## **ICMS Conference 2024 Program**



XVII International Conference on Molecular Spectroscopy

Monday

Chair: Halina Abramczyk

22-25.09.2024 Wojanów, Poland

22 Septeml	ber		Sunday
from 12.00 11.00–13.30			Registration Wrocław–Wojanów Bus Transfer
13.30–15.00			Lunch
15.00–15.10			Opening Ceremony
Session I: II	nteracti	ions and Calculat	ions Chair: Rui Fausto
15.10–15.40	I-1	Małgorzata Biczysko	Vibrational fingerprints of weak interactions from fully anharmonic computations: success and challenges
15.40–16.00	O-1	Ehud Pines	Structure of protonated water clusters in acetonitrile
16.00–16.20	0-2	Justinas Ceponkus	Conformations of valeric acid in noble gas and pH2 matrices
16.20–16.50			Coffee
Session II: Matrix Isolation		solation	Chair: Małgorzata Biczysko
16.50–17.20	I-2	Rui Fausto	Tunneling-driven and vibrationally-induced chemistries: Last news from Coimbra!
17.20–17.40	O-3	Magdalena Sałdyka	UV-induced photodecomposition of matrix isolated salicylhydroxamic acid: identification of new isocyanate complexes
17.40–18.00	O-4	Robert Medel	Matrix isolation spectroscopy of fluorine compounds
19.00–22.00			Barbecue

## 23 September

I-3

O-5

O-6

0-7

Session IV: Bioapplications II

9.00-9.30

9.30-9.50

9.50-10.10

10.10-10.30

10.30-10.50

Session III: Bioapplications I Chair: H. Michael Heise Halina A new modality for cancer tracking – Raman imaging, fluorescence and Abramczyk AFM studies combined with AI analysis Molecular spectroscopic studies of silylated graphene oxide interaction with Himanshu Ojha model proteins bovine serum albumin and pepsin Joanna Nowak-Oligonucleotide probe with 5-fluoro-4-thiouridine for photocrosslinking with Karnowska DNA target and binding to streptavidin support Aleksandra Multi-wavelength Raman studies of bactericidal coatings applied to fibrous substrates Wesełucha-Birczyńska Coffee

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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	0-11	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:	Session V: Earth Science and Cultural 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 ( <i>remote</i> )		
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 ( <i>Renishaw</i> )		
15.15–19.15			Jelenia Góra Tour		
19.30–20.30			Dinner		

Tuesday

## 24 September

Session VI:	Optica	l 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	Dobromiła 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		ials	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 ( $\gamma$ -Fe <sub>2</sub> O <sub>3</sub> -TEB) for efficient removal of cationic dye from wastewater: A sustainable and economical approach	
12.50–13.10	0-22	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: Maciej Sitarz			
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 $Y_3Al_5O_{12}$ 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 ( <i>Bruker</i> )
16.20–18.30			Coffee
16.30–18.30			Poster Session
19.30–20.30			Conference Dinner

## ISSSMC Conference 2024 Program



Galvna Puchkovska International School-Seminar Spectroscopy of Molecules and Crystals

24 Septem	24 September ISSSMC Online Tuesday				
Session online I: Molecules & Molecula			ular Interactions	Chair: Andriy Kadashchuk	
10.00–10.25	IGP-1	Mykhailo Bondar	Linear photophysics, fast vibronic relaxat absorption properties of new coumarin de		
10.25–10.50	IGP-2	Vytautas Klimavicius	Solid-state NMR of phosphate based functional materials		
10.50–11.05	OGP-1	Olena Gnatyuk	Vibrational and imaging markers of circulating metastatic cells based on the Lewis lung carcinoma cell line		
11.05–11.30			Coffee Break		
Session online II: Liquid Crystals & N			New Materials	Chair: Nataliia Bashmakova	
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 physicochemical properties and photocatalytic behavior of $\text{TiO}_2$ in hydrogen production reaction		
12.35–14.30			Lunch Break		
Session on	line III: I	Biological System	15	Chair: Taras Mykytiuk	
14.30–14.55	IGP-5	S. Yefimova	ROS-regulating nanomaterials		
14.55–15.20	IGP-6	G. Rudko	Luminophores for luminescent solar concentrators		
15.20–15.35	OGP-3	L. Brizhik	Soliton mediated long-range electron transport in donor—alpha-helix-acceptor systems		
15.35–15.50	OGP-4	Valeriia Ovdenko	Nonlinear optical properties of azo-naphthols with a pyridine nitrogen atom: theoretical and experimental study		
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 September Wednesday				
Session IX	: ISSSMO	C – New materials	s & Nanosystems	Chair: Svitlana Bugaychuk
8.30–8.55	IGP-7	Marek Drozd	Phases transition phenomena in highly sensi nanothermometry	tive luminescence
8.55–9.20	IGP-8	Alexander Krivchikov	Heat capacity of molecular crystals with diffe	rent types of disorder
9.20–9.45	IGP-9	Andriy Kadashchuk	Triplet-triplet annihilation mechanism of intri- generation in neat organic semiconductors	nsic charge-carrier
9.45–10.10	IGP-10	Galina Dovbeshko	War-derived air pollution based on carbon-connanoparticles with Fe and Cu metal compour property, and neurotoxicity risk assessment	
10.10–10.25	OGP-6	Yuriy Hizhnyi	Luminescence mechanisms in oxide glass-cerar electronic structure calculations	nic composites: insights from
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 w LC nanocomposites with gold nanoparticles	ith plasmonic resonance in
11.05–11.30	IGP-12	Taras Mykytiuk	Making 10nm nano-holes for trapping light b and silver nanoparticles	y mixing monolayers of gold
11.30–11.45	OGP-7	Nataliia Bashmakova	Spectral properties of two pyrrolopyridine derivation acid and urea	tives synthesized from citric
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 wi of purine nucleobases: model mass spectrometr study on molecular mechanisms of transmembra	y and quantum chemical
12.15–12.30			Closing Ceremony and Awards	
12.30–13.30			Lunch	
13.45–15.45			Wojanów–Wrocław Bus Transfer	