Poster Presentation

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Perovskites in low dimensional multi-layer structure types

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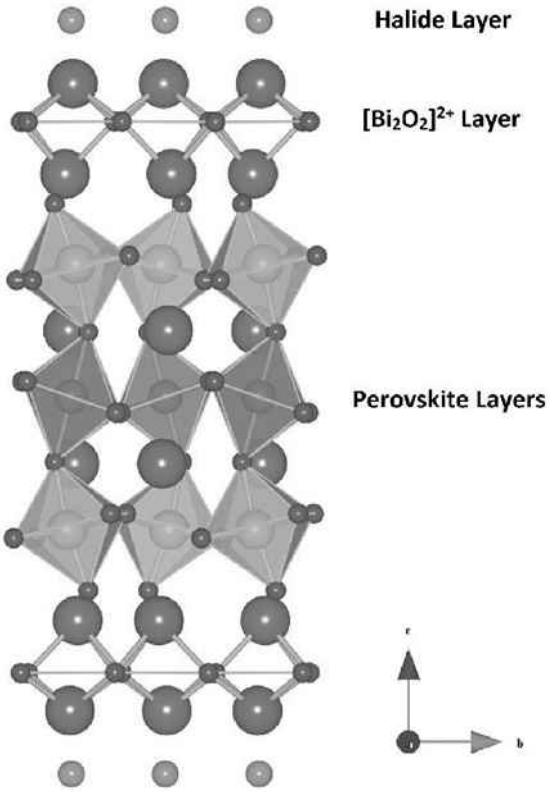
This study introduces examples of structure property relationships within the multi-layered Sillen-Aurivillius family (shown in Figure) and aims to investigate the effect of chemical doping and lattice matching effects. The first example involves doping 1/3 of the n = 3 ferroelectric perovskite layers with magnetic transition metal cations in $Bi_5PbTi_3O_{14}Cl$ [1] with charge balancing by removing Pb^{2+} for Bi^{3+}. A statistical 1:2 distribution of M^{3+} and Ti^{4+} across all three perovskite layers was found in $Bi_6Ti_2MO_{14}Cl$, M = Cr^{3+}, Mn^{3+}, Fe^{3+}, resulting in highly strained structures (enhancing the ferroelectricity compared to $Bi_5PbTi_3O_{14}Cl$) and pronounced spin-glass behavior below $T_{irr}(0)$ = 4.46 K. Ferroelectric transitions were observed at high temperature for each of the new compounds. Ferroelectric properties were also measured on $Bi_6Ti_2FeO_{14}Cl$ using piezoresponse force microscopy showing hysteretic phase behavior. A new n = 2 Sillen-Aurivillius compound $Bi_3Sr_2Nb_2O_{11}Br$, based on $Bi_3Pb_2Nb_2O_{11}Cl$ [2], was synthesized by simultaneously replacing Pb^{2+} with Sr^{2+} and Cl^- with Br^-. Inter-layer mismatch prevented the formation of $Bi_3Sr_2Nb_2O_{11}Cl$ and $Bi_3Pb_2Nb_2O_{11}Br$. Sr^{2+} doping reduces the impact of the stereochemically active $6s^2$ lone pair found on Pb^{2+} and Bi^{3+}, resulting in a stacking contraction in the lattice parameters by 1.22 % and an expansion of the a-b plane by 0.25 %, improving inter-layer compatibility with Br^-. X-ray Absorption Near Edge Structure spectra analysis shows that the ferroelectric distortion of the B-site cation is less apparent in $Bi_3Sr_2Nb_2O_{11}Br$ compared to $Bi_3Pb_2Nb_2O_{11}Cl$. Variable-temperature neutron diffraction data show no evidence for a ferroelectric distortion.

[1] *A. Kusainova, S. Stefanovich, J. Irvine, et al, Journal of Materials Chemistry, 2002, 12, 3413–3418,* ***[2]*** *A. Kusainova, P. Lightfoot, W. Zhou, et al, Chemistry of Materials, 2001, 13, 4731-4737*



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