

54th Heyrovský Discussion

**MOLECULAR
PHOTO-SPECTRO-ELECTROCHEMISTRY
MECHANISMS
AND ELECTROSYNTHESIS**



Castle Třešť (Czech Republic)

June 18-22, 2023

PROGRAMME

Sunday, June 18

- 10:00 Registration in **the entrance hall of the J. Heyrovský Institute**, refreshment, possibility to leave the luggage and walk in the town
- 15:00 Departure of a special bus from the J. Heyrovský Institute (Dolejškova 3, Prague 8 – Kobylisy)
- 17:30 Arrival, registration at the Castle Třešť
- 18:30 Welcome aperitif
- 19:00 Dinner

Monday, June 19 – morning

from
7:00 Breakfast

8:30

Opening of the 54th Heyrovský Discussion

Martin Hof, director of the J. Heyrovský Institute

Magdalena Hromadová, past-chair
of the ISE-Division 6 Molecular Electrochemistry

Douglas Grotjahn Commemoration of prof. Diane Smith

Technical notes

Chairman Jiří Ludvík

Topic: **General**

<i>Time</i>	<i>Chairman</i>	<i>Speaker</i>		<i>Title of presentation</i>
9:00	Flavio Maran	Kevin Moeller	US	From Molecules to Molecular Surfaces and Back Again. Exploiting the Synergy Between Electrochemistry and Synthesis <i>(Introductory lecture)</i>
to 10:00		Daniel Morales-Martinez	IT	Electrophotocatalysis: mechanistic insights into the electrochemical reduction of 9,10-dicyanoanthracene

10:00 Coffee break

<i>Time</i>	<i>Chairman</i>	<i>Speaker</i>		<i>Title of presentation</i>
10:30 to 12:15	Neso Sojic	Federico Polo	IT	ECL of Metal Complexes and Bifunctional Organic Dyes: Features, Applications, Pros and Cons <i>(Introductory lecture)</i>
		Guobao Xu	Ch	Single-electrode electrochemiluminescence
		Ludmila Šimková	CZ	(Spectro) Electrochemical Study of Phenyl- substituted Cibalackrot Derivatives – Potential Candidates for Singlet Fission
		Karol Lušpai	SK	Redox Behavior and Anion Radicals of Phenyl- substituted cibalackrot derivatives
12:30	Lunch			
Monday, June 19 – afternoon				
<i>Time</i>	<i>Chairman</i>	<i>Speaker</i>		<i>Title of presentation</i>
14:30 to 16:00	Douglas Grotjahn	Daniel Little	US	“Dual Behavior of a Redox Mediator. Oxidation or reduction depending upon the input energy source – electrochemical or photochemical” <i>(Introductory lecture)</i>
		Philippe Lainé	FR	Artificial Photosynthesis & Inversion of Redox Potentials
		Magdaléna Hromadová	CZ	Role of the Potential Inversion in the Reduction of 4,4'-Oligomethylenebipyridiniums. New Insights from a Combined Electrochemical, Spectro-electrochemical and Computational Studies
16:00	Coffee break			
Topic: Spectroelectrochemistry				
<i>Time</i>	<i>Chairman</i>	<i>Speaker</i>		<i>Title of presentation</i>
16:30 to 18:00	Peter Rapta	František Hartl	UK	Time-resolved infra-red spectroelectrochemistry: Recent achievements <i>(Introductory lecture)</i>
		Martin Pižl	CZ	Redox behaviour of Ru(II) polypyridyl biosensors: An experimental and theoretical study
		Romana Sokolová	CZ	Application of UV-Vis and IR spectroelectrochemistry in determination of redox mechanism
		Matěj Stočes	CZ	Metrohm: More than electrochemistry - novel possibilities for new discoveries
18:30	Concert (in the courtyard of the castle) Apollon Quartet			
19:30	Dinner			
21:00	Open fire sausage party in the park			

Tuesday, June 20 – morning			
from 7:00		Breakfast	
Topic: General			
<i>Time</i>	<i>Chairman</i>	<i>Speaker</i>	<i>Title of presentation</i>
8:30 to 10:00	Marie- Noëlle Collomb	Rainer Winter	GE A Personal Perspective on Mixed-Valent Compounds With Non-Identical Redox Sites: From Delocalization to Valence Tautomerism <i>(Introductory lecture)</i>
		Lars Vogelsang	GE Ferrocenyl-TATs – Platforms to probe the modification of a molecular switch
		Karolína Salvadori	CZ Nitro Group as Potential Switch and Probe in Urea-Based Receptors
10:00 Coffee break			
<i>Time</i>	<i>Chairman</i>	<i>Speaker</i>	<i>Title of presentation</i>
10:30 to 12:00	Jeanet Conradie	Peter Rapta	SK Redox mechanism of biologically active Cu(II) complexes studied by EPR, UV–vis–NIR spectroscopy and spectroelectrochemistry <i>(Introductory lecture)</i>
		Lucie Koláčná	CZ Electrochemical Study of Cu(II) Complexes of azamacrocyclic derivatives
		Tomáš Mikysek	CZ Electrochemical Study on Biomimetic Copper (II) Complexes
12:00 Lunch			
13:15 Departure of the bus for the trip:			
14:15 Gothic castle Lipnice			
16:30 historic town Havlíčkův Brod - Church tower and bells			
17:30 Traditional brewery "REBEL" (Havlíčkův Brod) - excursion and degustation			
19:30 Dinner in the brewery restaurant			
22:30 Expected arrival to the castle			

Wednesday, June 21 – morning				
from 7:00 Breakfast				
<i>Time</i>	<i>Chairman</i>	<i>Speaker</i>		<i>Title of presentation</i>
8:30 to 10:00	František Hartl	Marie-Noëlle Collomb	FR	Photo-induced redox catalysis for hydrogen production with molecular compounds: track intermediates by spectro-electrochemistry and transient absorption spectroscopy <i>(Introductory lecture)</i>
		Alice Barbero	IT	Electrochemical Reduction of CO ₂ with Organometallic Catalysts
		Aude Salamé	FR	Spectroelectrochemical evidences of Fe-CO intermediates in the CO ₂ catalytic reduction by Fe porphyrins
10:00 Coffee break				
<i>Time</i>	<i>Chairman</i>	<i>Speaker</i>		<i>Title of presentation</i>
10:30 to 12:15	Daniel Little	Douglas Grotjahn	US	Aspects of Molecular Electrocatalysis of Water Oxidation <i>(Introductory lecture)</i>
		Miguel Ibanez	US	Further studies on the effects of electron-donating and -withdrawing groups on water oxidation catalysts with phenanthroline sulfonate and terpyridine ligands on ruthenium
		Alexander Hildebrandt	GE	From electronic communication within bimetallic compounds to polymeric charge storage materials
		Anja Rehse	GE	Valence Tautomerism in (η^6 -Arene)chromium Triarylmethylidium Dyads
12:30 Lunch				
Wednesday, June 21 – afternoon				
Topic: New systems				
<i>Time</i>	<i>Chairman</i>	<i>Speaker</i>		<i>Title of presentation</i>
14:30 to 16:00	Kevin Moeller	Flavio Maran	IT	Thiolate Protected Gold Nanoclusters and the Hydrogen/Deuterium Puzzle <i>(Introductory lecture)</i>
		Mattia Reato	IT	Connecting Atomically Precise Nanoclusters
		Luka Pochkhua	US	Proton-coupled Electron Transfer in a Ring Hydrogen-bond System
16:00 Coffee break				

<i>Time</i>	<i>Chairman</i>	<i>Speaker</i>		<i>Title of presentation</i>
16:30 to 18:15	Olivier Buriez	James Becker	Isr	Anodic Oxidation of Cyclic OrganoSi Compounds <i>(Introductory lecture)</i>
		Hayati Celik	TR	Electroanalytical Investigation and Determination of Apixaban
		Alan Liška	CZ	Electrochemical investigation of the 14th group acyl compounds
		Alan Liška	CZ	PHREEQC plus: speciation modelling in your pocket
18:30	Walk around Třešť			
20:00	Farewell dinner			

Thursday, June 22 – morning

from

7:00 Breakfast

8:30 – 9:00 Please, leave the rooms – check out – put luggage in checkroom

<i>Time</i>	<i>Chairman</i>	<i>Speaker</i>		<i>Title of presentation</i>
9:00 to 10:30	Irena Hoskov- cová	Jeanet Conradie	SA	Ruthenium(II) complexes containing substituted 2,2':6',2"-terpyridines: is it possible to predict accurate redox potentials with density functional theory methods? <i>(Introductory lecture)</i>
		Rachel Staley	US	Degradation Mechanism of a Manganese Catalyst Electrocatalyst and Reporting of a Class of Pyridinium-Based Electrocatalysts
		Milan Sýs	CZ	The Electrochemical Oxidation of 17 β -Estradiol in Aqueous Organic Solvent Mixtures Gives Rise to Quinoid Derivatives, Known as Significant Breast Cancer Initiators
10:30	Coffee break			
Topic: New methodologies				
<i>Time</i>	<i>Chairman</i>	<i>Speaker</i>		<i>Title of presentation</i>
11:00 to 11:50	Rainer Winter	Olivier Buriez	FR	Development of Original Methodologies Combining Electrochemistry and Luminescence to Investigate Molecular Fluxes Through Phospholipid Membranes <i>(Introductory lecture)</i>
		Neso Sojic	FR	Ultrasensitive electrochemiluminescence microscopy of single biological entities: from cells to biomolecules

11:50	Closing remarks
12:00	Lunch
13:00	Departure to Prague
16:00	expected arrival at the Václav Havel Airport Prague
<p>38 oral presentations and 8 posters</p> <p>POSTERS SHOULD BE ON DURING THE WHOLE MEETING IN THE FOYER OF THE CONFERENCE HALL (No special poster session will be organized, discussion may proceed during coffee-breaks and after sessions)</p>	
POSTERS	
Soňa Boháčová CZ	Electrochemical and Mechanistic Study of Photoredox <i>N</i> -Arylation of Pyrazoles Catalyzed by New Acridinium-Derived Catalysts
Colton Breyer US	Methodology for the Analysis of Water Oxidation Electrocatalysts in Absence of Limiting Current
Joel Donkeng Dazie CM	Electrochemical properties of furfural and 5-hydroxymethylfurfural and their reactivity with aliphatic primary (di)amines
Viktoría Ebel GE	Redox Active Diruthenium Metallamacrocycles and their Molecular Conductances
Eliška Jiroušková CZ	Electrochemistry of stimulants 3-fluorophenmetrazine and 4-methylpentedrone
Dylan Karr US	Development of an Electrochemically-Reversible Hydride Transfer Mediator for Organic Synthesis
Jake Kerkhof US	Ruthenium water oxidation electrocatalysts with carboxylate and sulfonate groups in the active site
Alice Kulagová CZ	C ₃ N ₄ (X) electrochemical ammonia oxidation and functionalization with molecular catalysts