



Science&Progress 2021

Section I

Tuesday 9 Nov, moderator V.I. Chizhik
11:30-13:15

11:30-11:45	Vladimir Bazaykin	Diffusion of Toluol and Water in composopzite systeme: Poly-m-Phenyleneisophthalamide and MOF By Molecular Dynamics Simulations
11:45-12:00	Valerii Karpov	Kinetic Quantum Chemical Investigation of the GPx1 Catalytic Cycle using Crystal-based Model System
12:00-12:15	Milosh Ubovich	Orientation and Translational Mobility in Proton Ionic Liquid Propilammonium Nitrate
12:15-12:30	Alexander Selivanov	Diffusion Coefficients of Ionic Liquid [BMIM][SCN] Calculated by Molecular Dynamic Method
12:30-12:45	Darya Shvalyuk	DFT Study of Electronic Structure and Water Induced Phase Transition in the K ₂ La ₂ Ti ₃ O ₁₀ Photocatalyst
12:45-13:00	Milosh Ubovich	Molecular Mobility in Mixtures of Ethylammonium and Aluminum Nitrates. A Molecular Dynamics Simulation Study
13:00-13:15	Olga Kokh	Investigation of the molecular mobility of the ionic liquid BmpyrrNTF ₂ by NMR methods