ICMS Conference 2024 Program



22 September Sunday from 12.00 Registration 11.00-13.30 Wrocław-Wojanów Bus Transfer 13.30-15.00 Lunch **Opening Ceremony** 15.00-15.10 Session I: Interactions and Calculations Chair: Rui Fausto 15.10-15.40 1-1 Vibrational fingerprints of weak interactions from fully anharmonic Małgorzata Biczysko computations: success and challenges **Ehud Pines** 15.40-16.00 0-1 Structure of protonated water clusters in acetonitrile 16.00-16.20 Justinas Conformations of valeric acid in noble gas and pH2 matrices 0-2 Ceponkus Coffee 16.20-16.50 Session II: Matrix Isolation Chair: Małgorzata Biczysko 16.50-17.20 **Rui Fausto** Tunneling-driven and vibrationally-induced chemistries: Last news from **I-2**

identification of new isocyanate complexes

Matrix isolation spectroscopy of fluorine compounds

UV-induced photodecomposition of matrix isolated salicylhydroxamic acid:

Coimbra!

Barbecue

Magdalena

Sałdyka

Robert Medel

17.20-17.40

17.40-18.00

19.00-22.00

0-3

0-4

23 September Mond			
Session III: Bioapplications I			Chair: H. Michael Heise
9.00–9.30	I-3	Halina Abramczyk	A new modality for cancer tracking – Raman imaging, fluorescence and AFM studies combined with AI analysis
9.30–9.50	O-5	Himanshu Ojha	Molecular spectroscopic studies of silylated graphene oxide interaction with model proteins bovine serum albumin and pepsin
9.50–10.10	O-6	Joanna Nowak- Karnowska	Oligonucleotide probe with 5-fluoro-4-thiouridine for photocrosslinking with DNA target and binding to streptavidin support
10.10–10.30	0-7	Aleksandra Wesełucha- Birczyńska	Multi-wavelength Raman studies of bactericidal coatings applied to fibrous substrates
10.30–10.50			Coffee
Session IV: Bioapplications II			Chair: Halina Abramczyk
10.50–11.20	I-4	H. Michael Heise	ATR-FTIR spectroscopy of cells from a human monocyte cell line with stimulation by insulin – opportunities for a cellular-based insulin bioactivity assay
11.20–11.40	O-8	Dominika Święch	Comprehensive characterization of modified metallic surfaces for biomedical applications

11.40–12.00	O-9	Aleksandra Kurek	Analysis of red blood cells from individuals with allergy symptoms using Raman spectroscopy
12.00–12.20	O-10	Sylwester Mazurek	Diagnosing different types of arthritis using vibrational spectroscopy
12.20–12.40	O-11	Jakub Dybas	Interaction of endothelium-derived NO with red blood cells – tracking of hemoglobin adducts with resonance Raman spectroscopy
12.40–13.40			Lunch
Session V: Earth Science and Cultural Heritage Chair: A			ral Heritage Chair: Aleksandra Wajda
13.40–14.10	I-5	Rosa C. Ponterio	A step forward the sustainability: design and applications of flexible and low cost Surface Enhanced Raman Spectroscopy (SERS) sensors from waste cellulose
14.10–14.30	O-12	Maja Mroczkowska- Szerszeń	Application of statistical clustering methods in IR spectral discrimination of fossil resins of various provenance
14.30–14.50	O-13	Magdalena Gawęda	Amorphous silicon oxycarbide-based protective coatings for nuclear applications – spectroscopic and microstructural studies
14.50–15.05	O-14	Agnieszka Sozańska	Simultaneous in situ Raman and SEM imaging
15.15–19.15			Excursion: Sky Walk — Trail in the Clouds — Świeradów Zdrój
19.30–20.30			Dinner

24 September			Tuesday
Session VI: Optical Materials			Chair: Ivan Němec
9.00–9.30	I-6	Jan Zaręba	Monitoring structural phase transitions in hybrid compounds using nonlinear optical responses
9.30–9.50	O-15	Magdalena Leśniak	Structural study of the laser-induced crystalization in tellurite-phosphate glass
9.50–10.10	O-16	Robert Tomala	Preparation and luminescent properties of phosphors for high CRI white LED
10.10–10.30	O-17	Dominika Gruszkowska	Spectroscopic properties of cocomplexes of europium with phenanthroline family and diketone based ligands
10.30–10.50	O-18	Piotr Żemojtel	Tuning of the spectroscopic properties of semiconductor nanorings by size
10.50–11.20			Coffee
Session VII: Materials			Chair: Jan Zaręba
11.20–11.50	I-7	Ivan Němec	Spectroscopic, structural and optical characterization of molecular crystals based on heteroaromatic carries of NLO properties
11.50–12.10	O-19	Mirosław Mączka	Vibrational properties and mechanism of phase transitions in lead iodide perovskites comprising OH(CH ₂) _n NH ₃ ⁺ cations (n=2,3)
12.10–12.30	O-20	Kinga Suchorab	Oxidation kinetics of zirconium and its alloys – impact of stabilisation factors on the zirconium oxide polymorphs
12.30–12.50	O-21	Mallika Pathak	Magnetic <i>tagetes erecta</i> biochar (γ-Fe ₂ O ₃ -TEB) for efficient removal of cationic dye from wastewater: A sustainable and economical approach
12.50–13.10	O-22	Ewa Pięta	The role of adaptogens in cervical cancer therapy: High-definition vibrational spectroscopic imaging at the single-cell level
13.10–14.30			Lunch

Session VIII: Methods			Chair: Rosa C. Ponterio
14.30–15.00	I-8	Aleksandra Wajda	Vibrational Optical Activity – a unique tool for studying supramolecular systems
15.00–15.20	O-23	Łukasz Pięta	A novel approach for highly sensitive Raman spectroscopy – PIERS
15.20–15.40	O-24	Anna Kołodziej	The 2D correlation spectroscopy (2D-COS) study of polycaprolactone-hydroxyapatite composites bioactivity
15.40–16.00	O-25	Vitalii Boiko	Determination of structural transformation in transparent $\rm Y_3Al_5O_{12}$ ceramics in the process of chromium recharging
16.00–16.20	O-26	Karolina Haupa	FTIR spectrometers are like cars. Learn how to select the best for you (Bruker)
16.20–18.30			Coffee
16.30–18.30			Poster Session
19.30–20.30			Conference Dinner

ISSSMC Conference 2024 Program



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24 Septem	24 September ISSSMC Online Tuesda			
Session on	line I: M	lolecules & Molec	ular Interactions	Chair: Andrii Kadashchuk
10.00–10.25	IGP-1	Mykhailo Bondar	Linear photophysics, fast vibronic relaxation absorption properties of new coumarin der	-
10.25–10.50	IGP-2	Vytautas Klimavicius	Solid-state NMR of phosphate based function	ional materials
10.50–11.05	OGP-1	Olena Gnatyuk	Vibrational and imaging markers of circulating Lewis lung carcinoma cell line	metastatic cells based on the
11.05–11.30			Coffee Break	
Session on	line II: L	iquid Crystals & I	New Materials	Chair: Taras Mykytiuk
11.30–11.55	IGP-3	Longin N. Lisetskii	Induced and spontaneous nanostructuring systems for display and sensor application	
11.55–12.20	IGP-4	A. Demchenko	Molecular machines powered by electronic	excitation
12.20–12.35	OGP-2	E. Manuilov	Effect of tin and tin-carbon dopants on physical photocatalytic behavior of TiO ₂ in hydrogen pr	·
12.35–14.30			Lunch Break	
Session online III: Biological System			s	Chair: Nataliia Bashmakova
14.30–14.55	IGP-5	S. Yefimova	ROS-regulating nanomaterials	
14.55–15.20	IGP-6	G. Rudko	Luminophores for luminescent solar conce	entrators
15.20–15.35	OGP-3	L. Brizhik	Soliton mediated long-range electron transpor systems	t in donor—alpha-helix-acceptor
15.35–15.50	OGP-4	Valeriia Ovdenko	Nonlinear optical properties of azo-naphthols theoretical and experimental study	with a pyridine nitrogen atom:
15.50–16.05	OGP-5	Grygorii Monastyrskyi	WS ₂ and MoS ₂ 2D nanoparticles as inducers formation and spectroscopic properties	of changes in liposome

25 Septem	ber		Wednesday
Session IX: ISSSMC – New materials & Nanosystems Chair: Svitlana Bugaychuk			
8.30–8.55	IGP-7	Marek Drozd	Phases transition phenomena in highly sensitive luminescence nanothermometry
8.55–9.20	IGP-8	Alexander Krivchikov	Heat capacity of molecular crystals with different types of disorder
9.20–9.45	IGP-9	Andrii Kadashchuk	Triplet-triplet annihilation mechanism of intrinsic charge-carrier generation in neat organic semiconductors
9.45–10.10	IGP-10	Galina Dovbeshko	War-derived air pollution based on carbon-containing smoke nanoparticles with Fe and Cu metal compounds: physical chemical property, and neurotoxicity risk assessment
10.10–10.25	OGP-6	Yuriy Hizhnyi	Luminescence mechanisms in oxide glass-ceramic composites: insights from electronic structure calculations
10.25–10.40			Coffee
Session X:	ISSSMC	C – Methods & Ap	oplications Chair: Alexander Krivchikov
10.40–11.05	IGP-11	Svitlana Bugaychuk	Optical dielectric spectroscopy associated with plasmonic resonance in LC nanocomposites with gold nanoparticles
11.05–11.30	IGP-12	Taras Mykytiuk	Making 10nm nano-holes for trapping light by mixing monolayers of gold and silver nanoparticles
11.30–11.45	OGP-7	Nataliia Bashmakova	Spectral properties of two pyrrolopyridine derivatives synthesized from citric acid and urea
11.45–12.00	OGP-8	Mariia Kyrpa	Electronic structure and UV-Vis spectroscopy of mesoionic compounds
12.00–12.15	OGP-9	Vlada Pashynska	Noncovalent complexes of dimethyl sulfoxide with anti-cancer thioderivatives of purine nucleobases: model mass spectrometry and quantum chemical study on molecular mechanisms of transmembrane drug delivery facilitation
12.15–12.30			Closing Ceremony and Awards
12.30–13.30			Lunch
13.45–15.45			Wojanów-Wrocław Bus Transfer

ISSSMC-2024 Poster Session will be held online. The poster presentations will be available at https://isssmc.org.ua on September 22-25, 2024. Over those days, you will be able to look though the PDF presentations and submit your written questions to the authors by email; the authors will be asked to check it periodically and respond to your questions.