

ENERGYPOLIS SEMINAR

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Phase transitions in $A^{2+}B^{2+}PO_4$ zeolite-type compounds

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At the upcoming talk, recent structural investigations on $A^{2+}B^{2+}PO_4$ (A=K, Cs; B=Mg,Mn) phosphates will be presented.

Compounds with the general formula $A^{2+}B^{2+}PO_4$ (A = K, Rb; Cs,Tl,NH₄; B and X are tetrahedrally coordinated cations) belong to the tridymite structural family. Their oxygen framework is made up of corner-shared tetrahedra forming six-membered rings that host a large cation A [1]. These rings consist of BO₄ and PO₄ tetrahedra and may take different orientation. Despite the fact that PO₄ groups form rather rigid tetrahedra, the network is quite flexible because of rotation of PO₄ and MO₄ polyhedra. As a consequence, these types of structure undergo a series of phase transitions as the temperature is changed [2-6].

An interesting feature of this type of compounds is that many of them have the same orthorhombic prototype phase at high temperatures. It belongs to the centrosymmetric *Pnma* space group.

Despite the fact that many of the structures of these compounds have been already studied, there are still many open questions about structural transformations which motivate the present study.

References:

- [1] R.E. Gibbs, Proc. Roy. Soc. London. 63a (1926) 351
- [2] D. Blum, Ferroelectrics. 69 (1986) 283-292
- [3] A. Kruglik, M.Simonov, E. Zhelezin, N. Belov. Sov. Phys. Dokl. 24 (1979) 596-601
- [4] G. Wallez, F. Lukas, J.P. Souron, M. Quarton, Mater. Res. Bull. 34 (8) (1999) 1251-1261
- [5] L. Perez, L. Marcos, H. Schmid, Ferroelectrics. 175 (1), (1996) 41-50
- [6] M. Orlova et al., J. Solid State Chem. 221 (2015) 224-229



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Born 19. June 1981 in Nizhny Novgorod, Russia, Maria Orlova graduated in Chemistry at the University of Nizhny Novgorod (2003). From 2003 to 2007 she carried out her PhD work at the same institution in the field of Solid State Chemistry. In 2007-2008 she worked on hydrogen storage materials at the University of Geneva. She continued this topic at ESRF, France (2009-2011). Currently she is working at the University of Innsbruck, conducting her research in the field of phase transitions of functional phosphate materials, as well as performing diffraction studies for a project of the pharmaceutical company "Sandoz".