# Summer school on aqueous systems in theory and practice through workshops on MD simulations and/or food chemistry

### Location: Faculty of Chemistry and Chemical Technology, Ljubljana, Slovenia

#### Date: 04. 07. 2022 – 15. 07. 2022

	Monday, July 4	Tuesday, July 5	Wednesday, July 6	Thursday, July 7	Friday, July 8	Saturday, July 9	Sunday, July 10
Morning	Monday, July 4 10:00 - 11:20 prof. Janez Cerar University of Ljubljana Lecture Room 3 Presentation of the Summer School, CEEPUS network, UL FKKT 11:20 - 11:40 Coffee break 11:40 - 13:00	Tuesday, July 5 10:00 - 11:20 prof. Larisa Zoranić University of Split Lecture Room 3 Introduction to molecular dynamics 11:20 - 11:40 Coffee break 11:40 - 13:00	Wednesday, July 6 10:00 - 11:20 prof. Arbenita Hasani University of Pristina Lecture Room 3 Water treatment and quality requirements for drinking water 11:20 - 11:40 Coffee break 11:40 - 13:00	Thursday, July 7 10:00 - 11:20 prof. Zoltán Kovács MATE Budapest Lecture Room 3 Introduction to near- infrared spectroscopy (On-Line Lecture) 11:20 - 11:40 Coffee break 11:40 - 13:00	Friday, July 8 10:00 - 11:20 prof. Tomaž Urbič University of Ljubljana Comp. Classroom 3100 Use of QM software Zimere Musliji Lect. Room 3 (9:00→ Analyses of DNA 11:20 - 11:40 Coffee break 11:40 - 13:00	Saturday, July 9 10:00 - 11:20 prof. Davor Kovačević University of Zagreb Lecture Room 3 Polyelectrolyte complexation in solution and at the surface 11:20 - 11:40 Coffee break 11:40 - 13:00	
	Dominika Slabajna University of Ljubljana Lecture Room 3 Safety in laboratories	Larisa Zoranić Lecture Room 3 Introduction to molecular dynamics	Arbenita Hasani Lecture Room 3 Water treatment and quality requirements for drinking water	Zoltán Kovács Lecture Room 3 Introduction to near- infrared spectroscopy (On-Line Lecture)	Tomaž Urbič Comp. Classroom 3100 Use of QM software Zimere Musliji Analysis of extracted DNA Lab 32 $\rightarrow$ 12:00) Visit to UL BF (12 $\rightarrow$ 13:30)	Davor Kovačević Lecture Room 3 Polyelectrolyte complexation in solution and at the surface	F
	13:00 - 14:30 Lunch + ind. discussions 14:30 - 15:50 prof. Jaroslav Katona University of Novi Sad	13:00 - 14:30 Lunch + ind. discussions 14:30 - 15:50 Peter Ogrin University of Ljubljana	13:00 - 14:30 Lunch + ind. discussions 14:30 - 15:50 Peter Ogrin lab. exercises in MD	13:00 - 14:30 Lunch + ind. discussions 14:30 - 15:50 Larisa Zoranić Comp. Classroom 3100	13:00 - 14:30 Lunch + ind. discussions 14:30 - 17:30 Contact persons CEEPUS meeting	13:00 - 14:30 Lunch + ind. discussions 14:30 – 15:50 Comp. Classroom 3100 lab. exercises in MD	E
Afternoon	Lecture Room 3 Introduction to rheology of aqueous systems	Comp. Classroom 3100 lab. exercises in MD simulations Jaroslav Katona Laboratory 32 Applications of rheology in Food Science	simulations CC 3100 Zimere Musliji MSc Mother Teresa University Skopje Lecture Room 3 Molecular techniques in food technology	Proteins in water - exercise for molecular dynamics beginners Arbenita Hasani Lecture Room 3 Emerging trends and technologies in Food processing	<b>15:30 – 17:30</b> <b>Students</b> Guided tour to Ljubljana	simulations Zoltán Kovács Lecture Room 3 NIR spectroscopy (food science applications) (On-Line Workshop)	E
	15:50 – 16:10 Coffee break 16:10 - 17.30 Jaroslav Katona Lecture Room 3 Introduction to rheology of aqueous systems	15:50 – 16:10 Coffee break 16:10 - 17.30 Peter Ogrin lab, exercises in MD simulations CC 3100 Jaroslav Katona Applications of rheology in Food Science Lab 32	15:50 – 16:10 Coffee break 16:10 - 17.30 Peter Ogrin lab. exercises in MD simulations CC 3100 Zimere Musliji Extraction of DNA from different foods Lab 32	15:50 – 16:10 Coffee break 16:10 - 17:30 Larisa Zoranić Proteins in water- exercise CC 3100 Arbenita Hasani Lecture Room 3 Emerging trends and technologies	18:30 → Students and teachers Social evening and dinner at Union Pub in Ljubljana	15:50 – 16:10 Coffee break 16:10 - 17.30 lab. exercises in MD simulations CC 3100 Zoltán Kovács Lecture Room 3 NIR spectroscopy (food science applications) (On-Line Workshop)	

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	Monday, July 11	Tuesday, July 12	Wednesday, July 13	Thursday, July 14	Friday, July 15
Morning	10:00 - 11:20 dr. Jitka Krouská VUT Brno Lecture Room 3 Introduction to calorimetry 11:20 - 11:40 Coffee break 11:40 - 13:00 Jitka Krouská Lecture Room 3 Introduction to calorimetry	10:00 - 11:20 prof. Jan Jirsák University of Usti nad Labem Lecture Room 3 Liquids in strong electric fields - an MD perspective 11:20 - 11:40 Coffee break 11:40 - 13:00 Jan Jirsák Lecture Room 3 Liquids in strong electric fields - an MD perspective	10:00 -11:40prof. Dominik HegerMasaryk Univ. BrnoLecture Room 3Theoretical background of opticalspectroscopies11:40 - 12:00Coffee break12:00 -13:30Dominik HegerLecture Room 3Theoretical background of opticalspectroscopies	9:00 departure of bus for Žalec 10:00 arrival to Žalec - visit to Slovenian Institute of Hop Research and Brewing - visit to Eco-Museum of Hop- Growing and Brewing Industry in Slovenia - visit to Beer Fountain	10:00 - 11:20   Janez Cerar (moderator)   Lecture Room 3   Presentation of student reports   + discussions   11:20 - 11:40   Coffee break   11:40 - 13:00   Janez Cerar (moderator)   Lecture Room 3   Presentation of student reports   + discussions
	13:00 -14:00 Lunch + individual discussions 14:00 - 15:50 Peter Ogrin Computer Classroom 3100 lab. exercises in MD simulations Jitka Krouská Laboratory 32 Laboratory exercises: practical experiments in calorimetry	13:00 -14:30 Lunch + individual discussions14:30 -15:50 Peter Ogrin Computer Classroom 3100 preparation of student reportsJanez Cerar Lecture Room 3 preparation of student reports	13:30 - 14:30 Lunch + individual discussions 14:30 - 15:50 Jan Jirsák Computer Classroom 3100 tutorials in MD simulations of liquids in electric fields Lecture Room 3 + Laboratory 32 Dominik Heger, Janez Cerar Laboratory exercises in optical spectroscopies	13:00 - 14:30   Lunch (town of Žalec)   14:30   departure of bus for Celje Old   Castle (celjski Stari grad)   approx. at 14:50   arrival to Celje Old Castle   visit to Celje Old Castle   life in 15 <sup>th</sup> century (weapons, scriptorium, rooms, instruments	13:00-14:30 Lunch + individual discussions 14:30 - 15:50 Lecture Room 3 Closing of the Summer School + issuing Certificates of Attendance
Afternoon	15:50 – 16:10 Coffee break 16:10 - 17:30 Peter Ogrin Computer Classroom 3100 lab. exercises in MD simulations Jitka Krouská Laboratory 32 Laboratory exercises: practical experiments in calorimetry	15:50 – 16:10 Coffee break 16:10 - 17:30 Janez Cerar Lecture Room 3 Water, electrolytes, polyelectrolytes	15:50 – 16:10 Coffee break 16:10 - 17:30 Jan Jirsák Computer Classroom 3100 tutorials in MD simulations of liquids in electric fields Lecture Room 3 + Laboratory 32 Dominik Heger, Janez Cerar Laboratory exercises in optical spectroscopies	of torture) <b>17:30</b> departure of bus from Celje Old Castle for Ljubljana <b>18:30</b> arrival to Ljubljana	