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# Topological Edge Conduction Induced by Strong Anisotropic Exchange Interactions

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We predict that an interplay between isotropic and anisotropic exchange interactions in a honeycomb lattice structure can lead to topological edge conduction when the anisotropic interaction is at least twice the strength of the isotropic interaction. For materials like  $\text{Na}_2\text{IrO}_3$ , such a strong anisotropic exchange interaction simultaneously induces a zigzag type of antiferromagnetic order that breaks the time-reversal symmetry of the topological edge conductor. We show that the electronic transport in such topological conductors will exhibit a quantized Hall conductance without any external magnetic field when the Fermi energy lies within a particular energy range.

Recently, there is a growing interest in transition metal-based oxides and halides with honeycomb lattice structure [1–3] (see Fig. 1(a)) for exhibiting both isotropic and bond-dependent anisotropic exchange interactions [4]. An interplay between these exchange interactions can lead to quantum magnetism [5–11] and a spin liquid state [7, 12–14], which are modeled using the Kitaev-Heisenberg (KH) model as given by

$$\mathcal{H} = \sum K^\gamma S_i^\gamma S_j^\gamma + \sum J \vec{S}_i \cdot \vec{S}_j, \quad (1)$$

where  $\gamma \equiv \{x, y, z\}$ ,  $K^\gamma$  is the anisotropic exchange interaction along  $\gamma$  bond,  $J$  is the isotropic exchange interaction, and  $\vec{S}_i = \sum_{\gamma \equiv \{x, y, z\}} \hat{\gamma} S_i^\gamma$  is the spin- $\frac{1}{2}$  operator on the  $i^{\text{th}}$  lattice point.

In this letter, we predict that an interplay between the isotropic and anisotropic exchange interactions can form topological edge states when the anisotropic exchange interaction is at least twice the strength of the isotropic exchange interaction. Such an interplay will simultaneously induce an intrinsic magnetic order, specifically a zigzag antiferromagnetic (AFM) order, that breaks the time-reversal symmetry (TRS) of the edge conductor. We use a tight-binding model for such materials [15–17], the KH model, and a non-equilibrium Green's function (NEGF)-based quantum-transport model [18] to show that the exchange interaction induced topological edge conduction will exhibit a Hall conductance quantized to  $q^2/h$  (where  $q$  is the electron charge and  $h$  is the Planck's constant) when the current is running along the zigzag direction and the voltage is measured along the arm-chair direction. We further calculate the band structures and Hall conductances of  $\text{Na}_2\text{IrO}_3$  and  $\alpha\text{-RuCl}_3$  and show that  $\text{Na}_2\text{IrO}_3$  could be a model material to observe the phenomena predicted in this letter. Finally, using one-dimensional analytical arguments, we show that the topological edge state formation for high anisotropic exchange interaction is a property of Eq. (1).

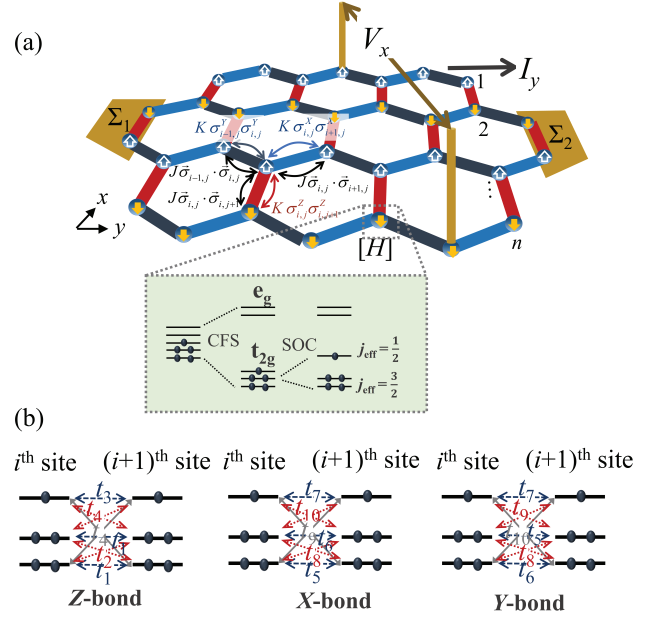


FIG. 1. (a) A honeycomb lattice with isotropic ( $J$ ) and bond-dependent anisotropic ( $K$ ) exchange interactions. Local  $d$ -orbital states on each lattice point in the presence of Coulomb interaction ( $U$ ), crystal field splitting (CFS), and spin-orbit coupling (SOC). (b) General nearest neighbor hopping scenario along different bonds.

Transition-metal-based oxides and halides with honeycomb lattice structures have a half-filled  $d^5$  ion (e.g.,  $\text{Ir}^{4+}$  or  $\text{Ru}^{3+}$ ) in each of the lattice points in an octahedral environment. The crystal field (CF) splits the  $d$ -orbital into a  $e_g$  (equally degenerate) pair and  $t_{2g}$  (triply degenerate) states, see Fig. 1(a), and all five electrons occupy the  $t_{2g}$  states. The presence of spin-orbit coupling (SOC) further splits the  $t_{2g}$  states into  $j_{\text{eff}} = \frac{1}{2}$  and  $\frac{3}{2}$ , states (see Fig. 1(a)), where the  $j_{\text{eff}} = \frac{3}{2}$  states are filled and the  $j_{\text{eff}} = \frac{1}{2}$  state is half-filled. Thus we have one hole per site. We describe the hole-mediated transport in such materials using a tight-binding Hamiltonian, given by

$$\mathcal{H} = H_U + H_{\text{CF}} + H_{\text{SOC}} + H_{\text{hop}}, \quad (2)$$

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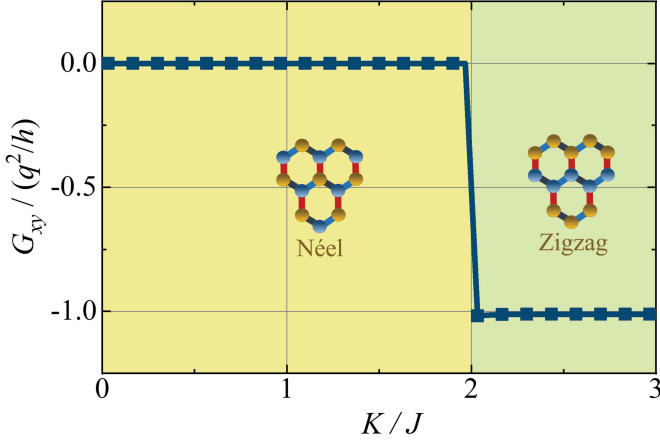


FIG. 2. The Hall conductance ( $G_{xy}$ ) and corresponding magnetic order as a function of  $K/J$ .

which is in the basis of the  $d_{xy}$ ,  $d_{yz}$ , and  $d_{zx}$  orbitals with each orbitals having two spin states, i.e.,  $\Psi \equiv \{\psi_{xy}^\uparrow, \psi_{xy}^\downarrow, \psi_{yz}^\uparrow, \psi_{yz}^\downarrow, \psi_{zx}^\uparrow, \psi_{zx}^\downarrow\}$ . Eq. (2) takes into account the static inter and intra-orbital Coulomb repulsion ( $H_U$ ), crystal field ( $H_{CF}$ ), spin-orbit coupling ( $H_{SOC}$ ), and hole-based hopping ( $H_{hop.}$ ) with bond-dependent hopping integrals ( $t_1$  to  $t_{10}$ ) shown in Fig. 1(b) [19]. The effective values of the hopping integrals are adopted from Ref. [15], which were obtained by fitting detailed DFT calculations considering electron-electron interactions.

The isotropic ( $J$ ) and anisotropic ( $K^z = K^x = K^y = K$ ) exchange interaction strengths in Eq. (1) are related to these hopping integrals as [15–17]

$$J = \delta (2t_1 + t_3)^2 - \xi \left\{ 9t_4^2 + 2(t_1 - t_3)^2 \right\}, \quad (3a)$$

$$K = \xi \left\{ 3t_4^2 + (t_1 - t_3)^2 - 3t_2^2 \right\}. \quad (3b)$$

where the coefficients  $\delta$  and  $\xi$  are determined by the Coulomb repulsion, Hund's coupling, and SOC strengths [15–17]. We have solved Eq. (1) in Fock space to find the ground energy state and corresponding intrinsic magnetic order for a particular combination of  $J$  and  $K$  calculated using the tight-binding parameters for  $\text{Na}_2\text{IrO}_3$  [15].

We use the tight-binding model in Eq. (2) to calculate the Green's function  $\mathcal{G} = [E\mathcal{I} - \mathcal{H} - \Sigma_0 - \Sigma_1 - \Sigma_2]^{-1}$  for the structure in Fig. 1(a), where  $E$  is the energy,  $\mathcal{I}$  is the identity matrix,  $\Sigma_{1,2}$  are the self-energy functions of the left and right contacts, respectively,  $\Sigma_0 = \mathcal{W}\mathcal{G}$  is the self-energy that takes into account the dephasing in the channel due to electron-electron interactions in a self-consistent manner. Here  $\mathcal{W}_{m,n} = \langle U_m U_n^* \rangle$  is calculated from the random potential at  $m^{\text{th}}$  and  $n^{\text{th}}$  lattices. We use Green's function [18, 19] to calculate the potential distribution on the  $xy$ -plane as

$$V(x, y) = V_0 \text{Re} \left\{ \frac{\mathcal{G}(\Gamma_1 f_1 + \Gamma_2 f_2) \mathcal{G}^\dagger}{\mathcal{G}(\Gamma_1 + \Gamma_2) \mathcal{G}^\dagger} \right\}, \quad (4)$$

where  $\Gamma_{1,2} = j(\Sigma_{1,2} - \Sigma_{1,2}^\dagger)$  are the broadening functions and represent the anti-Hermitian parts of the self-energy functions,  $f_{1,2}$  are the Fermi occupation factors of the left and right contacts respectively, and  $V_0$  is the applied potential. The Hall resistance is given by

$$R_{xy} = \frac{\Delta V_x}{I_y} = \frac{V(x=0, y) - V(x=w, y)}{\frac{q}{h} \int dE \text{Trace}[\text{Re}\{\Gamma_1 \mathcal{G} \Gamma_2 \mathcal{G}^\dagger\}](f_1 - f_2)}, \quad (5)$$

where the numerator represents the voltage difference between the two edges along  $x$ -direction and the denominator represents the current  $I_y$  flowing along the  $y$ -direction. Here,  $w$  is the channel width. The Hall conductance  $G_{xy}$  is calculated using  $R_{xy}$  and longitudinal resistance  $R_{xx}$  as  $G_{xy} = R_{xy}/(R_{xy}^2 + R_{xx}^2)$ .

In order to understand the effect of the intrinsic exchange interactions in the transport properties, we calculate  $G_{xy}$  and the magnetic order of the honeycomb lattice as a function of the relative strength between the anisotropic and isotropic exchange interactions (i.e.,  $|K/J|$ ), as shown in Fig. 2. We apply a current  $I_y$  along the zigzag chains ( $y$ -direction) and calculate the transverse voltage  $V_x$  along the armchair direction ( $x$ -direction), see Fig. 1(a). We change the  $|K|/|J|$  ratio by changing the hopping integral  $t_4$  and keep other parameters equivalent to the parameter values for  $\text{Na}_2\text{IrO}_3$ . The NEGF calculations show that  $|G_{xy}|$  is 0 when  $K < 2J$ ; however, becomes exactly  $q^2/h$  when the  $K \geq 2J$ , see Fig. 2. This phenomenon induced by a strong anisotropic exchange interaction in a two-dimensional (2D) channel is very similar to the popular signature of a quantum anomalous Hall (QAH) state [20–23] observed in band-inverted three-dimensional magnetic topological insulators with broken TRS.

The quantized Hall conductance in Fig. 2 is a combination of two effects: topological edge state formation when  $K \geq 2J$  and intrinsic magnetic ordering induced by the interplay between  $J$  and  $K$  that simultaneously breaks the TRS. In order to understand the edge state formation, we calculate the local density of states as

$$\mathcal{D} = \frac{1}{2\pi} \text{Re}(\mathcal{G} \Gamma \mathcal{G}^\dagger), \quad (6)$$

where  $\Gamma = j\{\Sigma_1 + \Sigma_2 - (\Sigma_1 + \Sigma_2)^\dagger\}$  is the broadening function. The spatial distribution of the local density of states is shown in Fig. 4(a) and (b) for tight-binding parameters that correspond to  $K < 2J$  and  $K > 2J$ , respectively. The density of states is non-zero everywhere throughout the 2D channel when  $K < 2J$  and there are no distinct edge states, as shown in Fig. 4(a) for the case  $|K|/|J| \approx 0.1$ . For  $K > 2J$ , the density of states in the middle of the 2D channel becomes zero, i.e., the middle of the 2D channel becomes insulating. However, the case of  $K > 2J$  exhibits edge states as shown in Fig. 4(b) for  $|K|/|J| \approx 2.5$ .

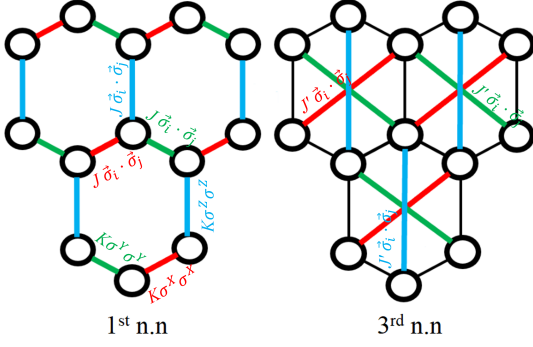


FIG. 3. Visual representation of all first and third nearest-neighbor (n.n) interactions.

To analyze the magnetic order in the honeycomb lattice considered here, we reduce Eq. (1) to a minimal model [15] as given by

$$H = \sum_{1\text{st nn}} \left( J \vec{S}_i \cdot \vec{S}_j + K S_i^x S_j^x \right) + \sum_{3\text{rd nn}} J' \vec{S}_i \cdot \vec{S}_j, \quad (7)$$

where  $J$  and  $K$  are the first nearest neighbor Heisenberg and Kitaev interaction coefficients, respectively, and  $J'$  is the third nearest neighbor Heisenberg interaction coefficient (see Fig. 3). We solve a 13-spin lattice system in a honeycomb structure containing 3 hexagons, as shown in Fig. 3. The ground state of the spin-lattice is obtained by sweeping the Hamiltonian parameter  $K/J$  from 0 to 4 and exactly diagonalizing. We use the nominal values  $(J', K) \sim (0.4, -1)$  meV typically used for  $\text{Na}_2\text{IrO}_3$  [15] and tune the  $J$  parameter for the  $K/J$  sweep. The ground-state solution is reasonably robust for the system size under consideration and in agreement with the previously reported results for  $\text{Na}_2\text{IrO}_3$  [15].

The honeycomb lattice considered here has a Néel type AFM order for  $K < 2J$ . Thus, the two-dimensional channel in the honeycomb lattice structure does not have an effective field that can produce an anomalous Hall effect and does not contribute to  $G_{xy}$ . Thus, we observe  $G_{xy} = 0$ . However, there is a sharp transition from Néel type AFM order to a zigzag type AFM order for  $K > 2J$ , see Fig. 2. A zigzag AFM order refers to the case where each of the zigzag atomic chains is a one-dimensional (1D) ferromagnetic chain; however, the ferromagnetic order alternates along the armchair direction (see Fig. 1(a)), giving rise to an overall AFM order. Thus, the edge atomic chains have a net magnetic order that breaks the TRS of the edge conductor. Note that the magnetic order for the case  $K = 2J$  is a superposition of a Néel and a zigzag AFM states.

Such systems may exhibit mixed-spin interaction terms arising from a pseudo-dipolar or Dzyaloshinskii-Moriya interaction [15, 20, 24]. However, magnetic phases in  $\text{Na}_2\text{IrO}_3$  and  $\alpha\text{-RuCl}_3$  can be described by a minimal model [15] consisting only of isotropic Heisenberg and

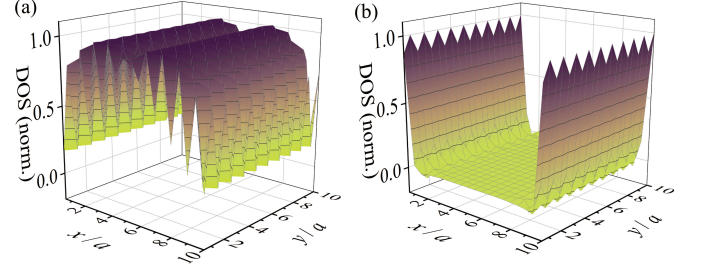


FIG. 4. Local density of states on the two-dimensional honeycomb lattice structure in Fig. 1(a) for (a)  $K = 0.1J$  and (b)  $K = 2.5J$ .

anisotropic Kitaev terms up to the 3<sup>rd</sup> nearest neighbor. Although, the magnetic order was calculated using a minimal model in Eq. (7), the transport calculations considered a general hopping among the  $t_{2g}$  states. We leave the study of such mixed-spin-interaction-induced magnetic order on the topological states for the future.

The zigzag AFM order has been observed in the transition metal oxides and halides, e.g.,  $\text{Na}_2\text{IrO}_3$  and  $\alpha\text{-RuCl}_3$ , at low temperatures [5–10]. We calculate the band diagram of  $\text{Na}_2\text{IrO}_3$  and  $\alpha\text{-RuCl}_3$  using Eq. (2), see Fig. 5(a)-(b), where the tight-binding parameters correspond to a zigzag AFM order. We observe the spin bands for the  $j_{\text{eff}} = \frac{1}{2}$  energy states show a small gap of  $\sim 26$  meV near the  $M$  symmetry point for both materials. We have calculated  $R_{xy}$  using Eq. (5) as a function of energy within the energy gap and found it to be quantized to  $h/q^2$  for  $\text{Na}_2\text{IrO}_3$ , as shown in Fig. 5(c). This indicates that the energy gap hosts non-trivial topological edge states. Interestingly, the calculated  $J \approx 3.4$  meV and  $K \approx -22.3$  meV, thus yields  $|K|/|J| \approx 6.6$  and satisfies the condition in Fig. 2. This phenomenon will be observed in Hall measurements on  $\text{Na}_2\text{IrO}_3$  at low temperatures where zigzag AFM forms and as long as the Fermi energy lies within the topological energy gap.

For  $\alpha\text{-RuCl}_3$ , we do not observe a quantized  $R_{xy}$  in the transport calculation within the energy gap, see Fig. 5(d). This is consistent with the condition in Fig. 2, as  $J$  and  $K$  are  $-2.02$  meV and  $-3.4$  meV based on the tight-binding parameters, respectively, which gives  $|K|/|J| \sim 1.68$ . A non-zero  $R_{xy}$  for a small energy range within the upper band is observed which corresponds to the anomalous Hall effect due to an uncompensated net magnetization in the lattice with a zigzag AFM order. Note that a half-integer quantized Hall effect has been observed for thermal transport [25, 26] in  $\alpha\text{-RuCl}_3$ , which is out of the scope of this letter. In this letter, we predict an anisotropic exchange interaction induced quantized Hall conductance due to charge transport in the topological edge state and we do not expect any topological conduction in  $\alpha\text{-RuCl}_3$ .

$\text{Na}_2\text{IrO}_3$  has been predicted to exhibit a quantum spin

Hall (QSH) state at the  $M$  symmetry point [27], which is equivalent to a 2D topological insulator with TRS [28] that exhibits a spin-momentum locked linear dispersion. Such a QSH state has not been observed yet [29, 30]; however, it has been pointed out that  $\text{Na}_2\text{IrO}_3$  exhibits a persistent energy gap [30]. Here, we point out that the energy band in Fig. 5(a) exhibits a small gap at the  $M$  symmetry point and an intuitive explanation is that the TRS protected linear dispersion predicted in Ref. [27] should exhibit a gap induced by TRS breaking with a net intrinsic magnetic order in the material. Note that this gap is similar to that observed in magnetic topological insulator [20–23, 31]; however, such a gap in  $\text{Na}_2\text{IrO}_3$  will be induced by the interplay between the isotropic and anisotropic exchange interactions.

Topological phases and QAH state have been theoretically discussed in various ferromagnetic oxides [32–34], and halides [35, 36] due to strong SOC. In this letter, we identify a new mechanism for topological edge conduction, which can be observed in specific oxides and halides known for exhibiting strong anisotropic exchange interactions [1, 3, 15]. We specifically discuss the Hall effect in the 2D channels with zigzag AFM order that will exhibit signatures similar to QAH.

We now show that the topological edge state formation for  $K \geq 2J$  is a property of the KH model in Eq. (1). For analytical simplicity, we start with a single atomic chain with  $N$  lattice points by retaining the zigzag nature of the anisotropic interaction [37, 38], as

$$\mathcal{H} = \sum_m \left( J \vec{S}_{m+1} \cdot \vec{S}_m + K^x S_{2m}^x S_{2m-1}^x + K^y S_{2m+1}^y S_{2m}^y \right). \quad (8)$$

We represent the  $S = \frac{1}{2}$  spin chains in Eq. (8) using fermionic operators,  $|\uparrow\rangle \equiv f^\dagger |\downarrow\rangle$  and  $|\downarrow\rangle \equiv f |\uparrow\rangle$  using the Jordan-Wigner transformation [39, 40], to get

$$\begin{aligned} \mathcal{H} = & \frac{1}{2} \left( J + \frac{K}{2} \right) \sum_m \left( f_{m+1}^\dagger f_m + f_m^\dagger f_{m+1} \right) - 2J \sum_m n_m \\ & - \frac{K}{4} \sum_m (-1)^m \left( f_{m+1}^\dagger f_m^\dagger + f_m f_{m+1} \right) + J \sum_m n_{m+1} n_m, \end{aligned} \quad (9)$$

where a constant term  $N/4$  is ignored. Here,  $n_m = f_m^\dagger f_m$  and we assume  $K^x = K^y = K$ .

We use Fourier transformation around the band minimum,  $f_m = \frac{1}{\sqrt{N}} \sum_{k'} s_{k'} e^{ik'm}$  to convert Eq. (9) from the real-space to the momentum space, as given by

$$\begin{aligned} \mathcal{H} = & \sum_{k'} \left\{ 2J - \frac{2J+K}{2} \cos k' \right\} s_{k'}^\dagger s_{k'} \\ & + \sum_{k'} \frac{K}{4} \sin k' \left( s_{k'} s_{-k'} - s_{-k'}^\dagger s_{k'}^\dagger \right) \\ & + \frac{1}{N} \sum_{k', q} J e^{-iqa} s_{k'-q}^\dagger s_{k'}^\dagger s_{k'-q} s_{k'}, \end{aligned} \quad (10)$$

where  $k' = k - k_0$ . Here,  $k, q$  are the wavevector,  $k_0$  is the wavevector at the band minimum, and  $s_{k'}^\dagger$  is the creation

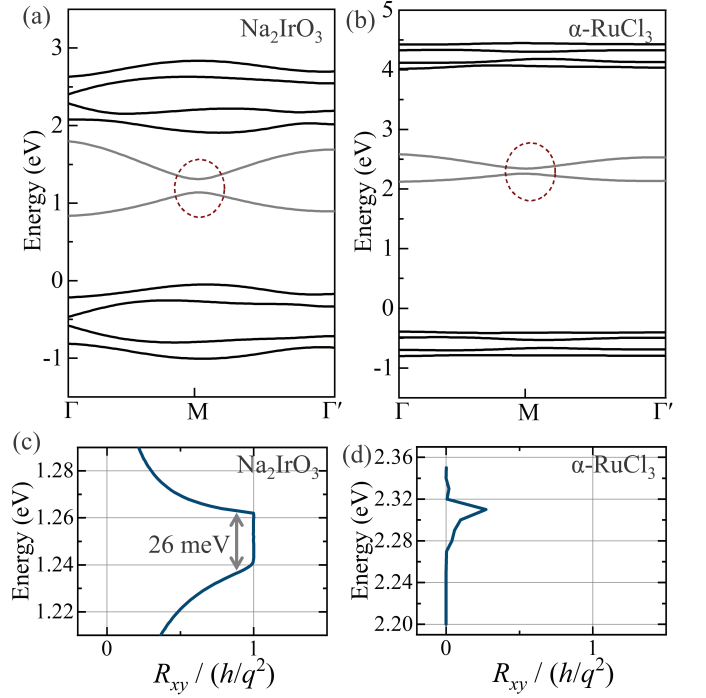


FIG. 5. Band diagram for (a)  $\text{Na}_2\text{IrO}_3$  and (b)  $\alpha\text{-RuCl}_3$ . Hall resistance is (c) quantized to  $h/q^2$  for  $\text{Na}_2\text{IrO}_3$  within the gap at  $M$  symmetry point. (d) No quantized Hall effect is observed for  $\alpha\text{-RuCl}_3$ .

operator in momentum-space. The third term in Eq. (10) represent the interaction term. Here, we consider a case where the atomic chain is a one-dimensional ferromagnet, corresponding to the case for the edge atomic chain for a zigzag AFM order. Under such approximation, the interaction term can be ignored for mathematical simplicity (see, e.g., Ref. [41]) to analyze a first-order dispersion relation.

We transform Eq. (10) into a  $2 \times 2$  matrix in the particle-hole basis using  $\mathcal{H} = \sum_k \Psi^\dagger \mathbf{H} \Psi$  with  $\Psi^\dagger \equiv \{s_{k'}^\dagger, s_{-k'}\}$ , which yields

$$\mathbf{H} = -J\sigma_z + \frac{2J+K}{4}\sigma_z \cos k' + \frac{K}{4}\sigma_x \sin k'. \quad (11)$$

Eq. (11) is in the basis of particle-hole; however, here particle represents an up spin, and the hole represents a down spin. Thus, Eq. (11) has the basis of up and down spins. The energy gap near the band minimum (i.e.,  $k \rightarrow k_0$ ) is given by  $|K - 2J|/2$  [19]. The energy gap near the  $M$  symmetry point in Fig. 5(a) for the  $\text{Na}_2\text{IrO}_3$  case is  $\sim 26$  meV, which is very close to the analytical estimation  $|K - 2J|/2 \approx 29$  meV. Note that the  $q^2/h$  plateau is observed within this energy gap (see Fig. 5(c)) since  $K$  and  $J$  satisfies the condition  $K \geq 2J$ .

We calculate the topological winding number [42, 43]

by obtaining the eigenfunction,  $\psi(k)$  of Eq. (11), as

$$W_Z = \frac{1}{j\pi} \int_0^{2\pi} dk \psi(k)^\dagger \partial_k \psi(k) = \begin{cases} 1; & \text{when } K \geq 2J, \\ 0; & \text{when } K < 2J, \end{cases} \quad (12)$$

Here,  $W_Z = 0$  for  $K < 2J$ , indicating a trivial state, while  $W_Z = 1$  for  $K \geq 2J$ , indicating topological edge states occurring for a strong anisotropic exchange interaction. Similar one-dimensional arguments for surface state formation in two and three-dimensional topological insulators have been discussed in the past [42]. The analytical conditions obtained from one-dimensional arguments in Eq. (12) exactly correspond to the full tight-binding model-based NEGF results in Fig. 2. Note that the full NEGF calculations consider a general case for the interactions.

In summary, we predict a strong anisotropic exchange interaction induced topological edge conduction in materials with honeycomb lattice structures. The topological edge conductor forms when the strength of the anisotropic interaction exceeds at least twice the strength of the isotropic interaction. For materials like  $\text{Na}_2\text{IrO}_3$ , such strong anisotropic exchange interaction simultaneously induces an intrinsic zigzag antiferromagnetic order that breaks the time-reversal symmetry of the edge conductor. We use a nearest-neighbor tight-binding model and the Kitaev-Heisenberg model to study the quantum transport in such materials and show that the existence of the time-reversal symmetry broken topological edge conductor will be exhibited as a quantized Hall conductance without any external magnetic field.

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