Nuclear shape evolution and shape coexistence in Zr and Mo isotopes

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Abstract The phenomena of shape evolution and shape coexistence in even-even $^{88-126}$Zr and $^{88-126}$Mo isotopes is studied by employing covariant density functional theory (CDFT) with density-dependent point coupling parameter sets DD-PCX and DD-PC1, and with separable pairing interaction. The results for rms deviation in binding energies, two-neutron separation energy, differential variation of two-neutron separation energy, and rms charge radii, as a function of neutron number, are presented and compared with available experimental data. In addition to the oblate-prolate shape coexistence in $^{96-110}$Zr isotopes, the correlation between shape transition and discontinuity in the observables are also examined. A smooth trend of charge radii in Mo isotopes is found to be due to the manifestation of triaxiality softness. The observed oblate and prolate minima are related to the low single-particle energy level density around the Fermi level of neutron and proton respectively. The present calculations also predict a deformed bubble structure in $^{100}$Zr isotope.

Keywords Covariant density functional · Shape coexistence · Charge radii · Single-particle levels · Bubble nuclei

1 Introduction

In nuclear physics, the study of exotic nuclei with large numbers of protons or neutrons is one of the most active areas of research, both theoretically as well as experimentally. The radioactive ion beam (RIB) facilities and sensitive detection technologies have extended our knowledge of nuclear physics far away from the $\beta$-stability line. The study of nuclear shape evolution in atomic nuclei is one of the fundamental quests in nuclear physics. The polarizing effect of added nucleons leads to a gradual increase of deformation in the nuclei away from spherical shell closures. However, an abrupt shape transition is seen in neutron-rich nuclei around $A \approx 100$ mass region. In the case of Zr isotopes, the ground states from $N = 50$ up to $N = 58$ are weakly deformed and a sudden shape transition is observed as $N = 60$ is approached. This sudden shape transition in Zr isotopes is evident from the irregularities in the two neutron separation energies\textsuperscript{[1]}, mean-square charge radii\textsuperscript{[2,3]}, and excitation energies of $2^+_1$ states and $B(E2)$ values\textsuperscript{[4,5]}. On the other hand, the shape transition is rather gradual in Mo isotopes\textsuperscript{[1,6]} showing characteristic signatures of triaxiality. This dramatic behavior makes the mass region $A \approx 100$ of special interest to test various theoretical models.

Nuclei at and near closed subshells are known to exhibit shape coexistence\textsuperscript{[7,8]}. Neutron rich zirconium ($Z = 40$) and molybdenum ($Z = 42$) isotopes are good examples of shape coexisting bands. The appearance of low-lying $0^+_2$ states is a feature of shape coexistence and shape transition in this mass region. Many experimental observations for shape transition and shape coexistence have been made in this mass region. The shape coexistence is seen in closed-subshell $^{94}$Zr nuclei where the role of subshells for nuclear collectivity is suggested to be important\textsuperscript{[9]}. The possibility of shape coexistence has been suggested in $^{98}$Zr and $^{100}$Zr nuclei by the analysis of yrast structure from the rotational band and transition strength through lifetime measurements\textsuperscript{[8,10,11,12]}. The shape coexistence in Mo isotopic chain was studied experimentally by using the Coulomb excitation technique\textsuperscript{[13,14,15]}. Very recently, J. Ha et al.\textsuperscript{[16]} have studied the shape evolution of $^{106}$Mo, $^{108}$Mo, and $^{110}$Mo isotopes through the energies and lifetimes of $2^+_1$
states. The quadrupole deformation parameter was obtained from these measurements suggesting the deformation is almost unchanged $N = 62$ to $N = 66$ and slightly decreases at $N = 68$.

Theoretically, various attempts have been made to study the phenomena of shape evolution in $Zr$ and $Mo$ isotopes. The structural evolution in even-even and odd-$A$ neutron-rich $Zr$ and $Mo$ isotopes is studied within self-consistent mean-field approximation based on D1S-Gogny interaction. A correlation between the isotopic shift of charge radii and shape transition in these isotopes has been suggested. The triple shape coexistence specific for the $0^+$ states and the evolution of the shape coexistence and mixing in the neutron-rich $N = 58$ $Zr$ isotopes are studied within the complex excited VAMPIR approach. The shape evolution and shape coexistence phenomena in neutron-rich nuclei at $N \approx 60$ is studied using the framework the covariant density functional theory (CDFT) with PC-PK1 interaction. They observed a rapid shape transition at $N = 60$ for $Zr$ nuclei while a smooth transition in $Mo$ isotopes. Many other theoretical studies with different formalisms are done to understand the evolution of structure in these nuclei, including the relativistic mean-field (RMF) model, the interacting boson model (IBM) model, and the self-consistent mean-field models with the Skyrme and the Gogny force.

2 Theoretical framework

Self-consistent mean-field (SCMF) models provide a very successful tool to study and analyze a variety of nuclear structure phenomena throughout the entire nuclear chart, from the valley of stability to exotic nuclei. These models are based on nuclear energy density functionals (EDF) that represents a unified approach to study the static and dynamic properties of finite nuclei quantitatively. The nucleons are treated as independent particles moving inside the nucleus under the influence of potentials derived from such functionals. The EDF is constructed as a functional of one-body nucleon density matrices that correspond to a single product state of single-particle states. This approach is analogous to Kohn-Sham density functional theory (DFT), which enables a description of quantum many-body systems in terms of a universal energy density functional.

2.1 Lagrangian density for the Point Coupling models

The relativistic mean-field representation is formulated in terms of point-coupling nucleon-nucleon interactions, without the inclusion of meson fields. The medium dependence of the interaction can be taken into account by terms of higher-order in the nucleon fields. The Lagrangian for density-dependent point coupling models includes the isoscalar-scalar, isoscalar-vector and isovector-vector four-fermion contact interactions in the isospace and can be written as (see Ref. for more details),

$$\mathcal{L} = \bar{\psi} (i\gamma.\partial - m) \psi - \frac{1}{2} \alpha_S (\rho) (\bar{\psi} \gamma^\mu \psi)(\bar{\psi} \gamma^\mu \psi) - \frac{1}{2} \alpha_V (\rho) (\bar{\psi} \gamma^\mu \psi)(\bar{\psi} \gamma^\mu \psi) - \frac{1}{2} \alpha_{TV} (\rho) (\bar{\psi} \gamma^\mu \psi)(\bar{\psi} \gamma^\mu \psi) - \frac{1}{2} \delta_S (\partial_\mu \bar{\psi} \gamma^\mu \psi) - e \bar{\psi} \gamma. A \frac{1}{2} \tau^3 \psi,$$

where $m$ is the mass of nucleon, $\alpha_S$, $\alpha_V$ and $\alpha_{TV}$ represent the coupling constants for four-fermion contact terms. In addition to free-nucleon terms and point-coupling
interaction terms, the Lagrangian density in above equation also includes the coupling of the protons to the electromagnetic field. In Eq. (1), the derivative terms accounts for the dominating effects of finite-range interactions and are necessary for a quantitative description of nuclear properties.

The microscopic density-dependent scalar and vector self-energies are computed by using following functional form of the couplings,

$$
\alpha_i(\rho) = a_i + (b_i + c_i x) e^{-d_i x}, \quad (i = S, V, T, V) \quad (2)
$$

where \( x = \rho / \rho_{sat} \) denotes the nucleon density in symmetric nuclear matter at saturation point \( \rho_{sat} \).

The point coupling CDFT model involve 10 parameters for and PC-PK1 can be found in Ref.[35] and the form factor

$$
\langle r \rangle = \frac{1}{2 \rho_{sat}} \int d^3r H(r), \quad (4)
$$

The pairing part of RHB functional is given by

$$
\mathcal{E}_{pair}[\kappa] = \frac{1}{4} \sum_{n_1' n_2'} \kappa_{n_1 n_1'} \kappa_{n_2 n_2'} \left( n_1 n_2 | V^{PP} | n_1' n_2' \right) (5)
$$

where \( \left< n_1 n_2 | V^{PP} | n_1' n_2' \right> \) are the matrix elements of the two-body pairing interaction, and indices \( n_1, n_1', n_2, \) and \( n_2' \) denote quantum numbers that specify the Dirac indices of the spinor.

The pairing force is separable in momentum space and in r-space has the form of

$$
V^{PP}(r_1, r_2, r_1', r_2') = -G \delta(R - R') P(r) P(r'), \quad (6)
$$

where \( R = \frac{1}{\sqrt{2}}(r_1 + r_2) \) and \( r = \sqrt{2}(r_1 - r_2) \) represent the center of mass and the relative coordinates, respectively and the form factor \( P(r) \) is of Gaussian form written as,

$$
P(r) = \frac{1}{(4\pi a^2)^{3/2}} e^{-r^2/2a^2}. \quad (7)
$$

The pairing force has a finite range and it also conserves translational invariance due to the presence of the factor \( \delta(R - R') \). Finally, the pairing energy in the nuclear ground state is given by

$$
\mathcal{E}_{pair} = -G \sum_N P_N^* P_N. \quad (8)
$$

### Table 1

The parameters of density-dependent point-coupling DD-PCX [37] and DD-PC1 [38] interactions in the Lagrangian. The value of saturation density is set to 0.152 fm\(^{-3}\) and mass of nucleon \( m = 939 \) MeV.

| Parameter | DD-PCX | DD-PC1 | Units |
|-----------|--------|--------|-------|
| \( a_S \) | -10.979243836 | -10.0432 | fm\(^2\) |
| \( b_S \) | -9.038250910 | -9.1504 | fm\(^2\) |
| \( c_S \) | -5.313008820 | -6.4273 | fm\(^2\) |
| \( d_S \) | 1.379087070 | 1.3724 | |
| \( a_V \) | 6.43014908 | 5.9195 | fm\(^2\) |
| \( b_V \) | 8.870626019 | 8.8637 | fm\(^2\) |
| \( d_V \) | 0.655310525 | 0.6584 | |
| \( b_{TV} \) | 2.963200654 | 1.8600 | fm\(^2\) |
| \( d_{TV} \) | 1.389081417 | 0.6403 | |
| \( \delta_S \) | -0.878850922 | -0.8149 | fm\(^2\) |

### 2.2 Covariant density functional theory with a separable pairing interaction

It is necessary to consider pairing correlations for a quantitative description of open-shell nuclei [35,10]. For nuclei far from stability, the BCS approximation presents a poor approximation. A unified and self-consistent treatment of mean-field and pairing correlations is necessary for an accurate description of weakly bound nuclei. This has led to the formulation and development of the relativistic Hartree-Bogoliubov (RHB) model. The formulation of RHB model is a relativistic extension of the conventional HFB framework in which mean-field and pairing correlations are treated self consistently. The RHB model gives a unified description of particle-hole (ph) and particle-particle (pp) correlations on a mean-field level by using the average self-consistent mean-field potential that encloses the long-range ph correlations and a pairing field potential which sums up the pp correlations. In the CDFT framework with pairing correlations, the density matrix can be generalized into two densities, the normal density \( \rho \) and pairing density \( \kappa \). The relativistic Hartree-Bogoliubov energy density functional can be written as

$$
\mathcal{E}_{RHB}[\rho, \kappa] = \mathcal{E}_{RMF}[\rho] + \mathcal{E}_{pair}[\kappa], \quad (3)
$$

where \( \mathcal{E}_{RMF}[\rho] \) is the nuclear energy density functional and is given by

$$
\mathcal{E}_{RMF}[\psi, \sigma, \omega, \rho, A] = \int d^3r H(r), \quad (4)
$$

The pairing part of RHB functional is given by

$$
\mathcal{E}_{pair}[\kappa] = \frac{1}{4} \sum_{n_1' n_2'} \kappa_{n_1 n_1'} \kappa_{n_2 n_2'} \left( n_1 n_2 | V^{PP} | n_1' n_2' \right) (5)
$$

where \( \left< n_1 n_2 | V^{PP} | n_1' n_2' \right> \) are the matrix elements of the two-body pairing interaction, and indices \( n_1, n_1', n_2, \) and \( n_2' \) denote quantum numbers that specify the Dirac indices of the spinor.

The pairing force is separable in momentum space and in r-space has the form of

$$
V^{PP}(r_1, r_2, r_1', r_2') = -G \delta(R - R') P(r) P(r'), \quad (6)
$$

where \( R = \frac{1}{\sqrt{2}}(r_1 + r_2) \) and \( r = \sqrt{2}(r_1 - r_2) \) represent the center of mass and the relative coordinates, respectively and the form factor \( P(r) \) is of Gaussian form written as,

$$
P(r) = \frac{1}{(4\pi a^2)^{3/2}} e^{-r^2/2a^2}. \quad (7)
$$

The pairing force has a finite range and it also conserves translational invariance due to the presence of the factor \( \delta(R - R') \). Finally, the pairing energy in the nuclear ground state is given by

$$
\mathcal{E}_{pair} = -G \sum_N P_N^* P_N. \quad (8)
$$

### 3 Results and Discussion

#### 3.1 Shape evolution in \(^{88-126}\)Zr and \(^{88-126}\)Mo isotopes

Shape is one of the most fundamental properties of nuclei and the quadrupole deformation parameter reflects the shape of the nuclei. The classification of deformed nuclei depends on the value of the quadrupole deformation parameter \( \beta_2 \). A positive value of \( \beta_2 \) corresponds to the prolate shape and the negative value to an oblate shape, while \( \beta_2 = 0 \) corresponds to spherical shape nuclei.

Fig. (1) displays the potential energy curves (PECs) of even-even \(^{88-126}\)Zr isotopes as a function of quadrupole
deformation parameter $\beta_2$, calculated using CDFT with DD-PCX and DD-PC1 parameters as given in Table 1. The energies in the PECs are normalized to the total energy of global minima. These calculations provide the results for the ground state of the nuclei. The calculations are performed systematically by taking constrained axial symmetry mapped by the quadrupole deformation parameter $\beta_2$. In both interactions, the isotopes with $N = 48 - 52$ show a spherical minimum which becomes shallow at $N = 54$, with $-0.2 \leq \beta_2 \leq 0.2$. An oblate minimum starts emerging at $N = 56$. Mean while, the prolate minima become deeper and the barrier height starts increasing on moving from $^{96}\text{Zr}$ to $^{98}\text{Zr}$. In case of DD-PCX interaction, a rapid increase in deformation parameter is observed as one move from $^{98}\text{Zr}$ ($\beta_2 = 0.290$) to $^{100}\text{Zr}$ ($\beta_2 = 0.428$). On moving from $^{100}\text{Zr}$, the ground state is seen to be stabilized with an almost constant prolate deformation, i.e., $\beta_2 \sim 0.45$, until $N = 70$. A sudden shape transition, from prolate to oblate, is seen at $N = 72$. On the other hand, the deformation parameter remains almost same for $^{98-102}\text{Zr}$ isotopes in case of DD-PC1 interaction. A sudden shape transition is observed on moving from $^{102}\text{Zr}$ (prolate) to $^{104}\text{Zr}$ (oblate) and the ground state remains oblate from $N = 64$ to $N = 76$ with a constant deformation around $\beta_2 \approx 0.2$. Fig. (1) shows an oblate-prolate shape coexistence with a very small energy difference in $^{96-110}\text{Zr}$ isotopes. The spherical shape is again restored on approaching neutron shell closure at $N = 82$. Thus, a dynamical shape transition is observed in the Zr isotope between two shell closures at $N = 50$ and $N = 82$. Fig. (2) presents the PECs of even-even $^{88-120}\text{Mo}$ isotopes as a function of $\beta_2$, with axially constrained CDFT calculations. The shape evolution for Mo isotopes is similar to that of Zr isotopes. The potential energy minima in PECs shows a spherical shape for Mo isotopes with $N = 48 - 52$ and prolate minima around $\sim 0.2$ for $N = 54 - 56$. In the meantime, the oblate minima start competing with the prolate minima and become deeper, with a small energy difference. In Fig. (2), a clear oblate-prolate shape coexistence is observed for $^{100-108}\text{Mo}$ isotopes for both parameter sets. On moving along the isotopic chain, there observed a single ground state oblate minima in $^{110-118}\text{Mo}$ isotopes. The shape again becomes spherical on reaching the neutron shell closure $N = 82$. However, it has been seen in the literature that many theoretical models predict a triaxial ground state between $N = 58$ and $N = 68$ in Mo isotopes. Also, the experimental charge radii have reproduced by taking the degree of triaxiality into account. Considering this fact, we have performed constrained triaxial calculations, mapped by triaxial parameter, $\gamma$, with a fixed value of $\beta_2$, in $^{100-110}\text{Mo}$ isotopes.

Fig. 1 (Color online) The potential energy curves (PEC), calculated using CDFT with DD-PCX and DD-PC1 interactions, as function of $\beta_2$ for $^{88-126}\text{Zr}$ isotopes. The energies are normalized with respect to the binding energy of the absolute minima.

Fig. 2 (Color online) The potential energy curves (PECs), calculated using CDFT with DD-PCX and DD-PC1 interactions, as function of $\beta_2$ for $^{88-126}\text{Mo}$ isotopes. The energies are normalized with respect to the binding energy of the absolute minima.

Figs. (3 & 4) show the PECs of $^{100-110}\text{Mo}$ isotopes as a function of triaxial deformation parameter, $\gamma$, for a fix value of $\beta_2$. The magnitude of $\beta_2$ values are taken as the minima in PECs in Figs. (1 & 2). It can be observed from the figures that, the PECs show a triaxial minima around $\gamma \approx 20^\circ$ and an oblate minima $\gamma \approx 60^\circ$ for the given value of $\beta_2$. In the present study, the triaxial min-
ima in $^{100-110}$Mo isotopes are the ground state minima with the highest total energy among the minimal observed in Figs. (1 & 2). The second ground state minima are oblate with a small energy difference, as presented in Table 2 and Table 3, respectively. Thus, we see the phenomena of shape coexistence in $^{100-110}$Mo isotope with triaxial ground-state that agrees with the predictions of various theoretical models [19,22], and the experimental results [3]. It is noted that the triaxial solution Mo isotopes above $N=66$ are almost same as the axial solution for both parameter sets. Hence, we have used the simple axial deformed calculation for these isotopes of Mo for the description of ground-state structural observables.

### Table 2 The location of the ground-state minima ($\beta, \gamma$) for $^{100-110}$Mo isotopes using DD-PCX parametrization.

| Nuclei | 1$^{st}$ minima | 2$^{nd}$ minima | $\Delta E_{\text{tot.}}$ (MeV) |
|--------|-----------------|-----------------|------------------|
| $^{100}$Mo | $(0.270,20^o)$ | $(0.230,55^o)$ | 0.041 |
| $^{102}$Mo | $(0.370,20^o)$ | $(0.230,60^o)$ | 0.224 |
| $^{104}$Mo | $(0.380,20^o)$ | $(0.230,60^o)$ | 0.287 |
| $^{106}$Mo | $(0.380,20^o)$ | $(0.230,60^o)$ | 0.307 |
| $^{108}$Mo | $(0.380,20^o)$ | $(0.230,55^o)$ | 0.067 |
| $^{110}$Mo | $(0.250,60^o)$ | - | - |

### 3.2 Systematics of average binding energy and two neutron separation energy

The stability of a nucleus is directly related to its binding energy and is also an important quantity to test a parameter set. The validity of a model can be judged by checking whether it can reproduce the experimental binding energy quantitatively or not. In Fig. (5), the rms deviation of binding energy, $\sigma_{\text{rms}}$, is calculated using CDFT formalism with DD-PCX and DD-PC1 parameters and compared with NL3 parameter set [21]. The rms deviation of binding energies is defined as

$$\sigma_{\text{rms}} = \sqrt{\frac{\sum_{i=1}^{n} (E_{i}^\text{Exp.} - E_{i}^\text{Cal.})^2}{n}}. \tag{9}$$

In Fig (5), the values of rms deviation of binding energies are given for each parameter set. We can see that the rms deviation of binding energies with both point-coupling parameter sets (DD-PCX and DD-PC1) are very close. It indicates that the parameter set DD-PCX is successful as DD-PC1 parameter set in reproducing...
the ground-state binding energies of the nuclei considered in the present study.

Another quantity that is related to the stability of a nucleus is two-neutron separation energy, \( S_{2n} \), defined as

\[
S_{2n}(Z, N) = E_b(Z, N) - E_b(Z, N-2). \tag{10}
\]

This quantity gives information on the stability of a nucleus against the emission of two neutrons, and thus define the neutron drip lines. Generally, the systematics of \( S_{2n} \) are known to decrease with the increasing number of neutrons. This decline in \( S_{2n} \) behavior is smooth except at magic number where a sharp change in the slope of \( S_{2n} \) is observed due to the presence of neutron shell closures. Fig. (6) presents the trend of \( S_{2n} \) behavior for Zr and Mo isotopic chains as a function of the neutron number. The theoretical results with DD-PCX and DD-PC1 parameter sets are calculated and compared with available experimental data\[41,42\] and theoretical NL3\[21\] results are shown.

The differential variation of the two-neutron separation energy \( (dS_{2n}(Z, N)) \) with respect to the neutron number \( (N) \) is defined as

\[
dS_{2n}(Z, N) = \frac{S_{2n}(Z, N+2) - S_{2n}(Z, N)}{2}. \tag{11}
\]

The \( dS_{2n}(Z, N) \) is an important quantity to investigate the rate of change of separation energy with respect to the neutron number. Here, we have calculated the systematics of \( dS_{2n}(Z, N) \) for Zr and Mo isotopic chains with DD-PCX and DD-PC1 parameter sets. We have also calculated the \( dS_{2n}(Z, N) \) from the experimental two-neutron separation energy. In Fig. (7), we compared the calculated \( dS_{2n} \) values for Zr and Mo isotopes with NL3\[21\] parameter set and with available experimental data\[11,12\]. Generally, the large and sharp deep fall in the \( dS_{2n} \) in an isotopic chain shows the signature of neutron shell closure. We can say that the deviation in the general trend may disclose some additional features of nuclear structure, like shape transition. An abnormal behavior in \( dS_{2n} \) trend at particular neutron number suggests the sudden change in ground state shape in Zr isotopic chain. On the other hand, the Mo isotopic chain shows a smoother behavior due to the occurrence of triaxiality. A sharp deep fall of \( dS_{2n} \) at \( N = 50 \) and \( N = 82 \) support the existence of robust shell closures.
3.3 Root-mean-square charge radius

The charge distributions in a nucleus are characterized by a fundamental property named as charge radii. Charge radii are considered among the most sensitive observables to explore the structural evolution in nuclei. Figs. (8 & 9) present the charge radii of Zr and Mo isotopes calculated using CDFT with DD-PCX and DD-PC1 parameter sets, as a function of neutron number. Comparison with experimental data[11,12] and theoretical results[21] are shown.

$$R_{ch} = \sqrt{R_p^2 + \langle r_p^2 \rangle + N \langle r_n^2 \rangle},$$  \hspace{1cm} (12)

where, $R_p$ denotes the rms radii of proton. Here $\langle r_p^2 \rangle = 0.833(10)$ $\text{fm}^2$[15] and $\langle r_n^2 \rangle = -0.1161(22)$ $\text{fm}^2$ are the mean-square charge radii of the proton and the neutron, respectively. In Figs. (8 & 9), the evolution of calculated rms charge radii in even-even $^{88-126}$Zr and $^{88-126}$Mo isotopes, as a function of neutron number, are plotted corresponding to the spherical, prolate, and oblate local minima in the PECs of these isotopes. In panel (a) of Fig. (8), a smooth increase in charge radii with almost similar slop is observed for the spherical and prolate shapes, with an exception from $N = 56$ to $N = 60$ in the Zr isotopes. This shows that the deformation of prolate minima in Zr isotopic chain is nearly the same as one move from $N = 60$ to $N = 70$. A sudden increase in charge radii from $N = 58$ to $N = 60$ is observed which is due to the increase in ground-state deformation from $\beta_2 = 0.290$ to $\beta_2 = 0.428$ (cf. Fig. (1)). A rapid fall in charge radii is also seen on moving from $N = 70$ to $N = 72$ which can be related to the sudden shape transition from prolate to oblate in Zr chain. However, such sharp rise at $N = 58$ is not seen with DD-PC1 force parameter, as seen in panel (a) of Fig. (9), rather a rapid increase in charge radii is observed on moving from $N = 56$ to $N = 58$. This dramatic rise is due to the shape transition from prolate to oblate as one move from $N = 56$ to $N = 58$. The value of charge radii shows a sharp fall from $N = 62$ to $N = 64$ due to the shape transition and then increase smoothly. Charge radii is again seen to decrease with neutron number which is due to the restoration of spherical shape at neutron shell closure $N = 82$. The calculated charge radii for Zr isotopes are well reproducing the experimental values[3]. A similar behavior of charge radii is observed with PC-PK1 point-coupling parameter[19], where a sharp rise in charge radii is seen from $N = 58$ to $N = 60$ in Zr isotopic chain. On the contrary, the charge radii in and Mo isotopes increase smoothly with the neutron number, as observed from panel (b) of Figs. (8 & 9). The experimental charge radii are reproduced well by taking triaxiality into account[6]. It can be observed from these figures that the ground-state in Mo isotopes become triaxial at $N = 58$ and an island of triaxiality is appearing from $N = 58$ up to $N = 66$. Similar behavior of charge radii in these isotopic chains was observed in the many theoretical studies[17,23,19]. A prominent characteristics of the isotopic evolution of charge radii in this region is probably the appearance of kink at $N = 82$ shell closure that was recently reported experimentally by laser spectroscopy technique in $^{132}$Sn isotope[46]. Also, the theoretical DFT calculations produce sharp kink at $N = 82$ using newly developed Fayans functional[47], which includes a gradient term in the pairing functional. In the present study, the sharp kink at $N = 82$ is absent in both Zr and Mo chains because of the non-flexibility of pairing functional in the present model, as explained in Ref. [48].

3.4 Single-particle energy levels

To understand the emergence of collectivity and shape coexistence phenomenon in Zr isotopes around $N = 60$, we plot the neutron and proton single-particle energy (SPE) levels in $^{100}$Zr, with DD-PCX parameter set, as functions of the axial deformation parameter $\beta_2$ in Fig. (10). Fermi levels are denoted by thick circles. Generally, the ground-state minima in the potential energy curve are associated with the effect of low-level density around the Fermi energy. According to Jahn-Teller effect[49], the regions of low-level density favor the onset of deformation. In the plot of neutron SPEs, a region of low-level density below the neutron Fermi energy level is observed around $-0.35 \leq \beta_2 \leq -0.15$ favoring an oblate shape. The panel (b) of Fig. (10) presents the plot of proton single-particle energy levels. A large
Fig. 8 (Color online) Nuclear charge radii in Zr and Mo isotopes as a function of neutron number. The calculated values with DD-PCX parameter set corresponding to the spherical (squares), prolate (down triangles), oblate (up triangles), and triaxial (diamonds). Experimental data are denoted by filled circles with error bars[3,6]. Open circles correspond to ground-state results.

Fig. 9 (Color online) Same as Fig. 8, but with different a parameter set DD-PC1.

shell gap is seen around $\beta_2 = 0.45$ below proton Fermi energy level which favors the onset of prolate deformation in $^{100}$Zr. This large shell gap is mainly formed by two levels split from the degenerate $\pi 1g_9/2$ state favoring the deformation[39]. A similar energy level diagram can be obtained using DD-PC1 parameter set. Thus, these ideas propose a simple comprehension of the several mechanisms leading to deformation in this mass region.

3.5 Contour plot for densities

In Figs. (11 & 12), the contour plots of axially deformed density distributions of neutrons in $^{90,100,114,122}$Zr isotopes are shown. These densities are plotted in the positive quadrant of the $xz$ plane, with $x = y$. The nuclear symmetry axis, $z$, is along the vertical axis and the coordinate $x$ or perpendicular axis is along the horizontal axis. A clear distinction between the spherical, prolate, and oblate shapes is seen for these isotopes corresponding to their ground-state $\beta_2$ values in the PECs (cf. Fig. (1 & 2)). In the figures, the red color corresponds to high density ($\sim 0.16$ fm$^{-3}$) and blue color to the lower density or zero density. Similar calculations for neutron and proton densities for $^{82,90,100,126}$Zr isotopes are done and plotted in Ref.[21]. From these figures, we observe a spherically symmetric neutron density distributions in $^{90}$Zr isotope and a prolate deformation in $^{100}$Zr indicating a shape transition from spherical to prolate as one moves away from $N = 50$. Again, a shape transition from prolate to oblate is observed as one reaches at $N = 74$ which can be seen from contour density plot for $^{114}$Zr. The spherically symmetric distribution of neutron densities are again restored on approaching neutron shell closure $N = 82$, as observed from figure. A close inspection of the density profile of $^{100}$Zr in both figures shows that the central part of the neutron density is less dense than the peripheral region, indicating the formation of a bubble. This result agrees with the study done in a recent paper on bubble structure nuclei in which a central depletion of neutron
density is observed for $^{100}$Zr. The occurrence of the bubble structure can be quantified by defining a term named as depletion fraction (DF). The depletion fraction for $^{100}$Zr calculated using CDFT formalism comes out to be 12.65% and 11.73% for DD-PCX and DD-PC1 parameter sets, respectively. This central depletion of density could be related to the unoccuency of 3s orbital. In present work, the occupencies of 3s$_{1/2}$ orbital are 0.0605 and 0.0379 for both parameter sets, respectively. However, a detailed study shall be carried out in future.

4 Conclusion

We have done self-consistent calculations using covariant density functional theory with density-dependent point-coupling DD-PC1 and recently developed DD-PCX force parameter in even-even $^{88–126}$Zr and $^{88–126}$Mo isotopes. We have studied the systematics of rms deviation of binding energy, two-neutron separation energy, differential variation of the two-neutron separation energy, rms charge radii, single-particle energy levels for these nuclei. The phenomena of structural change and shape coexistence have been observed in these isotopic chains. A sharp rise of charge radii in Zr isotopic chain from $N = 58$ to $N = 60$ is observed using new parameter set DD-PCX which can be related to the rapid increase in deformation parameter as one move from $^{98}$Zr to $^{100}$Zr. In this chain, a sudden shape transition from prolate to oblate has been seen at $N = 70$ whose signatures can be depicted in the systematics of two-neutron separation energies and rms charge radii. On the other hand, a smooth behavior in the evolution of charge radii is found in Mo isotopic chain due to the occurrence of triaxiality. This smoother increase in charge radii with neutron number is in good agreement with the available experimental data. Shape coexistence and triaxiality softness is seen for $^{100–108}$Mo isotopes. An oblate-prolate shape coexistence with almost degenerate energies is also seen for $^{96–110}$Zr isotopes. The observed oblate and prolate minimum are related to the low single-particle energy level density around the Fermi levels of neutron and proton respectively. We have also observed the depletion of central density in $^{100}$Zr isotope indicating a bubble structure. The overall results of the calculations for the ground-state properties in Zr and Mo isotopic mass chains, with new parameter set, are in good agreement with the available experimental data and with results obtained from different models.

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