Nuclear Structure and Dynamics in Relativistic Density Functional Theory

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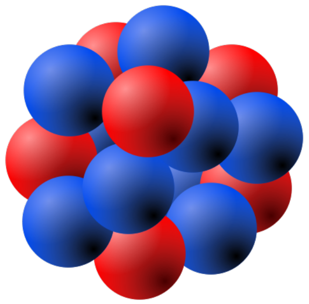
Outline

- Relativistic density functional theory on 3D lattice
- High-order deformation in atomic nuclei
- Time-dependent relativistic DFT for nuclear dynamics
- Towards relativistic *ab initio* calculations
- Summary

Relativistic nuclear many-body problem



Schrödinger Equation

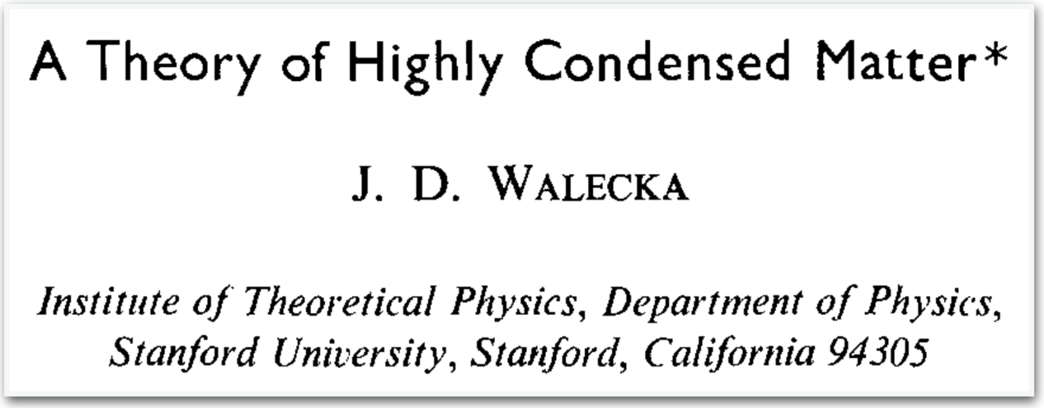
$$H|\psi\rangle = (T+V)|\psi\rangle$$

Relativistic QFT

$$L = L_N + L_\sigma + L_\omega + L_{\text{int}}$$

Walecka, Ann. Phys., 83, 491 (1974)

Mean-field approximation


A Theory of Highly Condensed Matter*

J. D. WALECKA

Institute of Theoretical Physics, Department of Physics, Stanford University, Stanford, California 94305

1. Mean-field approximation works surprisingly good !
2. Large mean fields *S ≈ -400 MeV, V ≈ 350 MeV*
3. Large spin-orbit splitting *predicts nuclear shell model, no adjustments to spin-orbit force*
4. Relativistic saturation *non-relativistic calculations lead to a collapse*

A covariant formulation provides an <u>efficient and comprehensive</u> explanation of observed bulk and single-particle systematics.

Density functional theory

The many-body problem is mapped onto a one-body problem

Hohenberg-Kohn Theorem

The exact ground-state energy of a quantum mechanical many-body system is a universal functional of the local density.

$$E[\rho] = T[\rho] + U[\rho] + \int V(\mathbf{r})\rho(\mathbf{r})\, d^3\mathbf{r}$$

Kohn-Sham DFT

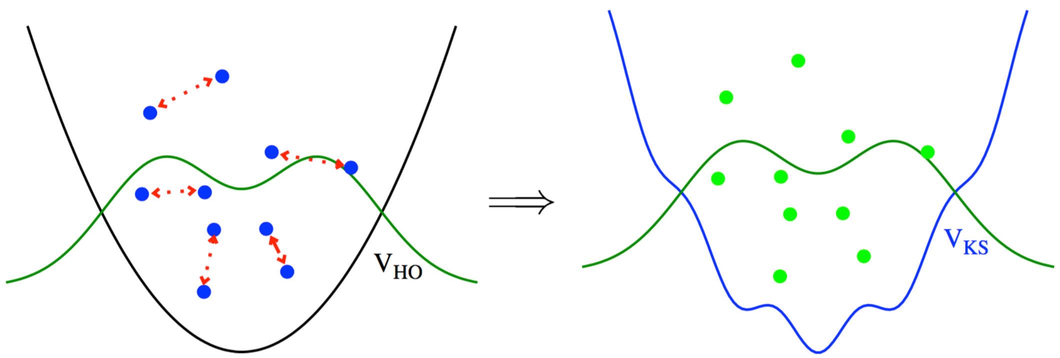


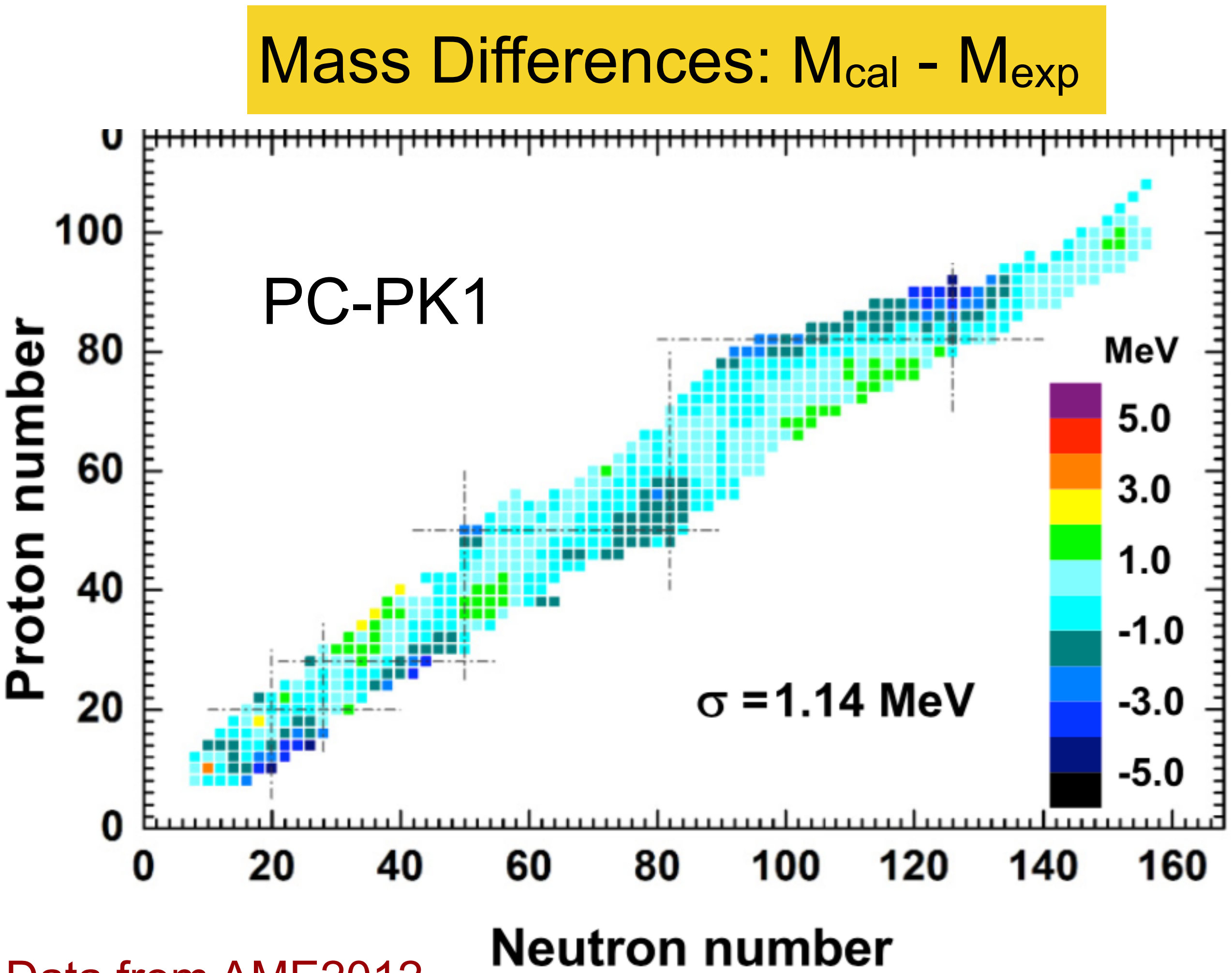
Figure from Drut PPNP 2010

$$T[\rho] \doteq \sum_{i=1}^{N} \left\langle \varphi_i \left| -\frac{\hbar^2}{2m}\nabla^2 \right| \varphi_i \right\rangle$$

$$E[\rho] \Rightarrow \boxed{\hat{h} = \frac{\delta E}{\delta \rho}} \Rightarrow \boxed{\hat{h}\varphi_i = \varepsilon_i \varphi_i} \Rightarrow \boxed{\rho = \sum_{i=1}^{A} |\varphi_i|^2}$$

The practical usefulness of the Kohn-Sham theory depends entirely on whether an **Accurate Energy Density Functional** can be found!

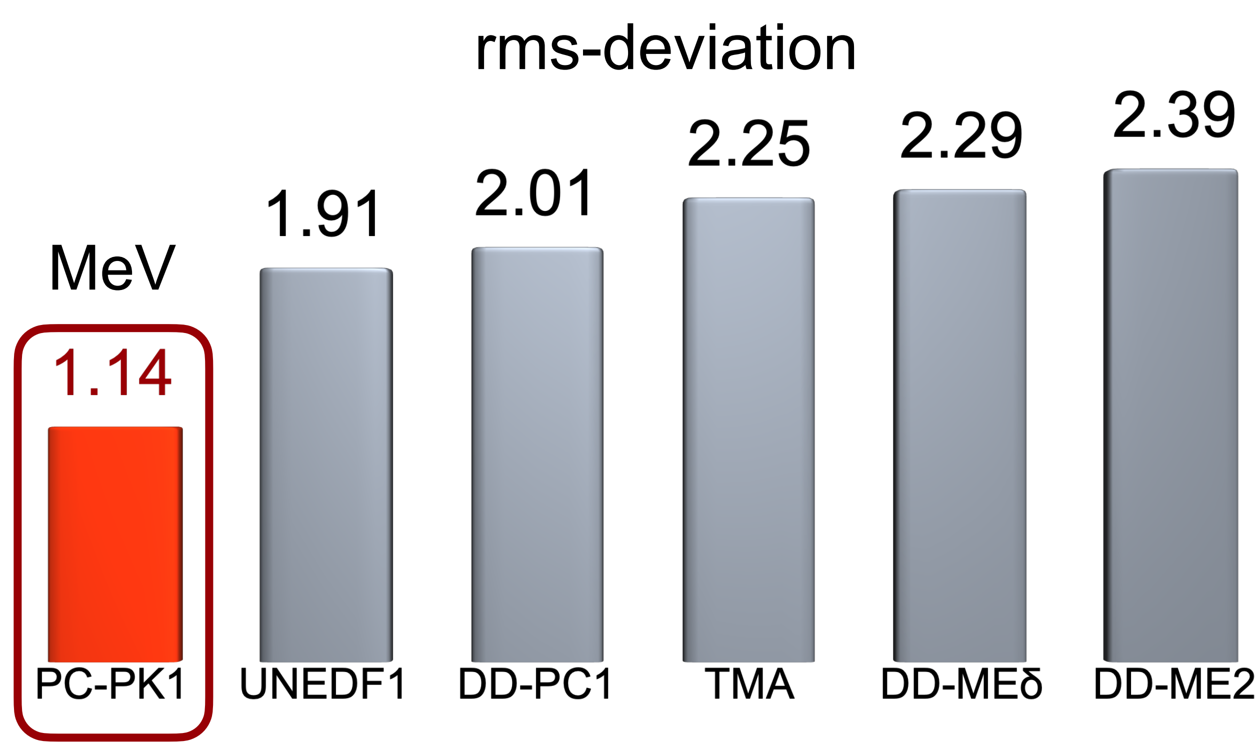
Covariant density functional： PC-PK1



Data from AME2012

PWZ, Li, Yao, Meng, PRC 82, 054319 (2010)

Lu, Li, Li, Yao, Meng, PRC 91, 027304 (2015)



http://nuclearmap.jcnp.org

Yang, Wang, PWZ, Li, PRC 104, 054312 (2021)

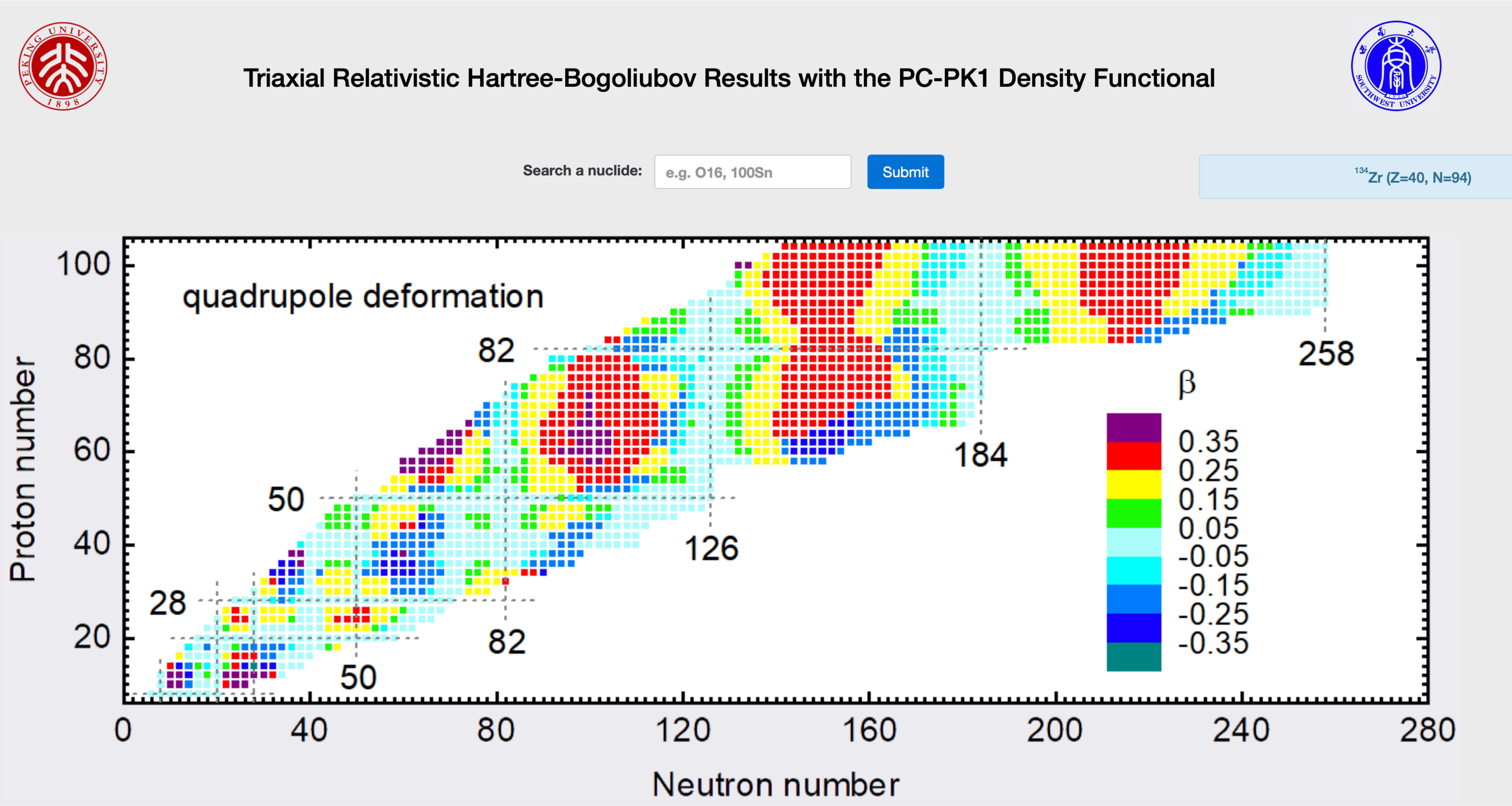
Yang, PWZ, Li, PRC 107, 024308 (2023)

Among the best density-functional description for nuclear masses!

How many nuclei are bound?

http://nuclearmap.jcnp.org/index.html

Triaxial RHB + 5DCH



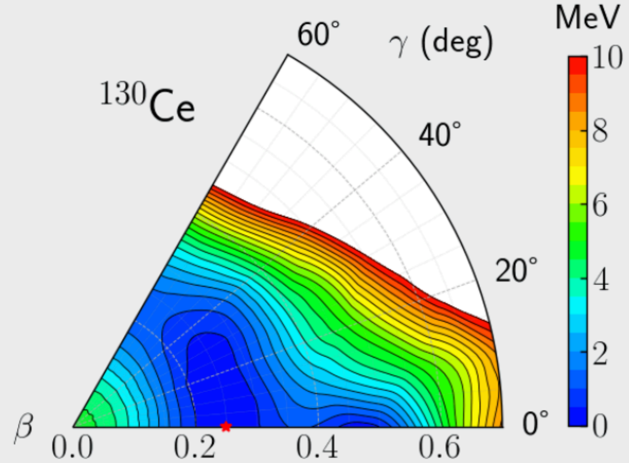
Yang, Wang, PWZ, Li, Phys. Rev. C 104, 054312 (2021)
Yang, PWZ, Li, Phys. Rev. C 107, 024308 (2023)

How many nuclei are bound?

http://nuclearmap.jcnp.org/index.html

Triaxial RHB + 5DCH

Results for Cerium 130 (Z=58, N=72)



Potential energy surface calculated by RHB theory with PC-PK1 density functional. All energies are normalized with respect to the binding energy of the absolute minimum. The contours join points on the surface with the same energy, and the energy difference between adjacent contours is 0.5 MeV.

Ground-state properties

Spectroscopy (coming soon)

E_{RHB} = -1079.46 MeV

E_{5DCH} = -1083.50 MeV

E_{exp} = -1083.32 MeV

β = 0.25

γ = 0°

To know the meaning of a quantity, please hold the mouse still on it.

Select a nuclide

Proton number

0

Neutron number

0

Submit

^{132}Nd

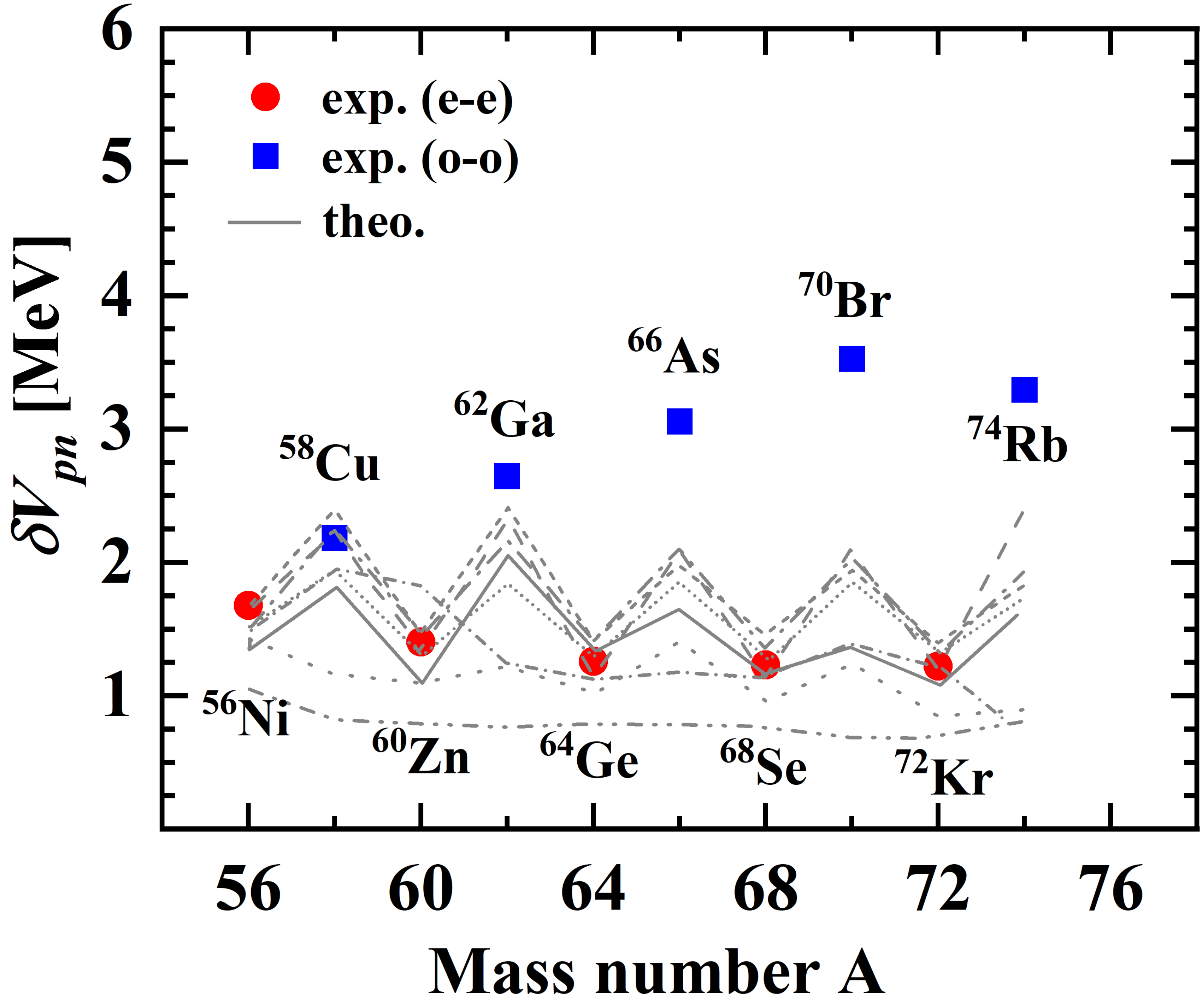
^{128}Ce ← → ^{132}Ce

^{128}Ba

Yang, Wang, PWZ, Li, Phys. Rev. C 104, 054312 (2021)
Yang, PWZ, Li, Phys. Rev. C 107, 024308 (2023)

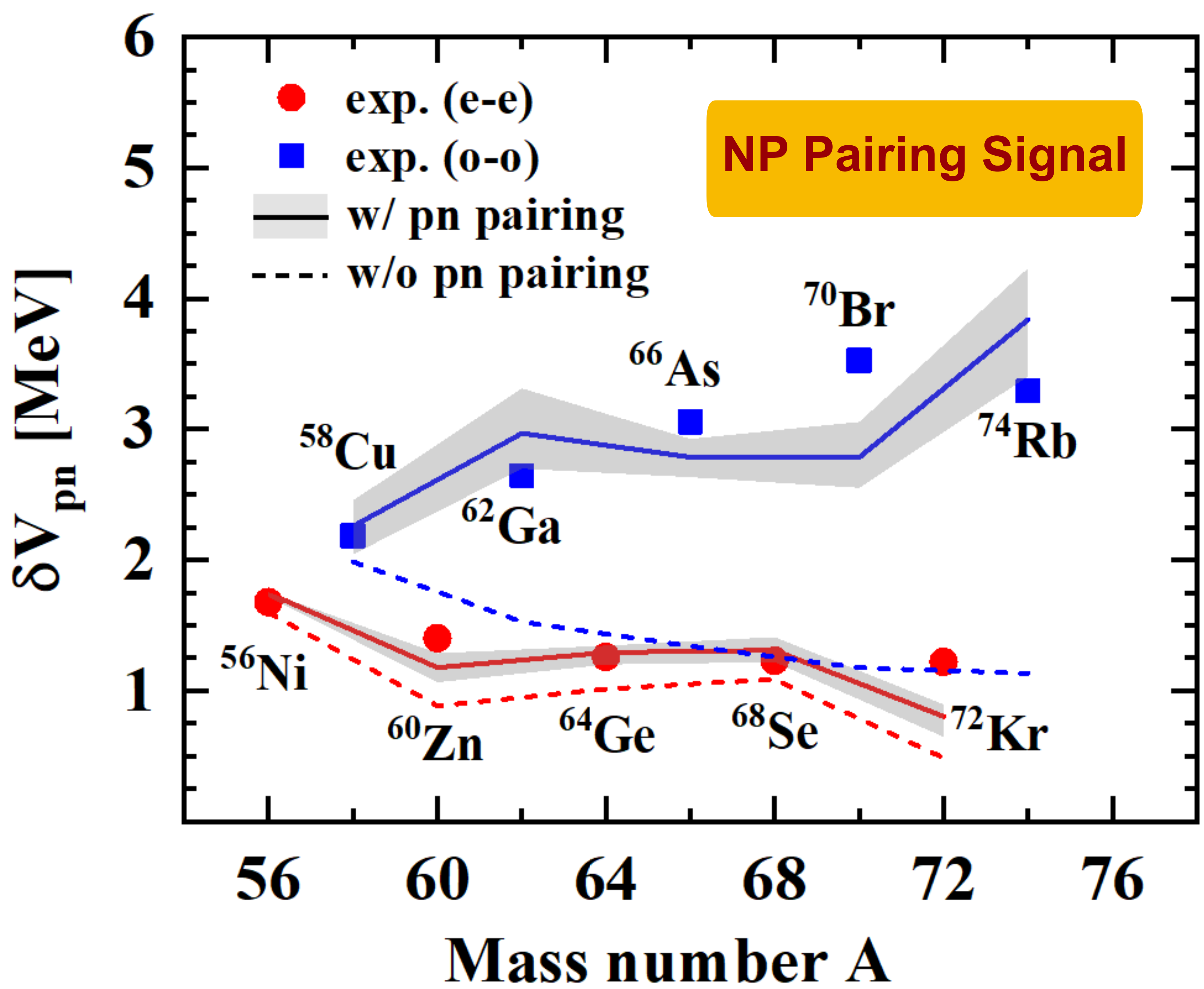
New mass measurement of upper fp-shell nuclei

This bifurcation in the double binding energy differences δV_{pn} cannot be reproduced by existing mass models.



Exp: M. Wang et al., PRL 130, 192501 (2023)

New mass measurement of upper fp-shell nuclei

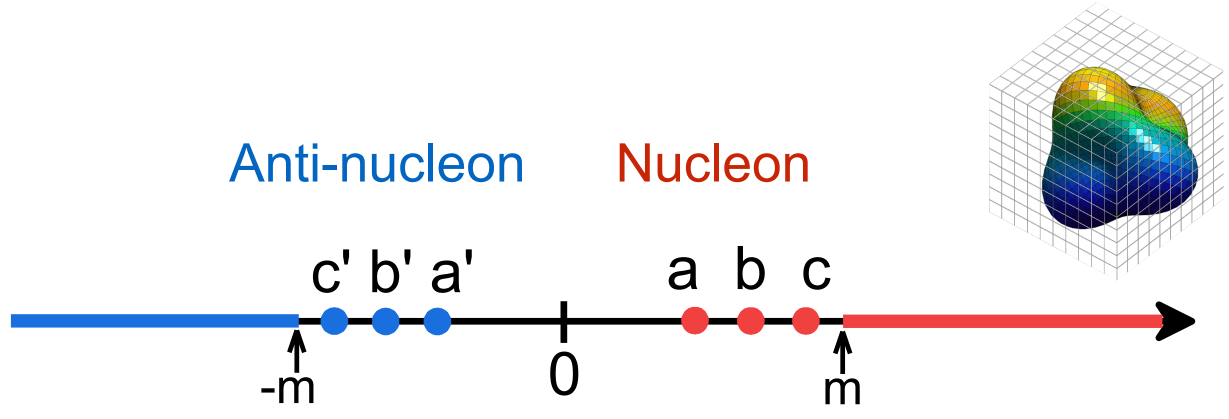


Exp: M. Wang et al., PRL 130, 192501 (2023)

Wang, Wang, Xu, **PWZ**, Meng, PRL 132, 232501 (2024)

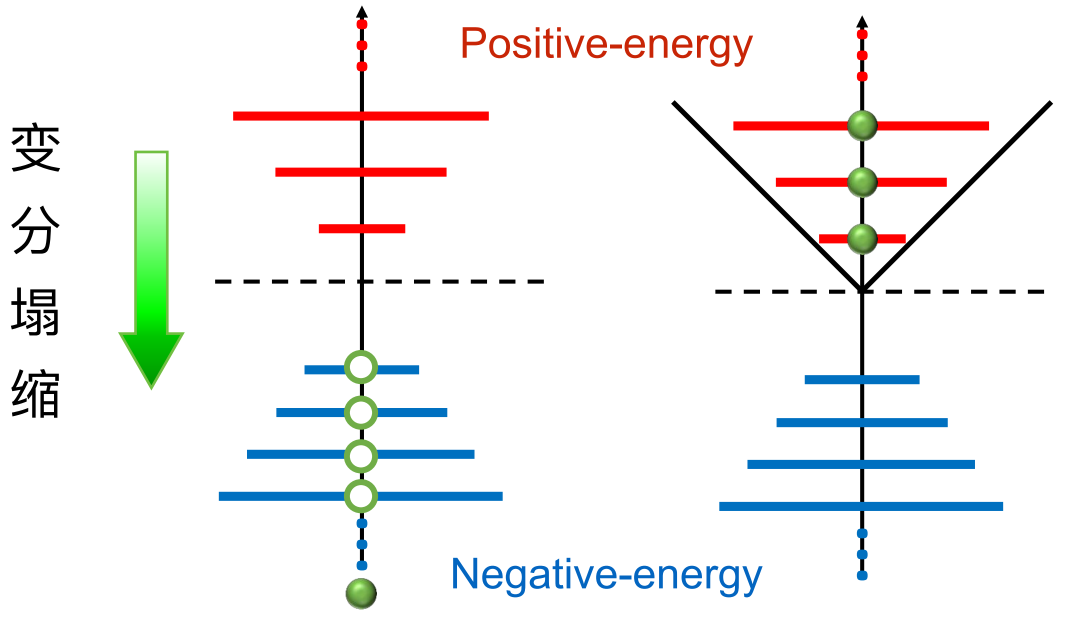
Lattice RDFT

- ✓ No spatial symmetry restriction
- ✓ A long-term challenge due to
  - a) variational collapse problem
  - b) fermion doubling problem



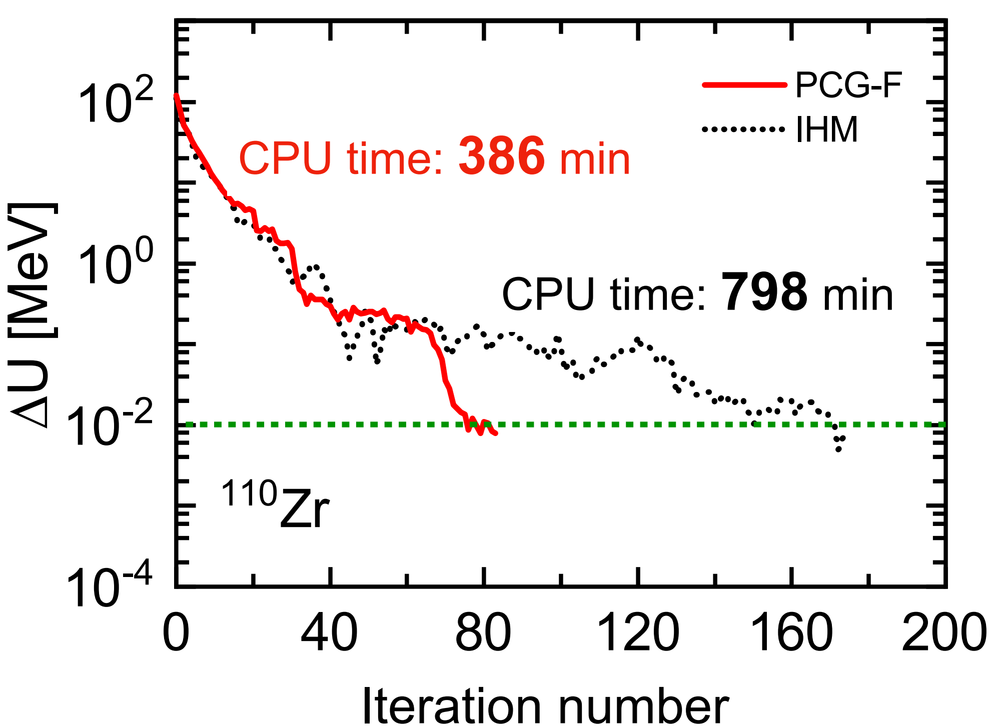
Hagino and Tanimura, PRC 82, 057301 (2010)

PCG-F Method



Li, Ren, **PWZ**, PRC 102, 044307 (2020)

PCG-F saves **~52%** of the CPU time



Xu, Li, Ren, **PWZ**, PRC 109, 014311 (2024)

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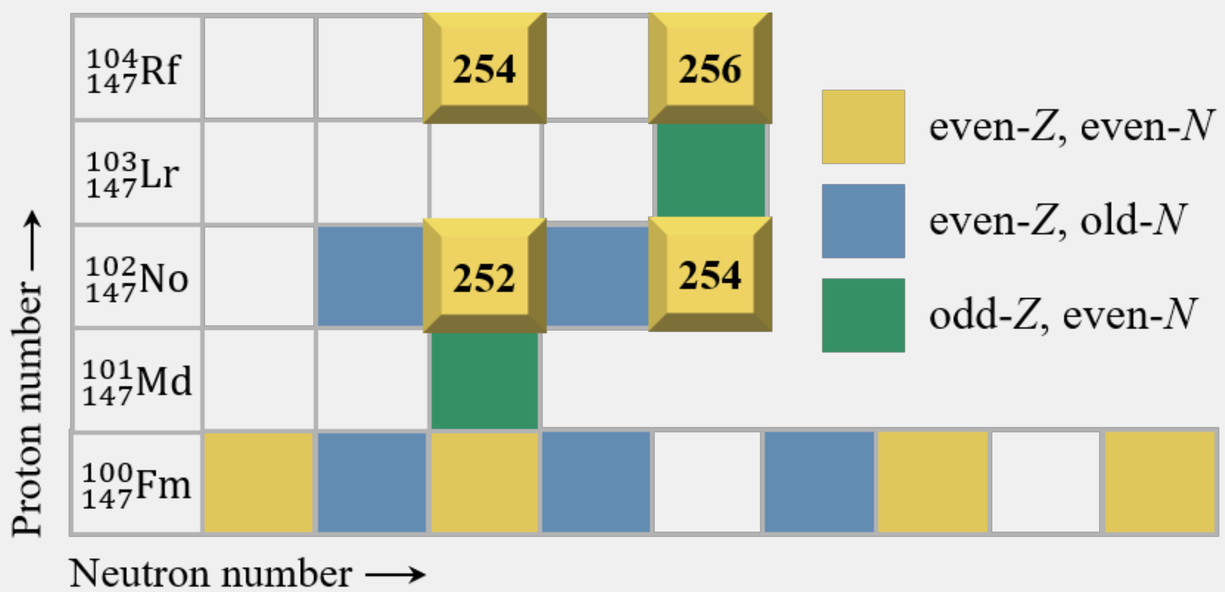
Transfermium nuclei

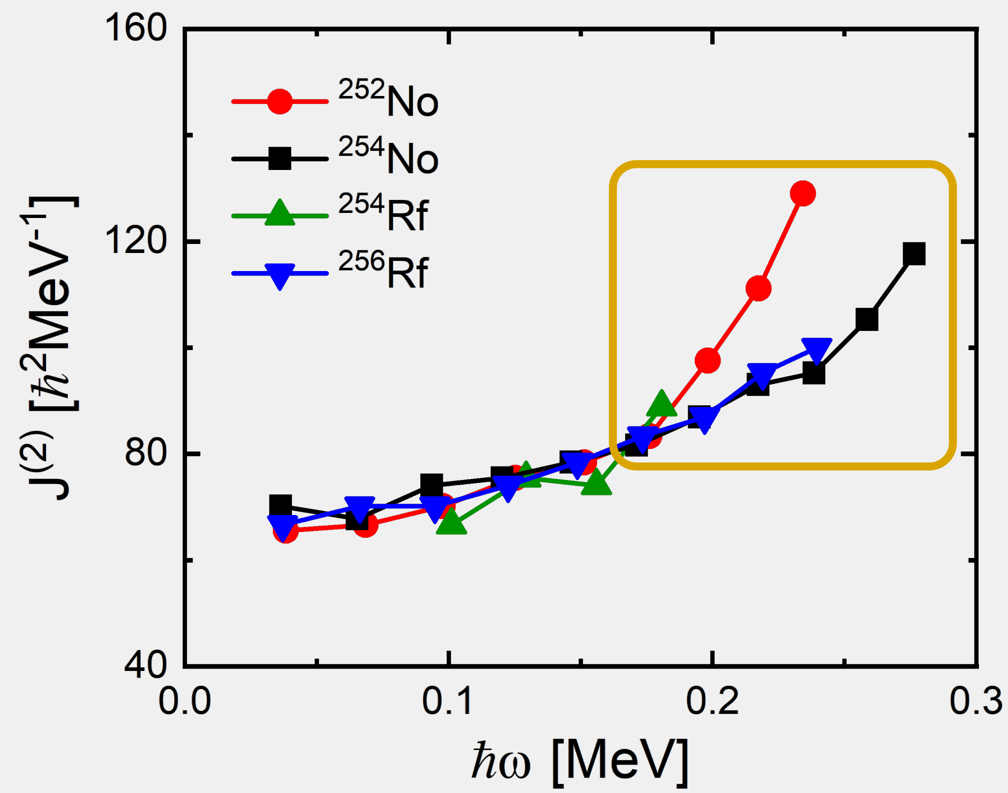
- **Transfermium nuclei** are the heaviest ones, whose rotational spectra have been measured experimentally; important for the location of the **"island of stability"**.

Herzberg, Greenlees, Prog. Part. Nucl. Phys. 61, 674 (2008); Ackermann, Theisen, Phys. Scr. 92, 083002 (2017)

ANL、FLNR、GANIL、GSI、JAEA、JYFL ...



PRL 82, 509 (1999) PRL 85, 1198 (2000) PRL 89, 202501 (2002)
PRL 95, 102502 (2005) PRL 95, 032501 (2005)
PRL 97, 082502 (2006) PRL 98, 132503 (2007)
PRL 102, 212501 (2009) PRL 109, 102501 (2012)
…



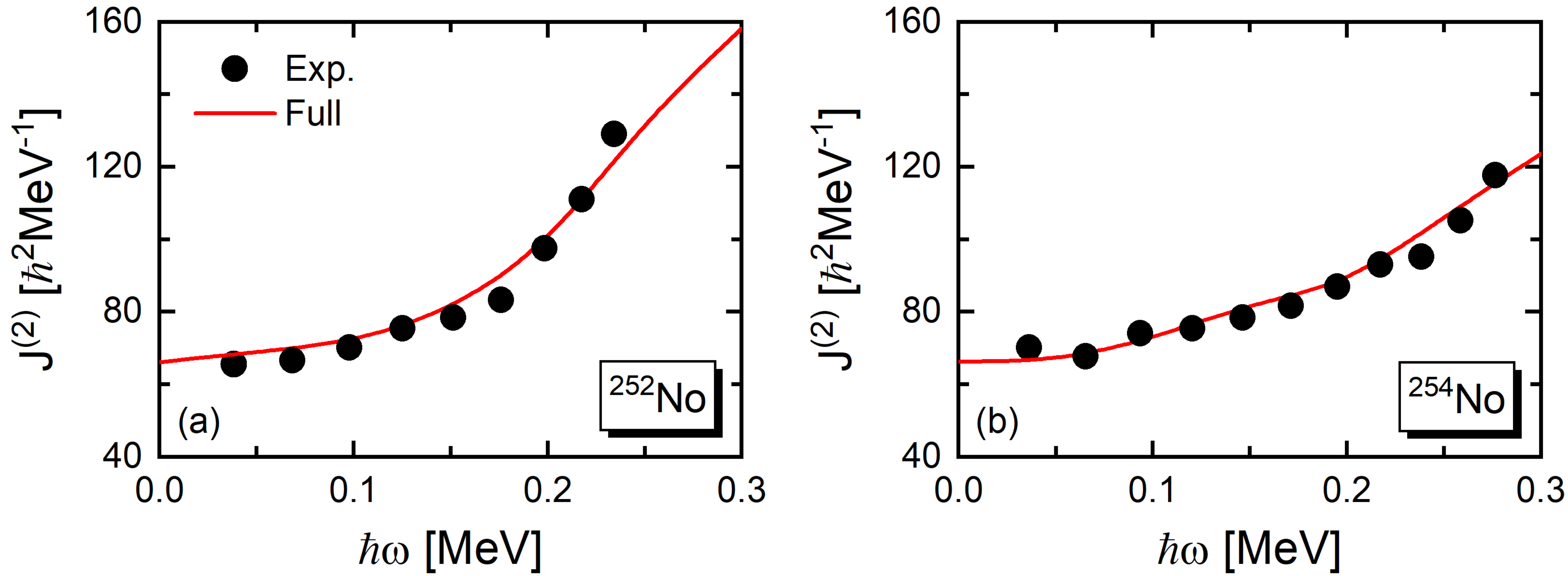
PRL 82, 509 (1999) PRL 109, 102501 (2012)
PRC 65, 014303 (2001) PRC 107, L061302 (2023)

The physical mechanism of the abnormal behavior in ^{252}No and ^{254}No?

Dynamic moments of inertia

Cranking CDFT in 3D lattice with a shell-model-like approach (SLAP):

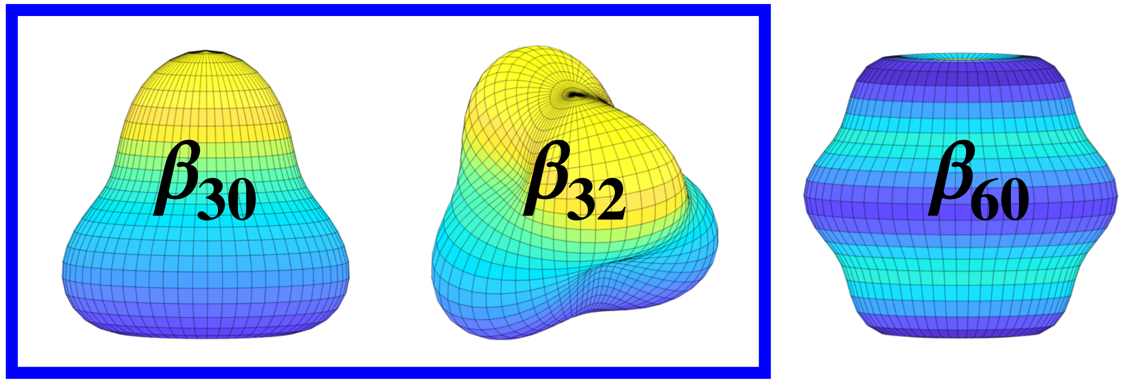
- ✓ self-consistent and microscopic description
- ✓ no adjustable parameter beyond a well-determined functional
- ✓ no spatial symmetry restriction
- ✓ pairing correlations is treated with particle number conservation

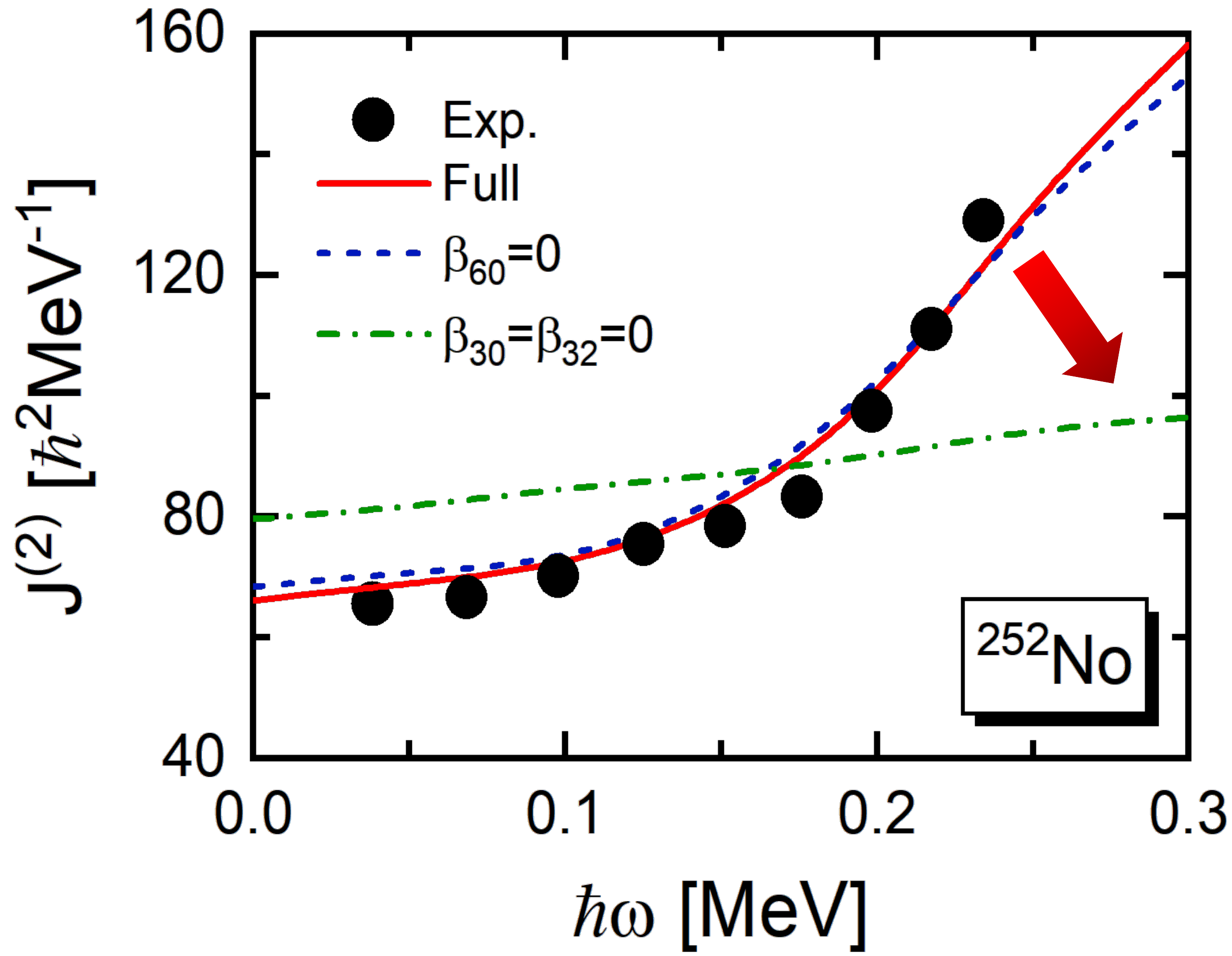


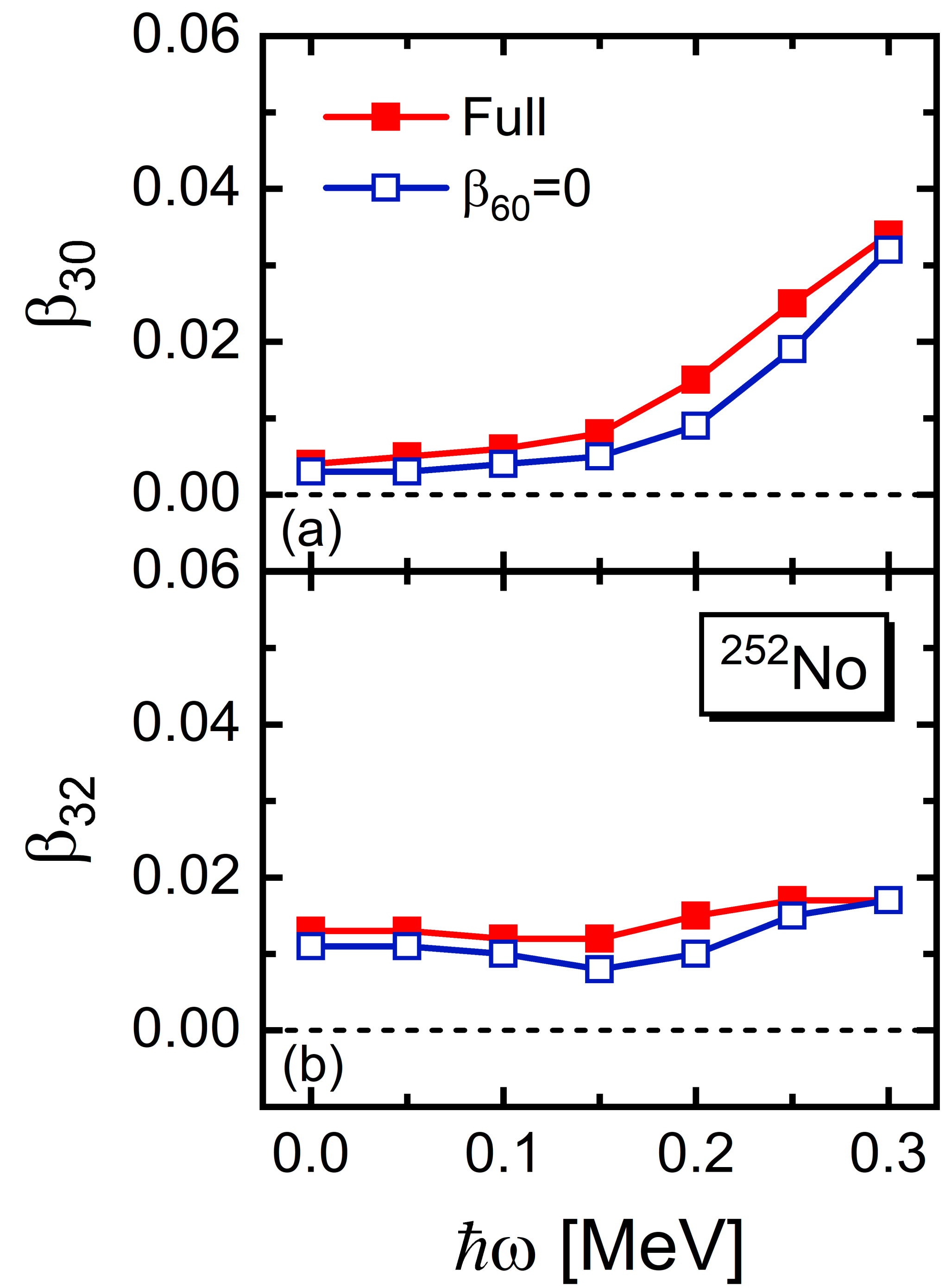
Xu, Wang, Wang, Ring, **PWZ**, PRL 133, 022501 (2024)

The experimental moments of inertia are well reproduced.

High-order deformation in ^{252}No



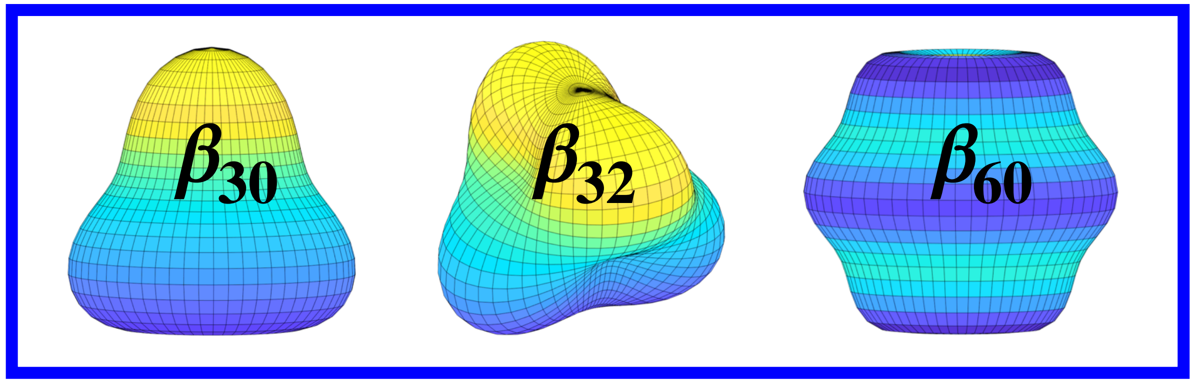


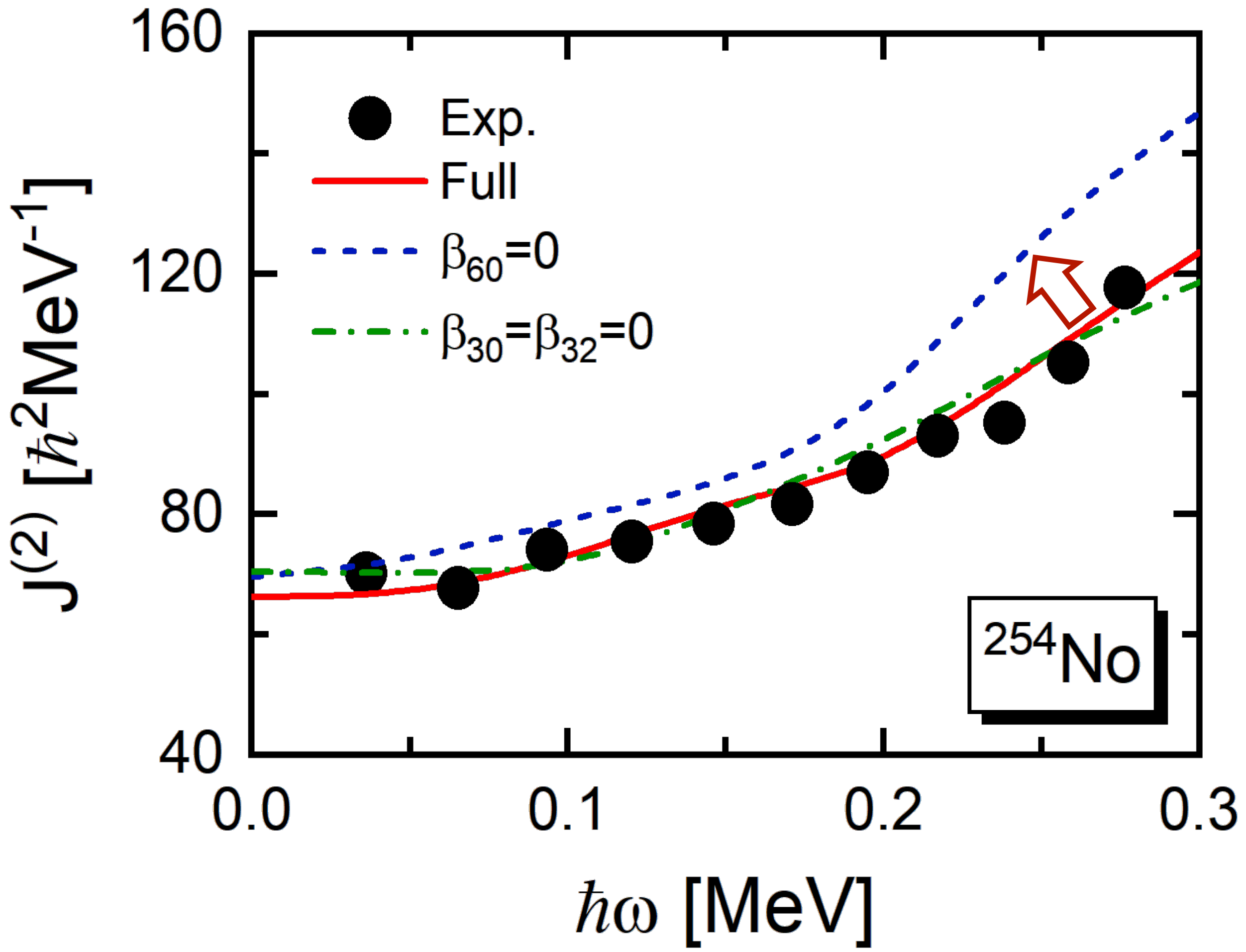


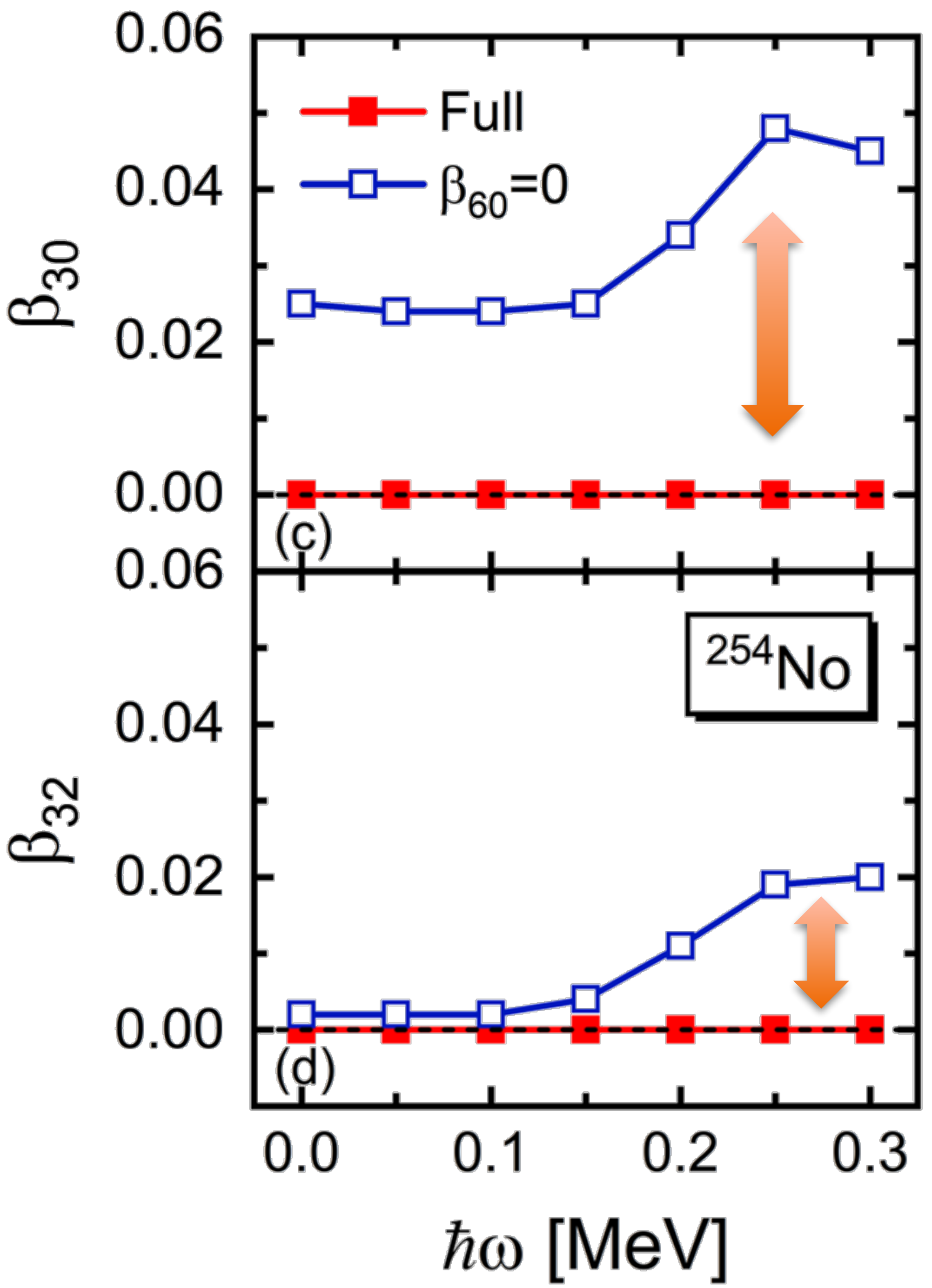
Xu, Wang, Wang, Ring, **PWZ**, PRL 133, 022501 (2024)

Octupole deformation is responsible for the upbending in ^{252}No.

High-order deformation in ^{254}No







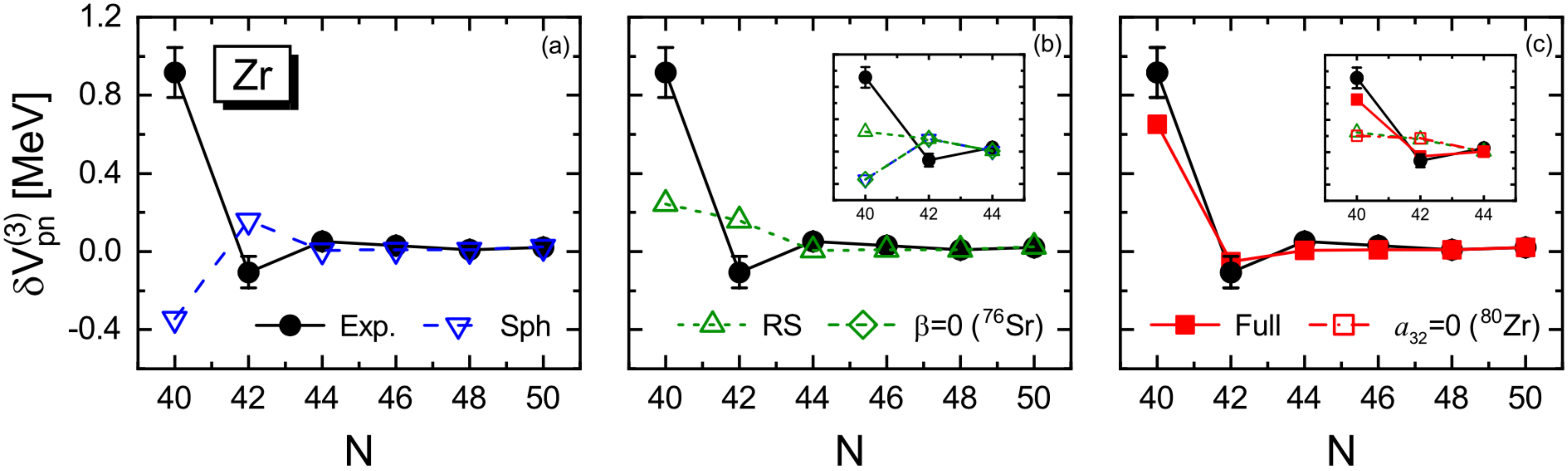
Xu, Wang, Wang, Ring, **PWZ**, PRL 133, 022501 (2024)

Octupole and β_{60} deformations are coupled with each other in ^{254}No.

Mass Probe of Tetrahedral Symmetry in ^{80}Zr

$$\delta V_{pn}(Z,N) = -\frac{1}{4}\left[E(Z,N) - E(Z,N-2) - E(Z-2,N) + E(Z-2,N-2)\right]$$

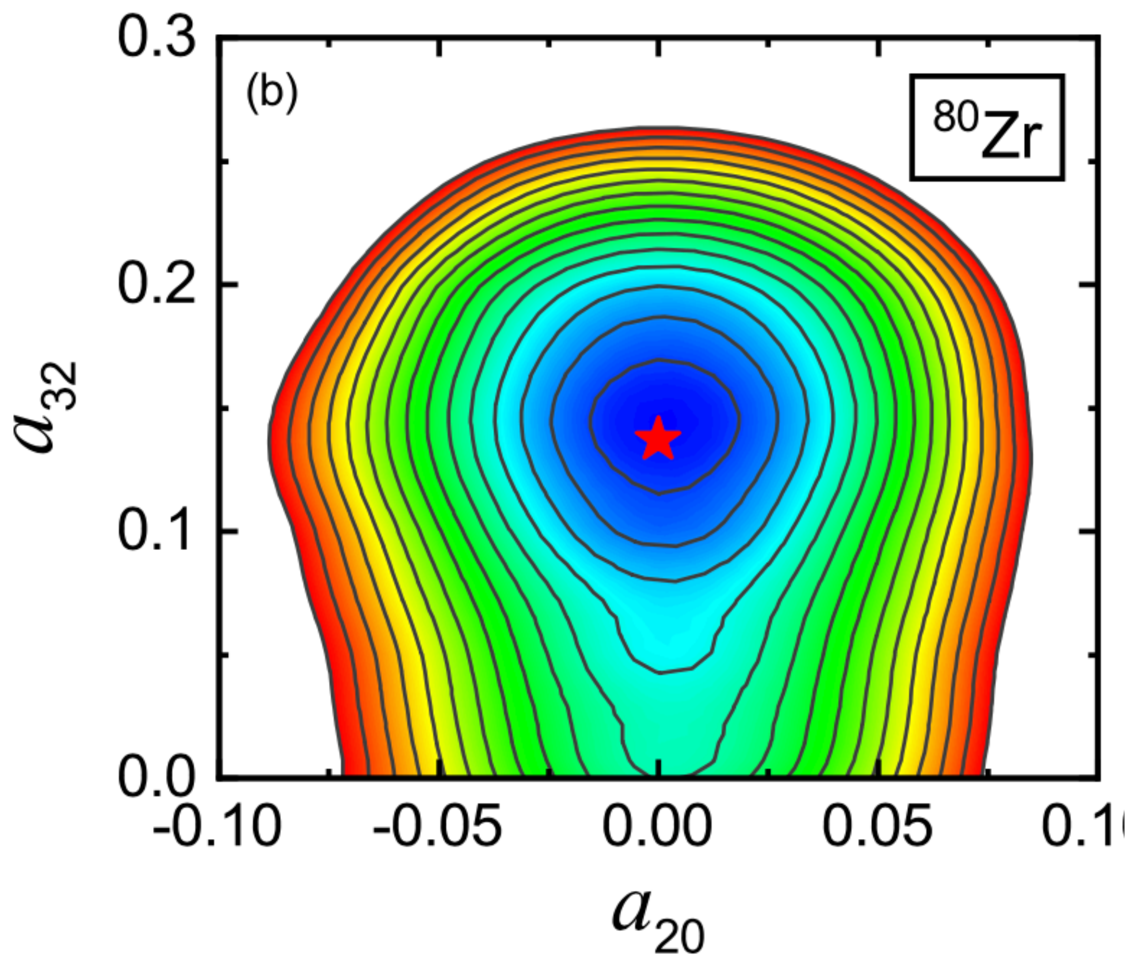
$$\delta V^{(3)}_{pn}(Z,N) = \delta V_{pn}(Z,N) - \delta V_{pn}(Z,N+2)$$

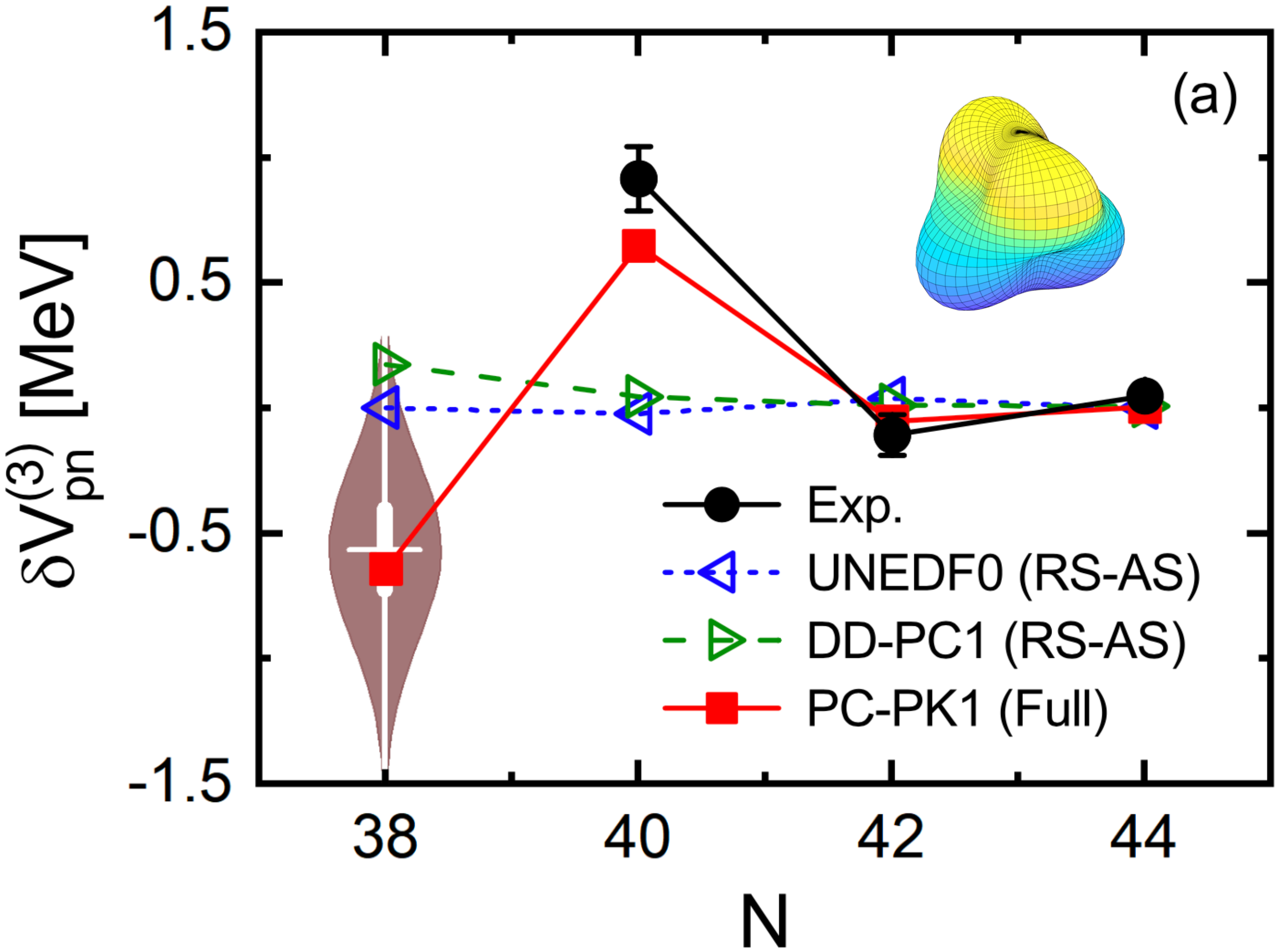


Xu and PWZ , submitted

Tetrahedral deformation of ^{80}Zr is revealed from nuclear masses.

Tetrahedral deformation of Zr-80





Xu and PWZ , submitted

Independent with the adopted density functional.

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Time-dependent RDFT

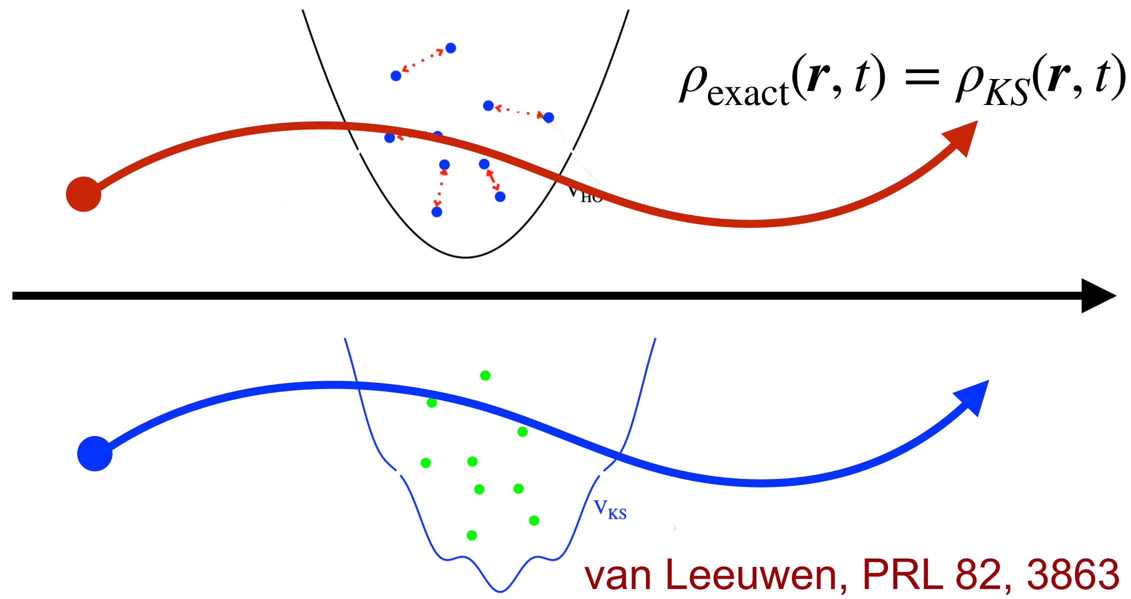
The many-body problem is mapped onto a one-body problem!

Runge-Gross Theorem

There is a unique mapping between the time dependent external potential and the density, for many body systems evolving from a given initial state.

Runge and Gross, PRL 52, 997 (1984)

Time-dependent Kohn-Sham DFT



van Leeuwen, PRL 82, 3863 (1999)

Ren, **PWZ**, Meng, PLB 801,135194 (2020)

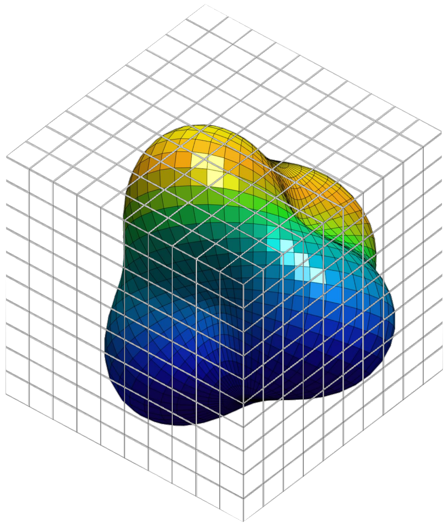
$$i\partial_t \begin{pmatrix} f \\ g \end{pmatrix} = \begin{pmatrix} m + V + S & \boldsymbol{\sigma}\cdot\boldsymbol{p} - \boldsymbol{\sigma}\cdot\boldsymbol{V} \\ \boldsymbol{\sigma}\cdot\boldsymbol{p} - \boldsymbol{\sigma}\cdot\boldsymbol{V} & -m + V - S \end{pmatrix} \begin{pmatrix} f \\ g \end{pmatrix}$$

$$\rho(\boldsymbol{r},t) = \sum_i^N f_i^2 + g_i^2$$

$$V[\rho](\boldsymbol{r},t)$$

No memory effects !

Applications of the TD-RDFT



3D Lattice: no spatial symmetry restriction

✓ Applications include:

- Linear alpha-chain — PRL 115, 022501 (2015) PLB 801,135194 (2020)
- Nuclear fission — PRL 128, 172501 (2022) PRC 111, L051302 (2025)
- Chiral dynamics — PRC 105, L011301 (2022) PLB 856, 138877 (2024)
- Nuclear reaction — PRC 102, 044603 (2020) PRC 109, 024614 (2024) PRC 109, 024316 (2024) Editors' Suggestion

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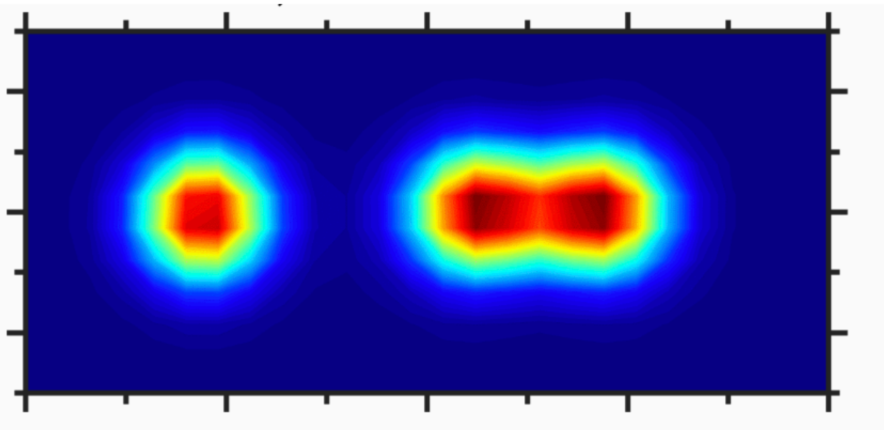
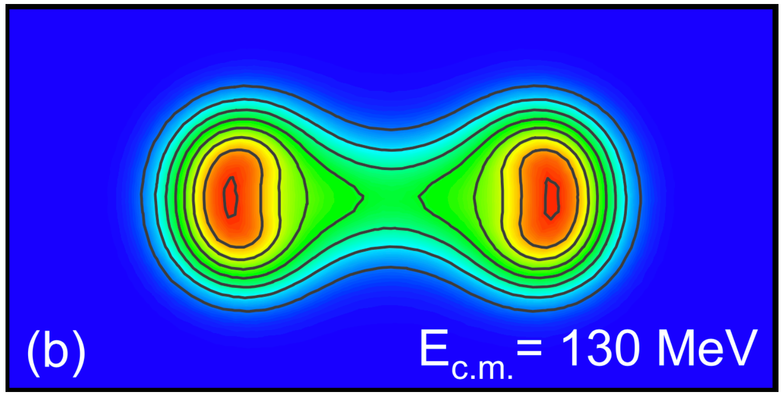
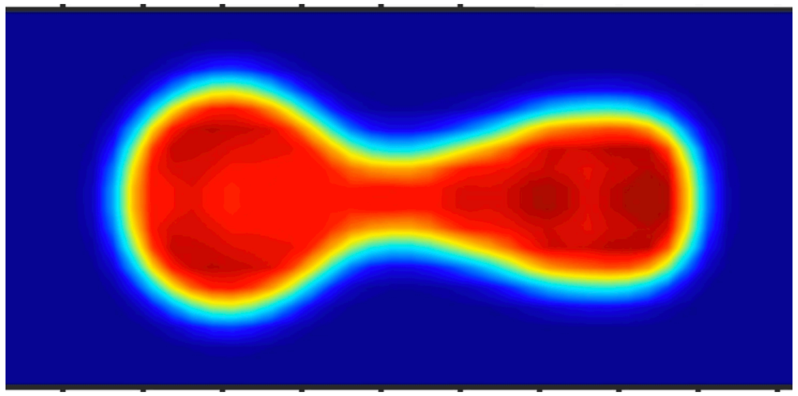




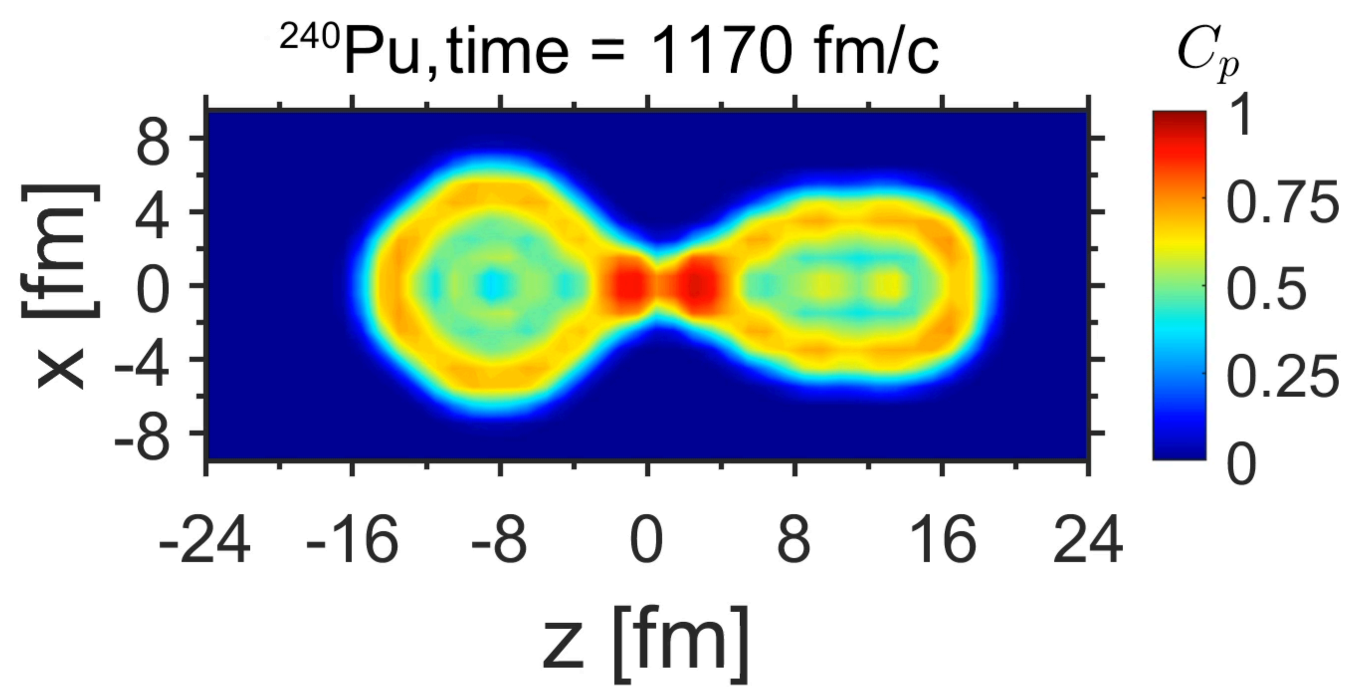


Nuclear fission dynamics

How do heavy nuclei split into two or more fragments?

Scission Mechanism :

- Geometrical definitions
- Nuclear forces / Coul. forces
- Statistical scission-point model
- Random neck rupture model
- Quantum localization method
- …



Ren, Vretenar, Nikšić, **PWZ**, Zhao, Meng
PRL 128, 172501 (2022)

New mechanism: *neck ruptures between two alpha-like clusters.*
Opens exciting possibilities for a microscopic study of ternary fission.

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Scission Mechanism :

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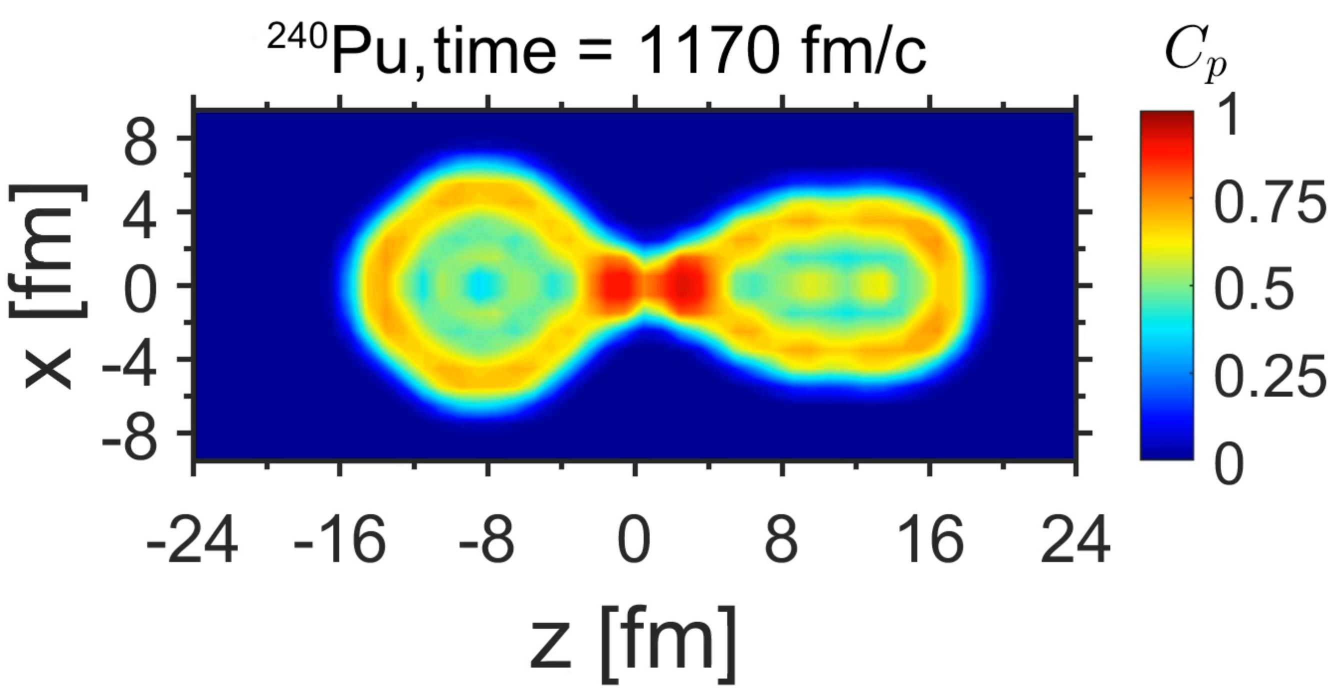
- … n localization method
- …

Ternary fission NOT explained !



Ren, Vretenar, Nikšić, **PWZ**, Zhao, Meng
PRL 128, 172501 (2022)

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Opens exciting possibilities for a microscopic study of ternary fission.

Collision of two ^{238}U nuclei

PRL **103**, 042701 (2009) PHYSICAL REVIEW LETTERS week ending 24 JULY 2009

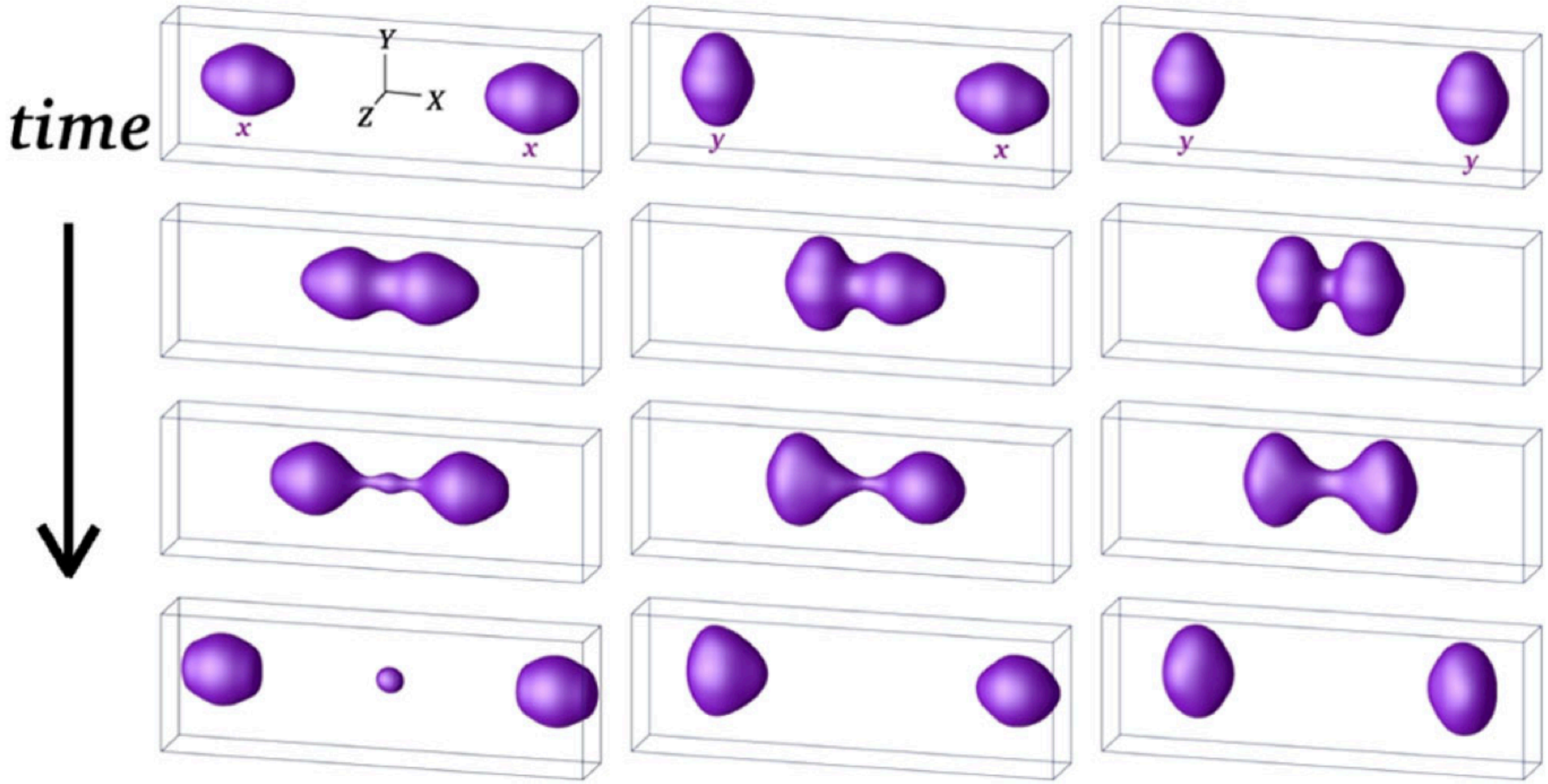
Collision Dynamics of Two ^{238}U Atomic Nuclei

Cédric Golabek
GANIL (IN2P3/CNRS - DSM/CEA), BP 55027, F-14076 Caen Cedex 5, France

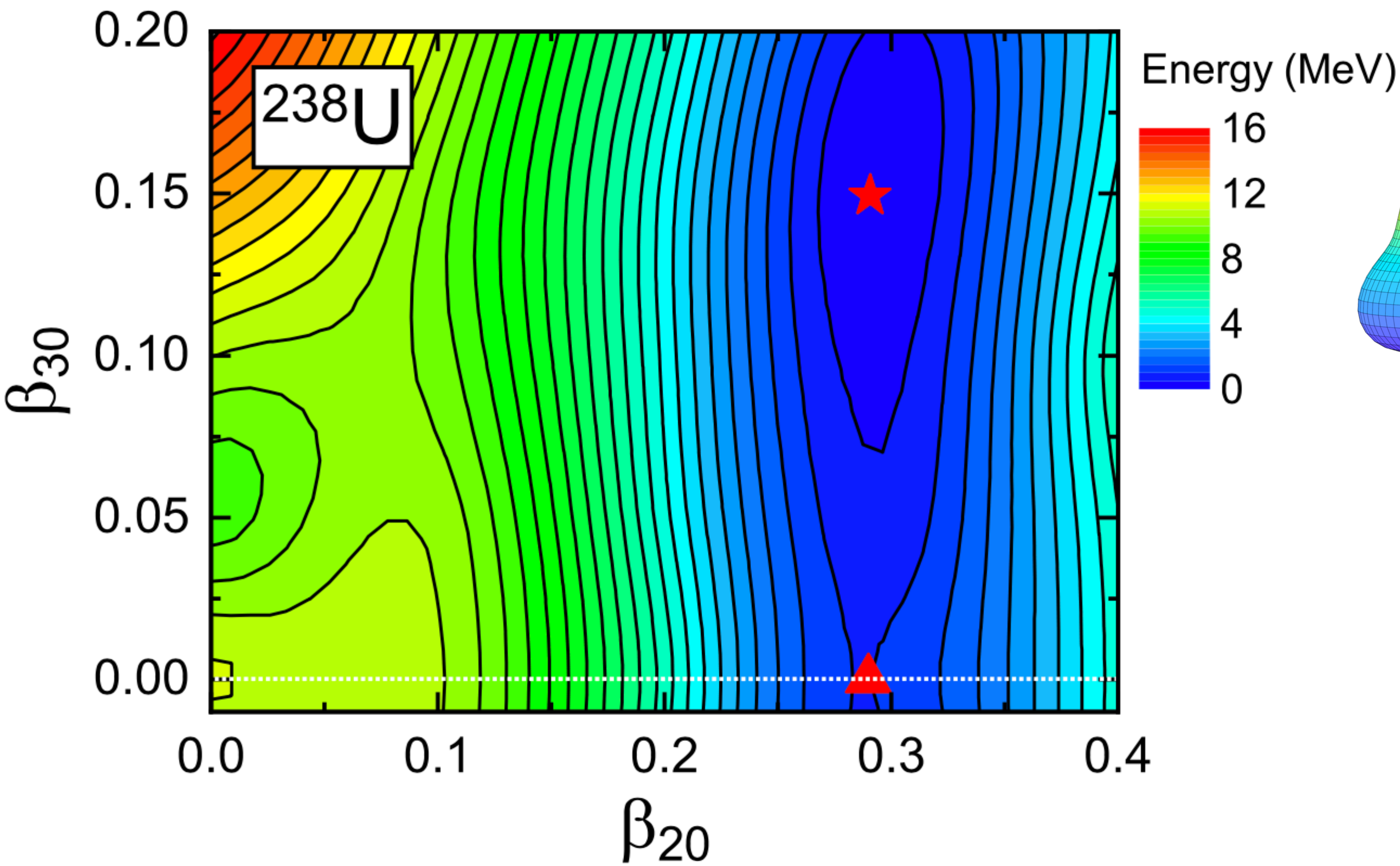
Cédric Simenel
CEA, Centre de Saclay, IRFU/Service de Physique Nucléaire, F-91191 Gif-sur-Yvette, France

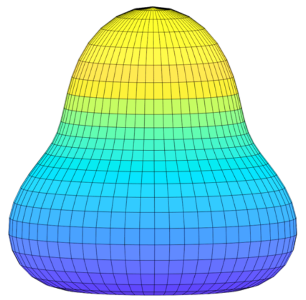
(Received 20 April 2009; revised manuscript received 19 May 2009; published 24 July 2009)

*“Surprisingly, we also observe **ternary fission** due to purely dynamical effects.”*



Octupole deformation of ^{238}U

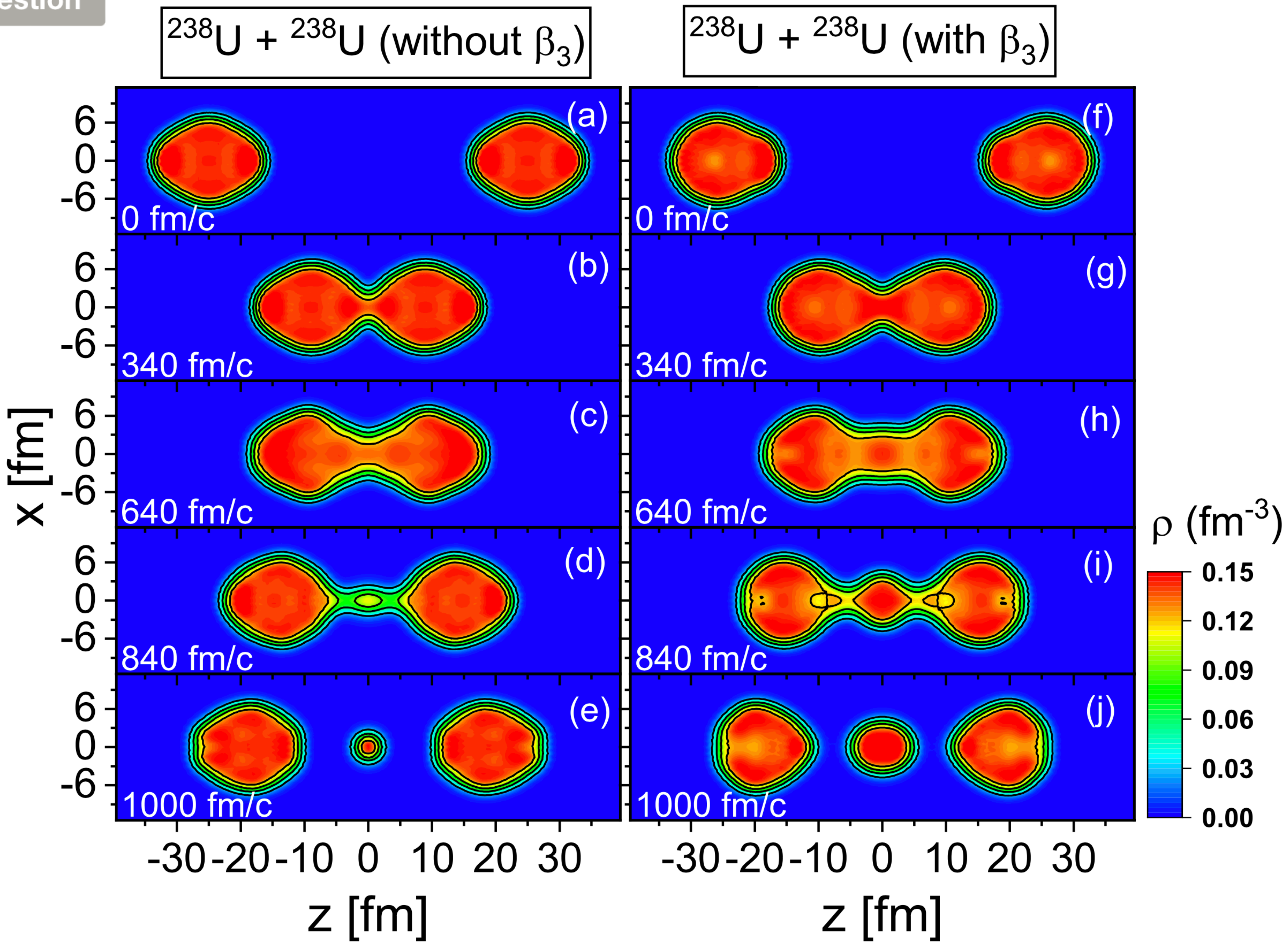




Zhang, Li, Vretenar, Nikšić , Ren, **PWZ**, Meng, PRC, 109, 024316 (2024)

Octupole effects

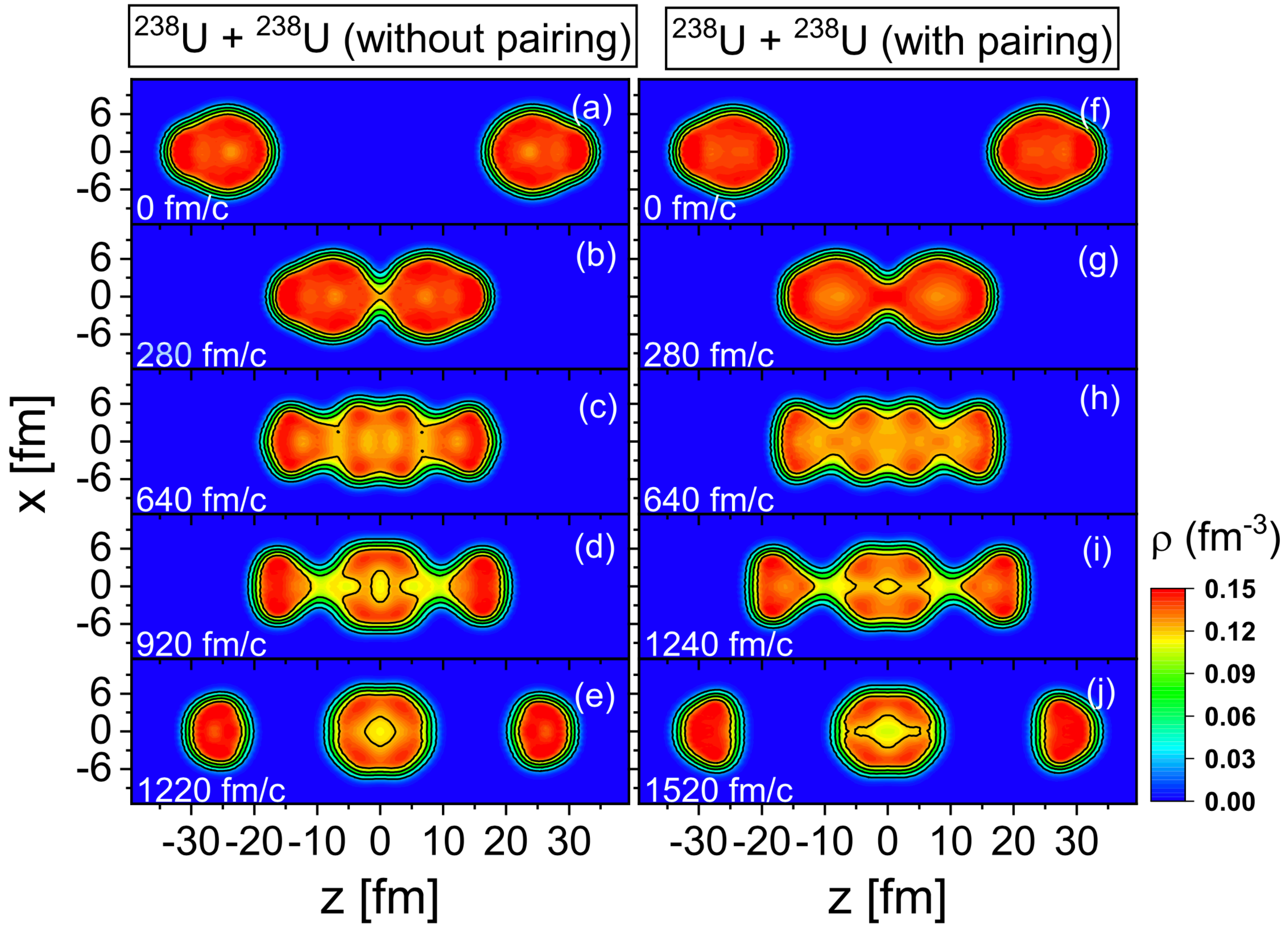
Editors' Suggestion



Zhang, Li, Vretenar, Nikšić , Ren, **PWZ**, Meng, PRC, 109, 024316 (2024)

Ternary quasifission

Editors' Suggestion

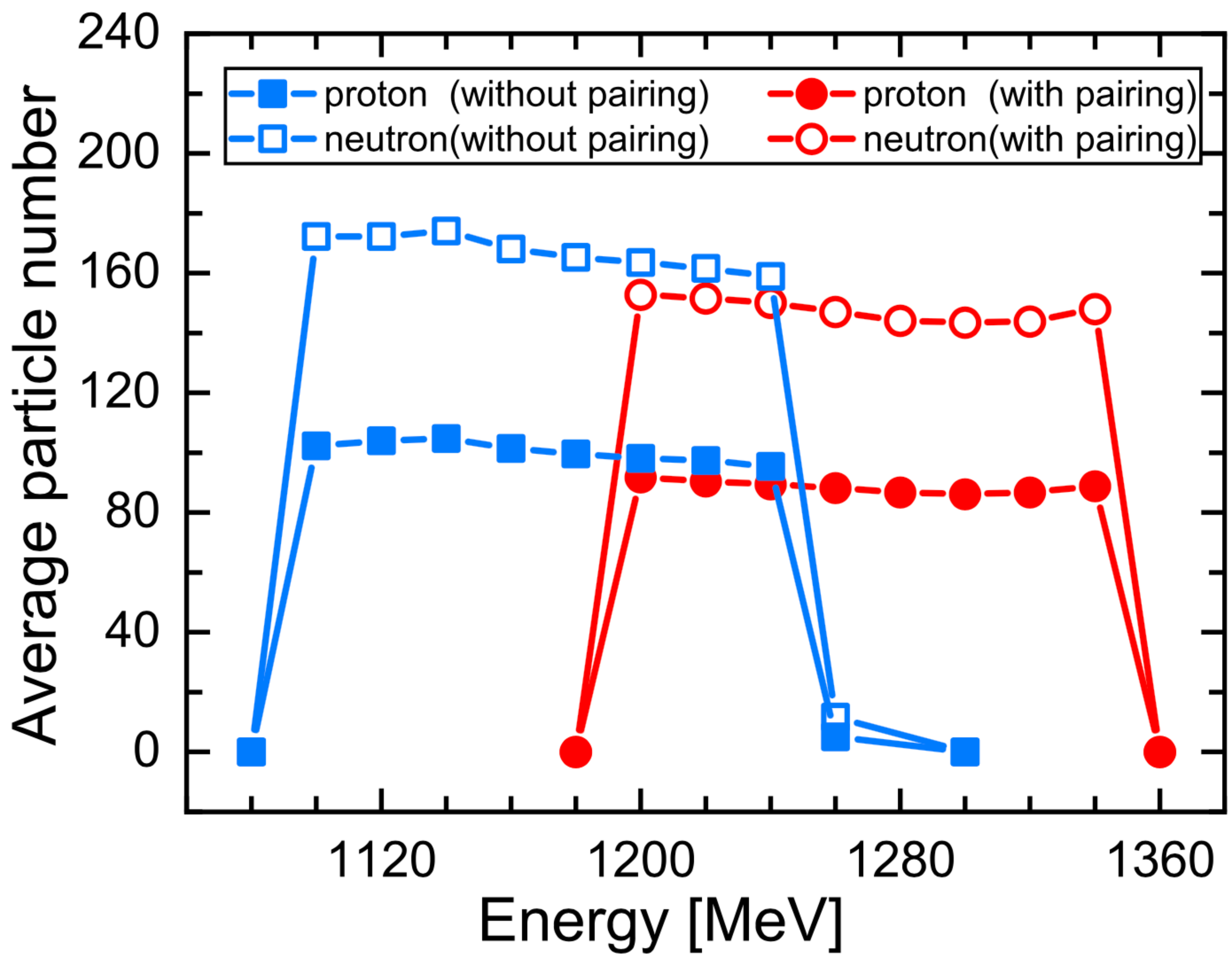


Zhang, Li, Vretenar, Nikšić , Ren, **PWZ**, Meng, PRC, 109, 024316 (2024)

Average particle number in the middle fragment

Editors' Suggestion

Zhang, Li, Vretenar, Nikšić , Ren, **PWZ**, Meng, PRC, 109, 024316 (2024)



without pairing

$95 \leq Z \leq 105$

$159 \leq N \leq 174$

with pairing

$86 \leq Z \leq 92$

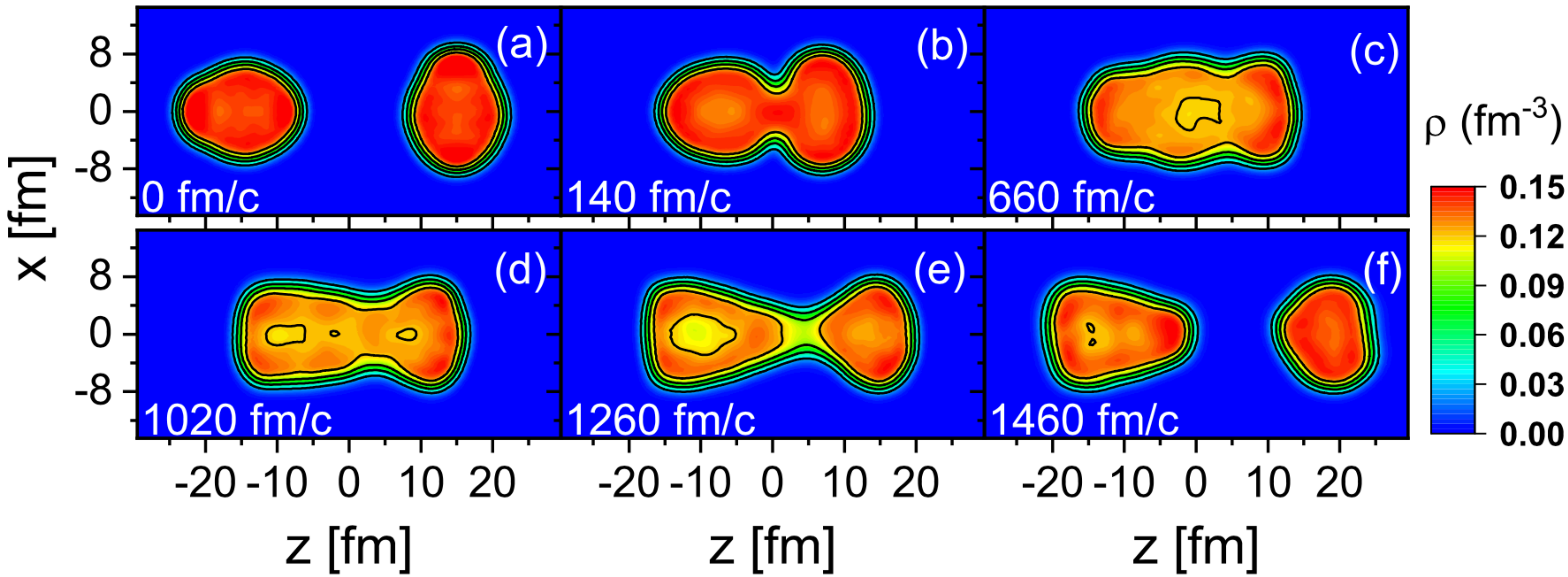
$144 \leq N \leq 153$

The formation of very heavy neutron-rich systems;

Synthesis of superheavy nuclei

Editors' Suggestion

Zhang, Li, Vretenar, Nikšić , Ren, **PWZ**, Meng, PRC, 109, 024316 (2024)



Heavy fragment: $111 \leq Z \leq 114 \quad 180 \leq N \leq 183$

Potentially interesting for the synthesis of superheavy elements.

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Where do the next ten years take us?

By 2030, a combination of **mean-field models** and **first-principles methods** will offer predictions — with quantified uncertainties— for nuclear structure and reactions in and, in some cases, **beyond medium-mass nuclei**.

—— Long Range Plan 2023

Progress in Particle and Nuclear Physics 109 (2019) 103713

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Review

Towards an *ab initio* covariant density functional theory for nuclear structure

Shihang Shen [a,b,c], Haozhao Liang [d,e], Wen Hui Long [f,g], Jie Meng [a,h,i,*], Peter Ring [a,j]

Progress in Particle and Nuclear Physics 64 (2010) 120–168

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Review

Toward *ab initio* density functional theory for nuclei

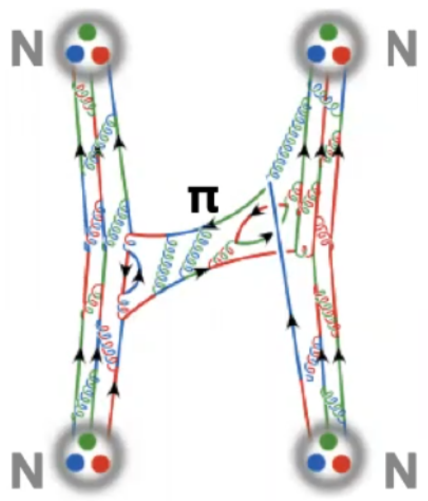
J.E. Drut, R.J. Furnstahl *, L. Platter

Department of Physics, Ohio State University, Columbus, OH 43210, United States

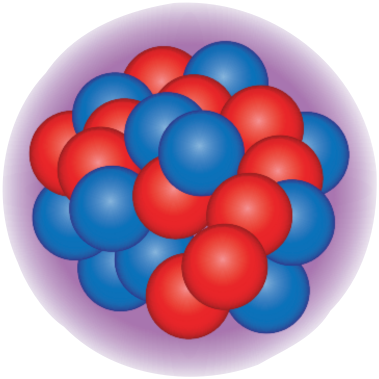
The goal of *ab initio* nuclear theory

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)



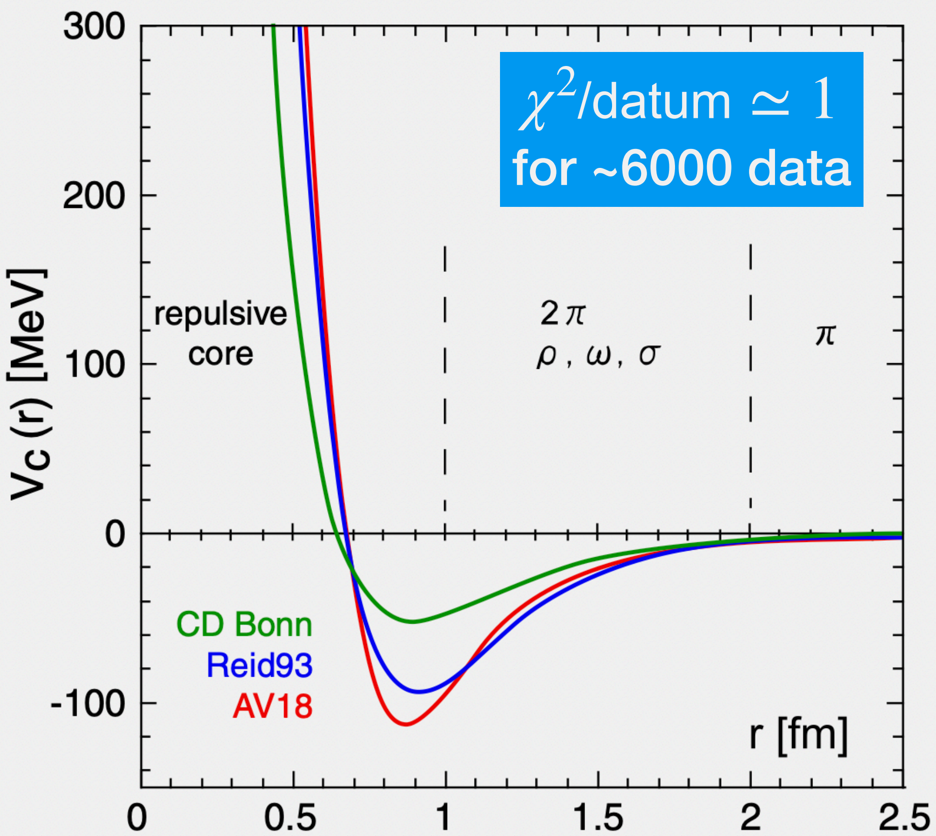
- **Solve the nuclear many-body problem**
  - Nuclear bulk properties: masses, radii, …
  - Nuclear spectra: energy levels, transitions, …
  - Nucleonic matter equation of state: neutron stars, …
  - New physics: $0\nu\beta\beta$, electric dipole moments, …
  - …



Ab initio calculations with *NN* forces

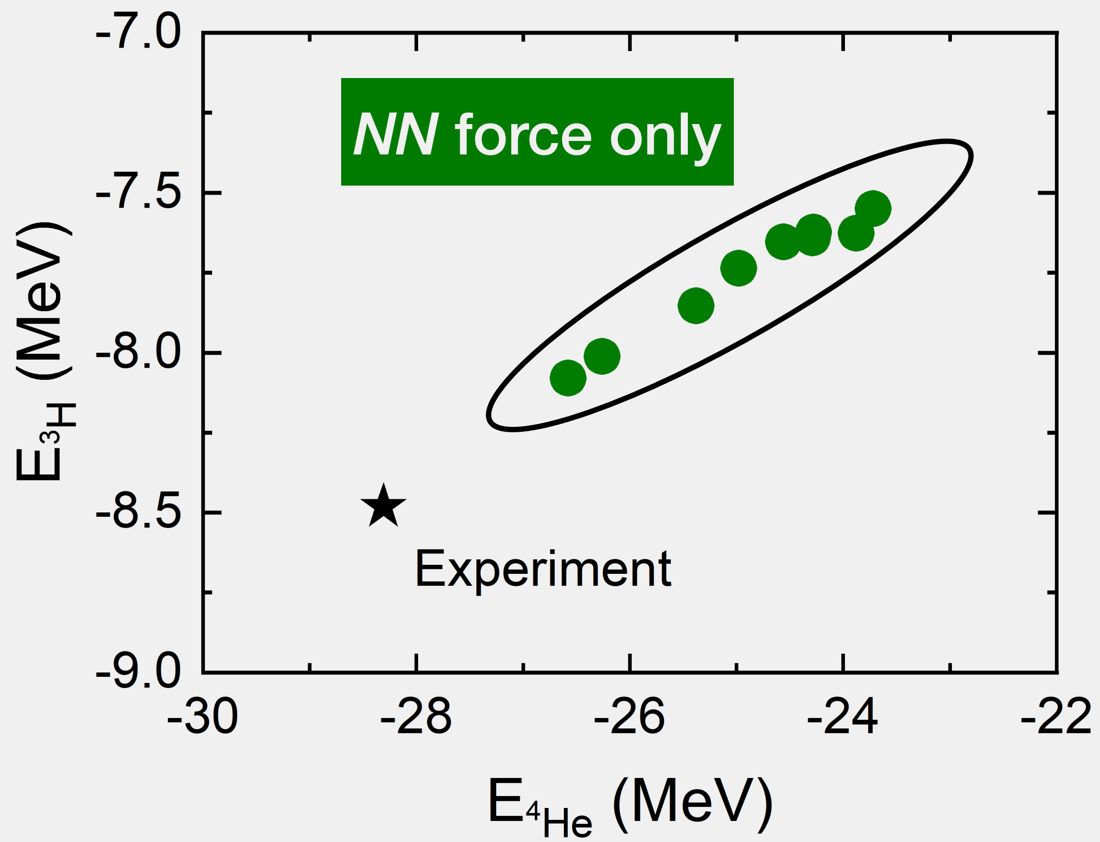
Many two-nucleon (NN) interactions, applied to nonrelativistic *ab initio* calculations, provide **insufficient binding** for light nuclei.

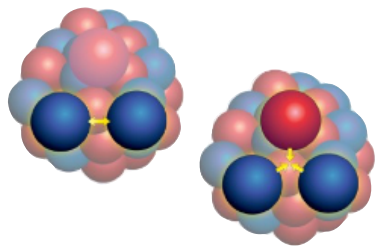
NN forces



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

^{3}H and ^{4}He

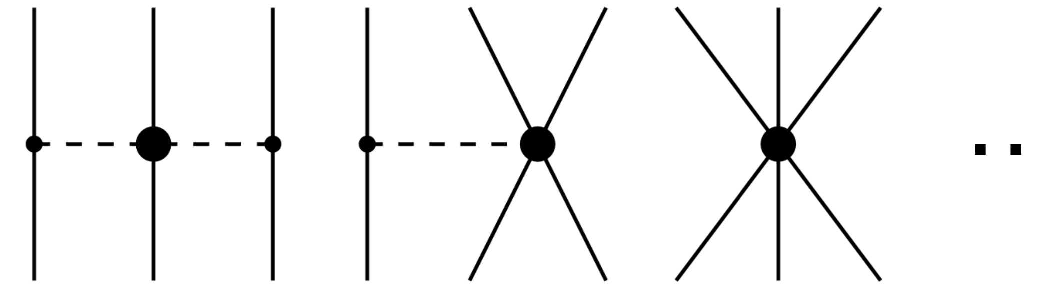




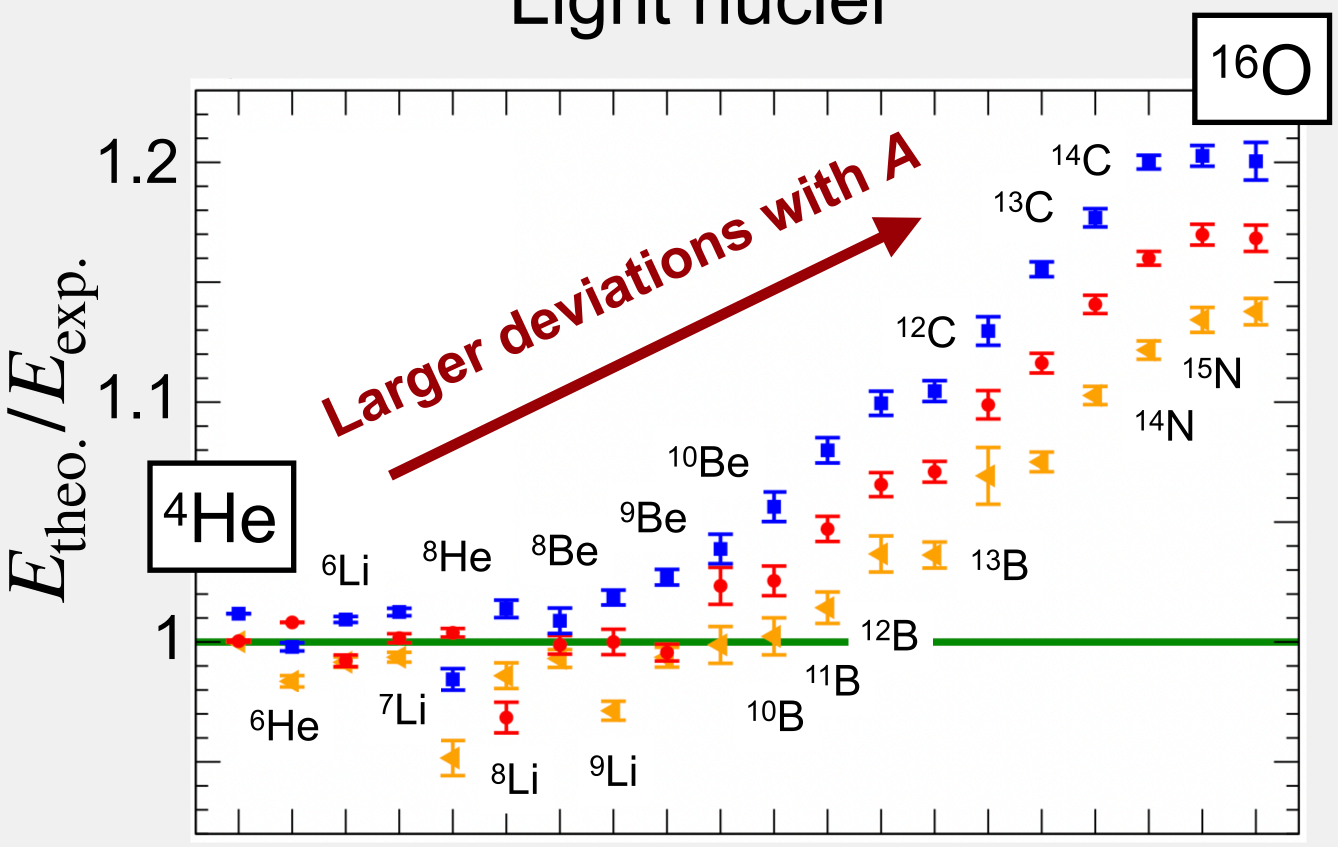
Three-nucleon forces are needed !

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

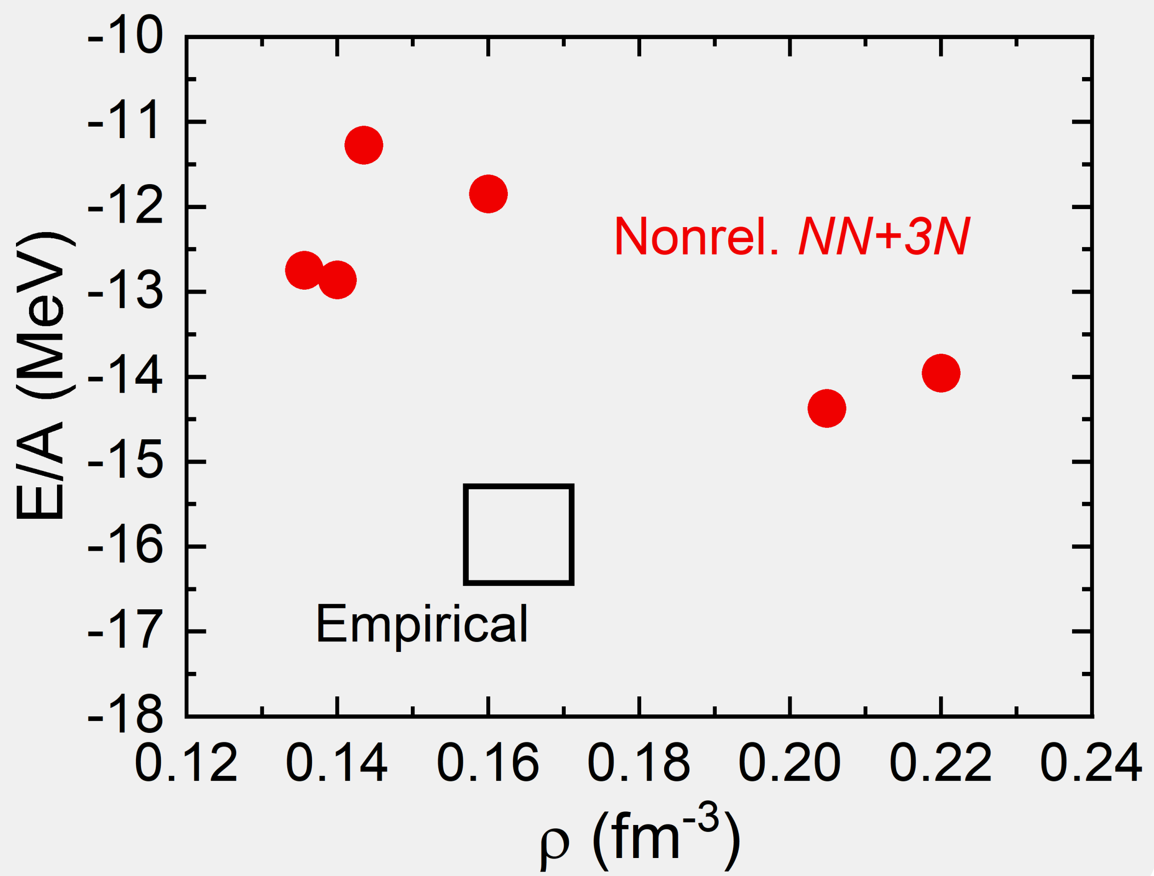
- **3*N*-force models fitting to**
  - $A = 3$ binding energy / beta decay
  - pd/nd scattering
  - …



Light nuclei



Nuclear matter



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

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

—— an outstanding problem in nuclear physics!

- **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.

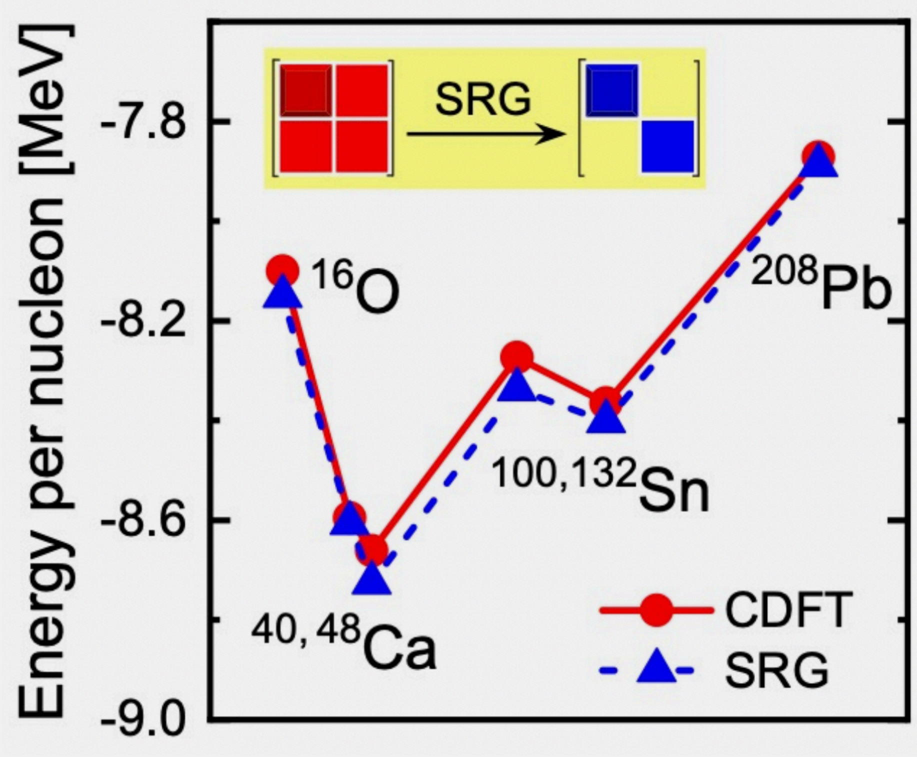
Our strategy: going for a relativistic *ab initio* framework

Relativistic effects

Bridge the Rel. and Nonrel. DFTs

$$4\pi r^2 \rho_v(r) = \rho_0 + \frac{d}{dr}\left[\frac{1}{4\tilde{M}^2}\frac{\kappa}{r}\rho_0\right] + \frac{d^2}{dr^2}\left[\frac{1}{8\tilde{M}^2}\rho_0\right] + O(\tilde{M}^{-3}),$$

Rel. Nonrel. (including high-order terms …)



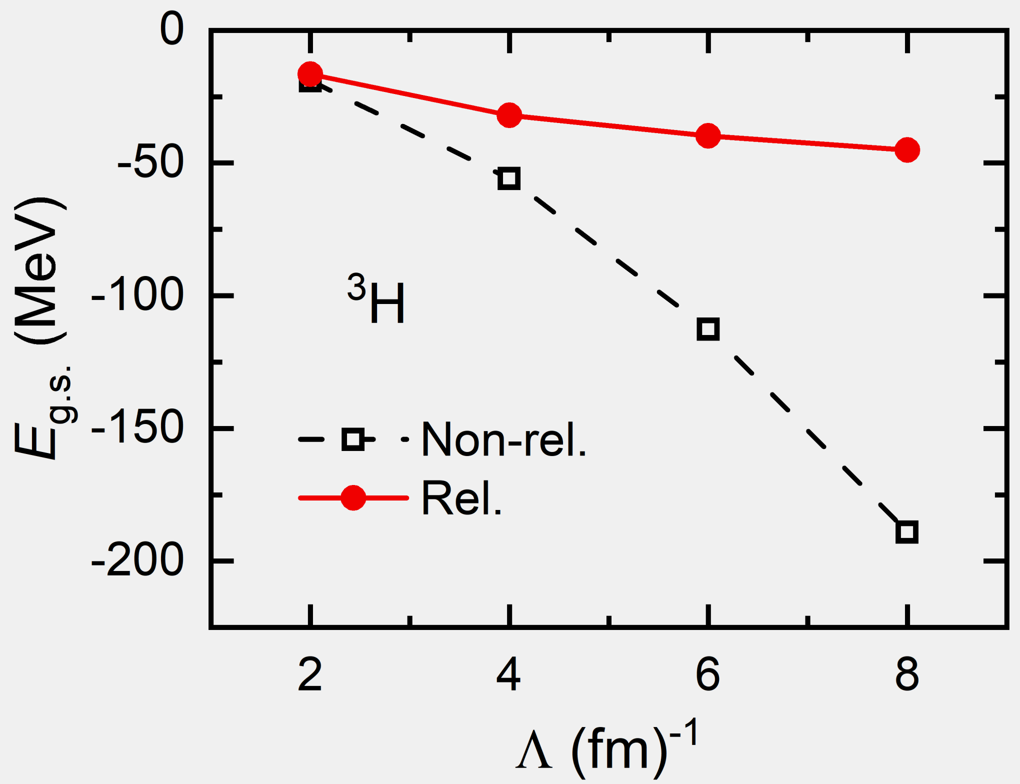
Ren and PWZ, PRC 102, 021301(R) (2020)
Editors' Suggestion

Rel. and Nonrel. VMC with LO forces

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

Nonrel Rel. corrections

Thomas collapse avoided !

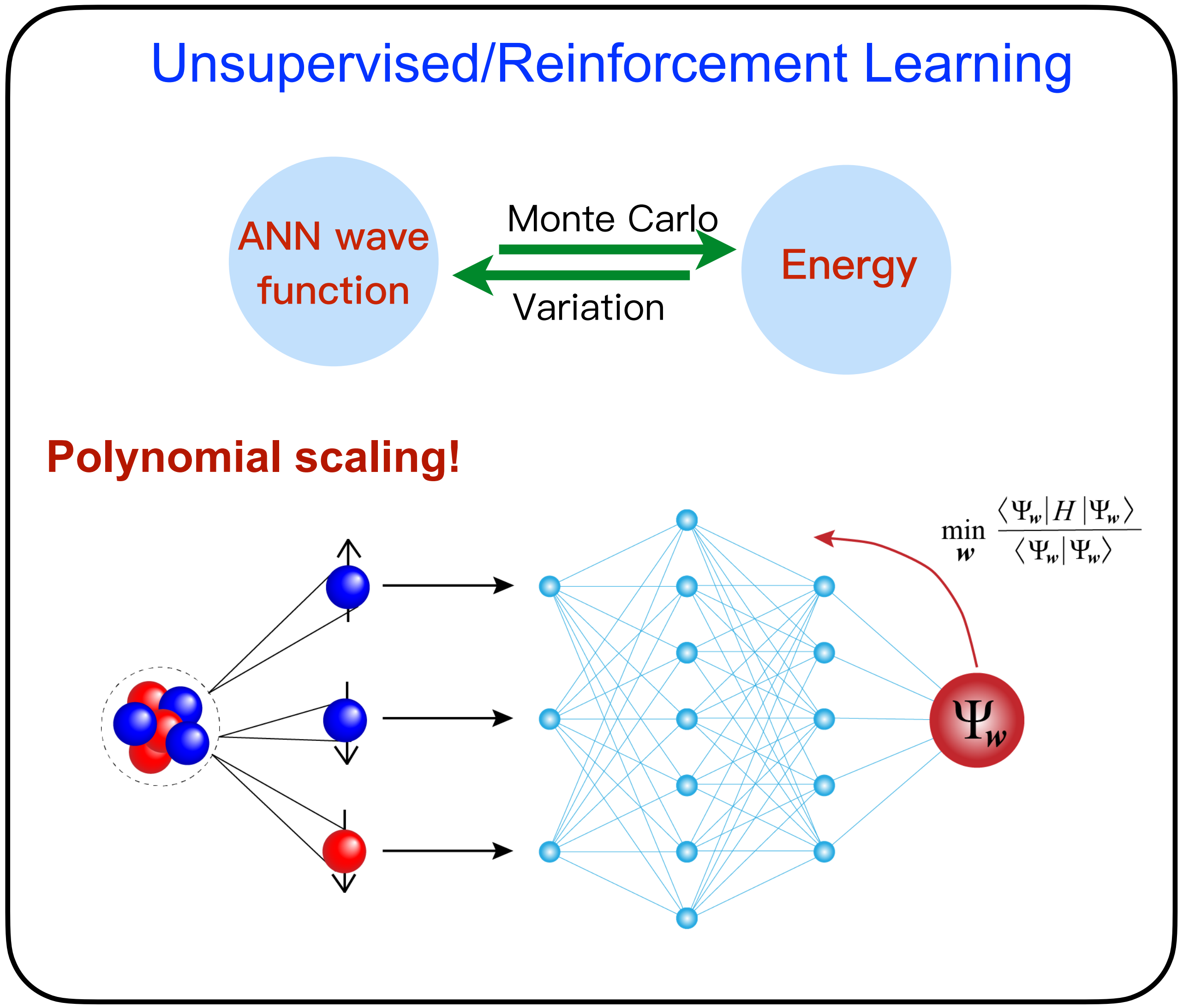


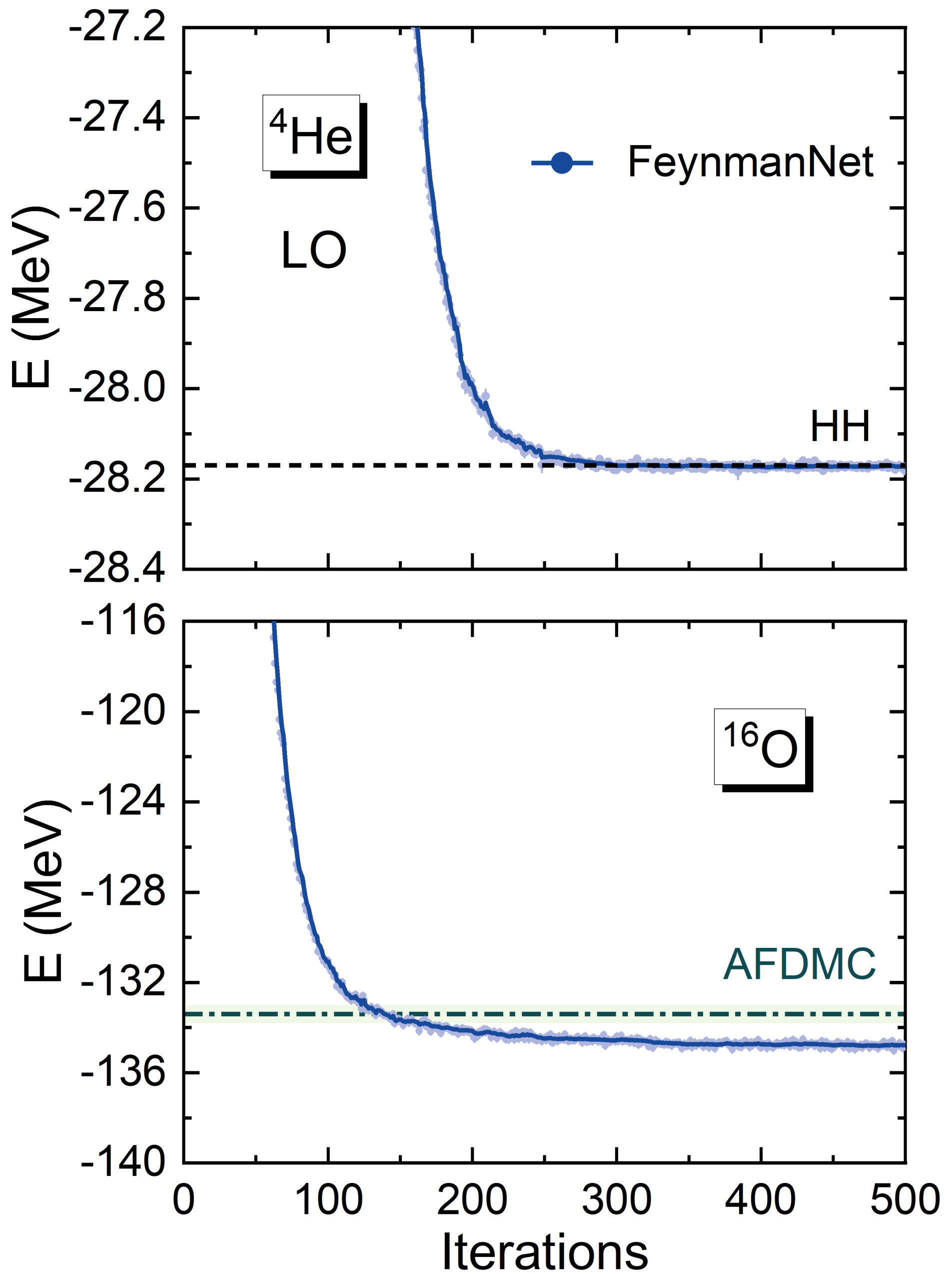
Yang and PWZ, PLB 835, 137587 (2022)

The relativity brings high-order effects …

Neural-network–based nuclear ab initio calculations

- **FeynmanNet:** Variational Monte Carlo + Deep Neural-Networks
- A deep-learning **high-precision** nuclear ab initio method

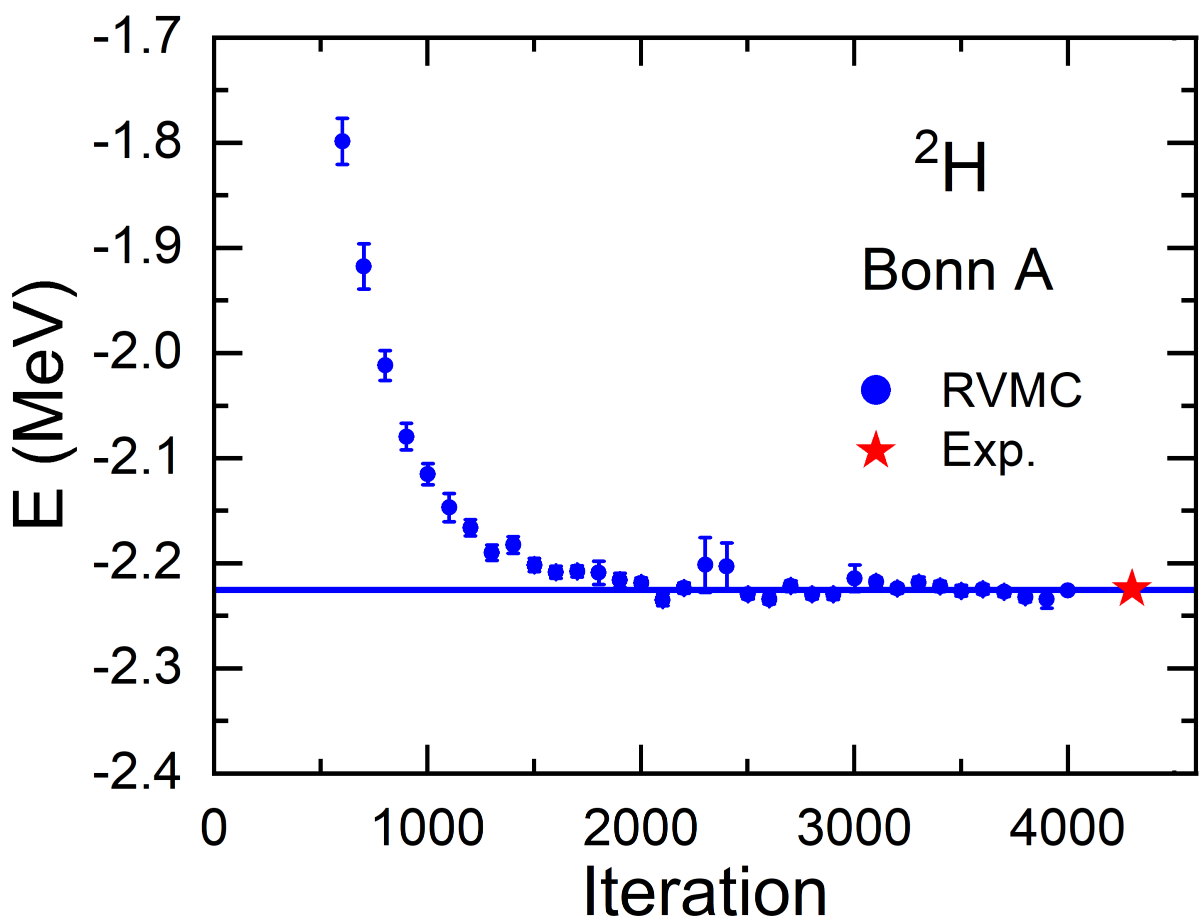


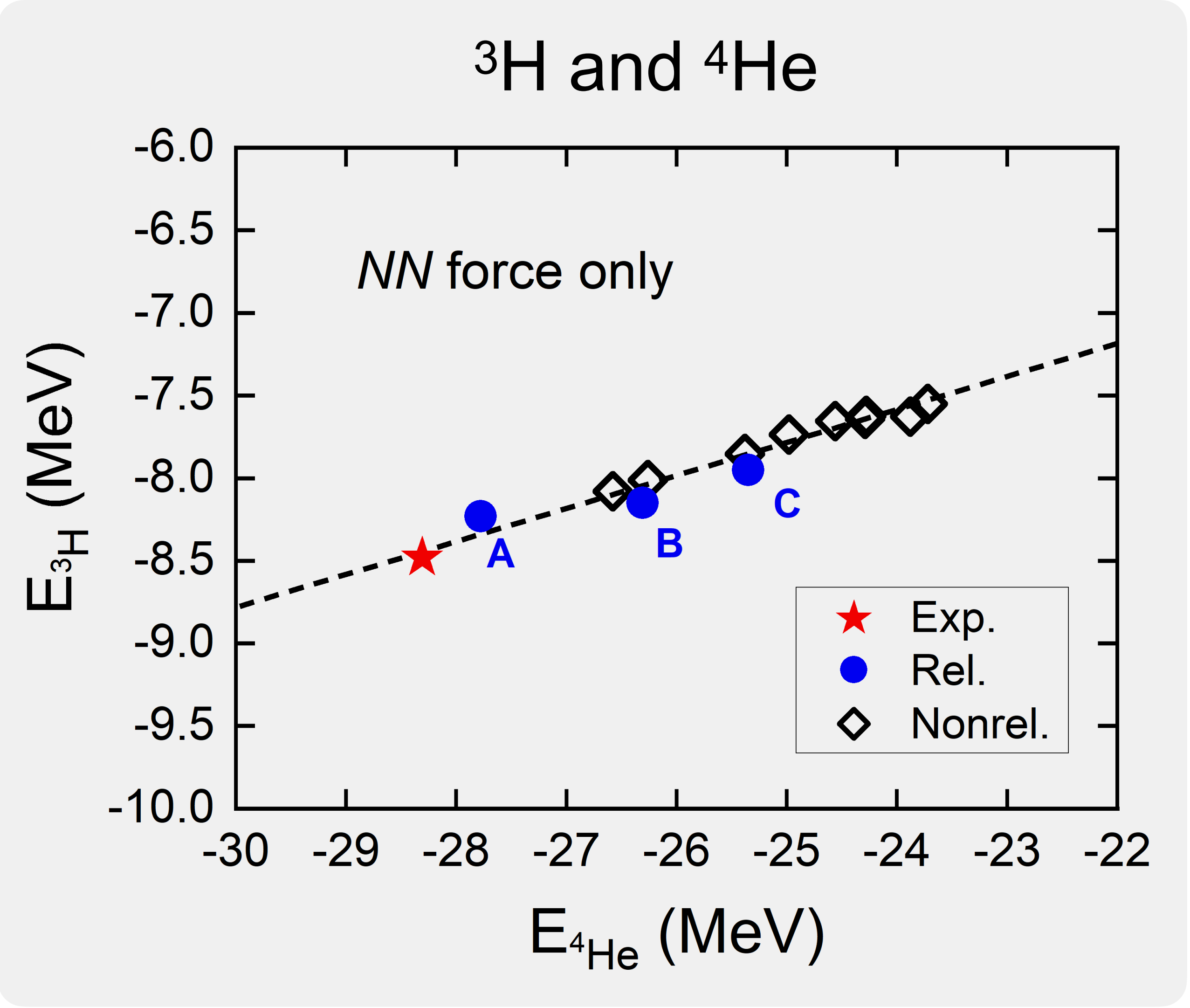


Yang and **PWZ**, PLB 835, 137587 (2022)
Yang and **PWZ**, PRC 107, 034320 (2023)
Yang, Epelbaum, Meng, Meng, **PWZ**, PRL 135, 172502 (2025)

Relativistic ab initio calculations with realistic forces

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



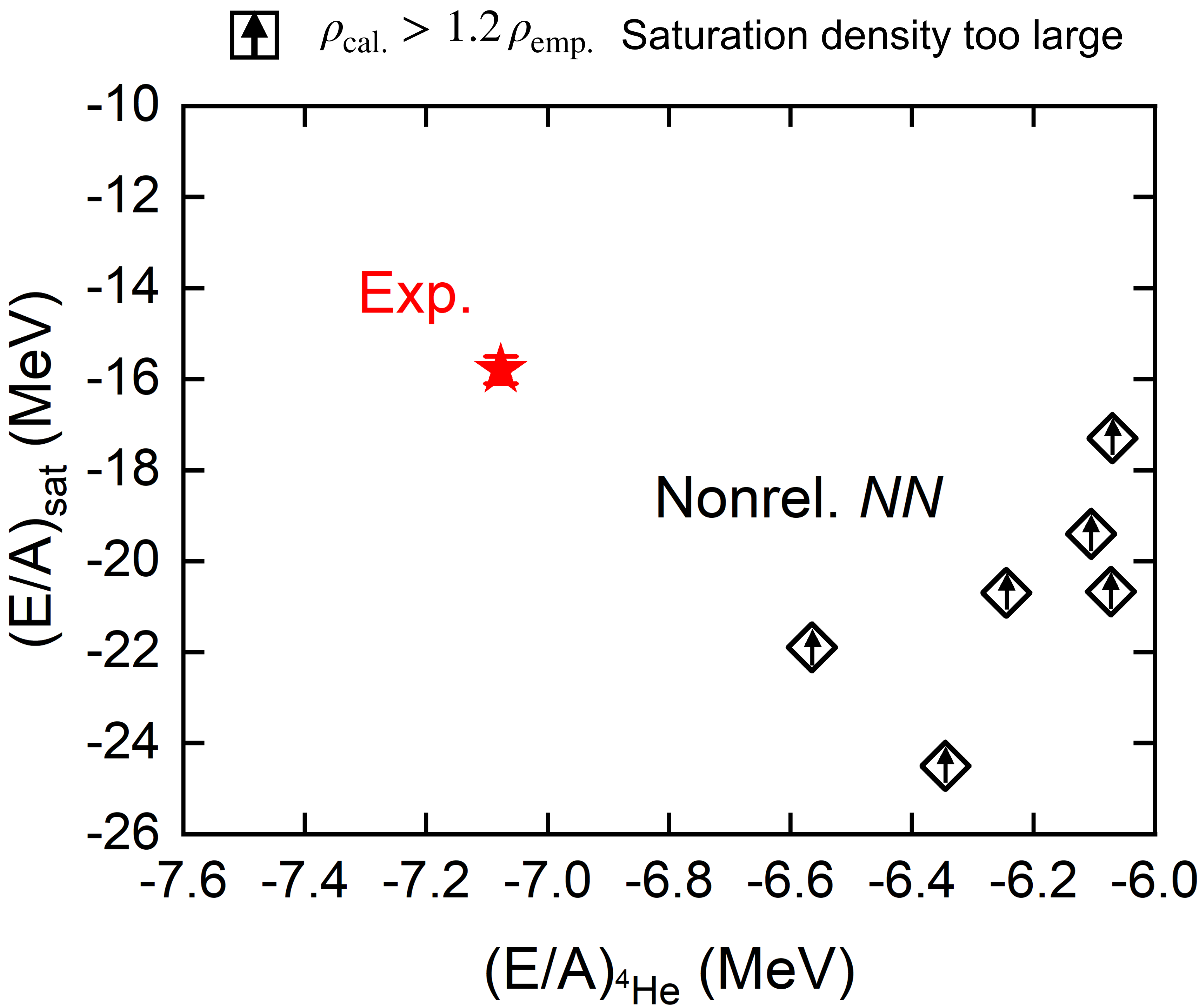


Yang and **PWZ**, CPL, 42 051201 (2025) "Express Letter"

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”



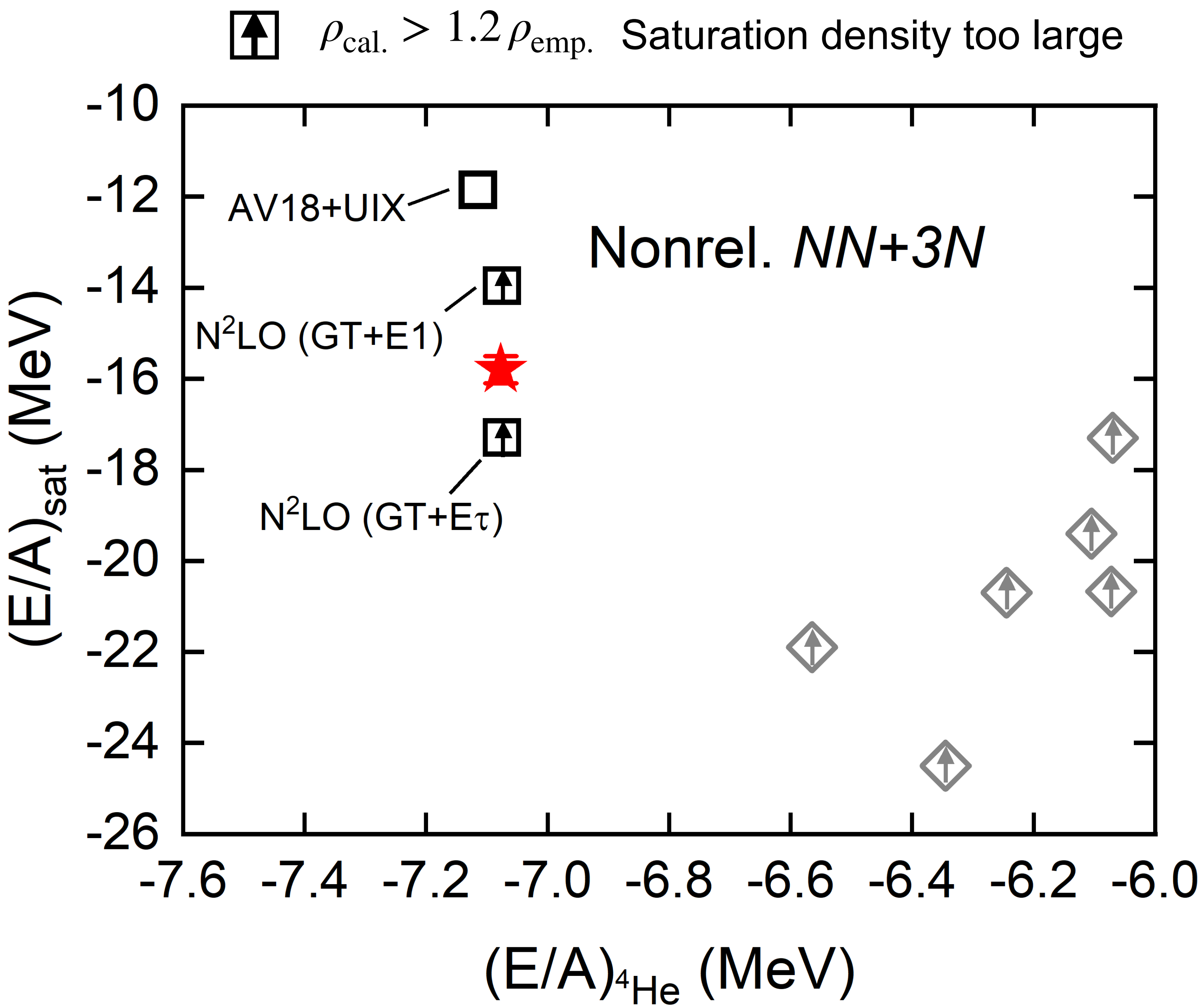
^{4}He	Nucl. Matt.

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"

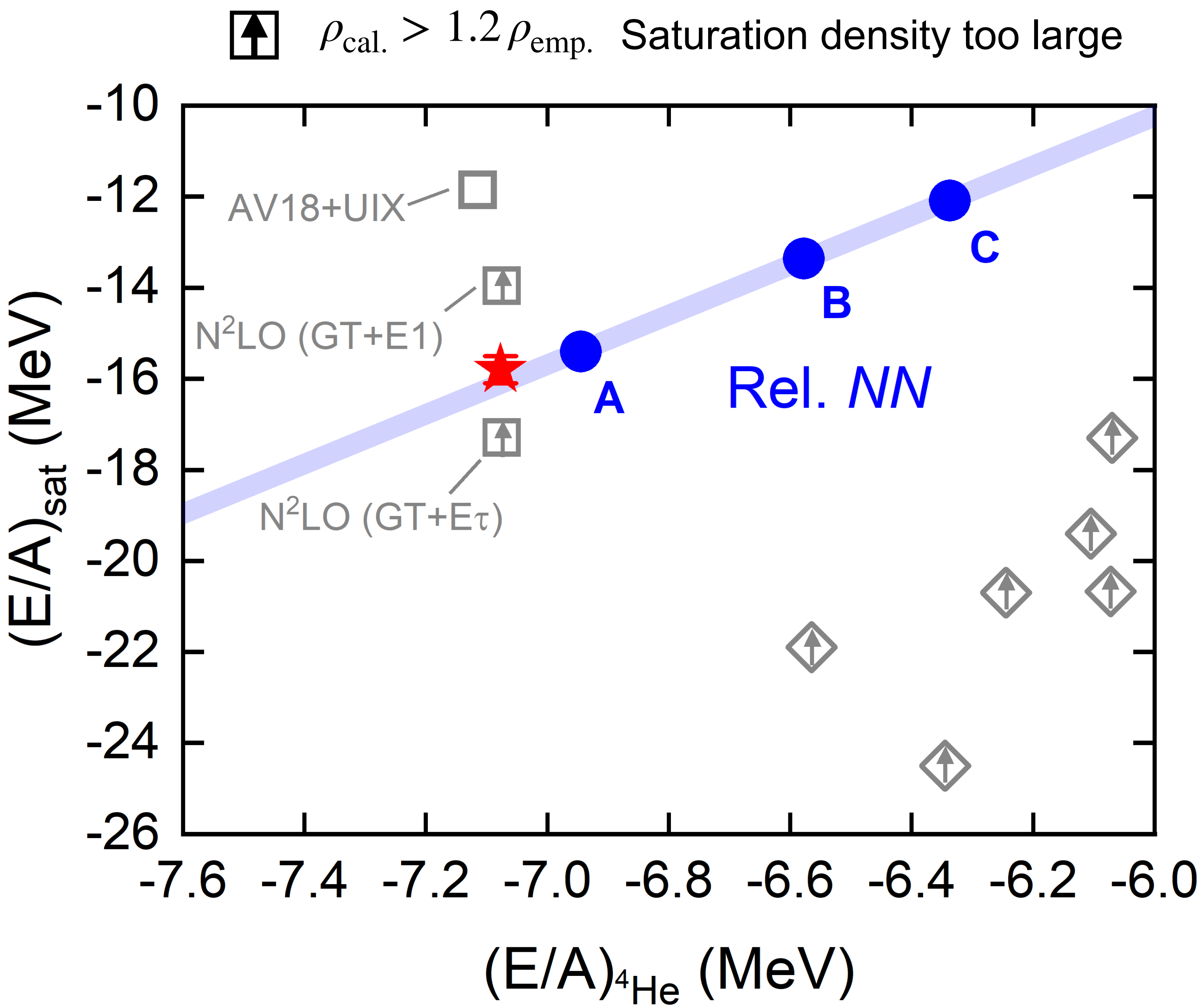


	^{4}He	Nucl. Matt.
NN	Underbind	Overbind
NN/3N	Fit	Diverse

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”



	^{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

Relativistic density functional theory (RDFT) has been solved in 3D lattice and extended to its time-dependent version for various nuclear structure and dynamics.

- Nuclear landscape with PC-PK1
  good performance for nuclear global properties
- High-order deformation in atomic nuclei
  octupole deformation effects in transfermium nuclei
  tetrahedral deformation in Zr-80
- Nuclear dynamics
  tail-to-tail collisions of U-238 could form very heavy neutron-rich systems
- Relativistic calculations for $A \leq 4$ nuclei with the Bonn potential
  Ground-state energies nicely reproduced
  Consistency between the light nuclei and nuclear matter achieved


Thank you.