We show how the shape evolution of the neutron-rich exotic Si and S isotopes can be understood as a Jahn-Teller effect that comes in part from the tensor-driven evolution of single-particle energies. The detailed calculations we present are in excellent agreement with known experimental data, and we point out of new features that should be explored in new experiments. Potential energy surfaces are used to understand the shape evolutions. The sub-shell closed nucleus, $^{42}$Si, is shown to be a perfect example of a strongly oblate shape instead of a sphere through a robust Jahn-Teller mechanism. The distribution of spectroscopic factors measured by $^{40}$Ca($e,e'p$) experiment is shown to be well described, providing a unique test on the tensor-driven shell evolution.

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Among the new frontiers of nuclear physics, one of the most important is the evolution of single-particle energies in nuclei far from stability, which is caused by dramatic changes in the location of magic numbers and types of collectivity relative to nuclei near stability [1]. One of the ingredients is the tensor-force driven changes in single-particle energies leading to tensor-force driven shell evolution [2, 3], with many experimental examples, e.g., [4].

We shall show in this Letter that tensor-driven shell evolution plays a critical role in the rapid shape change as a function of neutron and/or proton number, including triaxial and γ-unstable shapes. In particular, we show for the first time [2] how this shape change at low energy can be related to the Jahn-Teller effect [6, 7], where the degenerate intrinsic states led to a geometric distortion that removes the degeneracy and lowers the energy.

We study the structure of Si and S isotopes as examples, using shell-model calculation with SDPF-MU Hamiltonian to be described. The $sd$ and $pf$ cross-shell proton-neutron interaction is important, and is given by a monopole-based universal interaction ($V_{\text{MU}}$) [5] except for minor details. We show a test of this Hamiltonian by the spectroscopy of K isotopes. We then demonstrate that we can describe also the distribution of spectroscopic factors measured in the $(e,e'p)$ experiment [8], exhibiting the first theoretical reproduction of them. We then show levels, B(E2) values and potential energy surfaces (PES) of Si and S isotopes for even $N=22-28$ in comparison with experiments [8, 12], following an intuitive picture of the robust appearance of the oblate deformation in $^{42}$Si. We shall show that not only the property of $^{42}$Si but also the rapid change of structure of all these Si and S isotopes are naturally described.

We first outline the details of present shell-model calculations. The $sd$ and $pf$ shells are taken as the valence shell, whereas no excitation between them is included for the sake of simplicity. The interactions within each of these shells are based on existing interactions: USD [10] (GXPFI1B [14]) for the $sd$ ($pf$) shell. Regarding the monopole interaction $V_{\text{d}}$, as pointed out in Ref. [19], $V_{\text{d}}^{0\frac{1}{2}^+}$ must be corrected from its USD value. We made a shift, $\Delta V^{0\frac{1}{2}^+} = -3 \times \Delta V^{1\frac{3}{2}^+} = -0.7$ MeV, consistently with $V_{\text{MU}}$ and SDPF-M [20].

The monopole- and quadrupole-pairing matrix elements $\langle 0f_{7/2} 0f_{7/2} | V | 0f_{7/2} 0f_{7/2} \rangle_{J=0,2}$ are replaced with those of KB3 [18] for a better description of isotopes of $N \sim 20$. The cross-shell part, most essential for exotic nuclei of interest but rather undetermined so far, is given basically by $V_{\text{MU}}$ of [8] with small refinements stated below. The tensor-force component of $V_{\text{MU}}$ is nothing but the $\pi + \rho$ meson exchange force. In the experiments in many cases [2, 3], and has been accounted for microscopically under the new concept of Renormalization Persistency [21]. The central-force component is fine tuned from $V_{\text{MU}}$ with density dependence similar to the one in [22], so that its monopole part becomes closer to that of GXPFI1B [23]. We include the two-body spin-orbit force of the M3Y interaction [24]. Following USD and GXPFI1B, all of the two-body matrix elements are scaled by $A^{-0.3}$. The single-particle energies (SPE) of the $sd$ shell are taken from USD, and those of the $pf$ shell are determined by requesting their effective SPEs on top of $^{40}$Ca closed shell equal to the single-particle energies of GXPFI1B.

The Hamiltonian thus fixed is referred to as SDPF-MU hereafter, and is diagonalized by the mshell64 code [25].
Note that none of the cross-shell monopole interactions are fitted directly to experiment, in contrast to other recent interactions [20, 22].

We first study proton single-particle states of odd-A K (Z=19) isotopes. Figure 1 exhibits 1/2^+_1 levels for N\(=20\sim 28\). If valence neutrons occupy the lowest possible orbits (filling configuration), the 1/2^+_1 level relative to 3/2^+_1 corresponds to the 0d_3/2-1s^+_1/2 gap. Since this is the case with N\(=20\) and is almost so with N\(=28\), the lowering of the 1/2^+_1 level from N\(=20\) to 28 reflects considerable reduction of this gap. Experimentally observed reduction (∼3 MeV) is reproduced remarkably well by SDPF-MU Hamiltonian. This reduction is due to the proton-neutron monopole interaction \(V_{0fr/2,0d_{5/2}}\) that is more attractive than \(V_{0fr/2,1s_{1/2}}\); the difference is 0.44 MeV (at A\(=42\)), out of which the tensor and the central forces contribute, respectively, by 0.21 MeV and 0.22 MeV. The central force yields a stronger attraction between 0f_{7/2} and 0d_{3/2} because of the similarity of their radial wave functions [3].

We move on to the splitting between the 0d_{3/2} and 0d_{5/2} single-particle energies. The 0d_{5/2} single-particle strength is highly fragmented due to its large excitation energy (6-7 MeV). Spectroscopic factors of the proton sd-shell orbits have been measured for \(^{40}\text{Ca}\) by one-proton removal through \((e,e'p)\) reaction [8]. The left panel of Fig. 2 displays the experimental values in comparison to those obtained by the present calculation, where the usual overall quenching factor 0.7 is used [28]. The agreement is excellent both in positions of peaks and their magnitudes. However, this agreement is lost, if the tensor force is removed from the cross-shell interaction, as shown in the right panel of Fig. 2. For instance, the highest 0d_{3/2} peak is shifted in the wrong direction, and the main peak of 0d_{5/2} moves away towards higher energy. In the present calculation, as already stated, the ESPEs around \(^{40}\text{Ca}\) are consistent with experiments with a reasonably large 0d_{3/2}-0d_{5/2} gap ∼7 MeV. The proton shell structure evolves from \(^{40}\text{Ca}\) to \(^{48}\text{Ca}\), giving rise to the agreement with the fragmentation of spectroscopic factors. In particular, because only the tensor force can change the 0d_{3/2}-0d_{5/2} gap to this order of magnitude (by ∼2 MeV), the agreement shown in Fig. 2 provides us with the first evidence from electron scattering experiments to the tensor-force-driven shell evolution [2].

We now consider shape transitions driven by shell evolution, by taking as an example the exotic Si (Z=14) isotopes with even N\(=22\sim 28\). In a conventional view, Z=14 is a (sub-)magic number with a large 1s_{1/2}-0d_{5/2}
gap, as shown in Fig. 3(a). For a large gap, six protons occupy 0d_{5/2}, forming a closed shell. This should end up with a spherical shape particularly for a doubly magic nucleus, $^{42}\text{Si}$ ($N=28$), similar to that observed in $^{34}\text{Si}$ ($N=20$). The situation changes when many neutrons occupy the $0f_{7/2}$ orbital. Following the mechanism of Otuka et al. [2], the monopole interaction of the tensor force is strongly repulsive between a proton in $0d_{5/2}$ and a neutron $0f_{7/2}$. Hence, as neutrons occupy $0f_{7/2}$, the spin-orbit splitting decreases and the energy of proton $0d_{5/2}$ level comes closer to $1s_{1/2}$ level (The $1s_{1/2}$ energy is unaffected by this mechanism).

Figure 3(b) presents an intuitive illustration on the consequence of this change by taking a simple case comprised of $1s_{1/2}$ and $0d_{5/2}$ orbits. These orbits are mixed, like Nilsson orbits, due to the quadrupole deformation of the intrinsic state. Assuming an axially symmetric deformation, single-particle states of the same magnetic quantum numbers, denoted $m$, are mixed in the intrinsic states. Figure 3(b) indicates that this occurs for $m = \pm 1/2$ between $1s_{1/2}$ and $0d_{5/2}$, with amplitudes $\sin \theta$ and $\cos \theta$, respectively. A smaller $1s_{1/2}$-$0d_{5/2}$ gap results in more mixing, while the phase of mixing amplitude depends on $m$ as to whether the shape is prolate or oblate. In the present case, protons occupy the states of $m = \pm 5/2$, $\pm 3/2$, which yield in total a negative intrinsic quadrupole moment (i.e., a oblate shape). The total intrinsic quadrupole moment gains a larger magnitude, if the $1s_{1/2}$-$0d_{5/2}$ mixing gives a negative moment. The proton-neutron interaction, apart from its monopole part, can be modeled by a quadrupole-quadrupole interaction, and a similar mixing occurs for neutrons in $1p_{3/2}$ and $0f_{7/2}$, producing a negative intrinsic moment. Thus, by having the mixing leading to a negative intrinsic moment, the total magnitude of the moment becomes larger for both protons and neutrons, giving rise to stronger binding of the intrinsic state from the quadrupole-quadrupole interaction. The actual structure is determined by the competition between actual (effective) gaps and effects of the quadrupole-quadrupole interaction, implying that the shapes of Si isotopes depends on how the gaps are reduced by the tensor force.

We then examine this picture in the context of the shell-model calculations with the SDPF-MU Hamiltonian. Figure 4 exhibits yrast properties of even-$A$ Si and S isotopes. Effective charges are $(e_p, e_n) = (1.20e, 0.45e)$ fixed already by properties of lighter isotopes. The overall agreement to experiment is remarkable. For instance, in the present result, $2^+_1$ levels of Si isotopes keep coming down as $N$ increases consistently with experiment, whereas some increase is seen at $N = 28$ in other shell-model calculations [24, 27]. The nice agreement suggests that the intuitive picture above holds particularly towards $N=28$, resulting in strongly deformed shapes with low excitation energies consistent also with recent measurement by GANIL [12]. In fact, if the tensor force is omitted from the cross-shell interaction, $2^+_1$ level of $^{42}\text{Si}_{28}$ goes up. It is of much interest to see the missing experimental data in Fig. 4 as well as more precise $B(E2)$ values. Figure 4 exhibits results for S isotopes in good overall agreement.

The potential energy surface (PES) is useful to understand shapes contained in theoretical calculations. Figure 5 exhibits PES for Si isotopes obtained by the constrained Hartree-Fock method [29] for the SDPF-MU Hamiltonian. The full Hamiltonian is taken in Fig. 5 (a–d), whereas the cross-shell tensor force is removed in Fig. 5 (e–h). Shape evolutions are seen very clearly in both sequences (a~d) and (e~h), starting with similar patterns in $^{36}\text{Si}$. The shape evolves as more neutrons occupy pf-shell, with distinct differences between the two sequences. In (b,c), the deformation becomes stronger from (a) with triaxial minima, whereas the shape becomes more like modestly prolate in (f,g). In (d), one finds a strongly oblate shape with a sharp minimum, but the minimum is at the spherical shape in (h). This strong oblate deformation produces low $2^+$ level and large $B(E2)$ in Fig. 4 for the “doubly-closed” $^{42}\text{Si}$. Thus, the shape of exotic Si isotopes changes significantly within the range of $\Delta N \sim 6$. This is considered to be a manifestation of Jahn-Teller effect with varying shell structure driven by the tensor force. We note that the two sequences produce rather similar levels and $B(E2)$ in Fig. 4 for lighter isotopes, and the structure of $^{42}\text{Si}$ serves a key role in the study of the tensor-force effect.

Although more experiments are needed to clarify present issues, there are some hints of the triaxiality...
from $2^+_2$ level. The present calculations with (without) the cross-shell tensor force locates it at 0.62 (1.11) MeV above $2^+_2$ for $^{40}\text{Si}$. The extraordinary low-lying $2^+_2$ level caused by the tensor force appears to agree with a recent γ-ray experiment \[11\]: it is proposed that at least either 638(8) and 845(6) keV directly feeds the $2^+_1$ state.

With density-functional methods \[33, 34\], Si and S are discussed with somewhat less overall agreement with experiment, compared to the present calculation. It will be of interest to see single-particle properties given by these works in the view of Jahn-Teller effect. For instance, how much does the $1s_{1/2} - 0d_{5/2}$ gap change from $^{40}\text{Ca}$ to $^{48}\text{Ca}$?

In summary, we have presented more evidences of the tensor-force driven shell evolution, proposed by Otsuka \[2, 3\], in low-lying states of K isotopes and in distribution of spectroscopic factors measured by $^{48}\text{Ca}(e,e'p)$ experiment. Similarly, the levels and $B(E2)$'s of exotic Si and S isotopes are described well by the same Hamiltonian. The nuclear deformation at low excitation energy is a Jahn-Teller effect, which should be sensitive to the shell structure. The shell evolution driven by the tensor force plays a crucial role in rapid shape transitions, including a robust mechanism for the appearance of the stable oblate shape at subshell closures against prolate dominance of the nuclear deformation. In future, similarities and differences in $^{78}\text{Ni}$ will be of great interest.

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\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{potential_energy_surfaces}
\caption{(Color online) Potential energy surfaces of Si isotopes from $N = 22$ to $28$ calculated with (left) and without (right) the cross-shell tensor force. The energy minima are indicated by red circles.}
\end{figure}