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Diffraction study of doped apatite-type $\text{La}_{9.33+x}(\text{Si}_{1-y}\text{Al}_y\text{O}_4)_6\text{O}_{2+\square}$ ($A=\text{Fe, Al, Mg}$). Přemysl Beran^a, Ezhil Jothinathan^b, Jozef Vleugels^b, Omer van der Biest^b.

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Apatite type lanthanum silicates, $\text{La}_{9.33+x}(\text{SiO}_4)_6\text{O}_{2+3x/2}$, are a new class of electrolyte material reported to have better oxygen ion conductivity in the intermediate temperature (600–800°C). There is limited information on cation doping and defect processes at the local structural level, particularly the role of dopants on the Si site and the effect of vacancies in the La-occupied channels. It is known that it is possible to tailor the conductivity of these electrolytes by substitution either on silicon or on lanthanum site. In spite of their well established conductivity, the exact mechanism of conduction is still unclear. Two kinds of diffusion pathways have been proposed in the literature – a direct linear path along the hexagonal axis and non-linear, sinusoidal-like path through interstitial oxygen ions [1–4]. In this work we present the diffraction study of silicon site substituted lanthanum silicates by iron, aluminium, magnesium and as well both iron and aluminium at RT and also working temperature (800°C). The powders were prepared by using a modified sol-gel method [5] with appropriate cationic ratio. Phase purity and basic structural investigation were made using the laboratory X-ray powder diffraction. This shows that all samples present $P6_3/m$ symmetry. To describe the influence of doping on the Si site on the conducting channel and on the distribution of the mobile oxygen ions – diffusion pathways – we made Rietveld analysis of the neutron diffraction data not only at RT, where low conductivity is present, but also at working temperature, where the oxygen ion conduction occurs. Results are discussed from the point of view of structural changes of conducting channels and compared with the two diffusion pathways models proposed for these kinds of materials.

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Keywords: lanthanum silicate, fuel cells, neutron powder diffraction

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Structure and optical properties of natural low dimensional semiconductors. Robert S. Black^a, David G. Billing^a. ^aMolecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Private Bag 3, PO Wits 2050, Johannesburg, South Africa.

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Inorganic-organic hybrids have been of great interest from a crystal engineering point of view because of the ability to template metal halides into interesting structural motifs.

However, they have a much greater practical use. They can be used to template bulk materials into low dimensional semiconductors, by taking an inorganic semiconductor material, and intercalating organic amine cations to change the materials dimensionality, and in so doing, altering the optical properties of the material. The features most greatly affected by a change in dimensionality is, firstly, the band structure i.e., the tuning of the band gap, secondly, the electron mobility of the compound, and thirdly and most importantly, the ability confine the electron and hole orbit's (excitons), which drastically alters the materials recombination luminescence (Fig.1). A further advantage of inorganic organic hybrids is that they self assemble and are easily solution processed into thin films, this has positive implications regarding cost and the ease of processability for further technological applications such as LCD's displays [1]. Previously published results show the binding energy of the excitons increase as the dimensionality is decreased i.e. from 3D to 2D and from 2D to 1D. However there is a much larger increase in the binding energy from 2D to 1D systems as seen in Fig.1. Here we report the structure and optical properties of 1D hybrids with the general formula $(\text{RN}^+)\text{PbI}_3$, in which we further investigate the tunability of the band structure, the large binding energy associated with the excitonic behavior, and charge transfer effects between wires and spacers [3–5].

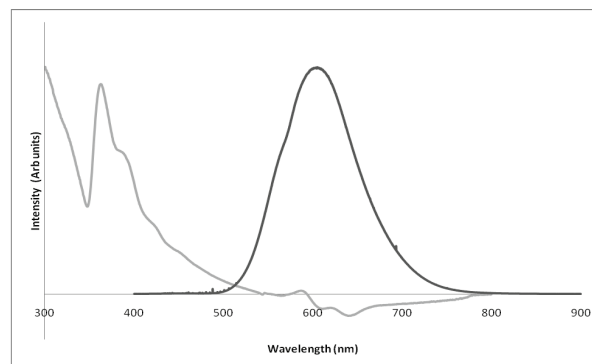


Fig.1. The binding energy effect as displayed in (piperidiumim)PbI₃ wires where we see the 1s exciton absorption peak at 365nm and the resultant 600nm photoluminescence emission both at 77K.

Keywords: Natural quantum wires, Inorganic-organic hybrids, Photoluminescence

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Crystalline compounds of the system glycine – ZnCl₂ – H₂O: crystal growth and optical properties. L. Bohaty^a, A.A. Kaminskii^b, P. Becker^a. ^aInstitute of Crystallography, University of Cologne, Germany. ^bInstitute of Crystallography, Russian Academy of Sciences, Moscow, Russia.

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In the system $\text{NH}_2\text{CH}_2\text{COOH}$ (= glycine) – ZnCl_2 – H_2O four structurally well characterised crystalline compounds are