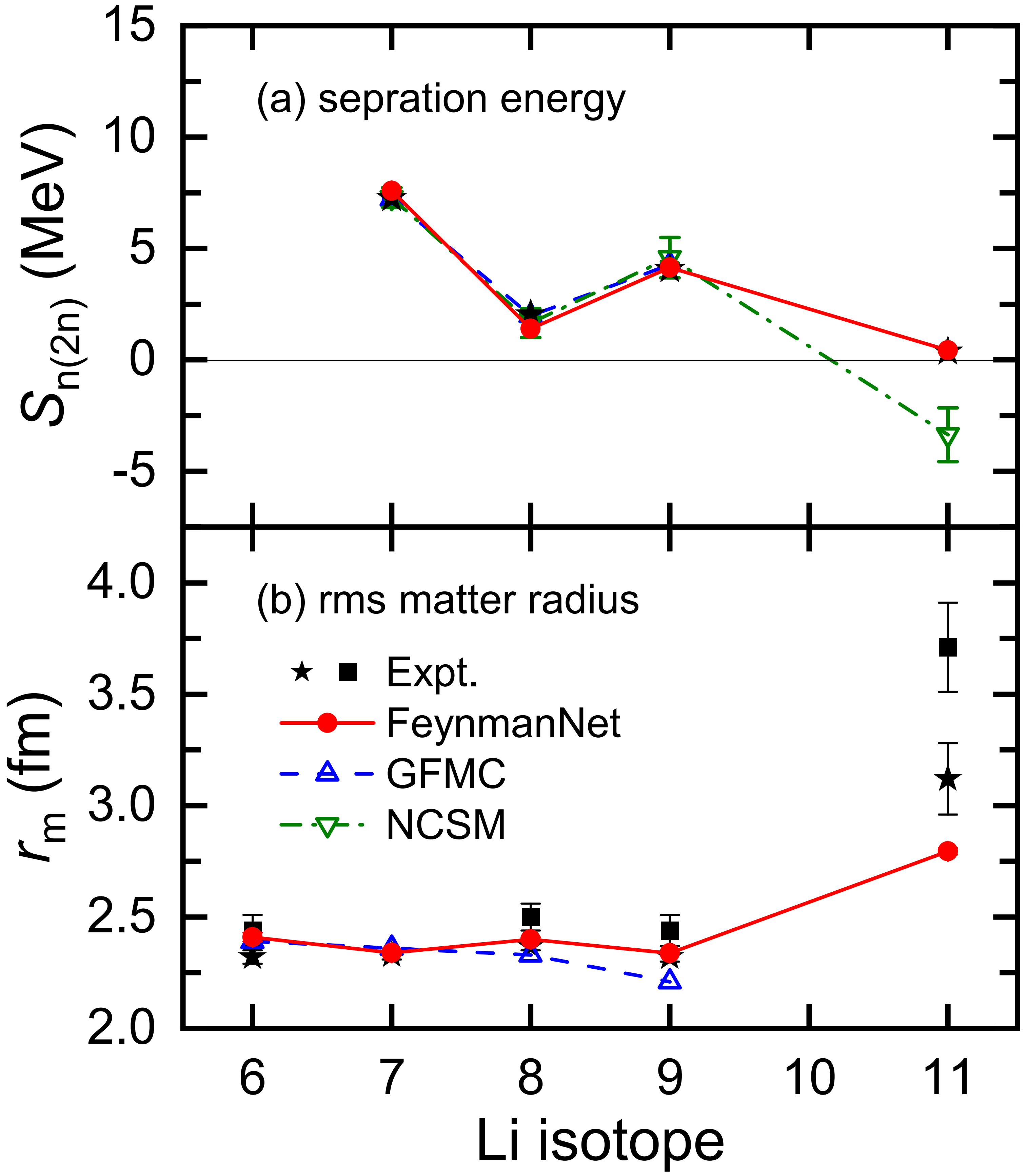
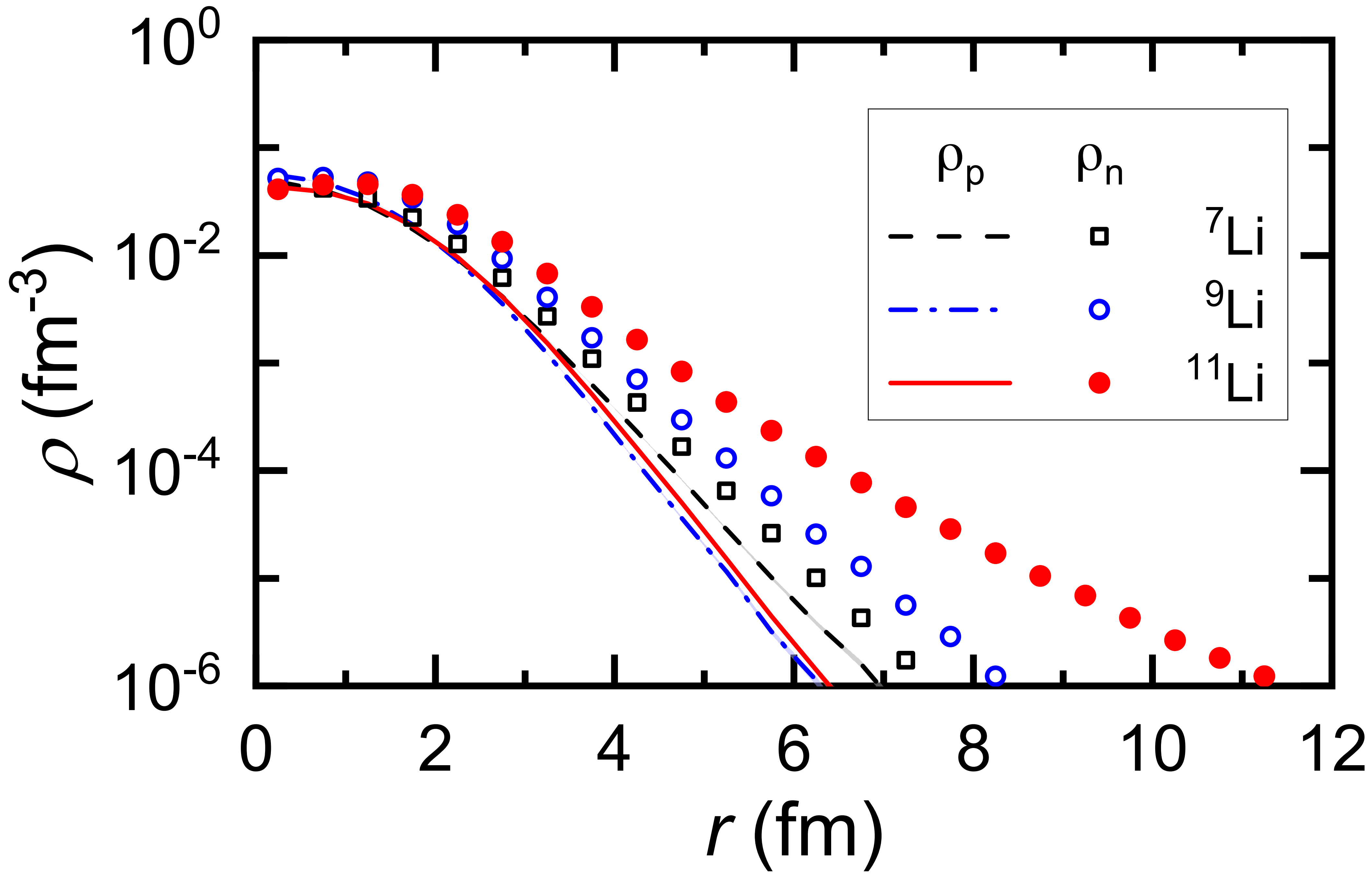
Nuclear polarizability: the dominant source for solving the puzzle

Yang, Epelbaum, Ji, **PWZ**, submitted

Halo of ^{11}Li

- ✓ Experimental radii and separation energies of Li isotopes are reproduced.
- ✓ **Halo emerges from full many-body dynamics.**

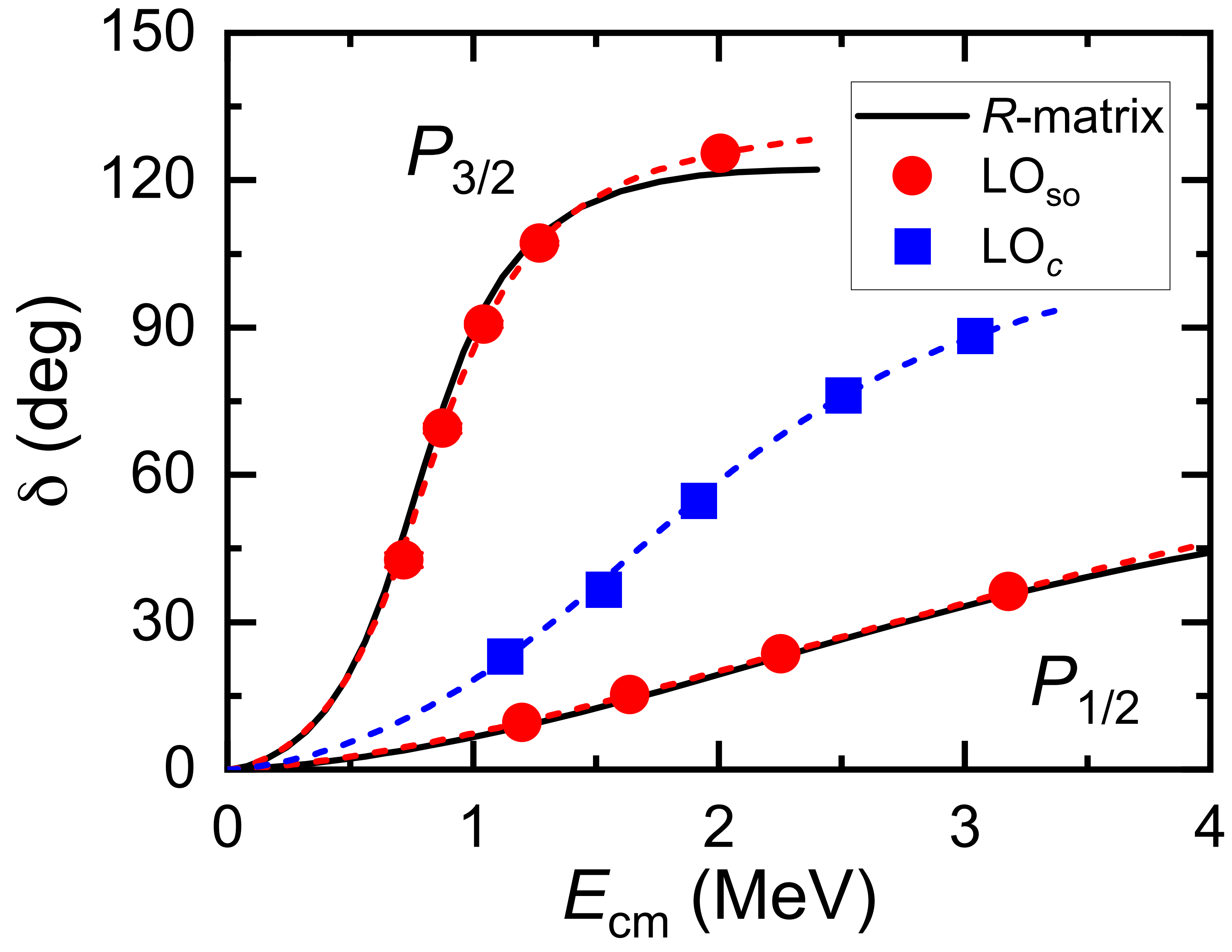


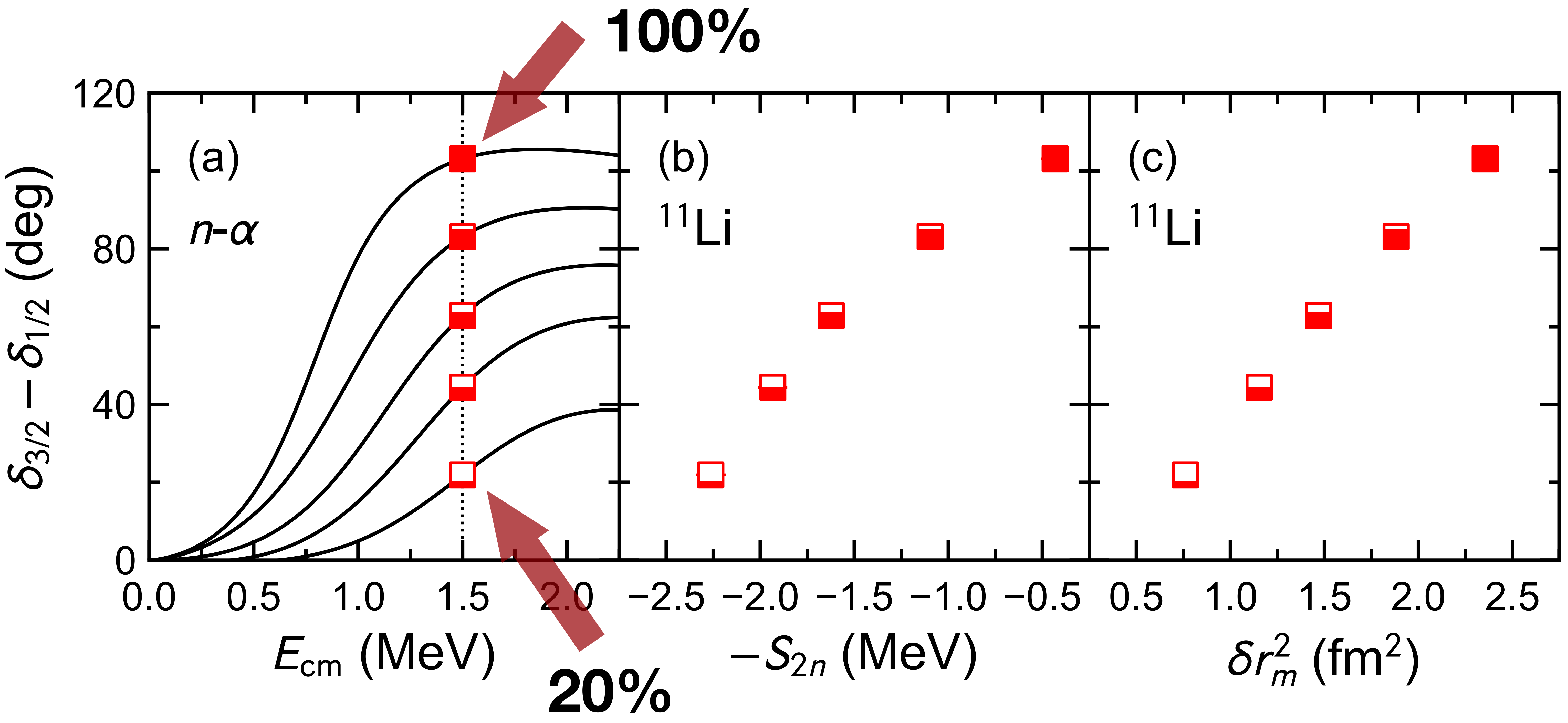


Yang, **PWZ***, submitted

Connecting the ^{11}Li halo to n-α scattering

The halo structure of ^{11}Li is closely related to the splitting of the neutron–alpha *P*-wave scattering phase shifts!



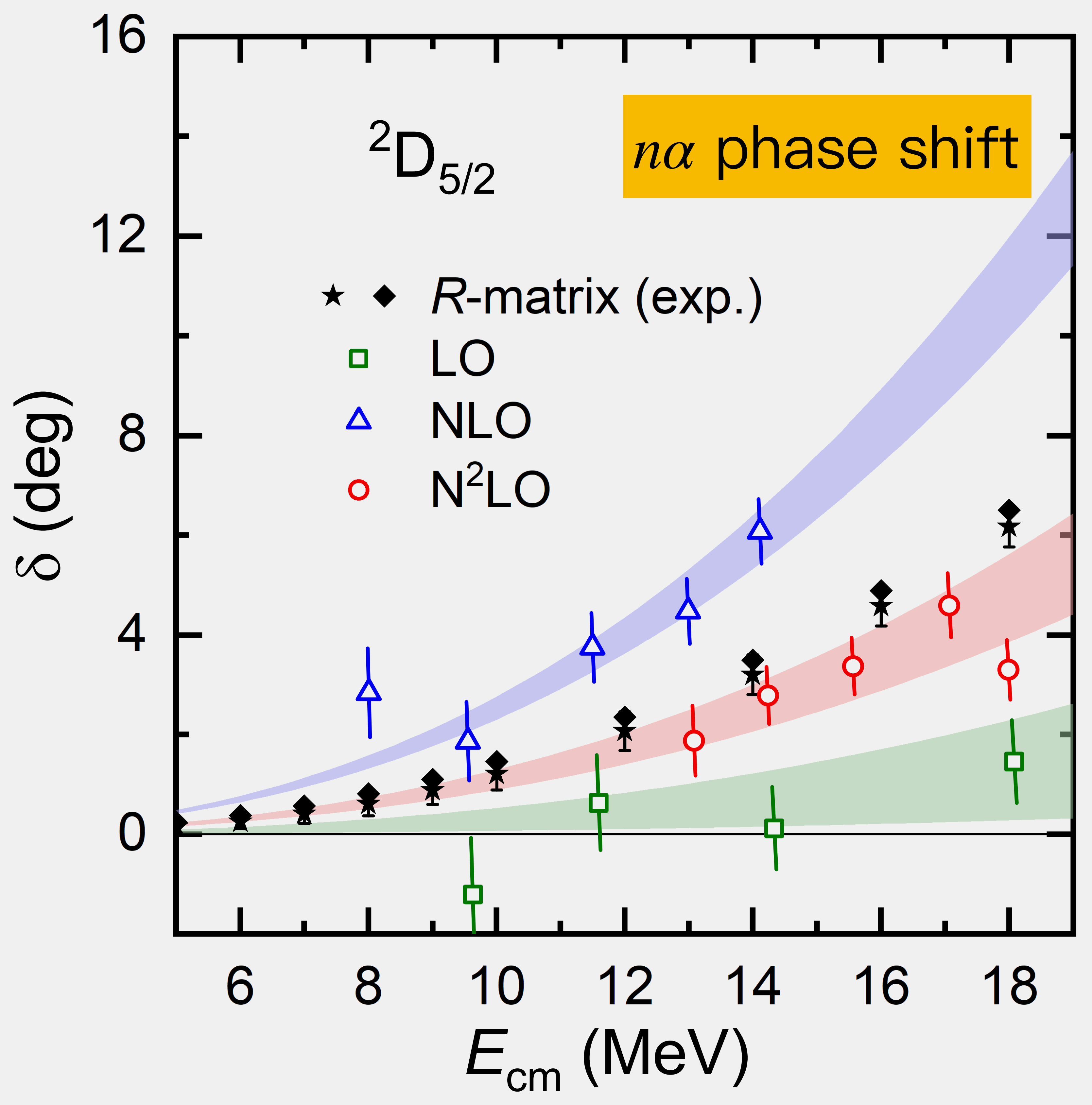


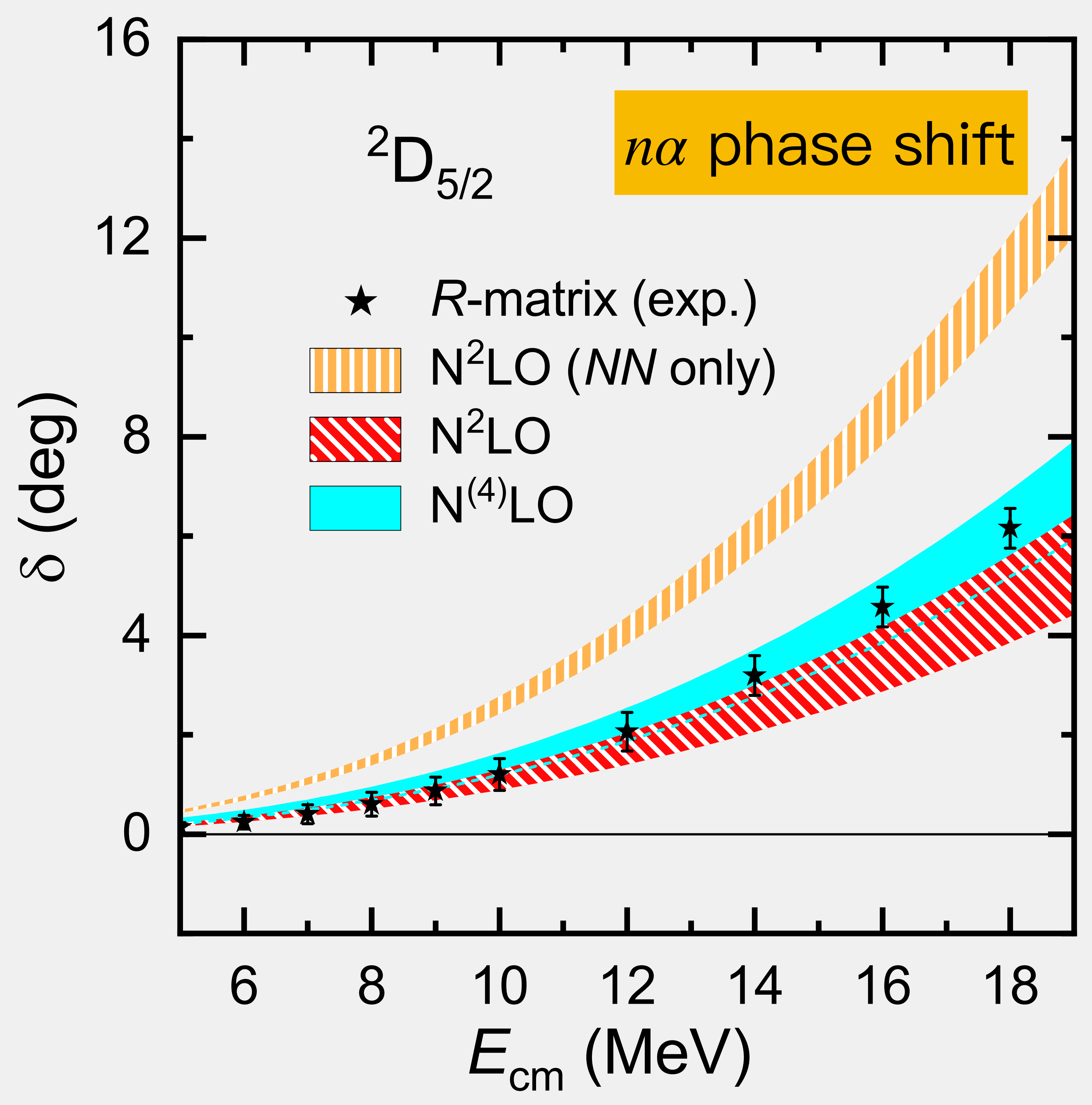
Yang, **PWZ***, submitted

Peripheral n-α scattering probes long-range 3N forces

✓ A **sensitive and clean probe** of the long-range 3N forces!

✓ A **highly nontrivial test** of chiral EFT in the few-nucleon sector!

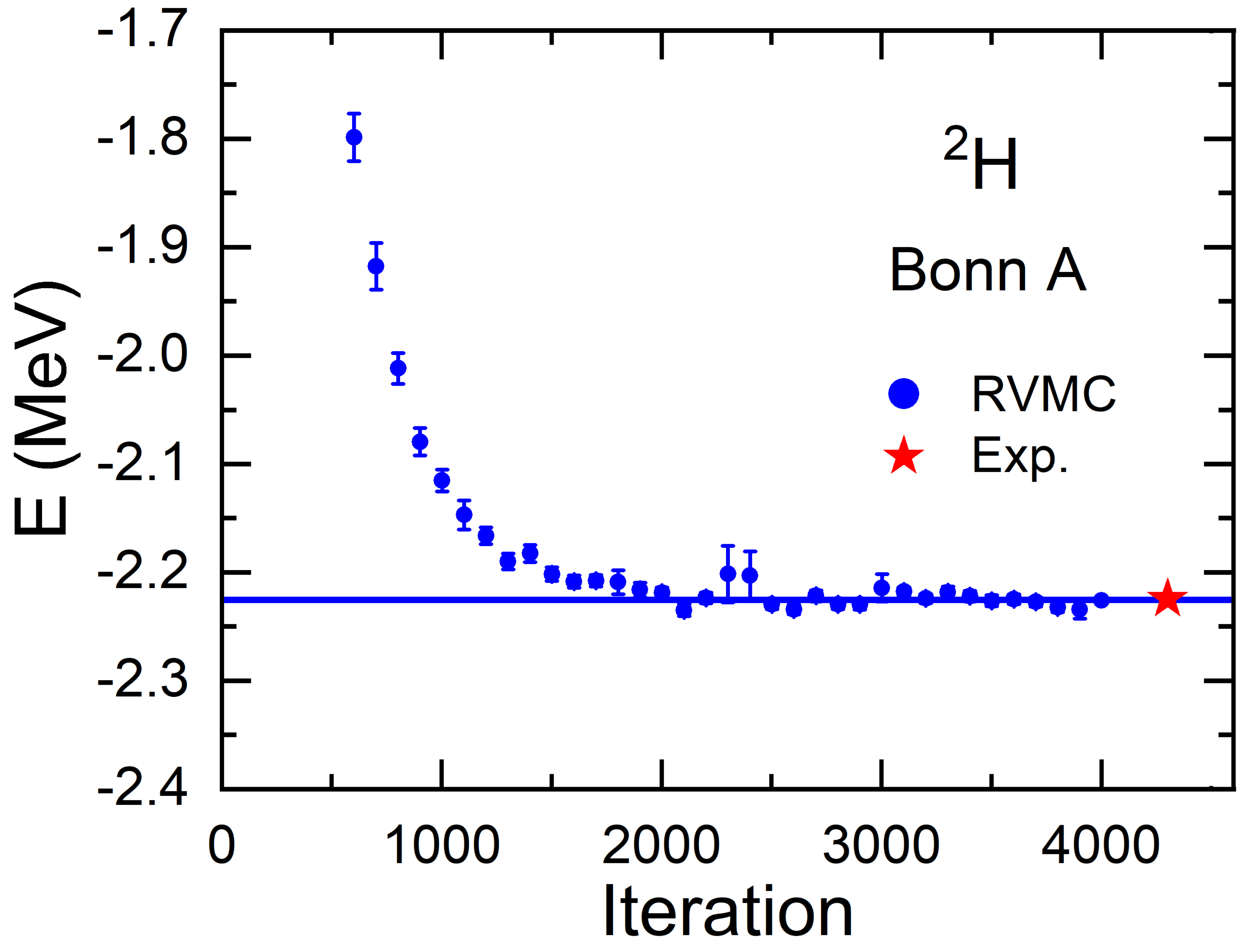


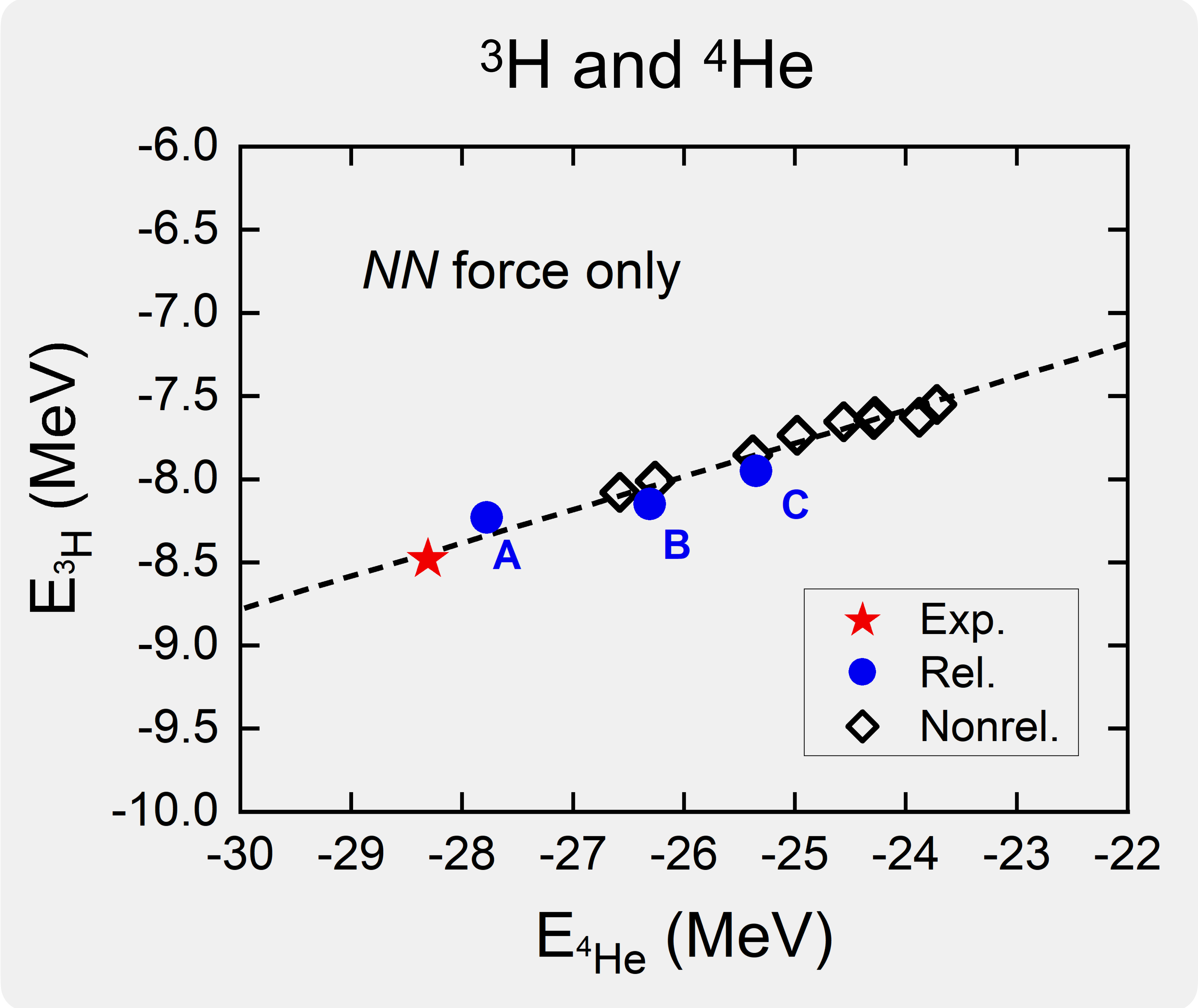


Yang, Epelbaum*, Meng*, Meng, **PWZ***, PRL 135, 172502 (2025)

Relativistic *ab initio* calculations

Relativistic results **improve the underbinding** of light nuclei without 3N forces.



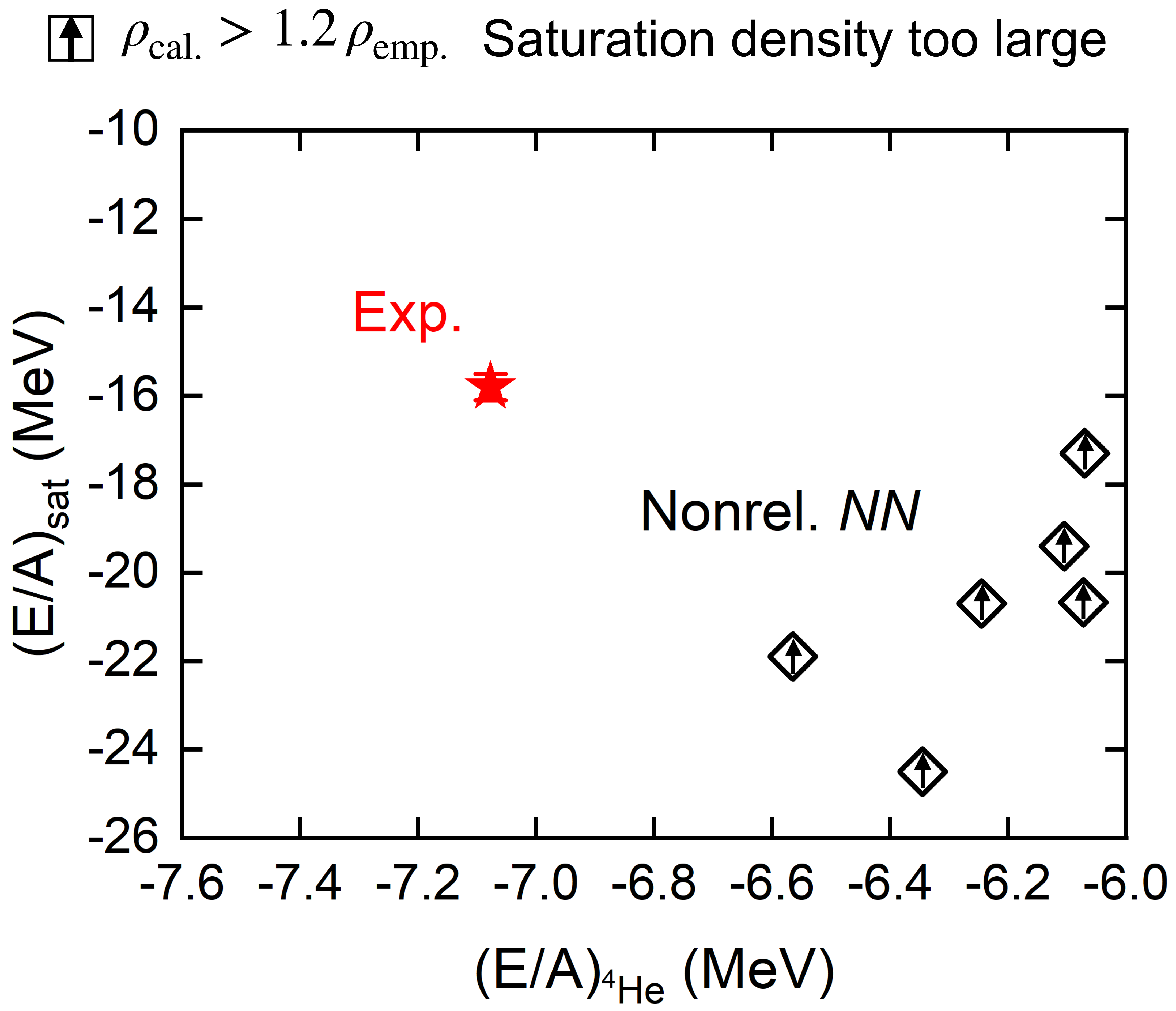


Yang and **PWZ***, CPL, 42 051201 (2025) "Express Letter"

Nonrel. calculations with AV18, CD-Bonn, Nijmegen I, II, Chiral forces

From light nuclei to nuclear matter

Yang, **PWZ***, CPL, 42 051201 (2025) “Express Letter”



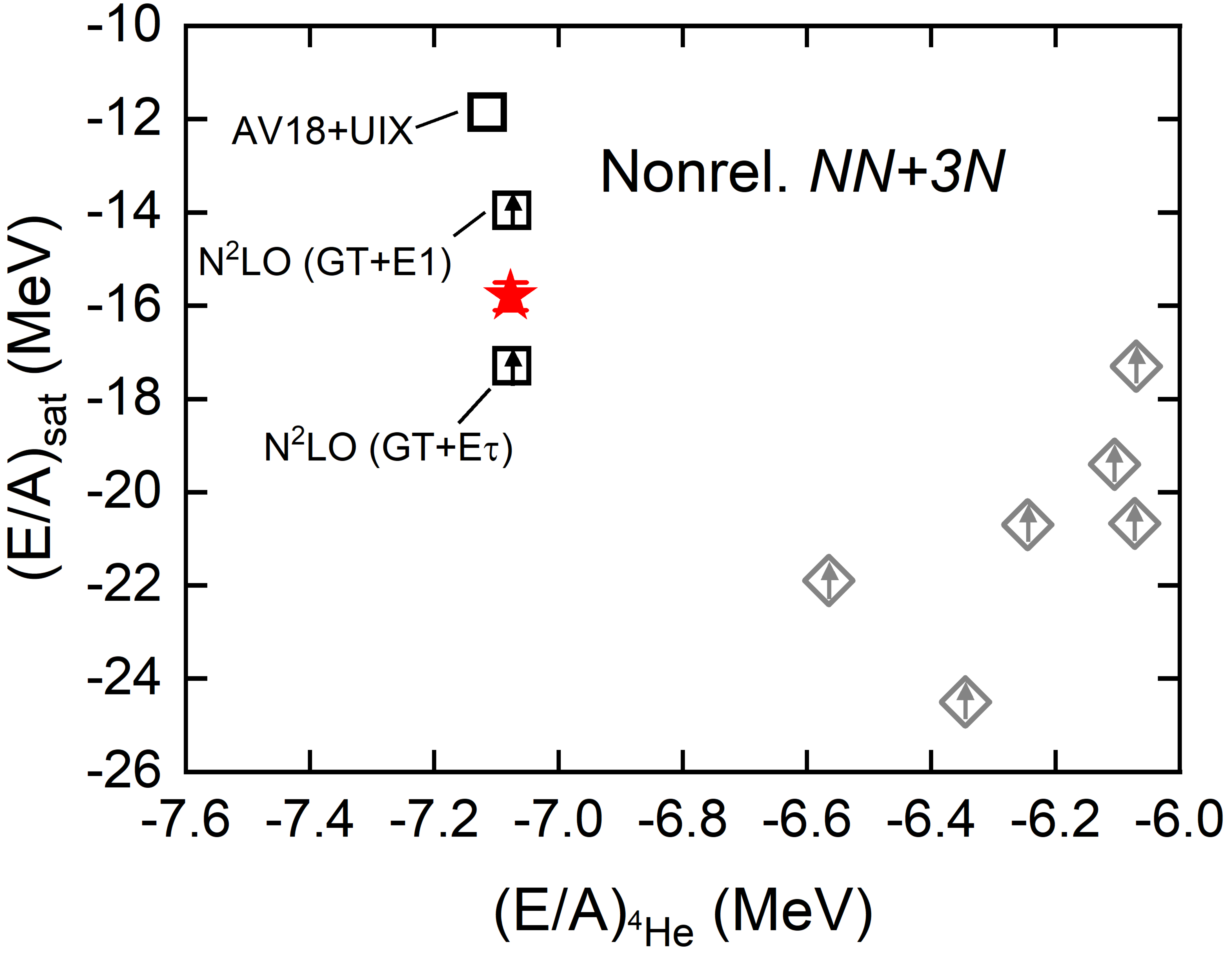
	^{4}He	Nucl. Matt.
NN	Underbind	Overbind

RBHF nuclear matter: from Wang, Zhao, Ring, Meng, PRC 103, 054319 (2021)

From light nuclei to nuclear matter

Yang, **PWZ***, CPL, 42 051201 (2025) “Express Letter”

$\rho_{\text{cal.}} > 1.2\,\rho_{\text{emp.}}$ Saturation density too large



	4He	Nucl. Matt.
NN	Underbind	Overbind
NN/3N	Fit	Diverse

RBHF nuclear matter: from Wang, Zhao, Ring, Meng, PRC 103, 054319 (2021)

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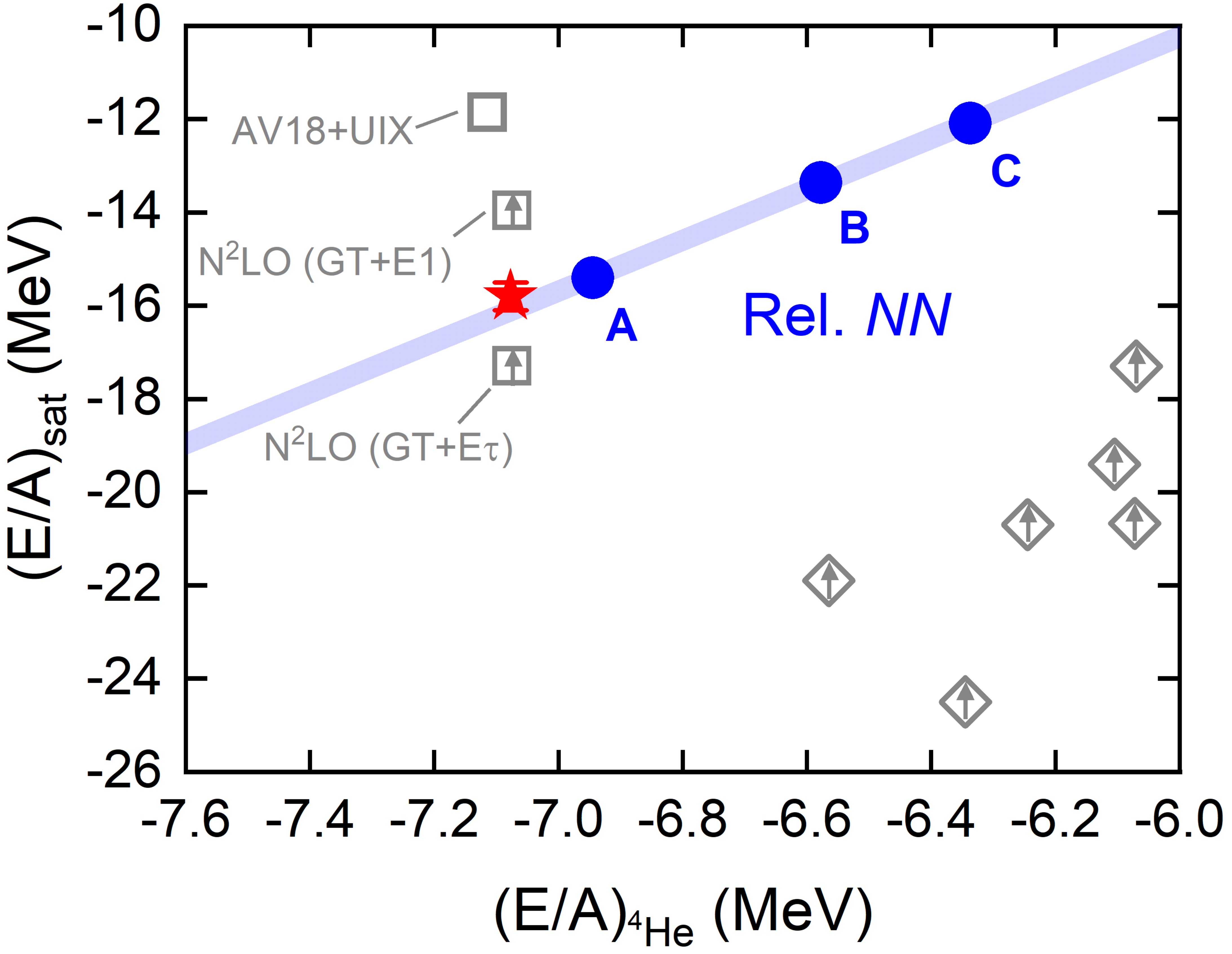


	^{4}He	Nucl. Matt.
NN	Underbind	Overbind
NN/3N	Fit	Diverse
Rel.	**Consistent !**	

RBHF nuclear matter: from Wang, Zhao, Ring, Meng, PRC 103, 054319 (2021)

Summary

Deep learning has been applied to solve the *ab initio* nuclear many-body problem.

- Many-body complexity

  FeynmanNet enables accurate many-body calculations with polynomial scaling.

- Exotic phenomena

  Nuclear polarizability is the dominant source for solving the puzzle of Lithium Zemach radii

  The **halo** of ^{11}Li is closely related to the splitting of n-α P-wave scattering phase shifts

  Peripheral n-α scattering probes **long-range 3N forces**

- From nuclei to nuclear matter

  Relativistic dynamics provides a promising route toward a consistent description from light nuclei to nuclear matter

Collaborations

- ✓ **Peking University:** Jie Meng, Yilong Yang
- ✓ **Beihang University:** Yakun Wang
- ✓ **Southeast University:** Lu Meng
- ✓ **Fudan University:** Wanbing He, Yugang Ma, Zixiao Zhang
- ✓ **Fuzhou University:** Xinhui Wu
- ✓ **Central China Normal University:** Chen Ji
- ✓ **Nankai University:** Zhengxue Ren, Fangfang Xu
- ✓ **University of Zagreb:** D. Vretenar, T. Nikšić
- ✓ **Ruhr University Bochum, Germany:** E. Epelbaum
- ✓ **Technical University of Munich, Germany:** P. Ring
- ✓ **Kyoto University, Japan:** K. Hagino
- ✓ **University of Milan, Italy:** G. Colò
- ✓ … …

Collaborations

- ✓ **Peking University:** Jie Meng, Yilong Yang
- ✓ **Beihang University:** Yakun Wang
- ✓ **Southeast University:** Lu Meng
- ✓ **Fudan University:** Wanbing He, Yugang Ma, Zixiao Zhang
- ✓ **Fuzhou University:** Xinhui Wu
- ✓ **Central China Normal University:** Chen Ji
- ✓ **Nankai University:** Zhengxue Ren, Fangfang Xu
- ✓ **University of Zagreb:** D. Vretenar, T. Nikšić
- ✓ **Ruhr University Bochum, Germany:** E. Epelbaum
- ✓ **Technical University of Munich, Germany:** P. Ring
- ✓ **Kyoto University, Japan:** K. Hagino
- ✓ **University of Milan, Italy:** G. Colò
- ✓ … …

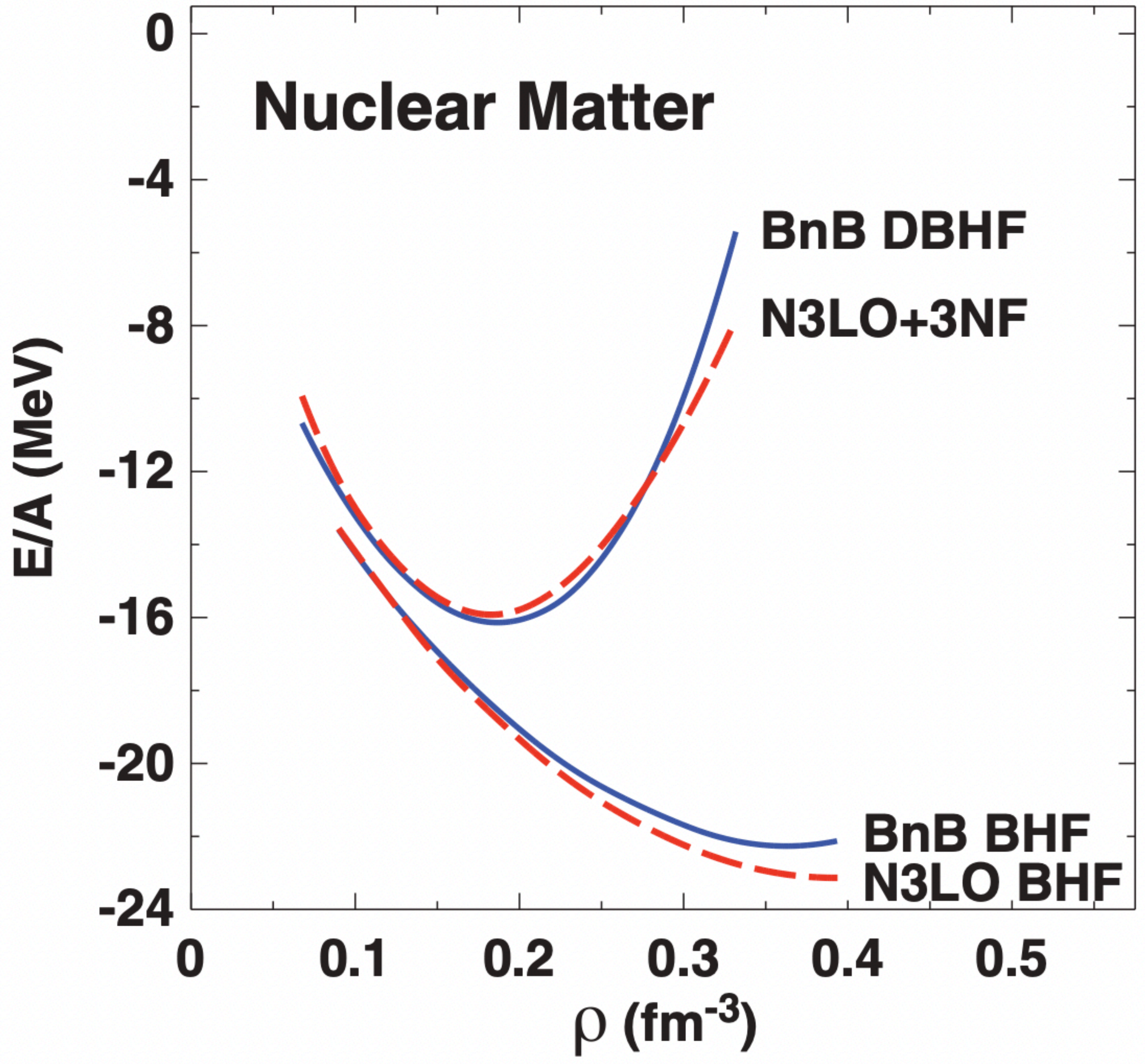
Thank you!

Relativistic Brueckner-Hartree-Fock

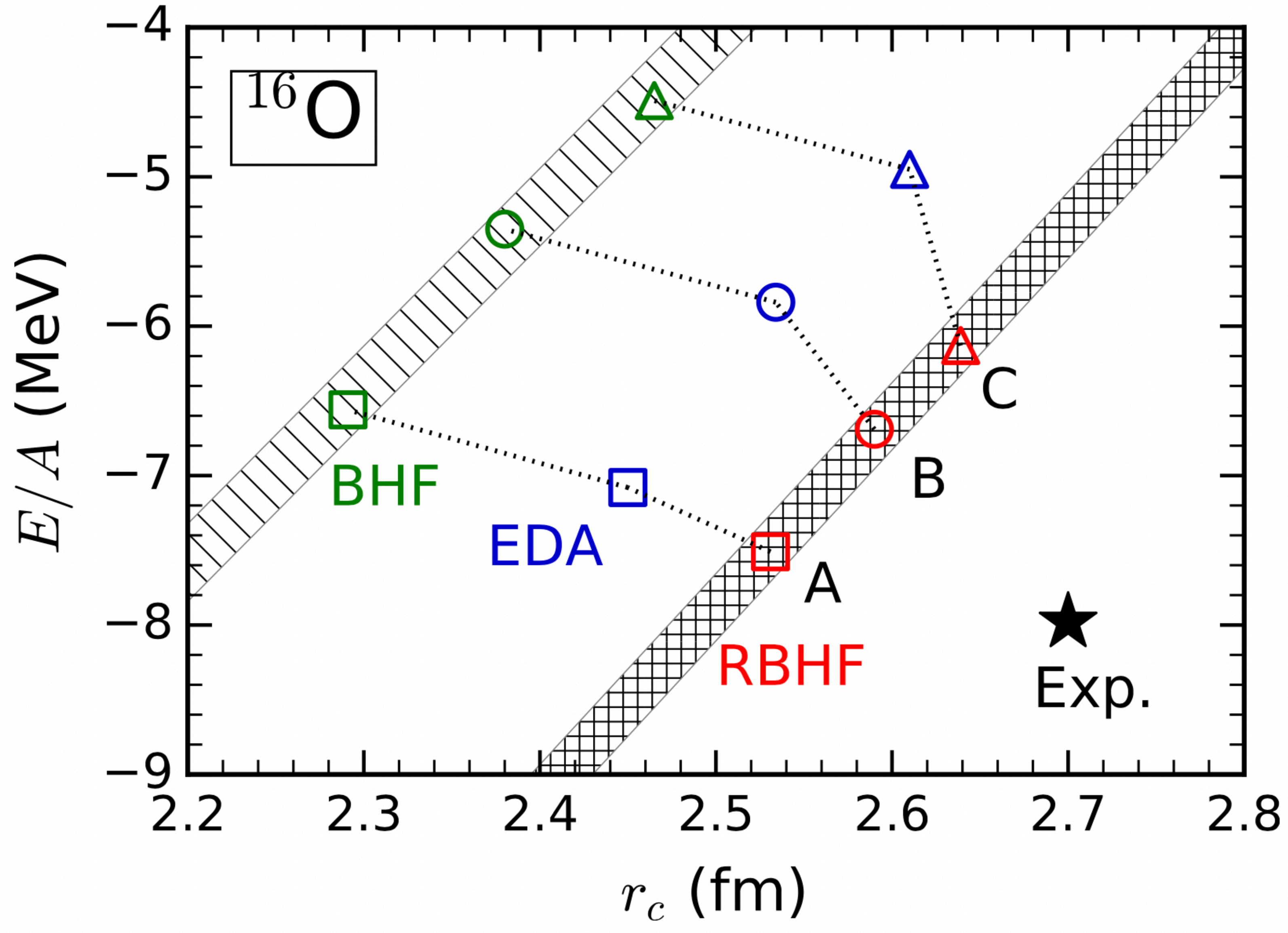
VOLUME 45, NUMBER 26 PHYSICAL REVIEW LETTERS 29 DECEMBER 1980

Nuclear Saturation as a Relativistic Effect

M. R. Anastasio, L. S. Celenza, and C. M. Shakin
Institute for Nuclear Theory and Department of Physics, Brooklyn College of the City University of New York, Brooklyn, New York 11210
(Received 18 June 1980)



Sammarruca, et al., PRC 86, 054317 (2012)



Shen et al., PPNP 109, 103713 (2019)

RBHF method is most suitable for nuclear matter and closed-shell nuclei.

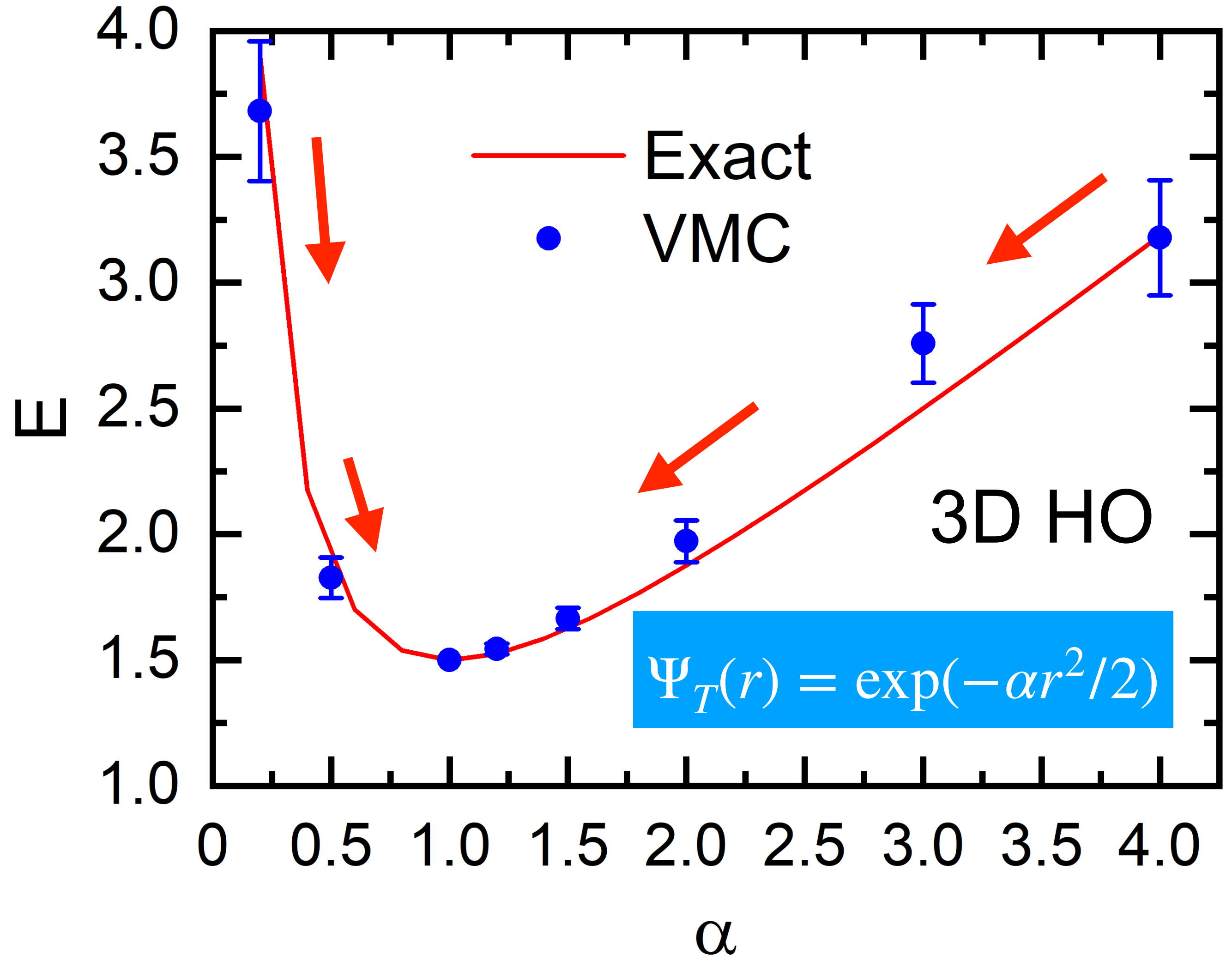
What is quantum Monte Carlo?

- **Monte Carlo:**
  solve multi-dimensional integrals by using random numbers.
- **Quantum Monte Carlo:**
  solve quantum mechanical problems using Monte Carlo methods.

Carlson et al., Rev. Mod. Phys. 87, 1067 (2015)

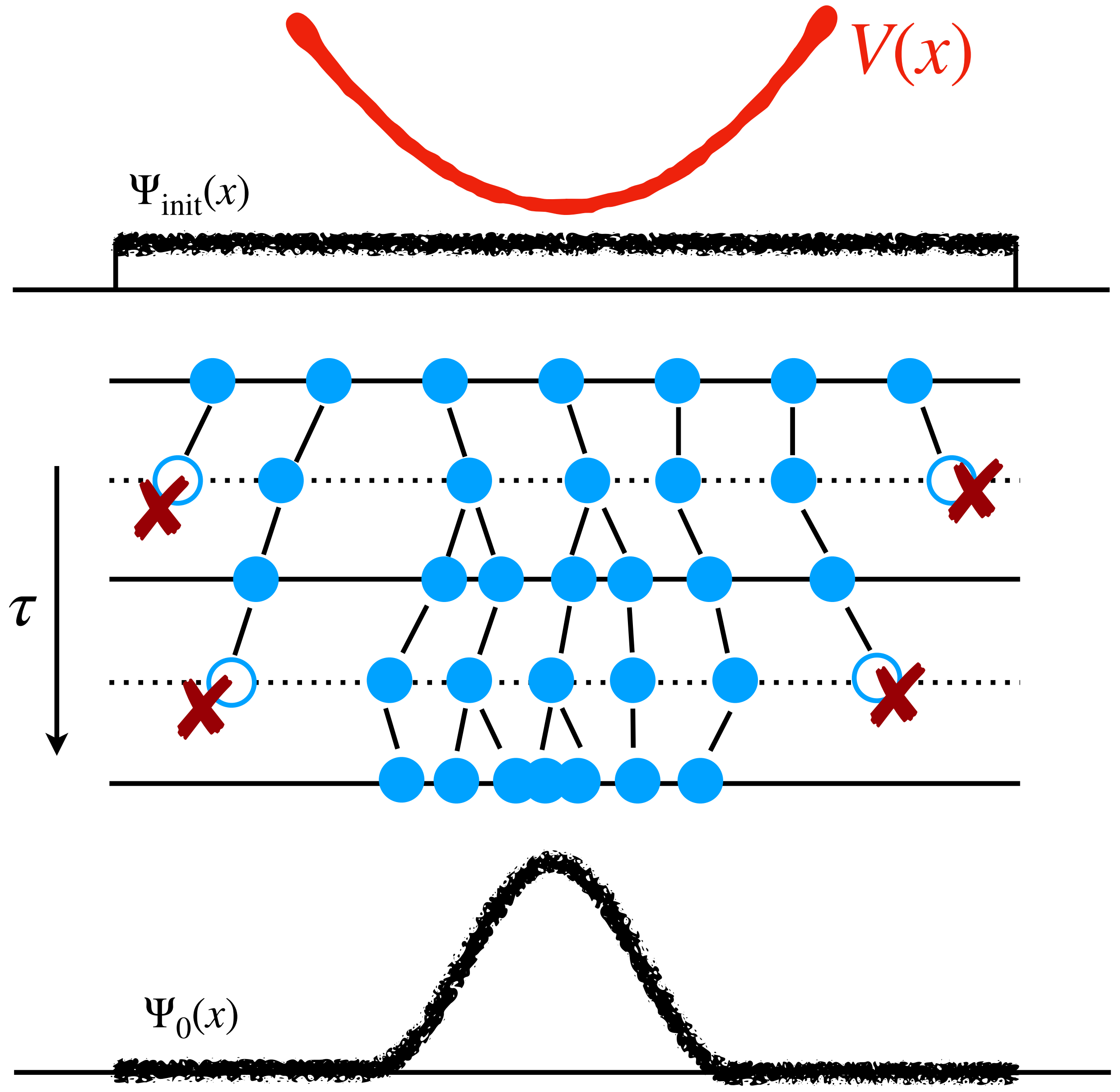
Variational Monte Carlo (VMC)

$$E_0 \leq E[\Psi_T] = \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle}$$



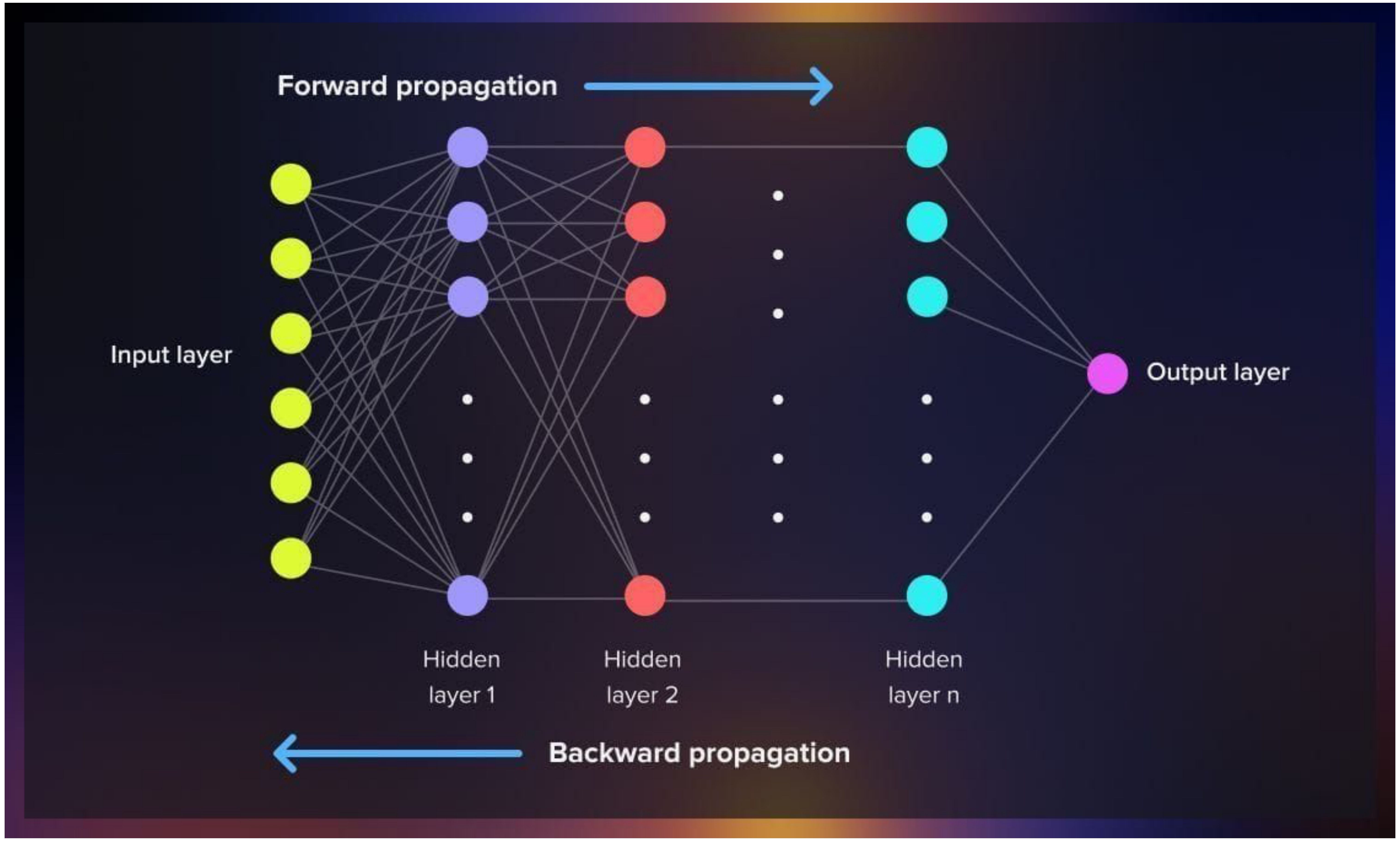
Diffusion Monte Carlo (DMC)

$$|\Psi_0\rangle = \lim_{\tau\to\infty} |\Psi(\tau)\rangle$$



Backpropagation

- ★ To create a training mechanism for neural networks
- ★ A method minimizing the cost function by updating the weights with the gradient descent.
- ★ It's fast, simple, and easy to program



FeynmanNet

$$\Psi(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_A) = \boxed{\Psi^{(\mathrm{R})}}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_A) + \mathrm{i}\boxed{\Psi^{(\mathrm{I})}}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_A)$$

Complexed valued network!

$$\Psi^{(\alpha)}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_A) = \mathrm{e}^{\mathcal{U}^{(\alpha)}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_A)} \sum_n w_n \det \boldsymbol{\Phi}^{(\alpha,n)}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_A), \quad \alpha = \mathrm{R}, \mathrm{I}\,.$$

$$[\boldsymbol{\Phi}^{(\alpha,n)}]_{i\mu} = \mathbf{f}^{(\alpha,n)}_{i\mu}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_A)\varphi_\mu(\boldsymbol{x}_i),$$

Slater 行列式：$\det \phi_{i\mu} = \det \varphi_\mu(\boldsymbol{x}_i)$

- Slater-Jastrow $\det[\varphi_\mu(\boldsymbol{x}_i)] \to \mathrm{e}^{\mathcal{U}(\boldsymbol{x}_1,\ldots,\boldsymbol{x}_A)} \cdot \det[\varphi_\mu(\boldsymbol{x}_i)]$ Jastrow correlator
- Slater-backflow $\det[\varphi_\mu(\boldsymbol{x}_j)] \to \det[f_\mu(\boldsymbol{x}_i; \{\boldsymbol{x}_j, j \neq i\})]$ Backflow correlations Feynman, Cohen, PR 102, 1189 (1956)
- **FeynmanNet**: Multi-determinant Slater-Jastrow-Backflow **+ ANN**

Yang and PWZ, PRC, 107, 034320 (2023)