

MS18. Thermoelectric materials - from fundamental science to applications

Chairs: Oliver Oeckler, Sylvie Hébert

MS18-P1 Interplay between structural transitions and thermoelectric properties in a Mn hollandite

Sylvie Hébert¹, Jesus Prado Gonjal¹, Hidefumi Takahashi¹, Denis Pelloquin¹, Antoine Maignan¹

1. Laboratoire CRISMAT, UMR6508 CNRS et ENSICAEN, 6 Bd du Maréchal Juin, 14050 Caen Cedex, France

email: sylvie.hebert@ensicaen.fr

Na_xCoO_2 and misfits are still the best p type thermoelectric oxides, with the combination of a large Seebeck coefficient, together with a metallic behaviour at 300K, and small values of thermal conductivities [1-3]. Their unique thermoelectric properties come from the presence of CoO_2 layers made of edge shared CoO_6 octahedra, with Co^{3+} and Co^{4+} in low spin states. New families of oxides have since then been investigated to find new potential thermoelectric materials. Among them, hollandites present an interesting crystallographic structure with (i) ribbons made of edge shared octahedra, and (ii) the presence of tunnels, in which large cations can be inserted. Several hollandites have been investigated, with both p and n type doping, and large power factors have been observed [4-5]. In this poster, the results obtained in the case of $\text{Ba}_x\text{Mn}_8\text{O}_{16}$ hollandite will be presented, with the evidence of a structural transition at high T. The impact of this structural transition on the transport properties will be discussed.

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J. Prado Gonjal, Present address : University of Reading
H. Takahashi, Present address : Nagoya University

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MS19. Topology of crystal structures

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MS19-P1 Crystal chemistry of Al-phosphate minerals with complex H-bond networks

Francesco Capitelli¹, Giancarlo Della Ventura², Fabio Bellatreccia², Maria Rosaria Ghiara³, Manuela Rossi³, Emanuela Schingaro⁴, Gennaro Ventrucci⁴, Angela Altomare⁵, Michele Saviano⁵

1. Istituto di Cristallografia – CNR Monterotondo (Rome, Italy)

2. Dipartimento di Scienze, Università Roma Tre (Rome, Italy)

3. Real Museo Mineralogico and Dipartimento di Scienze della Terra dell'Ambiente e delle Risorse, Università Federico II Naples (Naples, Italy)

4. Dipartimento di Scienze della Terra e Geoambientali, Università di Bari (Bari, Italy)

5. Istituto di Cristallografia – CNR Bari (Bari, Italy)

email: francesco.capitelli@ic.cnr.it

The (PO_4) oxyanion combines with over 30 elements to form natural phosphates, which are among the most complex and variegated compounds in all the mineral world, displaying a large number of recognized phases (about 300), most of them featuring hydrogen as hydroxyl groups and water molecules. Thus, hydrogen bond displays a crucial role in stabilizing the hydroxy-hydrated phosphate frameworks, providing the additional bond-valence contribution to the anions. Hence, the oxygen atoms of (PO_4) groups easily interact with neighbor cationic environments in the structure. For this reason, many phosphates are characterized by the presence of an intricate network of O-H...O interactions, joining the polyhedral units and making up the three dimensional framework (Humnicki & Hawthorne, 2002). In this sense, the study of such complex structures is achieved by means of Single-Crystal X-Ray Diffraction, with the contribute of powder FTIR spectroscopy, being the latter a powerful tool for the study of hydrogen in minerals, especially in presence of high OH/ H_2O contents.

In this work, we present the structure investigations of selected aluminum phosphates: vauxite $\text{FeAl}_2(\text{PO}_4)_2(\text{OH})_2 \cdot 6\text{H}_2\text{O}$, wardite $\text{NaAl}_2(\text{PO}_4)_2(\text{OH})_2 \cdot 2\text{H}_2\text{O}$, wavellite $\text{Al}_3(\text{PO}_4)_2(\text{OH},\text{F})_4 \cdot 5\text{H}_2\text{O}$, augelite $\text{Al}_2(\text{PO}_4)(\text{OH})_3$, whiteite $\text{CaFeMgAl}_2(\text{PO}_4)_4(\text{OH})_2 \cdot 8\text{H}_2\text{O}$ (Ventrucci *et al.*, 2015, and references therein). Main crystallographic features (bonds, angles, interactions) were examined and compared with those obtained from phosphate literature, and the networks of hydrogen bonds were further analyzed according to the Libowitzky (1999) relationship, for the range of D-H...A bond systems in the structure, in order to compare results of OH frequencies from FTIR spectra with those observed by X-ray refinement.

References