of oxygen atom of the cations. It is interesting that the structure of inorganic part is highly influenced by the existence of organic molecules in this type of inorganic-organic hybrid materials.

We have been studying the crystal structure and chemical bonding in the material by combining the data obtained by single crystal neutron and X-ray diffraction experiments. It is difficult to decide the atomic positions of organic part in the material from only X-ray diffraction data because heavy lead atom is coexisting in the structure. Neutron diffraction is suitable way to analyze the crystal structure of this type of materials. Neutron diffraction data was collected at 120K using time-of-flight single crystal neutron diffractometer "iBIX" constructed at J-PARC. X-ray diffraction data was also collected using imaging-plate single crystal X-ray diffractometer at 120K. From the obtained crystal structure, orientation of the cations and distortion tendency of $PbBr_6$ octahedra suggests the existence of chemical bonding between lead and oxygen atoms. In addition, the existence of hydrogen bonding between the nitrogen atoms of the cation and bromide atoms of inorganic chain is also suggested. Electron density distribution analysis by maximum entropy method was performed to investigate the nature of chemical bondings in the material. Overlapping of electron density is seen between lead and bromide atoms because of covalent characteristic of the bonding. On the other hand, because no overlapping of electron density is seen between lead and oxygen atoms, it is expected that the bonding has ionic characteristic. Each of inorganic chains is connected by electrostatic interaction through the cations.

Keywords: inorganic-organic, single crystal, bonding

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Synthesis, structural reinvestigation and physical properties of alkali hexatitanate

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The alkali hexatitanate having the tunnel structure form a class of compounds that can exhibit interesting physical properties such as bronze-type TiO_2, [1], [2] and Li ion conductor in ramsdellite-type $Li_2Ti_3O_7$, [3], [4] as well as their intriguing structural features. In the tunnel-type alkali and alkaline earth hexatitanate $A_2Ti_6O_{13}$ (A = H, Li, Na, K, Sr and Ba) systems, several compounds are reported until now. $H_2Ti_6O_{13}$ and $Li_2Ti_6O_{13}$ is known as metastable form by ion-exchange method. However, crystal structure and physical properties of $H_2Ti_6O_{13}$ and $Li_2Ti_6O_{13}$ has not been reported. In the present study, we successfully synthesized polycrystalline sample of $H_2Ti_6O_{13}$ and $Li_2Ti_6O_{13}$ by ion-exchange method from $Na_2Ti_6O_{13}$ [5]. The crystal structure was determined ab-initio structure determination by powder X-ray and neutron diffraction data. In addition, the structural validity was confirmed by bond valence sums calculation, and the data of MAS-NMR, and the results of the present first-principles calculation by the FLAPW method. The result of crystal structure on $Li_2Ti_6O_{13}$ showed LiO_4 plain tetra coordinates. This Li-O coordination is not normal, and different from that in other $A_2Ti_6O_{13}$ compounds. On the other hand, the crystal structure of $H_2Ti_6O_{13}$ showed OH-O hydrogen bonding, and ordered arrangement of proton is seen in the crystal structure.

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Keywords: oxide, structure solution, powder diffraction

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Critical behaviour of Ti doped manganite $La_{0,67}$ $Ba_{0,33}$ MnO_3

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The critical properties of Ti doped $La_{0,67}$ $Ba_{0,33}$ MnO_3 around the paramagnetic ferromagnetic phase transition were investigated based on the data of static magnetic measurement around Curie temperature T_c. It is found that the mean-field model is the best one to describe the critical phenomena around the critical point. The magnetic data analyzed in the critical region using the Kouvel-Fisher method yield the critical exponents in $La_{0,67}Ba_{0,33}Mn_{0,98}Ti_{0,02}O_3$ of β=0,589±0,015 with T_c=310,852±0.190 (from the temperature dependence of spontaneous magnetization below T_c) and γ=1,020±0,024 with T_c=310,111±0.143 (from the temperature dependence of inverse initial susceptibility above T_c) and δ=2.741 is determined separately from the isothermal magnetization at T_c. These critical exponent obtained by this method obey the Widom scaling relation $\delta=1+\gamma/\beta$, implying that the obtained values of β and γ are reliable.

Keywords: critical, perovskite, modelling

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The structure and magnetic properties of the solid-solution: $Na_2(Zn,Co)SiO_4$

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Na2ZnSiO4, a homeotype of wurtzite, is of interest as a host structure for the creation of potentially interesting magnetic materials. The solid-solution series Na2(Zn(1-x) ,Cox)SiO4 was synthesized by high temperature ceramic methods. The resulting blue compounds possessed band gaps of ~1.7 eV, independent of Co2+ doping percentage. Initial powder X-ray data were collected on a Rigaku Miniflex II diffractometer with copper Kα radiation and later high resolution data were collected on the 11-BM diffractometer at the Advanced Photon Source, Argonne National Laboratory with a wavelength of 0.413606 Å. The resultant data verified that the Co2+ and Zn2+ ions were randomly distributed forming a single Zn-Co phase from $0 < x < 0.50$. Rietveld analysis converged to X2 of 1.89 and R = 2.49 %. All atoms possessed tetrahedral environments, but those associated with the sodium ions were highly distorted. The high resolution data revealed a more complicated structure than predicted with evidence for aperiodicity in the crystal structure. Magnetic moment versus temperature data were collected from 2 K to 350 K under 1000 G field. The data conformed to a Curie-Weiss plot ($1/\chi$ vs. T), which represents primarily paramagnetic behavior although the positive Y intercept indicates the presence of short-range antiferromagnetic interactions at high temperature. At low temperatures, a paramagnetic-antiferromagnetic interchange occured with a Néel temperature at 5 K. Keywords: solid-solution, rietveld, anitiferromagnetism