

was heated under dynamic vacuum; at 130°C deuterium is released and LiMgAlD<sub>6</sub> is formed:  $\text{LiMg(AlD}_4)_3 \rightarrow \text{LiMgAlD}_6 + 2\text{Al} + 3\text{D}_2$ . At 180°C LiMgAlD<sub>6</sub> decomposes:  $\text{LiMgAlD}_6 \rightarrow \text{LiD} + \text{MgD}_2 + \text{Al} + 3/2\text{D}_2$ . The first reaction is endothermic; the second exothermic, indicating that LiMg(AlD<sub>4</sub>)<sub>3</sub> is not thermodynamic stable. LiMg(AlD<sub>4</sub>)<sub>3</sub> crystallizes in the monoclinic space group *P*2<sub>1</sub>/*c* with cell parameters:  $a = 8.37 \text{ \AA}$ ,  $b = 8.74 \text{ \AA}$ ,  $c = 14.30 \text{ \AA}$  and  $\beta = 124.83^\circ$ . The structure consists of isolated AlD<sub>4</sub> tetrahedra that are connected by octahedral Mg and Li atoms. LiMgAlD<sub>6</sub> crystallizes in the trigonal space group *P*321 with cell parameters:  $a = 7.98 \text{ \AA}$  and  $c = 4.38 \text{ \AA}$ . The structure consists of isolated AlD<sub>6</sub> octahedra tied together by hexa-coordinated Li and Mg atoms. A small amount of TiCl<sub>3</sub> was added to LiMg(AlD<sub>4</sub>)<sub>3</sub> and mixed using the ball milling technique. The effect of addition of TiCl<sub>3</sub> was also studied for LiMgAlD<sub>6</sub>.

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#### MS17 P11

##### Structural phase transitions in Sr<sub>2</sub>ScReO<sub>6</sub>

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In double perovskites A<sub>2</sub>MReO<sub>6</sub>, where A – an alkaline-earth ion and M – a non-magnetic two – or three-valence cation such as Zn<sup>2+</sup>, Mg<sup>2+</sup> or Sc<sup>3+</sup>, only the Re ion is relevant to the unusual magnetism in these compounds [1, 2]. Structural thermal behaviour of these compounds, which can be connected with magnetic and transport properties, is not yet investigated. In our work, high-temperature structure investigations of Sr<sub>2</sub>ScReO<sub>6</sub> were performed at beamline B2 (HASYLAB DESY, Germany) in Debye-Scherrer mode using the on-site readable image-plate detector OBI and a STOE furnace. All diffraction patterns have been analyzed by using the software package WinPLOTR [3]. Two phase transitions with a change of symmetry of the crystal structure from monoclinic (S.G. P<sub>2</sub><sub>1</sub>/*n*) to tetragonal (S.G. P<sub>4</sub>/*mnc*) and then to cubic (Fm-3m) have been detected at elevated temperatures. These phase transitions were also proved by DSC measurements. Low-temperature investigations of Sr<sub>2</sub>ScReO<sub>6</sub> are in progress.

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#### MS17 P12

**X-ray Induced Water Order-Disorder Transition in Hydrated Cesium Cobalt Oxide** Hwo-Shuenn Sheu<sup>a</sup>, Wei-Ju Shih<sup>a</sup>, Horng-Yi Tang<sup>b</sup>, Nien-Tsu Sun<sup>b</sup>, <sup>a</sup>National Synchrotron Radiation Research Center, Hsinchu, Taiwan <sup>b</sup> Department of Applied Chemistry, National Chi Nan

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Metal cobalt oxides, A<sub>x</sub>CoO<sub>2</sub> (A= Li, Na, K, Rb, Cs), with layered structure have been attracting wide attention for the past two decades. Li<sub>x</sub>CoO<sub>2</sub> is one of the most important intercalation compounds for secondary lithium ion batteries. Na<sub>x</sub>CoO<sub>2</sub> is recognized to be a potential candidate for thermal electric power materials and non-cuprites superconductors. A<sub>x</sub>CoO<sub>2</sub> compounds have a layered structure, with the CoO<sub>2</sub> layers consisting of CoO<sub>6</sub> octahedra sharing common edges and forming a triangular Co–O sublattice. Open and polarizable framework structure makes the compounds adaptable by chemical modification. The superconductivity of hydrated Na<sub>0.35</sub>CoO<sub>2</sub>·1.3H<sub>2</sub>O oxide was found and immediately targeted by research scientists owing to its unusual bilayer-hydrate (BLH) structure. In the coupling strength of CoO<sub>2</sub> layers might be varied by the replacement of different ionic size alkalis resulting in the change of c-axis lattice constant. The influence of coupling strength between CoO<sub>2</sub> layers on superconductivity, therefore, can be possibly studied when the process of controlling the interlayer spacing is developed. The bilayer-hydrate of Cs<sub>0.2</sub>CoO<sub>2</sub>·0.63H<sub>2</sub>O with a greatest interlayer spacing  $d = 10.0(2) \text{ \AA}$  among alkali cobalt oxides has been grown in crystal form. Magnetic susceptibility measurement of Cs<sub>0.2</sub>CoO<sub>2</sub>·0.63H<sub>2</sub>O displays a paramagnetic behavior down to 1.9 K. We find that X-ray powder diffraction patterns of Cs<sub>0.2</sub>CoO<sub>2</sub>·0.63H<sub>2</sub>O changed according to various X-ray dosages during the XRD measurement. The water ordering in Cs<sub>0.2</sub>CoO<sub>2</sub>·0.63H<sub>2</sub>O is sensitive to X-ray irradiation. The relative diffraction intensity vary is strongly dependent on the amount of water contain and the location at interfacial position. We will report the X-ray dosage dependent crystal structure of Cs<sub>0.2</sub>CoO<sub>2</sub>·0.63H<sub>2</sub>O in the meeting.

#### MS17 P13

**Investigation of K<sub>x</sub>Na<sub>1-x</sub>NbO<sub>3</sub> (KNN) near the Morphotropic Phase Boundaries** N. Zhang & A.M. Glazer, Department of Physics, University of Oxford, UK. D. Baker & P.A. Thomas, Department of Physics, University of Warwick, UK.

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**Keywords:** morphotropic phase boundary, sodium potassium niobate, neutron and X-ray scattering

PZT is commonly regarded as the leading piezoelectric material for a wide range of applications, and one which all others must be assessed against. However, there are growing concerns over the toxicity and environmental issues of lead-based substances, which is why attention has turned to other lead-free piezoelectric materials, one of which is Sodium Potassium Niobate (KNN).

The newer lead-free materials are united with PZT in that they exhibit a region in their phase diagrams where there appears to be a sudden change in crystal structure. This region has been termed the Morphotropic Phase Boundary (MPB) and appears to coincide with the maximum piezo-response of these materials. Of particular interest in K<sub>x</sub>Na<sub>1-x</sub>NbO<sub>3</sub> (KNN) is the presence of three morphotropic phase boundaries (MPB) that occur at  $x \sim 0.18$ ,  $x \sim 0.35$ , and  $x \sim 0.48$ [1].