



# Konferencja Użytkowników Komputerów Dużej Mocy - KUKDM 2024

## Thursday, 14 March 2024

### S2 - Contributed session (11:20 - 13:20)

time	[id] title	presenter
11:20	[6] Theoretical Studies of the Propylene Oxide Opening Reaction Mechanism in the Copolymerization of CO <sub>2</sub> with Epoxides Process Catalyzed by a Cobalt(III) Complex with Salen Ligand: Unraveling the Computational Complexity	ŻUROWSKA, Olga
11:35	[7] A Study of the Properties of Unsymmetrically Substituted 4,5-dialkoxy-2-nitroanilines by Spectroscopic and Theoretical Methods	SYNOWIEC, Karina
11:50	[8] Investigating the Mechanical Characteristics of Al <sub>2</sub> O <sub>3</sub> through Density Functional Theory and Molecular Dynamics	FATHALIAN, Mostafa
12:05	[10] Multi-scale Modeling of Texture Evolution in Deformed Metals	SUŁKOWSKI, Bartosz
12:20	[11] Studies on the Interaction of Nanoplastics with Lipid Systems	WŁODEK, Franciszek
12:35	[12] Theoretical Study of Copper Complexes in Artificial Photosynthesis	MIKŁAS, Alicja
12:50	[13] Hydrolysis as an Alternative Path of Nylon 6 and PHB Degradation: a Computational Study	DIDOVETS, Yuliia
13:05	[14] A Detail that Matters? Rotational Isomerism in Some Ortho-substituted Benzophenones	KAŁKA, Andrzej J.