



Institute for Materials Science
Universität Stuttgart



11th December
2023, 4:30 pm

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UCCS, University of Lille, France

Mixed oxy-fluoride anionic sublattice : A strategy for magnetic layered perovskites

The *Aurivillius* materials series of formula $(\text{Bi}_2\text{O}_2)(\text{A}_{n-1}\text{B}_n\text{O}_{3n+1})$ include perovskite slabs of variable thicknesses, $n = 1, 2, 3 \dots$ separated by Bi/O layers (where A is a large 12 coordinated cation, and B is a small 6 coordinated transition metals. They are generally limited to "high oxidation state" diamagnetic B cations such as Ti^{4+} , Nb^{5+} , W^{6+} . Due to the Bi^{3+} lone-pair effect, they mostly crystallize in polar space groups associated with attractive dielectric/ferroelectric properties. One way to access magnetically-active 3d transition metal oxide B ions is to partially substitute the O^{2-} anionic sublattice by F^- anions. Besides the limited number of reported *Aurivillius* ($n = 1$) diamagnetic oxyfluorides such as $\text{Bi}_2\text{Ti}^{4+}\text{O}_4\text{F}_2$, $\text{Bi}_2\text{Nb}^{5+}\text{O}_5\text{F}$, $\text{Bi}_2\text{V}^{4+}\text{O}_5\text{F}$ the recent synthesis of $\text{Bi}_2\text{Co}^{2+}\text{O}_2\text{F}_4$ opens wide potentialities to combine ferroelectric and magnetic properties. We prepared ($n = 1$) $\text{Bi}_2\text{M}(\text{O},\text{F})_6$ ($\text{M} = \text{Mn}^{2+}$, Fe^{2+} , Ni^{2+} , V^{4+}) as single crystals and/or polycrystalline samples, returning informative data on their accurate crystal structures, the O/F ordering in supercell, the plausible vacancies, the occurrence of various structural modulations ... etc. The segregation of antagonist O^{2-} and F^- anions in distinct sub-units of the structure has a significant impact on the bandgap and electronic properties. Electric and magnetic properties will be presented through the prism of their possible coupling into multiferroics.

COLLOQUIUM
MATERIALS SCIENCE

Winter Semester
2023/2024

Max-Planck-Institute
Werner-Köster Hall (2R4)
Heisenbergstr. 3
70569 Stuttgart

(Gummi Bears
served at 4:15)

Meeting-Link for TU Darmstadt:

<https://unistuttgart.webex.com/unistuttgart/j.php?MTID=mcaa017047150127142691>

