Conference Program

Tuesday, August 28, 2018	
18:00-21:00	**Registration**
18:30-20:30	**Dinner**
Wednesday, August 29, 2018	
08:00 - 09:00	**Registration**
09:00	**Opening Session**
09:15-11:15	**(S1) Session. Invited talks (*chaired by Anne-Marie Kelterer*)**
09:15	**Hong-Ming Lin** *"Bimetallic Electrocatalysts for Direct Liquid Formic Acid Fuel Cells"*
09:45	**Yi Hu** *"Formation of Silver Oxide Particles by Electrochemical Deposition"*
10:15	**Jacob Kongsted** *"Excited States in Complex Systems through Polarizable (Density) Embedding"*
10:45	**Poul Erik Hansen "***From Monomers to "Polymers". A Theoretical NMR Study Involving Charged Alkylpyrroles*"
11:15-11:45	**Coffee break**
11:45 – 13:15	**(S2) Session. Lectures (*chaired by Michal Jaszuński*)**
11:45	**Frank Jensen** *"Method Calibration or Data Fitting?"*
12:15	**Karol Jackowski** *"Influence of Paramagnetic Oxygen on Nuclear Magnetic Shielding of Small Molecules Studied by NMR Spectroscopy in the Gas Phase"*
12:45	**Tapas Kar "***Can Doping and Charge Modulation Make Boron-Nitrogen Nnano-Materials an Attractive Adsorbent for Toxic Gases?"*
13:15 – 14:30	**Lunch**
14:30 – 16:00	**(S3) Session. Lectures (*chaired by Hong-Ming Lin*)**
14:30	**Zbigniew Najzarek** *"Mechanochemical processes in fluidized bed mills"*
14:45	**Company presentation – Linegal Chemicals**
15:00	**Halina Szatyłowicz** *"Physical Interpretation of the Substituent Effect – the Quantum Chemistry Approach*"
15:30	**Szczepan Roszak** *"Metal Organic Frameworks - NewMaterials, New Chemistry"*
16:00 – 16:30	**Coffee break**
16:30 – 17:30	**Session. Lectures (*chaired by Tapas Kar*)**
16:30	**Jacek Korchowiec "***Modeling Monolayer Films at Air-Water Interface"*
17:00	**Anne-Marie Kelterer** *„Water-Mediated Reaction of Phenol Antioxidant with Peroxyl Radicals"*
17:15	**Teobald Kupka** *"Relativistic, Electron Correlation and Basis Set*

	Effects in the Calculation of Se Chemical Shifts"
19:00 – 20:30	**Dinner**
Thursday, August 30, 2018	
09:00 – 11:00	**(S5) Session. Lectures *(chaired by Frank Jensen)***
09:00	**Ioannis P. Gerothanassis** "*NMR in Natural Products: Chemical Analysis, Monitoring of Dynamic Changes, "in-cell" NMR and DFT Calculated Structures Based on NMR Chemical Shifts in Solution*"
09:30	**Michał Jaszuński** „*Nuclear Magnetic Dipole Moment from NMR Experiments: ^{209}Bi"*
10:00	**Peter Tolstoy** *"Outer Electronic Shell Visualization by NMR Chemical Shift Laplacian of a Helium Probe"*
10:30	**Kenneth Ruud** *"Phosphorescence and Triplet Lasing in Organic and Organometallic Systems"*
11:00 -11:30	**Coffee break**
11.30 - 13.00	**(S6) Session. Young scientists session *(chaired by Dawid Siodłak).***
11:30	**Marzena Szczepańska** „*Theoretical Investigation on Oxygen Rreaction with Palladium Porphyrin"*
11:45	**Nina Strasser** *"Hydrogen Bonding in the System 3-Aminopropanol-Water"*
12:00	**Kamini Mishra** *"Synthesis of Cyclohexanohemicucurbit[10-12]urils"*
12:15	**Anna Jezuita** *"Substituent Effect on the Electronic Structure of Meta- and Para-Substituted Nitrobenzene Derivatives"*
12:30 - 14:00	**Lunch**
14:00 - 15:15	**(S7) Session. Lectures *(chaired by Małgorzata Broda)***
14:00	**Jakub Kaminsky** "*Vibrational Optical Activity and Saccharides"*
14:30	**Robert Zaleśny** *"Partitioning of Interaction-induced Nonlinear Optical Properties of Molecular Complexes"*
14:45	**Tadeusz Pluta** *"Ground And Excited State Molecular Polarizability"*
15:00	**Joachim Włodarz** **„***Jupyter: God of Human-Centric Scientific Computing*
15:15	**Zofia Drzazga** *"UV-Vis Spectroscopy of Blood Serum in Efficiency Evaluation of Athletes in Normobaric Hypoxia"*
15:30 – 15:45	**Coffee break**
15:45 – 17:00	**(S8) Poster session:** **Jury of young scientist contest:** **Poul Erik Hansen, Małgorzata Biczysko, Peter Tolstoy** **P1.** Grzegorz Skrzyński and Tadeusz Pluta *„Dynamic polarizability of the Weakly Interacting Ar_2 Dimer"* **P2.** Nina Szczotka, Borys Ośmiałowski, Robert Zaleśny "*Two-Photon Absorption of Fluorescent Difluoroborates: in Silico Studies"* **P3.** Petrina Romana, Khomiyak Semen, Krvavych Anna, Konechna

Roksolana, Hamada Vira, Lupiy Khrystyna, Ilkiv Bohdan-Volodymyr, Novikov Volodymyr *"Biotechnology of Callus Biomass of Plants as an Alternative Method for the Production of Plant Raw Material"*

P4. Fedorova Olena, Petrina Romana, Zayarnyuk Natalia, Kurka Mariya, Mylyanych Andriy, Novikov Volodymyr *„Obtaining of a Combined Therapeutic Cosmetic Based on the Secret of the Snail and Biomass Panax Ginseng"*

P5. Christian Hebenstreit, Aneta Buczek, Małgorzata Broda, Anne-Marie Kelterer *"Interactions of 5-Fluorouracil with Water and beta-Cyclodextrin"*

P6. Bartłomiej Dec, Robert Bogdanowicz, Krzysztof Pyrchla, Mateusz Ficek, Michał Sobasze *"DFT Studies of Electrical Properties of Doped Diamond Films: Surface Termination Influence"*

P7. Małgorzata Leszczyńska, Krzysztof Ejsmont *"Substituent Effects in Heterocycling Fluorene Derivatives Substituted by Fulvene and Heptafulvene Systems"*

P8. Katarzyna Gajda, Karolina Jasiak, Agnieszka Kudelko, Błażej Dziuk, Bartosz Zarychta, Krzysztof Ejsmont *„Crystal, Molecular and Electronic Structures of N'-(2-hetarylmethylidene)-3-(3-pyridyl)acrylohydrazides"*

P9. Łukasz Gajda, Teobald Kupka, Aneta Buczek, Małgorzata A. Broda, Leszek Stobiński "*Vibrational and Electronic Spectra of Phthalocyanine-graphen Oxide Associates"*

P10. Andrzej Kałamarz, Zbigniew Najzarek, Teobald Kupka, Szymon Mycer *"From Egg Shell to Mechanochemical Preparation of Calcium Phosphates and Biomaterials"*

P11. Wioleta Edyta Śmiszek-Lindert, Elżbieta Chełmecka *"Spectroscopic and DFT Studies on Crystalline 3,4',5-Trihydroxystilbene – Plant Antibiotic"*

P12. Łukasz Kołodziej, Małgorzata Broda, Joanna Nackiewicz *„UV-VIS Spectra of Selected Phthalocyanines. Experimental and DFT Study"*

P13. Monika Staś, Dawid Siodłak, Małgorzata Broda *„Naturally Occurring Amino Acid Residues with Heterocyclic Rings"*

P14. Stadnytska Nataliya, Nakonachna Anna, Karpenko Olena, Shvets Volodymyr, Novikov Volodymyr, Lubenets Vira *„Influence of Tiosulphoesters and Compositions with Biosurfactants on the Efficiency of Tomato and Cereal Plants"*

P15. Stadnytska Nataliya, Diakon Iryna, Novikov Volodymyr *„New Metods of Fighting with Staphylococcus Aureus B Evcaliptus Viminalis and Cetraria Islandica"*

P16. Elwira Bisz, Michal Szostak „*Cyclic Ureas as Efficient, Sustainable Ligands in Iron-Catalyzed Cross-Coupling of Aryl Chlorides and Tosylates"*

P17. Yang Yi, Bożena Adrjan, Jun Li, Karol Jackowski, Szczepan Roszak **"***Chemical Shifts and Shielding Constants of Daidzein and Puerarin Using NMR Measurements and DFT Studies"*

P18. Aleksandra Piontek, Michal Szostak *"Iron-Catalyzed C(sp^2)–*

	C(sp^3) Cross-Coupling of Alkyl Grignard Reagents with Polyaromatic Hydrocarbons" **P19.** Luboš Plamitzer, Miroslav Hájek, Jakub Kaminský, Petr Pachl, Kamil Parkan, Marcela Pávová, Radek Pohl *"Enzymatically Stable Galectin Inhibitors"*
17:00 – 18:30	**Local art exhibition and show**
19:00 – 20:30	**Dinner**
Friday, August 31, 2018	
09:00 – 11:00	**(S9) Session. Invited talks (*chaired by Ioannis Gerothanassis*)**
09:00	**Małgorzata Biczysko** *"Computational Spectroscopy: from Astrochemistry to Biomolecules"*
09:30	**Andrzej Eilmes** *"Insight into Interactions in Condensed Phase from Vibrational Spectra Simulated via Ab Initio Molecular Dynamics"*
10:00	**Riina Aav** *„Templated Formation of Cyclohexanehemi-cucurbiturils"*
10:30	**Tatiana Korona** *„Exploring Point Defects in Hexagonal Boron-Nitrogen Monolayers"*
11:00 – 11:30	**Coffee break**
11.30 – 12.30	**Panel discussions and awards for young scientist**
12.30 – 12.45	**Conference end**
13.00 – 14.30	**Lunch**