



European Materials Research Society

Spring Meeting 2015

from May 11th to 15th
Lille Grand Palais - France

Call for papers
deadline for abstract submission:
15 January 2015

www.european-mrs.com

Symposium GG:

ANIM 2: Advances and enhanced functionalities of anion-controlled new inorganic materials

Anion-controlled functional materials present a wide range of applications due to their basic functionalities. This second edition ANIM 2 aims to cover a large domain from the synthesis to the understanding of the fundamental properties of novel devices based on enhanced properties offered by such inorganic mixed-anions materials. Based on the success of the first edition (E-MRS symposium T, spring 2013), this symposium will focus on the solid state chemistry and physics of such materials with interdisciplinary research and industrial applications, not yet widely known, but with vast application prospects.

Scope:

The present E-MRS symposium aims creating a European forum for the different types of researchers necessary for this field (physicists – experimentalists and theoreticians, materials scientists, solid state chemists, analytical scientists and device design engineers). The symposium will facilitate interdisciplinary discussions between these differing “core groups”, thereby stimulating collaboration and thus it will strengthen the European and Worldwide activities in this expanding field.

The symposium's main topics cover the following aspects:

- Theoretical fundamentals: theoretical concepts for novel physics expected to be derived from new functions and properties of coordinate covalent-bonding engineered ceramic material systems, epitaxial and polycrystalline thin films, glasses, single crystals, quantum size effects in nanoparticles and nanosized powders.
- Advances in synthesis that have enabled the development of N-containing materials using less toxic methods.
- Surveying the anion-substituted materials landscape: combined experimental and theoretical prediction investigations of various classes of materials systems, searches for new perovskite and related materials with a view to expand and optimize their functionalities and electronic properties (e.g. ferroelectric, ferromagnetic, semiconductive, thermoelectric, electroresistive, magnetoresistive, conductive transparent high temperature stable electrodes, solid state electrolytes, ionic conductors, photocatalytic, luminescent materials, nonlinear optical materials, dipole glasses, quasi-2-dimensional electron gases (Q2-DEG) in insulating hetero-interfaces).
- Overviewing of anion-substituted inorganic materials in device development activities: state-of-the-art characterization and electronic properties improvement based on heterostructures, interface phenomena, electrode interactions and various device prototypes demonstrations.

Hot topics to be covered by the symposium:

- Innovative synthesis routes for Anion-substituted New Inorganic Materials (ANIM) oxynitrides, oxyfluorides, oxyhydrides and other mixed anion materials (powders, nanomaterials, bulk ceramics, glasses, thin films and single crystals).
- Structural features and anion order of ANIM.
- ANIM-based (photo)catalyst materials.
- Optical properties: luminescence, nonlinear optical properties of ANIM materials.
- Ferromagnetic, paramagnetic; paraelectric, high-K gate, ferroelectric, multiferroic properties of ANIM materials. ANIM-type semiconducting and highly conducting electrode materials.
- ANIM-based energy materials for production and storage of energy: solid electrolytes, fuel cell materials electrode materials, supercapacitor materials, battery materials, hydrogen storage materials, ionic conductor and thermoelectric materials.
- Theory, simulations and combinatorial approaches for design of new anion-controlled materials and prediction of their functionalities.
- Technical challenges in the analytical and functional properties characterization of ANIM materials

Invited speakers:

- Alain Demourgues, ICMCB, Bordeaux, France
- Amparo Fuertes, ICMAB, Barcelona, Spain
- Shiv Halasyanami, University of Houston, Houston, USA
- Mike Hayward, University of Oxford, UK
- Hiroshi Kageyama, Kyoto University, Japan
- Ivoyl P. Koutsaroff, Murata Manufacturing Co., Ltd., Shiga, Japan
- Philip Lightfoot, University of St Andrews, UK
- Ru-Shi Liu, NTU, Taiwan
- Ram Seshadri, University of California, Santa Barbara, USA
- Anke Weidenkaff, University of Stuttgart, Germany

Scientific committee:

- Duncan Gregory, University of Glasgow, UK
- Takashi Hisatomi, The University of Tokyo, Japan
- Stéphane Jobic, IMN, Nantes, France
- Laurent Le Gendre, IETR, St Brieuc, France
- Thomas Lippert, Paul Scherrer Institut (PSI), Würenlingen, Switzerland
- Emma McCabe University of Kent, Canterbury, UK
- Yuji Masubuchi, Hokkaido University, Sapporo, Japan
- Alain Tressaud, ICMCB, Bordeaux, France

Publication:

High quality manuscripts will be published in a special issue of *Solid State Sciences (Elsevier)*

Symposium organizers:

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Deadline for abstract submission: January 15, 2015

E-MRS 2015 SPRING MEETING, May 11 - 15 – Grand Palais, Lille, France



2015 Spring Meeting
from May 11th to 15th Lille Grand Palais - France

SYMPOSIUM GG

ANIM 2: Advances and Enhanced Functionalities of Anion-controlled New Inorganic Materials

Symposium Organizers :

Franck Tessier, CNRS - Université de Rennes 1, France

J. Paul Attfield, University of Edinburgh, UK

Kenneth R. Poeppelmeier, Northwestern University, Evanston, USA

Shinichi Kikkawa, Hokkaido University, Sapporo, Japan

Published in a special issue of **Solid State Sciences (Elsevier)**



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ANIM 2: Advances and enhanced functionalities of anion-controlled new inorganic materials

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09:00	Welcome Address: Franck Tessier	
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2015 International year of light and light-based technologies (1) : Ivoyl P. Koutsaroff

09:15	<p>Rational approaches to anion-controlled phosphors for solid-state lighting Authors : Ram Seshadri Affiliations : Materials Department and Department of Chemistry and Biochemistry, Materials Research Laboratory, University of California, Santa Barbara CA 93106 Resume : In this contribution, I will address inorganic phosphors that play a key role in the now almost-mature solid-state white-lighting technologies based on combining a III-nitride-based near-UV or blue solid-state light source with down-conversion to longer wavelengths. These phosphors invariably comprise a crystalline oxide, nitride, or oxynitride host that is appropriately doped with either Ce³⁺ or Eu²⁺. Optical excitation into these states and concomitant reemission can be tuned into the appropriate regions of the visible spectrum by the crystal these ions are hosted in. Experimental studies of some of the best phosphor materials, employing state-of-the-art structural tools, have yielded guidelines for what are desirable structural features. The role of anion control, including substitution of oxygen by fluorine and by nitrogen will be emphasized. These substitutions call for new ways of thinking with regard to lattice rigidity and the band positions of the host vis-à-vis the levels on the activator ions.</p>	GG-1 1
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09:45	<p>Relation structure/luminescence in bismuth based compounds Authors : Jacob Olchowka, Marie Colmont, Houria Kabbour, Olivier Mentré, Claudia Wickeder Affiliations : Anorganische Chemie II, Universität Siegen, Germany; UCCS, Université de Lille1, France; UCCS, Université de Lille1, France; UCCS, Université de Lille1, France; Anorganische Chemie II, Universität Siegen, Germany Resume : Nowadays, energy saving context and high price of rare earth (RE) lead us to investigate new RE-free emitters as promising emitters. In this context, besides their interest for photocatalysis, the mixed-anionic Sillén compounds BiMO₂X (X = Cl, Br, I and M = metals) and novel related phases, also show an extremely bright luminescence at room temperature due to parity allowed, fast Bi³⁺: s₂ ↔ sp electronic transitions. Here the sizeable crystal field offered by mixed anionic (O, X) coordination sphere of Bi³⁺ together with M/M' cationic substitution influences luminescence properties and gives possibility to rationalize the effect of the first and second coordination sphere on Bi-optical properties. Here we present luminescence properties of a variety of Bi-based compounds with mixed-anionic lattice including (O,X) and (O, TO₄) (T=P,V) which all show RE-free bright room temperature luminescence. Experimental data combined with empirical and DFT calculations led to a full rationalization of the transition energies and show possibility for controlled tuning of the optical properties. For instance we show how excitation bands depends on the covalency of peripheral Bi-(O,X) though the well-known nephelauxetic effect, while the Stokes shift can be connected to the degree of Bi³⁺ lone pair stereoactivity in adequate Bi-phases. Finally, these compounds appear as ideal systems for the study of the structure luminescence relationships.</p>	GG-1 2
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Mixed-anions materials with electric properties : J. Paul Attfield

08:45 Recent Progress in Aliovalent Anion-substituted Perovskite Thin Film Dielectric Materials: Nanoscale characterization of ANIM materials and their functionalities

Authors : Ivoyl P. Koutsaroff

Affiliations : formerly at Murata Manufacturing Co., Ltd., Japan

Resume : In comparison to cationic substitutions or co-substitutions, anionic substitutions in perovskite materials are less systematically examined in regard to the dielectric properties of a given perovskite-type class compare to their oxide analogues. The exchange of the oxide ions for nitride ions can have a substantial influence on the structural (i.e., through rearrangement of B(O,N)₆ octahedra) and physical characteristics of perovskite materials and can allow creation of new mixed anion AB(O,N)₃ type perovskite derivatives. Very recently the oxynitride perovskites have been shown to exhibit ferroelectric behavior [1]. Typically studied oxynitride perovskite systems in regard to their dielectric properties in a bulk ceramic or as thin films are LaTiO₂N₁, SrTaO₂N₁, BaTaO₂N₁, and CaTaO₂N₁ [1-2]. The incorporation of N³⁻ results in a pronounced effects, such as elongated Ta(Ti)-N bond length and reduced electronegativity of the nitride ion, with respect to the oxide ion, will tend to increase the covalence of the cation-anion bonds. The increased covalence of the bonding can in turn increase the likelihood of cation displacements through a second order Jahn-Teller distortion of the d⁰ cation and could influence the paraelectric properties of the oxynitrides. Nanoscale characterization of ATiO_{3-x}N_x (A=Sr, Ba, Ca) perovskite films had been very limited and started less than half a decade ago[2]. 1. Oka, D. et al. Sci. Rep. 2014, 4, 4987. 2. <http://pubs.acs.org/page/cgdefu/vi/13.html>

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09:15 Origin of the anomalous thermoelectric properties in the rare earth borocarbonitrides

Authors : Takao Mori, Anastasiia Prytuliak, Walter Schnelle, Ulrich Burkhardt, Yuri Grin

Affiliations : NIMS, Univ. Tsukuba; NIMS; MPI-CPfS; MPI-CPfS; MPI-CPfS

Resume : The search for viable thermoelectric (TE) materials is intensifying [1]. Higher borides are attractive candidates for their stability, large Seebeck coefficients, S, and low thermal conductivity [2]. Higher borides are predominantly p-type and a counterpart to boron carbide was long sought after. Small additions of C and N were found to function as bridging sites resulting in new network structures, i.e. novel rare earth borocarbonitrides, which exhibited anomalous n-type [3]. We will report on several new developments in this series of compounds. Through transition metal doping, S of YB₂₂C₂N was increased by 220% while resistivity was reduced by ~10,000%, a striking overcoming of the conventional trade-off effect [4]. Small inclusions of boron carbide were shown to strongly affect the Seebeck coefficients of YB_{28.5}C₄ samples as a whole [5]. The origin of the anomalous n-type behavior in rare earth borocarbonitrides was indicated to be related to the pseudo-gap electronic structure formed mainly by the boron cluster framework, which gives guides on enhancing these materials further. [1] Thermoelectric Nanomaterials, ed. K. Koumoto and T. Mori (2013). [2] C. Wood et al, PRB 29 (1984) 4582, T. Mori et al, JAP 102 (2007) 073510,

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