Dzyaloshinskii-Moriya Interaction between Multipolar Moments in $5d^1$ Systems

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We propose a new type of Dzyaloshinskii-Moriya interactions which act on high-rank multipole moments such as quadrupole and octupole moments. Here we consider the $5d^1$ systems with broken spacial inversion symmetry, where the interplay of electron correlation, spin-orbit coupling, and inversion symmetry breaking plays a crucial role. Using numerical diagonalization on a two-site multiorbital Hubbard model, we reveal that anti-symmetric products of multipole operators have finite expectation values, indicating the existence of Dzyaloshinskii-Moriya interactions for multipoles. We also find that these expectation value have unusual dependence on a spin-orbit coupling.

Introduction.- Interplay of electron correlation and strong spin-orbit coupling (SOC) has attracted much interest due to its novel physical properties. For electrons in d orbitals, the SOC becomes larger as the main quantum number increases from $3d$ to $4d$, and to $5d$. In $5d$-based compounds, SOC becomes even comparable with electron correlation. Thus, they offer an ideal field to investigate the interplay of them.

Recently, $5d^5$ systems such as Ir-based magnets have been actively studied. Examples include Sr_2IrO_4, which shows an unconventional metal-insulator transition,[1] and Na_2IrO_3, which is proximity to the Kitaev spin liquid.[2–5] In these materials, Ir^{4+} ion is located at the center of the octahedral structure, thus fivefold $5d$ orbitals are split into threefold t_{2g} orbitals and twofold e_g orbitals due to the crystalline electric field.[6] Then, in the presence of strong SOC, the t_{2g} orbitals with pseudo orbital degrees of freedom ($L_{\rm eff} = 1$) form upper $J_{\rm eff} = 1/2$ doublet and lower $J_{\rm eff} = 3/2$ quartet, and only half-filled $J_{\rm eff} = 1/2$ doublet is active for $5d^5$ systems.[5,7,8]

In contrast to $5d^5$ systems, $J_{\rm eff} = 3/2$ quartet becomes active in $5d^1$ systems. Remarkably, the exchange interactions between $J_{\rm eff} = 3/2$ states contain not only a quadratic operators in $J_{\rm eff}$, but also biquadratic and triquadratic operators, due to its fourfold degree of freedoms.[10] Indeed, these interactions induce many exotic phases such as the quadrupolar ordered phase in a double-perovskite material Ba_2NaOsO_6.[9,10]

It is even more interesting if we consider the effects of spacial inversion symmetry breaking (ISB). If the system has magnetic dipole moments, the lack of spacial inversion symmetry induces the anti-symmetric exchange interaction, i.e. the Dzyaloshinskii-Moriya (DM) interaction.[11,12] For $3d$ systems, the DM inrteraction has been evaluated precisely by first principles calculations.[13] On the other hand, for $5d^1$ systems, which have the higher-rank multipole degrees of freedom, we naturally expect that there exist the analogues of DM interactions for the higher-rank multipoles, which can lead to novel phases with chiral multipole orders.

In this letter, we study exchange interactions between multipole moments by using numerical exact diagonalization method on two-site systems with three t_{2g} orbitals for each site. We discuss the perovskite crystal with the corner-sharing and the edge-sharing configurations, shown in Figs. 1(a) and 1(b), respectively, and ISB is taken into account through the displacement of oxygen sites. We show the existence of DM interaction between the dipoles of $J_{\rm eff} = 3/2$, as well as between higher-rank multipoles that consist of products of $J_{\rm eff}$-operators. To do this, we compute the expectation values of anti-symmetric products of multipole operators as a function of the SOC.

Model and method.- We consider the two-site problem

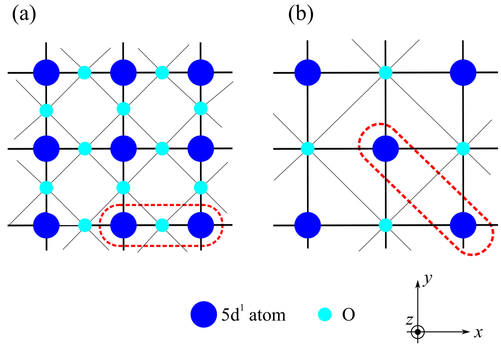

Fig. 1. (Color online) Schematic pictures of (a) corner-sharing configuration and (b) edge-sharing configuration. Blue circles denote $5d^1$ ions and light blue circles denote oxygen ions.

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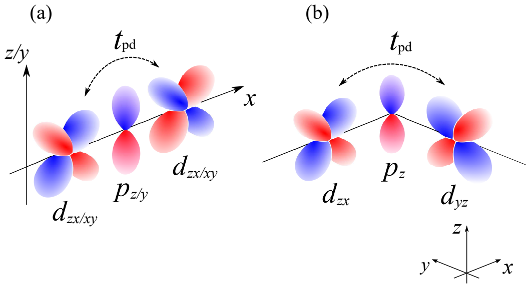

Fig. 2. (Color online) The schematic picture of transfer integral via oxygen's p orbitals in (a): corner-sharing configuration (b): edge-sharing configuration. $t_{\rm pd}$ denotes the oxygen-mediated transfer integral between d orbitals.

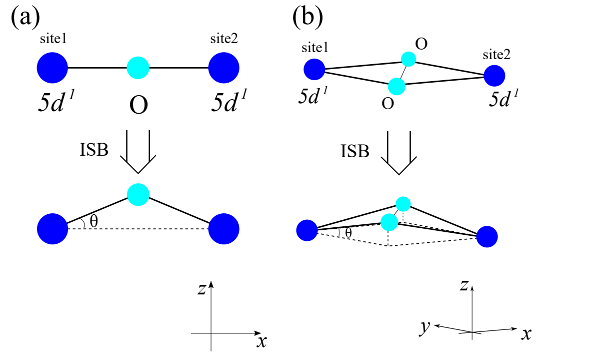

Fig. 3. (Color online) The schematic pictures of the configuration of the bond with and without the tilting for (a):corner-sharing configuration and for (b):edge-sharing configuration.

for $5d^1$ systems. The Hamiltonian is given as

$$H = H_t + H_{\rm ISB} + H_{\rm int} + H_{\rm SO}, \quad (1)$$

where H_t, $H_{\rm ISB}$, $H_{\rm int}$, $H_{\rm SO}$ represent the Hamiltonians of transfer integrals between t_{2g} orbitals for inversion-symmetric systems, transfer integrals induced by ISB, on-site Coulomb interactions, and SOC, respectively. The total electron number is set as two. As for the lattice structure, we study the perovskite crystal of the corner-sharing [Fig. 1(a)] and edge-sharing [Fig. 1(b)] configurations. The two-site systems considered here are encircled by red dotted lines in the same figures. As we will explain, the difference of lattice structure is reflected to the difference of oxygen-mediated transfer integrals in H_t.

For simplicity, we ignore the direct transfer integrals between d orbitals (t_{dd}), and consider the oxygen-mediated transfer integrals, shown in Figs. 2(a) and Figs. 2(b). As a result, H_t is given by

$$H_t^{(a)} = \sum_{\sigma=\uparrow,\downarrow} t(d^\dagger_{1,zx,\sigma}d_{2,zx,\sigma} + d^\dagger_{1,xy,\sigma}d_{2,xy,\sigma} + \text{h.c.}), \quad \text{(2-a)}$$

for a corner-sharing configuration, and

$$H_t^{(b)} = \sum_{\sigma=\uparrow,\downarrow} t(d^\dagger_{1,yz,\sigma}d_{2,zx,\sigma} + d^\dagger_{1,zx,\sigma}d_{2,yz,\sigma} + \text{h.c.}), \quad \text{(2-b)}$$

for an edge-sharing configuration. Here, $d^\dagger_{i,l,\sigma}(d_{i,l,\sigma})$ is a creation (annihilation) operator of the l-th orbital (l = 1,2, and 3 indicate yz,zx, and xy orbitals, respectively) with spin σ at the i-th site, and t is the amplitude of transfer integrals derived from the transfer integrals between d and p orbitals.

In addition to the above transfer integrals, we also consider transfer integrals, $H_{\rm ISB}$, induced by the distortion of oxygen atoms [Figs. 3(a) and 3(b)]. To be specific, we consider the situation where the oxygen between the two $5d^1$ atoms shifts slightly in the z-direction, giving rise to ISB of the system.[14–17] Then, new hopping processes appear which involve d_{xy} orbitals; they are given by

$$H_{\rm ISB}^{(a)} = \sum_{\sigma=\uparrow,\downarrow} t'(d^\dagger_{1,yz,\sigma}d_{2,xy,\sigma} - d^\dagger_{1,xy,\sigma}d_{2,yz,\sigma} + \text{h.c.}), \quad \text{(3-a)}$$

for a corner-sharing configuration, and

$$H_{\rm ISB}^{(b)} = \sum_{\sigma=\uparrow,\downarrow} t''(d^\dagger_{1,yz,\sigma}d_{2,xy,\sigma} - d^\dagger_{1,xy,\sigma}d_{2,yz,\sigma} - d^\dagger_{1,zx,\sigma}d_{2,xy,\sigma} + d^\dagger_{1,xy,\sigma}d_{2,zx,\sigma} + \text{h.c.}). \quad \text{(3-b)}$$

for an edge-sharing configuration. Microscopic derication of t' and t'' can be straightforwardly carried out by using the Slater-Koster formalism.[16,18]

The rest two terms, $H_{\rm int}$ and $H_{\rm SO}$, are given by

$$\begin{aligned} H_{\rm int} =& U_d \sum_{i=1,2}\sum_{l} n_{i,l,\uparrow}n_{i,l,\downarrow} \\ &+ \frac{U'_d - J_d}{2}\sum_{\substack{i=1,2\\ \sigma}}\sum_{\substack{l,m\\(l\neq m)}} n_{i,l,\sigma}n_{i,m,\sigma} \\ &+ \frac{U'_d}{2}\sum_{\substack{i=1,2\\ \sigma\neq\sigma'}}\sum_{\substack{l,m\\(l\neq m)}} n_{i,l,\sigma}n_{i,m,\sigma'} \\ &- \frac{J_d}{2}\sum_{i=1,2}\sum_{\substack{l,m\\(l\neq m)}} (d^\dagger_{i,m,\uparrow}d_{i,m,\downarrow}d^\dagger_{i,l,\downarrow}d_{i,l,\uparrow} \\ &+ d^\dagger_{i,m,\uparrow}d^\dagger_{i,m,\downarrow}d_{i,l,\uparrow}d_{i,l,\downarrow} + \text{h.c.}), \end{aligned} \quad (4)$$

and

$$H_{\rm SO} = \frac{\mathrm{i}\zeta}{2}\sum_{i=1,2}\sum_{\substack{lmn\\ \sigma,\sigma'}} \epsilon_{lmn} d^\dagger_{i,l,\sigma}d_{i,m,\sigma'}\sigma^n_{\sigma\sigma'}, \quad (5)$$

where $n_{i,l,\sigma}$ is number operator defined as $n_{i,l,\sigma} = d^\dagger_{i,l,\sigma}d_{i,l,\sigma}$, ϵ_{lmn} is the Levi-Civita symbol, σ^n is the n componet of the Pauli matrices, and U_d, U'_d, J_d, and ζ are the intra- and inter- Coulomb interactions, Hund's coupling, and the magnitude of SOC, respectively. Due to the cubic symmetry, U_d, U'_d and J_d satisfy $U_d - U'_d = 2J_d$.

We diagonalize the Hamiltonian in Eq. (1) numerically. Then, we pick up the ground state(s), and discuss the existence of anti-symmetric multipole-multipole interactions by directly calculating the expectation values of the anti-symmetric products of multipole operators. Namely, we assume that if those expectation val-

Table I. Multipole moments in $J_{\rm eff} = 3/2$ state. Bracket $[\cdots]$ denotes the symmetrized product of operators in the bracket, e.g. $[J_xJ_yJ_y] = J_xJ_y^2 + J_yJ_xJ_y + J_y^2J_x$.

Multipole	Symmetry	Operator
Dipole	T_{1u}	$J_x,\ J_y,\ J_z$
Quadrupole	T_{2g}	$Q_x=[J_yJ_z]/2$
		$Q_y=[J_zJ_x]/2$
		$Q_z=[J_xJ_y]/2$
	E_g	$Q_\alpha=J_x^2-J_y^2$
		$Q_\beta=(2J_z^2-J_x^2-J_y^2)/\sqrt{3}$
Octupole	A_{2u}	$T_{xyz}=\sqrt{15}/6\ [J_xJ_yJ_z]$
	T_{1u}	$O_x=J_x^3-1/2([J_xJ_yJ_y]+[J_xJ_zJ_z])$
		$O_y=J_y^3-1/2([J_yJ_zJ_z]+[J_yJ_xJ_x])$
		$O_z=J_z^3-1/2([J_zJ_xJ_x]+[J_zJ_yJ_y])$
	T_{2u}	$O'_x=\sqrt{15}/6([J_xJ_yJ_y]-[J_xJ_zJ_z])$
		$O'_y=\sqrt{15}/6([J_yJ_zJ_z]-[J_yJ_xJ_x])$
		$O'_z=\sqrt{15}/6([J_zJ_xJ_x]-[J_zJ_yJ_y])$

ues are finite, there exist corresponding interactions in the effective Hamiltonian that makes those expectation values finite. Possible single-site multipole operators for $J_{\rm eff} = 3/2$ states are summarized in Table I.[10] When the ground state is degenerate, we take the average over all the degenerated states. In what follows, we focus on ζ dependence of the coupling constants, and set other parameters as $U_d/t = 5.0$, $U'_d/t = 3.0$, $J_d/t = 1.0$, and $t'/t = t''/t = 0.0, 0.01, 0.05$, and 0.1, where t is the unit of parameters.

Results.- First, to see the crossover from L-S coupling regime to j-j copuling regime, we show in Fig. 4 ζ dependence of occupation number in $J_{\rm eff} = 3/2$ state and $J_{\rm eff} = 1/2$ state at $t'/t = 0.0$ for both configurations. We find that the occupation number of $J_{\rm eff} = 1/2$ state becomes almost zero for $\zeta/t \simeq 2$. This indicates that, for $\zeta/t \gtrsim 2$, j-j picture is better than L-S picture, and that our results for multipole interactions with respect to $J_{\rm eff}$ are valid in this regime. It should be noted that the occupation number is hardly dependent on t'.

Next, before discussing the DM interactions between multipoles, let us see the DM interaction for dipoles. We show in Fig. 5(a) ζ dependence of the expectation value $\langle \boldsymbol{J}_{1,\frac{3}{2}} \times \boldsymbol{J}_{2,\frac{3}{2}}\rangle_y$ for $t'/t = 0.01$, 0.05 and 0.1, where $\boldsymbol{J}_{i,\frac{3}{2}}$ $(i = 1, 2)$ indicates the $J_{\rm eff} = 3/2$ state at i-th site. Note that components other than y is 0 due to the symmetry requirement. In other words, the direction of $\boldsymbol{D}$ vector is determined by setting a lattice structure and a bond direction. Indeed, the expectation value $\langle \boldsymbol{J}_{1,\frac{3}{2}} \times \boldsymbol{J}_{2,\frac{3}{2}}\rangle_y$ is finite for all values of ζ, indicating that the DM interaction between $\boldsymbol{J}$ is induced by $t_{\rm ISB}$. Such a DM interaction of $\boldsymbol{J}$ also emerges in $5d^5$ systems with broken inversion symmetry.[17,19–21] We also see that the DM interaction for edge-sharing configuration becomes almost constant after the discontinuity around $\zeta/t \sim 3.5$. This result will be discussed later together with quadrupolar and octupolar DM interactions.

Interestingly, $\langle \boldsymbol{J}_{1,\frac{3}{2}} \times \boldsymbol{J}_{2,\frac{3}{2}}\rangle_y$ is nonzero even at $\zeta/t = 0$. This is because the orbital part, $\langle \boldsymbol{L}_{1,\rm eff} \times \boldsymbol{L}_{2,\rm eff}\rangle_y$, is finite due to the lattice distortion. To see this, we employ a perturbation theory with respect to $H_t + H_{\rm ISB}$ at $\zeta = 0$. For simplicity, we use $H_{\rm int} = U \sum_{i=1,2} \sum_{l,m(l\neq m)} n_{i,l}n_{i,m}$ as interaction term. Assuming that $U \gg t, t'$, we perform a second-order perturbation to obtain effective multipole-multipole interactions. As a result, we obtain

$$\mathcal{H} \sim \frac{t't}{U}(\boldsymbol{L}_1\times\boldsymbol{L}_2)_y - \frac{4t't}{U}(\boldsymbol{Q}_1\times\boldsymbol{Q}_2)_y + (\text{other interactions}). \tag{6}$$

This Hamiltonian is the origin of the finite expectation value of $\langle \boldsymbol{L}_1 \times \boldsymbol{L}_2\rangle_y$ and $\langle \boldsymbol{Q}_1 \times \boldsymbol{Q}_2\rangle_y$. The results in Fig. 5(a) indicates that the SOC enhances the DM interactions of orbital part, $\boldsymbol{L}_1 \times \boldsymbol{L}_2$, for small SOC regime.

To compare the contributions from spin and orbital parts, we plot the spin part of the DM interaction, $\langle \boldsymbol{S}_1 \times \boldsymbol{S}_2\rangle_y$, together with the total one in Fig. 5(b). Here we set $t'/t = 0.1$. For small ζ, although $\langle \boldsymbol{S}_1 \times \boldsymbol{S}_2\rangle_y$ increases as the SOC increases, its value is much smaller than that of $\boldsymbol{J}_{\rm eff} = 3/2$ for $\zeta/t \gtrsim 2.0$. This indicates that the orbital components mainly contribute to the DM interaction between $\boldsymbol{J}_{\rm eff} = 3/2$ states in this regime, as discussed in the above. For large ζ, in contrast, the spin part is almost same as the total one, meaning that the orbital part is almost vanishing in this regime.

Now, let us move on to the DM interactions for higher-rank multipoles. Figure 5(c) shows ζ dependence of the anti-symmetric product of quadrupoles, $\langle \boldsymbol{Q}_1 \times \boldsymbol{Q}_2\rangle_y$, for $t'/t = 0.01$, 0.05 and 0.1. ($\boldsymbol{Q}_1$ indicates the quadrupole moment with T_{2g} symmetry at i-th site; see Table I.) It is found that $\langle \boldsymbol{Q}_1 \times \boldsymbol{Q}_2\rangle_y$ is finite for both of two configurations (except for $\zeta/t > 3.5, t'' = 0.05, 0.1$ for an edge-sharing configuration). This indicates that the there exist quadrupole DM interactions, which are novel DM interactions among $5d$ systems.

We remark that the quadrupolar DM interaction is generally expected to lead to the lattice distortion beyond the mere displacement of oxygens, through the

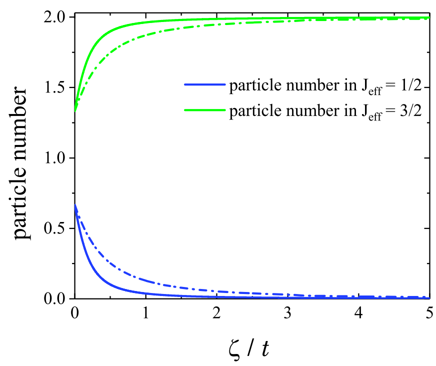

Fig. 4. (Color online) SOC dependence of occupation number in $J_{\rm eff} = 3/2$ and $J_{\rm eff} = 1/2$ states. The solid line shows that of corner-sharing configuration and the dotted line shows that of edge-sharing one.

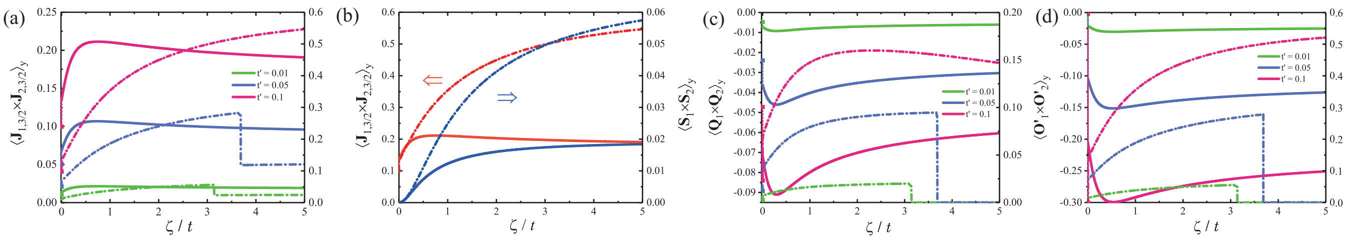

Fig. 5. (Color online) (a): The SOC dependence of the expectation value of y component of the DM interaction, $\langle \boldsymbol{J}_{1,\frac{3}{2}} \times \boldsymbol{J}_{2,\frac{3}{2}} \rangle_y$ for $t'/t = 0.01$, 0.05, and 0.1. The solid line corresponds to the corner-sharing configuration (left axis) and the dash-dotted line corresponds to the edge-sharing configuration (right axis). It is noted that we use this correspondence in the following figures. (b): The DM interaction between spins (blue) and that between $\boldsymbol{J}_{\rm eff} = 3/2$ states (red) at $t'/t = 0.1$. Each arrow shows the corresponding axises. (c): The SOC dependence of the y component of the interaction $\boldsymbol{Q}_1 \times \boldsymbol{Q}_2$. (d): The SOC dependence of the y component of the interaction $\boldsymbol{O'}_1 \times \boldsymbol{O'}_2$.

change of the charge distribution. In this letter, we discuss only the electronic state under fixed lattice structure, and lattice distortion induced by quadrupole DM interaction is the future problem.

The octupolar terms, $\langle \boldsymbol{O'}_1 \times \boldsymbol{O'}_2 \rangle_y$, is found to be finite and have similar ζ dependence to that for the qudrupole. ($\boldsymbol{O'}_1$ indicates the octupole moment with T_{2u} symmetry at i-th site; see Table I.) The only sharp difference is that octupolar DM interaction becomes exactly zero at $\zeta/t = 0$. This is because the highest rank of multipole for $\boldsymbol{L}_{\rm eff}$ is quadrupole, thus an octupole does not emerge at $\zeta/t = 0$.

Before closing this section, we discuss the reason why $\langle \boldsymbol{Q}_1 \times \boldsymbol{Q}_2 \rangle_y$ and $\langle \boldsymbol{O'}_1 \times \boldsymbol{O'}_2 \rangle_y$ vanish in the large SOC region in the edge sharing system with small distortion. In this region, we can calculate the wave function of the ground state. It is denoted as

$$
\begin{aligned}
|\mathrm{GS}\rangle = a e^{i\frac{\pi}{4}} \left(\left|\frac{3}{2}, \frac{1}{2}\right\rangle + \left|\frac{1}{2}, \frac{3}{2}\right\rangle - \left|-\frac{1}{2}, -\frac{3}{2}\right\rangle - \left|-\frac{3}{2}, -\frac{1}{2}\right\rangle \right) \\
- b \left(\left|\frac{3}{2}, -\frac{1}{2}\right\rangle + \left|-\frac{1}{2}, \frac{3}{2}\right\rangle \right) \\
- bi \left(\left|\frac{1}{2}, -\frac{3}{2}\right\rangle - \left|-\frac{3}{2}, \frac{1}{2}\right\rangle \right). \qquad (7)
\end{aligned}
$$

Here, we use the basis $|J_{1z}, J_{2z}\rangle$.The parameters a and b are independent of SOC, and b increases with lattice distortion. By using this state, it is found that $\langle \boldsymbol{J}_1 \times \boldsymbol{J}_2 \rangle_y = 48\sqrt{2}ab/25$, and $\langle \boldsymbol{Q}_1 \times \boldsymbol{Q}_2 \rangle_y = \langle \boldsymbol{O'}_1 \times \boldsymbol{O'}_2 \rangle_y = 0$. For example, in the $t'/t = 0.01$ case, we found $a \simeq 0.46, b \simeq 0.02$. Thus, we can estimate $\langle \boldsymbol{J}_1 \times \boldsymbol{J}_2 \rangle_y \simeq 0.025$ and this is consistent with the result of numerical calculation. From this calculation, it is found that if the wave function has symmetric form such as Eq. (7), multipolar DM interactions can be exactly zero even though the lattice is distorted.

Concluding remarks.- In conclusion, we have introduced the new type of DM interactions, namely the qudrupolar and octupolar DM interactions, on $5d^1$ systems with the structures of edge-sharing octahedra and corner-sharing octahedra.

These novel DM interactions may serve as a source of chiral multipolar orders, which have not yet been observed experimentally. Therefore, search for candidate materials for that will be an intriguing future problem. For instance, $KTaO_3$ with vacancy of oxygens has an inversion symmetry broken perovskite configuration,[22] and thus will be a good candidate. Another possibility is to make a surface/interface of $5d^1$ perovskite material,[16,17] on which ISB is artificially introduced.

Finally, we focus on the Mott insulating phase in this work, and the comparison with itinerant systems[23–25] will be an interesting perspective.

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