WELCOME

The Organizing Committee kindly welcomes you at the International Conference "Functional materials and nanotechnologies" **FM&NT-2012**. The conference is organised by Institute of Solid State Physics, University of Latvia in co-operation with National Research programme in Materials Science and Information Technologies of Latvia.

The purpose of the conference is to bring together scientists, researchers, engineers and students from universities, research institutes and related industrial companies working in the field of advanced material science, energy and materials technologies.

Scientific topics of the conference

Multifunctional Materials:

Advanced inorganic, organic and hybrid materials; ferroics; multiscale and multiphenomenal material modelling and simulation;

Nanotechnologies:

Progressive methods, technologies and design for investigation of nanoparticles, nanostructures, nanocomposites, thin films and coatings;

Energy:

Perspective materials and technologies for renewable and hydrogen energy, fuel cells, photovoltaics and developing diverse energy systems.

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The Organizing Committee sincerely hopes that the conference will give all the participants new insights into the wide spread development of functional materials and nanotechnologies and will enhance the circulation of information released at the meeting.

On behalf of FM&NT-2012 organizers thank you all for coming and we wish you most successful and enjoyable conference.

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Po-9

Hydroxyapatite OH-Channels for Proton Transferring Aimed to Surface Charging

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HAP is one of the most widely used materials in contemporary nanobiomedicine and nanotechnology. The interaction between HAP based biomaterials and living cells is improved, if the HAP surface is charged electrically [1]. The charge is inducible on HAP structures by the proton transport along the OH chains in columnar channels. These chains are formed by OH ions along c-axis and are surrounded by calcium triangles.

The results of computing simulation and studying of hydroxyapatite (HAP) properties and its hydrogen bonds and proton transfer peculiarities, surface and polarization properties [1] are presented. The reported data presents as *ab initio* quantum-chemical calculations (with Gaussian98 code, HF, 6-31G(d),), as well semi-empirical (PM3) and DFT by HyperChem 8.0, which clarify the double-well asymmetric potential energy profile and were held to investigate the energy barriers for proton transport along the columnar channel. The calculated values of barriers can explain long storage of polarization charge, which is observed in experiments, as electrets effect. A possibility to transfer proton via the barrier is supported due to the experiment. High pressure of hydrogen and followed electromagnetic stimulation induced transfer of the proton. In fact, the electron work function was altered for different kind of ceramics.

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