# *Lecture series and promotion of scientific cooperation on x-ray diffractometry and Rietveld method applications*

| Monday 11th of February | Tuesday 12th of February | Wednesday 13th of February | Thursday 14th of February | Friday 15th of February |
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| *Riga Technical University, Rudolfs Cimdins Riga Biomaterials Innovation and development Centre Pulka str. 3/3, Riga* | *University of Latvia, Faculty of Chemistry* <br><br> *Kr. Valdemāra street 48, Riga* | *University of Latvia, Faculty of Chemistry* <br><br> *Kr. Valdemāra street 48, Riga* | *Riga Technical University, Faculty of Materials Science and Applied Chemistry Āzenes street 14/24, Riga* | *University of Latvia, Faculty of Chemistry* <br><br> *Kr. Valdemāra street 48, Riga* |
| 9:00 Introduction of the project | 8:45 – 9:15 Installation of the software | 9:15 – 12:00 Practical work – Bruker D8 | 9:15 – 12:00 Practical work - PANalytical X'Pert PRO | 9:00 – 10:15 XRD analysis of thin solid films |
| 9:15 – 10:00 Introduction to XRD <br> ✓ Introduction <br> ✓ X-rays: Generation, Spectrum <br> ✓ Diffraction at crystal lattices <br> ✓ Basics of Powder diffraction | 9:15 – 10:00 Rietveld Refinement <br> ✓ Rietveld refinement: Principle <br> ✓ Modelling the Peak profile <br> ✓ Software overview, FPA vs. Classic approach <br> ✓ Example refinement | ✓ Practical work at the diffractometers: Sample preparation, data collection <br> ✓ Practical work: phase identification with PDF database <br> ✓ Practical work at the computer: data processing with BGMN | ✓ Practical work at the diffractometers: Sample preparation, data collection <br> ✓ Practical work: phase identification with PDF database <br> ✓ Practical work at the computer: data processing with BGMN | 10:15 – 10:30 Discussions |
| 10:00 – 10:15 Break | 10:00 – 10:15 Break | 10:30 – 10:45 Break | 10:30 – 10:45 Break | 10:30 – 10:45 Break |
| 10:15 – 11:00 Powder XRD <br> ✓ Powder diffractometer <br> ✓ Configurations (Detector types, DivSlits, Monochromators) <br> ✓ Peak profile <br> ✓ Phase identification <br> ✓ Databases (PDF, COD, AmMin) | 10:15 – 11:00 Introduction to BGMN <br> ✓ Introduction <br> ✓ Installation, Program structure <br> ✓ Structure files <br> ✓ Examples | List of samples: <br> 1) Hydroxyapatite and $\alpha$-tricalcium phosphate <br> 2) Polymorphic forms of organic substances <br> 3) Cocrystals and their forming substances | List of samples: <br> 1) Hydroxyapatite and $\beta$-tricalcium phosphate <br> 2) Silver doped Hydroxyapatite | 10:45 – 12:00 Measurement of residual stresses by XRD methods and discussions |
| 11:00 – 11:15 Coffee break | 11:00 – 11:15 Coffee break | | | |
| 11:15 – 12:00 Application and problems <br> ✓ Sample preparation <br> ✓ Graininess, ideal grain size <br> ✓ Micro-Absorption <br> ✓ Texture <br> ✓ Amorphous content <br> ✓ Crystallite size | 11:15 – 12:00 "HowTo" Session <br> ✓ Normal phase quantification <br> ✓ Textured sample <br> ✓ Anisotropic crystallite size <br> ✓ Non-existent phases <br> ✓ Micro-absorption | | | |
| Installation of the software <br> (**please bring your computers with you**) | | | | |

*The number of places available is limited, please register first by sending e-mail to*
*Arita.dubnika@rtu.lv*
*Agris.berzins@lu.lv (for LU students, researchers)*