

The IX International Summer School

“Modern Quantum Chemistry Methods in Applications”

Samara, Russia, 26.06.2023 – 26.07.2023

Session Program (Samara time, GMT+4)

June 26 th	
14⁰⁰-16⁰⁰ Samara University, Media Center, 204	Introductory lecture on using open-source software for molecular visualization and Gaussian 09 with supercomputer ‘Sergey Korolev’ Denis P. Porfiriev (Samara University, <i>Lebedev Physical Institute, Samara, Russia</i>)
17⁰⁰-19⁰⁰	“Introductory lecture on quantum chemistry calculations”, <i>Leading researcher of the field, videolecture</i>
June 27 th	
10⁰⁰-11⁰⁰ SB LPI Novo-Sadovaya, 221	<i>Lecture “To boldly look where no one has looked before: identifying primary photoproducts of acetylacetone”,</i> Ivan O. Antonov (<i>Lebedev Physical Institute, Samara, Russia, Sandia National Laboratories</i>)
13⁰⁰-16⁰⁰ Samara University	Training Session – individual assignments
June 28 th	
10⁰⁰-12⁰⁰ Samara University	Training Session
13⁰⁰-17⁰⁰ Samara University	Training Session
June 29 th	
10⁰⁰-12⁰⁰ Samara University	Training Session
13⁰⁰-17⁰⁰ Samara University	Training Session
June 30 th	
10⁰⁰-12⁰⁰ Samara University, Scient. build., 407	Open seminar of theoretical group <i>Speakers: A. Nikolaev (An unconventional way to form naphthalene in the reaction of the phenylethynyl radical with ethylene), V. Krasnoukhov</i>
13⁰⁰-17⁰⁰ Samara University	Training Session

July 3rd	
10⁰⁰-11⁰⁰ SB LPI Novo-Sadovaya, 221	Lecture "Modern Predictive Quantum Chemical Calculations for Thermochemistry and Kinetics: Procedures and Limitations", Vitaly G. Kiselev (<i>V.V. Voevodsky Institute of Chemical Kinetics and Combustion of the Siberian Branch of the RAS, Novosibirsk, Russia</i>)
11⁰⁰-13⁰⁰ SB LPI	Training Session
14⁰⁰-17⁰⁰ SB LPI	Training Session
July 4th	
10⁰⁰-12⁰⁰ SB LPI	Online Training Session
13⁰⁰-17⁰⁰	Online Training Session
July 5th	
10⁰⁰-12⁰⁰	Online Training Session
13⁰⁰-17⁰⁰	Online Training Session
July 6th	
10⁰⁰-11⁰⁰ Online	Lecture "Atomic data needed for stellar spectroscopic analyses" (Online) Ludmila I. Mashonkina (<i>INASAN, Moscow, Russia</i>)
11⁰⁰-13⁰⁰ Samara University	Training Session
14⁰⁰-17⁰⁰ Samara University	Training Session
July 7th	
10⁰⁰-12⁰⁰ Samara University Scient. build., 407	Open seminar of theoretical group <i>Speakers: M. Evseev "Theoretical study of the reaction of ethane radical with carbon monoxide", A. Astashova</i>
13⁰⁰-17⁰⁰	Online Training Session
July 10th	
10⁰⁰-11⁰⁰ Samara University, Media Center	Lecture "Modern Photoionization Tools to Explore the Formation of Complex Organics in Interstellar Ices", Ralf I. Kaiser (<i>University of Hawaii at Manoa, Honolulu, USA</i>)
11⁰⁰-13⁰⁰ Samara University	Training Session
13⁰⁰-17⁰⁰ Samara University	Training Session
July 11th	
10⁰⁰-12⁰⁰ Samara University	Training Session

13⁰⁰-17⁰⁰ Samara University	Training Session
July 12th	
10⁰⁰-12⁰⁰ Samara University	Training Session
13⁰⁰-17⁰⁰ Samara University	Training Session
July 13th	
10⁰⁰-12⁰⁰ Samara University	Training Session
13⁰⁰-17⁰⁰ Samara University	Training Session
July 14th	
10⁰⁰-12⁰⁰ Samara University Scient. build., 407	Open seminar of theoretical group <i>Speakers: O. Kuznetsov "Experimental study of the naphthalene formation reaction by the HACA mechanism", A. Pershin "Quantum chemical calculations in MOLPRO for atomic and molecular spectroscopy"</i>
13⁰⁰-17⁰⁰ Samara University	Training Session
July 17th	
10⁰⁰-12⁰⁰ Samara University	Training Session
14⁰⁰-17⁰⁰ Samara University	Training Session
July 18th	
10⁰⁰-12⁰ Samara University ⁰	Training Session
13⁰⁰-15⁰⁰ Samara University	Training Session
July 19th	
10⁰⁰-11⁰⁰ SB LPI Novo-Sadovaya, 221 Online translation	Lecture "Quantum chemistry as a tool of physicochemical research" (online) Nina P. Gritsan (V.V. Voevodsky Institute of Chemical Kinetics and Combustion of the Siberian Branch of the RAS, Novosibirsk, Russia)
13⁰⁰-17⁰⁰ Samara University	Training Session

July 20th	
10⁰⁰-12⁰⁰ Samara University	Training Session
13⁰⁰-17⁰⁰ Samara University	Training Session
July 21th	
10⁰⁰-12⁰⁰ Samara University Scient. build., 407	Open seminar of theoretical group <i>Speakers: P. Pivovarov, A. Nikolaev "The formation of the simplest methyl-substituted aromatic hydrocarbons via reactions involving the 1-propynyl radical"</i>
13⁰⁰-17⁰⁰ Samara University	Training Session
July 24th	
10⁰⁰-12⁰⁰ SB LPI Novo-Sadovaya, 221	Open seminar of theoretical group <i>Speakers: E. Batrakova "Numerical simulation of various types of radio frequency quadrupole ion traps", S. Tuchin "Optical pumping of rotational levels of the cao+ ground state at the 2[^]2p-x[^]2p transition by a broadband laser", D. Trufanov "Numerical simulation of a time-of-flight mass spectrometer with an ion mirror"</i>
13⁰⁰-17⁰⁰ Samara University	Training Session
July 25th	
10⁰⁰-11⁰⁰ Samara University, Media Center Online translation	<i>Lecture "Mechanisms of growth of large PAHs, hydrocarbon nanostructures and fullerenes"</i> Alexander M. Mebel (Florida International University, Miami, Florida, USA)
11⁰⁰-13⁰⁰ Samara University	Training Session
14⁰⁰-17⁰⁰ Samara University	Training Session
July 26th	
10⁰⁰-12⁰⁰ Samara University	Training Session
CLOSING OF THE SCHOOL	