Time	Saturday, 27.08	Sunday, 28.08	Monday, 29.08	Tuesday, 30.08	Wednesday, 31.08	Thursday, 1.09	Time
8:30		Registration					8:30
9:00		Opening	(Plenary Review) Köppel	(Plenary Review) Bersuker	(Invited Speaker) Chibotaru	Fishchev	9:00
9:10		(Plenary Review) Ceulemans					9:10
9:20						Zlatar	9:20
9:30					Koenis		9:30
9:40			Paz	(Invited Speaker) Ghosh		Ulak	9:40
9:50		(Plenary Review) Kresin			Dunn		9:50
10:00			(Invited Speaker) Eisfeld			Closing	10:00
10:10				Kugel	Nasrullahi		10:10
10:20							10:20
10:30		Coffee break	Reimers	Coffee break	Coffee break		10:30
10:40							10:40
10:50		(Invited Speaker) Kaldun	Coffee break	(Plenary Review) García-Fernández	(Invited Speaker) Kaplan		10:50
11:00							11:00
11:10			(Invited Speaker) Khomskii				11:10
11:20		Seibold			Joon		11:20
11:30				Polinger			11:30
11:40		Vargunin	Bussman-Holder		Nazipov		11:40
11:50				Kremer			11:50
12:00		Opalka	Adhikari		Lunch (12:00-13:10)		12:00
12:10				Baryshnikov			12:10
12:20		Lunch (12:20-13:30)	Lunch (12:20-13:40) (Meeting of the Steering Committee)				12:20
12:30							12:30
12:40							12:40
12:50							12:50
13:00				Excursion and Conference dinner (13:00-22:00)			13:00
13:10					Zolotaryuk		13:10
13:20							13:20
13:30		(Invited Speaker) Ernst			Perry		13:30
13:40			(Plenary Review) Tsukerblat				13:40
13:50					Kosevich		13:50
14:00		Gudkov					14:00
14:10					Yusupov		14:10
14:20		Glaum	(Invited Speaker) Polinger				14:20
14:30					Coffee break		14:30
14:40		Stroppa	Perić				14:40
14:50					Sato		14:50
15:00		Coffee break	Kovaleva				15:00
15:10					Sabovich		15:10
15:20		Kravchenko	Coffee break				15:20
15:30					Kamenskyi		15:30
15:40		Gorinchoy	Kojima				15:40
15:50					Kulik		15:50
16:00		Barta	Kokishnev				16:00
16:10					Morgan		16:10
16:20		Dovbeshko	Shelkov				16:20
16:30					Ursu		16:30
16:40		Hatanaka	Grachova				16:40
16:50							16:50
17:00			Poster Session (17:00-18:00)				17:00
18:00							18:00
19:00	Welcome reception / early registration (19:00-21:00)						19:00
20:00							20:00
21:00							21:00

UNIVERSITY OF TARTU
Institute of Physics

BOOK OF ABSTRACTS

XXIII INTERNATIONAL SYMPOSIUM ON THE JAHN-TELLER EFFECT

VIBRONIC COUPLING AND ELECTRON-PHONON INTERACTION IN MOLECULES AND CRYSTALS

BASIC JAHN-TELLER THEORY
JAHN-TELLER AND PSEUDO JAHN-TELLER COUPLING IN MOLECULES AND CRYSTALS
CONICAL INTERSECTIONS
SUPERCONDUCTIVITY
PEROVSKITES, FULLERENES, GRAPHENE, AND RELATED SYSTEMS

AUG 27–SEPT 1, 2016, TARTU, ESTONIA

Jahn-Teller Crystals – New Class of Smart Materials

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Smart materials are materials with properties that undergo significant and quick changes under environmental disturbances such as changes of temperature, pressure (hydrostatic and uniaxial), external magnetic and electric fields, light intensity, pH, and so on. Most of the material properties are defined by their electronic spectra. The electronic spectra undergo the most dramatic changes due to environmental forces when there is a degeneracy or pseudo degeneracy (small energy gaps) of the electronic states of the materials. In these materials, as a rule, the vibronic (electron-phonon) interactions are significant. All that leads to the conclusion that the Jahn-Teller systems are good candidates in the search for smart materials.

Different electronic and structural phase transitions are typical in the multicenter Jahn-Teller systems – Jahn-Teller crystals. If one accepts the fact that phase transitions are characterized by anomalously big material property changes, it becomes clear that Jahn-Teller multiferroics are especially good candidates for new smart materials and their applications.

While among the smart Jahn-Teller crystals there are representatives of all types of materials – metals, dielectrics, semiconductors, and superconductors, this presentation will concentrate on dielectric materials. Various old and new unusual smart properties will be analyzed.

Examples of practical applications of smart Jahn-Teller materials and corresponding patents will be discussed.

1. M. Kaplan, B. Vekhter, "Cooperative Phenomena in Jahn-Teller Crystals", Plenum Press, New York/ London (1995).
2. M. Kaplan, G. Zimmerman, "Elastic Anomalies in Jahn-Teller Crystals with Competing Orderings", J. of Phys.: Conf. Ser., **428**, 012033 (2013).
3. M. Kaplan, "Jahn-Teller Crystals – New Class of Smart Materials", 4th Annual World Congress of Advanced Materials, p.81, Chongqing, China (2015).

Two-level behavior of Ti^{3+} *d*-orbitals in $NaTiSi_2O_6$

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$NaTiSi_2O_6$ is a spin ½ member of quasi one-dimensional magnets of the pyroxene family. It is a Mott insulator, which crystallizes in the monoclinic space group *C2/c* at high temperatures [1, 2]. Its crystal lattice consists of slightly distorted TiO_6 octahedra, which are skew edge connected into zigzag chains, bridged by SiO_4 tetrahedra. In coordinates used in [3], the threefold t_{2g} level of Ti^{3+} splits due to distortion and crystal field into low-lying doublet with d_{xy} and d_{yz} orbitals and a single d_{xz} orbital removed to 0.3 eV higher energy. This orbital degeneracy causes cooperative Jahn-Teller (JT) effect through strong electron-lattice coupling [3]. At T_c= 210 K the lattice undergoes structural phase transition into triclinic $P\bar{1}$ space group [1, 2] with dimerization of Ti zigzag chains. The phase transition is actually orbital ordering and the creation of d_{xy} dimers with spin singlet ground state, which is the orbital analogue of spin-Peierls transition. As a result a spin-gap of order 500-700 K [1, 4] and 53 meV [5] opens and the magnetic susceptibility starts rapidly to decrease. Theoretical calculation for the pyroxene family magnets in [6] gives for Ti-Ti dimer in $NaTiSi_2O_6$ antiferromagnetic exchange coupling J_{intra}= 396 K and weak exchange between the dimers J_{inter} 5K, close to the experimental data.

In order to gain more insight on local spin dynamics of the compound, we have performed ^{29}Si NMR spin-lattice relaxation study on $NaTiSi_2O_6$, [7]. We have found that at low temperature the magnetization recovery curve is nonexponential, with initial increase of the magnetization as square root of the time, which is characteristic to relaxation on paramagnetic impurities with no spin diffusion [8, 9]. Detailed analysis of the magnetization recovery gives a concentration of such impurities [9], which are in the present case mostly undimerized Ti^{3+} ions. We have found that temperature dependence of this concentration *c(T)* follows activation type behaviour $c(T) = c_0 \exp(-E_a/T)$, with the energy $E_a = 300 \pm 20K$. We ascribe this activation energy to the splitting of the lower *d*-orbital doublet. We note that E_a is very close to phonon Raman modes 221 and 209 cm^{-1}, which anti-cross at T_c, when the dynamic JT phase changes into the static one [3]. We show that the concentration of the unpaired Ti^{3+} ions and the magnetic susceptibility data can be well described within a two level model, with 300 K splitting between the levels and the additional singlet-triplet energy gap of order 650 K.

1. M. Isobe *et al.*, Novel phase transition in spin-1/2 linear chain systems: $NaTiSi_2O_6$ and $LiTiSi_2O_6$, J. Phys. Soc. Japan 71, 1423 (2002).
2. G. J. Redhammer, *et al.*, Single-crystal structure refinement of NaTiSi2O6 clinopyrexene at low temperatures (298 < T < 100K), Acta Crystallogr., sect.B: Struct. Sci B59, 730 (2003).
3. M. J. Konstantinovic *et al.*, Orbital dimerization in $NaTiSi_2O_6$: An orbital analogue of the spin-Peierls phase transition, Phys. Rev. B69, 020409(R) (2004).
4. P. J. Baker *et al.*, Muon-spin relaxation on the dimerized spin-1/2 chains $NaTiSi_2O_6$ and TiOCl, Phys. Rev. B75, 094404 (2007).
5. H. J. Silverstein *et al.*, Direct measurement of the spin gap in a quasi-one-dimensional clinopyroxene: $NaTiSi_2O_6$, Phys. Rev. B90, 140402(R) (2014).
6. S. V. Streltsov and D. I. Khomskii, Electronic structure and magnetic properties of pyroxenes $(Li,Na)TM(Si,Ge)_2O_6$: Low-dimensional magnets with 90° bonds, Phys. Rev. B77, 064405 (2008).
7. R. Rästa *et al.*, ^{29}Si NMR study of $NaTiSi_2O_6$, this conference.
8. W. E. Blumberg, Nuclear spin-lattice relaxation caused by paramagnetic impurities, Phys. Rev. 119, 79 (1959).
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