MS13-P9 **Crystal Structure Analysis of Layered Compounds Cr_xTiS_2** Ken-ichi Ohshima, Shou Ikeda, Takuro Kawasaki, Miwako Takahashi *Institute of Materials Science, University of Tsukuba, Tsukuba 305-8573, Japan*
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Single-crystals of Cr_xTiS_2 (x=0.22, 0.31, and 0.72) were prepared, where the chemical vapor transport method using iodine as the transport gas was adopted. The X-ray structure analysis at room temperature has been performed to investigate the ordered atomic arrangements of intercalated Co atoms and their site occupancies. The superstructures of the Co atoms are observed to be $2a$x$2a$x$2c$ unit cells for x=0.22, and $\sqrt{3}a$x$\sqrt{3}a$x$2c$ unit cells for x=0.31 and 0.72. Furthermore,the electron density distribution (EDD) was obtained by the maximum entropy method for understanding the nature of the chemical bond.The overlapping of EDDs between Cr and S atoms and Ti and S atoms corresponds to the covalent bonding in the van der Waals gap layer and TiS_2 layer. It is found that the nature of the covalent bonding between Cr and S atoms causes a decrease in the interatomic distance. In addition, the theoretical EDD by full-potential linearized argumented-plane-wave (FLAPW) method was calculated and compared with the observed one. The agreement between the two EDDs was quite good.

Keywords: layered compound, Cr_xTiS_2, EDD

MS13-P10 **Proton conduction in geometrically frustrated lanthanum tungstate** Tobias Scherb,[a] Simon A.J. Kimber,[b] Christiane Stephan,[a] Paul F. Henry,[ca] Gerhard Schumacher,[a] Sonia Escolastico,[d] Jose M. Serra,[d] *[a]Helmholtz-Zentrum Berlin, Germany, [b]European Synchrotron Radiation Facility, France, [c]European Spallation Source, Sweden, [d]Instituto de Tecnología Química, Spain*
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Ln_6WO_{12} (Ln = Lanthanide or Yttrium) compounds are due to their mixed protonic/electronic conduction properties and their superior stability in acidic atmospheres highly potential materials for the use as gas separation membranes. We prepared pure samples of $La_{5.5}WO_{12-\delta}$ which showed exceptional device performance and stability, and studied the crystal structure in detail by the complementary use of neutrons and photons. The performance at temperatures above T = 600 °C is better than reported for other mixed conductors, and the comparable tiny water uptake (< 0.2 weight %), measured by thermogravimetry, suggests an unusually effective mechanism for proton transport. To date, the crystal structure of this compound is unknown with contradictory reports about cubic, pseudo-cubic or tetragonal symmetry. The results here show a cubic symmetry for the studied compound with a remarkable degree of disorder around the W sites. Moreover, we identified a splitting of one La site into two 50 % occupied sites which have average 7-fold oxygen coordination. The disorder of octahedral units and metal displacements finds a natural explanation in a combination of local structural constraints and frustrated geometry. We find that topological defects are strongly implicated in the mechanism for proton conductivity, which is apparently similar to that seen in water ice. The presentation will thus provide a robust example of chemical functionality through frustration and a compelling avenue for designing new functional solid state materials.

Keywords: proton conductivity; lanthanum tungstate; frustration