Konferencja Użytkowników Komputerów Dużej Mocy - KUKDM 2023

Thursday, 20 April 2023

Session 2 (11:15 - 13:00)

time	[id] title	presenter
11:15	[11] Ab Initio Molecular Dynamics Studies of Hydrogen Bonding and IR Spectra in EMIM-TFSI/H2O Systems	WRÓBEL, Piotr
11:30	[12] Vibrational Spectra from Molecular Dynamics: Seeking for an Efficient Computational Method	EILMES, Andrzej
11:45	[13] Computational Modeling of Intermolecular Interactions in Supramolecular Crystals: Towards Automated Explorations of Chemical Spaces	NIEDZIELSKI, Grzegorz
12:00	[14] Molecular Modeling of Cisplatin Derivatives: the Relationship Between Structure and Potential Bioactivity	ŁACH, Wojciech
12:15	[15] Solvent Molecules Impact on the Nylon 6 Thermal Degradation Process: the Ab Initio Molecular Dynamics and DFT Study	DIDOVETS, Yuliia
12:30	[16] Molecular Modeling of Selected Perovskites with Possible Application in Photovoltaics	MIKŁAS, Alicja
12:45	[17] Computational Studies on Structural and Photophysical Properties of a 2,4-Dihydroxyphenyl-Substituted 1,3,4-Thiadiazole	KACZMARCZYK, Dominika