

International conference

Functional Inorganic Materials



FIM 2022

Abstract book



VILNIUS UNIVERSITY PRESS



Vilnius
University



CENTER
FOR PHYSICAL SCIENCES
AND TECHNOLOGY



kaunas
university of
technology



Lithuanian
Chemical
Society



CONFERENCE PROGRAMME

5th of October. Arrival day.

17:00–20:00 Participant meeting at Vilnius Airport.

6th of October

Vilnius University seminar room 239, Universiteto St. 3 (live or online).

Time	Presenter	Institution	Title of the Lecture
8:00–9:00	Participant registration		
9:00–9:10	Welcome speech from the vice rector of Vilnius University Prof. (HP) Dr. Edita Sužiedelienė		
9:10–9:20	Welcome speech from Prof. Habil. Dr. Jūras Banys , the president of the Lithuanian Academy of Sciences		
9:20–9:30	Information from the chairman of the organizational committee Prof. Habil. Dr. Aivaras Kareiva		
Oral session (Chairperson Prof. Dr. Simas Šakirzanovas)			
9:30–10:00	Invited Speaker Prof. Dr. Pierre Rabu	University of Strasbourg, <i>France</i>	Insertion-Grafting to Exfoliation in Layered Functional Systems
10:00–10:30	Invited Speaker Prof. Dr. Aleksej Žarkov	Vilnius University, <i>Lithuania</i>	Phase Transformations in Calcium Phosphates
10:30–11:00	Invited Speaker Dr. Simonas Ramanavičius	Center for Physical Sciences and Technology, <i>Lithuania</i>	Formation and Applications of Nonstoichiometric Titanium Oxides and MXenes (Ti ₃ C ₂ T _x) Nanostructures
11:00–11:30	Coffee break		
11:30–12:00	Invited Speaker Prof. Dr. Koichiro Hayashi	Kyushu University, <i>Japan</i>	Carbonate Apatite Honeycomb Scaffolds for Bone Regeneration
12:00–12:30	Invited Speaker Prof. Dr. Artūras Katelnikovas	Vilnius University, <i>Lithuania</i>	Inorganic CsPbX ₃ (X = Cl, Br, I) Perovskite Quantum Dots: Synthesis, Properties, and Applications
12:30–14:00	Lunch break		
Oral session (Chairperson Prof. (HP) Dr. Aldona Beganskienė)			
14:00–14:30	Invited Speaker Prof. Dr. Vytautas Getautis	Kaunas University of Technology, <i>Lithuania</i>	Advanced Organic Molecules for New Generation Solar Cells
14:30–15:00	Invited Speakers Prof. Habil. Dr. Wojciech	Nicolaus Copernicus	The Properties of Polymeric and Ceramic Membranes in Gas and Liquid Separation

Phase Transformations in Calcium Phosphates

A. Zarkov^{1,*}, D. Griestiute¹, A. Kizalaite¹, E. Raudonyte-Svirbutaviciene¹,
V. Klimavicius², A. Kareiva¹

¹ Institute of Chemistry, Vilnius University, Naugarduko 24, LT-03225 Vilnius,
Lithuania

² Institute of Chemical Physics, Vilnius University, Sauletekio 3, LT-10257, Vilnius,
Lithuania

*Corresponding author, e-mail: aleksej.zarkov@chf.vu.lt

Calcium phosphates (CPs) are a family of materials widely used in biomedical applications and especially bone regeneration due to their structural and compositional similarity to natural bone [1]. The compositional and structural variety of CPs leads to their different physicochemical, mechanical and biological properties, which allows the application of these materials in medicine in various forms from cements to ceramics and coatings [2].

While some CPs can be prepared directly by precipitation from aqueous solution, some phases can only be obtained by employing thermal treatment. Conventionally, for thermally induced synthesis, Ca and P salts are thoroughly mixed and annealed at an appropriate temperature. This approach is commonly applied for the preparation of CP phases such as calcium hydroxyapatite (HA, $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$), tricalcium phosphate (TCP, $\text{Ca}_3(\text{PO}_4)_2$) or calcium pyrophosphate (CPP, $\text{Ca}_2\text{P}_2\text{O}_7$). It should be underlined that the Ca/P ratio in starting materials and final products is expected to be identical and precursors are used in strictly stoichiometric ratios. It is generally assumed that only the structural components such as H^+ , OH^- , H_2O , and CO_3^{2-} are removed during annealing in the form of volatile species.

Another way to obtain some CPs considers the thermal conversion of less stable phases. For instance, calcium-deficient hydroxyapatite (Ca/P ratio 1.5:1) is commonly used for the preparation of β -TCP. Thermal treatment at higher temperature allows the α -TCP polymorph to be synthesized as well. Depending on the annealing temperature, amorphous CP (Ca/P ratio 1.5:1) can be converted to both TCP polymorphs, moreover, it is a suitable precursor for the preparation of low-temperature metastable α -TCP. Additionally, phase transformations in CPs can occur in aqueous medium, where the presence of other ions and medium pH are the most important factors. Overall, the phase transformations in CPs highly depend on the origin of starting material, the presence of impurities and processing conditions.

Acknowledgements

This research was funded by a grant WHITCERAM (No. S-LJB-22-1) from the Research Council of Lithuania.

References

1. W. Habraken, P. Habibovic, M. Epple and M. Böhner, *Mater. Today*, **19** (2016) 69–87.
2. S. V. Dorozhkin and M. Epple, *Angew. Chem., Int. Ed.*, **41** (2002) 3130–3146.