Magnetic properties of $S = 5/2$ anisotropic triangular chain Bi$_3$FeMo$_2$O$_{12}$

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Abstract

Competing magnetic interactions in low-dimensional quantum magnets can lead to the exotic ground state with fractionalized excitations. Herein, we present our results on an $S = 5/2$ quasi-one-dimensional spin system Bi$_3$FeMo$_2$O$_{12}$. The structure of Bi$_3$FeMo$_2$O$_{12}$ consists of very well separated, infinite zig-zag $S = 5/2$ spin chains. The observation of a broad maximum around 10 K in the magnetic susceptibility $\chi(T)$ suggesting the presence of short-range spin correlations. $\chi(T)$ data do not fit to $S = 5/2$ uniform spin chain model due to the presence of 2$^\text{nd}$ nearest-neighbor coupling ($J_2$) along with the 1$^\text{st}$ nearest-neighbor coupling ($J_1$) of the zig-zag chain. The electronic structure calculations infer that the value of $J_1$ is comparable with $J_2$ ($J_2/J_1 \approx 1.1$) with negligible inter-chain interaction ($J'/J \approx 0.01$) implying that Bi$_3$FeMo$_2$O$_{12}$ is a highly frustrated triangular chain system. The absence of magnetic long-range ordering down to 0.2 K is seen in the heat capacity data, despite a relatively large antiferromagnetic Curie-Weiss temperature $\theta_{\text{CW}} \approx -40$ K. The magnetic heat capacity follows nearly a linear behavior at low temperatures indicating that the $S = 5/2$ anisotropic triangular chain exhibits the gapless excitations.

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I. INTRODUCTION

Investigating the exotic magnetic properties of low-dimensional and geometrically frustrated spin systems is one of the active research fields in modern condensed matter physics $^1$-$^4$. Mermin-Wagner theorem states that the system with dimensionality $d \leq 2$ and finite range interactions preserve continuous symmetry $^5$. The quantum fluctuations, in general, originated from quantum effects, are intrinsic and significant in low-dimensional magnetic systems (LDMS). These are further prominent for low spin ($S = 1/2$) magnetic materials. The physics of $S = 1/2$ LDMS is quite rich, and they offer a viable ground for the experimental realization of correlated quantum states with exotic fractional excitations $^1$, $^2$. The algebraic spin-spin correlation decay in $S = 1/2$ uniform spin chain systems suggests that the ground state is gapless $^6$, $^8$. Further, the introduction of geometric frustration through the presence of 2$^\text{nd}$ nearest neighbor (NN) interaction ($J_2$) along with that of 1$^\text{st}$ NN interaction ($J_1$) to the $S = 1/2$ uniform spin chain leads to a gapped excitation spectrum in the ground state as per the exactly solvable Majumdar-Ghosh (MG) chain model $^9$. The MG chain model states that $J_2/J_1 = 0.5$ opens a spin-gap and forms a singlet ground state $^{10}$.

On the other hand, the LDMS with large spin (i.e., $S = 5/2$) has not been studied extensively as the quantum effects are not prominent in these materials. A few examples with $S = 5/2$ systems are SrMn$_2$V$_2$O$_8$ $^{11}$, SrMn(VO$_4$)(OH) $^{12}$, Ba$_3$Fe$_2$Ge$_2$O$_{14}$ $^{13}$, and Bi$_2$Fe(SeO$_3$)OCl$_3$ $^{14}$. For example, the Mn-based linear chain system SrMn$_2$V$_2$O$_8$ exhibits a broad maximum ($T_{\text{max}}$) in the susceptibility data $\chi(T)$ around 200 K. However, due to the presence inter-chain couplings ($J'/J_1 \approx 0.6$), this material shows a magnetic long-range order (LRO) at 45 K. The Fe-based zig-zag chain Bi$_2$Fe(SeO$_3$)OCl$_3$ system shows $T_{\text{max}}$ around 130 K in the $\chi(T)$ data and LRO at 13 K, even in the presence of magnetic frustration with $J_2/J_1 \approx 0.2$. All these $S = 5/2$ spin systems undergo LRO at finite temperature due to the inter-chain coupling and insufficient magnetic frustration. It is pertinent to ask whether a correlated dynamic ground state is realizable or not in low dimensional systems with large spin. In this context, exploring novel low dimensional spin systems with large spin $S = 5/2$ promising to host quantum spin liquid with exotic fractional excitations set an attractive setting.

In this paper, we report the magnetic properties and electronic structure calculations on Bi$_3$FeMo$_2$O$_{12}$ $^{15}$. This material comprises the very well separated $S = 5/2$ zig-zag chains passing along the c-axis. The magnetic moments ($S = 5/2$) interact antiferromagnetically with Curie-Weiss temperature $\theta_{\text{CW}} \approx -40$ K. No magnetic LRO or spin freezing is observed down to 0.2 K. From the electronic structure calculations, the estimated ratio

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of 2nd NN and 1st NN couplings between Fe atoms is close to 1.1, and negligible inter-chain coupling ($J'/J_1 \approx 0.01$), which suggests that the Bi$_3$FeMo$_2$O$_{12}$ is a unique material with very well separated $S = 5/2$ triangular chains with a small anisotropy. Interestingly, heat capacity shows a nearly linear behavior with a finite value of the linear coefficient, suggesting the gapless excitations in the $S = 5/2$ triangular chains, unlike the $S = 1/2$ triangular chains that host a spin-gap ground state $[16]$. 

II. EXPERIMENTAL DETAILS

The polycrystalline samples of Bi$_3$FeMo$_2$O$_{12}$ and the non-magnetic analog Bi$_3$GaMo$_2$O$_{12}$ were synthesized by solid-state reaction method using the respective chemicals of Bi$_2$O$_3$, Fe$_2$O$_3$, Ga$_2$O$_3$, and MoO$_3$. These chemicals are mixed in stoichiometric ratio and thoroughly grounded in agate mortar and pestle. The pellets were made using the hydraulic press and heated at different temperatures from 400°C to 800°C. Finally, the sample was fired at 800°C for 72 hours with a few intermediate grindings to obtain the single phase of the samples Bi$_3$FeMo$_2$O$_{12}$. Neutron powder diffraction (NPD) experiments were performed using the neutron powder diffractometer PD-I ($\lambda = 1.094$ Å) with three linear position-sensitive detectors at Dhruva reactor, Bhabha Atomic Research Center, India. Magnetization ($M$), and heat capacity ($C_p$) measurements were performed on the polycrystalline sample pellets using the Physical Properties Measurement System (PPMS) with the corresponding attachments of Vibration Sample Magnetometer (VSM) and heat-capacity measurement option, respectively, in the temperature range from 2 K to 300 K and in the magnetic fields up to 160 kOe. Low-temperature heat capacity data was measured using a dilution fridge on a flat pellet of Bi$_3$FeMo$_2$O$_{12}$. 

III. RESULTS

A. Structural details

Bi$_3$FeMo$_2$O$_{12}$ crystallizes in a monoclinic structure with a space group $C2/c$ and holds the Scheelite-type structure with ABO$_4$ family $[15]$. The Bi atoms are located at the A-site, while B-site is occupied by Fe and Mo atoms in Bi$_3$FeMo$_2$O$_{12}$ structure. Interestingly, the Fe and Mo atoms are ordered at the B-site. The unit cell consists of FeO$_4$, MoO$_4$ tetrahedral, and BiO$_6$ polyhedral units (see Fig. 1(a)). The obtained lattice parameters from the Rietveld refinement of XRD pattern are $a = 16.91$ Å, $b = 11.65$ Å, and $c = 5.25$ Å, $\alpha = \gamma = 90^\circ$, $\beta = 107.1^\circ$. The Fe$^{3+}$ ($S = 5/2$) ions form an infinite zig-zag chain running along the c-axis, as shown in Fig. 1(b). The 1st NN distance of Fe-Fe is 3.79 Å with a possible exchange path of Fe-O1-O1-Fe. The 2nd NN distance of Fe-Fe is 5.25 Å, and its possible exchange path could be through Fe-O2-O2-Fe interactions. The bond lengths and bond angles are shown in the table 1. These chains are very well separated by a relatively large distance of 8.64 Å, suggesting that the compound might have nearly isolated $S = 5/2$ zig-zag spin chains.

B. Neutron diffraction measurements

The data were recorded at different temperatures from 6 K to 50 K. Rietveld refinement of NPD data was performed using the FullProf Suite software package as shown in Fig. 2(a), (b), and (c). The observed neutron diffraction pattern could be fitted by considering only the nuclear phase. We have subtracted the intensities of 50 K from 6 K data, i.e., $I$ (50 K) – $I$ (6 K). We do not see any signs of new Bragg intensities or diffuse background patterns from the subtracted data as shown in Fig. 2(d). We have also compared the difference plot of $I$ (50 K) – $I$ (6 K) with the difference plot of $I$ (50 K) – $I$ (20 K), and there is no difference seen between these two plots. Neither additional magnetic Bragg peaks nor an enhancement in the intensity of the fundamental nuclear Bragg peaks has been observed down to 6 K (see Fig. 2(d)), indicating the absence of magnetic long-range order and rule out the presence of a phase transition at 11 K as was reported in reference $[17]$. 

C. Magnetization measurements

Temperature-dependent magnetic susceptibility $\chi(T)$ measurements were performed on the polycrystalline sample Bi$_3$FeMo$_2$O$_{12}$ in the $T$ range from 2 – 300 K in $H = 10$ kOe (see Fig. 3(a)). The fit of the $\chi(T)$ data to Curie-Weiss law yields the temperature-independent susceptibility $\chi_0 \approx -2.0 \times 10^{-4}$ cm$^3$/mol, Curie-Weiss temperature $\theta_{CW} \approx -40$ K, and Curie constant $C \approx 4.3$ cm$^3$ K/mol. Diamagnetic susceptibility is estimated to be $\chi_{dia} \approx 2.4 \times 10^{-4}$ cm$^3$/mol from the individual ions in the formula Bi$_3$FeMo$_2$O$_{12}$. After the subtraction of
Figure 2: (Color online) Rietveld refinement of Neutron diffraction (ND) data measured at different temperatures 50 K, 20 K, and 6 K are shown in (a), (b), and (c), respectively. Red pluses represent the calculated diffraction pattern (Ical), the black line represents the diffraction pattern (Iobs), the blue line represents the difference (Iobs - Ical), and the green vertical lines represent the Bragg positions. (d) The ND intensities of 6 K and 20 K after subtracting the ND intensities at 50 K.

\( \chi_{\text{dia}} \) from the obtained value of \( \chi_0 \), the calculated Van Vleck susceptibility is \( \chi_{\text{VV}} \approx 4.2 \times 10^{-5} \text{cm}^3/\text{mol} \). From the value of \( C \), the effective magnetic moment of Fe\(^{3+} \) is calculated to be 5.90 \( \mu_B \) (= \( \sqrt{8C} \mu_B \)), well consistent with the expected value of 5.91 \( \mu_B \) for \( S = 5/2 \). The absence of splitting in zero-field-cooled (ZFC) and field-cooled (FC) susceptibility rules out the spin-glass transition in this compound, as shown in the inset of Fig. 3(a). Fig. 3(b) represents the magnetization isotherm at 2 K was measured up to 160 kOe. The \( M(H) \) follows linear behavior, indicating the absence of ferromagnetic components in the samples. \( M(H) \) data do not saturate up to 160 kOe field. The large magnetic field is required to reach saturated magnetization \( M_{\text{sat}} = gS = 5\mu_B \) for \( S = 5/2 \) magnetic moments.

At low-\( T \), \( \chi(T) \) shows a broad maximum around \( T_{\text{max}} \approx 10 \) K, indicating the presence of short-range correlations [16,18,20,21]. We tried to analyze \( \chi(T) \) with \( S = 5/2 \) uniform spin chain model by Bonner and Fisher (BF) [21,22] and found that this model could not reproduce our experimental data. According to the \( S = 5/2 \) uniform spin chain, the broad maximum would appear at \( k_B T_{\text{max}} / J = 10.6 \) [22]. From our experimental observation of \( T_{\text{max}} \) position, the \( J/k_B \) value expected to be about \(-1 \) K [22]. We have then compared the experimental data with the \( S = 5/2 \) uniform chain model with \( J/k_B \approx -1 \) K. As shown in the inset of Fig. 3(b), the experimental value of magnetic susceptibility is much smaller than the simulated data, suggesting the presence of significant additional antiferromagnetic exchange couplings. From this analysis, we anticipated the presence of a significant value of 2\(^{nd} \) NN coupling along with 1\(^{st} \) NN coupling qualitatively. This is further quantitatively confirmed from the first-principle density functional theory (DFT) electronic structure calculations discussed later in the paper. The presence of 2\(^{nd} \) NN exchange coupling accounts for the large magnetic frustration in this material since \( J_1 \) and \( J_2 \) form a triangular network (see Fig. 4(b)).

D. Heat capacity measurments

The heat capacity \( C_p(T) \) data of \( \text{Bi}_3\text{FeMo}_2\text{O}_{12} \) and \( \text{Bi}_3\text{GaMo}_2\text{O}_{12} \) were investigated in zero field (see Fig. 4). At low-\( T \), there is a large difference seen between the \( C_p \) of \( \text{Bi}_3\text{FeMo}_2\text{O}_{12} \) and \( \text{Bi}_3\text{GaMo}_2\text{O}_{12} \) indicating the dominance of magnetic contribution. Interestingly, no sharp peak is observed down to 0.2 K in the \( C_p(T) \) data of \( \text{Bi}_3\text{FeMo}_2\text{O}_{12} \), suggesting the absence of magnetic LRO. The frustration parameter \( f = | \theta_{\text{CW}} | /T_N \) value
To understand the magnetic behavior of Bi$_3$FeMo$_2$O$_{12}$, spin-polarized DFT calculations in the local-spin density approximation (LSDA) and LSDA+$U$ (Hubbard $U$) approach were carried out by means of a full-potential linearized muffin-tin orbital (FP-LMTO) method [28, 29] as implemented in the RSPt code [30]. We have considered on-site Coulomb interaction $U = 2$ eV combined with Hund’s exchange $J_H = 0.8$ eV within the fully rotationally invariant LSDA+$U$ approach [31] to treat the electronic correlation effects of Fe-$d$ states. Such choices of $U$ are guided by a previous report on a correlated oxide containing high-spin Fe$^{3+}$ ions [32]. From both LSDA and LSDA+$U$ calculations, the lowest energy state is identified for the pattern with the antiferromagnetic couplings between the $1^{st}$ NN and $2^{nd}$ NN Fe-spins in the isolated zig-zag-chain.
The computed total and orbital-decomposed density of states (DOS) in this lowest-energy magnetic state as obtained from LSDA+U are shown in Fig. 6(a). The DOS of Fe-3d clearly shows that the majority spin states are fully filled up, and the minority spin states are empty (see Fig. 6(b)). This is consistent with the picture of the high-spin ground state of Fe$^{3+}$ ions (3d$^6$). The Mo-d states (see Fig. 6(c)) are found to be completely empty, indicating the nominal d$^0$ non-magnetic state of these ions. The O-p states are also delocalized and spread in the entire valence band. The insulating gap of 1.7 eV is found between O-p and the Fe-d states, making this system a member of the charge-transfer insulator in the Zaanen, Sawatzky, and Allen (ZSA) scheme \[33, 34\].

We next estimated the various magnetic exchange couplings ($J_1$ and $J_2$) as marked in Fig. 6(d) based on the converged lowest energy magnetic state. Here we employed the formalism of Ref. \[35\], where the total converged energies of the magnetic system are mapped onto a Heisenberg Hamiltonian, and magnetic force theorem \[36, 37\] is applied to extract the inter-atomic magnetic exchange interactions. Our calculations, as summarized in Table I reveal that both $J_1$ and $J_2$ are antiferromagnetic. The $J_1$ and $J_2$ exchange interactions are mediated through Fe-O-O-Fe super-exchange paths with varied Fe-Fe distances (3.79 Å and 5.25 Å), as mentioned in Table I. Interestingly, the magnitudes of both the exchanges come out to be almost equal ($J_2/J_1 \approx 1.1$) although the corresponding Fe-Fe distances are very different. We also note that such a conclusion is very robust and independent of the adopted methods and independent of U choice within the LSDA+U approach.

The highly delocalized nature of O-p orbitals promotes such super-super exchange interaction. Interestingly, the Fe-O-O angles that connect the two 2nd NN Fe are equal while these angles are different for 1st NN. The peculiar character of the crystal symmetry is responsible for the reason of having $J_1$ and $J_2$ to be nearly equal, despite having a difference in the Fe-Fe bond distances.

The nature of the exchange could also be qualitatively understood within the framework of the extended Kugel-Khomskii model \[38, 39\]. It is well established that half-filled orbitals promote antiferromagnetic super-exchange since virtual hopping between Fe orbitals is allowed only if they possess anti-parallel alignments. Importantly, the antiferromagnetic nature, together with the comparable exchange interactions ($J_1 \approx J_2$), causes strong spin-frustration in the zig-zag-shaped triangular Fe$^{3+}$ chains. The estimated $\theta_{CW} \approx -37.5$ K agrees very well with the experimental value of $-40$ K, providing further credence to the theoretically computed values of the exchange interactions. The ratio of the inter- to intra-chain magnetic exchange coupling $J'/J_1$ is estimated at about 0.01. Thus, we can conclude that the present system is an example of a nearly isolated $S = \frac{5}{2}$ triangular spin chain.

### IV. DISCUSSION

Triangular antiferromagnets offer a promising ground for realizing the unusual states of matter. In $S = \frac{5}{2}$ triangular systems, a few 2D magnets were investigated AFeO$_2$ (A=Cu, Li, and Na) \[40, 41\]; however, the quantum ground state without magnetic LRO has not been identified. Achieving the disordered quantum state in $S = \frac{5}{2}$ systems probably requires a material with ideal one-dimensionality. Our experimental observations on $S = \frac{5}{2}$ triangular chain material Bi$_3$FeMo$_2$O$_{12}$ ($J_2/J_1 \approx 1.1$ and $J'/J \approx 0.01$) revealed that it exhibits large magnetic frustration ($f > 200$). Besides, the observation of the linear behavior of $C_m(T)$ suggests the presence of gapless excitations. Strikingly, the physics of $S = \frac{5}{2}$ triangular chain behavior is entirely different from that of the $S = 1/2$ triangular chain, where one can expect a robust spin-gap ground state \[17\]. As an example, $S = 1/2$ zig-zag chain system Sr$_{0.5}$Ca$_{0.1}$CuO$_2$ has shown the spin-gap ground state due to the randomness.

![Figure 6: Total and orbital-decomposed density of states (DOS) for the lowest energy magnetic state. Fermi energy is set to zero.](image_url)

**Table I: The details of exchange coupling strengths using LSDA approach with U**

| Exchange path | $J_1$   | $J_2$   |
|---------------|---------|---------|
| Fe-Fe distance | 3.8Å    | 5.3Å    |
| Fe-O1-O1-Fe (Fe-O1-O1=128.5° & O1-Fe=71.9°) | Fe-O2-O2-Fe (Fe-O2-O2=111.8° & O2-Fe=111.8°) |
| LSDA+U        | -1.52 K | -1.66 K |
All the results support that the titled compound might be a possible candidate for gapless spin liquid. Muon spin relaxation and inelastic neutron scattering experiments in sub-Kelvin temperature may shed microscopic insights into the ground state and spin dynamics of the titled material.

V. CONCLUSION

Our investigation reveals that the titled compound Bi$_3$FeMo$_2$O$_{12}$ is a nearly ideal quasi-one-dimensional $S = 5/2$ triangular chain system with a small anisotropy ($J_2/J_1 \approx 1.1$). The presence of strong magnetic frustration and negligible inter-chain interactions preclude magnetic LRO down to 200 mK. $C_m(T)$ data show a linear behavior reflecting the gapless excitations in the ground state. These results will stimulate both theoretical and experimental interests to examine whether our $S = 5/2$ triangular chain Bi$_3$FeMo$_2$O$_{12}$ can host the spin liquid ground state.

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