$J = 0$ nonmagnetic insulating state in $K_2\text{Os}X_6$ ($X = \text{F, Cl, and Br}$)

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In 4$d$/5$d$ transition-metal systems, many interesting physical properties arise from the interplay of bandwidth, electronic correlations, and spin-orbit interactions. Here, using ab initio density functional functional theory, we systematically study the double-perovskite-like system $K_2\text{Os}X_6$ ($X = \text{F, Cl, and Br}$) with a 5$d^4$ electronic configuration. Our main result is that the $J = 0$ nonmagnetic insulating state develops in this system, induced by strong spin-orbit-coupling (SOC). Specifically, the well-separated Os$X_6$ octahedra lead to the cubic crystal-field limit and result in dramatically decreasing hoppings among nearest neighbor Os-Os sites. In this case, the three degenerate $t_{2g}$ orbitals are reconstructed into two “effective” $j_{\text{eff}}$ ($j_{\text{eff}} = 1/2$ and $j_{\text{eff}} = 3/2$) states separated by the strong SOC, opening a gap with four electrons occupying the $j_{\text{eff}} = 3/2$ orbitals. Furthermore, the hybridization between the Os $5d$ orbitals and the $X$ ($X = \text{F, Cl, and Br}$) $p$ orbitals increases from F to Br, leading the electrons in $K_2\text{OsF}_6$ to be more localized than in $K_2\text{OsCl}_6$ and $K_2\text{OsBr}_6$, resulting in a smaller bandwidth for $K_2\text{OsF}_6$ than in the Cl- or Br-cases. Our results provide guidance to experimentalists and theorists working on this interesting family of osmium halides.

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In the past decade, material systems with 4$d$ or 5$d$ transition-metal (TM) atoms, such as iridium and osmium, have attracted growing attention due to the exotic physical phenomena induced by the strong spin-orbit coupling (SOC) [1–5]. Compared to the nearly negligible SOC in 3$d$ atoms, the strength of the SOC $\lambda$ is substantially enhanced in those 4$d$/5$d$ systems, leading to comparable values between $\lambda$, the hopping parameter $t$, the Hubbard repulsion $U$, and the Hund coupling $J_H$, resulting in several intriguing electronic phases arising from their competition, such as topological phases [6–9], the orbital-selective Peierls phase [10,11], “spin-orbit Mott” insulating state [12,13], Rashba-like splitting [14,15], the anomalous Hall effect [16,17], and quantum spin liquid ground states [18,19].

In an octahedral 5$d^4$ system, under a cubic crystal-field condition, the five degenerate $d$ orbitals split into two sets of bands (the higher $e_g$ and lower $t_{2g}$ bands) separated by a large crystal-field splitting energy $\Delta$ ($\sim 10Dq$) [20] [Fig. 1(a)]. Due to the competition among $\Delta$, $J_H$, and $\lambda$, many electronic states are possible for a 5$d^4$ system, such as $S = 2$, $S = 1$, and $J = 0$ states. For the 4$d$/5$d$ system with 5$d^4$ configuration, such as Ru$^{4+}$, Os$^{4+}$, and Ir$^{5+}$, the four electrons will occupy the three degenerate $t_{2g}$ orbitals, leading to a metallic state [Fig. 1(b)] because the $t_{2g}$ orbitals are not fully occupied (four electrons in three $t_{2g}$ orbitals). Then, by introducing the SOC effect, the three $t_{2g}$ orbitals reconstruct into two “effective” $j_{\text{eff}}$ ($j_{\text{eff}} = 1/2$ and $j_{\text{eff}} = 3/2$) states separated by the SOC [Fig. 1(a)]. Returning to the case $U = 0$, and considering the SOC with $\lambda > 0$, this system with a 5$d^4$ electronic configuration is expected to be a nonmagnetic (NM) insulator made of local two-hole $J = 0$ singlets [22,23], where the band gap is opened by the strong SOC between the $j_{\text{eff}} = 1/2$ and $j_{\text{eff}} = 3/2$ states [Fig. 1(c)].

Recently, neutron scattering experiments revealed a soft longitudinal magnon mode in $\text{Ca}_2\text{RuO}_4$ with the 4$d^4$ configuration, which has been considered as a hallmark of a $J = 0$ singlet state quantum phase transition [24,25]. In theory, this could lead to an exotic magnetically ordered state induced by the condensation of spin-orbit excitons [22,23,26–32]. Most searches for the $J = 0$ state have mainly focused on the 5$d^4$ iridates systems. However, they display the $S = 1$ magnetic ground state or weak moments, instead of the NM insulator with the $J = 0$ singlets, such as the 5$d^4$ iridates $\text{Ba}_3\text{YIr}_2\text{O}_9$ [33] and $\text{Ba}_3\text{ZnIr}_2\text{O}_9$ [34,35]. Furthermore, the $J = 0$ state is still under debate for some double-perovskite iridates with quite small noncubic crystal-field effect, such as $\text{Sr}_2\text{YIrO}_6$ [36,37] and $\text{Ba}_2\text{YIrO}_6$ [38,39]. Hence, the $J = 0$ state is still rare in real materials.

In general, the 4$d$/5$d$ orbitals are much more spatially extended than the 3$d$ orbitals, leading to an enhanced hopping $t$ in the 4$d$/5$d$ case, corresponding to a large bandwidth $W$ in these systems (with the hopping $t$ providing the scale). In this case, the large bandwidth $W$ would induce the breakdown of the $J = 0$ singlet state [37,40,41], where an $S = 1$ state is obtained because $W \gg \lambda$. Furthermore, the $J = 0$ singlet ground state could also be suppressed by the large crystal-field splitting energy (between $d_{x^2−y^2}$ and $d_{z^2}$ orbitals) [40,41], resulting in $S = 1$ or $S = 0$ states induced by Jahn-Teller distortion $Q_3$ [42]. Hence, a 5$d^4$ system with a strong SOC effect, small bandwidth $W$, and cubic crystal-field splitting becomes the best candidate to obtain the $J = 0$ NM singlet insulator.

$K_2\text{Os}X_6$ ($X = \text{F, Cl, and Br}$) has a double-perovskite-like structure, which is known to display the required conditions. This system has a 5$d^4$ electronic configuration with strong SOC Os$^{4+}$ ions, where the Os$X_6$ octahedra are at sufficiently...
large distance that they can be considered isolated from one another (Fig. 2). K$_2$OsF$_6$ has the space group $P\overline{3}m1$ (No. 164) while both K$_2$OsCl$_6$ and K$_2$OsBr$_6$ have the space group $Fm\overline{3}m$ (No. 225) [44]. In this family, due to the well-separated OsX$_6$ octahedra, the Jahn-Teller distortion is suppressed, leading to six equal Os-X bonds in this system, resulting in a nearly cubic crystal-field environment. In this case, the crystal-field splitting (between $d_{x^2-y^2}$ and $d_{xy}$ orbitals) is suppressed. In addition, the hopping $t$ between nearest-neighbor (NN) Os-Os sites should be small due to the Os-X-X-Os super-super exchange caused by the geometric structure of isolated OsX$_6$ octahedra. Hence, by considering the SOC in Os atoms, the $J = 0$ NM insulating state could possibly be stabilized in this family.

Based on the density functional theory (DFT) within the generalized gradient approximation (GGA) method and the Perdew-Burke-Ernzerhof revised for solids (PBEsol) exchange potential [45–49], we obtained that the relaxed crystal lattices are $a = b = 5.786$, and $c = 4.569$ Å for K$_2$OsF$_6$, close to experimental values ($a = b = 5.777$ and $c = 4.544$ Å) [50]. We also found that the lattice constants of K$_2$OsCl$_6$ and K$_2$OsBr$_6$ ($a = b = c = 9.608$ Å for the Cl case, and $a = b = c = 10.184$ Å for the Br case) are in agreement with experiments ($a = b = c = 9.719$ Å for the Cl case, and $a = c = 10.300$ Å for the Br case) [51,52]. To save computing resources, we used the unit cell structure of K$_2$OsCl$_6$ and K$_2$OsBr$_6$ [Fig. 2(b)] in the calculations below. In addition, we also calculated the phononic dispersion, finding that these structures are dynamically stable (see Fig. S1 of the Supplemental Material [42]).

Next, we calculated the density of states (DOS) of K$_2$OsX$_6$ ($X = F$, Cl, and Br) in the NM state without SOC [42]. According to the DOS, the states near the Fermi level are mainly contributed by the Os-5$d$ $t_{2g}$ orbitals, partially hybridized with $X$-$p$ orbitals, while most other X’s $p$ states are located below the Os-$5d$ energy states [Figs. 3(a)–3(c)]. Note that the K’s 4$s$ states are located at high-energy bands (unoccupied states) while the K’s 3$p$ states occupy low-energy states below the X’s 3$p$ states.

As shown in Figs. 3(a)–3(c), the $X$-$p$ orbitals become closer to the Fermi level when $X$ changes from F to Br. With increasing atomic radius from F to Br, the $p$ components near the Fermi level become larger, leading to an increase in the $p$-$d$ hybridization tendency from F to Br. In this case, the Os’s $t_{2g}$ bands are more extended in K$_2$OsCl$_6$ ($W \sim 0.7$ eV) and K$_2$OsBr$_6$ ($W \sim 0.8$ eV) than in K$_2$OsF$_6$ ($W \sim 0.3$ eV), as shown in Figs. 3(a)–3(c), suggesting stronger electronic correlations ($U/W$) in K$_2$OsF$_6$. Furthermore, the energy splitting between the $t_{2g}$ and $e_g$ orbitals decreases from F ($\sim 3.3$ eV) to Br ($\sim 2.6$ eV) by estimating the weight-center positions of the energy bands. In addition, we also calculated the electron localization function (ELF) [53] for K$_2$OsF$_6$, K$_2$OsCl$_6$, and K$_2$OsBr$_6$, respectively, as displayed in Fig. 3(d). The ELF picture indicates that the charges are more localized inside the Os-F bonds than the Os-Cl or Os-Br bonds, resulting in more hybridized $p$-$d$ bonds in K$_2$OsF$_6$ than in K$_2$OsCl$_6$ or K$_2$OsBr$_6$. For this reason, the bandwidth of OsX$_6$ increases from F to Br, by considering the super-super exchange coupling (Os-$X$-$X$-Os) between two NN sites of Os. Furthermore, the stronger $p$-$d$ hybridization tendencies would also reduce the SOC constants of Os atoms in the Cl or Br cases. This reduction was also experimentally observed in K$_2$IrX$_6$ ($X = F$, Cl, and Br) with the 5$d^5$ configuration (572/444/420 meV for F/Cl/Br, respectively) [54].

To understand qualitatively the possible $J = 0$ state based on the maximally localized Wannier functions (MLWFs) method [55], we obtained the on-site energies and hoppings for different Os’s $t_{2g}$ orbitals [56]. The spreads of $t_{2g}$
However, this is not the case we studied here. In addition, the electronic correlations play the dominant role.

For K\textsubscript{2}Os\textsubscript{2}Cl\textsubscript{6} and K\textsubscript{2}Os\textsubscript{2}Br\textsubscript{6}, the t\textsubscript{2g} bands of Os are not separated and keep metallic behavior. By introducing SOC in K\textsubscript{2}Os\textsubscript{2}Cl\textsubscript{6} and K\textsubscript{2}Os\textsubscript{2}Br\textsubscript{6}, the t\textsubscript{2g} states begin to separate and reconstruct into the j\textsubscript{eff} = 1/2 and j\textsubscript{eff} = 3/2 states, opening a gap. In this case, the SOC plays the key role in deciding the nature of the insulating state, by separating the empty j\textsubscript{eff} = 1/2 and fully occupied j\textsubscript{eff} = 3/2 states. The almost undistorted OsX\textsubscript{6} (X = F, Cl, and Br) octahedra are ideally separated, leading to a dramatic decrease in the hopping between Os-Os sites. In this quasisdisconnected geometry, the weak Os-X-Os superexchange interaction leads to the decreasing connectivity of the OsX\textsubscript{6} octahedra, resulting in a case close to the atomic limit. In the F case, the large SOC effect achieves a J = 0 NM state by comparison with the small hopping (∼40 meV) and quenched crystal-field splitting.

Without SOC and U effects, the band structures of K\textsubscript{2}Os\textsubscript{2}Cl\textsubscript{6} and K\textsubscript{2}Os\textsubscript{2}Br\textsubscript{6} show metallic behavior due to the partially occupied t\textsubscript{2g} orbitals, as shown in Figs. 4(c) and 4(e). By introducing the SOC in K\textsubscript{2}Os\textsubscript{2}Cl\textsubscript{6} and K\textsubscript{2}Os\textsubscript{2}Br\textsubscript{6}, the t\textsubscript{2g} bands begin to separate and reconstruct into the j\textsubscript{eff} = 1/2 and j\textsubscript{eff} = 3/2 states [see Figs. 4(c) and 4(e)]. Different from the results for K\textsubscript{2}Os\textsubscript{2}F\textsubscript{6}, a band gap is not obtained with the SOC effect in both K\textsubscript{2}Os\textsubscript{2}Cl\textsubscript{6} and K\textsubscript{2}Os\textsubscript{2}Br\textsubscript{6}, keeping a metallic state. Some Os 5d electrons partially occupy the j\textsubscript{eff} = 1/2 states, contributing to the conductivity in both the Cl and Br cases. This can be understood intuitively. Due to the stronger p-d hybridization tendencies in the Cl or Br cases than in the F case, the bandwidth increases, and the SOC constants of Os atoms are reduced. Then, the hopping t could compete with the strong SOC λ, leading to a metallic phase with partially occupied j\textsubscript{eff} = 1/2 states crossing the Fermi level. In this region, λ > t, the J states are not totally separated. Then, if the strength of the SOC could continue to increase, the gap should finally open. Furthermore, similar to the results for K\textsubscript{2}Os\textsubscript{2}F\textsubscript{6}, the electronic correlation U would not separate the t\textsubscript{2g} states and open a gap [Figs. 4(d) and 4(f)].

To better understand the SOC effect, we also calculated the band gaps within the GGA + SOC approximation by selecting various SOC strengths. As displayed in Fig. 5, the gap increases by enhancing the SOC strength [60]. Due to the small bandwidth of K\textsubscript{2}Os\textsubscript{2}F\textsubscript{6}, the gap can be opened by a small SOC strength (~50%). On the other hand, the insulating gap can be obtained for a higher SOC strength (~150%) for K\textsubscript{2}Os\textsubscript{2}Cl\textsubscript{6} and K\textsubscript{2}Os\textsubscript{2}Br\textsubscript{6} because the larger bandwidths of the Cl or Br cases leads to a competition between hopping t
and SOC $\lambda$. Because the energy gap between the Os’s $j_{d\pi}$ = 1/2 and $j_{d\delta}$ = 3/2 states is about 3$\lambda$/2, we can estimate the SOC values by calculating the changes in the value of this energy gap under very small modifications in the SOC strength. In addition, we also estimated that the SOC values are about 0.467, 0.405, and 0.367 eV for K$_2$OsF$_6$, K$_2$OsCl$_6$, and K$_2$OsBr$_6$, respectively. This reduced tendency of SOC values in K$_2$OsX$_6$ is quite similar to the case of the K$_2$IrX$_6$ system with $d^5$ configuration [54]. By comparing the induced hoppings from F to Cl, this could explain the metallic behavior in Cl and Br cases. By continuing increasing the strength of the SOC, the gaps increase in K$_2$OsCl$_6$ and K$_2$OsBr$_6$, as expected. In the strong SOC condition, the entire K$_2$OsX$_6$ ($X = F$, Cl, and Br) family could be considered to be a potential $J = 0$ NM insulator. The insulating vs metallic character of the correlated system under study is decided by several factors related to different parameters (primarily $t$, $\lambda$, $J_H$, and $U$). As described in the text, the $J = 0$ state can be stabilized in a $d^5$ system only in a special range of parameters, namely under severe limitations, at least according to our calculations. For a complete physical picture, it would be important to study how the $J = 0$ state evolves by varying those many different parameters. Such effort will demand considerable computational resources and discussion, and they should be based on model calculations, beyond the scope of our present paper.

For the spin-orbital-entangled $J = 0$ NM insulating compounds, the excitonic $J = 1$ triplet state displays interesting magnetic order caused by the condensation of mobile spin-orbit excitons [22,23]. The ordered moment is dependent on the competition between exchange interactions and the energy gap caused by the SOC. Furthermore, some possible interesting features can be obtained near the quantum critical point (QCP) in the $J = 1$ excitonic state, such as a Higgs mode [24] and magnons [5]. Our results for the K$_2$OsX$_6$ ($X = F$, Cl, and Br) family provide a starting point for experimentalists and theorists to work on the $j_{d\pi}$ = 0 state or the $J = 1$ triplet excitations on this 5$d^5$ system, such as in inelastic neutron scattering (INS) or resonant inelastic x-ray scattering (RIXS) experiments. In fact, the $K$ site could be replaced by other 1+ ions [61], such as Rb$^+$, Cs$^+$ and (NH$_4$)$^+$, where the same $J = 0$ physics should be obtained. Due to the “zero-dimensional” geometry structure, the $K$ site may be replaced by 2+ ions, such as in the $d^3$ configuration, where the spin-orbital Mott state could be obtained. Hence, our results clearly provide a potential candidate system for experimentalists and theorists to work on this $K$ system and related materials.

In summary, we presented a systematic study of the K$_2$OsX$_6$ ($X = F$, Cl, and Br) family with a 5$d^5$ electronic configuration by using DFT first-principles calculations.

**FIG. 4.** Band structures of the NM state based on GGA, GGA + SOC, and GGA + $U$ + SOC for (a,b) K$_2$OsF$_6$, (c,d) K$_2$OsCl$_6$, and (e,f) K$_2$OsBr$_6$, respectively. Here, the correlation effects were considered by the Liechtenstein formulation within the double-counting term [58], where the on-site Coulomb interaction used was $U = 2$ eV, and the Hund coupling was $J_H = 0.4$ eV for the Os atoms [59]. The Fermi level is the horizontal dashed line. (a,b) For K$_2$OsF$_6$, the coordinates of the high-symmetry points in the Brillouin zone (BZ) are given by $\Gamma = (0, 0, 0), M = (0.5, 0, 0), K = (1/3, 1/3, 0), A = (0, 0, 0.5), L = (0.5, 0, 0.5)$ and $H = (1/3, 1/3, 0.5)$. (e,f) For K$_2$OsCl$_6$ or K$_2$OsBr$_6$, the coordinates of the high-symmetry points in the BZ are given by $\Gamma = (0, 0, 0), X = (0.5, 0, 0.5), U = (0.625, 0.25, 0.625), K = (0.375, 0.375, 0.75), L = (0.5, 0.5, 0.5)$, and $W = (0.5, 0.25, 0.75)$.

**FIG. 5.** Band gaps as a function of SOC strength for K$_2$OsF$_6$, K$_2$OsCl$_6$, and K$_2$OsBr$_6$, respectively, within GGA + SOC calculations. Here, we do not introduce the Hubbard interaction $U$ on Os sites because the SOC plays the key role to open the gap.
Due to the isolated geometry of the well-separated OsX₆ octahedra, this system is close to the cubic crystal-field limit and results in dramatically decreasing hoppings for nearest-neighbor Os-Os sites, providing a fertile condition for obtaining the $J = 0$ NM insulator. By introducing the SOC, the three degenerate configuration fully occupy the lower tile condition for obtaining the pings for nearest-neighbor Os–Os sites, providing a ferromagnetism limit and results in dramatically decreasing hop-octahedra, this system is close to the cubic crystal.

Due to the isolated geometry of the well-separated OsX₆ the Os 5e₃ orbitals and X (X = F, Cl, and Br) p orbitals split into two separated “effective” $j_{eff}$ ($j_{eff} = 1/2$ and $j_{eff} = 3/2$ states) states. In K₂OsF₆, due to the small bandwidth of the Os 5d orbitals (∼0.3 eV), the SOC effect is sufficiently strong to open a gap. Hence, four electrons on the Os 4d (5d³ configuration) fully occupy the lower $j_{eff} = 3/2$ quadruplet, leading to an unoccupied $j_{eff} = 1/2$ doublet, resulting in a $J = 0$ NM insulator.

Furthermore, the hybridization between the Os 5d orbitals and X (X = F, Cl, and Br) p orbitals increases from F to Br, leading the electrons in K₂OsCl₆ and K₂OsBr₆ to be less localized than in K₂OsF₆, resulting in a larger bandwidth for the Cl or Br cases (∼0.7, 0.8 eV for K₂OsCl₆ and K₂OsBr₆, respectively) than in the F case. In these compounds, the SOC λ competes the hopping $t$ in K₂OsCl₆ and K₂OsBr₆, and the combination is not enough to open a gap because some electrons would occupy the $j_{eff} = 1/2$ states. By increasing the SOC strength to ∼150%, the $j_{eff} = 1/2$ and $j_{eff} = 3/2$ states become totally separated, obtaining the $J = 0$ NM insulator in K₂OsCl₆ and K₂OsBr₆. Hence, our results should encourage experimentalists and theorists to continue working on this interesting family of osmium halides to achieve the $J = 0$ state, and also $J = 1$ triplet excitations and excitonic magnetism.

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[20] $Dq$ means deci (ten) quanta of energy, where $10Dq$ represents the empirical octahedral crystal field splitting energy.
[21] In the large $U$ limit, the system (four electrons in three orbitals) should be a Mott insulator, where the gap is opened by the Hubbard $U$. However, the real system could be metallic or insulating depending on the competition of bandwidth $W$ (corresponding to hopping $t$ scale) and Hubbard interaction $U$. For example, see L. F. Lin, Y. Zhang, G. Alvarez, A. Moreo, and E. Dagotto, Phys. Rev. Lett. 127, 077204 (2021).
In K2OsCl6 and K2OBr6, the OsF6 or OsBr6 octahedra are ideal cubic structure (No. 225). Without any distortion, leading to the ideal 90° bond angles of the F-Os-F bond not being strictly 90°. The octahedra have a slightly distorted octahedron-like behavior, resulting in the angle of the F-Os-F bond not being strictly 90°. Bonds in the\( J_{HF}/U \) case of the Os site, especially for F case. For example, cRPA calculation indicates that the \( U \) of the Os site is smaller than 1 eV; see B. Kim, P. Liu, Z. Ergönenc, A. Toschi, S. Khmelevskyi, and C. Franchini, Phys. Rev. B 94, 241113(R) (2016). However, in our case of the \( J = 0 \) state, the SOC plays the key role to open the gap, not \( U \).

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