



Nuclear chiral rotation within **R**elativistic **C**onfiguration-
interaction **D**ensity functional theory

Yakun Wang (王亚坤)

Collaborators: Jie Meng, Pengwei Zhao

Outline

- Chirality and its emergence in atomic nuclei
- Theoretical framework of ReCD theory
- Chiral rotation of ^{130}Cs within ReCD theory
- Summary and perspective

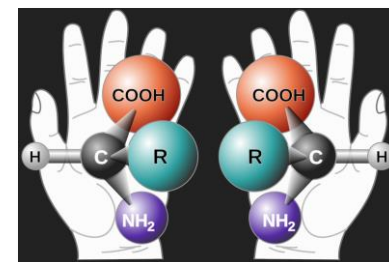
Chirality in nature

□ Chirality exists **commonly** in nature

- ✓ Macroscopic spirals of snail shells and human hands
- ✓ Biochemistry molecules
- ✓ Elementary particles

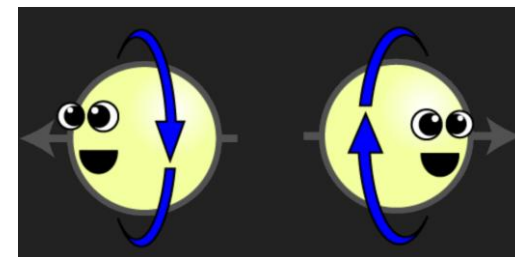


□ An object is chiral if it cannot be mapped to its **mirror image** by rotations and translations



□ Chirality and its **simultaneous breaking** is important in several branches of science:

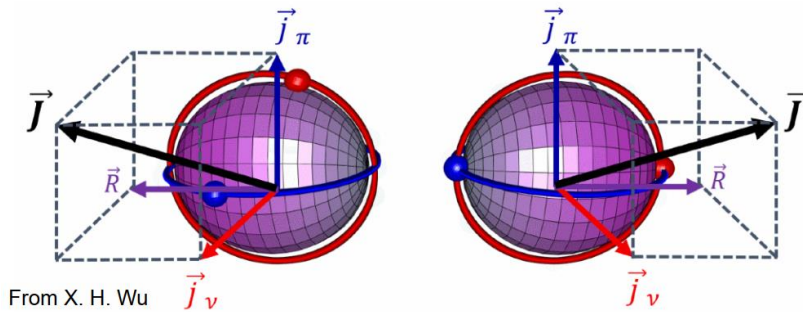
- ✓ Enantiomer of chiral drugs has **different pharmacology activity**
- ✓ Chiral materials exhibit **unique optical properties**
- ✓ **Breaking of chiral symmetry** leads to **mass generation of particles**



Chirality in atomic nuclei

- Three-dimensional rotation of triaxial nucleus presents **chiral geometry**

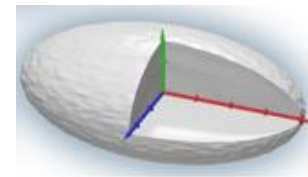
Frauendorf and Meng, NPA 617, 131 (1997)



From X. H. Wu

Left-handed $|L\rangle$

Right-handed $|R\rangle$



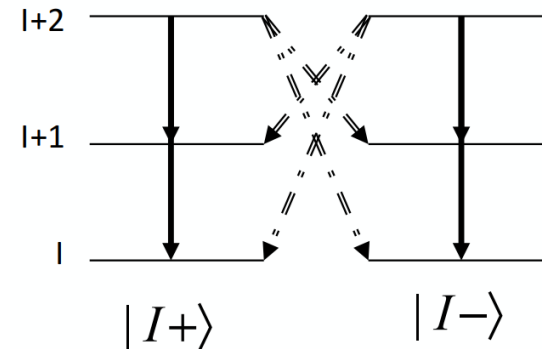
Triaxial nucleus

Intrinsic frame

Laboratory frame

Chiral symmetry restoration

$$|I+\rangle = \frac{1}{\sqrt{2}}(|L\rangle + |R\rangle), \quad |I-\rangle = \frac{i}{\sqrt{2}}(|L\rangle - |R\rangle)$$



- Degenerate energies, **similar transition probabilities** \Rightarrow **Chiral doublet bands**

First experimental evidence of chiral doublet bands

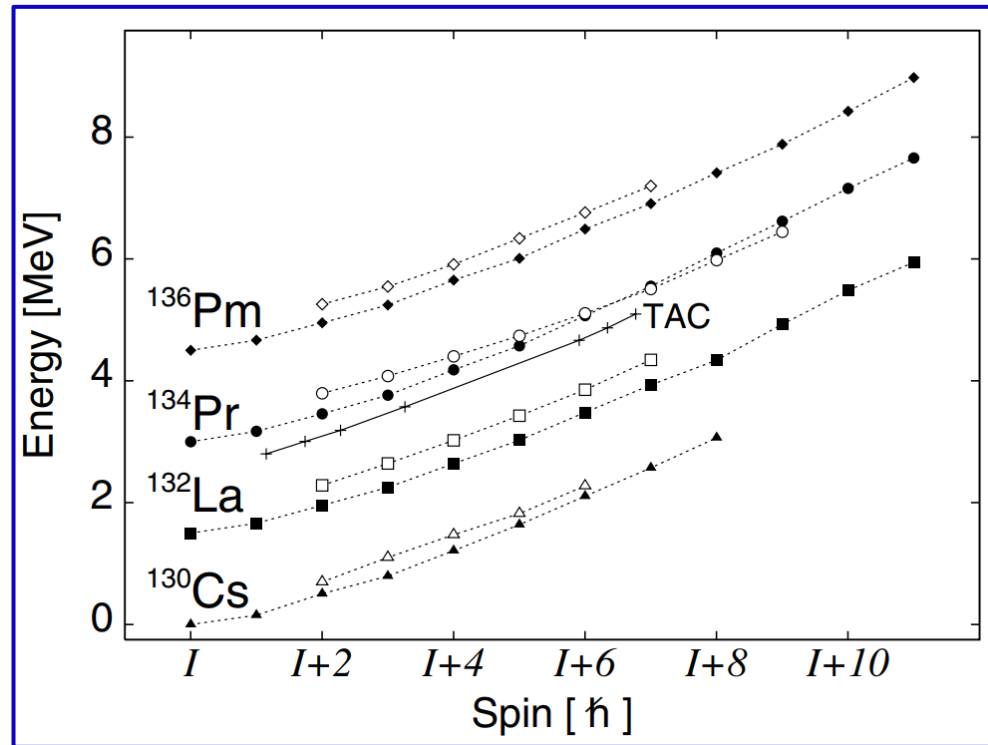
VOLUME 86, NUMBER 6

PHYSICAL REVIEW LETTERS

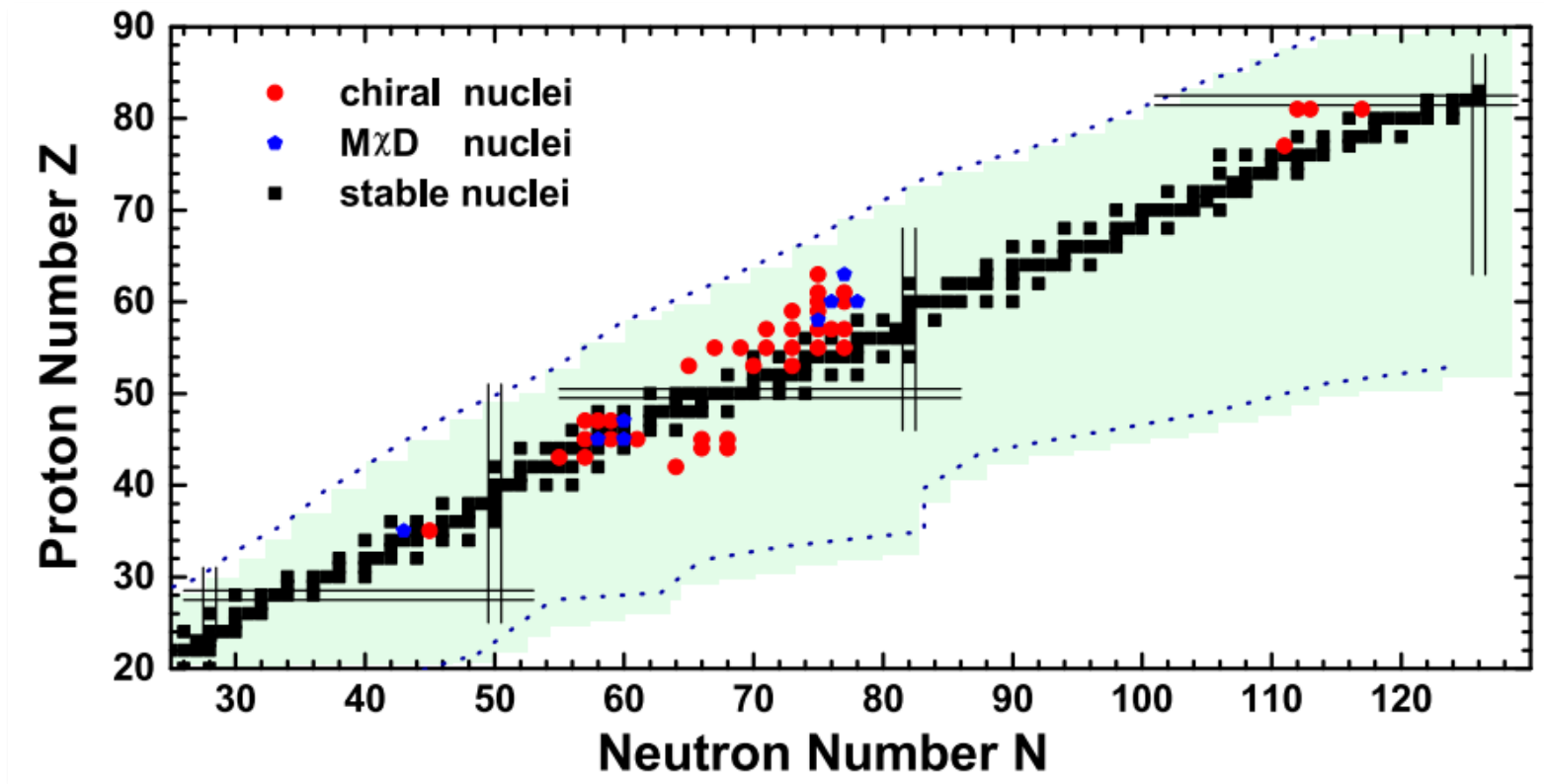
5 FEBRUARY 2001

Chiral Doublet Structures in Odd-Odd $N = 75$ Isotones: Chiral Vibrations

K. Starosta,^{1,*} T. Koike,¹ C. J. Chiara,¹ D. B. Fossan,¹ D. R. LaFosse,¹ A. A. Hecht,² C. W. Beausang,² M. A. Caprio,² J. R. Cooper,² R. Krücken,² J. R. Novak,² N. V. Zamfir,^{2,†} K. E. Zyromski,² D. J. Hartley,³ D. L. Balabanski,^{3,‡} Jing-ye Zhang,³ S. Frauendorf,⁴ and V. I. Dimitrov^{4,‡}



Experimental progress



□ More than 60 chiral doublet bands have been reported in mass regions 80, 100, 130, and 190

Xiong and Wang, ADNDT 125, 193-225 (2019)

Theoretical progress

□ Phenomenological models

✓ Particle rotor model

Frauendorf and Meng, NPA 617, 131 (1997)

Koike et al., PRL 93, 172502 (2004)

Zhang et al., PRC 044307 (2007)

Qi et al., PLB 675, 175 (2009)

✓ Generalized coherent state model

Raduta et al., JPG 43, 095107 (2016)

✓ Interacting boson fermion-fermion model

Tonev et al., PRL 96, 052501 (2006),

Brant et al., PRC 78, 034301 (2008)

Phenomenological assumptions,
parameters fitted to the data

□ Microscopic models

✓ Tilted axis cranking (TAC) model

Frauendorf and Meng, NPA 617, 131 (1997)

Dimitrov et al., PRL 84, 5732 (2000)

✓ TAC+random phase approximation, and collective Hamiltonian

Mukhopadhyay et al., PRL 99, 172501 (2007)

Almehed et al., PRC 83, 054308 (2011)

Q. B. Chen et al., PRC 87, 024314 (2013)

Q. B. Chen et al., PRC 94, 044301 (2016)

✓ Triaxial projected shell model

F. Q. Chen et al., PLB 785, 211 (2018)

YKW et al., PRC 99, 054303 (2019)

Single-j or PPQQ Hamiltonian,
limited predictive power

Nuclear chirality in density functional theory

□ Nonrelativistic density functional theory (DFT) + TAC

Olbratowski et al., PRL 93, 052501 (2004)

Olbratowski et al., PRC 73, 054308 (2006)

□ Relativistic DFT (RDFT)+ TAC

Zhao, PLB 773, 1 (2017)

Zhao et al., PRC 99, 054319 (2019)

Wang and Meng, PLB 841, 137923 (2023)

□ Time-dependent RDFT+TAC

Ren et al., PRC 105, L011301 (2022)

✓ Self-consistent method based on more realistic interactions

✓ Core polarization + nuclear currents

✗ Only the **lower energy band** can be described

✗ Transition probabilities and spin treated in a **semiclassical** way

✓ Simultaneous description for the energies of lower and upper bands

✗ **Semiclassical** treatment of transition probabilities and spin

Description of nuclear chirality in a fully **microscopic** and **quantal** way based on the DFT is highly desirable!

The present work

- Relativistic Configuration-interaction Density functional (ReCD) theory is adopted to study the nuclear chirality:
 - ✓ ReCD combines the advantages of configuration-interaction shell model and relativistic DFT \Rightarrow Simultaneous description of chiral doublet bands based on microscopic two-body interactions
 - ✓ The broken rotational symmetry is restored by three-dimensional angular momentum projection technique \Rightarrow quantal description of spectra and transition probabilities

RDFT

Relativistic Lagrangian density and Hamiltonian:

$$(\bar{\psi} \mathcal{O} \Gamma \psi), \quad \mathcal{O} \in \{1, \tau\}$$

$$\Gamma \in \{1, \gamma_\mu, \gamma_5, \cancel{\gamma_\mu \gamma_5}, \sigma_{\mu\nu}\}$$



$$\mathcal{L} = \mathcal{L}^{\text{free}} + \mathcal{L}^{4f} + \mathcal{L}^{\text{der}} + \mathcal{L}^{\text{hot}} + \mathcal{L}^{\text{em}}$$

$$\hat{H} = \int d\mathbf{r} \mathcal{H}(\mathbf{r})$$

Relativistic density functional:

$$E \equiv \langle \Phi | \hat{H} | \Phi \rangle = \int d\mathbf{r} \left\{ \sum_{i=1}^A \psi_i^\dagger (\boldsymbol{\alpha} \cdot \mathbf{p} + \beta m) \psi_i + \frac{1}{2} \alpha_S \rho_s^2 + \frac{1}{3} \beta_S \rho_s^3 + \frac{1}{4} \gamma_S \rho_s^4 + \frac{1}{2} \delta_S \rho_s \Delta \rho_s \right.$$

$$\left. + \frac{1}{2} \alpha_V j_\mu j^\mu + \frac{1}{4} \gamma_V (j_\mu j^\mu)^2 + \frac{1}{2} \delta_V j_\mu \Delta j^\mu + \frac{1}{2} \alpha_{TV} \vec{j}_\mu \vec{j}^\mu + \frac{1}{2} \delta_{TV} \vec{j}_\mu \Delta \vec{j}^\mu + \frac{1}{2} e^2 A_\mu j^\mu \right\}$$

Relativistic Hartree-Bogoliubov (RHB) equation:

$$\begin{pmatrix} h_D - \lambda & \Delta \\ -\Delta^* & -h_D^* + \lambda \end{pmatrix} = E_k \begin{pmatrix} U_k \\ V_k \end{pmatrix}$$

$$h_D = \boldsymbol{\alpha} \cdot \mathbf{p} + \beta(m + S) + V$$

$$\Delta_{\mu\nu} = \frac{1}{2} \sum_{\delta\gamma} \langle \mu\nu | V^{pp} | \delta\gamma \rangle \alpha_\kappa \delta_{\delta\gamma}$$

Intrinsic ground-state for odd-odd nucleus: $|\Phi_{\pi_0\nu_0}\rangle = \hat{\beta}_{\pi_0}^\dagger \hat{\beta}_{\nu_0}^\dagger |\Phi_0\rangle$

ReCD theory

□ Configuration space:

$$|\Phi_\kappa\rangle \in \{|\Phi_{\pi_0\nu_0}\rangle, \hat{\beta}_{\pi_i}^\dagger \hat{\beta}_{\nu_j}^\dagger |\Phi_0\rangle, \hat{\beta}_{\pi_i}^\dagger \hat{\beta}_{\nu_j}^\dagger \hat{\beta}_{\nu_k}^\dagger \hat{\beta}_{\nu_l}^\dagger |\Phi_0\rangle, \hat{\beta}_{\pi_i}^\dagger \hat{\beta}_{\nu_j}^\dagger \hat{\beta}_{\pi_k}^\dagger \hat{\beta}_{\pi_l}^\dagger |\Phi_0\rangle\}.$$

□ Wavefunction in ReCD theory:

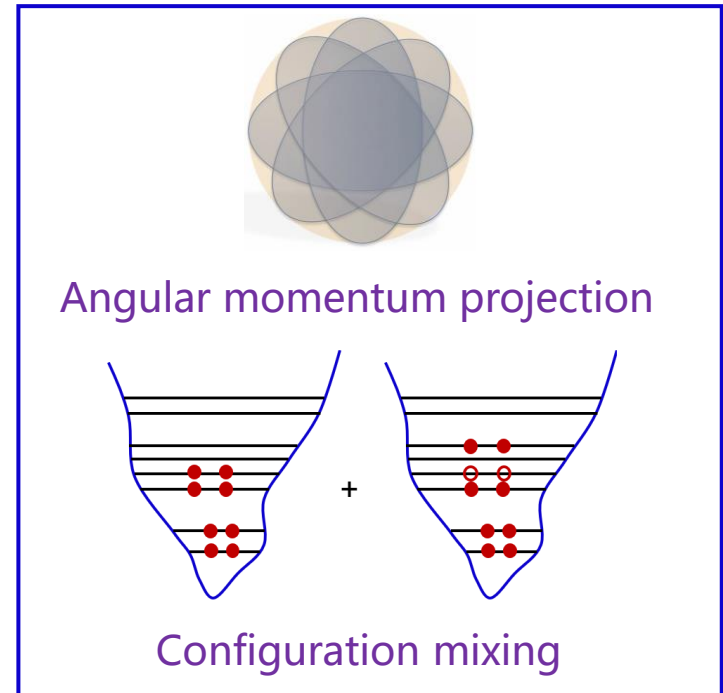
$$|\Psi_\alpha^I\rangle = \sum_{K=-I}^I \sum_{\kappa} f_{K\kappa}^{I\alpha} \hat{P}_{MK}^I |\Phi_\kappa\rangle$$

□ Hill-Wheeler equation:

$$\sum_{K'\kappa'} \{ \mathcal{H}_{KK';\kappa\kappa'}^I - E_\alpha^I \mathcal{N}_{KK';\kappa\kappa'}^{I\alpha} \} f_{K'\kappa'}^{I\alpha} = 0$$

□ Transition probabilities:

$$\frac{1}{2I_i + 1} |\langle \Psi^{I_f} | \hat{O}_\lambda | \Psi^{I_i} \rangle|^2$$



ReCD theory: residual interaction and the intrinsic states come from a universal density functional, and no truncation is adopted to the model space

The applications of ReCD theory

□ Spectroscopic properties

Zhao, Ring, Meng, PRC 94, 041301 (R) (2016)

YKW, Zhao, Meng, PRC 105, 054311 (2022)

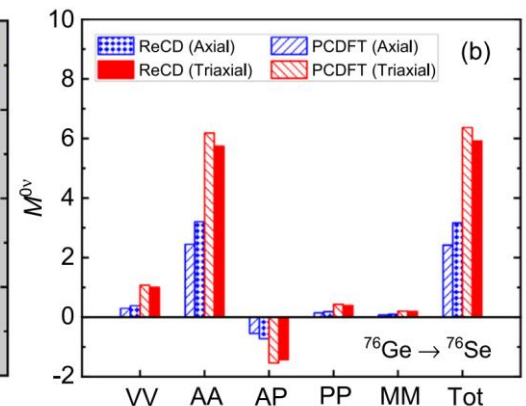
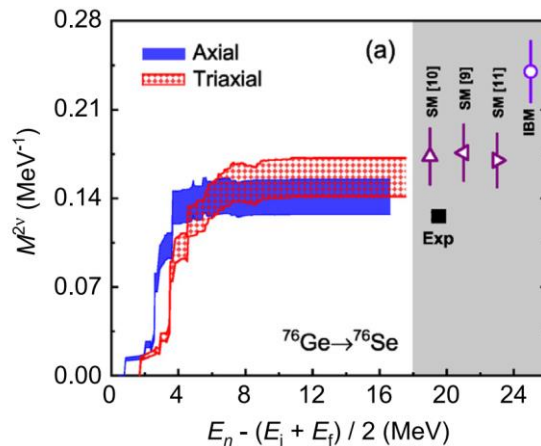
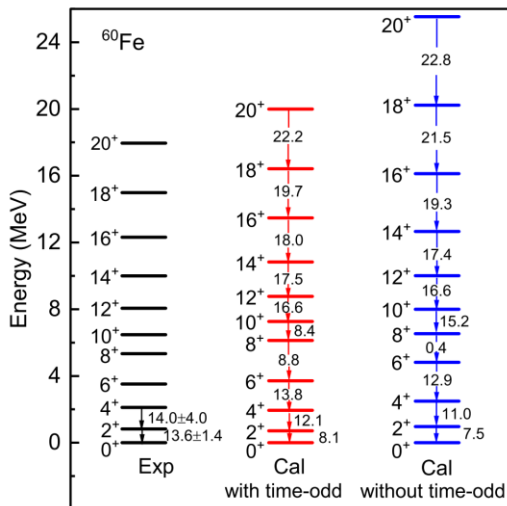
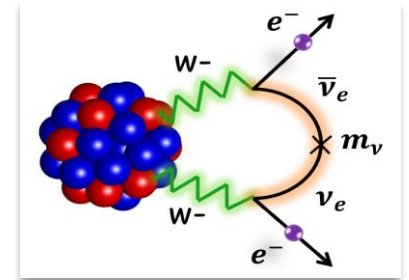
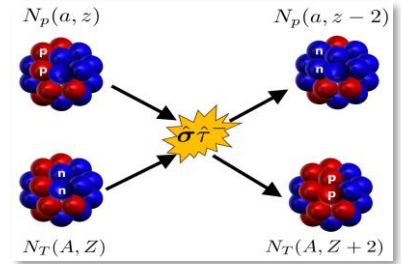
YKW, Zhao, Meng, PLB 848, 138346 (2024)

□ Double Gamow-Teller transitions

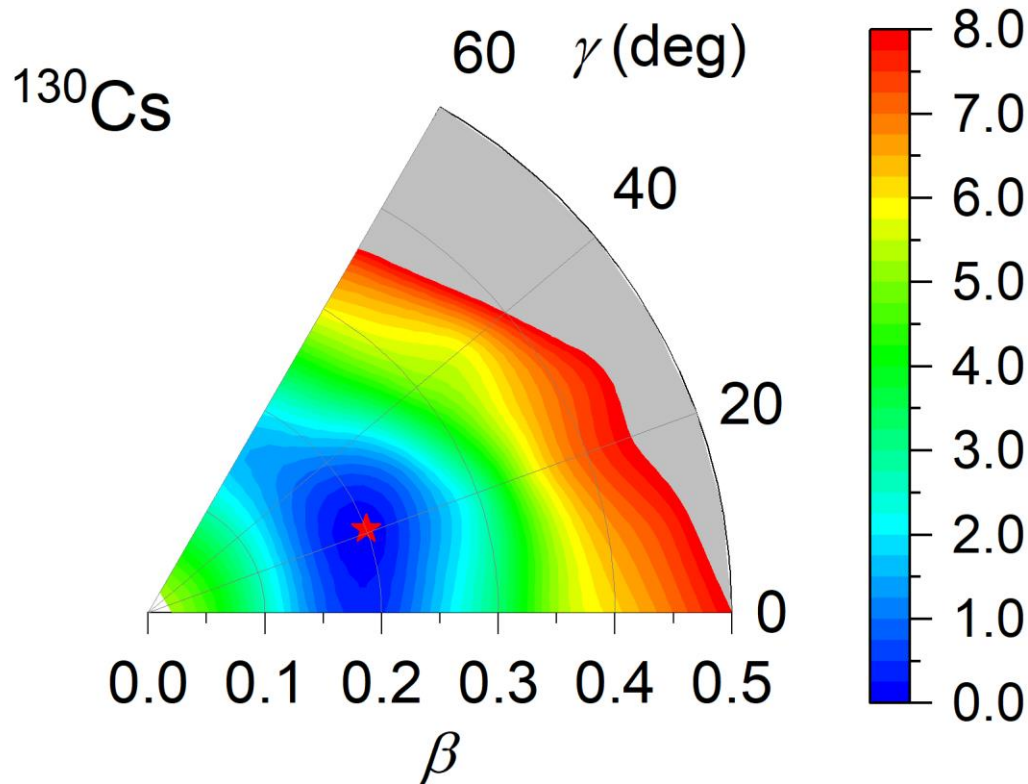
YKW, Zhao, Meng, PLB 855, 138796 (2024)

□ Two neutrino and neutrinoless $\beta\beta$ decay

YKW, Zhao, Meng, SB 69, 2017-2020 (2024)

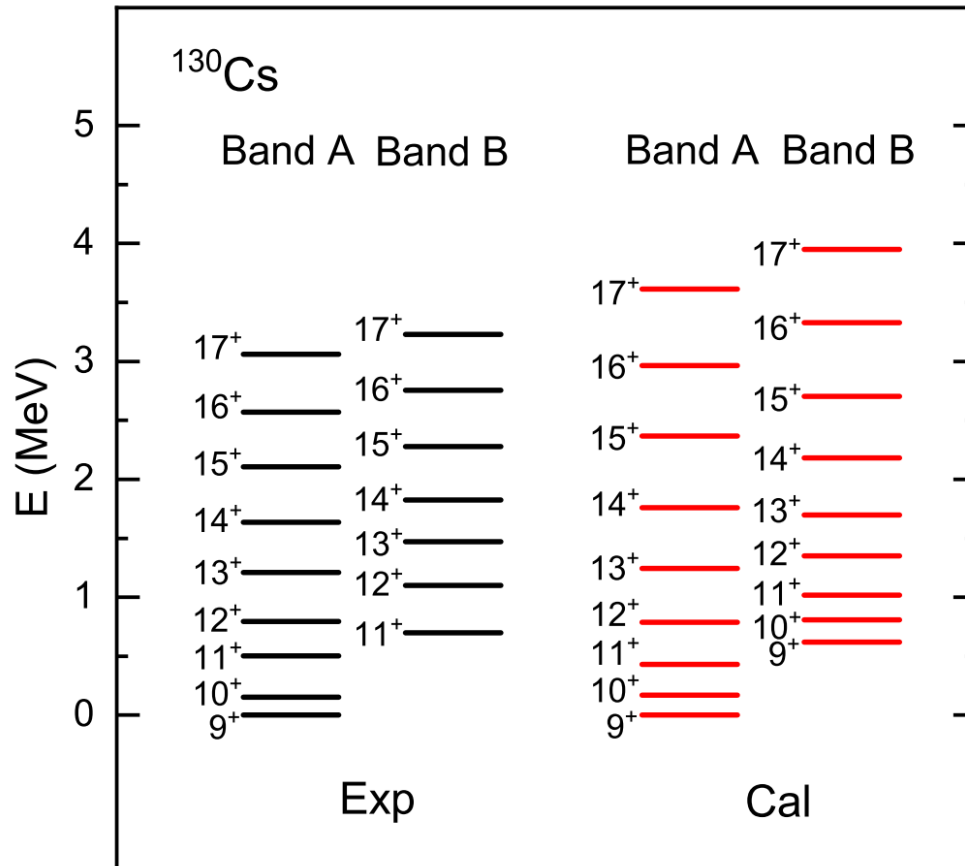


Potential energy surface



- Deformation parameters β and γ of odd-odd nucleus ^{130}Cs are predicted to be 0.20 and 21°

Energy spectra



YKW, Zhao, Meng, PLB 848, 138346 (2024)

✓ Intrinsic model space:

$$|\Phi_{\pi_0\nu_0}\rangle$$

$$\hat{\beta}_{\pi_i}^\dagger \hat{\beta}_{\nu_j}^\dagger |\Phi_0\rangle$$

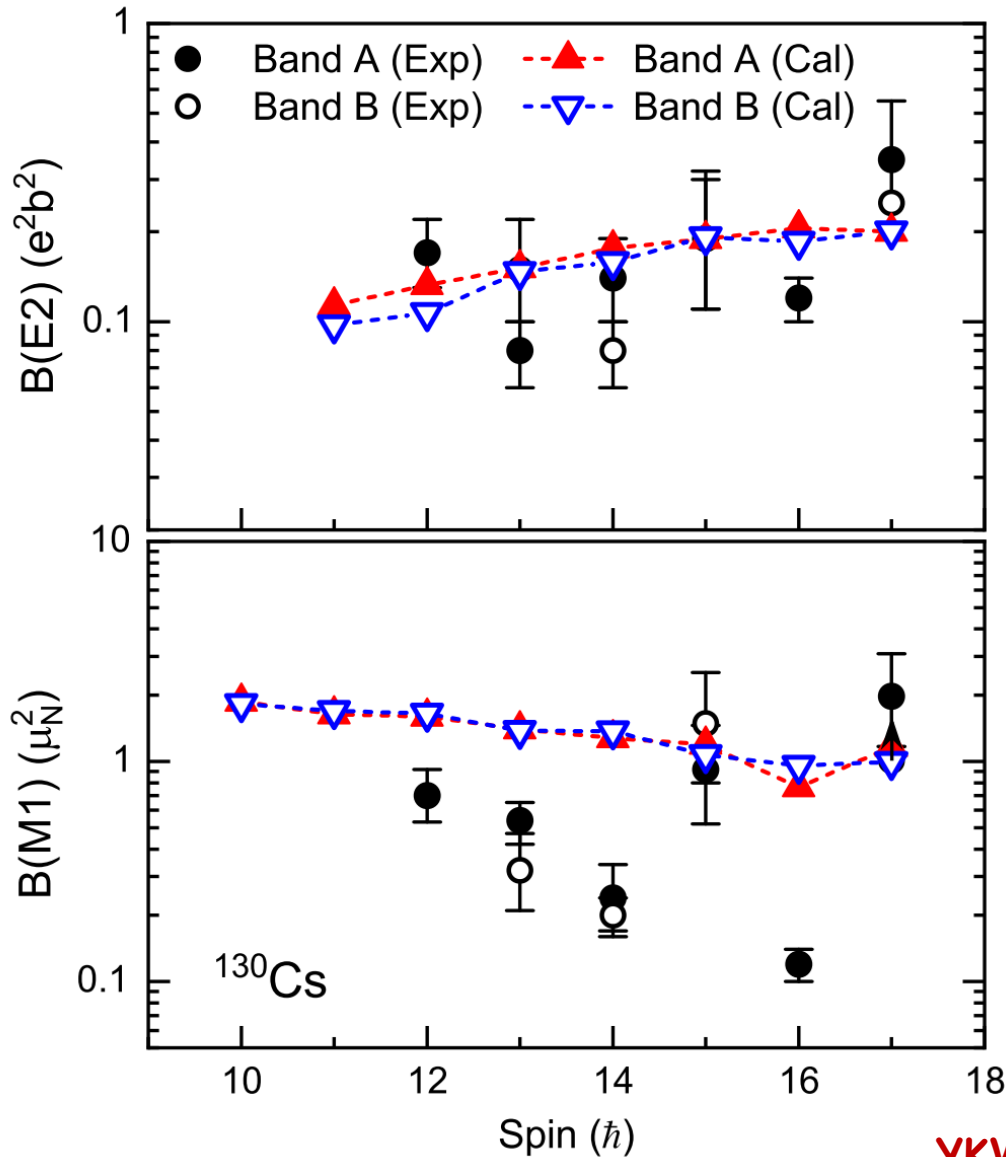
$$\hat{\beta}_{\pi_i}^\dagger \hat{\beta}_{\nu_j}^\dagger \hat{\beta}_{\nu_k}^\dagger \hat{\beta}_{\nu_l}^\dagger |\Phi_0\rangle$$

$$\hat{\beta}_{\pi_i}^\dagger \hat{\beta}_{\nu_j}^\dagger \hat{\beta}_{\pi_k}^\dagger \hat{\beta}_{\pi_l}^\dagger |\Phi_0\rangle\}$$

✓ Energy cutoff: 5.0 MeV

- The energy spectra for both the yrast and side bands in ^{130}Cs are reproduced satisfactorily by the ReCD calculations

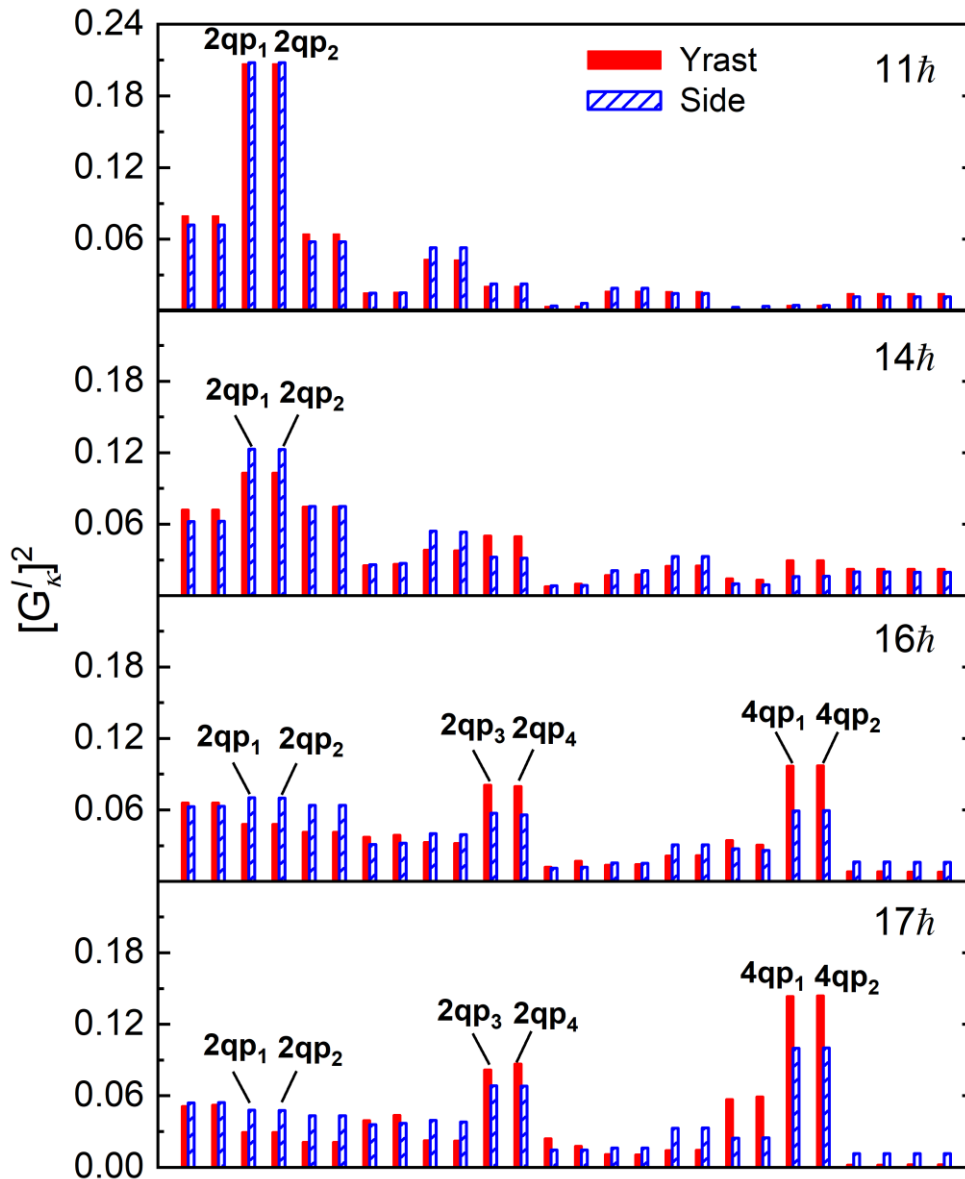
Transition probabilities



- The $B(E2)$ and $B(M1)$ values are reproduced satisfactorily
- Transition probabilities for yrast and side bands are predicted to be similar
- No effective charges are used in the calculation
- The calculated staggering behaviors for $M1$ transitions for states with spin larger than $14\hbar$ are much weaker than data

YKW, Zhao, Meng, PLB 848, 138346 (2024)

Composition of wavefunctions



$$G_{\kappa}^I = \sum_K \sum_{\kappa' K'} N_{\kappa K; \kappa' K'}^{1/2} F_{\kappa' K'}^I$$

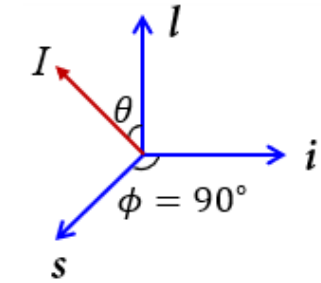
Label	Configuration
2qp ₁	$\pi(h_{11/2;1/2}) \otimes \nu(h_{11/2;9/2})$
2qp ₂	$\pi(h_{11/2;1/2}) \otimes \nu(h_{11/2;-9/2})$
2qp ₃	$\pi(h_{11/2;1/2}) \otimes \nu(h_{11/2;5/2})$
2qp ₄	$\pi(h_{11/2;1/2}) \otimes \nu(h_{11/2;-5/2})$
4qp ₁	$\pi(h_{11/2;1/2}) \otimes \nu(h_{11/2;9/2}h_{11/2;7/2}h_{11/2;-7/2})$
4qp ₂	$\pi(h_{11/2;1/2}) \otimes \nu(h_{11/2;-9/2}h_{11/2;7/2}h_{11/2;-7/2})$

Four qp configurations begin to play dominant roles for states with $I = 16\hbar$ and $17\hbar$

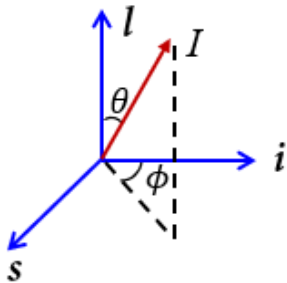
YKW, Zhao, Meng, PLB 848, 138346 (2024)

Chiral geometry: A-plot

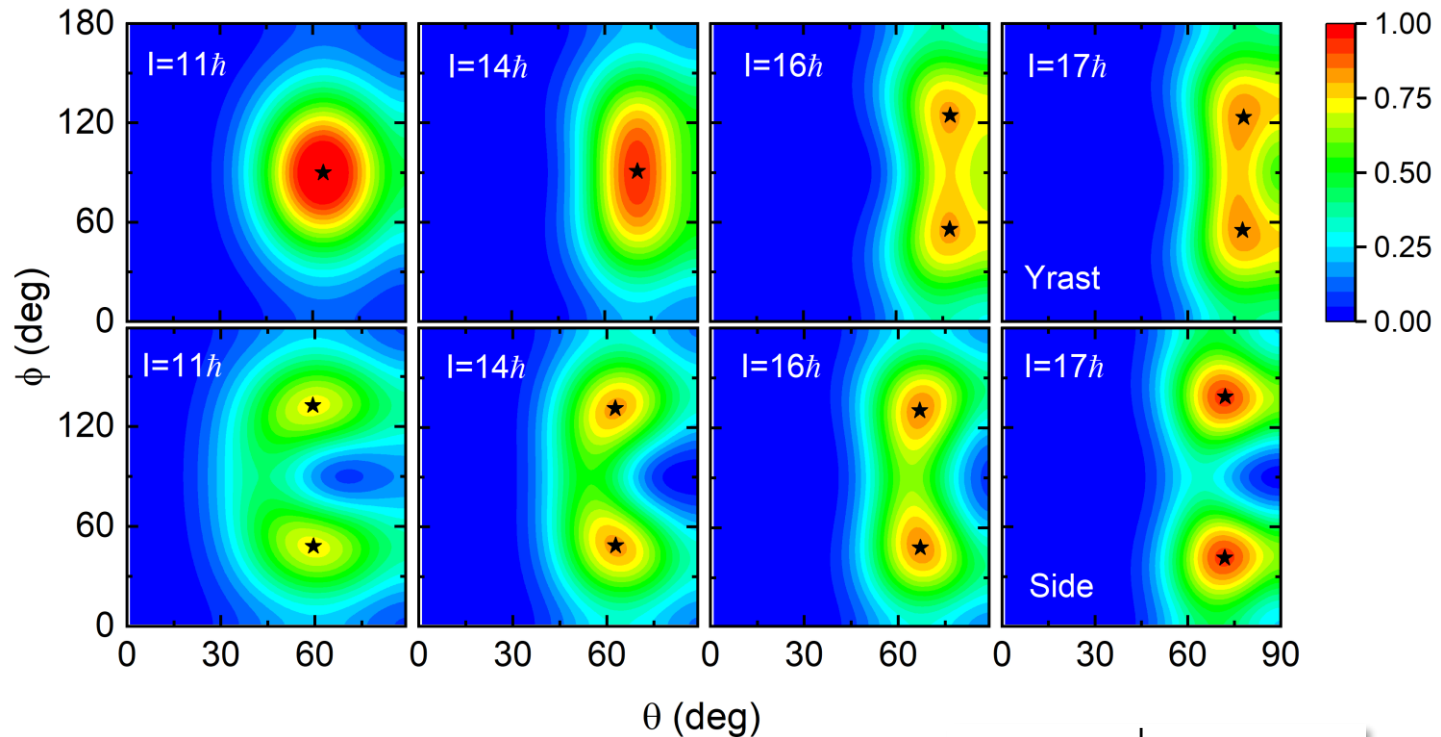
Azimuthal plot (A-plot): *the probability distribution for the orientation of the angular momentum on the (θ, ϕ) plane* F. Q. Chen et al., PRC 96, 051303 (R) (2017)



Planar rotation

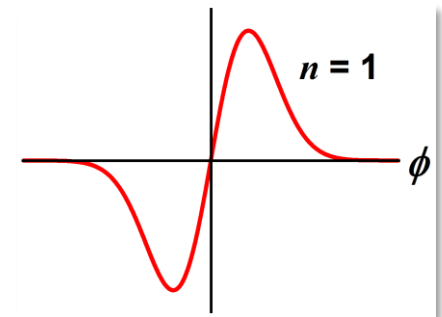


Aplanar rotation



YKW, Zhao, Meng, PLB 848, 138346 (2024)

□ The evolution from chiral vibration to static chirality is clearly shown by exploring the A-plot

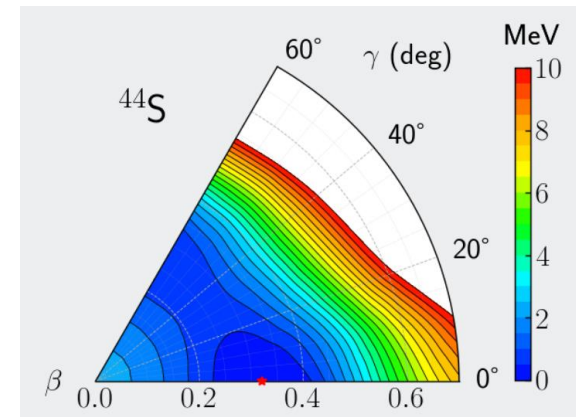
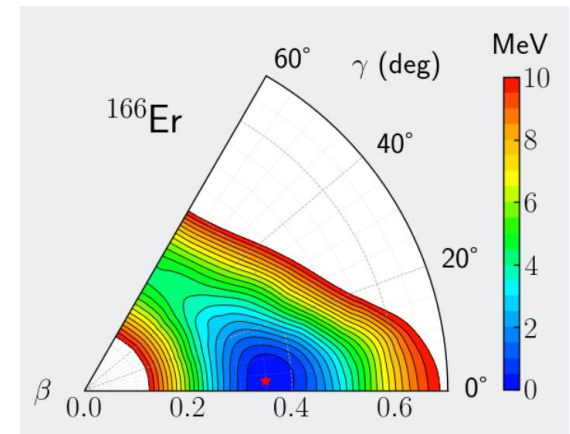


Summary

- ReCD theory is adopted to study the nuclear chirality in ^{130}Cs :
 - ✓ The spectroscopic properties of chiral doublets are reproduced satisfactorily
 - ✓ The chiral geometries from **chiral vibration** to **static chirality** are illustrated through the A-plot
 - ✓ The present work provides the **first microscopic and quantal description** for the chirality in atomic nuclei within the framework of DFT

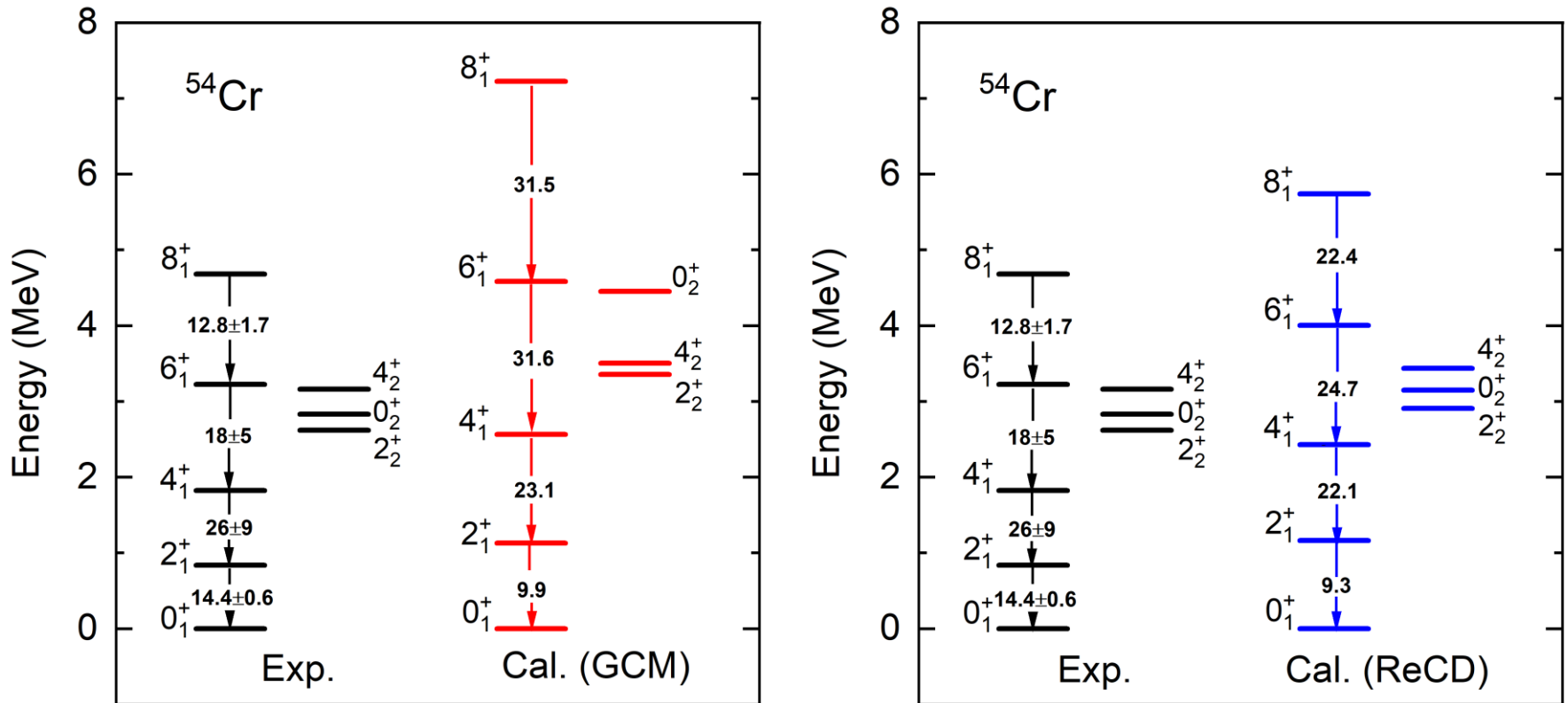
Perspectives

- The present ReCD calculations is performed based on an intrinsic ground state $|\Phi_0\rangle$ with a single deformation parametrized by $(\beta_{\min}, \gamma_{\min})$.
- From this point of view, the ReCD theory is most suitable for describing nuclei with stiff potential energy surfaces.
- For nuclei with soft shapes or shape coexistence, ReCD theory may not be a good choice, and one needs to turn to (for example) GCM method.
- However, GCM is limited to low-lying states and correlations induced by single-particle motion are missing.



ReCD theory + GCM \Rightarrow Collective + noncollective correlations, low-lying and high-spin states

Perspectives



- ✓ Compared to the GCM calculation, the extended ReCD calculation provides a much better description of data.
- ✓ The description could be further improved by including more quasiparticle states in the configuration space.