



**International Union of
Crystallography**
**Commission on Mathematical
and Theoretical Crystallography**



International School on Fundamental Crystallography
Sixth MaThCryst school in Latin America
Workshop on the Applications of Group Theory in the Study
of Phase Transitions

Abstracts of some poster presentations

SYNTHESIS AND CHARACTERIZATION OF PEROVSKITE CERAMICS FOR CATALYSIS & SOFC APPLICATIONS

Natasha Di Benedetto, Joaquín Grassi y Leopoldo Suescun

Laboratorio de Cristalografía, Química del Estado Sólido y Materiales, DETEMA, Facultad de Química, UdeLaR, Montevideo, Uruguay
ndibenedetto@fq.edu.uy - joaquingrassi@fq.edu.uy

The ideal perovskite structure has the general stoichiometry ABX_3 , where A (A=Ln, AE), is a larger cation than B (transition metals), and X is an anion (e.g.: oxo). Despite the simplicity of the crystalline structure, the fact that A and B can be almost any cation of the periodic table, generates an immense structural variety and gives place to numerous properties of interest such as multiferroic properties (magnetic, electric, elastic, etc.). The oxides of this family are probably the most studied materials in the last decades since comprehension of this type of structures and the correlation between their structure and properties is of fundamental and technological interest, it is the deviations respect the ideal structure through changes in the system's symmetry what leads to the appearance of the properties mentioned above. At the moment, the most interesting properties that exhibit these structures are: energy conversion (photovoltaic cells and fuel cells), adsorption and catalysis (mainly heterogeneous).

Volatile organic compounds (VOCs) are a group of carbon-based chemicals considered not only as major contributors to air pollution but also the main hazardous substances for human health. An additional complication of VOCs is that this category includes a wide range of compounds with very different chemical properties; this makes it difficult to find a single catalyst for the effective elimination of the majority of them. A few years ago, the catalytic oxidation combustion process involving perovskite-based catalysts –especially manganites– arose as an interesting alternative to traditional methods for VOCs elimination.

We have synthesized, characterized and tested the catalytic oxidation of acetone for LaMnO_3 and the $\text{La}_{0.8}\text{A}_{0.2}\text{MnO}_3$ series (A= Mg, Ca, Sr, Ba). All of the compounds of the series were obtained as unique phases (except when A=Mg) and performed similarly when tested for acetone catalytic oxidation (the new materials proved to be active even at low temperatures: 17% at 100°C for LaMnO_3), showing values comparable to those obtained in literature. $\text{La}_{0.8}\text{Ca}_{0.2}\text{MnO}_3$ was the one which exhibited the biggest difference between the as-obtained powder and the calcined one, the utilization of other techniques to understand deeply the microstructure and its relation with the catalytic properties might be the key to explain these variations.

Fuel Cells (FC) are electrochemical devices that convert chemical energy into electrical energy with high efficiency from fuel oxidation. Among the various types of FC, several aspects of Solid Oxide Fuel Cells (SOFCs) catch the eye, such as fuel flexibility, a complete solid structure, high power density and low greenhouse effect gas emissions. Currently, the interest in those devices is focused especially in the so-called Intermediate Temperature Solid Oxide Fuel Cells (IT-SOFC) that operate between 500-800°C which creates the necessity for new materials with higher electrochemical activity in this temperature range. The higher cathodic activities have been reported for materials with $\text{ABO}_{3-\delta}$ perovskite type structure with oxygen vacancies ($\delta > 0$).

We proposed the study, synthesis and structural and electrochemical characterization of the high-TC superconductors $\text{REBa}_2\text{Cu}_3\text{O}_{7-\delta}$ (RE = La, Y, Nd, Sm, Pr and Gd) as potential SOFC cathodes. The results obtained show that some of the members of the series (Y, Sm and Gd) present an O - T phase transition which could compromise the mechanical stability of the cell. While for La, Nd and Pr this transformation does not occur and they have moderate polarization resistances.

Expression, Purification and Crystallization of PKS involved in formation of Ebelactona from *Streptomyces aburaviensis*

Cardoso, T. P.¹, Huang, F.³, Leadlay, P.³, Dias, M.V.B.^{1 2}

¹Programa de Pós-Graduação em Microbiologia, IBILCE-UNESP, São José do Rio Preto-SP;

²Departamento de Microbiologia, ICB-USP; São Paulo-SP; ³Department of Biochemistry, University of Cambridge, Cambridge-UK.

tabataperes@hotmail.com

Macrocyclization of polyketides generates arrays of molecular architectures that are directly linked to biological activities. The four-membered ring in oxetanones (β-lactones) is found in a variety of bioactive polyketides (for example, lipstatin, hymeglusin and ebelactone). Ebelactones are produced by the actinomycete, *S. aburaviensis*. They are known inhibitors of esterases, lipases, cutinases, homoserine transacetylase and cathepsin A.

This wide range of biological activities has triggered interest in the synthesis of these natural compounds. The origin of the oxygen atoms in Ebelactona was not determined, and with it the biosynthesis of the most intriguing component of these molecules, the β-lactone ring, was left unresolved. The biosynthesis of a number of macrocyclic polyketide lactones has been extensively studied and many polyketide synthases (PKSs) gene clusters identified.

Bacterial modular Type I PKSs are multienzymes that govern the biosynthesis of diverse complex polyketide natural products, including clinically useful antibiotics, immunosuppressants, and antitumor compounds. They follow a remarkable assembly-line paradigm, in which each cycle of polyketide chain extension is accomplished by a different set or module of vertebrate fatty acid synthase (FAS)-related enzyme domains.

The present study aims to obtain and structurally analyze of Ebe G PKS enzyme, in order to improve the knowledge about the physiological processes in which this protein act.

Expression and purification of the enzyme Ebe G by immobilized nickel affinity column and size molecular exclusion were realized

We subjected the protein sample to the Oryx 6 crystallization robot by testing crystallization kits from Jena Bioscience. Crystals of Ebe G were obtained in two conditions at 20°.

We have successfully expressed and purified of Ebe G. For a first screening, we obtained crystals which will be taken to X-ray diffraction. We are still working to purify and getting proteins crystals data of the structure of Ebe G. Analysis of this possible structure will reveal details of the specificity for its substrates.

Morphology and orientation in mesostructured systems based on small quiral molecules.

Federico Movilla, DQIAQF/INQUIMAE-Universidad de Buenos Aires

In this work we present a new family of quiral amino acid derivatives showing a rich supramolecular chemistry mainly, due to the presence of certain functional groups. Their molecular and supramolecular structure and properties were studied by different spectroscopic techniques, X-ray diffraction (XRD), polarized light microscopy (POM) and scanning electron microscopy (SEM). A variety of crystalline material was obtained employing different crystallisation procedures. In particular, the mesostructured material was analysed using powder X-ray diffraction employing a 2D detector to compare the differences in the azimuthal intensities produced by the preferred orientation originated by the self-assembly of the nano crystalline particles. Moreover, supramolecular organogels were also obtained when certain solvents and temperature control were applied. Results showed that these new compounds are excellent building blocks either for formation of supramolecular gels, as for the obtaining of crystalline material. Furthermore, the properties and identity of the resultant material could be modulated by tuning the intermolecular interactions given by the presence of functional groups in the compounds and by controlling the experimental conditions employed during the synthesis, both key features for the rational design of new materials.

X-RAY STUDY OF CRYSTALLOGRAPHIC TEXTURE IN Ti/MgB₂ WIRES

Mauro Melone, IB/UNCuyo - CNEA - CCT Patagonia /CONICET

In this work the Powder-in-Tube (PIT) method has been used for the conformation of wires. The sheath was conformed of Grade 2 Ti and the core of a mixture 95 at.% MgB₂ con 5 at.%SiC (20 – 30nm). The crystallographic texture of the sheath and the core have been determined by pole figures taken by x-ray diffraction. The critical current density (J_c) has been determined by magnetization loops in two different orientations whit a SQUID magnetometer. An increment of J_c anisotropy with the increment of the texture is presumed.