Machine Learning Density Functional Theory for Atomic Nuclei

Pengwei Zhao 赵鹏巍

Peking University

Outline

- Nuclear density functional theory
- Machine learning orbital–free DFT for nuclei
- Nuclear deformation from orbital–free DFT
- Summary

Quantum Many-Body Problem

$$H\psi = E\psi$$

QM

Hohenberg-Kohn

$$\min_{\rho} E[\rho(\boldsymbol{r})]$$

EDF

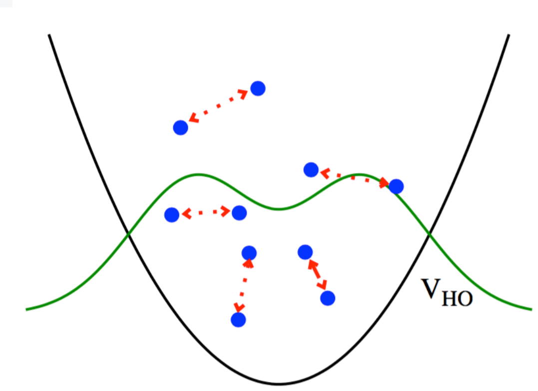
$$E[\rho] = T_s[\rho] + E_H[\rho] + E_{xc}[\rho]$$

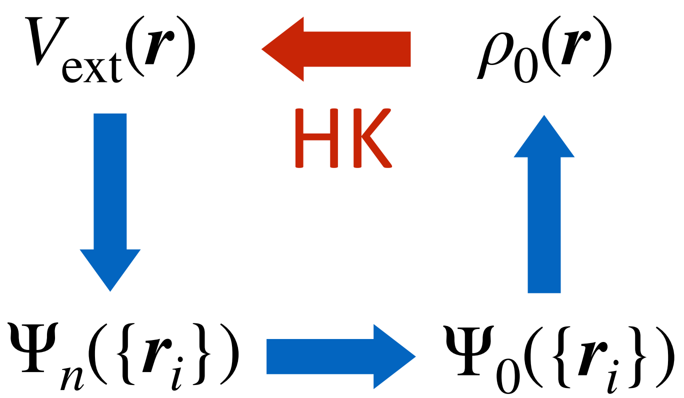
Hohenberg-Kohn Theorem

Hohenberg-Kohn Theorem Phys. Rev. 136 B864 (1964)

- ✓ There exists a universal energy functional defined in terms of the density.
- ✓ The exact ground state is determined by the global minimum value of this functional.

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





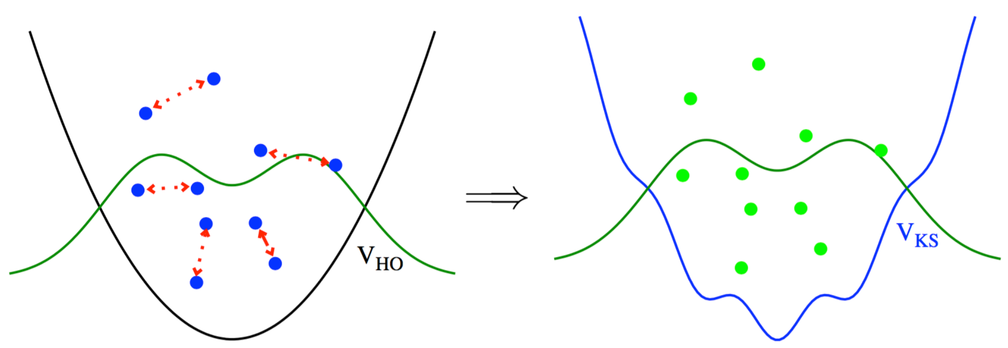
Walter Kohn
1998 Nobel Prize

- ◉ The many-body problem is reformulated in terms of the density but is not actually solved.
- ◉ The HK functional is a priori unknown, e.g., *no direct link from the density to the kinetic energy.*
- ◉ HK-DFT is in principle exact but impractical.

—> Kohn-Sham approach

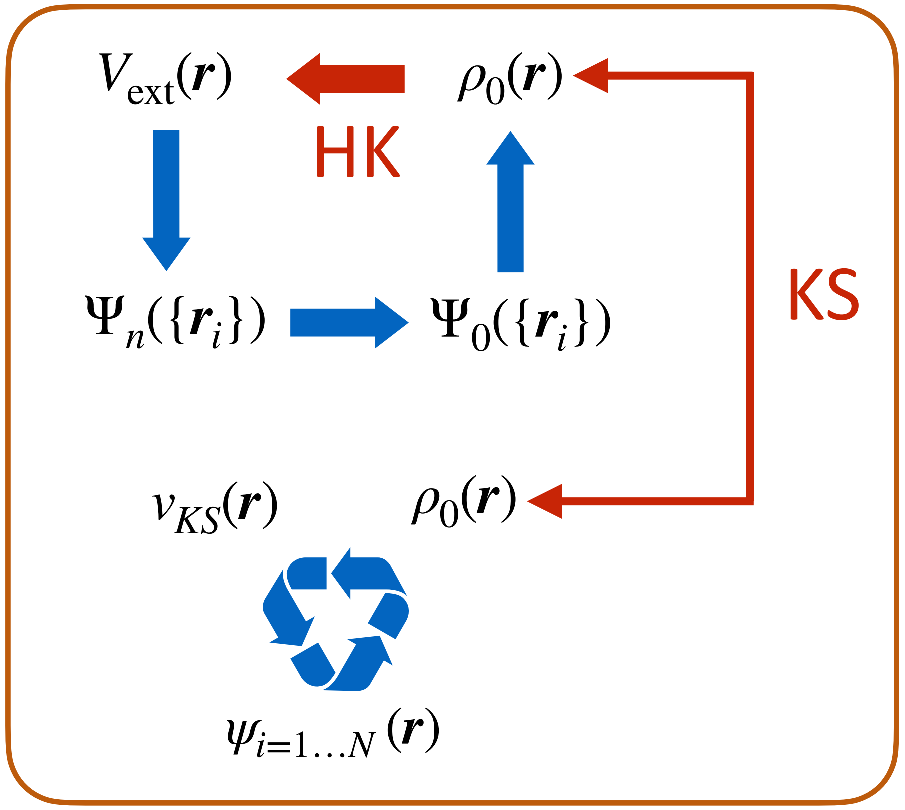
Kohn-Sham density functional theory

The KS-DFT separates contributions that are (in principle) possible to compute from contributions that are much more complicated!



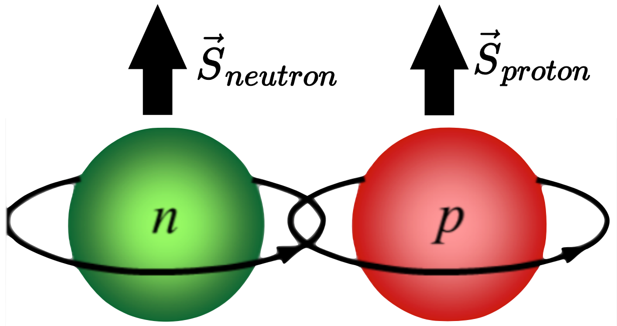
$$E[\rho] = T_0[\rho] + \int V(\mathbf{r})\rho(\mathbf{r})\,\mathrm{d}^3\mathbf{r} + E_H[\rho] + E_{xc}[\rho]$$

$$T_0[\rho] \doteq \sum_{i=1}^{N} \left\langle \varphi_i \middle| -\frac{\hbar^2}{2m}\nabla^2 \middle| \varphi_i \right\rangle$$



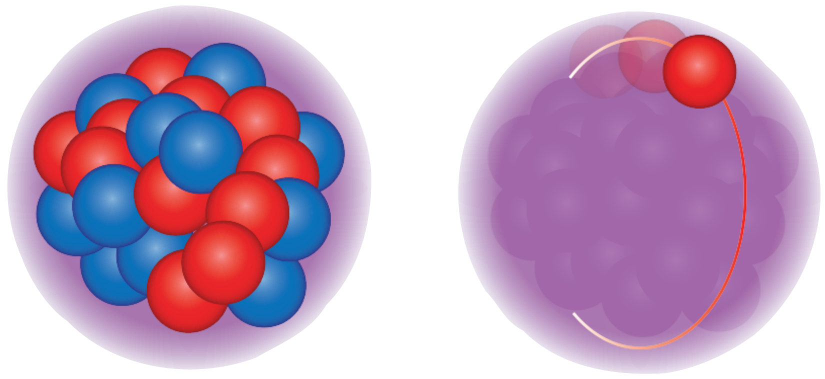
- KS orbitals are used to evaluate the kinetic energy.
- The number of orbitals increase with the particle number.
- Orthonormalization constraint must be enforced for the orbitals.
- Scales with $O(N^3)$.

Density functional theory for nuclei



- ✓ The nuclear force is complicated
- ✓ More degrees of freedom: spin, isospin, pairing, …
- ✓ Nuclei are self-bound systems

  DFT for the intrinsic density



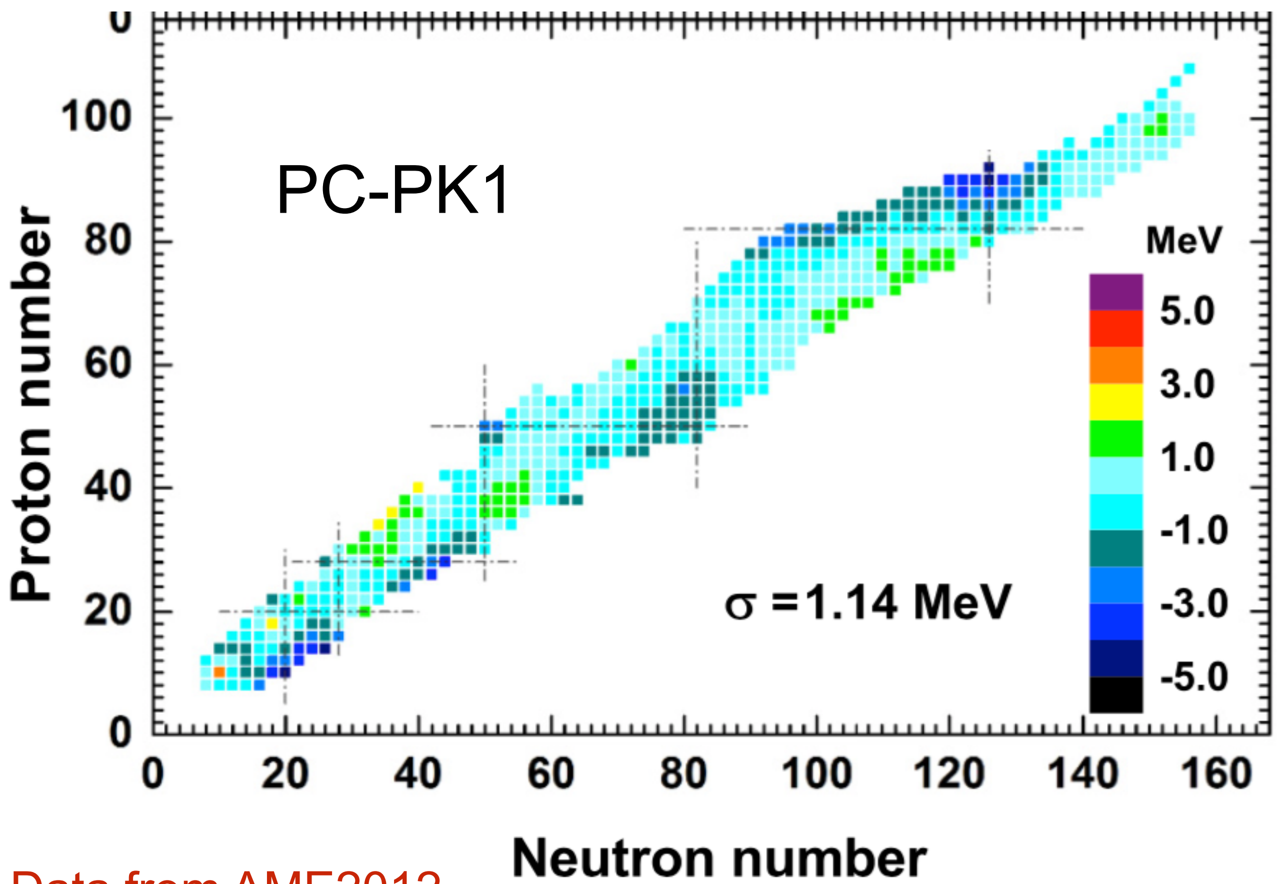
- ✓ At present, all successful functionals are phenomenological

  not connected to any NN- or NNN-interaction
- ✓ Adjust to properties of nuclear matter and/or finite nuclei,

  and (in future) to ab-initio results

Covariant density functional：PC-PK1

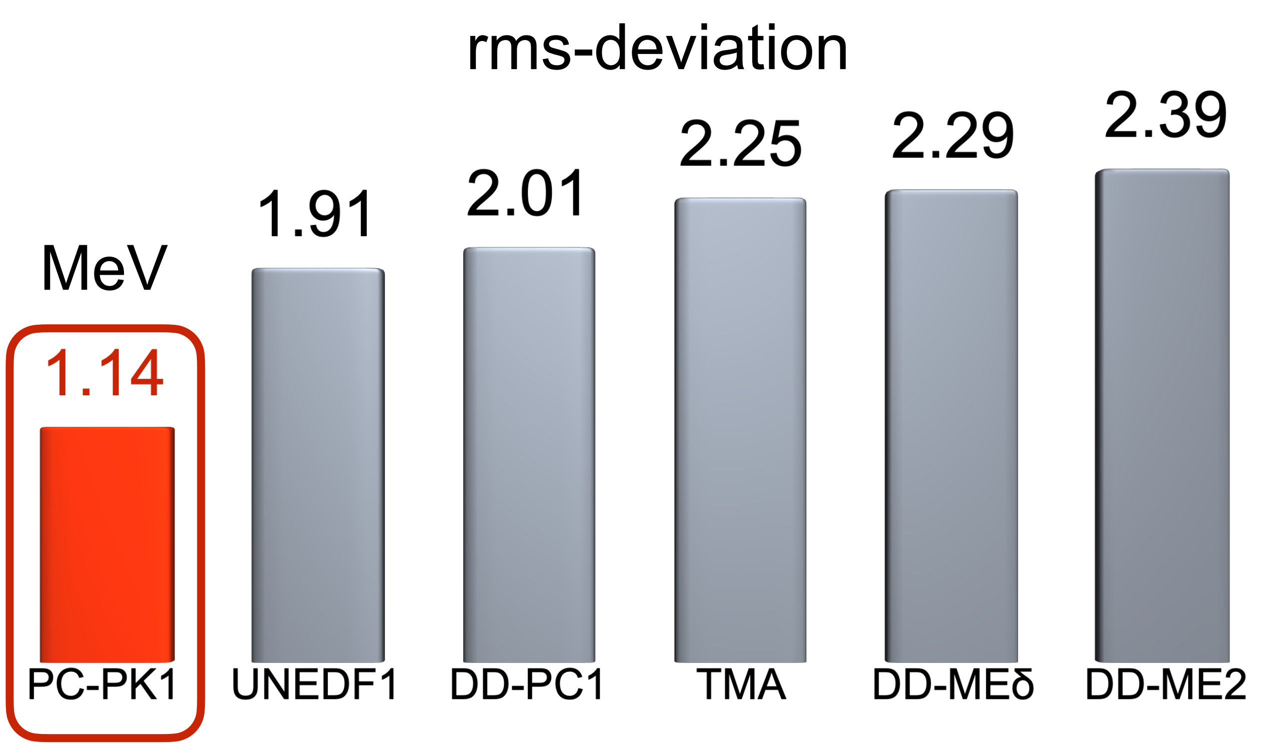
Mass Differences: M_{cal} - M_{exp}



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)

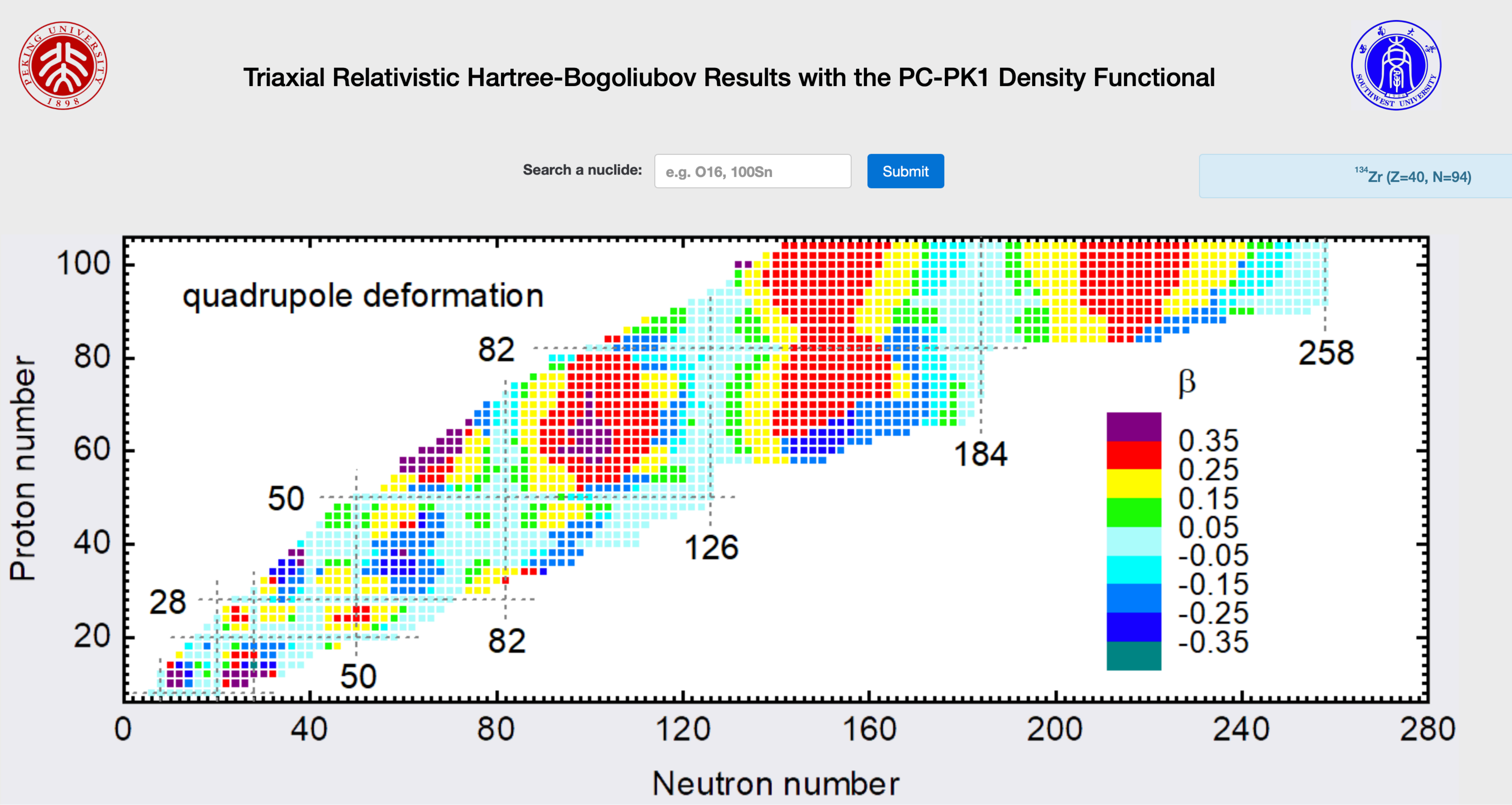
Yang, PWZ, Li, PRC 107, 024308 (2023)

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?

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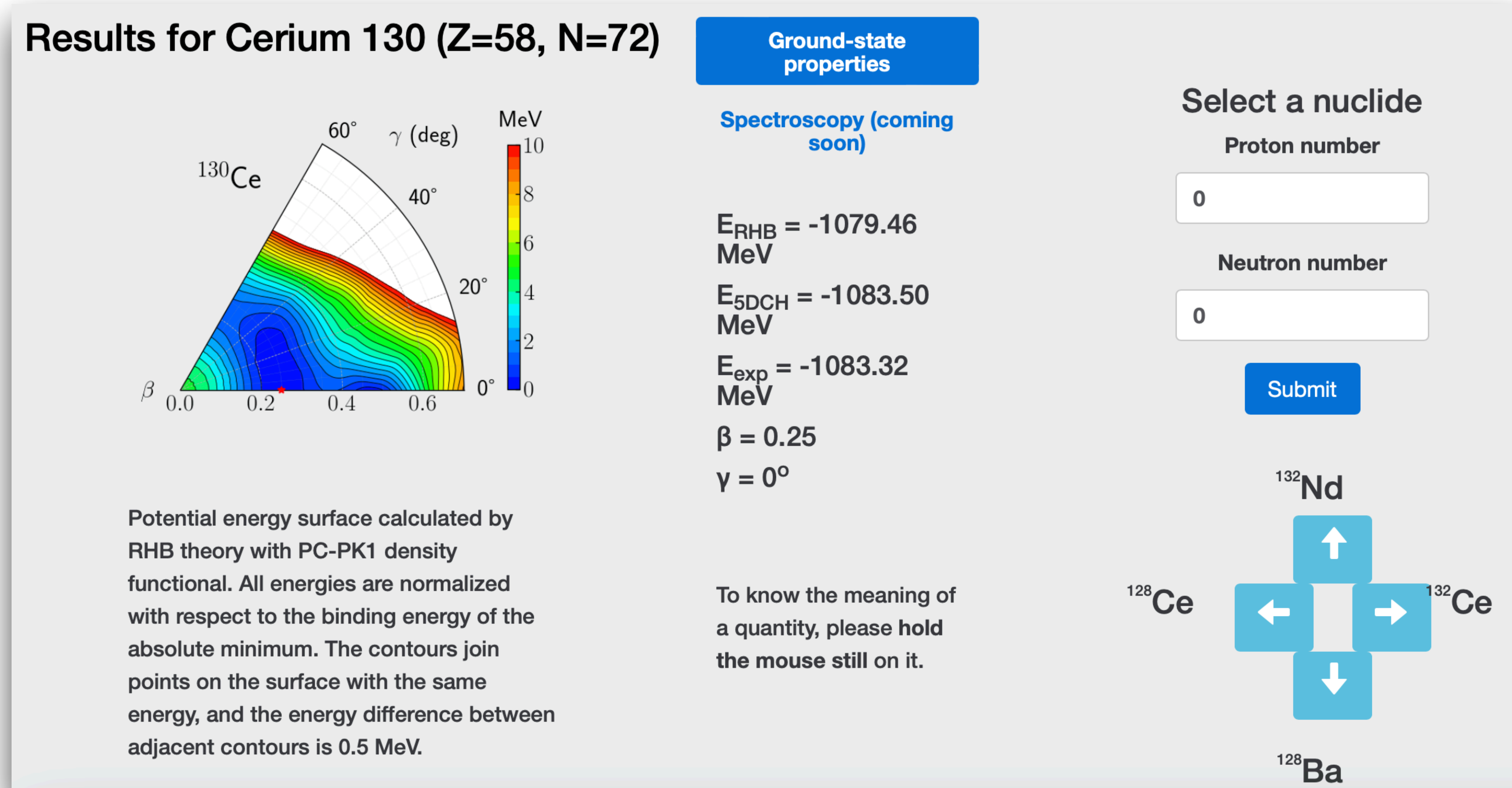
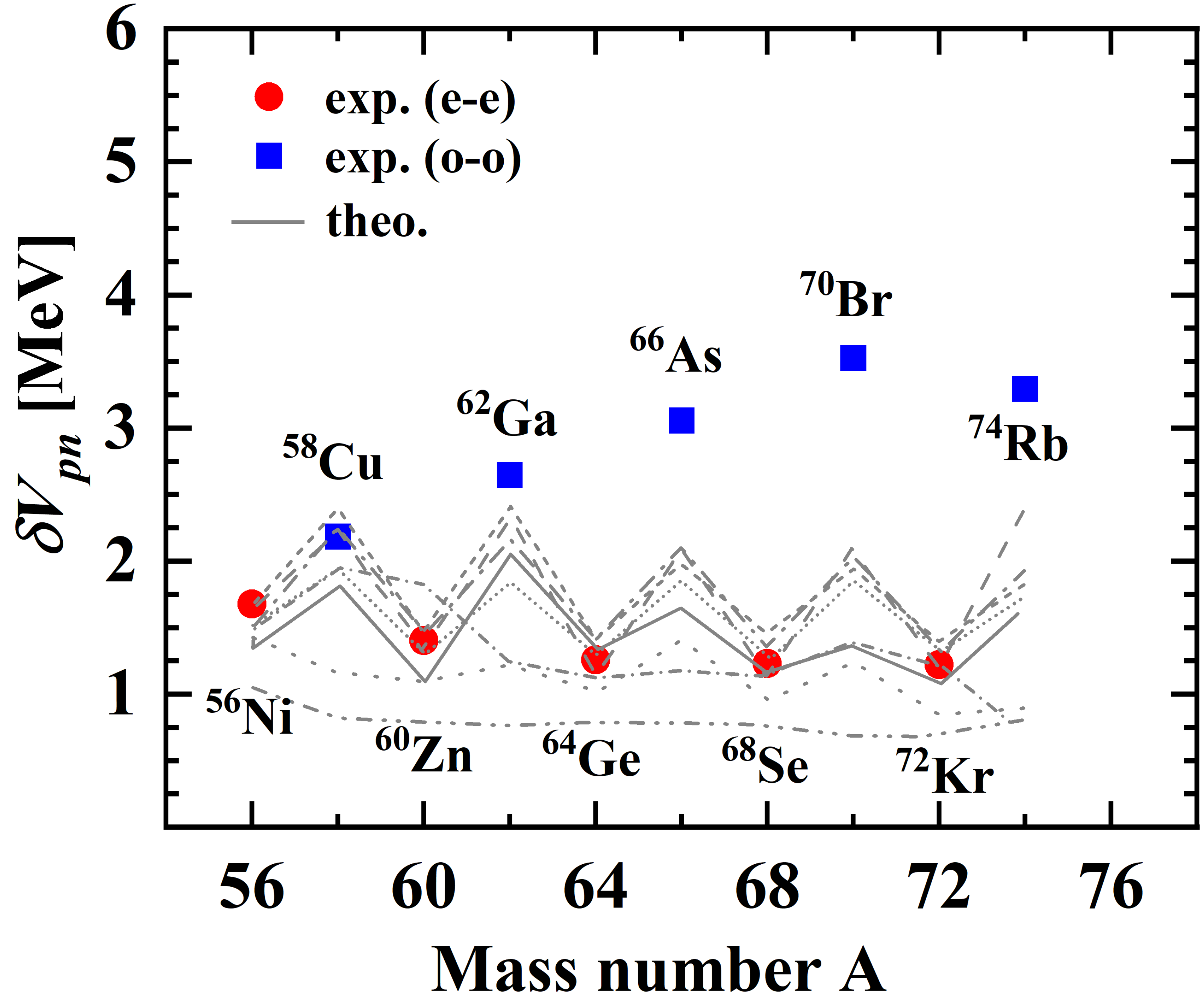


Yang, Wang, **PWZ**, Li, Phys. Rev. C 104, 054312 (2021)
Yang, **PWZ**, Li, Phys. Rev. C 107, 024308 (2023)

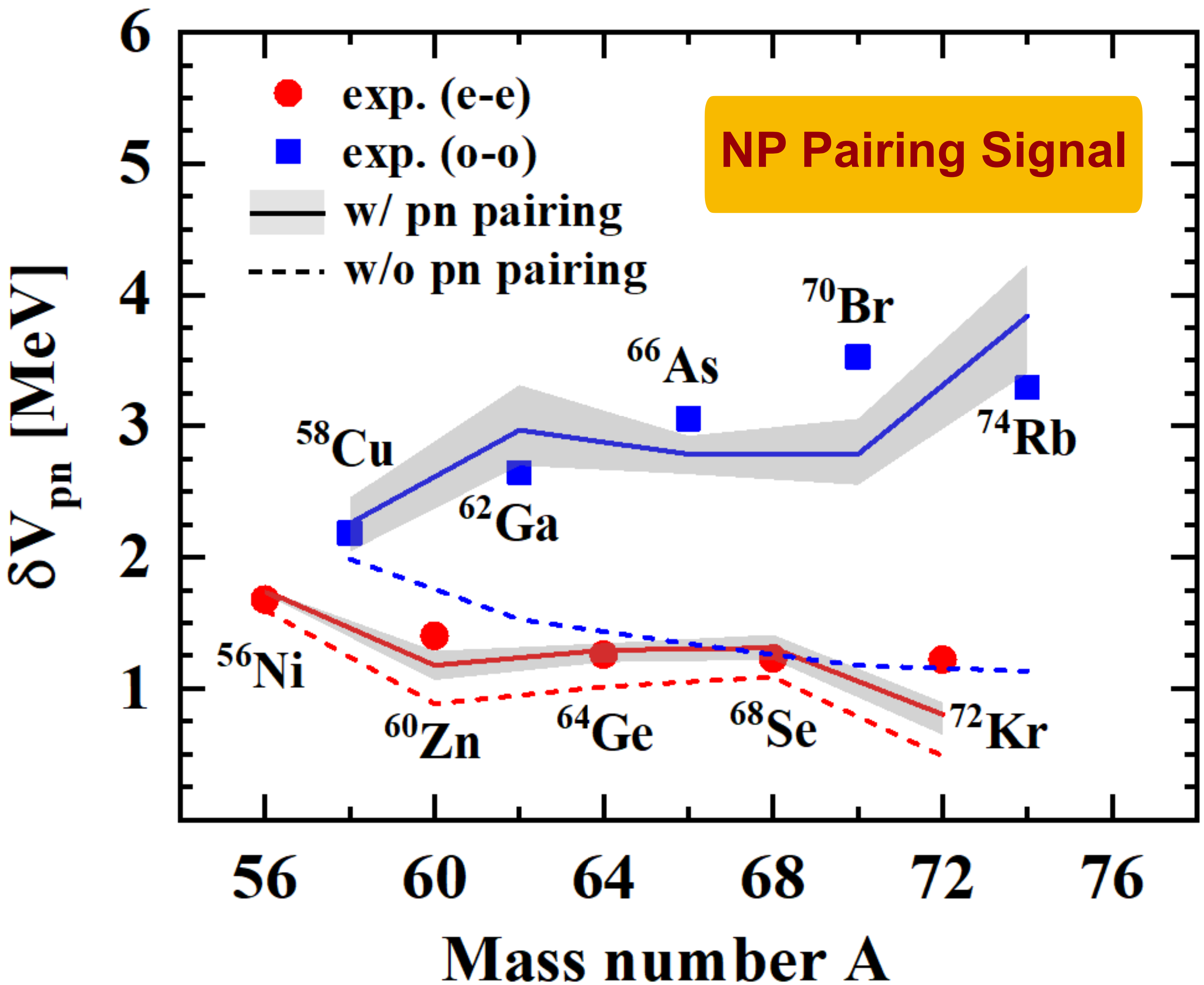
New mass measurement of upper fp-shell nuclei

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)

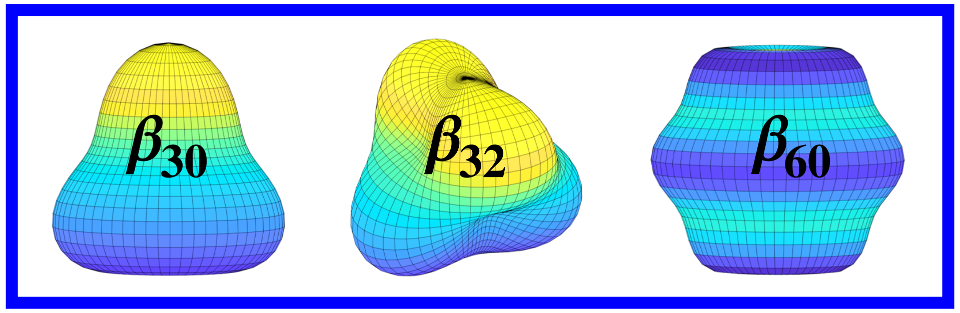
New mass measurement of upper fp-shell nuclei

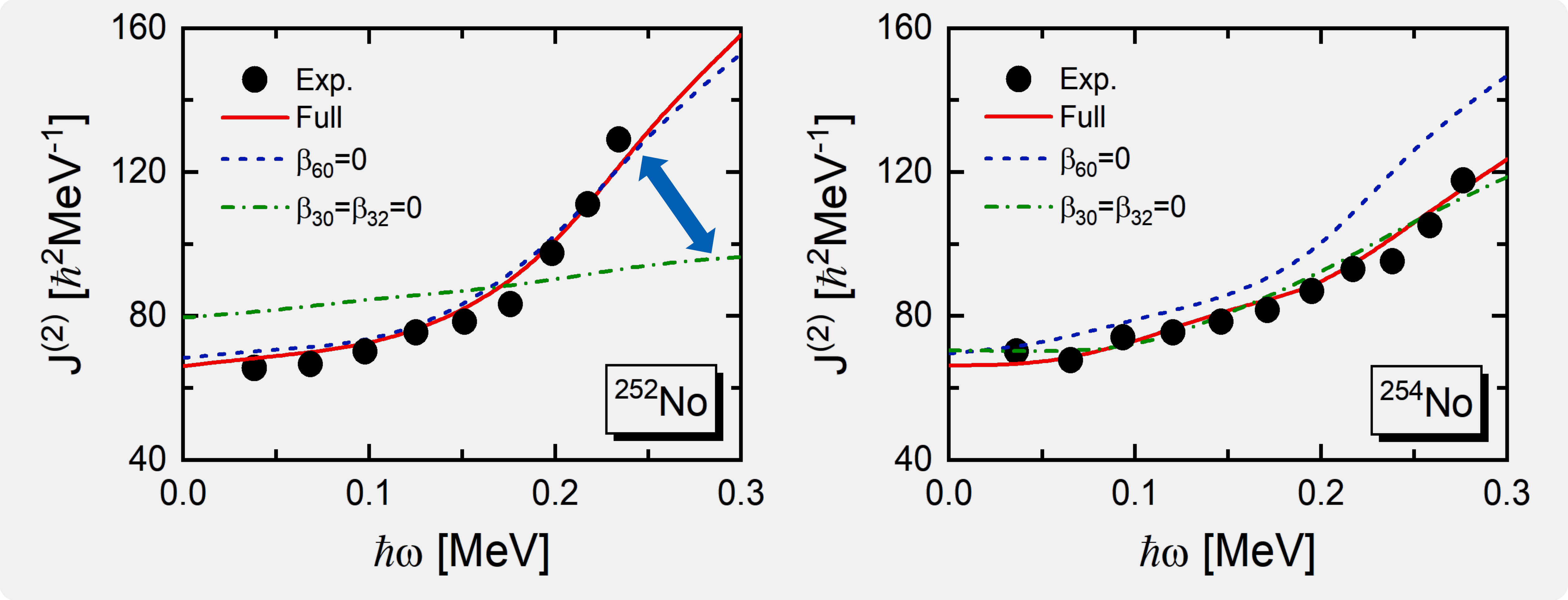


Exp: M. Wang et al., PRL 130, 192501 (2023)

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

High-order deformation in transfermium nuclei





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

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

Orbital-free density functional theory

✓ Energy depends solely on the density,

$$E[\rho] = \boxed{T_s[\rho]} + \int V(\mathbf{r})\rho(\mathbf{r})\,\mathrm{d}^3\mathbf{r} + E_H[\rho] + E_{xc}[\rho]$$

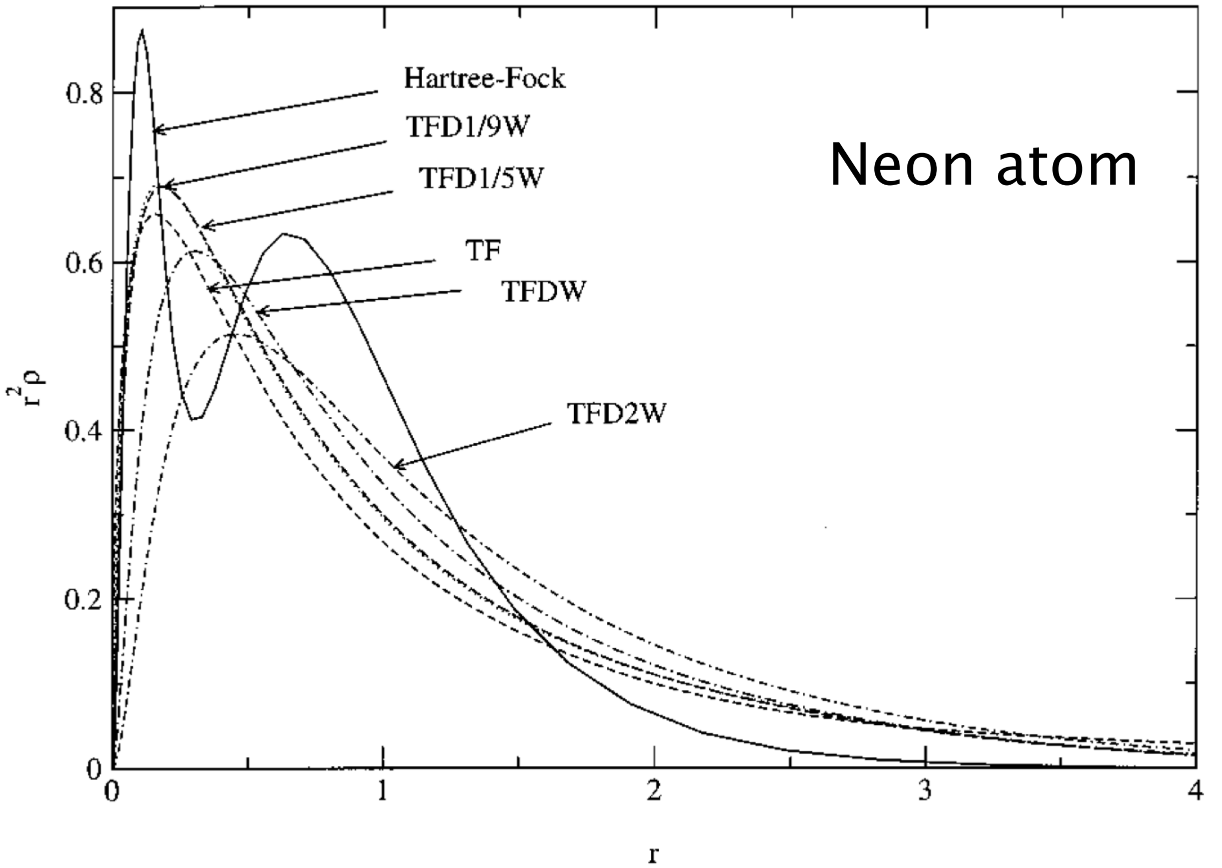
✓ No KS orbitals needed (no costly orthonormalization, scales with $O(N \log N)$.

✓ Accurate kinetic energy density functional is needed.
T_s is of the same order as the total energy.

Thomas-Fermi functional and extended …

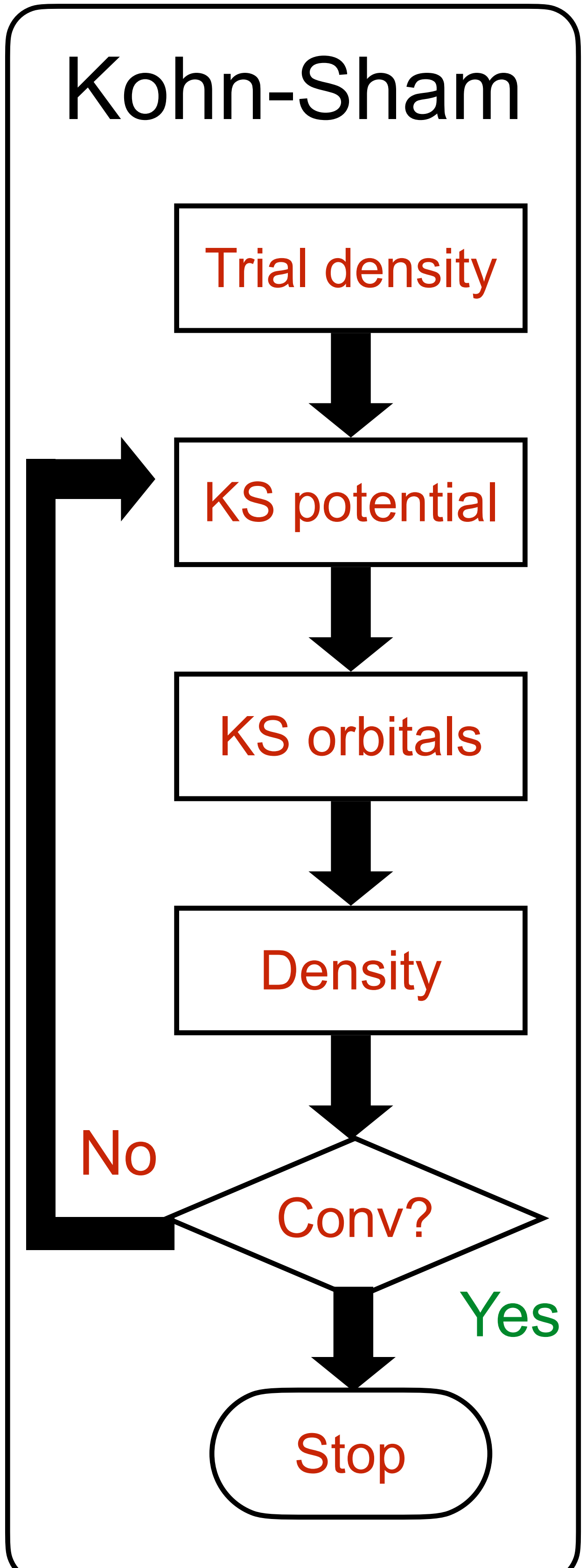
$$E[\rho] = \int d^3\boldsymbol{r} \frac{\hbar^2}{2m}\frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{2/3} \rho^{5/3} + \dots$$

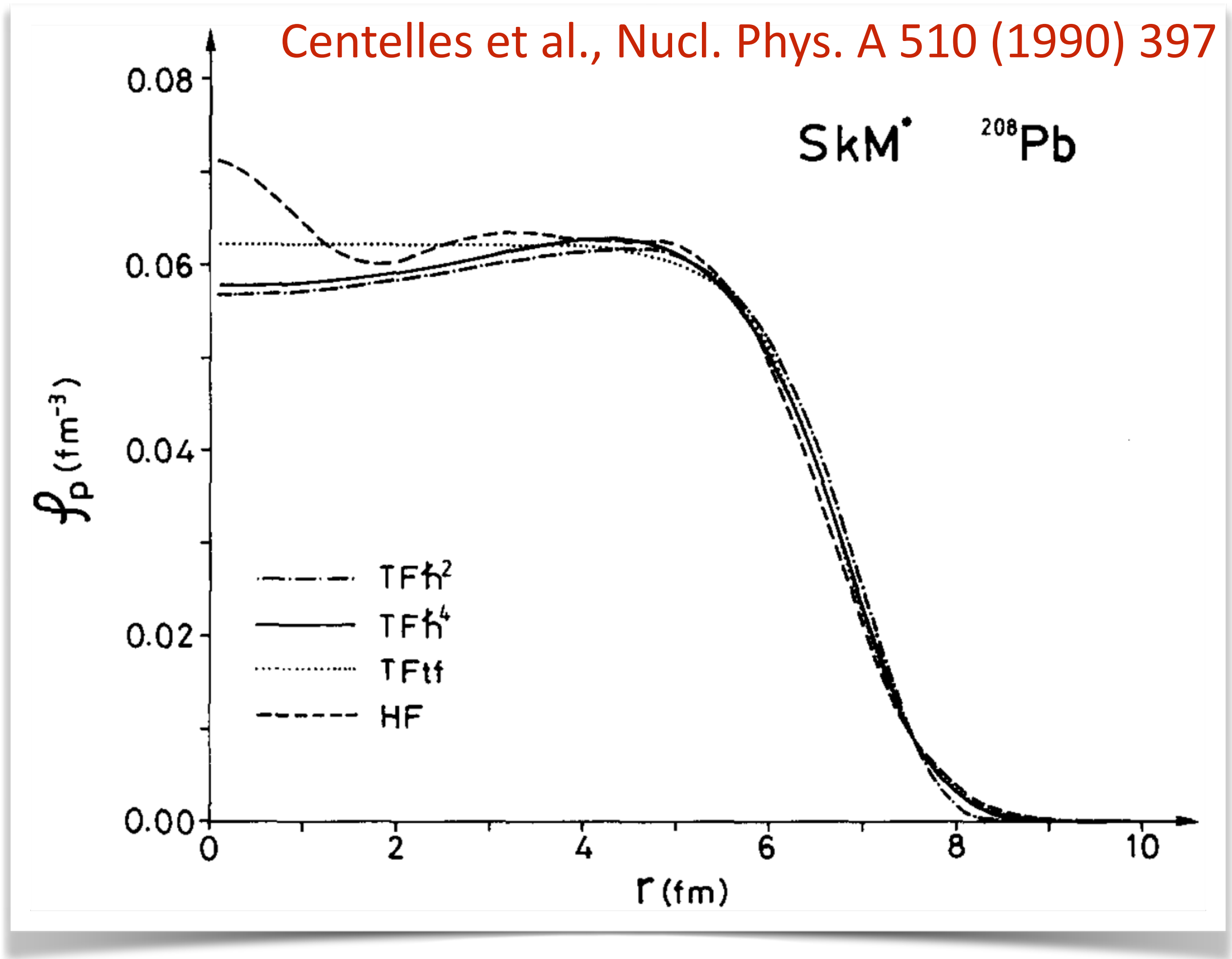
No shell effects …

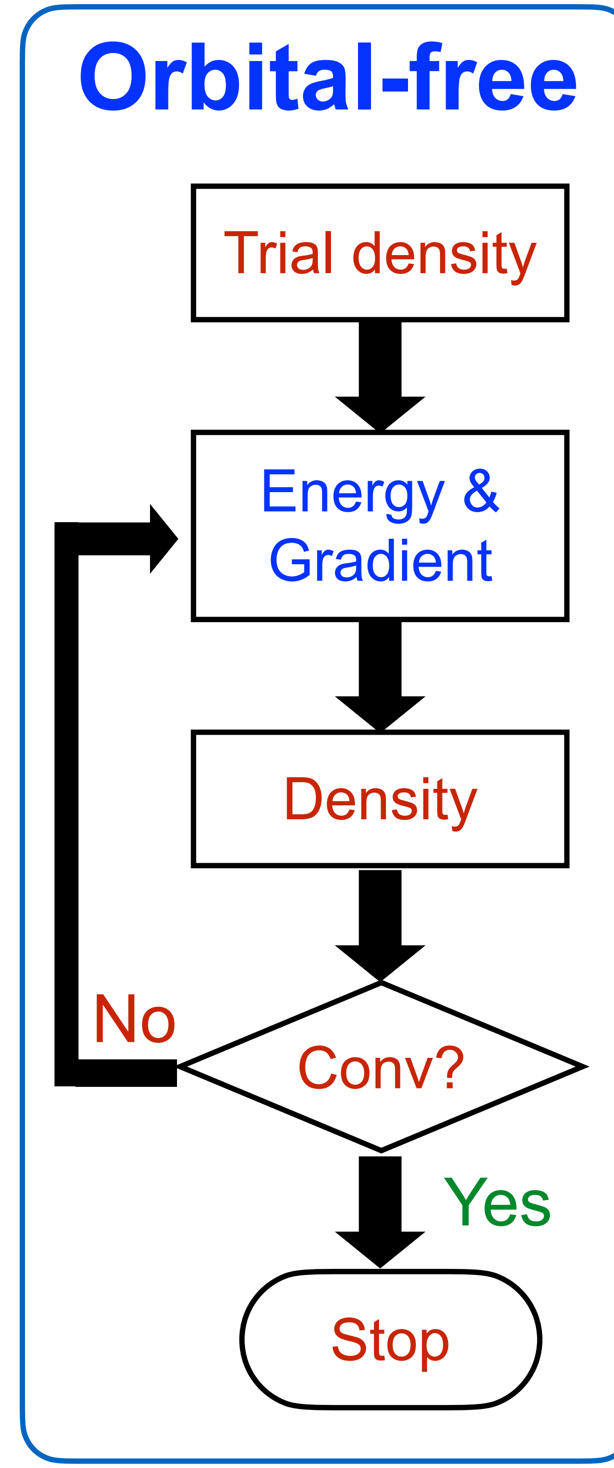


J. Chem. Phys., 114 (2001) 631

Kohn-Sham vs orbital-free for nuclei







A high accuracy orbital-free DFT?

Colò and Hagino, PTEP **2023** 103D01 (2023)

Machine learning and DFT

Condensed Matter Physics

✓ A proof of principle

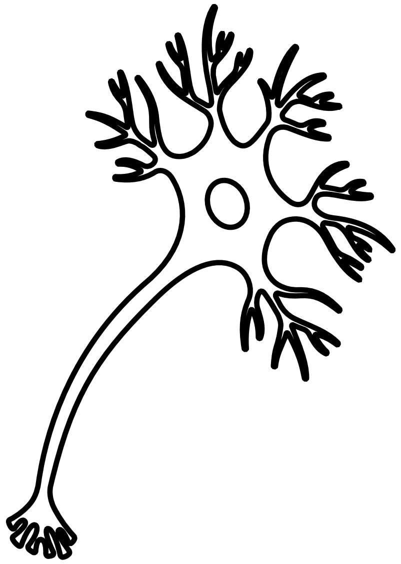
Snyder et al. PRL 108, 253002 (2012)

✓ Realistic examples for certain systems

Brockherde et al. Nat. Commun. 8, 872 (2017) …

✓ Generalization across various systems.

Li et al. PRL 126, 036401 (2021); Kirkpatrick et al. Science 374, 1385 (2021) …



Nuclear Physics

PHYSICAL REVIEW C **105**, L031303 (2022)

Letter

Nuclear energy density functionals from machine learning

X. H. Wu (吴鑫辉), Z. X. Ren (任政学), and P. W. Zhao (赵鹏巍)*

State Key Laboratory of Nuclear Physics and Technology, School of Physics, Peking University, Beijing 100871, China

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Other works: Hizawa, Hagino, Yoshida, PRC 108, 034311 (2023)

Yang, Fan, Naito, Niu, Li, and Liang PRC 108, 034315 (2023) …

Nuclear density functional from machine learning

Hohenberg-Kohn Theorem Phys. Rev. 136 B864 (1964)

✓ There exists a universal energy functional defined in terms of the density.

✓ The exact ground state is determined by minimizing this functional.

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

Walter Kohn
1998 Nobel Prize

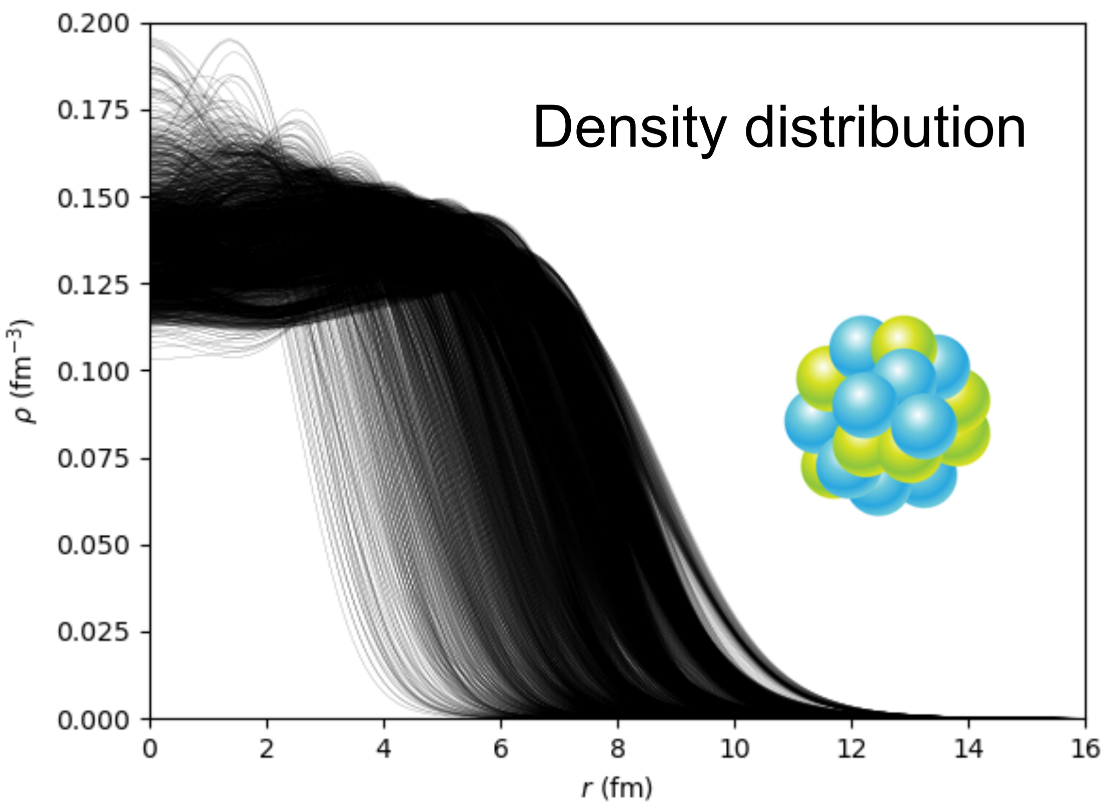
Challenges for DFT:

- ☐ The HK functional is **a priori unknown.**
- ☐ HK-DFT is in principle exact but impractical.
- ☐ Thomas-Fermi functionals are **not accurate.**

ML for DFT:

- ☑ **Regression in functional space !**
- ☑ **Interpolation !**
- ☑ **Existence theorem !**

$$\rho \rightarrow E[\rho]$$



Data set

$$E_{\text{tot}}[\rho] = E_{\text{kin}}^{\text{ML}}[\rho] + E_{\text{int}}[\rho]$$

Machine Learning Skyrme functional: SkP

We know exact kinetic energy for non-interacting systems …

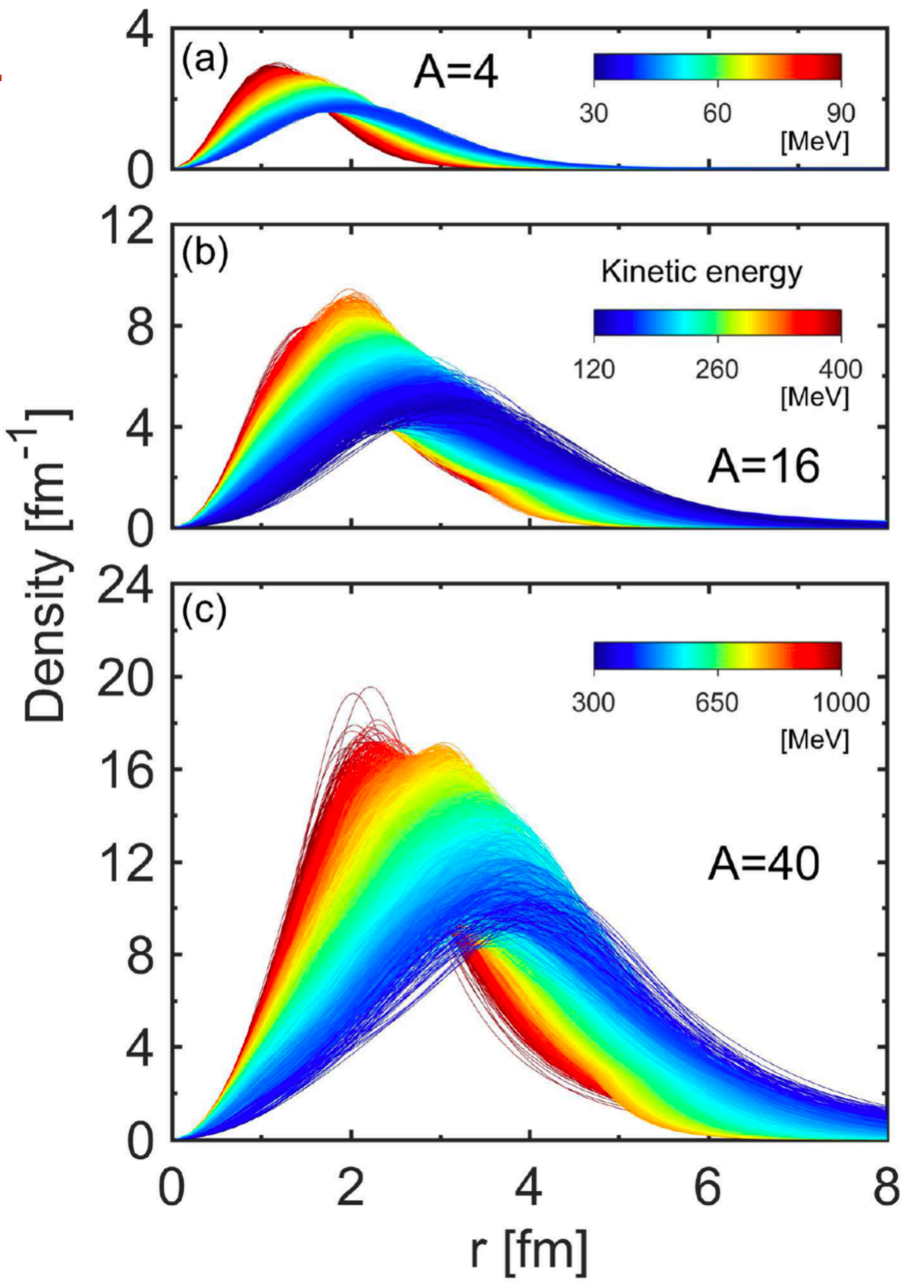
Rather than provide all available (raw) data in an unbiased way, **nuclear physics knowledge** is used to pre-process and select relevant data.

$$\rho_{sat} \simeq 0.15\,\text{fm}^{-3} \qquad \bar{T} \simeq 20\,\text{MeV}$$

Dataset:

- Training: 3×10k samples
- Validation: 3×1k samples
- Test: 3×1k samples

Wu, Ren, PWZ, PRC, 105, L031303 (2022)



Architecture

Kernel ridge regression

$$E_{\text{kin}}^{\text{ML}}[\rho(\boldsymbol{r})] = \sum_{i=1}^{m} \omega_i K(\rho_i, \rho) \qquad K(\rho, \rho') = \exp[-||\rho(\boldsymbol{r}) - \rho'(\boldsymbol{r})||^2/(2AA'\sigma^2)]$$

$$L(\boldsymbol{\omega}) = \sum_{i=1}^{m} \left(E_{\text{kin}}^{\text{ML}}[\rho_i] - E_{\text{kin}}[\rho_i]\right)^2 + \lambda||\boldsymbol{\omega}||^2$$

Loss function

$$\boldsymbol{\omega} = (\boldsymbol{K} + \lambda \boldsymbol{I})^{-1} \boldsymbol{E}_{\text{kin}}$$

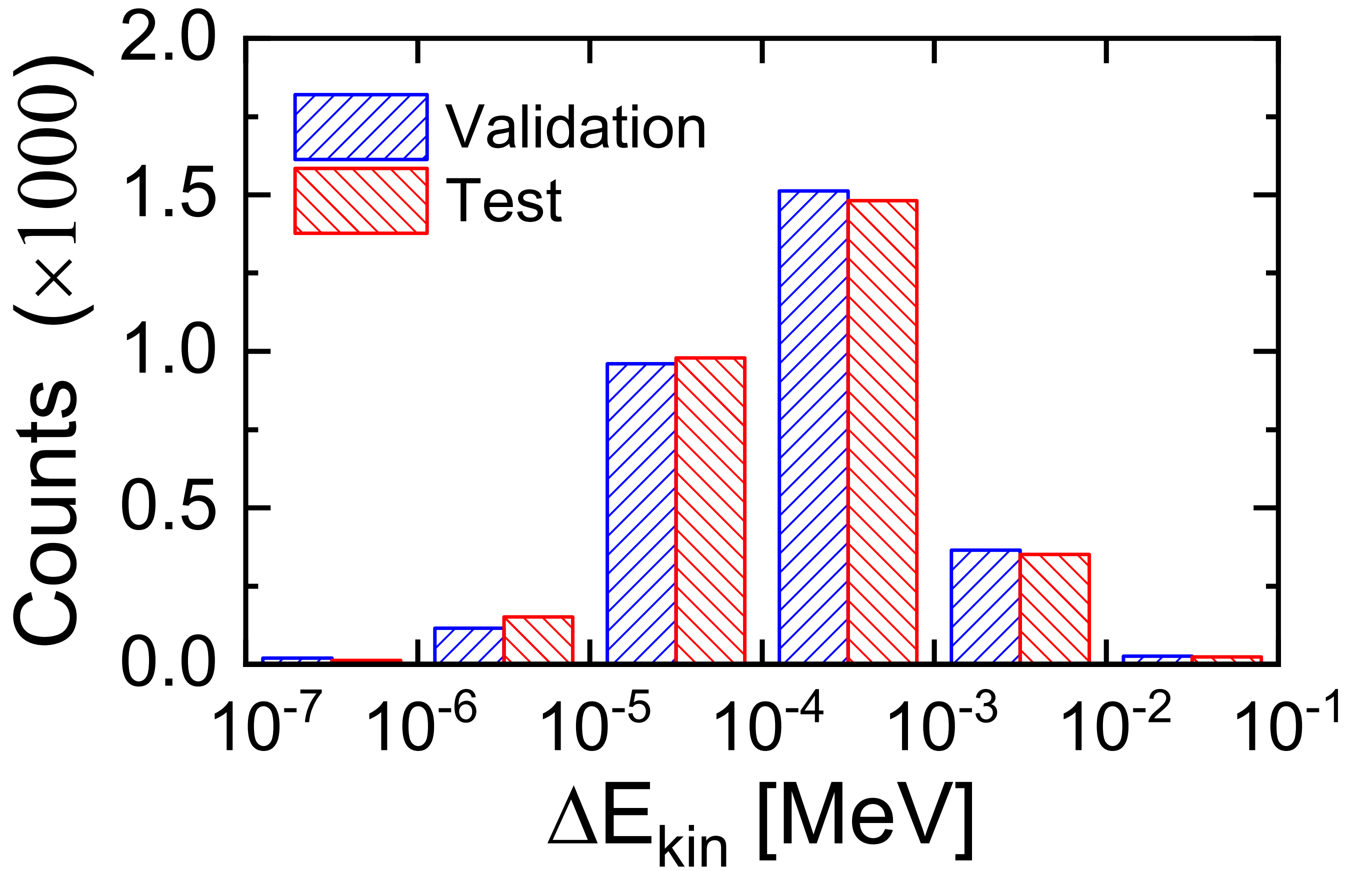
Input: ρ_i , $E_{\text{kin}}[\rho_i]$

Output: ω_i

Training set

Hyperpara. λ, σ

Validation set

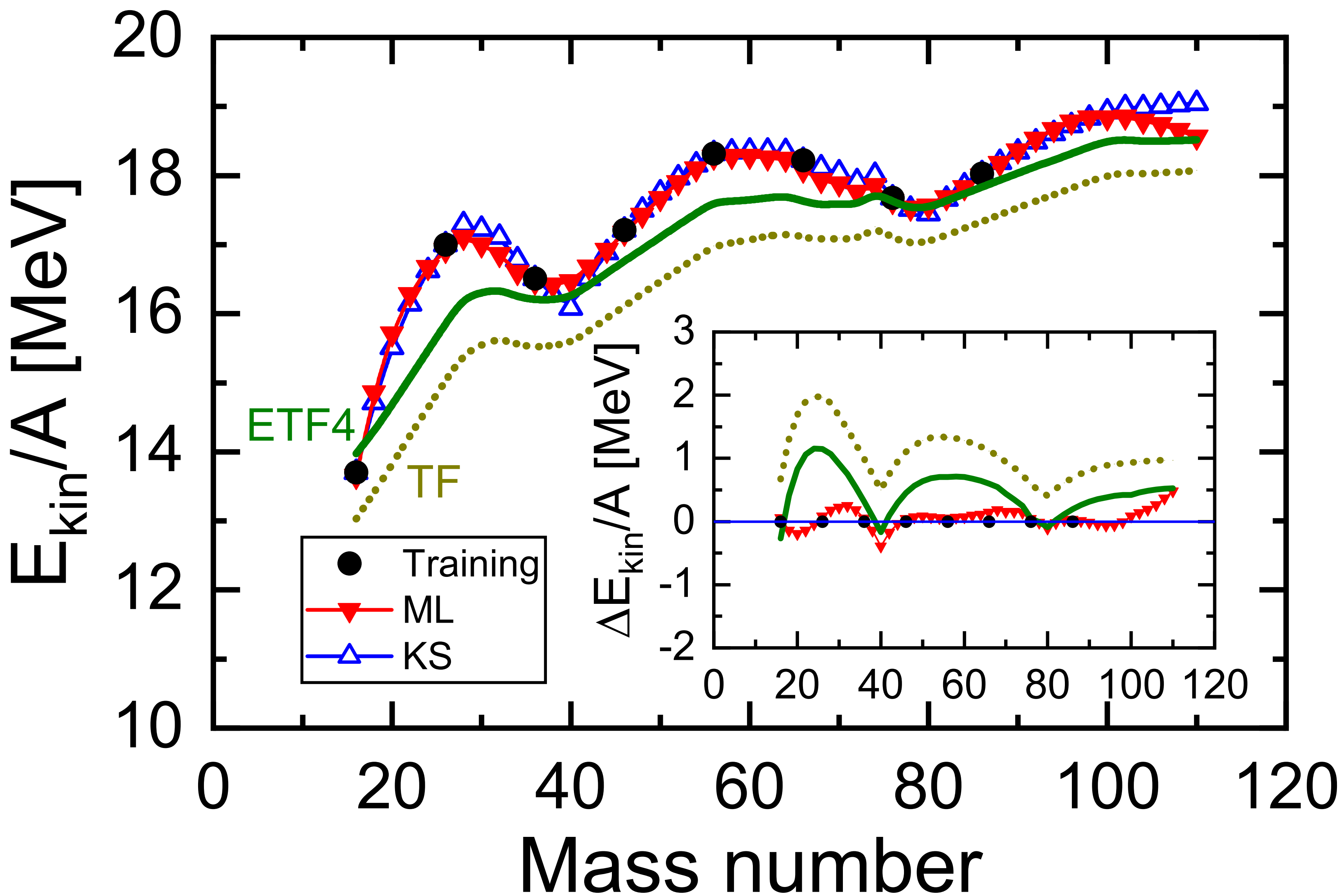


Wu, Ren, PWZ, PRC, 105, L031303 (2022)

Generalization

Trained on a small representative dataset, the model should **generalize to unseen data**.

In particular, the model has to be valid for **arbitrary system sizes**.

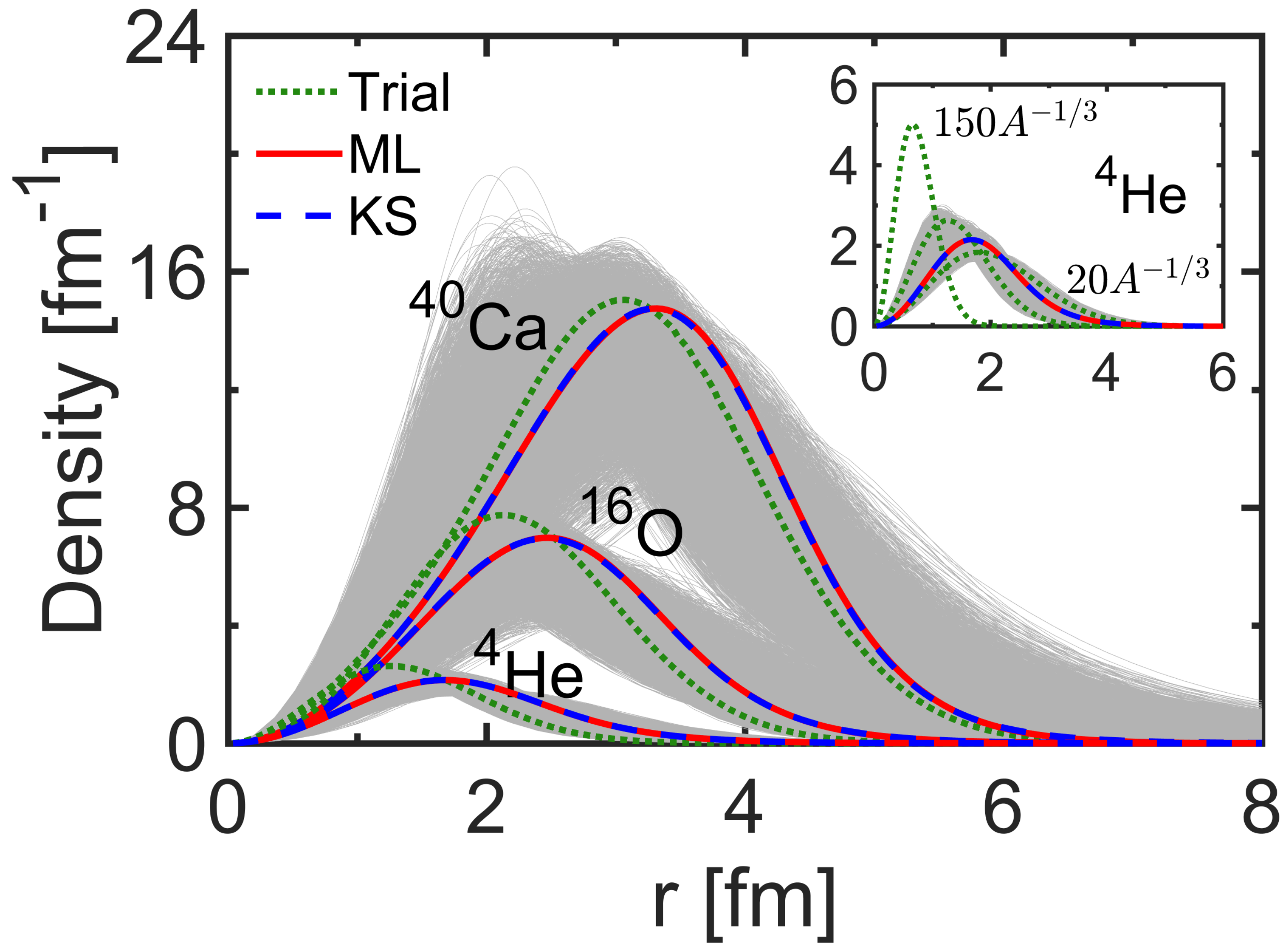


Wu, Ren, PWZ, PRC, 105, L031303 (2022)

Self-consistent ground-state density

$$E_{\text{tot}}[\rho] = E_{\text{kin}}^{\text{ML}}[\rho] + E_{\text{int}}^{\text{SkP}}[\rho]$$

Robust self-consistent solution



Wu, Ren, **PWZ**, PRC, 105, L031303 (2022)

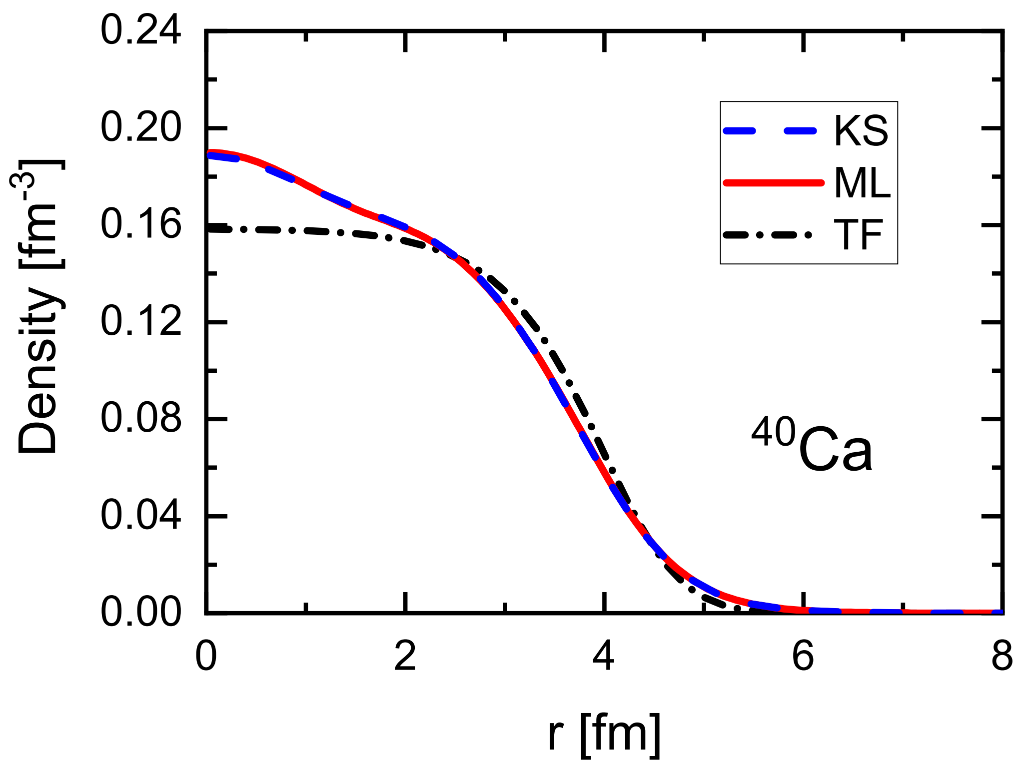
Ground-state energies and radii

Most accurate orbit-free DFT for nuclei !

Wu, Ren, PWZ, PRC, 105, L031303 (2022)

		Kohn-Sham	Machine-Learning	Experiment
^{4}He	E_{tot}	-26.3700	-26.3931 (0.0012)	-28.2957
	E_{kin}	35.2138	35.2044 (0.0056)	/
	$\langle r^2 \rangle$	2.1626	2.1628 (0.0002)	1.6755
^{16}O	E_{tot}	-127.3781	-127.1622 (0.1584)	-127.6193
	E_{kin}	219.2875	218.3458 (0.6882)	/
	$\langle r^2 \rangle$	2.8077	2.8113 (0.0047)	2.6991
^{40}Ca	E_{tot}	-342.0645	-341.8027 (0.5724)	-342.0521
	E_{kin}	643.1100	642.9145 (1.6875)	/
	$\langle r^2 \rangle$	3.4677	3.4652 (0.0055)	3.4776

TF
-372.3350
651.2168
3.3843



Extended TF results from Centelles et al., Nucl. Phys. A 510 (1990) 397

Total energies (in MeV) and neutron and proton r.m.s. radii r_n and r_p (in fm) obtained with SkM*

	E (TF$\hbar^2$)	E (TF$\hbar^4$)	E (TFtf)	E (HF)
^{40}Ca	−366.8	−349.8	−346.5	−341.1
^{90}Zr	−818.3	−792.2	−787.8	−783.0
^{208}Pb	−1671.2	−1631.9	−1626.3	−1636.6

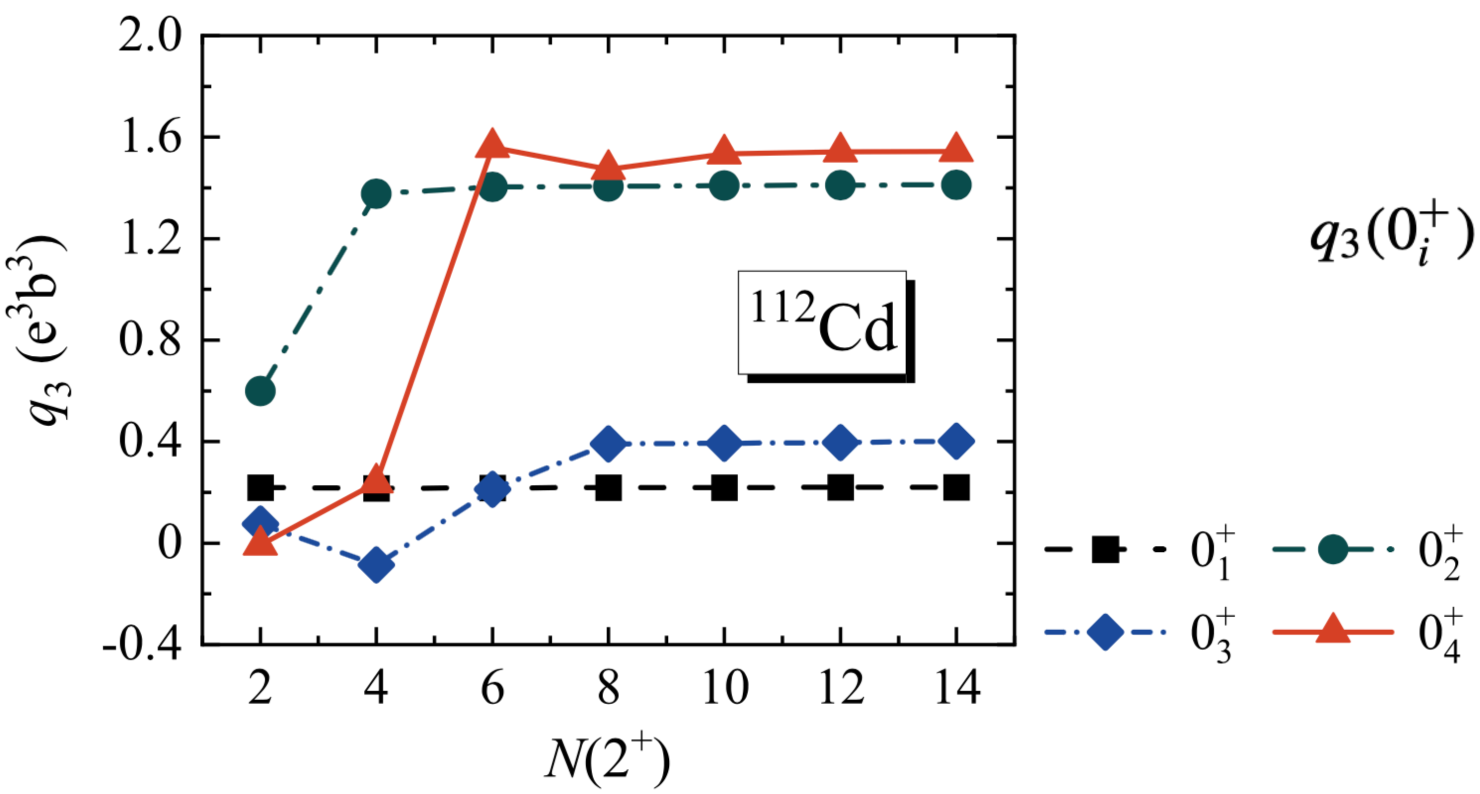
Deformed nuclei ?

Nuclear shape

- Nuclear states are the eigenstates of **Hamiltonian**, **Angular momentum**, and **Parity**.
- Nuclear states are NOT the eigenstates of **Multiple moment** $\hat{Q}_{\lambda\mu}$
- One observes only the **expectation value** and **fluctuations**

$$q_1 = \langle \hat{Q}_{2\mu} \rangle \sim \beta; \quad q_2 = \langle \hat{\boldsymbol{Q}} \cdot \hat{\boldsymbol{Q}} \rangle \sim \beta^2; \quad q_3 = \langle [\hat{\boldsymbol{Q}} \times \hat{\boldsymbol{Q}}]^{(2)} \cdot \hat{\boldsymbol{Q}} \rangle \sim \beta^3 \cos 3\gamma; \quad q_4 = \cdots\cdots$$

- Nuclear deformation influences many observables, but is not directly measured.

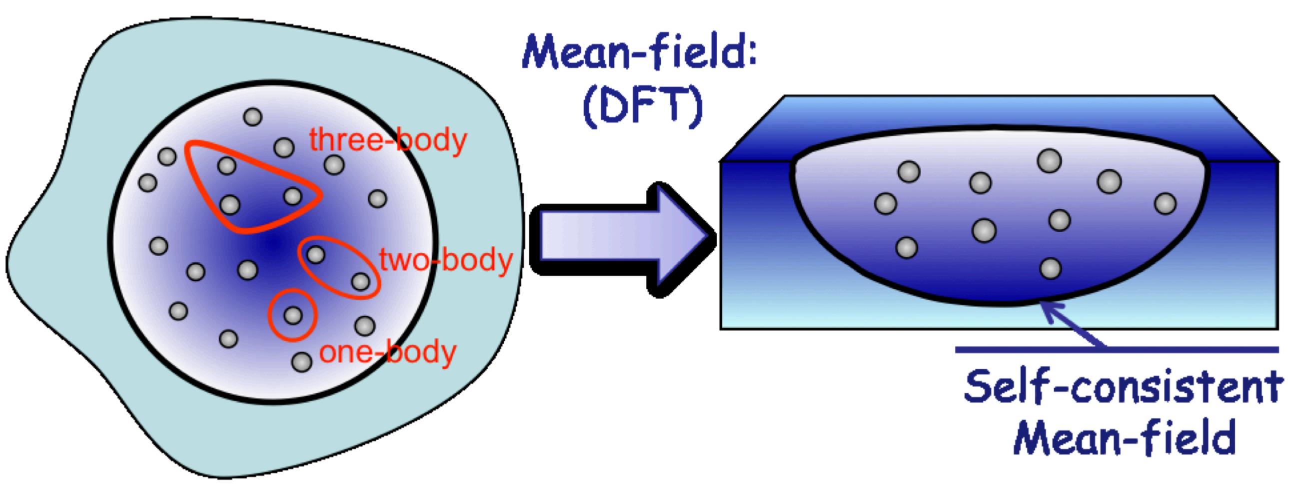


$$q_3(0_i^+) = -\sqrt{\frac{7}{10}} \sum_{jk} \langle 0_i^+ || \hat{Q}_2 || 2_j^+ \rangle \langle 2_j^+ || \hat{Q}_2 || 2_k^+ \rangle \times \langle 2_k^+ || \hat{Q}_2 || 0_i^+ \rangle,$$

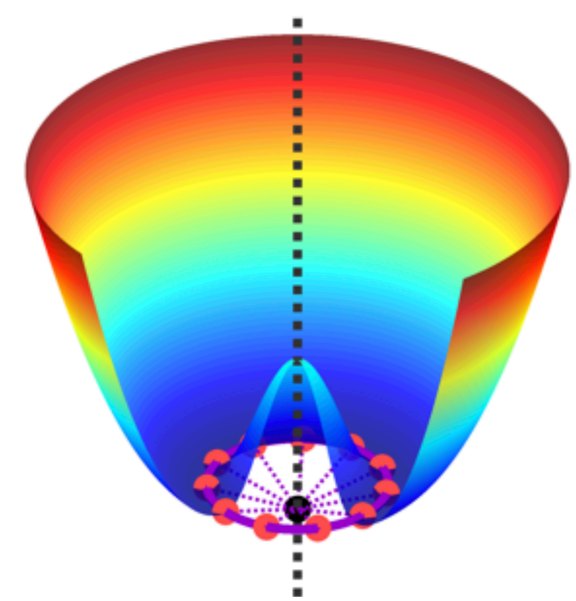
Yang, **PWZ**, Li, PRC 107, 024308 (2023)

Deformation in DFT

- Nuclei are described with the local density, introducing a **mean field**.
- Energy variation leads to a deformed density profile, which may break the symmetry of the Hamiltonian, i.e., **spontaneous symmetry breaking (SSB)**.
- **SSB:** the mean-field density breaks the Hamiltonian's symmetry to lower the total energy. The true physical ground state must **restore the symmetry**.
- **Shell effects** provide the driving force for such breaking in open-shell nuclei.

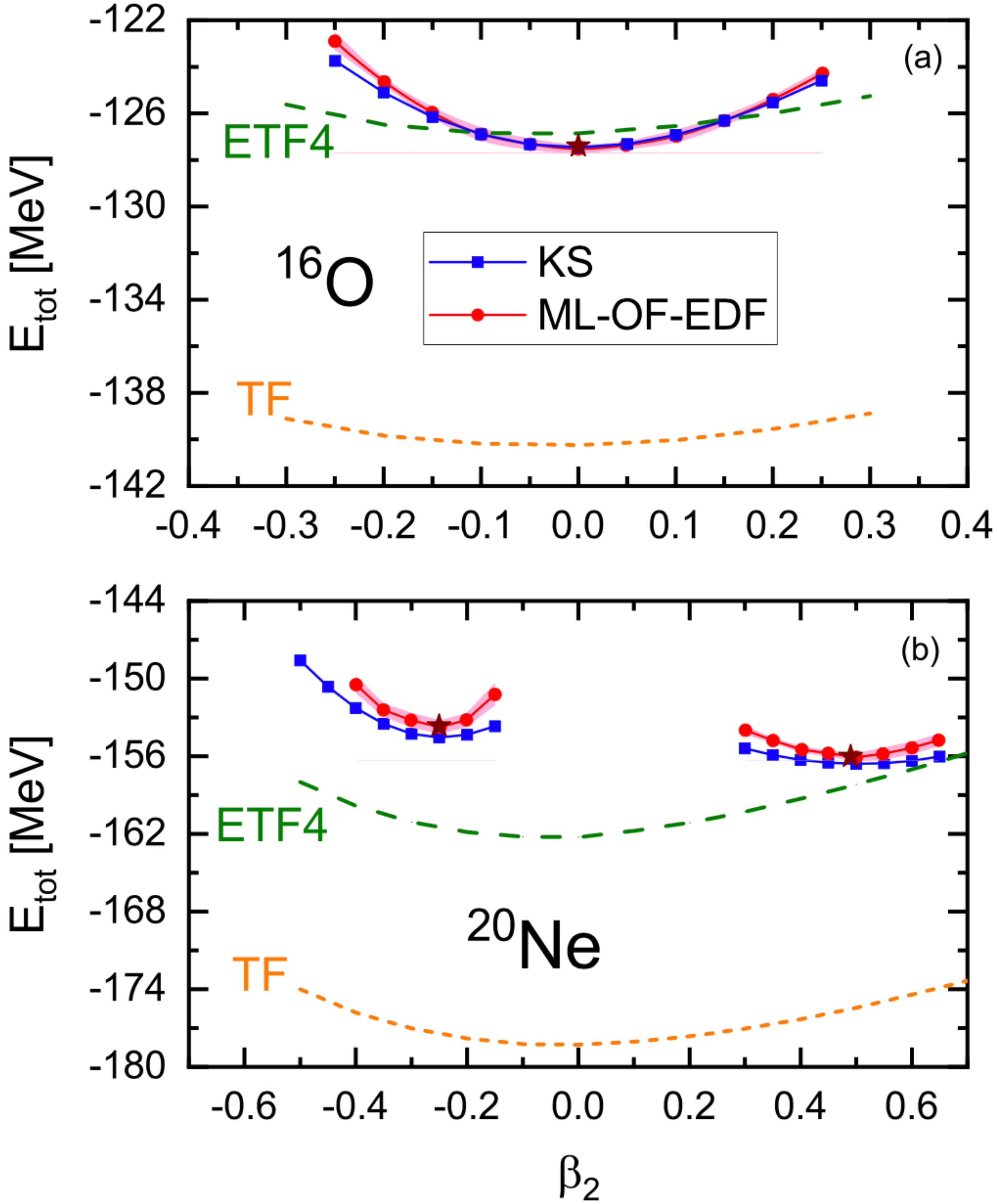


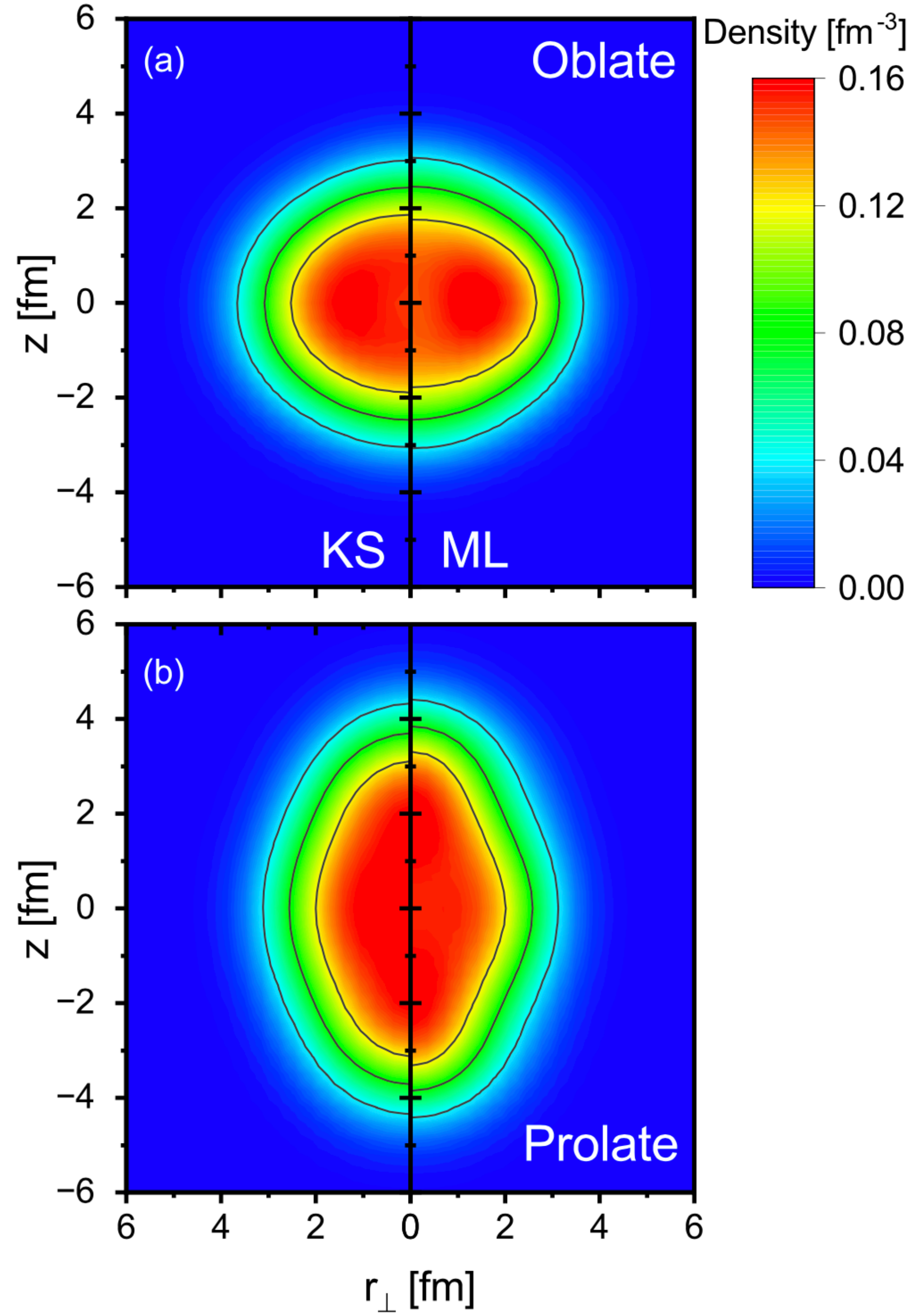
Jahn–Teller effects



赵鹏巍, 物理 48, 773 (2019)

From spherical to deformed nuclei





Wu, Ren, **PWZ**, Communications Physics 8, 316 (2025)

Summary

Machine learning has been applied to build orbital-free density functional theory for atomic nuclei.

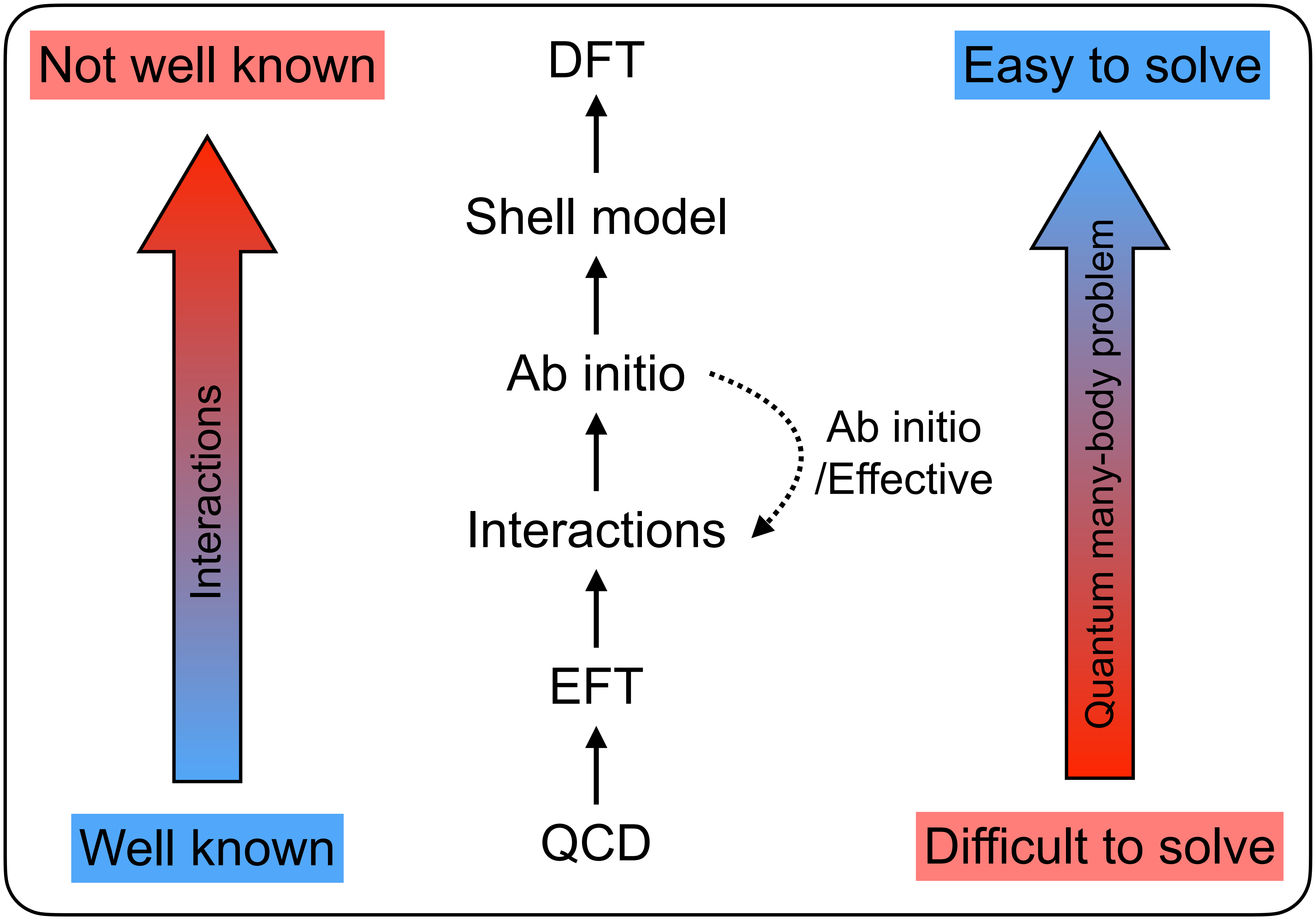
- ➢ The existing orbital-free density functional is not accurate due to the missing of quantum shell effects. **No deformation**!
- ➢ Machine Learning orbital-free DFT for nuclei.
  - ✓ robust and most accurate ever
  - ✓ works for both spherical and deformed nuclei
  - ✓ computationally efficient

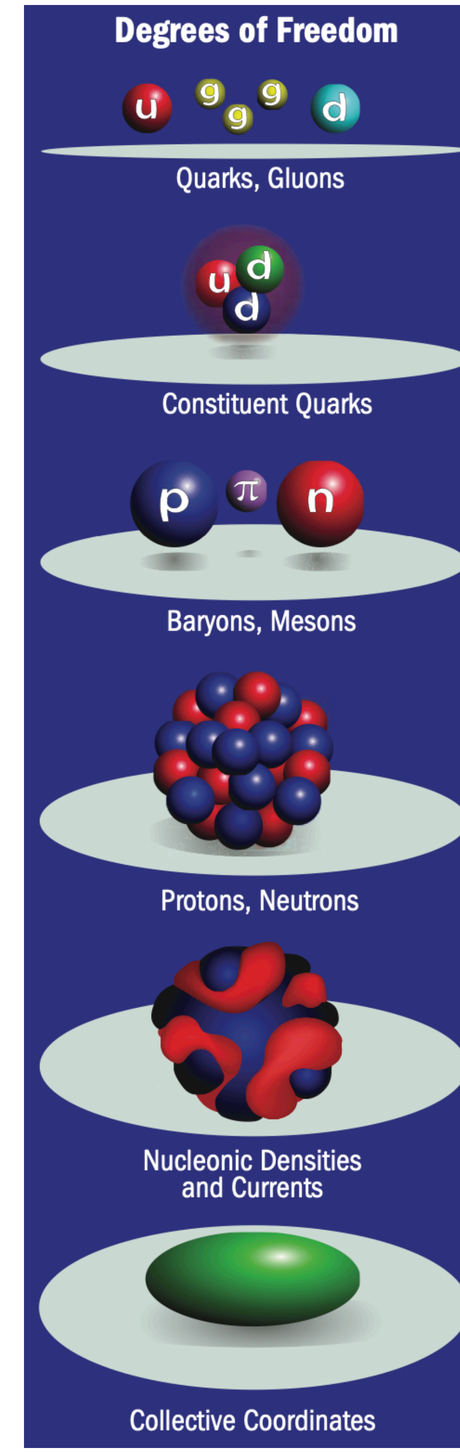
⬇ Global calculations ? Time-dependent ? Relativistic ?


Thank you.

Nuclear many-body problem

Overarching goal: *understand nuclear properties from a unified theoretical view rooted in the forces among nucleons*.





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

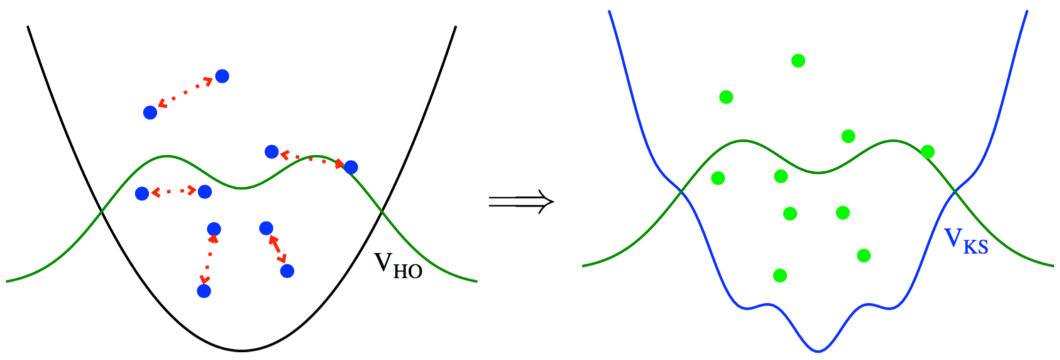


Figure from Drut PPNP 2010

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

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

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