北京大学
PEKING UNIVERSITY

Laser spectroscopy of $^{81\text{-}82}$Zn at CRIS

Xiaofei Yang，Yongchao Liu

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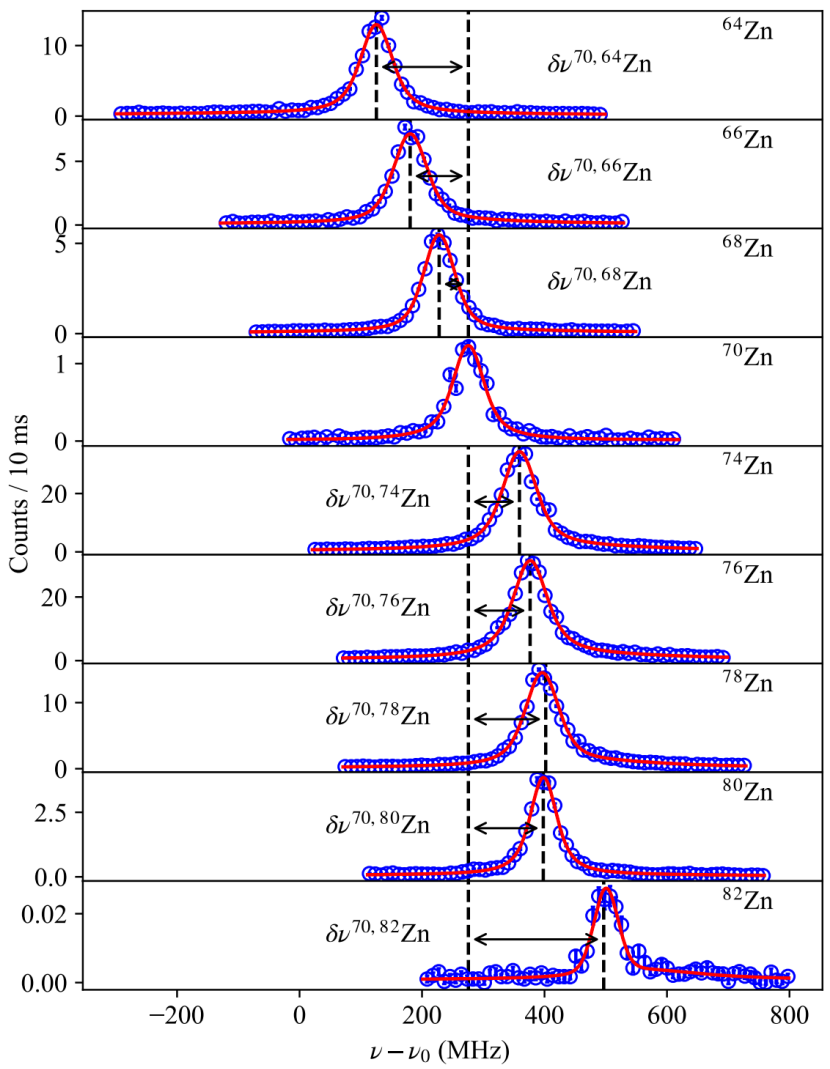
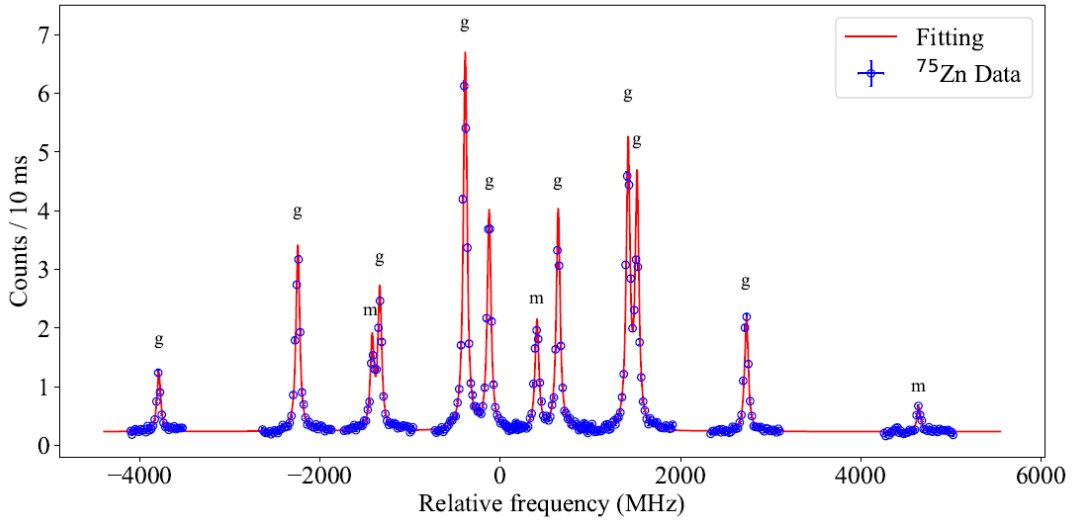
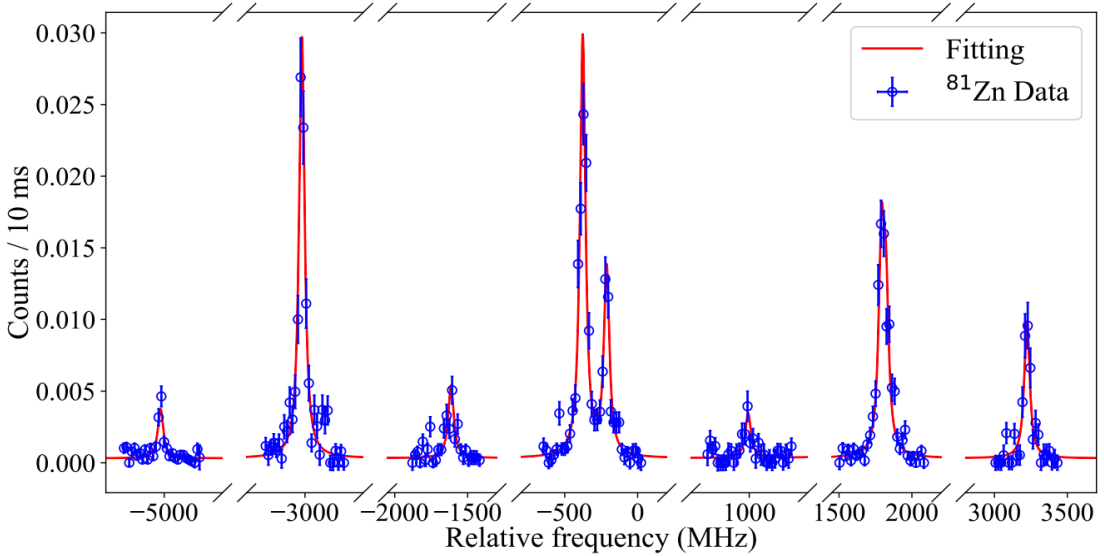
HFS spectra and data of Zn isotopes at CRIS



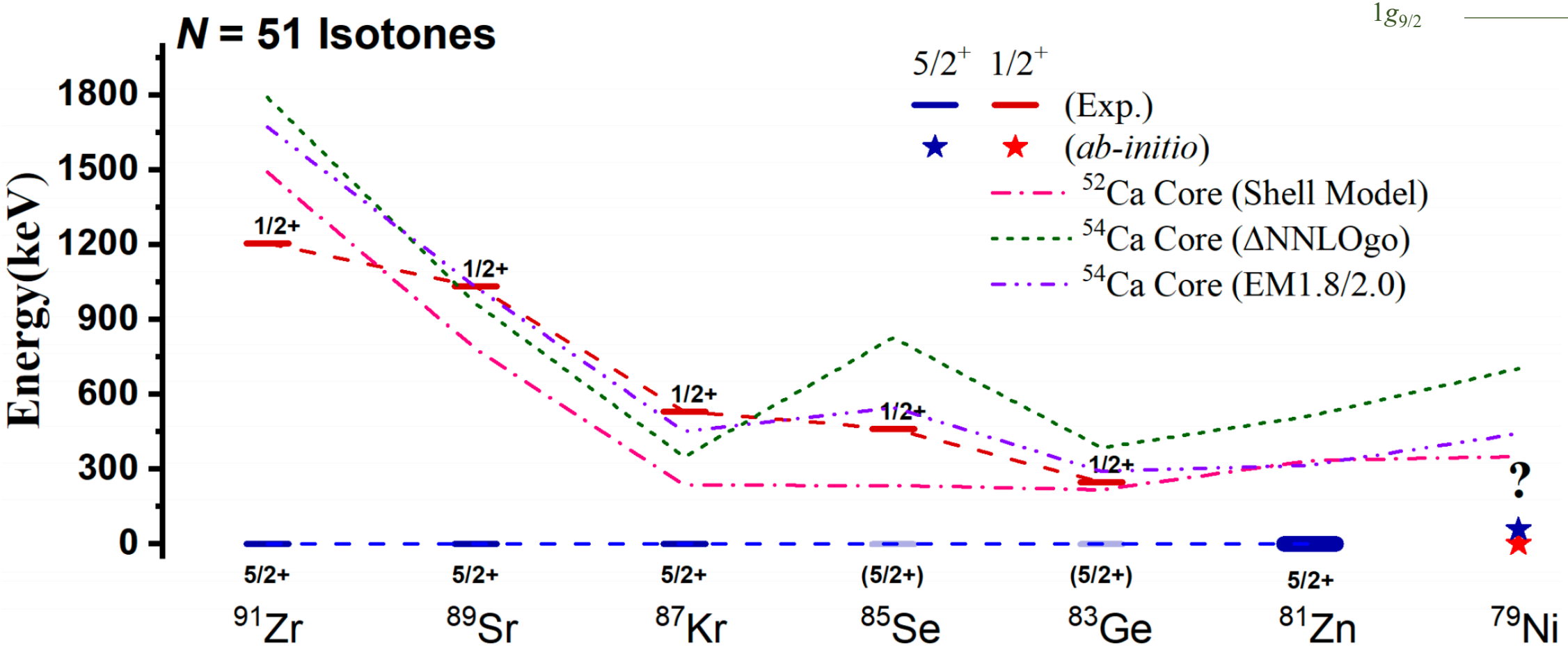


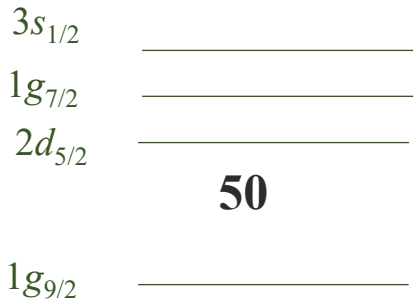


Data obtained: I, μ, Q : ^{81}Zn; $\langle r^2 \rangle$: ^{81,82}Zn

1. I, μ, Q : ^{81}Zn

1. Firm assignment of $5/2^+$ for ^{81}Zn, no shell inversion at Z=30

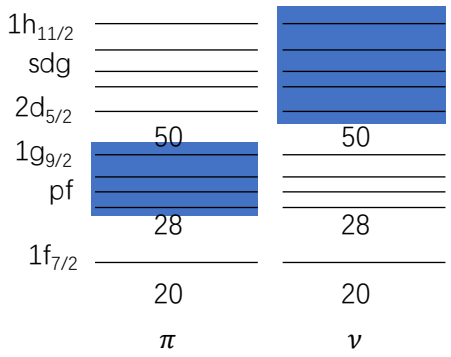




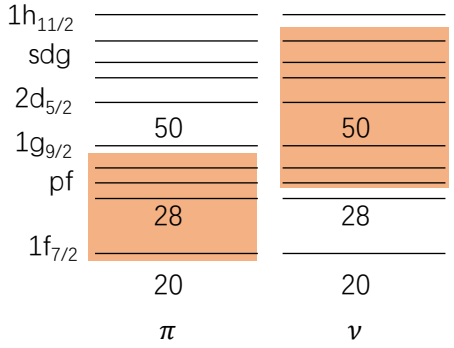
1. I, μ, Q : ^{81}Zn

2. Core excitations of ^{78}Ni is necessary to reproduce the moments of ^{81}Zn

^{78}Ni core

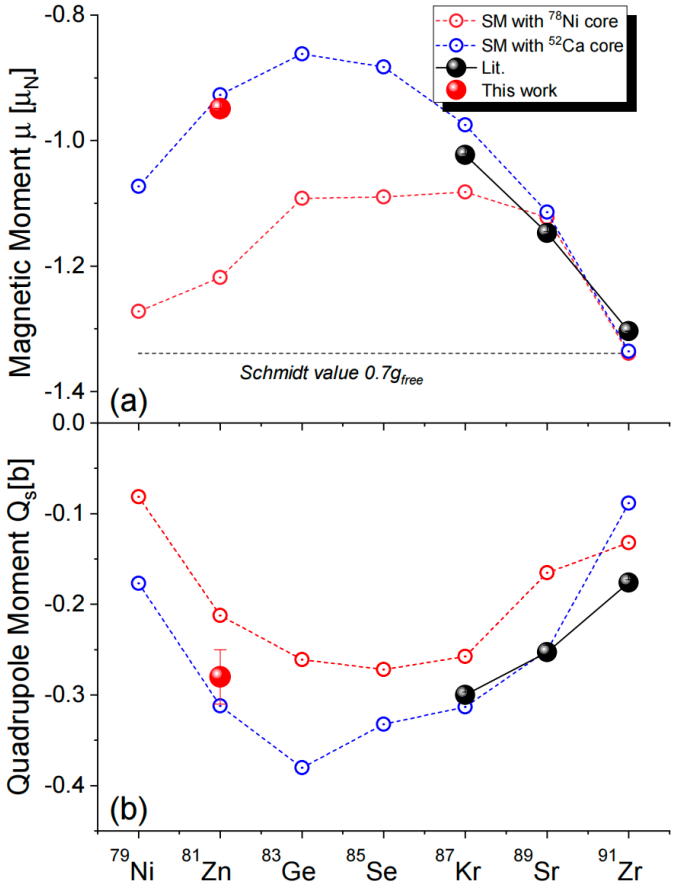


^{52}Ca core

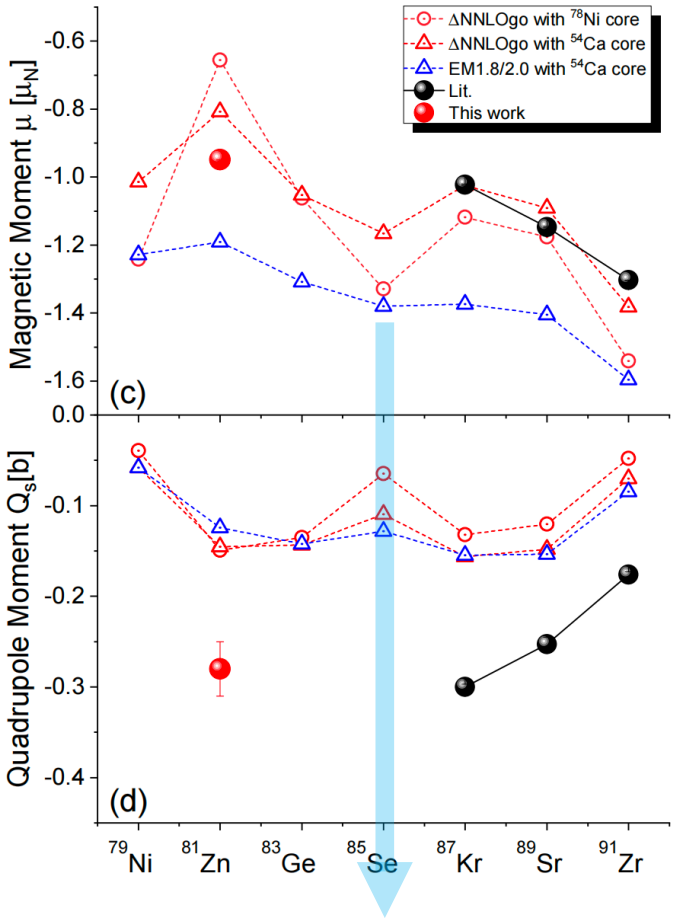


J.G. Li, PLB 840 (2023) 137893

Shell model



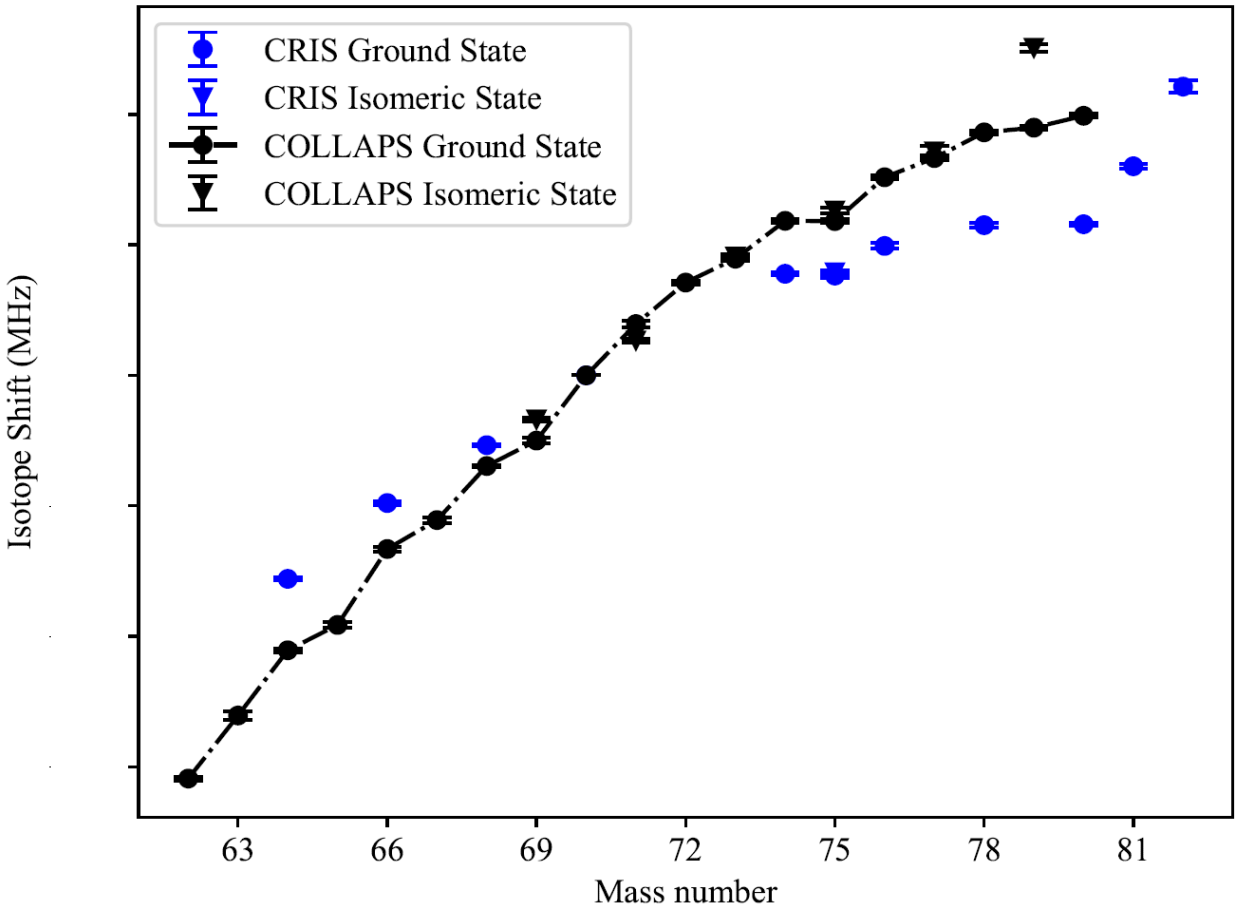
VS-IMSRG(+MEC)

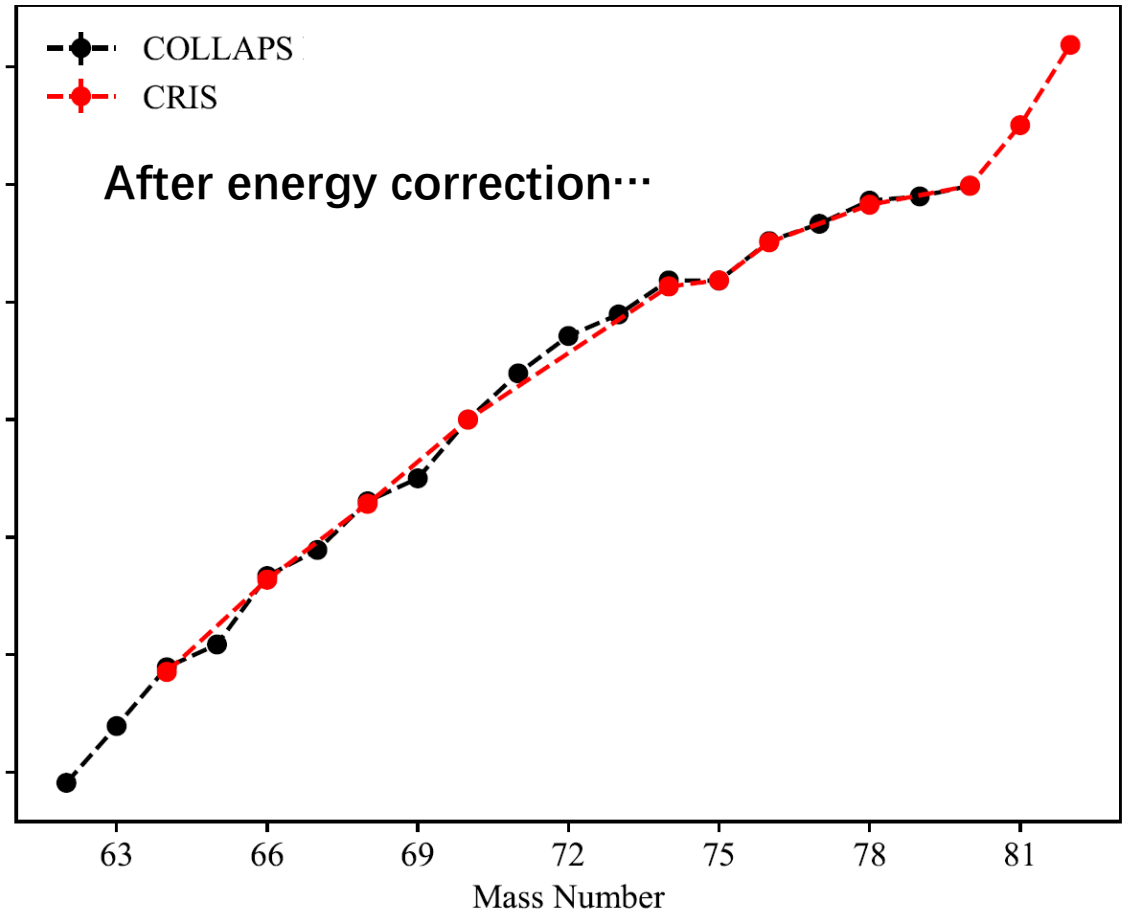


Status of the paper: Preliminary draft

Theoretically check is on going

2. Radii of ^{81,82}Zn



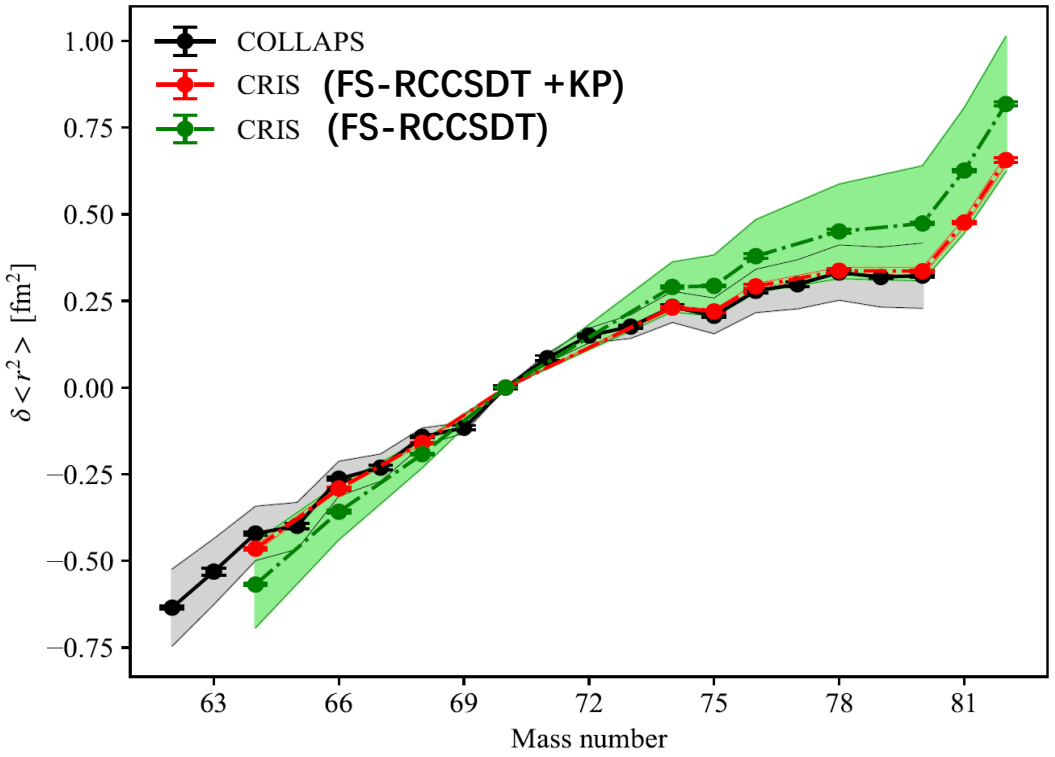


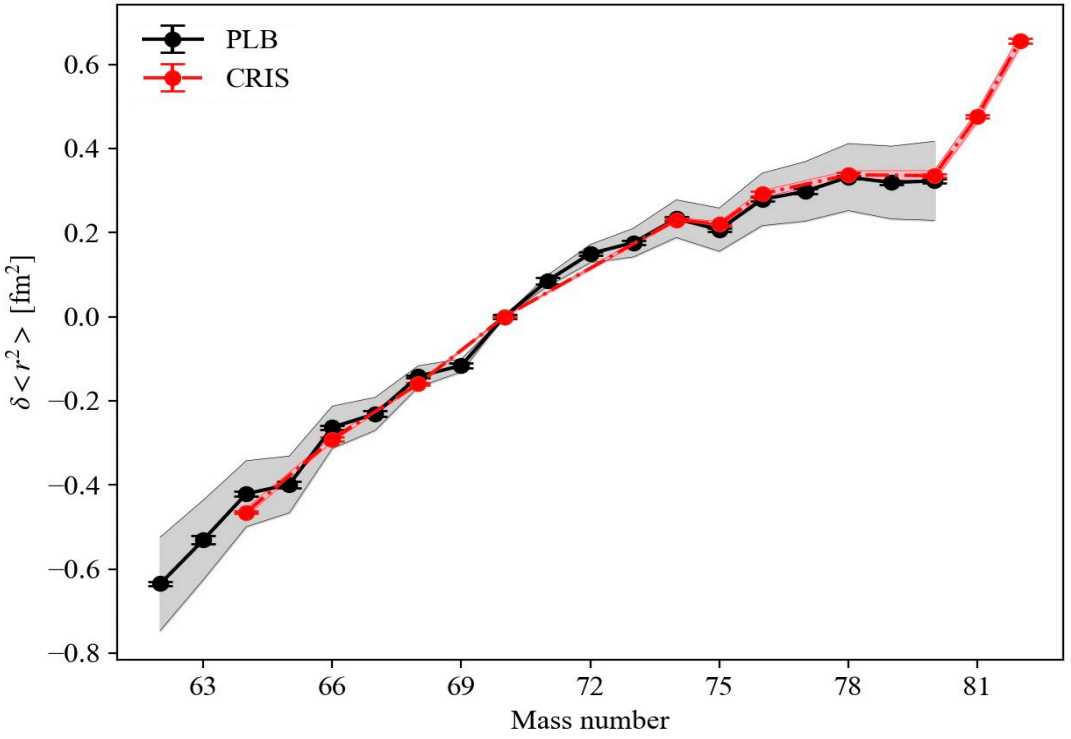
2. Radii of ^{81,82}Zn

:

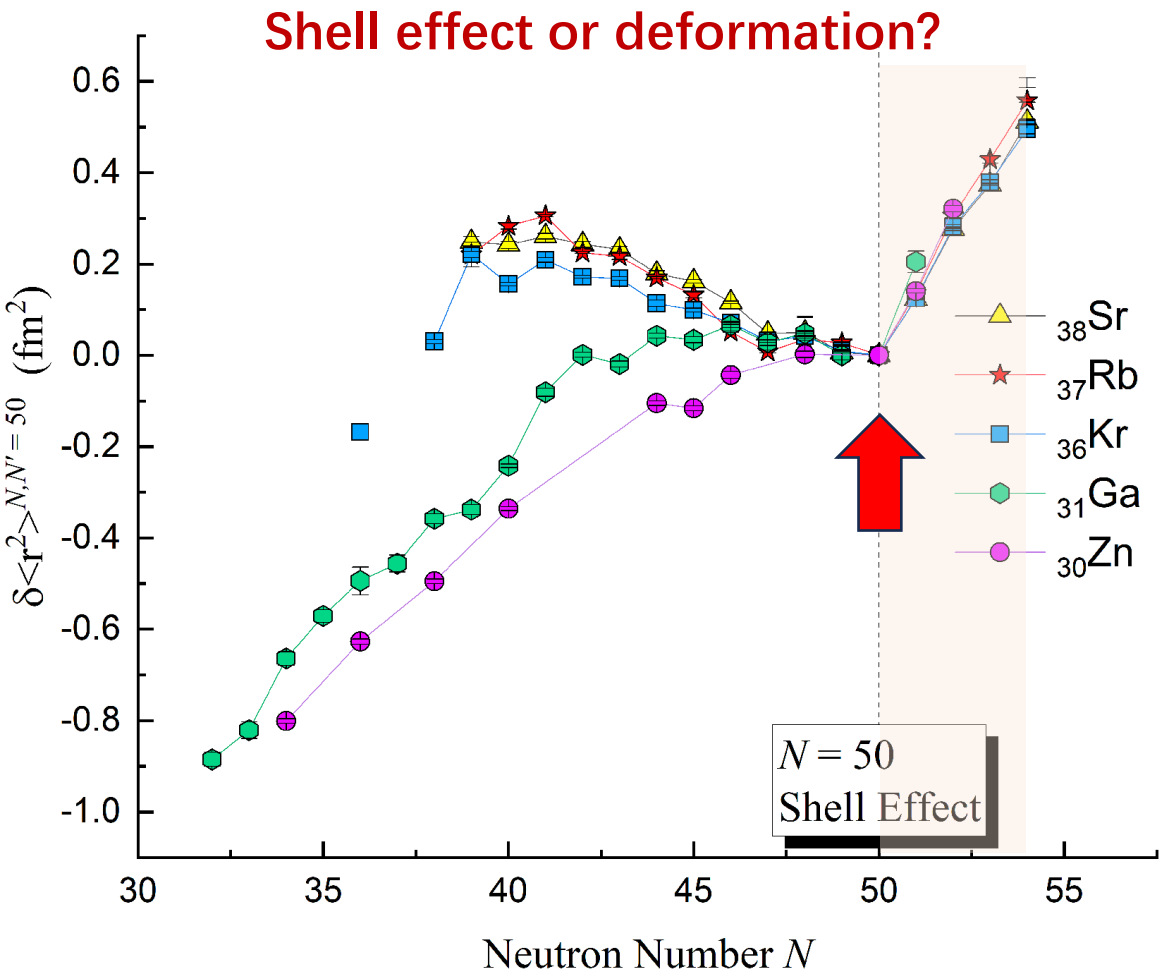
	F (MHz fm^{-2})	M (GHz u)	Method
2019 COLLAPS	+346(3)	+14(7)	MCDHF
2019 COLLAPS	+346(35)	+49(17)	MCDHF + KP
2023 CRIS	**+324(3)**	**-21(30)**	**FS-RCCSDT**
2023 CRIS	**+324(3)**	**+3.9(21)**	**FS-RCCSDT+KP**

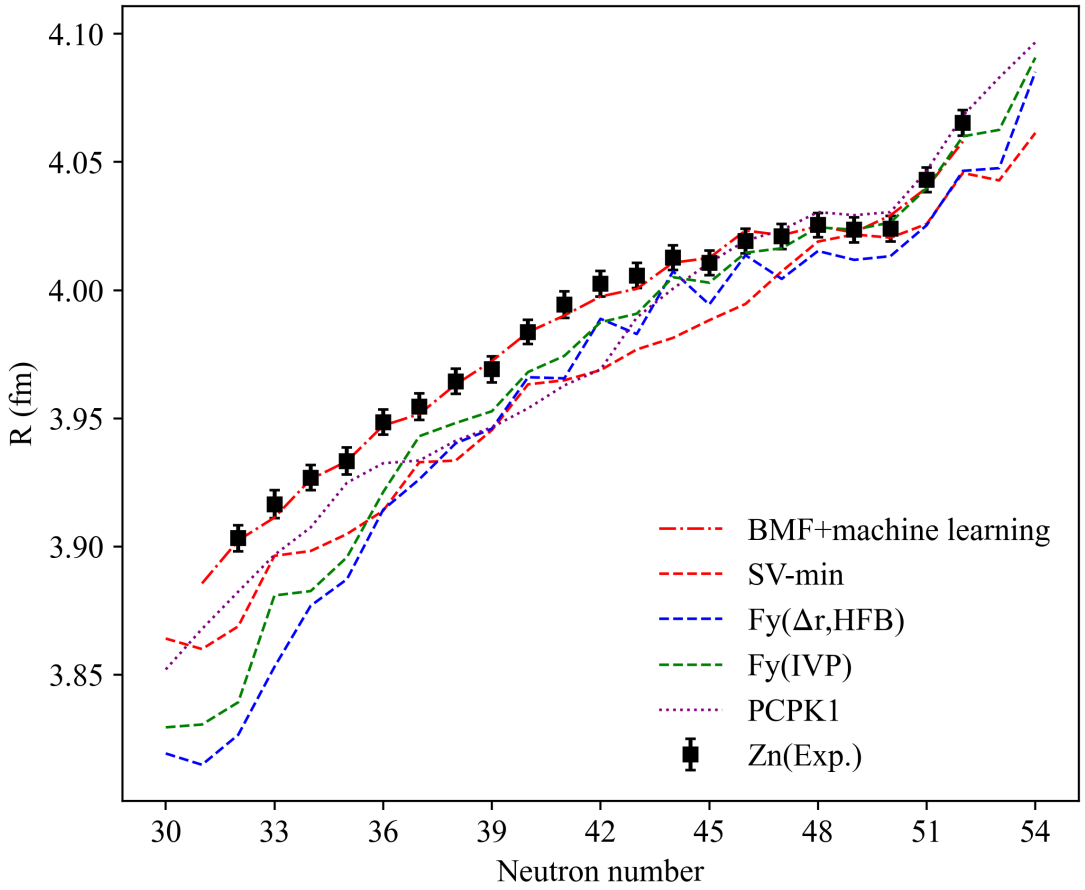
A. V. Oleynichenko; L. V. Skripnikov





2. Radii of ^{81,82}Zn

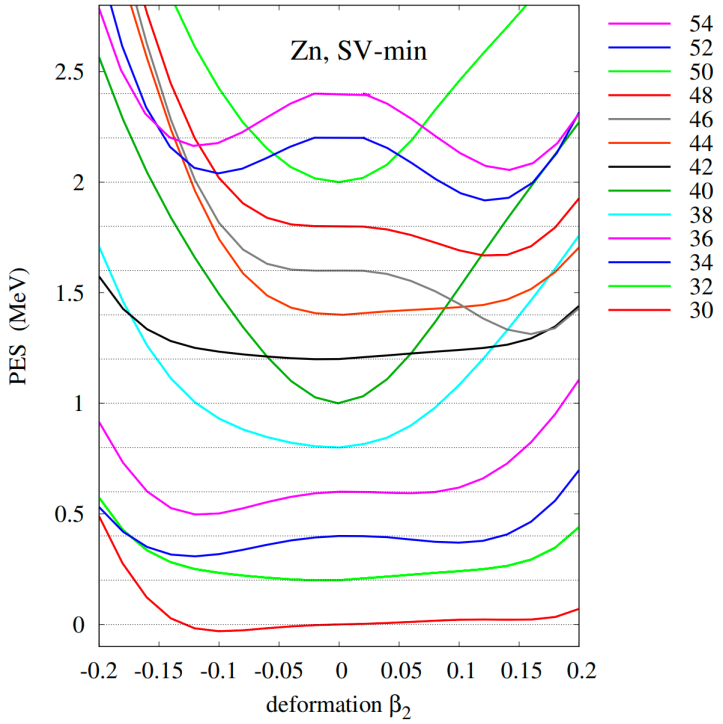




- Unexpected （？） large kink is observed at $N = 50$
- As large as those in Kr($Z = 36$), Rb($Z = 37$), Sr($Z = 38$)
- Current theoretical calculation

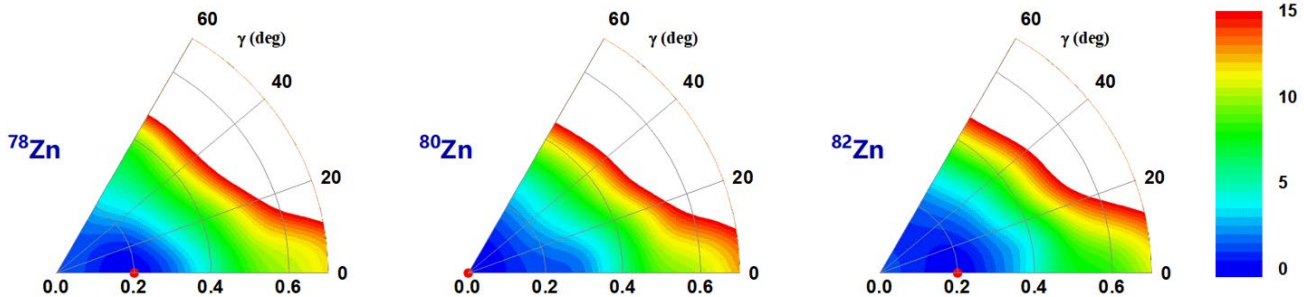
2. Radii of ^{81,82}Zn

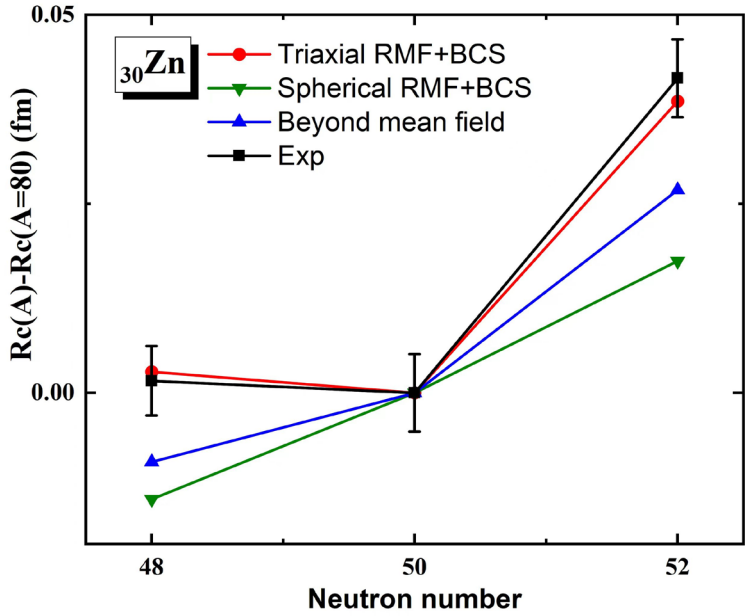
SV-min

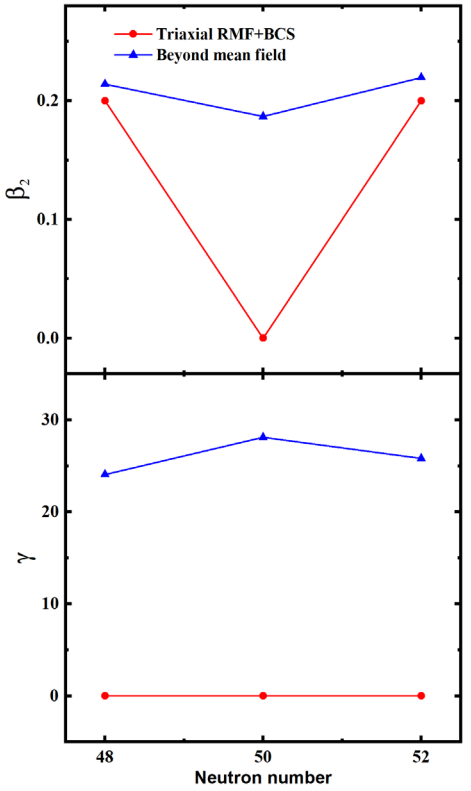


g.s. deformations		
N	β_2	γ
30	0.000	-
32	0.000	-
34	0.086	52.8
36	0.087	60.0
38	0.006	0.2
40	0.000	-
42	0.005	14.1
46	0.010	8.4
48	0.001	-
50	0.000	-
52	0.067	0.0
54	0.086	60.0

BMF



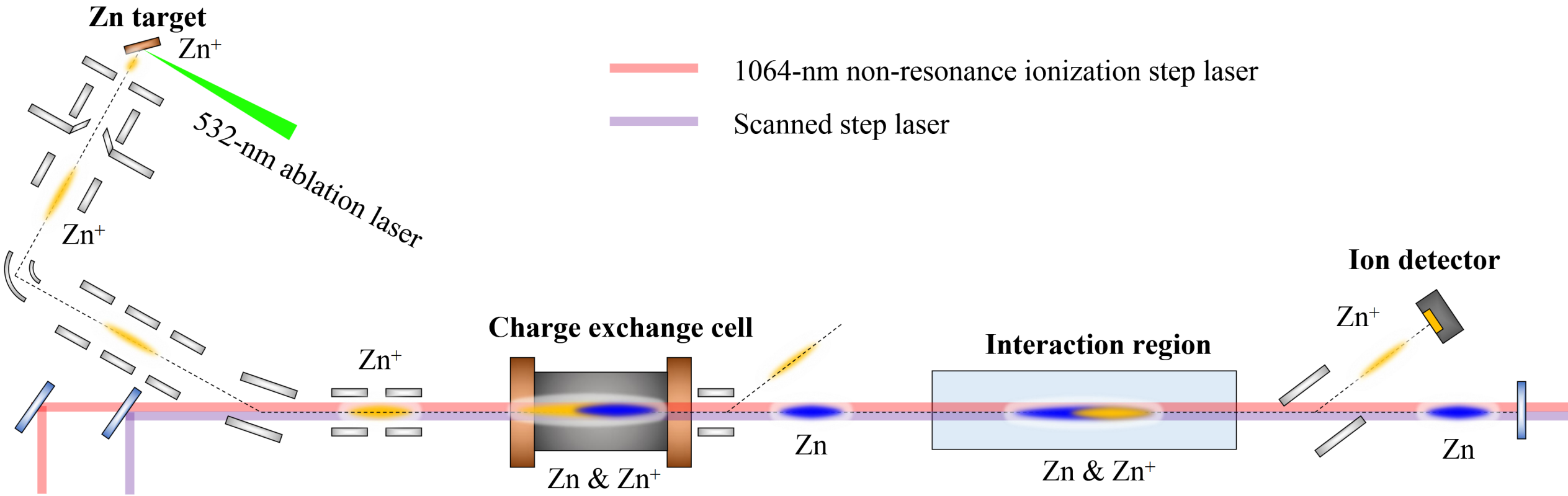




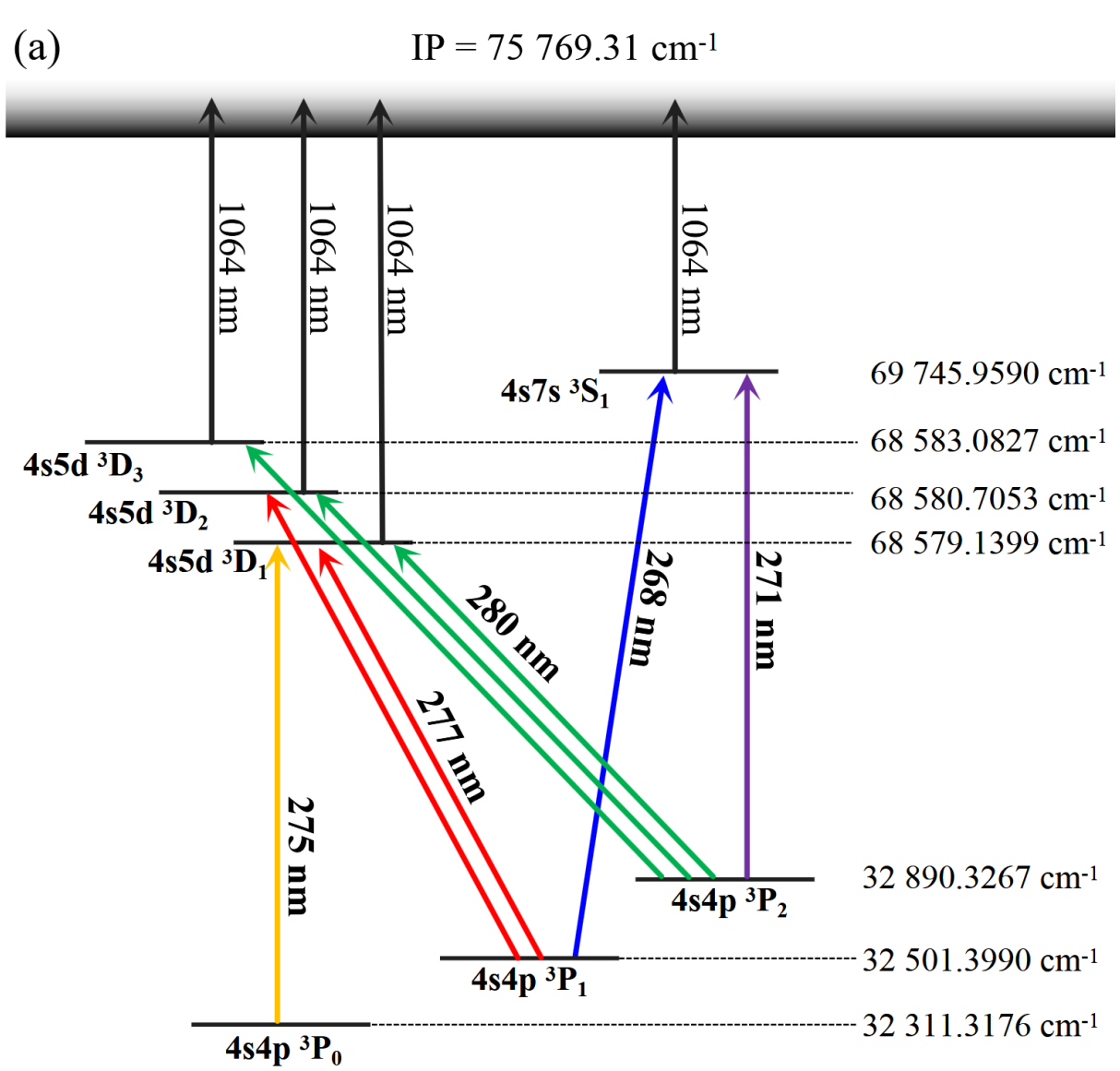
Status of the paper: Needs more discussion with theorist

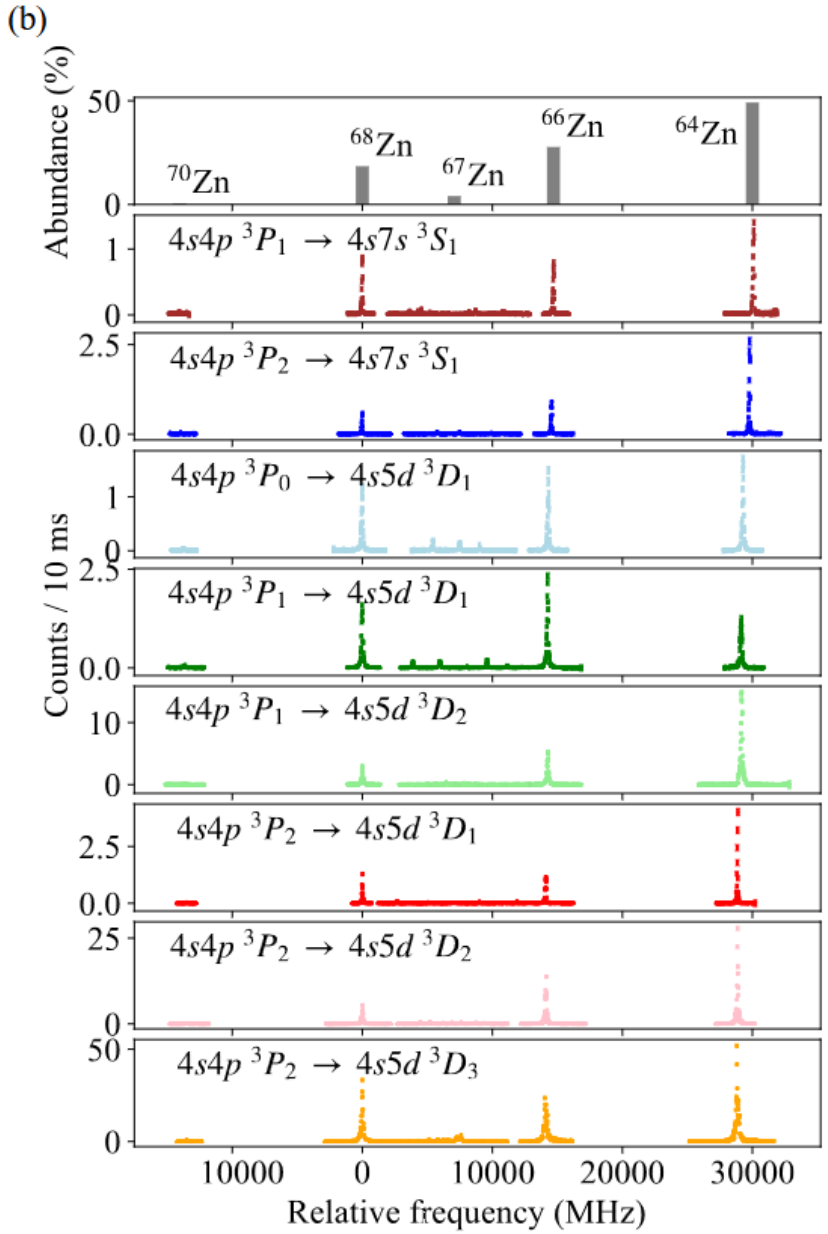
Offline Zn data @ 2019

Yongchao, Shiwei, Jordan, Xiaofei, Alex (atomic theory), Leonid (atomic theory), and ……

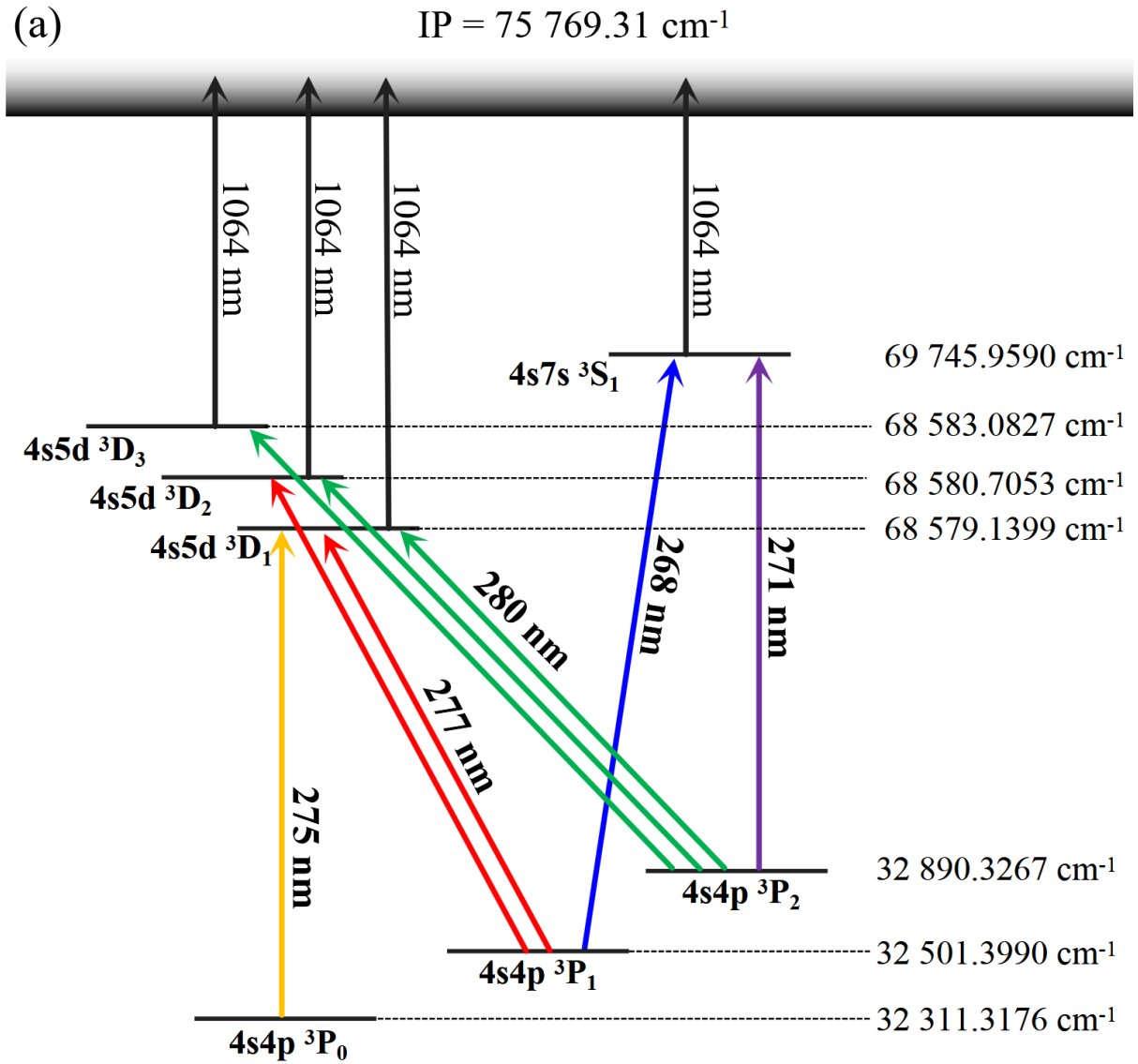


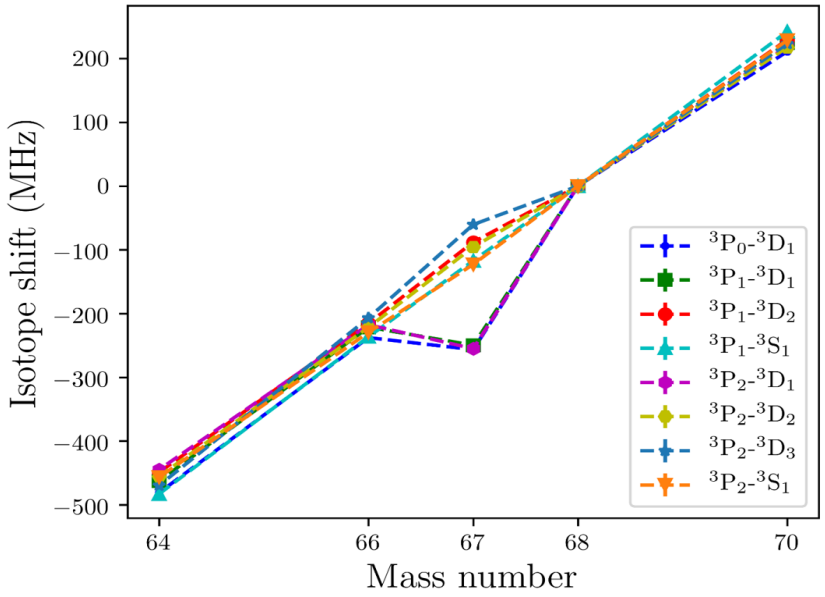
Offline Zn data





Offline Zn data





Offline Zn data

Hyperfine structure constants of the Zn atom

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[2] *Moscow Institute of Physics and Technologies (National Research University), Institutskij pereulok 9, Dolgoprudny Moscow region 141700, Russia*

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(Dated: April 18, 2024)

Hyperfine interaction matrix elements were calculated using the relativistic Fock-space coupled cluster (FS-RCC) theory [1–3]. To obtain the basic value of the property matrix element, the CCSD approximation was used, and the intermediate Hamiltonian (IH) technique formulated for incomplete main model spaces was used to bypass the intruder states problem and ensure stability of the solution of CC amplitude equations [4]; energy denominators corresponding to excitations from buffer state determinants were shifted to the frontier energy chosen to be equal to -1.3 a.u. (this approximately corresponds to the energy of the $4s^2$ determinant). The active space comprised $4spdf$, $5spdf$, $6spd$, $7sp$ spinors of the Zn^{2+} ion. The main model space in the target $0h2p$ Fock space sector (two particles over closed shells) were composed of Slater determinants corresponding to the $4s^2$, $4s5s$, $4s6s$, $4s4p$, $4s5p$, $4s6p$, $4s4d$, $4s5d$, $4s4f$ configurations. At the IH-FS-RCCSD stage all electrons of Zn were correlated, the virtual spectrum cutoff was chosen to be 2000 Hartree. Corrections for connected triple excitations were calculated as the differences between the values of matrix elements obtained at the FS-RCCSDT [5] and FS-RCCSD levels for the reduced problem with the $1s2s2p3s3p$ shells of Zn excluded from correlation calculation and virtual space cutoff equal to +1.0 a. u. Such an approach, further denoted as FS-RCCSD+ΔT, was previously applied to calculate electric field gradient at nucleus in atomic bismuth [6]. Calculations with triples were performed not within the IH framework, but the dynamical energy denominator shift technique [3, 7] was used to achieve convergence of amplitude equations (in this particular case, the intruder state problem is the most severe for CCSDT calculations in the $0h1p$ Fock space sector). The uniform values of the shift parameters $S_2 = -1.0$ a. u. and $S_3 = -1.5$ a. u. were used for double and triple excitation amplitudes, respectively, in the $0h1p$ and $0h2p$ Fock space sectors; the real simulation of an imaginary shift formula from [8] with the attenuation parameter $n = 3$ was used. Note that the final values of A and B constants (Tab. I) were found to be quite stable with respect to the IH and shifting parameters (see below for the discussion on uncertainty estimates).

Basic FS RCCSD values of diagonal hyperfine interaction matrix elements were calculated using the finite-difference approach. The second-order analytic connected expression for effective one-electron operators [9] was used to calculate matrix elements within the FS RCCSDT approximation. The same second-order method was also employed to calculate off-diagonal hyperfine matrix elements.

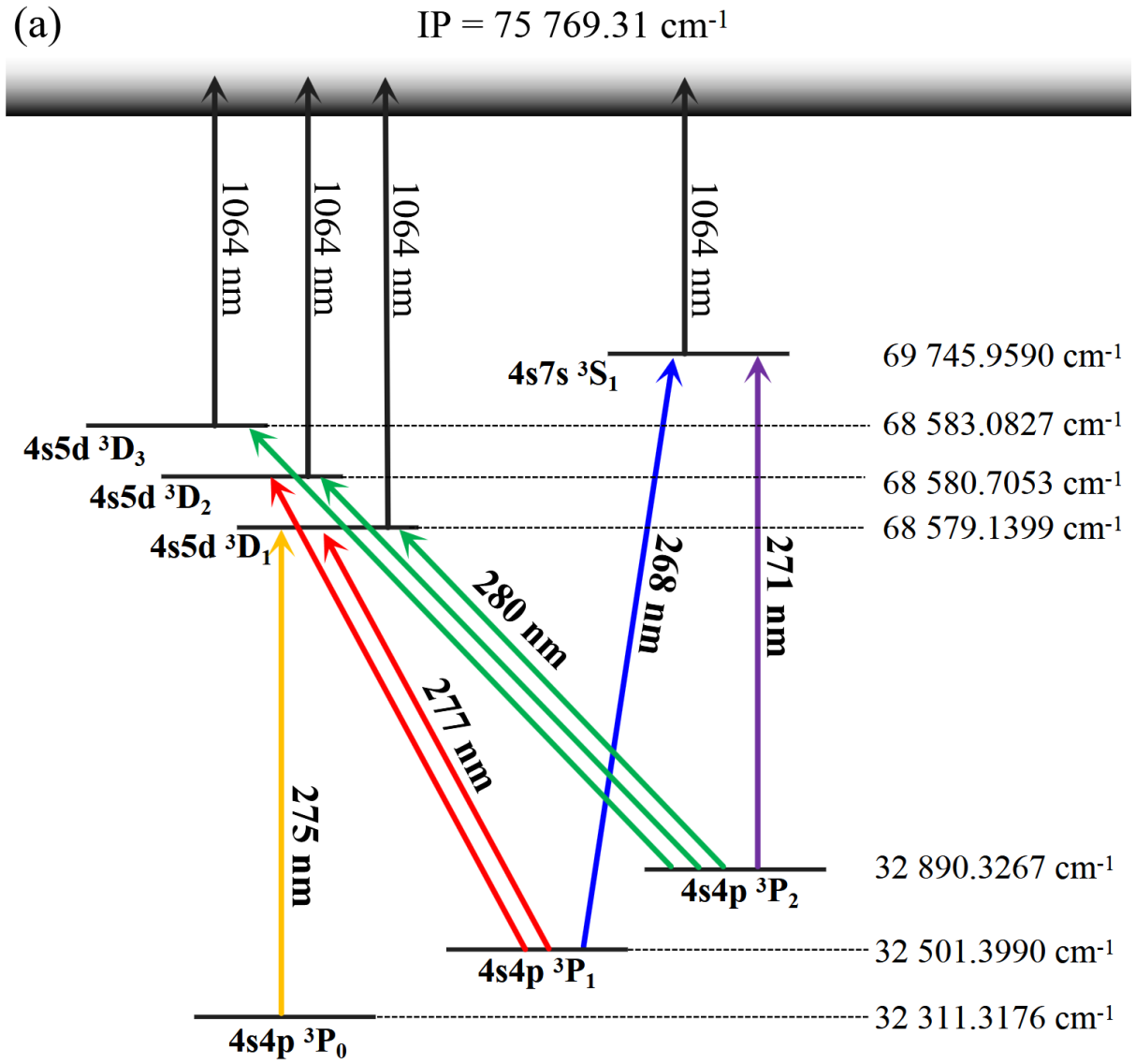
The four-component Dirac-Coulomb Hamiltonian was used in all calculations. Basis set was based on the Dyall's ae4z basis set [10] extended by additional functions; it comprised $(33s25p21d12f5g3h3i)$ primitive Gaussian functions. All coupled cluster calculations were carried out using the EXP-T program package [11, 12], while the DIRAC software [13, 14] was used to obtain transformed molecular integrals.

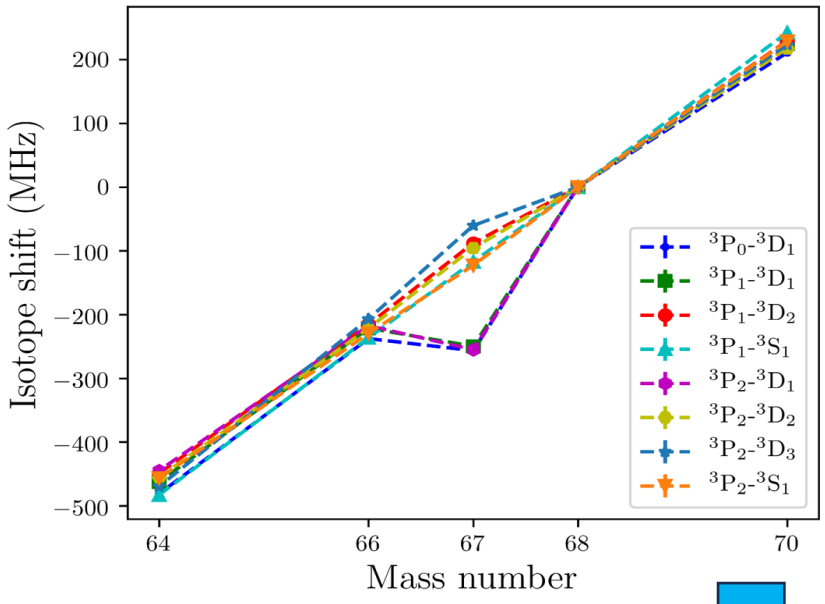
There are three main sources of uncertainties which may influence the overall accuracy of calculation. The first one arises from the intermediate Hamiltonian approach employed in CCSD calculations. To estimate the IH error the series of calculations with different parameters of IH (attenuation parameter n, frontier energy $\overline{E}$) varying in wide ranges ($n = 1 - 5$ and $\overline{E} = -1.3... - 0.9$) were employed and the maximum deviation between the obtained matrix elements was regarded as an estimate of the uncertainty arising from IH. The second uncertainty is associated with an incomplete accounting for triple and higher excitations and it was estimated to be equal to half the correction for triple excitations (note that for diagonal elements the lack of higher excitations is a dominating source of error). The third uncertainty is specific for off-diagonal matrix elements and is due to the lack of higher-order contributions in the second-order analytic scheme employed; corresponding uncertainty was estimated based on the differences between finite-order and finite-field values obtained for corresponding diagonal elements. The final uncertainty was calculated as a root of the sum of squares of uncertainties described above.

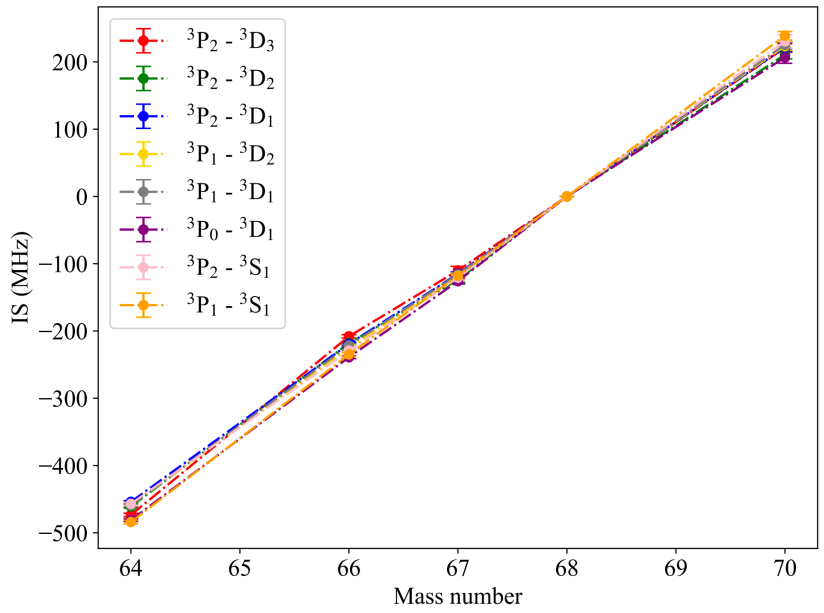
FS-RCCSD(FF)+ΔT:
a new technique for calculating off-diagonal matrix elements at the FS-CCSDT level.

	3D_1, MHz	3D_2 , MHz	3D_3 , MHz
dA	-11.3(2)	-9.8(2)	-2.2(1)
dB	30.1(7)	-146.4(4.1)	-86.9(2.6)
dCOG	-132.0(2.9)	26.0(2.3)	38.0(1.1)

Offline Zn data

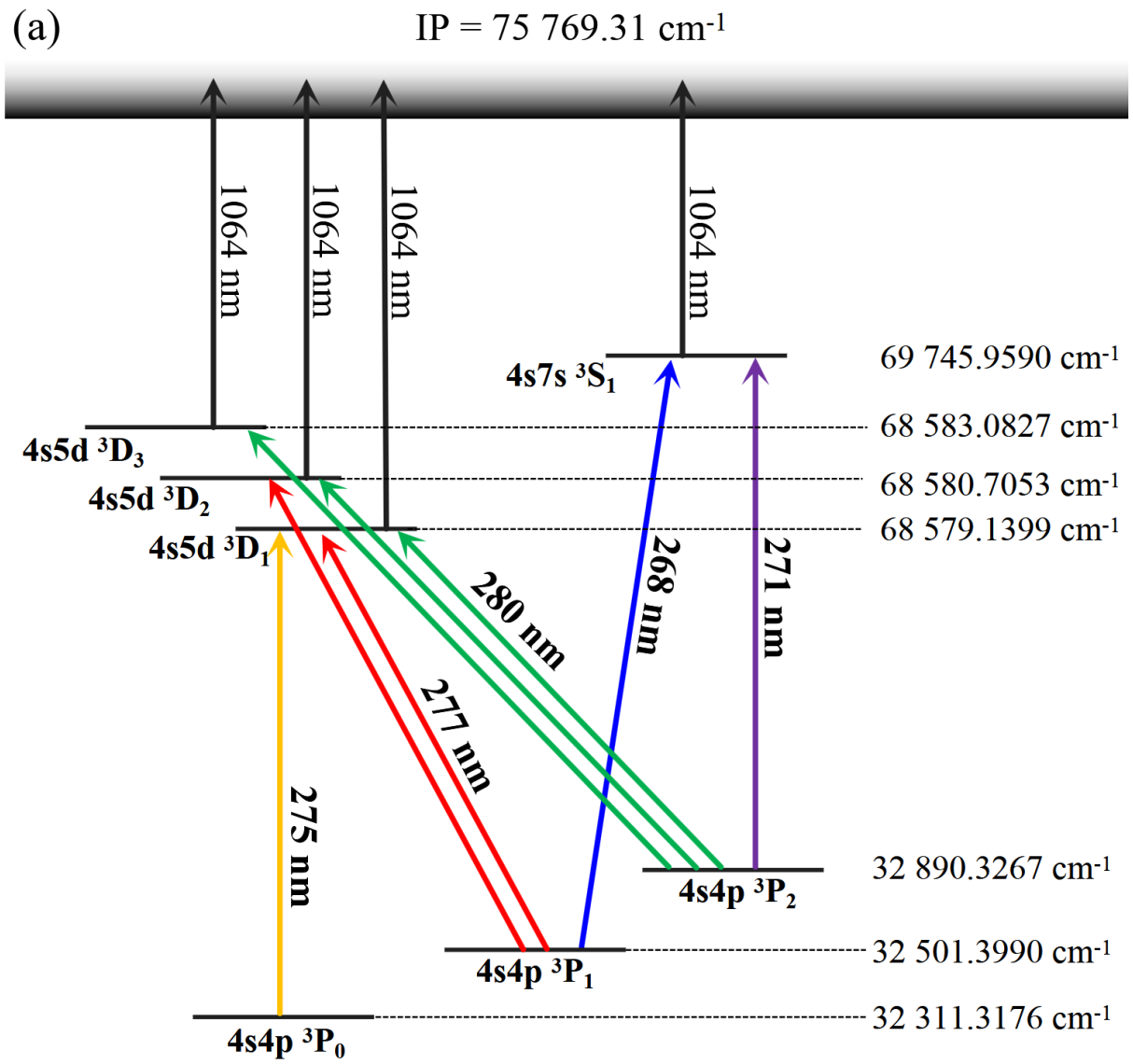


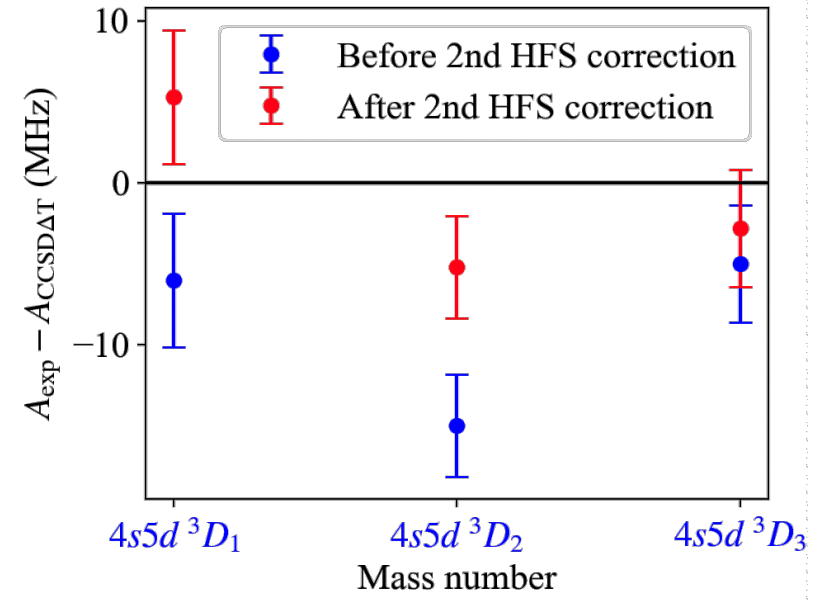


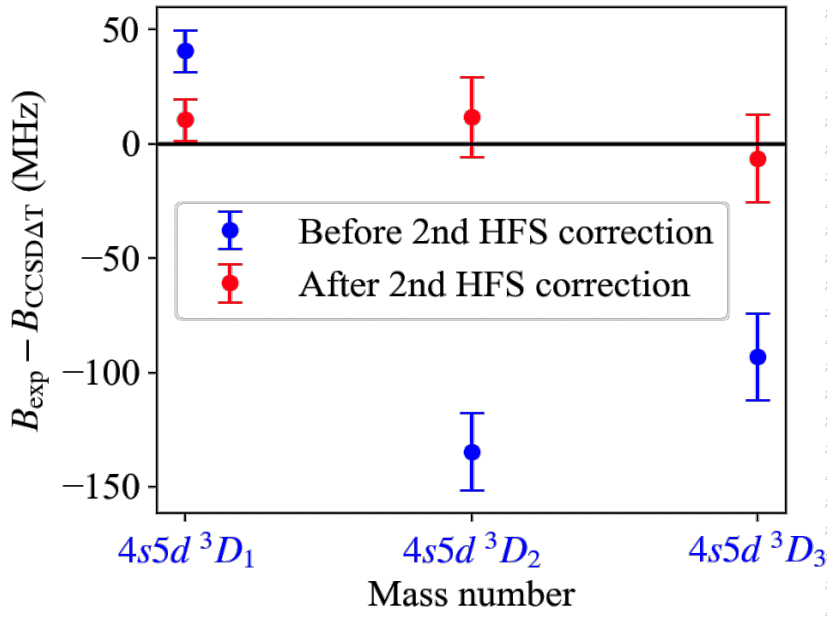


FS-RCCSD+ΔT
for
2nd order HFS

Offline Zn data







Status of the paper: A very preliminary draft

Thank you!

CRIS collaboration

CERN

MANCHESTER 1824
The University of Manchester

PEKING UNIVERSITY
北京大學

KU LEUVEN

UNIVERSITY OF GOTHENBURG

Massachusetts Institute of Technology

sckcen

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