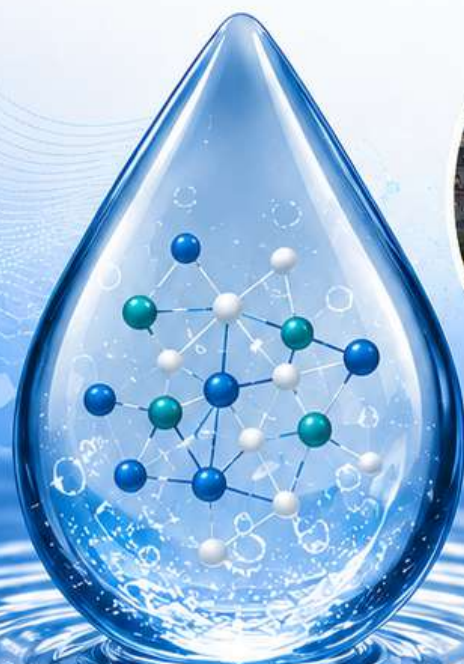


I S S P 22

22nd International Symposium on Solubility Phenomena and Related Equilibrium Processes

31 Aug – 3 Sep 2026

Sofia, Bulgaria



with satellite workshop

“Tailored Properties of
Ionic Liquid Electrolytes
for Sustainable
Energy Storage Applications”



ABSTRACT BOOK



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 *Institute of General and Inorganic Chemistry,
Bulgarian Academy of Sciences*

 *Burgas State University “Prof. Dr. Assen Zlatarov”, Bulgaria*

22nd International Symposium on Solubility Phenomena and Related Equilibrium Processes

with

satellite workshop “Tailored Properties of Ionic Liquid Electrolytes for Sustainable Energy Storage Applications”



Endorsed by IUPAC



31 Aug - 03 Sep 2026, Sofia, Bulgaria

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PROGRAM

30.08.2026, Sunday

10:00 – 16:00

Annual Meeting of the IUPAC Subcommittee on Solubility and Equilibrium Data

31.08.2026, Monday

8:30 – 17:00	Registration
Opening session Chairperson: Prof. Radostina Stoyanova	
9:00 – 9:45	Opening Ceremony
9:45 – 10:00	IUPAC Representative Clara Magalhaes
10:00 - 10:45	PL1 Michael Steiger Crystallization in confinement: Solubility issues in the conservation of cultural heritage
10:45 - 11:15	Coffee break
Session 1: Solubility Phenomena - theories, experimental and analytics Chairperson: Prof. Clara Magalhaes	
11:15 - 11:30	OP1 Clemente Bretti R.A.L.S. Santos, C. Bretti, M.C.F. Magalhães, C.M.P.G. Amorim, D. Milea and D.C. G.A. Pinto, Study on the coordination of N-hydroxyamides with iron(II) and iron(III)
11:30 - 11:45	OP2 Nese Cevirim-Papaioannou N. Cevirim-Papaioannou, P. Q. Fürst, F. E. Furcas, K. Dardenne, T. Prüßmann, J. Rothe, M. Altmaier, X. Gaona, Stability and solubility of Fe(II)-CO ₃ phases
11:45 - 12:00	OP3 Ivayla Pantcheva I. Pantcheva, Solution behaviour of Ni(II) mixed-ligand complexes containing polyether ionophore and glycine
12:00 - 12:15	OP4 Andrija Vukov A. Vukov, B. Šarac, D. Goste, S. Papović, T.T. Borović, S. Belić, S. Gadžurić, M. Vraneš, Micellization behavior of newly synthesized surfactant nicotine-based ionic liquids
12:15 - 14:00	Lunch time
Session 2: Solubility Phenomena - theories, experimental and analytics Chairperson: Prof. Silvana Mattedi	
14:00 - 14:15	OP5 Yordan Georgiev Y. Georgiev, M. Olech, M. Yaneva, V. Smilkova, H. Yemendziev, M. Yordanova, M. Ognyanov, P. Denev, Phytochemical composition and <i>in vitro</i> inhibitory activity of herbal extracts against medically relevant enzymatic biological systems

14:15 - 14:30	OP6 Glenn Hefter G. Hefter, J. Hungerb, R. Buchner, Dielectric Spectroscopy and the 'Wicked' Problem of Electrolyte Solubilities
14:30 - 14:45	OP7 Paul Fürst P. Q. Fürst, N. Cevirim-Papaioannou, X. Gaona, S. Hagemann, M. Altmaier, H. Geckeis, Solubility, Speciation, and Thermodynamic Modeling of Fe(II) in Repository-Relevant Systems from Near Neutral to Hyperalkaline Conditions
14:45 - 15:00	OP8 Earle Waghorne W. Earle Waghorne, Solvent Parameters from Computational Chemistry
15:00 - 15:30	Coffee break
Session 3: Advances in Computational Modeling Chairperson: Prof. Wolfgang Voigt	
15:30 - 16:15	PL2 José Palomar J. Palomar, P. Navarro, J. Lemus, A. Belinchón ¹ , A. Pereira, S. Moreno, S. Delgado, Using computational modelling to explore thermodynamic challenges in chemical process development
16:15 - 16:30	OP9 Christian Kiefer C. Kiefer, D. Fellhauer, M. Altmaier, X. Gaona, Thermodynamic Reference Database (THEREDA): Pitzer Activity Model for Tc(IV) Solubility and Complexation in the Tc(IV)–Na ⁺ –Cl [–] –HCO ₃ [–] –CO ₃ ^{2–} –OH [–] –H ₂ O(l) System
16:30 - 16:45	OP10 Jiangping Liu J. Liu, N. Kovalenko G. Das, A. Anderko, Thermodynamic Modeling of Rare Earth Solvent Extraction
16:45 - 17:00	OP11 Miriam Guimarães M. D. Guimarães, S. F. M. Costa, D. O. Abranches, A. M. Ferreira, J. A. P. Coutinho, S. P. Pinho, O. Ferreira, M. A. R. Martins, Integrated computational and experimental screening of solvents for polylactic acid recycling
Poster Session 1 Chairperson: Prof. Diana Rabadjieva	
17:15 – 17:30	Flash Oral Presentation - P9, P16, P17, P18, P19
17:30 – 20:30	POSTER SESSION 1 / Welcome drink

01.09.2026, Tuesday

Session 4: Solubility Phenomena in Pharmaceuticals and Biological Systems Chairperson: Prof. Demetrio Milea	
9:00 - 9:45	PL3 Zahari Vinarov Z. Vinarov, The role of solubility and solubilization in pharmacy: from drug discovery to drug development
9:45 - 10:00	OP12 Tatjana Verbić T. Verbić, A. Serajuddin, A. Avdeef, M. Kuentz, Understanding Drug Salt Solubility: Mechanistic Complexities and Practical Approaches

10:00 - 10:15	OP13 Olivera Markovic O. Marković, M. Pešić, A. Avdeef, A. Serajuddin, T. Verbić, Tricyclic antidepressants solubility study: Role of Competing Counterions in Aggregation and Solid-Phase Transformations
10:15 - 10:30	OP14 Mónia Martins L. B. Corso, I. W. Cordova, I. Morais, F. Nogueira, A. C. S. Pais, S. A. O. Santos, J. A. P. Coutinho, A. Zuber, O. Ferreira, S. P. Pinho, M. A. R. Martins, Green chemistry solutions for antimalarial drug extraction and solubility enhancement
10:30 - 11:00	Coffee break
Session 5: Solubility Phenomena in Pharmaceuticals and Biological Systems Chairperson: Assoc. Prof Zahari Vinarov	
11:00 - 11:15	OP15 Silvana Mattedi R. Simões, G. Teixeira, A.C.M. Silva, A.S. Lima, S. Mattedi, Menadione's solubility in fatty acids predicted by the COSMO-SAC CS25 model
11:15 - 11:30	OP16 Viktoriya Smilkova V. Smilkova, Y. Georgiev, M. Ognyanov, A. Veli, N. Atanasova, L. Dobрева, M. Yaneva, S. Simova, S. Danova, K. Vasilev, L. Gonsalvesh, A. Petrova, Isolation, chemical characterization and modification with ferric ions of natural prebiotic herbal polysaccharides
11:30 - 11:45	OP17 Simão Pinho S. P. Pinho, P. C. Hamasaki, C. A. Piske, O. Ferreira, M. A. R. Martins, D. O. Abranches, J. A. P. Coutinho, Salt Effects on Amino Acid Solubility: Experimental, Molecular, and Data-Driven Perspectives
11:45 - 12:00	SP1 Ivayla Sopotenska, Aurubis AD, Company presentation
12:00 - 12:15	SP2 Todor Todorov, AQUACHIM, Company presentation
12:15 - 12:30	Official Conference Group Photo
12:30 - 14:00	Lunch time
14:15	Conference tour

02.09.2026, Wednesday

Session 6: Solubility Phenomena in the Environment Chairperson: Assoc. Prof. Pedro Carvalho	
9:00 - 9:45	PL4 Vera Slaveykova Vera I. Slaveykova, Inès Segovoa-Campos, Arin Kantarcyian, Rocco Gasco, Arturo A. Keller, Solubility at the Nanoscale: Environmental Fate and Impact of Engineered Nanomaterials
9:45 - 10:00	OP18 Anastasiia Kuzenkova A. Kuzenkova, T. Plakhova, A. Romanchuk, S. Kalmykov, How cation

	composition controls the structure and solubility of Pu(V) and Np(V) double carbonates
10:00 - 10:15	OP19 Antonina Kovacheva, A. Kovacheva, D. Rabadjieva, Chemical equilibrium models for calculation of metal chemical species in different type surface waters
10:15 - 10:45	Coffee break
Session 7: Solubility Phenomena in Industrial Applications Chairperson: Prof. José Palomar	
10:45 - 11:30	PL5 Wolfgang Voigt W. Voigt, Lithium recovery for batteries from primary and secondary sources
11:30 - 11:45	OP20 Bence Kutus E. Hajdú, B. Kutus, Synthesis of lithium hydroxide using barium hydroxide
11:45 - 12:00	OP21 Inês C. M. Vaz I. C. M. Vaz, M. Bastos, L. M. N. B. F. Santos, J. A. P. Coutinho, N. Schaeffer, Understanding and quantifying the thermodynamics of lanthanide extraction in hydrophobic eutectic solvents
12:00 - 12:15	OP22 Lama Mzek L. Mzek, M. Atanassova, Ligand – Diluent Interplay in the Extraction and Separation of Fe(III) ion by β -Dicarbonyl N-Heterocyclic Chelators
12:15 - 14:00	Lunch time
Session 8: Chemical synthesis of nanosized materials Chairperson: Prof. Svetlana Zheleva	
14:00 - 14:30	IL1 María Pascual L.Fernández-Rodríguez, M.Sedano, R. Sánchez, M.Álvarez, M.J.Pascual, Corrosion of borosilicate glasses in molten salts
14:30 - 15:00	IL2 Peter Petrov Ryan Bower, David Owen, Bruno Rente, Ming Fu, Thomas Smith, Arutiun P. Ehasarian, Rupert Oulton, Peter K Petrov, Nanostructured Titanium Nitride Thin Film Arrays for Photocatalytic Applications
15:00 - 15:15	OP23 Ivaylo Tankov I. Tankov, R. Yankova, S. Delibaltova, N. Todorov, R. Nikolova, Catalytic, electronic and spectroscopic properties of imidazolium hydrogen squarate
15:15 - 15:45	Coffee break
Award Session Chairperson: Prof. Slobodan Gadzuric	
15:45 - 16:05	Franzosini Prize OP24 Glenn Hefter- the recipient of the 2026 Solute, Solvents, Solutions, Solubilities & Stabilities
16:05 - 16:45	Balarew Award OP25 Bence Kutus - the recipient of the 2026 Complexation and precipitation reactions of Ca^{2+} ions in strongly alkaline media

	OP26 Monia Martins - the recipient of the 2025 Solubility without Borders OP27 Lyuben Borislavov - the recipient of the 2025 for Bulgaria Machine-learning aided metal-ion battery cyclic stability prediction
Poster Session 2 Chairperson: Prof. Albena Bachvarova-Nedelcheva	
16:45 – 17:00	Flash oral presentation - P21, P22, P28, P32, P36
17:00 - 18:30	POSTER SESSION 2
20:00 – 24:00	Conference dinner Restaurant PRINCIPI DI PIEMONTE (hall Sofia), INTERPRED building, 36 Dragan Tsankov str.

03.09.2026, Thursday

WORKSHOP

Tailored Properties of Ionic Liquid Electrolytes for Sustainable Energy Storage Applications"
IUPAC project Ref: Proposal 2025-032-1

Session 9 Chairperson: Assoc. Prof. Simão Pinho	
9:00 - 9:45	PL W1 Gero Frisch Measuring What Matters? Speciation and Chemical Behaviour of Ionic Liquids and Deep Eutectic Solvents in Energy Storage Applications.
9:45 - 10:00	OP W1 Şefik Süzer Şefik Süzer, Tapping into Electrical-Double Layer Formation in Ionic Liquid/Carbon Interfaces using DC/AC/Pulsed X-Ray Photoelectron Spectroscopy
10:00 - 10:15	OP W2 Snežana Papović S. Papović, T.T. Borović, M. Vraneš, M.E. di Pietro, A. Rossetti, A. Roganović Improving the thermal stability of lithium-ion battery electrolytes safety
10:15 - 10:45	Coffee break
Session 10 Chairperson: Prof. Earle Waghorne	
10:45 - 11:30	PL W2 Xinpei Gao Xinpei Gao, Heterogeneous Colloid Electrolytes: Ionic Liquids, Plastic Crystals, and Liquid Crystals

11:30 - 11:45	OP W3 Pedro Carvalho Beatriz F. Esteves, Rita Nunes , Bruna R. M. Ferreira, Pedro J. Carvalho, Ionic Liquid-based Composite Membranes for Efficient Greenhouse Gases Separation
11:45 – 12:00	OP W4 Slobodan Gadžurić S. Gadžurić, N. Cakó Bagány, S. Belić, T. T. Borović, M. Vraneš, S. Papović F. Dian, B. Šarac, D. Goste, A. Melchior, Tailoring the Properties of Ionic Liquids for Targeted Applications
12:00 – 12:30	Closing remarks
14:00 – 15:00	Round table - IUPAC project Ref: Proposal 2025-032-1 Working Group on Standardized Measurement and Properties of Ionic Liquid Electrolytes for Sustainable Energy Storage Applications

*Legend: PL – plenary lecture; IL – invited lecture; OP – oral presentation

POSTERS

POSTER SESSION 1

P1	<u>E. N. Tsurko</u> , D. Touraud and W. Kunz	Solubility Thermodynamics of Sodium Ferulate in Aqueous Solutions at Temperatures 276.15 - 363.15 K
P2	<u>S. Belić</u> , T. T. Borović, A. Vukov, D. Goste, B. Šarac, M. Vraneš, S. Papović, N. Cakó Bagány and S. Gadžurić	Synthesis and Physico-Chemical Characterisation of Phosphonium and Ammonium Ionic Liquids for Rare Earth Recovery from Permanent Magnets
P3	<u>N. Izhbehova</u> , Z. Vladimirova, D. Danalev, Ivan Iliev, Rositza Hristova and V. Karadjova	Antitumoral activity of novel Cu(II)–peptide complexes
P4	<u>Tian-Lan ZHANG</u>	Understanding solubility product (K _{sp}) from the perspective of pseudo-equilibrium
P5	<u>J. Sohr</u> , H. C. Moog, M. Altmaier, F. Bok, V. Brendler, D. Freyer, X. Gaona, S. Hagemann, G.-D. Miron, M. Pannach, W. Voigt and L. Wissmeier	THEREDA - Thermodynamic reference database
P6	<u>Chr. Tzvetkova</u> , V. Georgiev, I. Karadjova, A. Stoyanova-Ivanova, L. Ivanova and A. Detcheva	Comparative Assessment of Corrosion Dynamics and Metal Ion Release from Orthodontic Archwires in Biomimetic Oral Environments
P7	<u>K. Sezanova</u> , R. Gergulova, R. Shterinska, A. Kovacheva and D. Rabadjieva	Dissolution of (Cu, Zn) Doped Calcium Phosphates in Solution with Demineralization Activity
P8	<u>R. Gergulova</u> , K. Sezanova, D. Rabadjieva, P. Shestakova	Insights into the Thermodynamics and Kinetics of Double-Doped Amorphous Calcium Phosphate Formation and Its Response in Artificial Saliva

P9	T. Biver, C. Castelli, M. Vable, G. D. G. Santonoceta, S. Muscarella, G. Barone, C. Sgarlata	Spectroscopic data treatment for the binding of small molecules to nucleic acids and proteins
P10	K. Bitchikh, N. Smakghi, A.H. Meniai	Modeling Solid–Liquid Equilibria to Predict Drug Solubility in Pharmaceutical Solvents
P11	V. Georgieva, L. Gonsalvesh, S. Mileva, D. Asamova and S. Genieva	Thermodynamic Aspects of Cd(II) Adsorption onto Vine Rod-Derived Biochar
P12	S. Stefanova, Y. Ivanova, P. Vassileva, I. Uzunov, D. Voykova, Y. Dimitrova and P. Konova	Cellulose-Based Adsorbent for Wastewater Dye Treatment
P13	A. Kovacheva, M. Nedyalkov and D. Rabadjieva	Comparative assessment of the hydrochemical characteristics of Pomorie lake (Bulgaria)
P14	M. Trayanova, A. Kovacheva, S. Kolev, A. Benderev, D. Rabadjieva	Lithium in thermal mineral waters in Southern Bulgaria
P15	V. Petkova, E. Serafimova, K. Mihaylova, S. Panova	The effect of chemical extraction reagents on the determination of plant-available forms of P ₂ O ₅ in High energy milled Phosphorite
P16	E. Encheva-Mircheva, K. Chakarova, J. Zaharieva and M. Tsvetkov	Effect of Ce-doping on the photocatalytic activity of SrTiO ₃
P17	G. Vassilev, S. Holzmann, S. Harizanova, M. Kalapsazova, U. Krewer, A. Tadjer, R. Stoyanova	In-situ monitoring of gas evolution in symmetric cells for sodium-ion batteries
P18	K. Tumbalova, S. Todorova, I. Yordanova, Z. Geshkova, S. Delibaltova, H. Kolev, T. Todorova, Y. Kalvachev, R. Velinova, P. Konova, G. Ivanov, P. Markov, D. Voykova, M. Anchina, A. Liutcanova and Anton Naydenov	Synthesis and characterization of Pd–Co modified ZSM-5 zeolite catalysts for methane oxidation-influence of Si/Al ratio
P19	S. Petrova, E. Vasileva, N. Danchova, V. Petrov, A. Bachvarova-Nedelcheva	Synthesis and characterization of NPs-modified multifunctional cotton material

POSTER SESSION 2

P20	V. Mihalkov, J. Mateeva and R. Genova-Koleva	Optimizing synthesis parameters of decorated TiO ₂ and TiO ₂ nanotubes
P21	K. Ivanova, E. Vassileva, I. Ivanova and A. Bachvarova-Nedelcheva	Synthesis, Characterization and Antimicrobial Behavior of TiO ₂ /TeO ₂ /CuO Sol–Gel Nanopowders
P22	H. Lalkovski, L. Aleksandrov and A. Bachvarova-Nedelcheva	Sol-Gel preparation of TiO ₂ /SiO ₂ /CeO ₂ nanopowders
P23	R. Kukeva, M. Kalapsazova, M. Shipochka and R. Stoyanova	EPR Evidence of Structural Degradation and Particle Size Reduction in Cycled P2- and P3-Layered Oxides

P24	<u>S. Bencheva</u> , Y. Kostova, R. Dimitrova, Z. Yordanova, A. Bachvarova-Nedelcheva	Synthesis and Characterization of Spirulina/Silica Hybrids via Sol–Gel Processing
P25	<u>S. Mileva</u> , A. Veli, R. Nikolova, H. Kolev, I. Tankov	Surface and structural features of asphaltene-based activated carbon
P26	<u>Al. Stoilova</u> , N. Penov, E. Valcheva, G. Rusev, I. Karadashka	Green Synthesis and Evaluation of Nanomaterials
P27	<u>T. Koseva</u> , S. Genieva and G. Rusev	Hydrothermal Synthesis of Novel Functional Materials Based on Rare Earth Elements
P28	<u>T. Tushev</u> , V. Koleva, J. L. Tirado, P. Lavela, S. Lavela, S. Harizanova, R. Stoyanova	TiO ₂ Dry Coating Na ₄ Fe ₃ (PO ₄) ₂ P ₂ O ₇ to Improve its Sodium Energy Storage at Different Temperatures
P29	<u>Ts. Gerasimova</u> , I. Uzunov, N. Rangelova, M. Kalapsazova and R. Stoyanova	Solubility of lignocellulosic components in phosphoric acid: approach for tuning the electrochemical performance of walnut shells-derived hard carbon
P30	<u>T. Yotova</u> , R. Yankova and A. Kostadinova	DFT Insights into the Electronic Structure and Reactivity of Potassium Hexaaquanickel (II) Diselenate
P31	<u>Y. Kyoybashieva</u> , Y. Kostova, I. Boyadzhieva, L. Kabaivanova and A. Bachvarova-Nedelcheva	Structural and Antibacterial Properties of Sol-Gel-Prepared Si–Chitosan-Ag Hybrids
P32	<u>V. Kondova</u> , D. Tsekova, G. Staneva	Self-Assembling L-Glu Derivatives to Nanosized Complexes in Solution
P33	<u>Ts. Lazarova</u> , K. Tumbalova, D. Kichukova, C. Rosmini, G. Theochari, D. Kovacheva, I. Spassova	Sonochemically prepared high-entropy spinel oxides (CoMnFeNiX ₃) ₄ , where X=Cr, Zn, Al, for methanol decomposition
P34	S. Harizanova, M. Kalapsazova, D. Jugović, M. Milović, S. Mentus, R. Stoyanova	Influence of Crystal Structure and Cu Substitution on Sodium Storage in NaFeO ₂ -based Electrodes
P35	<u>D. Ivanova</u> , N. Kaneva	Tribocatalytic degradation of antibiotics in waters with varying hardness using nanoflowers
P36	<u>M. Nedyalkov</u> , R. Nikolova, R. Kukeva, P. Tzvetkov, R. Stoyanova	Phase Transitions Inducing Changes in the Luminescent Properties of Manganese(II) Coordination Complexes
P37	<u>V. Stoeva</u> , D. Marinova, L. Borislavov, and R. Stoyanova	Li/Na competition in naphthalimide electrochemical matrix
P38	<u>S. Stanchovska</u> , M. Kalapsazova, S. Harizanova, V. Koleva, R. Stoyanova	Hydrothermal Synthesis of Sodium Titanates as High-Capacity Electrodes in Sodium-Ion Batteries



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Crystallization in confinement: Solubility issues in the conservation of cultural heritage

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Keywords: Salt damage, Cultural heritage, Porous materials, Solubility calculation

It is generally recognized that crystal growth in the porous structures of materials such as stone, brick, ceramics and concrete is a major cause of damage limiting the durability of the world's architectural heritage (Figure 1a) [1]. Crystal growth is related to phase changes in pore solutions including the crystallization of the solvent (frost damage) or of the solutes (salt damage). They are induced by variation of ambient temperature and relative humidity (Figure 1b). Unfavorable conditions of temperature and RH may result in repeated cycles of crystallization–deliquescence, hydration–dehydration and freezing–thawing, respectively. This leads to rapid decay of building materials, dramatically limiting the durability of cultural heritage objects.

There is a number of different sources of salt enrichment in old buildings which lead to a variety of crystalline salts and complex parent brines. Typically, these brines are mixtures of chlorides, nitrates, and sometimes carbonates of sodium, potassium, magnesium and calcium. A huge number of crystalline phases including single salts in different hydrated states and a number of double salts may form from these brines.

Understanding solubilities in these complex mixtures at relevant temperatures is essential to predict the behavior of salt mixtures and to define safe ranges of climatic conditions to avoid salt damage (e.g., Figure 1c). Moreover, in the confinement of small pores, solubility equilibria are also affected by pore size [2]. Finally, understanding the damage mechanism of growing crystals requires an understanding of solubility under non-hydrostatic, anisotropic stress [3]. The talk will focus on all aspects of solubilities in porous building materials including their size dependence and attempts and challenges in model predictions with the ion interaction (Pitzer) approach [4].

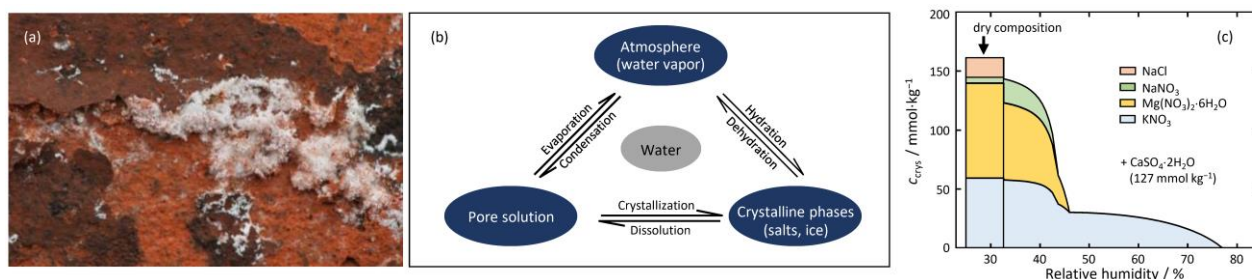


Figure 1. (a) Salt efflorescences on brick building at the North Sea coast. (b) Phase equilibria of water–salt systems in porous building materials. (c) Model predicted crystallization sequence of salt mixture in sandstone building (Bavaria).

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- [3] A. Tuluk, E. Ronde, M. Steiger, B. Lubelli, H. Meekes, E. Vlieg, *J. Cryst. Growth* **2026**, 691, 128669, <https://doi.org/10.1016/j.jcrysgro.2026.128669>
- [4] M. Steiger, *J. Chem. Eng. Data* **2025**, 70, 4856, <https://doi.org/10.1021/acs.jced.5c00166>

Using computational modelling to explore thermodynamic challenges in chemical process development

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Keywords: Molecular design, process simulation, carbon capture and utilization, ionic liquid

First stages of chemical process development can be successfully guided by computational modelling – the thermodynamics drawing the exploring dimensions – to simultaneously design i) new chemical products with enhanced properties, and ii) new chemical process with optimized key performance indicators (KPIs). In this work, some illustrative examples on how multiscale computational research strategies can contribute to the development of new efficient and cost-effective carbon capture and utilization (CCU) technologies based on ionic liquids are presented. CCU solutions involve a wide range of industrial carbon sources (postcombustion, hydrogen production, biogas upgrading, etc. or direct air capture, DAC) and added-value chemical products (chemicals, fuels, building materials, etc.). The process performance of CCU technologies is determined for several factors, highlights the CO₂ partial pressure of treated gas streams, the sorbent/catalyst material properties, the operating conditions, the process configuration and used utilities [1]. Integrated system & material & process computational design is applied to optimize the sustainability and competitiveness of innovative CCU technologies, minimizing energy/chemical requirements, process cost, and environmental impacts [2]. Additional advances through the development of digital twin prototype allow operating pilot demonstration plants, optimizing the process and accelerating technology scale-up and market implementation.

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The role of solubility and solubilization in pharmacy: from drug discovery to drug development

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Keywords: drug solubility; micellar solubilization; surfactants; bile salts; supersaturation

Drug solubility and the associated phenomena of dissolution, solubilization, supersaturation, crystallization and precipitation, is a cornerstone in pharmaceutics. These processes influence the selection of lead compounds during drug discovery and guide formulation strategy, excipient selection, and dosage-form design during drug development.

At the discovery stage, drug aqueous solubility is one of the properties which can limit selection. Drug candidates with very poor solubility in water present significant challenges in drug development, including poor or highly variable oral bioavailability, difficult parenteral administration etc. Therefore, solubility is increasingly considered together with potency, safety, permeability, metabolic stability, and other physicochemical properties when selecting compounds for further development. As a result, considerable efforts are still aimed at creating accurate models for prediction of drug solubility, including physics-based and data-driven machine learning methods.

During drug development, the focus shifts from solubility as a selection criterion to solubility as a formulation challenge. As highlighted by the Biopharmaceutics Classification System, solubility is one of the two most important factors which determine the bioavailability of oral drugs. However, most new drug candidates have very poor solubility in water, often limited by crystal-lattice stability, unfavorable solvation, or both. In some cases, this gives rise to pronounced positive food effects, where lipids and digestion products generate colloidal solubilizing phases in the gastrointestinal tract and increase the apparent solubility of the drug.

Formulation science applies the same concepts. Surfactant micelles, lipid-based systems, and other colloids may enhance apparent solubility, but their rational use requires understanding the structure–function relationships that govern solubilization, including the effects of surfactant chain length, headgroup chemistry, aggregation behavior etc. Another powerful strategy, particularly for solid-state-limited compounds, is drug amorphization. However, such systems have low storage stability, form unstable supersaturated solutions and can crystallize and precipitate after intake. Advances in the use of polymers that stabilize the amorphous solid state and inhibit crystallization or precipitation during dissolution has allowed the commercial application of this approach.

Overall, solubility provides a unifying framework for connecting drug molecular properties, formulation design and gastrointestinal behavior. Mechanistic understanding of these phenomena supports rational decisions from early drug discovery to advanced pharmaceutical development.

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Solubility at the Nanoscale: Environmental Fate and Impact of Engineered Nanomaterials

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Keywords: Silver nanoparticles, dissolution, aggregation, bioaccumulation, toxicity

Solubility is a central, but often underestimated, driver of contaminant behavior in aquatic environments, governing bioavailability, transformation, and ecological impact. For engineered nanomaterials, solubility extends beyond classical dissolution to include dynamic interconversions among dissolved ions, primary nanoparticles, transformed and aggregated particulate species.

This work examines how physicochemical speciation governs the environmental fate and impacts of engineered silver nanomaterials (nAg) in freshwater phytoplankton species. Extracellular polymeric substances (EPS), released by phytoplankton, play an important role in shaping nanoparticle “identity”. EPS adsorption enhances colloidal stability via steric repulsion while reducing Ag⁺ release, thereby simultaneously stabilizing particulate forms. Microscopic and spectroscopic analyses reveal that EPS covers nAg surfaces forming ecocorona, altering dissolution and aggregation behavior. Comparative studies of citrate- and lipoic acid-coated nAg show that EPS can either mitigate or enhance nanoparticle reactivity depending on primary coating type. While EPS generally increases colloidal stability, it reduces Ag⁺ release and toxicity for citrate-coated particles but can enhance dissolution and biological effects for lipoic-acid-coated particles.

At the organismal level, solubility-driven transformations strongly nAg influence uptake and toxicity. Studies on the freshwater diatom *Cyclotella meneghiniana* reveal that Ag uptake depends on speciation and particle size. Dissolved Ag⁺ leads to rapid accumulation, whereas nAg shows slower, sustained uptake. Metabolomic and physiological analyses further demonstrate that both Ag⁺ and nAg induce significant metabolic reprogramming, affecting amino acid metabolism, glutathione pathways, nucleotide metabolism, and energy production. Notably, nAg exerts stronger and more specific effects on central metabolic pathways, including the TCA cycle and oxidative stress responses, compared to ionic silver.

Together, these results demonstrate that at the nanoscale, particles occupy an intermediate domain between dissolved and particulate matter, where size and surface chemistry fundamentally reshape solubility-controlled processes. This framework provides new insight into the environmental behavior of engineered nanomaterials and supports more realistic risk assessment.

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Lithium recovery for batteries from primary and secondary sources

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Keywords: Lithium recovery, salt-lake brines, solubility, DLE processes, lithium hydroxide

The increasing demand for lithium compounds for battery production is well-known. A review of the various types of lithium resources available worldwide will be given. One type is mineral-based, and the other is brine-based, which requires totally different extraction and purification technologies. In recent and future times, the recycling of lithium from batteries represents a new requirement.

The battery producers need high-purity lithium hydroxide or lithium carbonate, which one depends on the battery type and the market conditions.

After a chemical and mineralogical characterization of the source types for lithium, a survey on the main recovery processes with their pros and cons for mineral-based and brine-based resources.

All processes end up with an aqueous lithium salt solution, from which all other metals (sodium, potassium, calcium, magnesium, heavy metals) and anions (chloride, sulfate, fluoride, etc.) have to be removed. The final processing step consists in the conversion of the lithium salt into hydroxide ($\text{LiOH} \cdot \text{H}_2\text{O}$) and its crystallization.

In mineral technologies, the lithium salt solution is generated through a liberation and separation of the lithium mineral from the rocks (flotation, density separation), with a subsequent pyrometallurgical treatment and a leaching step.

In the case of salt-lake brines, the concentrated lithium salt solution (5 - 10 g/L Li) is obtained after a solar pond evaporation (South America, West China) to enhance the concentration and separation by stepwise crystallization of other salts in the order of their solubility in the multicomponent system Li^+ , Na^+ , K^+ , Mg^{++} , Ca^{++} // Cl^- , SO_4^{--} , borate – H_2O . This technology is discussed critically because of the water loss in arid areas. Several of companies and institutions are offering direct liquid extraction (DLE) processes to concentrate and separate lithium from dilute brines, avoiding the evaporation process. The principles and limits of these technologies will be discussed in relation to “classical” evaporation and crystallization techniques. A perspective view on the application of advanced solar evaporation and crystallization techniques for brines will be outlined, where no water is used or lost in the separation of lithium salts. It will be shown that modern evaporation and crystallization technology, based on a knowledge of multicomponent solubility data of the respective salt mixtures, gives rise to process developments adapted to the chemistry of the lithium source, the local environmental requirements (water, wastes), and the availability of reagents. Different from the DLE processes, the company is not dependent on specialist companies for membranes or adsorbents.

Corrosion of borosilicate glasses in molten salts

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Keywords:

The objective of this work is the development of borosilicate glasses with high chemical resistance to corrosion by molten salts, particularly nitrates, for potential application as protective coatings in storage tanks used in concentrated solar power (CSP) plants. Current storage tanks are typically manufactured from stainless steel and externally insulated. The refractory insulating material lining the walls of tanks containing molten nitrate salts does not require particularly high operating temperatures, since the salts generally operate below 500 °C. However, these refractory materials usually exhibit a residual porosity of approximately 12–15%, which may facilitate the penetration of molten salts and promote corrosion processes.

To address this issue, the application of vitreous enamel coatings on the concrete walls of the tanks has been proposed. Such enamels must exhibit strong adhesion, high chemical compatibility with the substrate, and the ability to seal the surface porosity effectively. In addition, the glass enamel must provide excellent resistance to corrosion by molten nitrate salts under operating conditions.

This work includes a comprehensive review of the state of the art concerning corrosion mechanisms and degradation processes associated with molten salts, together with the development of new borosilicate glass compositions. The glass compositions were designed and thermally characterized, and their corrosion resistance was evaluated through immersion tests in molten salts at temperatures around 500 °C, including analyses of reaction kinetics and corrosion products. Wettability studies on different concrete substrates were also carried out to assess adhesion and densification behaviour, enabling the selection of the most suitable glass compositions for this application.

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Nanostructured Titanium Nitride Thin Film Arrays for Photocatalytic Applications

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Keywords: Plasmonic metasurfaces, titanium nitride, scalable fabrication, light-activated anti-bactericidal surfaces

Nanostructured titanium nitride (TiN) thin films are emerging as promising platforms for plasmon-enhanced photocatalysis, offering a robust and scalable alternative to noble metals. In this work, we present TiN thin-film arrays engineered to enhance photocatalytic performance through strong light absorption, localised surface plasmon resonances, and hot-carrier generation. Their high-aspect-ratio geometry maximises surface area and electromagnetic-field localisation, thereby promoting efficient light-driven surface reactions.

We develop a scalable fabrication approach that preserves nanoscale structural fidelity and plasmonic functionality across large areas, overcoming limitations of electron beam lithography. Optical characterisation confirms strong plasmonic response in the visible–near-infrared range, suitable for photocatalytic applications.

As an example, we demonstrate a photocatalytically enhanced metasurface exhibiting antimicrobial activity under illumination, illustrating the multifunctional potential of these nanostructured TiN systems.

This work highlights a pathway toward durable, large-area plasmonic photocatalytic surfaces for applications in environmental and biomedical technologies.

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Study on the coordination of *N*-hydroxyamides with iron(II) and iron(III)

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Keywords: siderophores; stability constants; chemical speciation; solution equilibria; sequestration

The *N*-hydroxyamides are siderophores present in nature with significant implications in agriculture and medicine [1-2]. These compounds form metal complexes, particularly with iron(III), thereby influencing the overall concentration and chemical speciation of such cations in aqueous systems. Consequently, predictive models that include *N*-hydroxyamides must account for their coordination to iron(III) in water, typically expressed through stability constants, $\log \beta$. In this study, the stability constants of two *N*-hydroxyamides, namely *N*-hydroxyacetamide and *N*-hydroxybenzamide, with both iron(III) and iron(II) were determined. Measurements were carried out by potentiometric titrations in KCl(aq) at $I = 0.15 \text{ mol dm}^{-3}$ and at $T = 298.2 \text{ K}$. Experimental potentiometric titration data were analyzed using the BSTAC computer program [3], while speciation and sequestration diagrams were obtained by the PyES software [4].

From preliminary analyses, four distinct coordination species were identified for *N*-hydroxyamides with iron(III), and two with iron(II), each characterized by specific stoichiometries and stability constants, as reported in Table 1. Altogether, these results are essential for understanding their chemical behavior and biological relevance. In this contribution, the influence of the two investigated ligands on the chemical speciation of iron(III) and iron(II) in aqueous solution is discussed in terms of both species formed and their sequestering ability.

Table 1. Stability constants of *N*-hydroxyacetamide and *N*-hydroxybenzamide with iron(III) and iron(II) in KCl(aq) at $I = 0.15 \text{ mol} \cdot \text{dm}^{-3}$ and $T = 298.2 \text{ K}$

<i>N</i> -hydroxyacetamide		<i>N</i> -hydroxybenzamide	
Species	$\log \beta^{a, b}$	Species	$\log \beta^{a, b}$
iron(III)		iron(III)	
$[\text{Fe}(\text{L})]^{2+}$	12.22 ± 0.05	$[\text{Fe}(\text{L})]^{2+}$	9.80 ± 0.10
$[\text{Fe}(\text{L})(\text{OH})]^+$	9.24 ± 0.05	$[\text{Fe}(\text{L})(\text{OH})]^+$	6.93 ± 0.09
$[\text{Fe}(\text{L})(\text{OH})]_2$	5.87 ± 0.05	$[\text{Fe}(\text{L})(\text{OH})]_2$	3.28 ± 0.05
$[\text{Fe}(\text{L})_2]^+$	22.26 ± 0.05	$[\text{Fe}(\text{L})_2]^+$	19.30 ± 0.04
iron(II)		iron(II)	
$[\text{Fe}(\text{L})]^+$	8.93 ± 0.03	$[\text{Fe}(\text{L})]^+$	8.28 ± 0.02
$[\text{Fe}(\text{L})_2]$	16.29 ± 0.07	$[\text{Fe}(\text{L})_2]$	14.40 ± 0.06

^a $\log \beta$ refer to equilibrium: $p \text{ M} + q \text{ L} + r \text{ H} = \text{M}_p\text{L}_q\text{H}_r$, charges omitted for simplicity, negative p values refer to the formation of hydroxo-species; ^b $\pm$ standard deviation.

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Stability and solubility of Fe(II)-CO₃ phases

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Keywords: Solubility and phase stability, siderite, chukanovite, anoxic iron corrosion, carbonate systems

Steel and other iron-based alloys are widely used as container materials within the context of nuclear waste disposal. In the case of groundwater intrusion into underground repositories, aqueous systems are expected to develop. In such systems, the anoxic corrosion of iron and steel components, and the consequent generation of hydrogen gas play a significant role in determining the reducing geochemical conditions that influence the mobility of radionuclides.

In reducing systems containing carbonate, the primary Fe phases expected to form under near-neutral and alkaline conditions are siderite (FeCO₃) and chukanovite (Fe₂(OH)₂CO₃), respectively. The latter is reported to be metastable in comparison to siderite, and a slow transformation to FeCO₃ is expected [1]. The presence of thick layers of chukanovite in archaeological artefacts suggests that this transformation process may take up to several thousands of years [2].

Siderite solubility was systematically investigated at 25 °C in 0.1 M NaClO₄ media, under slightly acidic to alkaline conditions (6 ≤ pH ≤ 9) and at different partial CO₂(g) pressures (pCO₂ = 0.01 and 0.05 atm) [3]. The thermodynamic data provided in this study were evaluated and selected by major databases (e.g., NEA-TDB, Thermochemie, PSI-Nagra TDB) [4,5,6].

A number of studies have focused on the influence of the concentration ratios [Fe²⁺]/[OH⁻] and [CO₃²⁻]/[OH⁻] to assess the conditions favoring the formation of chukanovite [1,2,7]. These investigations have shown that chukanovite commonly co-exists with siderite or Fe(OH)₂, depending on the pH conditions as well as the total carbonate concentration. Some studies have suggested that chukanovite can be stabilized under specific conditions. However, thermodynamic data reported in the literature are often derived from a very limited solubility dataset [7,8] and no thermodynamic data have been selected by major databases to date.

Chukanovite was successfully synthesized by mixing oxygen-free Na₂CO₃, NaOH and FeCl₂ solutions, as confirmed by XRD. All experiments were performed under Ar atmosphere at T = (22 ± 2)°C. Individual batch samples were prepared from undersaturation conditions with approximately 10 mg of chukanovite. Batch solubility experiments were conducted in 0.5 M NaCl – NaHCO₃ – Na₂CO₃ systems with C_{tot} = 0.005 – 0.1 M. Systematic solid phase characterization of samples aged under different conditions was performed using XRD. ICP-MS was used to quantify total Fe concentrations. The pH and [Fe] were monitored at regular time intervals. EXAFS measurements

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were carried out with both pure and mixed solid phases in order to gain insight on the structure as well as the solid-phase transformation. Fe K-edge X-ray absorption spectra of Fe(II) solid phases were measured at the INE-Beamline at the KIT Light Source, operated by the Institute for Nuclear Waste Disposal at KIT.

XRD measurements indicate the transformation of chukanovite to siderite or Fe(OH)₂ depending on C_{tot} and pH, even after short equilibration time. Experimental data suggest that chukanovite influences the solubility in some of the investigated systems, particularly during the early stages of equilibration. Nevertheless, the measured Fe concentrations generally agree well with siderite solubility after prolonged equilibration time. A preliminary fit based on the experimental data indicates $\log K_{s,0} \approx -10.8$ for siderite, which is in good agreement with the selected value in NEA-TDB and Thermochimie ($\log K_{s,0} = -10.68 \pm 0.21$) [4,5] and PSI-Nagra TDB ($\log K_{s,0} = -10.9$) [6]. Evaluation of the EXAFS data, as well as the derivation of thermodynamic and activity models are currently on-going and will be discussed in this contribution.

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Solution behaviour of Ni(II) mixed-ligand complexes containing polyether ionophore and glycine

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Keywords: monensin A, glycine, mixed-ligand Ni(II) complexes

The polyether ionophores (PIH), monensin (MonH) and salinomycin (SalH), are natural antibiotics that form various coordination species. In the presence of divalent metal cations, both ionophores exist as neutral bis complexes $[M(PI)_2(H_2O)_2]$ when the metal-to-ligand molar ratio varies from 1-10 to 1-2 (MeOH solutions). Circular dichroic spectral studies reveal also the possibility of the formation of positively charge mono species $[M(Mon)]^+$ with an additional amount of M(II) in solution (from 1 to 10 equivalents compared to monensinate). The coordination mode of the ionophore in the bis complexes has been unambiguously determined by single crystal X-ray diffraction, but its conformation in the mono species has not yet been elucidated.

To neutralize the charged mono species and to isolate them as a neutral compound, we chose glycine (GlyH) as a secondary ligand to obtain possibly mixed-ligand complexes $[M(PI)(Gly)]$. Ni(II) was selected as a target metal ion due to its optical activity since the spectral changes in Ni(II)-containing monensinate and/or glycinate systems can be monitored by electron spectroscopy. Briefly, we prepared $[Ni(PI)]^+$ *in situ* in methanol and added increasing amounts of glycinate (Fig. 1, left, monensin case is presented; $NiCl_2 \cdot 6H_2O$ was used as a metal source). The matrix rank analysis (MRA) of the spectral data reveals that the system is complicated and can be described by the formation of at least five optically active particles, among which are the starting mono complex $[Ni(Mon)]^+$, and mixed-ligand species $[Ni(Mon)(Gly)]$ / $[Ni(Mon)(Gly)_2]^-$. Probably some additional ligation processes take place at high excess of glycinate anions that cause the constantly increasing absorbance of the system. The behaviour of $NiCl_2 \cdot 6H_2O$ under the analogous conditions (Fig. 1, right) follows the same trend. The reason for the observed hyperchromic effect in both reaction mixtures is still unresolved and needs to be clarified in the future.

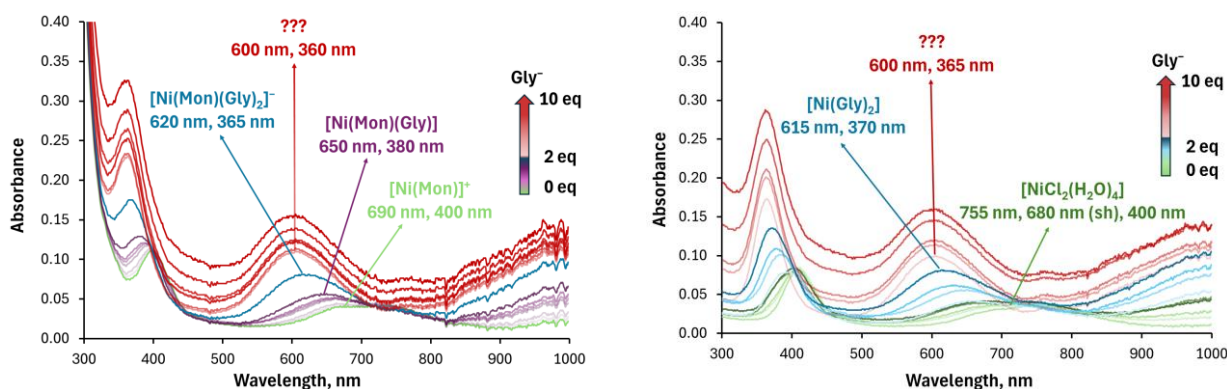


Figure 1. Titration of $[Ni(Mon)]^+$ (left) and $NiCl_2 \cdot 6H_2O$ (right) with glycinate in methanol

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Micellization behaviour of newly synthesized surfactant nicotine-based ionic liquids

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Keywords: Ionic Liquids, Nicotine, Surfactant

Ionic liquids, ionic compounds with melting points below 100 °C, are of particular interest both as additives and alternative solvents due to their tunable properties. A subset of these compounds, are surface-active ionic liquids (SAILs), whose long alkyl chain substituents give them an amphiphilic character. Due to their surfactant nature, SAILs have interesting interactions in a water medium and give rise to distinct chemistry compared to traditional molecular solvents [1]. Nicotine is a naturally occurring pyridine alkaloid, composed of a pyridine and a pyrrolidine ring. The tertiary nitrogen on the pyrrolidine ring is particularly susceptible to alkylation, allowing for the attachment of a long alkyl side-chain and resulting in a quaternary ammonium SAIL [2].

In this work, four nicotine-based ionic liquids with a series of alkyl side-chain lengths are synthesized: N-octylnicotinium bromide, N-decylnicotinium bromide, N-dodecylnicotinium bromide and N-tetradecylnicotinium bromide (Figure 1). Conductivity measurements in aqueous solutions of the investigated SAILs provided information about their critical micelle concentrations, showing similar values to analogous imidazolium SAILs. Tensiometric measurements were also performed to further investigate the micellization behaviour of these SAILs. ITC measurements were performed to analyze the thermodynamic parameters related to micellization and DLS was utilized to explore the size and shape of the micelles.

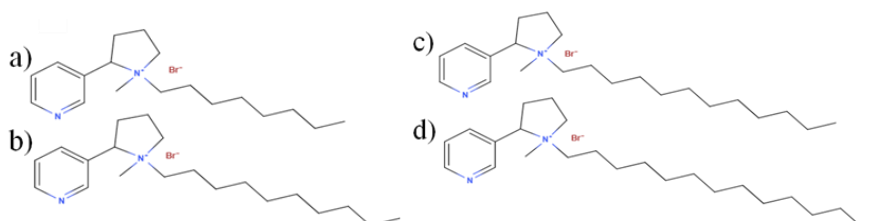


Figure 1. Structures of: a) N-octylnicotinium bromide, b) N-decylnicotinium bromide, c) N-dodecylnicotinium bromide, d) N-tetradecylnicotinium bromide

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Phytochemical composition and *in vitro* inhibitory activity of herbal extracts against medically relevant enzymatic biological systems

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Keywords: herbal extracts, LC-ESI-MS/MS, antioxidant phenolics, lipoxygenase and α -amylase inhibitors

The aim of the present study was to investigate the phytochemical composition, *in vitro* antioxidant activity, lipoxygenase and salivary α -amylase inhibitory effects of selected herbal extracts. Twenty-four extracts with boiling water and 70% (v/v) aqueous ethanol were obtained from *Tilia cordata* Mill., *Lavandula angustifolia* Mill., *Matricaria chamomilla* L., *Urtica dioica* L., *Sideritis scardica* Griseb., *Salicornia europaea* L., *Sambucus nigra* L., *Cistus incanus* L., and *Bistorta major* S. F. Gray. The yields of the aqueous or ethanolic extracts varied between 18.7 and 42% (w/w) or between 13.7 and 45.1%, respectively. The 70% ethanolic extracts of *B. major* rhizomes and *C. incanus* stems were characterized with the highest total phenolic content of 504 $\pm$ 4 and 343 $\pm$ 5 mg gallic acid equivalents/g extract among all samples. The content of total flavonoids in the same samples of *B. major* and *C. Incanus* was 3.60 $\pm$ 0.05 and 33.4 $\pm$ 0.2 mg quercetin equivalents (QE)/g extract, respectively. The total tannins in the two samples in the same order were 33 $\pm$ 1 and 89 $\pm$ 7.5 mg tannic acid equivalents (TAE)/g extract. The most potent CUPRAC antioxidant activity of 7893.8 $\pm$ 9.6 and 5267.1 $\pm$ 17.7 μ mol trolox equivalents (TE)/g extract were also expressed by the ethanolic *B. major* and *C. incanus* samples, which was mainly attributed to the phenolic constituents. Similarly, the best ABTS antioxidant activity was demonstrated by the ethanolic *B. major* and *C. incanus* extracts with values of 6621.9 $\pm$ 176.2 and 4596.3 $\pm$ 39.4 μ mol TE/g extract, respectively. Catechin, chlorogenic and gallic acids were the major identified phenolic compounds in the *B. major* ethanolic extract on the basis of the LC-ESI-MS/MS analysis, representing 1.3, 0.7, and 0.5% of the sample. Gallic (0.3%) and protocatechuic (0.05%) acids were found in the highest amounts in a 70% ethanol extract of *C. incanus*, as well as myricetin (0.2%), catechin (0.15%), quercetin (0.1%), and isocupperide (0.01%). The *C. incanus* aqueous extract and *B. major* ethanolic extract exhibited meaningful inhibitory activities against a soybean lipoxygenase (EC 1.13.11.12) of 80.0 $\pm$ 1.6% and 80.2 $\pm$ 1.2% at 71.4 μ g/mL, which were lower than that of indomethacin at 60 μ g/mL (90.4 $\pm$ 2.9%). The 70% ethanol extract of *B. major* expressed a distinct inhibitory activity against human salivary α -amylase (EC 3.2.1.1) from 49.8% to 98.2% in the concentration range of 143 to 714 μ g/mL. Some antioxidant phenolics derived from *B. major* and *C. incanus* could be useful lipoxygenase and salivary α -amylase inhibitors in the supplementary therapy of diabetes and other inflammatory diseases.

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Dielectric Spectroscopy and the 'Wicked' Problem of Electrolyte Solubilities

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Keywords:

Prediction of the solubilities of solid electrolytes in water (or any other solvent for that matter) without the use of empirical parameters is a 'wicked' problem in chemistry; even after hundreds of years of investigation, there is little sign of an imminent breakthrough. Nevertheless, the basic principles of this problem are well understood: the solubility of any solid solute in any solvent reflects the difference in the stability of that solute in the solid state and in its saturated solution. This talk will focus on the latter, utilizing dielectric spectroscopy to study the behaviour of the aqueous solutions of two archetypal 2:2 electrolytes: MnSO_4 and FeSO_4 . Broadband dielectric spectroscopy is a powerful technique for investigating both the ion-solvent (solvation) and ion-ion (association) interactions that dominate the behaviour of electrolytes in solution. The interplay between these two phenomena has a major effect on the solution speciation and hence the solubilities of these electrolytes. The complexity of such interactions helps to explain why the prediction of electrolyte solubilities is likely to remain a 'wicked' problem in chemistry for some time yet.

Solubility, Speciation, and Thermodynamic Modeling of Fe(II) in Repository-Relevant Systems from Near Neutral to Hyperalkaline Conditions

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Keywords: Anoxic Iron Corrosion, Solubility and Phase Stability, Ferrous Iron Hydroxide, Hibbingite, Thermodynamic Modeling

Iron is a ubiquitous element in geological environments and plays a pivotal role in controlling redox conditions in deep underground repositories for nuclear waste disposal. In such repositories, metallic iron is extensively used as structural and container material, and its anoxic corrosion shapes the near-field geochemical environment, influencing pH, E_h , and hence the mobility of safety-relevant radionuclides. Accurate knowledge of Fe(II) speciation, solubility, and the stability of corrosion products is essential for evaluating the long-term behavior of actinides, fission and activation products. In this work we focus on conditions associated with water intrusion and cement degradation, which are expected to produce reducing alkaline to hyperalkaline aquatic systems.

Despite extensive research on iron's aquatic chemistry, significant uncertainties remain regarding Fe(II) behavior in chloride-rich, alkaline and hyperalkaline systems relevant to repository safety assessments. In particular, the lack of high-quality thermodynamic data for Fe(II) solid phases (e.g., $\text{Fe}(\text{OH})_2(\text{cr})$, $\text{Fe}_2(\text{OH})_3\text{Cl}(\text{cr})$) and aqueous hydrolysis species (e.g., $\text{Fe}(\text{OH})_2(\text{aq})$, $\text{Fe}(\text{OH})_3^-$, $\text{Fe}(\text{OH})_4^{2-}$) impacts the accuracy of geochemical models that underpin predictions of repository evolution, as recognized in the reviews conducted for the Thermochemical Database (TDB) project of the Nuclear Energy Agency (NEA).^[1,2]

To address these gaps, comprehensive solubility experiments were performed with well-characterized Fe(II) solid phases, including $\text{Fe}(\text{OH})_2(\text{cr})$ and $\text{Fe}_2(\text{OH})_3\text{Cl}(\text{cr})$, over a broad range of conditions: near-neutral to alkaline pH ($7.5 \leq \text{pH}_m \leq 10.5$) at constant ionic strengths ($0.01 \text{ M} \leq I_m \leq 4.0 \text{ M}$) using KCl/KOH as background electrolyte^[3] as well as dilute to concentrated MOH ($\text{M} = \text{Na}, \text{K}$) systems ($0.10 \text{ m} \leq \text{KOH} \leq 4.20 \text{ m}$; $1.06 \text{ m} \leq \text{NaOH} \leq 22.73 \text{ m}$)^[4]. All experiments were performed under argon atmosphere ($<1 \text{ ppm O}_2$, $25 \pm 2 \text{ }^\circ\text{C}$). Solid phase characteristics and composition were confirmed by detailed X-ray diffraction (XRD) analyses, including Rietveld refinement. E_h , pH, and aqueous Fe concentrations were monitored over extended equilibration periods up to 258 days, with Fe(II)/Fe(III) redox speciation validated by capillary electrophoresis coupled with ICP-MS.

Experimental results were combined with selected literature to derive chemical, thermodynamic, and activity models (SIT, Pitzer) for the $\text{Fe}^{2+}\text{--K}^+\text{--H}^+\text{--Cl}^-\text{--OH}^-\text{--H}_2\text{O}(\text{l})$ system. The solubility products obtained for $\text{Fe}(\text{OH})_2(\text{cr})$ ($\log^*K_{s,0}^{\circ} = 12.32 \pm 0.05$) and $\text{Fe}_2(\text{OH})_3\text{Cl}(\text{cr})$ ($\log^*K_{s,0}^{\circ} = 16.38 \pm 0.20$) are notably lower and more robust than values previously selected in principal databases, reflecting improved solid phase characterization and larger particle size. Under hyperalkaline conditions, systematic experiments confirm $\text{Fe}(\text{OH})_3^-$ as the predominant Fe(II) species up to around 1 m NaOH/KOH, with $\text{Fe}(\text{OH})_4^{2-}$ dominating at higher alkalinity, thereby

clarifying Fe(II) speciation in repository relevant aquatic systems and advancing models beyond the limitations of past studies.

We have derived thermodynamic and activity models that demonstrably improve upon past data and can be implemented in geochemical calculations. The results highlight the critical influence of solid phase properties (e.g., crystallinity, particle size) on Fe(II) stability and solubility and provide new insights into the mechanisms of solid phase transformations under relevant conditions. Overall, this research provides fundamental data and robust models for Fe(II) chemistry, enabling more accurate predictions of redox evolutions, radionuclide retention, and the safety of nuclear waste repositories under alkaline and hyperalkaline scenarios.

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Solvent Parameters from Computational Chemistry

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Keywords: solvent parameters, solubility, linear free energy relationship, computational chemistry

Understanding and predicting the effects of changes in solvent on chemical processes is one of the classical problems in solution chemistry and linear free energy relationships are well established for these purposes. Thus one writes:

$$Y = \sum a_i P_i \quad (1)$$

where Y is some property and the P_i are parameters representing solvent properties that are relevant to the solvation process. The coefficients, a_i represent the response of Y to P_i and the $a_i P_i$ terms represent the contributions of the different interactions, i , to Y .

Traditionally, experimental solvent parameters, such as those of Kamlet and Taft, Gutmann, Dimroth and Reichardt, Hansen and Catalan, have been used and, in general the P_i reflect the hydrogen bond acidity and basicity of the solvent and non-specific electrostatic interactions, denoted solvent polarity/polarizability (for example, Kamlet and Taft's α , β and π^* , respectively).

Correlations of these parameters against properties of solvent molecules, determined by computational chemistry, have shown that there are marked consistencies in the molecular properties that contribute to the P_i [1]. These consistencies suggest that solvent parameters based on calculated molecular properties could be used in eq. (1).

This was demonstrated for the solubility of thioxanthen-9-one in a range of organic solvents [2]. In this case the fits to eq. (1) using computer generated solvent parameters were comparable to those using experimental parameters.

This talk will extend these studies to other compounds and discuss the differences between, and relative merits of, the experimental and computer based solvent parameters.

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Thermodynamic Reference Database (THEREDA): Pitzer Activity Model for Tc(IV) Solubility and Complexation in the Tc(IV)–Na⁺–Cl[–]–HCO₃[–]–CO₃^{2–}–OH[–]–H₂O(I) System

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Keywords: Tc(IV), carbonate, solubility, Pitzer model, THEREDA.

⁹⁹Tc is a β -emitting fission product of ²³⁵U and ²³⁹Pu, produced with high-yield in nuclear reactors. Because of its large inventory in high-level nuclear waste, long half-life ($t_{1/2} = 2.11 \cdot 10^5$ a), and redox-sensitive character, ⁹⁹Tc is an important radionuclide in the context of nuclear waste disposal. Under the reducing conditions expected in underground repositories for nuclear waste, Tc(IV) will be the predominant oxidation state of technetium, which forms sparingly soluble hydrous oxides TcO₂ · xH₂O^[1].

Carbonate is a ubiquitous component of pore water in both clay and crystalline host rock formations investigated for deep geological repositories. It also constitutes a major component of cementitious materials used as backfill and geotechnical barriers in a repository. Carbonate forms strong complexes with hard Lewis acids such as, e.g., tetravalent metals (An(IV), Zr(IV), Tc(IV), ...), leading to the formation of ternary hydroxo-carbonato complexes (M–OH–CO₃) in alkaline to hyperalkaline pH conditions. Therefore, carbonate plays an important role in the aquatic chemistry of radionuclides^[2].

The Thermodynamic Reference Database (THEREDA)^[3] is designed for geochemical calculations in the context of radioactive waste disposal. THEREDA focuses on solubilities of radionuclides, fission products and matrix elements under high ionic strength conditions. Therefore, THEREDA uses the Pitzer approach for ionic strength corrections. The present work provides an extension of the previous Tc(IV) database in THEREDA by inclusion of carbonate-containing systems.

A chemical, thermodynamic, and Pitzer activity model for Tc(IV) solubility and complexation in the system Tc(IV)–Na⁺–Cl[–]–HCO₃[–]–CO₃^{2–}–OH[–]–H₂O(I) was derived based on the previous THEREDA dataset on Tc (Release 10, 2016), our previous work^[4] on Tc(IV) in chloride systems, the newest NEA-TDB book on Tc^[1], and the work of Baumann *et al.*^[5] in NaCl–NaHCO₃–Na₂CO₃ systems. The species Tc₂O₃²⁺, TcO(OH)₂(aq), TcO(OH)₃[–], Tc(OH)₂CO₃(aq), and Tc(OH)₃CO₃[–] were considered. New Pitzer parameters for the interaction between Na⁺ and Tc(OH)₃CO₃[–] were derived. Results from model calculations for $I = 5$ mol/L (5.609 mol/kg) NaCl–NaHCO₃–Na₂CO₃ with different total carbon (TC) contents 0.01 mol/L < TC < 0.5 mol/L are shown in Figure 1 (top). For 4 < pH_m < 12 a strong increase of Tc(IV) solubility is observed with increasing TC due to the formation of Tc(OH)₃CO₃[–]. The results of the model calculations were compared with experimental literature data from Baumann *et al.* at different ionic strengths (0.3 mol/L < I < 5 mol/L) and various total carbon concentrations (0.01 mol/L < TC < 0.5 mol/L) (Figure 1 bottom). The present model shows the ability to describe the experimental data well. The results of this work will be included in an upcoming THEREDA release.

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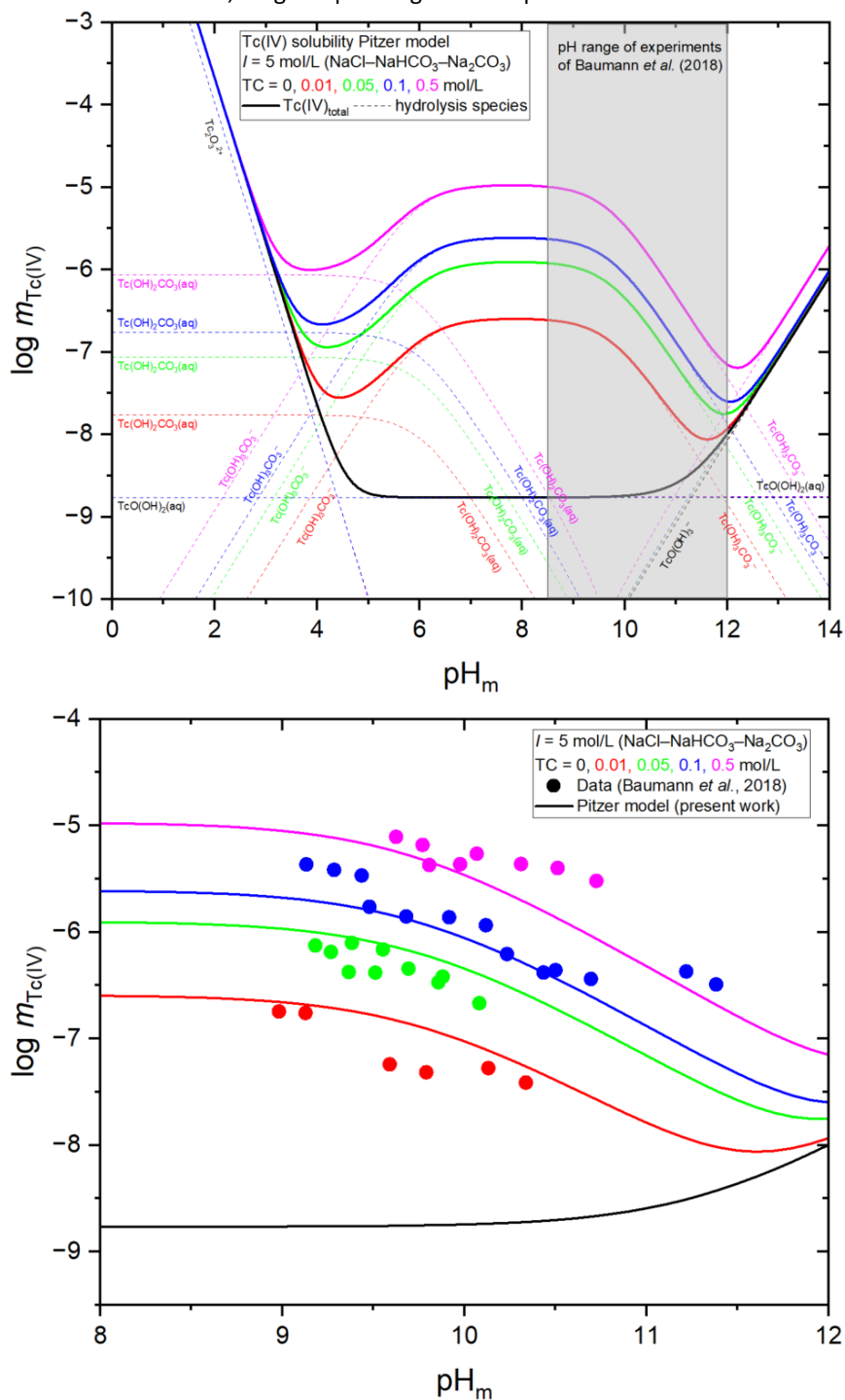


Figure 1. Results of Pitzer model calculations for Tc(IV) solubility in 5 mol/L (5.609 mol/kg) NaCl–NaHCO₃–Na₂CO₃ with different total carbon concentrations (TC = 0, 0.01, 0.05, 0.1, 0.5 mol/L). Species concentration with dotted lines (top). Comparison with experimental data from Baumann *et al.*^[5] (bottom).

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Thermodynamic Modeling of Rare Earth Solvent Extraction

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Keywords: rare earth elements, solvent extraction, TODGA, thermodynamic modeling, MSE

Rare earth elements (REEs) are critical to modern technologies, yet their separation remains a significant challenge due to their similar chemical behavior and sensitivity to process conditions. Solvent extraction (SX) is the primary industrial method for REE separation, but its design is complicated by the interplay of aqueous speciation, acidity, and extractant chemistry. In particular, solvation-based extractants such as N,N,N',N'-tetraoctyl diglycolamide (TODGA) require detailed mechanistic understanding to enable predictive process modeling.

In this work, a thermodynamic model for REE solvent extraction using TODGA has been developed within the OLI Mixed Solvent Electrolyte (MSE) framework. The model rigorously describes chemical speciation in both aqueous and organic phases across a wide concentration range. Special emphasis is placed on the solvation mechanism of TODGA, including the formation of metal–ligand complexes in the organic phase and their equilibrium with aqueous REE species.

The model is parameterized using experimental data such as distribution ratios and nitric acid dependence, ensuring accurate representation of extraction equilibria. By explicitly accounting for fundamental chemical interactions, the framework enables reliable prediction of REE extraction behavior under varying conditions, including acid concentration, metal loading, and extractant composition.

The validated model provides a predictive tool for process design and optimization, allowing simulation of separation performance and guiding the selection of operating conditions to enhance efficiency and selectivity. This work demonstrates the capability of thermodynamic modeling to reduce experimental effort and improve the development of advanced SX systems based on TODGA.

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Integrated computational and experimental screening of solvents for polylactic acid recycling

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Keywords: 3D printing, green solvents; plastic recycling; machine learning

By 2029, global production of polylactic acid (PLA) is expected to exceed 2.4 million tonnes per year, a figure that reflects the material commercial success, with much of this demand driven by additive manufacturing, commonly known as 3D printing, where PLA has established itself as the dominant raw material. However, with the growth of this technique has also come an increase in waste generated by failed prints, support structures and end-of-life components, which accumulate in large volumes that current disposal and recovery strategies are not equipped to handle [1,2,3].

This work proposes a dissolution-based recycling route able to selectively recover PLA and separate additives and copolymers through the use of lower-hazard solvent systems. To identify effective solvents and to minimize the need for trial-and-error screening, a combined computational-experimental strategy was employed. In an initial stage, Hansen solubility parameters and the predictive model COSMO-RS were employed to classify conventional and emerging solvents, including bio-derived candidates. The most promising solvents were validated experimentally through PLA dissolution tests conducted under moderate thermal conditions, both above and below the polymer glass transition temperature. The resulting dataset was then used to train machine learning models, which demonstrated high predictive accuracy in distinguishing between effective and ineffective solvents and in identifying promising new candidates.

By integrating molecular thermodynamic screening, experimental validation, and AI-guided selection, this approach supports the development of a scalable polymer recycling process with reduced reliance on hazardous solvents.

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Understanding Drug Salt Solubility: Mechanistic Complexities and Practical Approaches

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Keywords: drug salts, solubility product, solubility–pH profile, disproportionation, aggregation

Drug salt formation is a widely used strategy to improve the solubility and dissolution rate of poorly water-soluble active pharmaceutical ingredients (APIs). [1] However, despite its routine application, the underlying physicochemical principles governing salt solubility are often oversimplified, leading to inconsistencies in experimental data and misinterpretation of results. Our work revisits the fundamental concepts of drug salt solubility with a focus on mechanistic understanding and practical implications.

We highlight the distinction between thermodynamic and kinetic solubility and emphasize the central role of the solubility product (K_{sp}) as the true equilibrium descriptor of salt systems. Through analysis of solubility–pH profiles, we demonstrate that real systems frequently deviate from classical Henderson–Hasselbalch behavior due to factors such as spontaneous salt disproportionation, buffer–drug interactions, and the formation of water-soluble molecular aggregates. These effects can significantly alter the apparent solubility and complicate data interpretation.

Common experimental pitfalls are critically assessed here, including the influence of buffer composition, ionic strength, solid-state transformations, and equilibration conditions on the results. Based on these insights, we propose practical recommendations for harmonized solubility measurement protocols to improve reproducibility and data transparency across laboratories.

In addition, the current approaches for predicting salt solubility are evaluated. While substantial progress has been made in modeling intrinsic solubility, [2,3] predictive frameworks for salt solubility remain limited due to the scarcity of reliable K_{sp} datasets and the complexity of ionization equilibria.

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Tricyclic antidepressants solubility study: Role of Competing Counterions in Aggregation and Solid-Phase Transformations

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Keywords: Solubility, Tricyclic antidepressants, Solubility product, pH-Ramp *shake-flask* method

Quantitative determination of solubility and comprehensive characterization of solution and solid-phase equilibria in drug systems are essential for predictive understanding of *in vivo* performance and for rational design of pharmaceutical formulations, particularly for poorly soluble, ionizable and surface-active compounds. This study systematically investigates the influence of competing counterions on solubility, aggregation and solid-phase transformations of selected tricyclic antidepressants (TCAs), revealing equilibria not previously identified in the literature. Solubility–pH profiles were determined using the pH-Ramp *shake-flask* method^{1–3} in the presence of both chloride and phosphate ions and in chloride-free and phosphate-free suspensions. Using the computer program *pDISOL-X*, concentration thermodynamic constants ($I_{ref} = 0.15$ M, 25°C) including intrinsic solubilities, solubility products and aggregation constants were refined. Distinct solubility behaviors were observed depending on the nature and concentration of counterions. Drug–phosphate aggregates and self-aggregates significantly elevated solubility of TCA, depending on pH and counterions concentration. In some cases, solubility could be reduced *via* the common-ion effect by increasing ionic strength in the system. Multiple solid-phase transformations, driven by the Gibbs phase rule “hard” or “soft” constraints, were characterized by PXRD, DSC and TGA. Solid-phase composition, transition pH values and the width of the $pH_{max} - pH_{min}$ range were strongly dependent on the suspension composition, direction of pH change in titrations and drug mass/suspension volume ratio. Besides, partial degradation in alkaline suspensions was also influenced by counterions. These findings demonstrate that neglecting counterion effects can lead to misinterpretation of solubility data and unreliable predictions in drug development, especially in complex systems where multiple, previously unrecognized equilibria govern drug solubility.

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Green chemistry solutions for antimalarial drug extraction and solubility enhancement

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Keywords: Artemisinin, COSMO-RS, Green solvents, Eutectic systems, Terpenes

Malaria remains a life-threatening disease, particularly in sub-Saharan Africa, where it continues to cause hundreds of thousands of deaths annually. Artemisinin-based combination therapies are among the most effective treatments; however, their performance is often limited by the low aqueous solubility of key active pharmaceutical ingredients (APIs), including artemisinin, pyrimethamine, and quinine. This limitation affects dissolution and overall drug performance.

This work explores the use of green, bio-derived solvents to enhance the solubility and extraction efficiency of antimalarial compounds. Predictive thermodynamic models, including COSMO-RS and Hansen Solubility Parameters, were employed to screen and rationalize solute-solvent interactions for artemisinin and related APIs. Promising candidates, particularly terpene-based systems, were experimentally validated through solid-liquid extraction from *Artemisia annua* and compared with conventional halogenated solvents.

In parallel, the formation of eutectic systems using natural green excipients was investigated as a strategy to enhance drug solubility and enable direct formulation. The combined approach, integrating extraction and eutectic formation, demonstrates the potential to bypass complex purification steps while improving overall process efficiency. Selected terpene systems increased artemisinin recovery by approximately 15% while eliminating hazardous solvents, and the resulting extracts exhibited biological activity comparable to pure compounds.

Overall, this study highlights how computationally guided solvent selection and eutectic design can address solubility limitations while supporting safer and more sustainable pharmaceutical processes. The proposed strategies align with green chemistry principles and offer scalable pathways for improved antimalarial drug extraction and formulation.

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Menadione's solubility in fatty acids predicted by the COSMO-SAC CS25 model

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Keywords: Solid-liquid equilibrium, Vitamin K3, Fatty acids, COSMO-SAC CS25.

Menadione, the synthetic form of vitamin K, plays a fundamental role in the coagulation cascade and is essential for restoring natural forms of this vitamin in some organisms. This compound, also known as vitamin K3, can be converted into vitamin K2 (menaquinone) and acts as an intermediate in the metabolic conversion of vitamin K1 (phyloquinone) into vitamin K2 [1]. Menadione, a lipophilic molecule, typically requires environmentally harmful organic solvents during synthesis, which can also contaminate vitamin supplements. Fatty acids, in turn, are lipids formed by long hydrocarbon chains with terminal carboxylic groups found in oils and fats. Due to the possibility of forming similar intermolecular interactions, fatty acids appear as greener alternative solvents for menadione, providing a greener route and a safer product.

Currently, the use of computational chemistry tools is an essential ally in the development of preliminary studies, as it provides an economical and time-saving way to investigate reactions. COSMO (Conductor-like Screening Model) based models employ a dielectric continuum approach to calculate, in energetic terms, the interactions between charged surfaces of compounds present in a system. Thus, it can be used to predict thermodynamic properties of phase equilibria by the use of quantum descriptors that partition the molecule into solvated surface segments.

In this work, COSMO-SAC CS25 was used to calculate, through a solid-liquid equilibrium, the activity coefficient and the solubility of menadione in fatty acids that compose the most common oils in Brazil, in order to establish a solubility order for these solvents. First, Avogadro was used to obtain the molecular geometry of menadione and each fatty acid. Then, the charged surfaces of each molecule were obtained through ab-initio quantum mechanical calculations using NWChem through the hybrid functional B3LYP and the def2-SVPD basis set [2]. Finally, the interactions between menadione and the fatty acids were simulated using the COSMO-SAC CS25 model, and solubility predictions were obtained. These interactions were also analyzed in terms of activity coefficients, in order to study the ideality deviation of the mixture's behavior. The results obtained by this simulation showed that, among the fatty acids analyzed, lauric acid, linolenic acid, and linoleic acid were the best candidates to be used as a solvent for menadione.

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Isolation, chemical characterization and modification with ferric ions of natural prebiotic herbal polysaccharides

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Keywords: *Bistorta major*, polysaccharides, prebiotics, anti-biofilm activity

The aim of the present study was to investigate the structural features, *in vitro* prebiotic and antibacterial activities of water- (WE), alkali-extractable (AE) and ferric ion-modified (Fe³⁺) polysaccharides (PSs), isolated from the leaves and rhizomes of *Bistorta major* S. F. Gray. The yields of WEPS from leaves (BML-WEPS) and rhizomes (BMR-WEPS) were 6.4% and 2.6%, and of AEPS from leaves (BML-AEPS) and rhizomes (BMR-AEPS) were 4.8% and 4.3%. The total carbohydrate content of the Ps was above 74%. BML-WEPS and BMR-WEPS contained methylesterified and acetylated pectins, with BML-WEPS being richer in the acidic homogalacturonan fragment (42.7±0.5% total uronides) and with a higher molecular weight (Mw= 85.0×10⁴ g/mol). BMR-WEPS had more arabinogalactan (AG) chains, abundant in α-L-1,3,5-linked arabinans, than BML-WEPS, based on 2D NMR analyses. BML-AEPS contained acidic AGs and xylans, and BMR-AEPS was an α-(hetero)glucan. No condensed tannins were found in BML-WEPS, but BMR-WEPS, BML-AEPS and BMR-AEPS contained 3.0%, 0.5% and 1.2% total condensed tannins, respectively. All PSs (20 mg/mL) stimulated the growth and biofilm formation of pure or mixed cultures of *Clostridium beijerinckii* 4.3A1 and 6A, and in combination with *Lactobacillus helveticus* 611, as the sole carbon source. PSs (20 mg/mL) did not significantly inhibit the growth of *Escherichia coli*, *Staphylococcus aureus*, *Streptococcus mutans* and *Pseudomonas aeruginosa* strains, but some inhibited statistically significantly biofilmogenesis by *P. aeruginosa* and *E. coli*. FTIR, HPSEC-RID and spectrophotometric analyses confirmed the binding of Fe³⁺ to PSs. Fe³⁺-WEPS exhibited a better prebiotic activity than the original WEPS and reduced biofilmogenesis in pathogens. PSs and their ferric derivatives can be tested in synbiotic products for future application in functional nutrition and supplementary therapy of socially significant diseases characterized by dysbiosis.

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Salt Effects on Amino Acid Solubility: Experimental, Molecular, and Data-Driven Perspectives

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Keywords: Electrolyte Solutions, Consistency, Uncertainty, Gaussian Processes, Molecular Dynamics

Electrolyte aqueous solutions constitute the natural environment of biomolecules and play a fundamental role in regulating their structure, function, and physicochemical behaviour. Understanding how salts influence the solubility of amino acids, peptides, and proteins is therefore essential for biological, pharmaceutical, food, and biotechnological applications. Despite extensive experimental studies and the long-standing insights provided by the Hofmeister series, significant inconsistencies in solubility datasets and the absence of a unified molecular interpretation continue to limit predictive capability [1].

This work presents a framework for understanding ion-specific effects on amino acid solubility by integrating systematic experimental measurements, molecular dynamics simulations, and modern data-driven modelling approaches. A large diversity of amino acids is considered, as well as salts including fluoride, chloride, bromide, nitrate, sulfate, or thiocyanate anions, as well as sodium, potassium, ammonium, magnesium, and calcium cations.

The results reveal distinct ion- and charge-dependent salting-in and salting-out mechanisms, highlighting the dominant role of specific ion- functional group interactions rather than bulk water structuring. Molecular-level analyses, supported by radial distribution functions obtained from molecular dynamics simulations, provide insight into the preferential interactions between ions and amino acid functional groups. Additionally, the influence of optical isomerism, pH, peptides, and glycine derivatives is discussed to extend the understanding of solvation phenomena in increasingly complex systems.

To address long-standing inconsistencies in literature data, Gaussian Process modelling is employed to critically evaluate and reconcile experimental solubility measurements, enabling the identification of unreliable datasets and supporting the rational design of new experiments. By combining thermodynamic measurements, molecular-scale interpretation, and statistical learning tools, this work establishes a robust framework for describing salt effects on biomolecular solubility and contributes to the development of predictive models for complex biological and industrial applications.

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How cation composition controls the structure and solubility of Pu(V) and Np(V) double carbonates

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Keywords: solubility, structure, plutonium, neptunium

The development of nuclear energy as an environmentally clean technology requires the creation of reliable radioactive waste (RW) disposal methods. A key challenge is ensuring the long-term safety of repositories to prevent the migration of radionuclides into the environment. The most radiotoxic components of RW are plutonium and neptunium, which have long half-lives and are highly toxic. To predict their behavior in the environment, accurate data on the physicochemical forms they adopt upon interaction with natural inorganic components are needed, including the most common carbonate anions and alkali and alkaline earth cations. Currently, thermodynamic and structural data for such systems are extremely limited, which hinders scientifically based safety modeling of disposal sites.

In the present work, the structures of double carbonates of Pu(V) and Np(V) with alkali and alkaline earth metal cations were investigated. It was found that compounds of the composition KAnO_2CO_3 (An = Pu, Np) consist of hexagonal anionic layers $[\text{AnO}_2\text{CO}_3]^-$ with K^+ cations located between them. In contrast, the structure of $\text{NaNpO}_2\text{CO}_3 \cdot 3\text{H}_2\text{O}$ is significantly different, featuring alternating orthorhombic layers $[\text{NpO}_2\text{CO}_3]_n^{n-}$ and interlayer cationic species $[\text{Na}(\text{H}_2\text{O})_3]_n^{n+}$ [1, 2]. Using the ion exchange method, the double carbonate compounds $\text{Mg}_{0.5}\text{NpO}_2\text{CO}_3 \cdot 6\text{H}_2\text{O}$ and $\text{Ca}_{0.5}\text{NpO}_2\text{CO}_3 \cdot 4\text{H}_2\text{O}$ were obtained and characterized. It was established that in the series of Np(V) double carbonates, cations with a small ionic radius (less than 1 Å) Na^+ , Ca^{2+} , Mg^{2+} – lead to a rhombic layer motif in the neptunium-containing layers, whereas larger radius cations (K^+ , NH_4^+) result in a hexagonal layer motif. Using slow chemical precipitation from a Pu(VI) solution, the compound $\text{Mg}_{0.5}\text{PuO}_2\text{CO}_3 \cdot x\text{H}_2\text{O}$ was obtained for the first time, and its possible existence under environmental conditions was confirmed.

Solubility experiments were conducted under undersaturation conditions for the obtained double carbonate compounds of Np(V) and Pu(V) in solutions of various compositions within the pH range of 6–11. Thermodynamic modeling of the experimental data was performed taking into account all possible physicochemical forms of the components in solution. Based on the modeling, the solubility products were determined: $\log K_{\text{sp}}(\text{Mg}_{0.5}\text{NpO}_2\text{CO}_3 \cdot 6\text{H}_2\text{O}) = -15.9 \pm 0.2$, $\log K_{\text{sp}}(\text{KNpO}_2\text{CO}_3) = -16.5 \pm 0.1$, and $\log K_{\text{sp}}(\text{Ca}_{0.5}\text{NpO}_2\text{CO}_3 \cdot 4\text{H}_2\text{O}) = -15.4 \pm 0.2$ [3]. The stability region of the KPuO_2CO_3 phase is also described. The results demonstrate that double carbonates of Np(V) and Pu(V) with a hexagonal layer structure exhibit the highest thermodynamic stability.

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Chemical equilibrium models for calculation of metal chemical species in different type surface waters

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Keywords: Chemical equilibrium models, Surface water, Chemical species, Bioavailability

In natural surface waters, metals are present as free metal ions and as inorganic and organic complexes at different concentrations. Their chemical species identification is essential for assessing the bioavailability and potential impact on aquatic ecosystems. Thermodynamic modeling is a widely used approach for studying processes in natural water systems and for calculating and predicting metal chemical species. The specificity of the thermodynamic models used is determined by the different ionic strengths of the studied water.

In this study, various thermodynamic models were applied to calculate the chemical species of Al, Fe, Mn, Co, Ni, Cu, Zn, Cd, and Pb in different types of surface water. Experimental data for the total concentrations of major and trace metals, dissolved organic carbon, and pH were used as input data for the calculations. The combined models of ion interaction (IIM) and ion association (IAM) were applied to calculate the inorganic chemical species in saline marine waters with a high ionic strength ($I > 0.1$). The IIM was used to calculate the chemical interactions with major ions, while the IAM was used to calculate the chemical species of trace metals. Just the IAM was used to calculate the inorganic chemical species of metals in surface fresh water with low mineralization and low ionic strength ($I < 0.1$). Accounting for the complexation reactions of metals with organic matter in both types, saline and freshwater, was done with the discrete ligand Stockholm Humic Model (SHM).

The results showed that Al, Fe, Mn, Co, Ni, Cu, Zn, Cd, and Pb formed a wide variety of complexes, the distribution of which depends on the nature of the metal, the physicochemical characteristics, and the chemical composition of the medium, and the concentrations of all present elements. In all studied surface waters, the metal-organic complexes are dominant for Fe, Cu, and Pb, while Al forms stable inorganic complexes, mainly $\text{Al}(\text{OH})_4^-$. Regarding Mn inorganic species, the dominant ones were free Mn^{2+} , MnCO_3^0 , and MnSO_4^0 . Significant differences in the distribution of chemical species of the elements are observed for Ni, Co, Zn, and Cd, where the ratio of inorganic and organometallic species varies depending on the medium composition.

In addition, the bioavailability of Al, Fe, Cu, Zn, Cd, and Pb in surface river water calculated by the combined ion-association - Stockholm humic model (IA-SHM) was compared with calculations using the biotic ligand model (BLM). It was established that when inorganic species (free ions, hydroxy, and carbonate) were dominant, species distribution differed. These differences are due to the mutual competition of metals accounted for by IA-SHM, which makes it more effective for estimating microelement bioavailability.

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Synthesis of lithium hydroxide using barium hydroxide

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Keywords: Li-ion battery, lithium hydroxide, barium hydroxide, causticization, solubility

In the coming years, lithium hydroxide monohydrate ($\text{LiOH} \cdot \text{H}_2\text{O}$) is expected to become the dominant precursor for the synthesis of NMC mixed-oxide cathodes, as it allows lower synthesis temperature thus higher structural stability [1]. On the industrial scale, LiOH is produced via reacting Li_2CO_3 with $\text{Ca}(\text{OH})_2$, yielding sparingly soluble CaCO_3 (causticization). The reaction however suffers from poor reaction yields if concentrated suspensions are used, decreasing to $\sim 35\%$ for suspensions of an initial Li^+ concentration of 30 g L^{-1} [2]. To this end, we studied the causticization process using $\text{Ba}(\text{OH})_2$ as an alternative agent.

We have found that at 1:1 $\text{Ba}(\text{OH})_2\text{:Li}_2\text{CO}_3$ molar ratio and 5 g L^{-1} initial concentration of Li^+ (c_{Li^+}), the reaction yield is 97% already after 30 minutes, whereas the reaction rate becomes slower above this concentration, due to the limited solubility of $\text{Ba}(\text{OH})_2$ and slow precipitation of BaCO_3 . Nevertheless, yields after 2 hours of reaction are markedly greater than those with $\text{Ca}(\text{OH})_2$ at all Li^+ concentrations, varying from 97% vs. 92% ($c_{\text{Li}^+} = 5 \text{ g L}^{-1}$) to 70% vs. 35% ($c_{\text{Li}^+} = 30 \text{ g L}^{-1}$). Increasing the reaction time to 2 days, the reaction is essentially quantitative (98%) even at $c_{\text{Li}^+} = 30 \text{ g L}^{-1}$, corresponding to 3.2 mol L^{-1} LiOH , significantly exceeding the limit of the traditional lime causticization (1.5 mol L^{-1}) [2].

Further, the $\text{CO}_3^{2-}\text{:OH}^-$ molar ratio remains below 1.5% for all Li^+ concentrations and reaction times, whereas the $\text{Ba}^{2+}\text{:Li}^+$ ratio shows a clear time-dependence, decreasing below 0.5% after two days of reaction. Yet, higher ratios after the onset of reaction necessitate the application of further methods to decrease the Ba^{2+} concentration to a level acceptable for the preparation of battery-grade $\text{LiOH} \cdot \text{H}_2\text{O}$ in a reasonable time-window.

That is, the higher solubility of $\text{Ba}(\text{OH})_2$ compared to $\text{Ca}(\text{OH})_2$ as well as the lower solubility of the precipitating BaCO_3 as compared to CaCO_3 both increase the efficiency of the $\text{Li}_2\text{CO}_3 \rightarrow \text{LiOH}$ transformation, rendering the $\text{Ba}(\text{OH})_2$ reaction a viable alternative to the traditional causticization process.

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Understanding and quantifying the thermodynamics of lanthanide extraction in hydrophobic eutectic solvents

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Keywords: Solvent extraction; Lanthanides Separation; Thermodynamics; Eutectic solvents.

The growing demand for critical metals in modern technologies calls for more sustainable extraction strategies. Solvent extraction (SX) is widely used for metal recovery through selective ion partitioning between immiscible phases. In this context, hydrophobic eutectic solvents (HES) have emerged as promising alternatives to conventional organic diluents, offering advantages such as reduced volatility, elimination of inert solvents, and mitigation of third-phase formation. However, their non-ideal and highly structured nature poses challenges for understanding the factors governing metal transfer ^[1].

In this work, the solvent extraction of lanthanides is investigated using tri-*n*-octylphosphine oxide (TOPO) as extractant, incorporated within a HES formed with decanoic acid. The biphasic transfer of trisnitrato complexes of lanthanides ($M(NO_3)_3$) is studied over a range of temperatures, enabling a thermodynamic analysis of the extraction process. Temperature-dependent distribution data are interpreted through a van't Hoff approach to access the overall enthalpic and entropic contributions governing metal partitioning and results are compared with a conventional SX system (TOPO in toluene).

To directly quantify the enthalpy of extraction, an isothermal titration calorimetry (ITC) methodology was developed and optimized for HES-based biphasic systems. The experimental setup was carefully designed to ensure effective phase contact and reliable heat measurements. Systematic studies involving varying metal concentrations and phase ratios yielded consistent and reproducible calorimetric data, being validated through independent performance tests with conventional SX systems already reported^[2].

The combined van't Hoff and calorimetric analyses provide complementary insights into the energetic landscape of lanthanide extraction in eutectic media, offering a robust basis for understanding the driving forces underlying metal ion partitioning and for designing more efficient and sustainable extraction systems.

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Ligand – Diluent Interplay in the Extraction and Separation of Fe(III) ion by β -Dicarbonyl *N*-Heterocyclic Chelators

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Keywords: Fe(III) ion; solvent extraction; ionic liquid; β -dicarbonyl chelators; ligand–diluent interactions

The influence of ligand structure and solvent environment on Fe(III) ion extraction was investigated using a series of β -dicarbonyl ligands containing saturated *N*-heterocyclic moieties (HL5–HL8) [1,2]. The extraction behavior was evaluated in chloroform and imidazolium-based ionic liquid media in order to examine the effect of the organic phase on metal transfer and complex stabilization. The synthesized ligands exhibited pronounced affinity toward Fe(III) ion, while the extraction efficiency strongly depended on ligand architecture and solvent nature. Comparative studies revealed enhanced Fe(III) ion distribution in ionic liquid systems relative to chloroform [1,3], indicating more favorable stabilization of the extracted species in ionic media. Competitive extraction experiments involving transition, rare-earth, and platinum-group metal ions demonstrated clear selectivity toward Fe(III) ion, whereas most competing ions showed considerably lower extraction under identical experimental conditions. The obtained results emphasize the important role of ligand–diluent interactions in controlling extraction efficiency and separation behavior. These findings demonstrate that β -dicarbonyl *N*-heterocyclic chelators combined with tunable organic media represent promising solvent systems for selective Fe(III) ion separation.

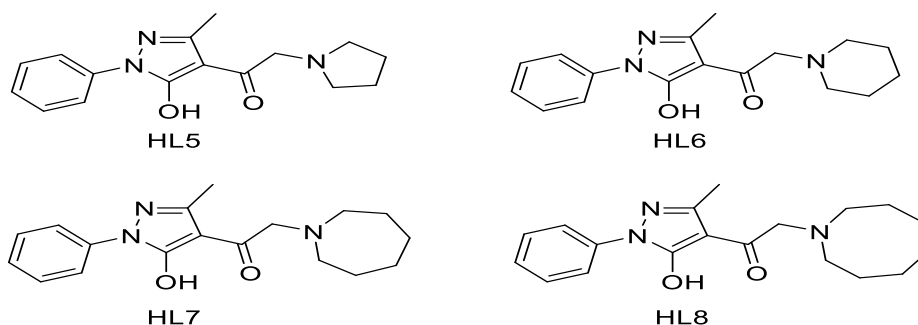


Figure 1. Chemical structures of chelating extractants HL5–HL8.

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Catalytic, electronic and spectroscopic properties of imidazolium hydrogen squarate

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Keywords: Imidazolium hydrogen squarate, Catalytic performance, Spectroscopic properties

Compounds composed of organic cations and anions represent a particularly promising class of organocatalysts. Although organocatalysis offers significant advantages for the selective synthesis of target compounds, important challenges still include minimizing by-product formation and facilitating catalyst separation from the final reaction mixture [1]. In this context, the squaric acid-based organic ion pair imidazolium hydrogen squarate ($[\text{C}_3\text{H}_5\text{N}_2]^+[\text{C}_4\text{O}_4\text{H}]^-$) was investigated in terms of its catalytic performance for butyl acetate production. The acidity (Hammett function, H_0), electronic structure (analyzed through molecular electrostatic potential (MEP) and natural population (NPA) analysis) and spectroscopic (FT-IR, Raman, UV-Vis, XPS) features of $[\text{C}_3\text{H}_5\text{N}_2]^+[\text{C}_4\text{O}_4\text{H}]^-$ were evaluated as well.

FT-IR and Raman techniques identified vibrational bands associated with intramolecular hydrogen bonding ($\text{C}=\text{O}\cdots\text{H}-\text{N}[\text{C}]$) between $[\text{C}_3\text{H}_5\text{N}_2]^+$ and $[\text{C}_4\text{O}_4\text{H}]^-$. These interactions affected the UV-Vis behavior of the title compound, resulting in strong absorption within 250–270 nm region. XPS analysis confirmed the FT-IR, Raman and UV-Vis findings by detecting signals attributed to organic carbon ($\text{C}=\text{C}$), protonated nitrogen (N^+-H) and highly reduced oxygen ($\text{O}\cdots\text{H}$) in the C 1s, N 1s and O 1s lines, respectively. MEP and NPA showed that the $\text{C}=\text{O}\cdots\text{H}-\text{N}[\text{C}]$ bonds also influenced the electronic structure of $[\text{C}_3\text{H}_5\text{N}_2]^+[\text{C}_4\text{O}_4\text{H}]^-$, rendering a hydrogen atom in the imidazolium cation the most positively charged (electrophilic) center. The latter indicated the acidity ($H_0 = 1.909$) of $[\text{C}_3\text{H}_5\text{N}_2]^+[\text{C}_4\text{O}_4\text{H}]^-$, highlighting its role as an acidic organocatalyst in the synthesis of butyl acetate (yield of 36.2% at 80°C after 6 h reaction time). Using kinetic and thermodynamic calculations, the following values for the forward reaction were generated: ΔH_r° (16.2 kJ/mol), ΔS_r° (62.4 J/mol $\times$ K), E_{A_f} (30.1 kJ/mol), A_f (767.1 l/mol $\times$ h), $\Delta H_f^\ddagger$ (27.2 kJ/mol) and $\Delta S_f^\ddagger$ (–199.2 J/mol $\times$ K). Based on the results obtained, the butyl acetate synthesis was stated as an endothermic reaction, proceeding through the formation of an activated complex. A plausible reaction mechanism was also proposed.

Acknowledgements: This work was financially supported through the Research Institute at Burgas State University "Prof. Dr. Assen Zlatarov", project NI-14/2025.

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Franzosini Award 2026

Solutes, Solvents, Solutions, Solubilities & Stabilities

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Keywords: Solutes, Solvents, Solutions, Solubilities, Stabilities

Emeritus Professor Hefter will briefly comment on various aspects of his research in solution chemistry over the last 50 or so years. He will also review his interactions with IUPAC via the Sub-Committee on Solubility and Equilibrium Data (SSED) and its predecessor bodies in the Analytical Chemistry Division.

Complexation and precipitation reactions of Ca^{2+} ions in strongly alkaline media

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Keywords: calcium hydroxide, tricalcium aluminate hexahydrate, complexation, solubility

$\text{Ca}(\text{OH})_2$ is an important reagent in numerous industrial processes associated with strongly alkaline aqueous media. During alumina production (known as the Bayer process), it is used for the causticization of spent liquors (i.e. partially carbonated $\text{NaOH}/\text{NaAl}(\text{OH})_4$ solutions), aided by polyhydroxy carboxylates. In this reaction, tricalcium aluminate hexahydrate (TCA) may be formed, which is considered as a major solid phase contributing to the alkalinity of bauxite residue (BxR), the by-product of the Bayer process. Further, $\text{Ca}(\text{OH})_2$ is used for the industrial-scale production of lithium hydroxide monohydrate, the precursor of modern lithium-ion battery cathodes. Since Ca^{2+} speciation in the solution phase and its distribution between the solution and solid phases are important factors governing the above reactions, detailed understanding of the underlying complexation and precipitation reactions is indispensable.

We have found that in strongly alkaline NaOH solutions saturated with $\text{Ca}(\text{OH})_2$, Ca^{2+} primarily exists in its dihydroxido complex form, $\text{Ca}(\text{OH})_2^0$, which gives rise to a lower limit of $\text{Ca}(\text{OH})_2$ solubility, in contrast to previous models. Addition of polyhydroxy carboxylates (such as gluconate and heptagluconate) induces the formation of stable chelate complexes via ligand deprotonation, with a trinuclear species ($\text{Ca}_3\text{L}_2\text{H}_{-4}^0$) being the most prominent one in concentrated Ca^{2+} solutions. Interestingly, the same species is formed with Mg^{2+} ions; however, ligand deprotonation does not occur.

Upon addition of various amounts of HCl to TCA suspensions, TCA completely transforms to a layered double hydroxide hosting Cl^- ions, i.e. Friedel's salt, instead of simple dissolution. Due to this conversion, the TCA/LDH system acts as pH buffer at around $\text{pH} = 11$, before further dissolution yielding $\text{Al}(\text{OH})_3$ and CaCl_2 . Strikingly, the presence of silicate hinders the formation of LDH, altering the buffering range and apparent acid consumption of TCA.

During the causticization of Li_2CO_3 with $\text{Ca}(\text{OH})_2$ yielding LiOH and CaCO_3 , we found that the yield decreases significantly with increasing amounts of reactants, due to their limited solubility. The commonly quoted maximum concentration of LiOH , 1.5 mol L^{-1} , appears to be governed by the vaterite polymorph of CaCO_3 , whereas in the presence of pure calcite, 2.3 mol L^{-1} can be attained.

The above findings highlight the peculiar behavior and industrial significance of Ca^{2+} ions in strongly caustic aqueous solutions.

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Solubility without Borders

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Keywords: Liquid-liquid equilibrium; Solid-liquid equilibrium; Greener solvents; Sustainable separation processes

Solubility has been the central theme of my scientific career, guiding both fundamental research and the development of sustainable chemical processes. In this lecture, I will present my scientific journey, following the evolution of my research from solution thermodynamics and liquid-liquid equilibria involving ionic liquids to solid-liquid equilibria of eutectic systems, and later to the design of sustainable solvents and separation processes. Particular emphasis will be given to the development of new experimental methodologies for equilibrium measurements, the characterization of novel solvent systems, and the use of thermodynamic modelling to understand molecular interactions and guide solvent selection. I will also present examples showing how these fundamental studies support applications in greener separation processes, sustainable agriculture, biomass valorization, and plastic recycling. Overall, I hope to show the central role of solubility in addressing challenges across many applied fields and in enabling more efficient and sustainable chemical technologies.

Acknowledgements: This lecture reflects the work of many people who have been part of my scientific journey and whom I would like to thank: first, my PhD supervisors, Simão P. Pinho and João A. P. Coutinho, who taught me how to do good science; all my colleagues from the University of Aveiro, the Polytechnic University of Bragança, and the many institutions that welcomed me during my many research stays, especially in the Czech Republic, Poland, Brazil, India, and China. A special thank you to all my students, the most rewarding part of my scientific journey. If this lecture tells a story, it is a story about people.

Machine-learning aided metal-ion battery cyclic stability prediction

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Keywords: machine learning, statistics, redox-active materials

Recently, the data-driven methods for discovery have gained a significant popularity in the field of materials science. These methods rely on the processing of large amounts of experimental or theoretically-derived data and thus the access to well-structured datasets plays a crucial role for the successful application of such methods. Since the number of openly available datasets for metal-ion battery materials is fairly limited [1], the present study aims to utilize a previously developed energy-storage materials relational database for building different time-series machine learning models for cyclic stability prediction based on the cell performance during the first ten cycles.

All models were trained and validated on electrochemical data acquired by galvanostatic and potentiostatic cycling of redox-active organic compounds in lithium- and sodium-ion model electrochemical cells. This class of redox-active materials was chosen due to gainful properties in terms of energy density per unit of mass, environmental compatibility and structure tunability (i.e., organic compounds can be synthetically modified to attain maximal specific capacity) [2].

All of the proposed time-series machine learning algorithms were compared to select the most robust protocol for cyclic stability estimation.

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Solubility Thermodynamics of Sodium Ferulate in Aqueous Solutions at Temperatures 276.15 - 363.15 K

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Keywords: sodium ferulate, dissolution Gibbs energy, enthalpy, specific ion effects, salting-out, antioxidant

Determination of thermodynamic and antioxidative properties of natural or natural based mostly hydrophilic molecules such as polyphenols is necessary because of their bioactivity and bioavailability and paramount importance in green [1] and edible formulations, food chemistry, flavour and aroma chemistry, cosmetic and pharmaceutical industries. Hydrocynamic acid derivative - sodium ferulate – is important phenolic compound present in several plants with claimed beneficial effects in prevention and treatment of disorders linked to oxidative stress and inflammation. Sodium ferulate is constructed 5- HT-Receptor as a Target, the study In vitro [2,3] has shown inhibitory effect of sodium ferulate at the transcriptional level on the expression of some inflammatory mediators; in the studies In vivo possible antidepressant-like effect is shown, it's possible contribution of the serotonergic system (5- HT-Receptor subtypes). In this work solubility of sodium ferulate in water has been determined in the temperature range 276.15 - 363.15 K. The dependence of solubility of sodium ferulate at different pH adjusted from physiological (pH=7.4) to pH = 10.1 – 10.5 is measured and analyzed. The dissolving kinetics of commercial sodium ferulate and sodium ferulate received from ferulic acid is compared. Thermodynamic functions of dissolution (Gibbs energy, enthalpy and entropy) of sodium ferulate are analyzed in comparison with those ones of other natural phenolic compounds. The antioxidant effect of ferulate as radical-scavenging agent with high bond dissociation enthalpy on stabilization of oils of different oil groups such as vegetable oils, processing oils, and fragrance oil is studied. Ferulic acid has been shown to be classified as specific antioxidant: it is almost ineffective in peanut and linseed oil and very effective in Polyalphaolefine. Its effectiveness is comparable with effectiveness of lauryl gallate or propyl gallate in lubricants and exceeds considerably the effect of synthetic antioxidants as BHA, BHT, TBHQ. Specific ion effects to understand biophysical phenomena related to the Hofmeister series [4,5] of sodium ferulate are investigated in aqueous solutions of Poly(N-isopropylacrylamide) (PniPam) and egg white and compared with salting-out and salting-in properties of other polyphenols and aromatic compounds.

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Synthesis and Physico-Chemical Characterisation of Phosphonium and Ammonium Ionic Liquids for Rare Earth Recovery from Permanent Magnets

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Keywords: ionic liquids; rare earth elements; recycling; hydrometallurgy; permanent magnets

The growing demand for rare earth elements (REEs) in green technologies, combined with the environmental challenges of their primary production, has created an urgent need for sustainable recycling methods. One promising solution lies in the use of ionic liquids (ILs) as environmentally friendly extracting agents for REE recovery from permanent magnet waste. Furthermore, these ILs are intended for incorporation into polymer inclusion membranes (PIMs), where they will serve as selective carriers for the enhanced separation and transport of target REEs. In this work, we investigate a series of novel ILs designed for selective complexation of neodymium, praseodymium and dysprosium – key REEs in end-of-life magnets.

The following ILs were synthesised and comprehensively characterised: tetrabutylphosphonium salicylate, tetrabutylphosphonium thiosalicylate, tetrabutylphosphonium 8-hydroxyquinolate, tetrabutylphosphonium o-picolinate, tetrabutylphosphonium anthranilate, tetrabutylammonium 8-hydroxyquinolate and benzyltrimethylammonium 8-hydroxyquinolate. Structural characterisation was performed by NMR and FTIR spectroscopy. Thermal behaviour was investigated by differential scanning calorimetry (DSC). Key physico-chemical properties – density, viscosity and speed of sound – were determined, providing essential insight into intermolecular interactions and structure–property relationships.

Phosphonium-based ILs with salicylate, thiosalicylate and 8-hydroxyquinolate anions show particularly promising complexation behaviour, positioning them as viable candidates for replacing conventional hazardous organic solvents in future separation processes.

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Antitumoral activity of novel Cu(II)–peptide complexes

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Keywords: Cu(II)-peptide complexes, antitumor activity, cytotoxicity, antiproliferative activity, phototoxicity

Copper(II)-based coordination compounds have emerged as promising candidates for the development of novel anticancer agents, due to their favorable biological properties and the ability to form stable complexes with bioactive ligands. In the present study, novel Cu(II)-peptide complexes were synthesized and structurally characterized by FTIR spectroscopy, ICP analysis, elemental analysis, and powder X-ray diffraction.

The biological activity of the complexes was evaluated by evaluating their cytotoxic and antiproliferative effects on human breast cancer cell lines (MCF-7 and MDA-MB-231) and non-tumorigenic breast epithelial cells (MCF-10A). Cytotoxicity was further determined using the BALB/3T3 Neutral Red Uptake assay. All compounds showed concentration-dependent biological activity. Phototoxicity tests show that the Photo-Irritation Factor (PIF) values are below the phototoxicity threshold, indicating a favorable safety profile.

The results obtained indicate that complexation of peptide ligands with Cu(II) ions is a promising approach for the development of new metal compounds with antitumor potential and low phototoxic risk.

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Understanding solubility product (K_{sp}) from the perspective of pseudo-equilibrium

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Keywords: ion product; structural unit; multi-unit particle; particle surface; precipitation reaction

Here we present a way of describing the precipitation reaction of sparingly soluble electrolytes, applicable to both pseudo-equilibrium and equilibrium systems.

Let $A_{rm0}B_{m0}$ ($m_0 \geq 1$) be the structural unit of a multi-unit particle $(A_{rm0}B_{m0})_u$, where $u \geq 1$ is the number of structural units in the particle. Then the precipitation reaction and relevant dissociation constant are expressed as follows:



$$K_{d,u} = (IP)_0^{m_0} / [(A_{rm0}B_{m0})_u]^{1/u} \quad (2)$$

$$(IP)_0 = [A]^r \cdot [B] \quad (3)$$

Given the relationship $(A_{rm0}B_{m0})_u = u(A_{rm0}B_{m0})$ in solution chemistry, we rewrite eqn (1) as eqn (4). The relevant dissociation constant ($K_{d,m0}$, eqn (5)) relates the ion product to the structural unit. By convention, the structural unit represents the whole particle.



$$K_{d,m0} = (IP)_0^{m_0} / [A_{rm0}B_{m0}] \quad (5)$$

But, as found in the pseudo-equilibrium systems, the ion product responds directly to the particle surface, rather than to the whole particle.^[1] To account for the fact, we designate $A_{rm}B_m$ ($0 < m \leq m_0$) as the surface proportion per structural unit and express the reaction of the entire surface of a particle as follows:



$$K_{d,m} = (IP)_0^m / [A_{rm}B_m] \quad (7)$$

$$\ln[A_{rm}B_m] = m \cdot \ln(IP)_0 - \ln K_{d,m} \quad (8)$$

The slope (m) of a $\ln[A_{rm}B_m]$ vs. $\ln(IP)_0$ plot decreases with increasing structural units (u) during crystal growth, consistent with the prediction made by the particle-surface equation^[1]:

$$u \left(\frac{m}{m_0} \right)^d = 1 \quad (\text{the dimension of the particle } d = 3) \quad (9)$$

When the reaction attains equilibrium, the parameter m approaches a small value; the u value is accordingly large enough to reduce eqn (2) to eqn (10), where K_{sp} may be related to the $\Delta G^\ominus$ of $(A_{rm0}B_{m0})_u$ formation. Because the precipitate at this stage differs from that initially emerging from solution, the inequality “ion product $> K_{sp}$ ” is not the apposite criterion for precipitation occurrence.

$$K_{sp} = K_{d,u} \big|_{u \rightarrow \infty} = (IP)_0^{m_0} = \text{solubility product} \quad (10)$$

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THEREDA – Thermodynamic Reference Database

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Keywords: Thermodynamic database, Nuclear waste management, Oceanic salts, Pitzer approach Speciation, Solid-liquid phase equilibria

The Thermodynamic Reference Database (THEREDA) is designed for geochemical calculations in the context of repositories for radioactive waste under high-saline conditions. For this purpose, it adopts the Pitzer ion-interaction approach. THEREDA is currently the only database worldwide that allows comprehensive polythermal calculations (up to at least 100 °C) of the hexary system of the oceanic salts Na-K-Mg-Ca-Cl-SO₄-H₂O, including acids, bases, and CO₂/carbonates. Its validity is documented primarily, yet not exclusively, by application to solubility data. THEREDA's potential to predict the development of the geochemical environment, e.g. in the event of an intrusion of solution, constitutes a prerequisite for the engineering design of a nuclear waste repository with regard to the selection and placement of plug and sealing system components.

The focus of THEREDA lies on the calculation of solubilities of radionuclides (actinides, fission and activation products), chemotoxic and matrix elements e.g., canister materials, and compounds having an impact on the overall geochemical milieu in the near field of a repository under high-saline conditions.

Special features of THEREDA besides its focus on high-saline solutions are procedures for testing prior to any release combined with intercode-comparison, extensive and publicly available validation against published experimental data, and systematic application of a scheme to mark data with regard to quality, reliability, and origin. Traceability of data and validated experimental results to published sources is also emphasised. This documentation is in part realised in ready-to-use parameter files for users, and in part on the website (www.thereda.de). Another feature is the possibility for operation of THEREDA by several institutions in a net-worked manner.

To highlight THEREDA's potential, examples for applications of the database and a detailed description are given in [1].

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Comparative Assessment of Corrosion Dynamics and Metal Ion Release from Orthodontic Archwires in Biomimetic Oral Environments

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Keywords: Orthodontic archwires, Saliva models, Ion release, Trace element analysis, Multivariate analysis

The long-term biocompatibility of orthodontic archwires depends heavily on their corrosion resistance and subsequent ion release within the environment of the oral cavity. To evaluate such dynamics, the present study compared the degradation profiles of five commercially available orthodontic archwires – specifically Stainless Steel (Cr-Ni-Fe), Ni-Ti, Cu-Ni-Ti, a complex multi-force Cr-Ni-Ti-Fe, and Ti-Nb – exposed to two distinct environments over a 7-day incubation period: a high-salinity electrolyte model (Saliva 1, pH 7.0) and a biomimetic model enriched with mucin and organic compounds, including urea, glucose and ascorbic acid (Saliva 2, pH 6.4).

Due to nanogram-range analyte concentrations, direct quantification required Total Reflection X-Ray Fluorescence (TXRF) with a Ga internal standard to overcome matrix effects. For Saliva 2, an organic matrix digestion with HNO₃ was performed and verified by Flame Atomic Absorption Spectrometry (FAAS). Principal Component Analysis (PCA) on z-scores was then used to isolate subtle matrix-alloy interactions.

Released concentrations of Cr, Ni, Fe, and Cu remained low (0.005 mg L⁻¹ – 0.08 mg L⁻¹), while Ti fell below detection limits (< 0.01 mg L⁻¹), confirming passivating TiO₂ stability. Saliva-dependent variations mostly fell within experimental uncertainty, indicating high baseline stability. However, PCA (81.6% variance expanded) isolated a significant matrix effect for Ni-Ti: the slightly acidic, organic-rich Saliva 2 accelerated Ni dissolution (0.009 ± 0.001 mg L⁻¹) compared to Saliva 1 (0.006 ± 0.001 mg L⁻¹), driven by glycoprotein bio-complexation and organic molecule interactions at pH 6.4. The multi-force Ni-Ti-Fe-Cr archwires showed the lowest corrosion resistance, yielding peak concentrations of Fe (0.08 mg L⁻¹) and Cr (0.03 mg L⁻¹) regardless of the media.

Based on a standard salivary flow rate of 1.5 L/day, the maximum daily systemic exposure was 13.5 µg/day for Ni and 46 µg/day for Cr. These values are orders of magnitude below the 300 µg/day Tolerable Daily Intake (TDI) limit established by the WHO and EFSA. In conclusion, the minimal ion release poses no toxicological risk, confirming the excellent clinical biocompatibility of the tested archwires.

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Dissolution of (Cu, Zn) Doped Calcium Phosphates in Solution with Demineralization Activity

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Keywords: Dissolution, (Cu, Zn) Doped ACP, modified β -TCP, calcium phosphates

Calcium orthophosphates exhibit chemical and structural similarities to the inorganic component of biological apatite, making them suitable for the development of biomaterials for dental and regenerative medicine. Ion modification of calcium phosphates improves their biological properties.

In the present study, the behavior of double-doped (Zn, Cu) amorphous calcium phosphate (ACP) and its calcined product obtained at 600 °C was investigated in a demineralization-active solution. The aim was to evaluate the response of as-synthesized calcium phosphates in a biomimetic, low-pH environment that simulates conditions associated with bacterial sugar metabolism in the oral cavity, a process that can promote tooth demineralization and caries formation. A solution composed of 0.1 mol·L⁻¹ lactic acid, 2.2 mmol·L⁻¹ NaH₂PO₄, 2.2 mmol·L⁻¹ CaCl₂, and 0.005 mmol·L⁻¹ NaF, with the pH set to 4.5, was chosen as a demineralizing agent, as this solution has been used in literature to simulate artificial lesions on extracted teeth. ACP was prepared by continuous precipitation from initial solutions containing CaCl₂, CuCl₂, ZnCl₂, and K₂HPO₄, followed by 1 h maturation, washing, and lyophilization. The calcined phase was obtained after a one-hour stay at 600 °C. The results showed that ACP transformed into a biphasic mixture of (Cu, Zn)- β -tricalcium phosphate (TCP) and hydroxyapatite (HA) during the heating.

Kinetic studies of the dissolution of the (Cu, Zn)-ACP in demineralization active solution showed that during the first 10 min of immersion, the concentrations of all three cations increased sharply in the solution, with the most pronounced increase observed for Ca ions, followed by Cu and Zn ions. Subsequently, their concentrations decrease by the 6th hour and plateau by the 72nd hour. The behavior of the biphasic mixture was different, as evidenced not only by an increase in the concentration of ions in the solution, but also by higher concentrations of Cu²⁺ and Zn²⁺ released from the biphasic mixture than from the ACP. We explain this phenomenon by the different local structure of the two materials. In ACP, Cu²⁺ and Zn²⁺ ions can be incorporated into a highly disordered calcium-phosphate network, thus being able to bind them more strongly. After heat treatment, local rearrangement occurs, copper and zinc coordination changes, and some ions become more exposed to the solution. As a result, they may become kinetically more readily leached out despite the matrix becoming more crystalline.

Acknowledgments: The authors thank the Bulgarian Ministry of Education and Science for the financial support under the project KP-06-H99/7/2025.

Insights into the Thermodynamics and Kinetics of Double-Doped Amorphous Calcium Phosphate Formation and Its Response in Artificial Saliva

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Keywords: calcium phosphate, simulated body fluid, artificial saliva, doped calcium phosphates

The effects of the electrolyte environments of simulated body fluid (SBF) and artificial saliva (AS), as well as the inclusion of low-molecular-weight organic acids, on the chemical and phase composition of biomimetic precipitated calcium phosphates double-doped with Mg and Zn were studied. Glycine (Gly) and valine (Val) were chosen as organic additives because amino acid residues are involved in the structure of non-collagen proteins and have also been found to be present in blood plasma. Two complementary approaches are applied: a thermodynamic approach to predict system behavior and various experimental synthesis routes. Thermodynamic modeling of chemical equilibria in the SBF/AS-NaCl-CaCl₂-MgCl₂-ZnCl₂-K₂HPO₄-H₂O and SBF/AS-NaCl-CaCl₂-MgCl₂-ZnCl₂-K₂HPO₄-Gly/Val-H₂O systems at pH 6.5, close to the AS, pH 7.5, close to the SBF, and 8.5 allows us to predict that the same calcium phosphates will precipitate in both biomimetic media, irrespective of electrolyte environment and the presence of Gly and Val. The latter affects the chemical composition of the precipitates.

The results of the thermodynamic prognosis were proved experimentally. The experimental study shows only the precipitation of X-ray amorphous, cation-deficient calcium phosphate at pH 8–8.2, independent of the electrolyte medium, the presence of organic molecules, and the sequence of initial solution mixing. The constant pH during the syntheses and kinetic rather than thermodynamic factors are decisive for the precipitation of amorphous products. The concentration of Mg in the amorphous phase varies from 5.86 to –8.85 mol% and of Zn from 0.71 to –2.84 mol%, being the lowest in the sample obtained in the presence of Gly. The content of doped ions depends on complexation in solution. The greater the number and more stable complexes formed in the solution, the lower the concentration of Zn and Mg in the solid phase.

Furthermore, the release of Ca²⁺, Mg²⁺, and Zn²⁺ ions from selected samples into an artificial saliva solution was analyzed to assess their potential to promote enamel remineralization. Upon contact with artificial saliva, the amorphous product dissolves during the first 6 h, releasing ions, after which reverse deposition and recrystallization begin. The higher concentrations of Zn and Mg stabilize the amorphous phase and slow its transformation into hydroxyapatite. Thirty days are not enough for a complete phase transformation into nanocrystalline hydroxyapatite.

Our research can serve as a basis for further in-depth in vitro studies of the remineralization potential of calcium phosphates double-doped with Zn and Mg.

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Spectroscopic data treatment for the binding of small molecules to nucleic acids and proteins

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Keywords: inner filter effects, binding constant, software, metal complexes, fluorescence

Transforming metal ions and Low-cost Ligands into next generation metallodrugs (TRILLI) is a national project that aims at unveiling key aspects for a rational design of new metal complexes (MCs) and boost their development as metallodrugs. TRILLI will, inter alia, determine the binding of several selected low-cost MCs to biomolecules, examine the relationships between the biological activity and thermodynamic stability of the MCs and investigate the role of the organic ligands. Essential elements such as iron [1], copper [2] and zinc [3], that are currently being tested, are considered. We present here the results obtained for the binding of a panel of metal complexes made from different metal centers (Cu^{2+} , Zn^{2+} , Fe^{3+}) and the ligands shown below (Figure 1) to bovine serum albumin (BSA) and to DNA G-quadruplexes of different topologies.

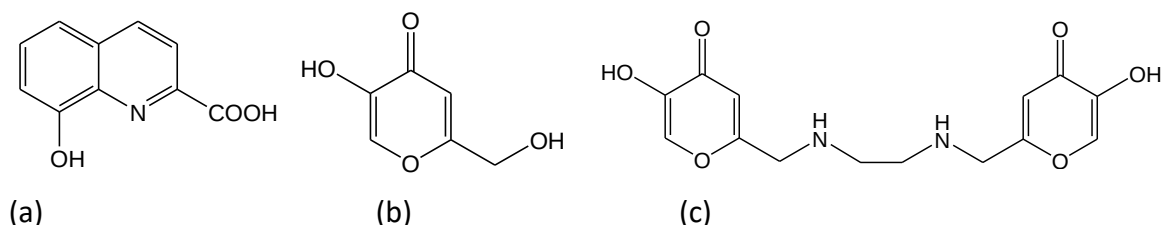


Figure 1. The ligands considered in this study: (a) 8-hydroxyquinoline-2-carboxylic (8-HQA); (b) kojic acid (KA); (c) 2,2'-(ethane-1,2-diylbis(iminomethanediyl))bis(5-hydroxy-4H-pyran-4-one) (S2).

The contribution will talk about the practical aspects of data treatment connected to fluorescence measurements, done to investigate the binding of the MCs to albumin protein and to DNA G-quadruplexes. Check and correction for inner-filter effects and use of software for the evaluation of the binding constant will be discussed.

Acknowledgements: Project PRIN2022 - Prot. 2022APCTNA "TRILLI" is gratefully acknowledged. The ISMeC Group (International Group for the Thermodynamics of Metal Complexes, www.ismecgroup.org) is acknowledged for fruitful discussion, scientific exchanges and support.

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Modeling Solid–Liquid Equilibria to Predict Drug Solubility in Pharmaceutical Solvents

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Keywords:

This study focuses on the modeling of solid–liquid equilibria (SLE) in binary systems across a range of solvents and temperatures, using advanced thermodynamic models such as NRTL and UNIFAC. Two solutes, namely 2-hydroxybenzoic acid and N-(4-hydroxyphenyl)acetamide, were investigated in various solvents, including Ethyl Acetate, Acetone, Water, Acetic Acid, Methanol, Propanol, and Butanol. The application of the NRTL model requires interaction parameters, which are often unavailable in the literature; therefore, this work calculated these parameters for the considered systems. Comparison of the modeled phase diagrams with experimental data from the literature demonstrated excellent agreement, particularly for the NRTL model, whereas the UNIFAC model, which is based on the group contribution concept, provided only approximate predictions due to its inherent assumptions.

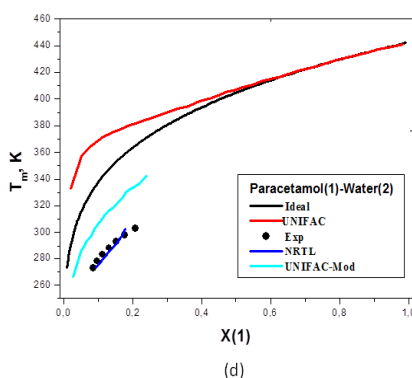


Figure 1 Solubility of Paracetamol in Water

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Thermodynamic Aspects of Cd(II) Adsorption onto Vine Rod-Derived Biochar

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Keywords: vine rod biochar; Cd(II) adsorption; thermodynamic analysis

Cadmium contamination of aquatic systems remains an important environmental concern due to the toxicity and persistence of Cd(II) ions. In recent years, biochar materials derived from agricultural residues have attracted increasing attention as sustainable adsorbents for heavy metal removal from aqueous solutions [1–3]. In the present study, thermodynamic aspects of Cd(II) adsorption onto vine rod-derived biochar were investigated. The adsorbent was obtained by slow pyrolysis of lignocellulosic vine rod residues and applied for Cd(II) removal from aqueous media under different temperature conditions. The experimental workflow of biochar preparation, adsorption procedure, filtration, and ICP-MS determination of Cd(II) ions is illustrated in Figure 1.

Thermodynamic parameters were evaluated to assess the energetic characteristics and spontaneity of the adsorption process. Thermodynamic parameters obtained by nonlinear evaluation were additionally compared with values previously determined using linear adsorption analysis [4], allowing assessment of the influence of the calculation approach on the thermodynamic interpretation of the adsorption process. The obtained results indicate favorable interaction between Cd(II) ions and the porous carbonaceous structure of the investigated biochar. The study confirms the applicability of vine rod-derived biochar as a low-cost and environmentally sustainable adsorbent for water purification purposes.

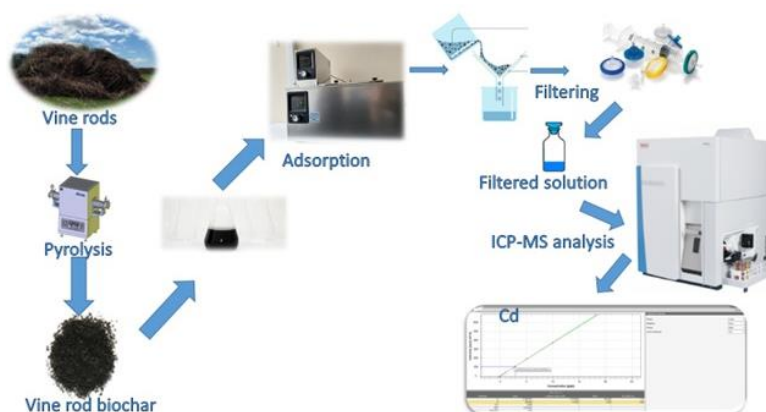


Figure 1. Experimental workflow for Cd(II) adsorption onto vine rod-derived biochar and ICP-MS analysis

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Cellulose-Based Adsorbent for Wastewater Dye Treatment

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Keywords: Wastewater treatment; azo dye removal; modified cellulose; adsorption thermodynamics; adsorption kinetics; agricultural biomass

The textile industry is a major source of highly contaminated wastewater, posing serious environmental concerns due to the presence of synthetic dyes that are frequently discharged after incomplete fixation during dyeing processes. Orange G, an anionic azo dye, is known for its high chemical stability and potential toxicity, making its efficient removal from aqueous media essential.

Among various treatment methods, adsorption is considered one of the most efficient, cost-effective, and environmentally friendly approaches for dye removal. In this study, a novel cellulose-based adsorbent was developed for the removal of Orange G from aqueous solutions. Einkorn husks were used as a renewable raw material for cellulose extraction through alkaline treatment and bleaching. The extracted cellulose was chemically modified with N, N-dimethyl-1-octadecylamine, resulting in surface cationization and enhanced affinity toward negatively charged dye molecules. The structural and surface properties of the modified material were characterized by XRD, DTA, FTIR, SEM, and low-temperature nitrogen adsorption analyses. The results confirmed increased porosity and successful grafting of quaternary ammonium groups onto the cellulose structure.

The adsorption performance was evaluated through batch experiments by investigating the effects of contact time, pH, temperature, and initial dye concentration. Adsorption equilibrium was reached within approximately 30 minutes, indicating favorable kinetics. Experimental data were analyzed using pseudo-first-order, pseudo-second-order, and intraparticle diffusion kinetic models, while equilibrium data were fitted to Langmuir, Freundlich, and Dubinin–Radushkevich isotherms.

The adsorption process was best described by the pseudo-second-order kinetic model and the Langmuir isotherm, suggesting chemisorption and monolayer adsorption. Thermodynamic analysis indicated that the adsorption process is spontaneous and exothermic.

In conclusion, the developed cationized cellulose material demonstrates strong potential as an efficient and sustainable adsorbent for Orange G removal from aqueous media, while also highlighting the value of converting agricultural waste into functional materials for wastewater treatment.

Acknowledgements: Research equipment of the Distributed Research Infrastructure INFRAMAT, part of the Bulgarian National Roadmap for Research Infrastructures, supported by the Bulgarian Ministry of Education and Science, was used in this investigation.

Comparative Assessment of the Hydrochemical Characteristics of Pomorie Lake (Bulgaria)

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Keywords: Pomorie Lake; hydrochemistry; hypersaline lake; major ions; nutrients;

Pomorie Lake is one of the largest coastal hypersaline lagoons along the Bulgarian Black Sea coast and represents a unique ecosystem of high ecological and economic importance. This study presents a comparative assessment of the hydrochemical characteristics of the lake based on monitoring data collected during 2014–2016 and 2024–2026, with emphasis on salinity dynamics, physicochemical parameters, major ions, and nutrient concentrations.

The results reveal pronounced temporal variations in salinity, primarily controlled by climatic conditions and the hydrological regime. Salinity decreased from 27‰ in December 2014 to 14.4‰ in June 2015 following intense precipitation and remained relatively low (approximately 16‰) in April 2016. During 2024–2026, salinity gradually recovered from an average of 26.6‰ in November 2024 to approximately 36‰ in May 2026, corresponding to the characteristic salinity of the lake. Throughout the investigated periods, the water remained slightly alkaline (pH 7.24–8.93), while alkalinity increased considerably during 2024–2026 (128–266 mg CaCO₃ L⁻¹).

The concentrations of major ions (Na⁺, K⁺, Ca²⁺, Mg²⁺, Cl⁻, and SO₄²⁻) closely followed salinity fluctuations, with the highest sodium (13,317 mg L⁻¹) and chloride (23,854 mg L⁻¹) concentrations recorded during the high-salinity period in May 2026. No significant differences were observed between surface (10 cm) and deeper (100 cm) water samples, indicating efficient vertical mixing of the water column.

The most pronounced changes were found in nutrient concentrations. During 2014–2016, nitrogen species remained low and generally below environmental limits. In contrast, monitoring during 2024–2026 revealed substantial enrichment with ammonium nitrogen, with concentrations exceeding the regulatory limit by up to twelve times at several sampling sites, indicating increasing anthropogenic influence. Phosphate concentrations, which were previously low or only slightly elevated, increased markedly by May 2026, reaching values up to four times above the permissible limit in coastal areas.

The comparison demonstrates that while the major ionic composition of Pomorie Lake remains relatively stable and primarily reflects natural salinity variations, nutrient enrichment has intensified in recent years, suggesting increasing anthropogenic pressure and deterioration of water quality

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Lithium in Thermal Mineral Waters in Southern Bulgaria

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Keywords: lithium, thermal waters, mineral waters, geological factors, chemical species

Over the past decade, lithium has established itself as a strategically important element, critical to the production of batteries for electric vehicles and energy storage systems. Its chemical properties and relatively low abundance in the Earth's crust (Li Clarke, according to various authors, 20–65 g/t) make it difficult to discover economically important deposits and extract it. Traditional methods for extracting lithium from rock formations are associated with significant environmental damage and high economic costs. An alternative approach is the extraction of waters with an increased concentration of lithium - a technology that is assessed as more environmentally friendly and more sustainable.

The present study aims to analyze and systematize data on the content of lithium in the thermal waters of Southern Bulgaria, by tracing the factors determining its solubility, migration and chemical species in the aquatic environment. Over 400 results of chemical analyses of thermal waters from 146 deposits and water manifestations have been processed. The results obtained enable the localization of zones with increased lithium concentrations (Fig. 1) and the assessment of the influence of geological factors on their distribution. An assessment of the chemical composition of the waters and the physicochemical conditions governing lithium behavior was conducted. Through thermodynamic modeling, the chemical species of lithium migration in the thermal waters were determined, along with the conditions for the dissolution and possible deposition of lithium-containing mineral phases.

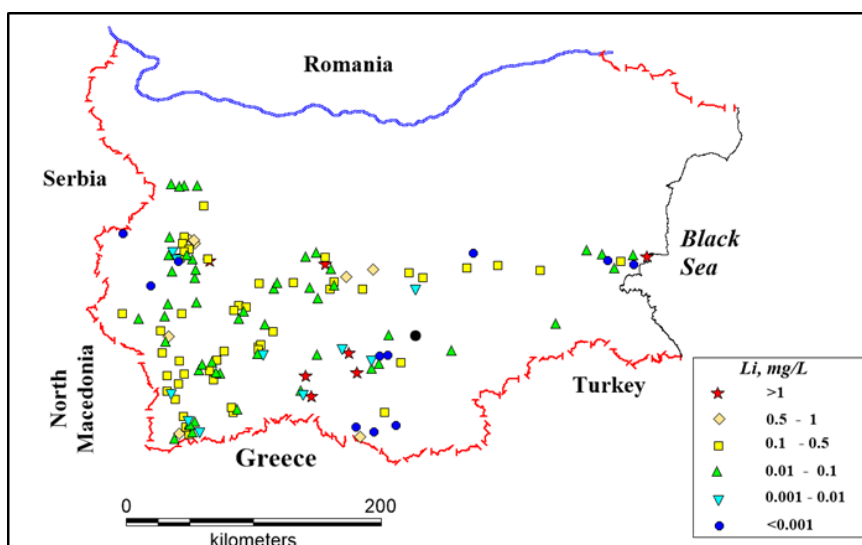


Fig. 1. Lithium content in the thermal mineral waters of southern Bulgaria

Acknowledgments: The authors thank the Bulgarian Ministry of Education and Science for the financial support under the project KP-06-H94-2/2025.

The effect of chemical extraction reagents on the determination of plant-available forms of P_2O_5 in High energy milled Phosphorite

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Keywords: Phosphorite, Ecological processing, High energy milled activation, Extraction reagents

Under the European Union's Critical Raw Materials Act (CRMA), which entered into force in 2024 and remains the governing framework for 2025, the EU recognizes 34 Critical Raw Materials (CRMs) and a subset of 17 Strategic Raw Materials (SRMs) that are considered especially important for the green transition, digital technologies, defense, and aerospace. The CRMA group includes P and phosphate rocks.

Phosphate-rich rocks like phosphorite have strategic significance, particularly due to their wide application in the agricultural sector. They are primarily used for the extraction of phosphorous for fertilizer production, essential for food production and plant growth. However, traditional processing methods require the use of acids, which in turn leads to the production of greenhouse gases and solid waste such as phosphogypsum.

The object of this study is a phosphate rock originating from Western Asia (Syria) with CaO- P_2O_5 -SiO₂ contents as follow: 46.5–48.4% CaO, 29.0–29.6% P_2O_5 , and 7.3% SiO₂. The samples were activated with 5, 10, and 20 mm Fe milling balls using a planetary ball mill (Pulverisette–5, Fritsch Company, Germany) for varying durations ranging from 30 to 300 minutes. The effect of HEM activation was evaluated by determining the available forms of P_2O_5 using different extractants—2% citric acid and Petermann's solution.

The aim of the research in this study is to investigate the influence of the extractants on the determination of the mobile forms of P_2O_5 in HEM-activated samples of natural calcium phosphate—phosphorite. Solving this problem will allow, on the one hand, an assessment of the effectiveness of the method used for P_2O_5 extraction and the effectiveness of the activation parameters during the treatment of the phosphate rock.

The results obtained show that the method applied for treating the natural raw material increases the conversion rate of total P_2O_5 into a form available to plants, with 2% citric acid demonstrating better effectiveness as an extraction reagent.

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Effect of Ce-doping on the photocatalytic activity of SrTiO₃

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Keywords: water purification, perovskites, photocatalysis

Environmental pollution and the need for effective removal of contaminants from air, soil, and water remain among the most pressing challenges in modern scientific research. In particular, water contamination with organic compounds poses a serious problem due to their persistence and slow degradation. Photocatalytic processes have emerged as a promising and efficient approach for water purification. In this context, significant efforts are directed toward the development of new catalysts that are capable of degrading model organic pollutants such as dyes and antibiotics under various conditions. Materials based on SrTiO₃ have attracted considerable attention in this field. Therefore, the development of cost-effective and reliable methods for achieving tailored properties and better catalytic activity is of great importance.

In this study, a series of perovskite-based catalysts with the general formula Sr_{1-x}Ce_xTiO₃ were synthesized using a Pechini method. The incorporation of Ce³⁺ ions into the structure leads to the formation of various types of defects within the crystal lattice. The obtained materials were characterized by various physicochemical techniques. Subsequently, the catalytic performance was evaluated for the degradation of organic pollutants. The influence of the aqueous matrix on the catalytic process was also investigated, and based on the experimental results, a reaction mechanism was proposed.

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In-situ monitoring of gas evolution in symmetric cells for sodium-ion batteries

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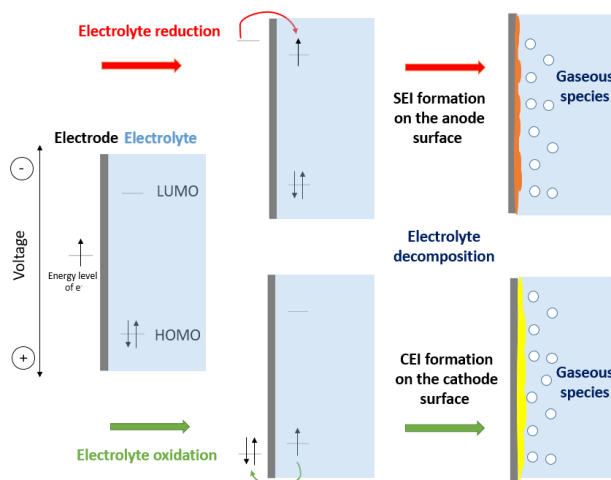
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Keywords: Na-ion batteries, OEMS, Symmetrical cell, Layered oxides

Layered sodium transition-metal oxides are among the most widely investigated cathode materials for Sodium-ion batteries (SIBs) because of their ability to provide high specific capacities by operation at high voltages. At elevated potentials, during the first charging of the cell, a protective solid layer, known as cathode electrolyte interphase (CEI) is formed on the surface of the electrode. In general, CEI in SIBs is considered to be less robust than the one formed in lithium-ion batteries (LIBs) due to its higher solubility in the electrolyte and the lower redox potentials of Na. Such instability can initiate parasitic interfacial reactions, leading to gas evolution, which in turn cause cell swelling and increased risk of the safety issues. The present study aims to investigate the gaseous species formed during the operation of symmetrical electrochemical cells utilizing Online Electrochemical Mass Spectrometry (OEMS) instrumentation. The cathode material $\text{Na}_{0.67}\text{Ni}_{0.5}\text{Mn}_{0.5}\text{O}_2$ was synthesized in P3-layered structure and was employed simultaneously as positive and negative electrode in the cells. This methodology ensures that the detected gases are limited only to the interaction between the target material and the electrolyte. Two different electrolytes composed of 1 M NaPF_6 and 1 M NaClO_4 both dissolved in propylene carbonate were investigated. The observed gasses at 25°C were H_2 , CO_2 and propene (C_3H_6) during charging of the cell and O_2 during discharging. The most pronounced gas detection was attributed to the CEI formation above 4.0V (vs Na^+/Na). No major differences in the gas evolution between the two electrolytes was noticed.



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Synthesis and characterization of Pd–Co modified ZSM-5 zeolite catalysts for methane oxidation-influence of Si/Al ratio

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Keywords: synthesis, Pd–Co modified ZSM-5 zeolite catalysts, methane, oxidation

Catalytic methane combustion is an efficient and more environmentally sustainable alternative to traditional thermal combustion processes, offering a way to reduce greenhouse gas emissions. Among the most commonly used catalysts for this reaction are Pd/Al₂O₃ systems, which are highly active but suffer from deactivation, particularly in the presence of water vapour. On the other hand, zeolites have emerged as promising catalyst supports due to their large surface area, thermal stability, and their ability to effectively disperse active metal particles, thereby improving catalytic efficiency.

In this study, monometallic and bimetallic catalysts were synthesized using ZSM-5 supports with different Si/Al ratios (15, 23, 40, and 50) and silicalite-1 via impregnation with Co(NO₃)₂·6H₂O and Pd(NO₃)₂·2H₂O solutions. Both metals were simultaneously deposited in the bimetallic catalysts by co-impregnation. The palladium content in all samples was approximately 0.5 wt%, while the cobalt loading in the bimetallic catalysts was 0.25 wt%. The catalysts were further characterized by N₂-physisorption, X-ray diffraction (XRD), temperature-programmed reduction in hydrogen (H₂-TPR) and methane (CH₄-TPR), temperature-programmed oxygen desorption (O₂-TPD), X-ray photoelectron spectroscopy (XPS), and high-resolution transmission electron microscopy (HRTEM). Detailed kinetic studies were also performed to gain a better understanding of the reaction mechanism and catalytic behavior of the system.

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Synthesis and Characterization of NPs-Modified Multifunctional Cotton Materials

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Keywords: sol-gel, nanoparticles, cotton

The development of smart textiles offers innovative solutions for protective clothing, environmental remediation, and healthcare. This study demonstrates a facile, efficient sol-gel methodology for the synthesis and subsequent deposition of pure and rare-earth-doped titanium dioxide nanoparticles (NPs) onto cotton fabrics. To investigate the effects of lanthanide incorporation, four samples were prepared: pure TiO₂, 2% Gd-TiO₂, 2% Ho-TiO₂, and 2% La-TiO₂.

The modified textile materials were successfully characterized to confirm their structural, optical, and morphological properties. X-ray diffraction (XRD) confirmed the crystalline phases of the TiO₂ and cellulose matrices, while Fourier Transform Infrared spectroscopy with Attenuated Total Reflectance (FTIR - ATR) verified the successful immobilization and chemical interaction of the NPs with the cotton cellulose fibres. UV-Visible diffuse reflectance spectroscopy (UV-Vis) was successfully utilized to investigate the optical properties and reflectance behaviour of the modified textiles, demonstrating the influence of Gd, Ho, and La incorporation on the light-absorption profile of the fabrics. Scanning Electron Microscopy coupled with Energy Dispersive X-ray Spectroscopy (SEM-EDS) confirmed the homogenous distribution of the nanoparticles across the fabric surface alongside accurate elemental composition.

Ultimately, the successful integration of these tailored nanoparticles via a straightforward processing route yields modified cotton materials with significant potential for possible practical applications in photocatalytic self-cleaning, UV radiation shielding, and antimicrobial textiles.

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Optimizing synthesis parameters of decorated TiO₂ and TiO₂ nanotubes

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Keywords: TiO₂ nanoparticles, TiO₂ nanotubes, hydrothermal synthesis, BaTiO₃ nanocrystals, surface decoration, interrupted hydrothermal treatment

This study investigates a strategy for the surface decoration of TiO₂ nanoparticles and TiO₂ nanotubes with BaTiO₃ nanocrystals by optimizing the key synthesis parameters governing nanotube formation and subsequent BaTiO₃ deposition. Although hydrothermal synthesis of TiO₂ nanotubes and BaTiO₃/TiO₂ heterostructures has been widely reported, limited attention has been given to optimizing interrupted hydrothermal synthesis routes for nanotube formation prior to surface modification.

TiO₂ nanoparticles were synthesized by the controlled hydrolysis of TiCl₄, while TiO₂ nanotubes were prepared via alkaline hydrothermal treatment followed by proton exchange. An interrupted hydrothermal synthesis strategy was explored by varying the number of treatment cycles and the hydrothermal temperature to optimize nanotube formation, morphology, structural integrity, and yield.

As a subsequent step, preliminary experiments on the in situ deposition of BaTiO₃ nanocrystals onto TiO₂ nanoparticles and TiO₂ nanotubes will be initiated to assess the feasibility of the proposed surface modification strategy and to guide further optimization.

Acknowledgements: Project No. 59-14, "Synthesis and Investigation of Inorganic Nanoporous Materials".

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Synthesis, Characterization and Antimicrobial Behavior of TiO₂/TeO₂/CuO Sol–Gel Nanopowders

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Keywords: sol-gel, characterization, nanopowders, antimicrobial activity

This research aims to advance the development of metal-based antimicrobial materials by investigating how synthesis parameters and chemical composition influence the functional properties of sol–gel-derived TiO₂/TeO₂/CuO powders. The integration of the sol–gel method with controlled heat treatment provides a versatile and tunable approach for engineering nanomaterials suitable for healthcare applications and antimicrobial surface coatings.

Two samples were investigated: a ternary one with the nominal composition 80TiO₂/10TeO₂/10CuO and a binary one - 80TiO₂/20CuO. Following gel drying, both samples were thermally treated at 600 °C for 2 hours. Their structural and optical characteristics were examined using X-ray diffraction (XRD), scanning electron microscopy (SEM), UV–Vis spectroscopy, and infrared (IR) spectroscopy. Surface morphology and homogeneous elemental distribution were further assessed through SEM imaging and EDX mapping. Antibacterial activity against *Escherichia coli* ATCC 25922 was evaluated using minimum inhibitory concentration (MIC) assays and spot tests. This Gram-negative bacterium is frequently associated with antibiotic resistance and hospital-acquired infections, providing additional motivation for its selection as a test organism.

The observed antibacterial response against *E. coli* confirms the functional activity of the synthesized powders and supports their potential for further development as antimicrobial materials.

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Sol – Gel Preparation of TiO₂/SiO₂/CeO₂ Nanopowders

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Keywords: sol-gel, powders, characterization

The sol–gel synthesis of nanopowders has attracted significant attention due to the enhanced structural, optical, and thermal properties of mixed oxide nanomaterials. In this study, yellow-colored TiO₂/SiO₂/CeO₂ nanopowders were successfully prepared using the sol–gel method by employing suitable metal alkoxides and cerium nitrate as precursors under controlled hydrolysis and condensation reactions. The main objective of this work was to establish a correlation between the synthesis method and the resulting properties of the powders. In order to obtain useful information regarding phase formation and thermal stability, the as-prepared powders were calcined at elevated temperatures.

Structural characterization by X-ray diffraction (XRD) confirmed the amorphous nature of the powders up to 600 °C, while nanocrystalline mixed oxide phases were formed at higher temperatures. Differential thermal analysis (DTA) revealed the thermal stability, and decomposition stages of the prepared gels. UV–Visible spectroscopy (UV–Vis) studies indicated shifting of the absorption edge to the higher wavenumbers. Fourier Transform Infrared (FTIR) spectroscopy confirmed the presence of Ti–O–Ti, Si–O–Si, and Ce–O bonding vibrations, demonstrating the successful formation of the composite structure. The results confirmed that the sol–gel method is an effective route for producing homogeneous TiO₂/SiO₂/CeO₂ nanopowders with enhanced structural and optical characteristics, making them promising candidates for advanced photocatalytic and optoelectronic applications.

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EPR Evidence of Structural Degradation and Particle Size Reduction in Cycled P2- and P3-Layered Oxides

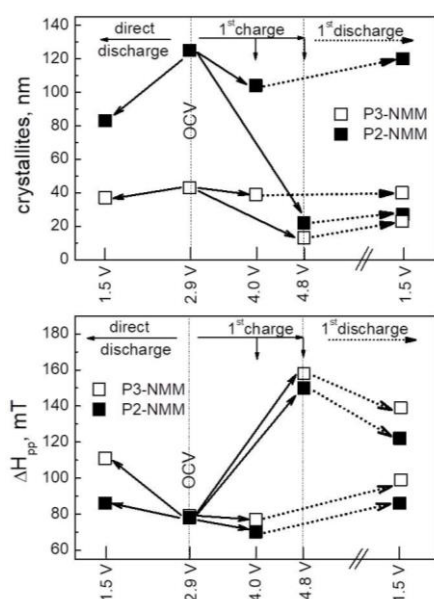
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Keywords: EPR, EPR linewidth correlations, electrochemistry, phase transitions, electrochemical "pulverization"

Layered oxides with chemical composition $\text{Na}_{2/3}\text{Mg}_{1/3}\text{Mn}_{2/3}\text{O}_2$ were synthesized in two polymorphic structures, specifically P2 and P3. Galvanostatic analysis was performed within a narrow voltage window (1.5-4.0 V), where severe phase transitions were avoided, and within an extended window with an upper voltage of up to 4.8 V. While the extended window enhanced the gravimetric capacity, severe structural degradation was triggered. We used Electron Paramagnetic Resonance (EPR) and X-ray powder diffraction (XRPD) to evaluate structural changes in electrodes cycled under different galvanostatic conditions across both voltage ranges.



The focus of the current study was set on the fragmentation process that accompanies phase transitions. This process is more pronounced in electrodes operated up to an upper cut-off voltage of 4.8 V. Removing sodium ions causes a major drop in layer spacing (shrinking from ~ 5.6 Å to ~ 4.7 Å). This severe "squeeze" generates significant internal stress, which damages the crystal structure.

The linewidth EPR parameter reflects the structural changes in close proximity of the paramagnetic centers. The broadening is due to the appearance of random deviations in the structural parameters of Mn^{4+} ion coordination.

We found a strong correlation between crystallite size and EPR linewidth in both pristine and tested electrodes.

Фиг.1. Crystallite sizes and EPR line width (ΔH_{pp}) for P3-NMM and P2-NMM after direct charging to 4.0 V and 4.8 V, followed by discharging to 1.5 V. For comparison, the data for P3-NMM and P2-NMM after the direct discharge to 1.5 V are also shown.

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Synthesis and Characterization of *Spirulina*/Silica Hybrids via Sol–Gel Processing

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Keywords: sol-gel, *Spirulina*, hybrids, characterization

Microalgae have gained significant attention in recent years as a versatile and renewable resource for food, feed, chemicals, and biofuels. Among them, *Spirulina* (*Arthrospira* sp.) is a well-known species of unicellular blue green algae that has attracted considerable scientific interest due to its rich biochemical composition and diverse functional properties. However, large scale applications remain limited by slow growth rates, high cultivation costs, and challenges associated with their integration into inorganic matrices.

Immobilizing microalgae through encapsulation within a silica matrix offers a promising strategy to enhance their stability, usability, and compatibility with various technological processes, including heavy metal detection and environmental remediation. To the best of our knowledge, *Spirulina*/SiO₂ hybrid materials prepared via a sol–gel approach has not yet been reported, underlying the novelty of the present work.

In this study, *Arthrospira* sp. biomass was incorporated into a silica network through a sol–gel process using tetraethyl orthosilicate (TEOS) as the precursor and agar as an additional organic additive. To catalyze the hydrolysis step, different catalysts (hydrochloric acid and ethanol) were employed, enabling the preparation of a series of hybrid compositions. The resulting materials were characterized using X ray diffraction (XRD), UV–Vis spectroscopy, infrared (IR) spectroscopy, optical microscopy, and 3D X-ray tomography. Their antioxidant properties were also evaluated.

The obtained hybrids exhibited good cross linking, uniform morphology, and high structural homogeneity, confirming the successful incorporation of the biomass into the silica matrix. These findings indicate that the developed SiO₂/*Spirulina* hybrid materials hold strong potential for future environmental and biotechnological applications.

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Surface and structural features of asphaltene-based activated carbon

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Keywords: Asphaltenes, Activated carbon, Structural features, Surface chemistry

Converting asphaltenes into activated carbon (AC) is a highly effective way to upcycle petroleum industry waste into advanced, high-value carbon materials. Because asphaltenes are carbon-rich and highly aromatic, they are an excellent precursor for producing nanoporous materials with massive surface areas and tunable electrochemical properties [1,2]. This study investigates the structure and surface properties of asphaltene-based activated carbon via a number of analytical techniques such as infrared (FT-IR) spectroscopy, Raman spectroscopy, X-ray powder diffraction (XRD), ultraviolet-visible (UV-Vis) spectroscopy, porosimetry (BET) analysis, X-ray photoelectron spectroscopy (XPS), thermogravimetric (TGA) analysis and differential scanning calorimetry (DSC).

XRD analysis revealed broad diffraction peaks centered at 25° and 42°, indicating the formation of an amorphous carbon structure. Additional reflections at 27°, 28° and 47° were observed in the XRD pattern of the synthesized activated carbon and were attributed to the ZnS phase formed through the interaction between the chemical activator (ZnCl₂) and the sulfur naturally present in the raw asphaltenes. Structural calculations indicated that the synthesized activated carbon consists of layers with a diameter of approximately 35 Å, composed of about 13 condensed aromatic rings. The presence of structural disorder, commonly associated with porous carbon materials, was further confirmed by the relatively high intensity ratio ($I_D/I_G = 1.092$) between the D band (1336 cm⁻¹) and G band (1598 cm⁻¹) in the Raman spectrum. FT-IR spectroscopy identified functional groups related to O-H stretching/deformation vibrations and Zn-S bonds, supporting the XRD findings. Similar conclusions were drawn from the analysis of the S 2p, Zn 2p_{3/2} and O 1s regions. In addition, several oxygen-containing functional groups, including carboxylic acids, ethers, ketones and sulfate species, were detected. Sulfur was predominantly present in the form of sulfate groups and thiophene-like structures. Analysis of the C 1s and N 1s spectra showed that carbon species were mainly associated with alkyl chains and condensed aromatic rings, while nitrogen-containing functionalities were assigned to pyrrole-, pyridine- and carbazole-type structures. Nitrogen adsorption-desorption isotherms demonstrated that the asphaltene-derived activated carbon possesses a specific surface area of 535 m²/g and a total pore volume of 0.24 cm³/g. TGA/DSC analysis revealed an endothermic effect accompanied by a 2.5% mass loss, which was attributed to the removal of adsorbed water, in agreement with the FT-IR results, where O-H vibrations are clearly detected.

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Green Synthesis and Evaluation of Nanomaterials

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Keywords: green synthesis; copper nanoparticles; walnut shells; UV-Vis spectroscopy; SEM; FTIR; Raman spectroscopy

This study focuses on the eco-friendly green synthesis of copper Cu(II) nanoparticles using an aqueous extract of walnut shells (*Juglans regia*) as a reducing and stabilizing agent, and copper sulfate pentahydrate ($\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$) as the metal precursor. The nanoparticle formation process was monitored in real-time using UV-Vis spectroscopy. The influence of key reaction parameters, including process temperature and the volume ratio of plant extract to precursor, was systematically investigated. The resulting nanoparticles were evaluated using a comprehensive suite of physicochemical techniques – FTIR, SEM and Raman spectroscopy. The results demonstrate that optimizing the temperature and component ratio allows for effective control over the material properties, highlighting walnut shells as a promising bio-resource for sustainable nanotechnology.

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Hydrothermal Synthesis of Novel Functional Materials Based on Rare Earth Elements

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Keywords: Hydrothermal synthesis, Rare-earth oxotellurates,

Oxotellurates(IV, VI) are intensively investigated due to their promising applications in optoelectronics, energy technologies, and advanced materials science. Rare-earth oxotellurates have been studied as phosphor materials for light-emitting diode (LED) fabrication because of their efficient luminescent properties [1]. Other compounds exhibit potential as ionic conductors in solid oxide fuel cells and oxygen-permeable membranes [2]. In addition, some oxotellurates demonstrate nonlinear optical properties suitable for photonic and laser applications, including frequency-doubling devices [3].

In the present work, rare-earth oxotellurates(IV, VI) with probable compositions $\text{La}_2\text{Te}_3\text{O}_9$, $\text{Er}_2\text{Te}_3\text{O}_9$, CeTeO_5 , Er_2TeO_6 , and Dy_2TeO_6 were synthesized via a hydrothermal method at 220°C. The synthesis was carried out using $\text{La}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$, $\text{Er}(\text{NO}_3)_3 \cdot 5\text{H}_2\text{O}$, $\text{Ce}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$, metallic Dy treated with concentrated HNO_3 , TeO_2 , H_6TeO_6 , acetic acid, and CsBr employed as a fluxing agent. The obtained solid phases were characterized by powder X-ray diffraction (PXRD) and infrared (FTIR) spectroscopy in order to evaluate their phase composition and structural features.

The PXRD analysis revealed the formation of crystalline phases for the synthesized oxotellurates(IV) $\text{La}_2\text{Te}_3\text{O}_9$ and $\text{Er}_2\text{Te}_3\text{O}_9$, as well as for the cerium oxotellurate(VI) CeTeO_5 . In contrast, the synthesized Er_2TeO_6 and Dy_2TeO_6 compounds exhibited predominantly amorphous character under the applied hydrothermal conditions. The observed differences in crystallinity may be associated with the specific coordination behavior of the rare-earth ions, as well as with the influence of the synthesis conditions on nucleation and crystal growth processes.

The FTIR spectra of the synthesized compounds indicated the presence of crystallization water and characteristic absorption bands attributed to stretching and bending vibrations of O–H bonds originating from water molecules. Additional bands corresponding to deformation vibrations of Te–OH groups and vibrations of Te–O bonds were also observed. Vibrational modes associated with Ln–O bonds are generally located in the far-infrared region below 400 cm^{-1} .

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TiO₂ Dry Coating Na₄Fe₃(PO₄)₂P₂O₇ to Improve its Sodium Energy Storage at Different Temperatures

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Keywords: Sodium-ion Batteries, Dry Metal Oxide Coating, Electrochemical Techniques, Sodium Diffusion Kinetics

Sodium-ion batteries (SIBs) have emerged as a promising alternative to lithium-ion technology for large-scale energy applications owing to the abundance and low cost of sodium resources. Among the investigated cathode materials, the mixed phosphate-pyrophosphate Na₄Fe₃(PO₄)₂P₂O₇ (NFPP) has attracted a considerable attention due to its high theoretical capacity, excellent structural stability, and ability to reversibly intercalate up to three Na⁺ ions per formula unit. However, the electrochemical properties of NFPP are limited by its intrinsically low electronic conductivity and sluggish charge-transfer kinetics, which result in poor electrochemical performance. To address these limitations, the present work explores the surface modification of NFPP with 1 wt.% TiO₂ through a dry-coating method.

The electrochemical behavior of both NFPP/TiO₂ modified and non-modified NFPP materials was systematically investigated and compared in sodium half-cells using electrolyte 1 M NaPF₆:PC at 20 and 40 °C. Galvanostatic charge-discharge measurements were performed to evaluate the reversible capacity, cycling stability, and Coulombic efficiency. The kinetic response of the modified material was investigated by electrochemical impedance spectroscopy (EIS), cyclic voltammetry (CV), and galvanostatic intermittent titration technique (GITT). The contributions of Faradaic and capacitive charge-storage mechanisms were quantified from the CV data, while Na⁺ diffusion coefficients were determined using EIS, CV, and GITT analyses. Particular attention was paid to the influence of the TiO₂ coating on the electrolyte/electrode interfacial resistance, charge-transfer resistance, and sodium-ion transport properties.

The results reveal a significant enhancement of the electrochemical performance of NFPP after TiO₂ modification, whereas non-modified NFPP exhibits poor electrochemical behavior under identical conditions. The improved properties of NFPP/TiO₂ are attributed to the beneficial effect of the TiO₂ surface layer on interfacial charge-transfer processes, electrode kinetics, and Na⁺ diffusion. These findings demonstrate that the dry-coating approach using electroconductive TiO₂ modifier represents an effective strategy for enhancing the electrochemical performance of Na₄Fe₃(PO₄)₂P₂O₇ as a promising cathode material for next-generation sodium-ion batteries.

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Solubility of lignocellulosic components in phosphoric acid: approach for tuning the electrochemical performance of walnut shells-derived hard carbon

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Keywords: Hard carbon; sodium-ion batteries; dissolving of lignocellulosic components; acid pretreatment

Hard carbon (HC) is a technologically promising and inexpensive electrode material with practical applications in sodium-ion batteries. In recent years, there have been numerous research examining both the influence of the raw materials and the methods for its production. Most studies have focused on post-synthesis methods, such as ash removal [1], hydrothermal expansion, mechanochemical defect creation etc.

Herein, we evaluate pre-synthesis approach consisting of the treatment of the raw material with phosphoric acid (PA) aiming partially dissolving of lignocellulosic components. We selected raw material with an approximately equal content of the three main lignocellulosic components (hemicellulose, cellulose, and lignin, each at about 33%), i.e., walnut shells (WSs). After soaking for 48 h in phosphoric acid, WSs were rinsed and dried, then carbonized at 800 °C, follow pyrolysis in an argon atmosphere at 1100 and 1300 °C. The obtained hard carbons were characterized by differential thermal analysis (DTA-TG), powder X-ray diffraction (XRD), BET and CHNS analyses. To evaluate the effect of 48h-pretreatment with PA on the electrochemical properties, we additionally obtained hard carbon samples produced without acid pretreatment, as well as those produced after prolonged acid treatment (72h). The electrochemical properties of all HCs were carried out in model half cells consist of sodium metal as a counter electrode and carbonate-based sodium electrolyte, i.e. 1 M NaPF₆:PC. To quantify the Na-storage performance three parameters were determined: first sodiation, first irreversible capacity and cycling stability. Based on the electrochemical results, the approach for tuning the properties of hard carbon through PA-pretreatment was discussed.

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DFT Insights into the Electronic Structure and Reactivity of Potassium Hexaaquanickel (II) Diselenate

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Keywords: Potassium Hexaaquanickel (II) Diselenate, DFT, Cytotoxic activity

The present study investigates the electronic structure, physicochemical characteristics, and biological reactivity of potassium hexaaquanickel (II) diselenate (KNiSe) through density functional theory (DFT) analysis combined with experimental cytotoxic evaluation against the human lung adenocarcinoma cell line A549. The obtained results reveal a pronounced dose-dependent cytotoxic effect of KNiSe after 24 h exposure. Cell viability gradually decreased from approximately 72% at 2.5 µg/mL to only 7% at 20 µg/mL, while the calculated half maximal inhibitory concentration (IC₅₀) was approximately 7 µg/mL, indicating high biological activity and promising antitumor potential. Statistical analysis demonstrated significant reductions in viability at concentrations ≥5 µg/mL ($p < 0.05$), becoming highly significant at concentrations ≥10 µg/mL ($p < 0.01$ – 0.001), with good reproducibility of the experimental data.

Microscopic examination following crystal violet staining confirmed the dose-dependent cytotoxic effect of KNiSe. Untreated A549 cells showed typical epithelial morphology with dense monolayer formation, while treated cells exhibited loss of intercellular contacts and structural elongation at low concentrations. Concentrations above the IC₅₀ induced severe monolayer disruption, cytoplasmic shrinkage, cell rounding, and detachment from the substrate, indicating apoptotic cell death.

The observed biological activity is correlated with the nanoscale physicochemical properties of the synthesized material. Transmission electron microscopy (TEM) revealed ultrasmall primary nanoparticles with dimensions of approximately 6–9 nm, favoring efficient cellular uptake and enhanced reactivity. Dynamic light scattering (DLS), however, indicated a substantially larger hydrodynamic diameter (~370 nm), high polydispersity index (PDI = 0.69), and low zeta potential (–6.6 mV), suggesting aggregation and limited colloidal stability in suspension. Despite aggregation, the strong cytotoxic response implies that the biological activity is predominantly governed by the ultrasmall primary nanoparticles and the synergistic interaction between nickel and selenium species, which likely stimulate reactive oxygen species (ROS) generation, oxidative stress, and apoptosis [1].

Overall, the combined theoretical and experimental findings demonstrate that potassium hexaaquanickel (II) diselenate possesses significant cytotoxic activity toward A549 cells and represents a promising candidate for further anticancer investigations. Additional mechanistic studies, selectivity evaluation, and in vivo experiments are required to fully elucidate its therapeutic potential.

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Structural and Antibacterial Properties of Sol-Gel-Prepared Si–Chitosan–Ag Hybrids

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Keywords: Silica-chitosan hybrids; structure; antibacterial properties

Antibacterial hybrid materials are of growing interest for applications in wound dressings, medical coatings, packaging, and water purification systems. Si–chitosan–Ag hybrids are especially attractive for these purposes because they combine the natural bioactivity of chitosan with the structural stability of silica and the strong antibacterial properties of silver nanoparticles.

Si–chitosan–Ag hybrid materials were synthesized using the sol–gel method with different solvents, such as distilled water and phosphate buffer. After aging, the obtained gels were characterized by XRD, DTA-TG, FTIR, Raman, UV–Vis, SEM, TEM, EPR, and XPS analyses. XRD confirmed the amorphous structure of the gels, while a weak peak associated with metallic silver was also observed. DTA-TG revealed that the presence of silver influenced the thermal stability of the as-prepared hybrids. FTIR and Raman spectroscopies provided complementary information about the functional groups present in the hybrids, confirming the characteristic vibrations of chitosan and the formation of the silica network. UV–Vis spectroscopy confirmed the presence of a silver surface plasmon resonance band at around 350–400 nm. SEM and TEM analyses revealed the morphology of the hybrids, the distribution of silver particles, and nanoparticle sizes of approximately 10–15 nm. EPR and XPS analyses established the presence of both Ag⁰ and Ag⁺ species.

The antibacterial activity of the Ag-free and Si–chitosan–Ag hybrid composites was evaluated against the Gram-positive strain *Bacillus subtilis* (NBIMCC 1709 / ATCC 6633) and the Gram-negative strain *Escherichia coli* (ATCC 25922). The obtained results showed good antibacterial activity for the Ag-containing hybrids, making these materials promising candidates for applications in biomedicine and nanotechnology.

Acknowledgements: The research equipment used was from the distributed research infrastructure INFRAMAT, which was supported by the Bulgarian Ministry of Education and Science under contract.

Self-Assembling L-Glu Derivatives to Nanosized Complexes in Solution

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Keywords: L-Glutamic acid (L-Glu), complexes in solution, self-assembling, nanoscale

This study is related to the design and synthesis of a series of derivatives of the L-glutamic acid (L-Glu) that tend to form nanosized complexes in solution under specific conditions. The structures of the newly-synthesized compounds correspond to double-chained (Fig. A and B) and gemini (Fig. 1C and D) α -amino acids-based surfactants. Some of them are part of the non-ionic surfactants (Fig. 1A and C), while others belong to the group of the anionic surfactants (Fig. 1B and D). All newly-synthesized compounds are characterized with melting points, ¹H and ¹³C NMR spectra, IR-FTIR spectra, UV-Vis spectra, circular dichroism (CD) spectra and mass-spectra.

In our research we discovered that the sodium salts of the anionic surfactants self-assemble in supramolecular complexes. Critical aggregation concentrations (CAC) and concentrations of stability of some representatives were determined at pH 7.4 in 0.1 M Hepes buffer by using a fluorescence spectrophotometer and pyrene as a fluorescent agent.

The hydrodynamic size and zeta potential of the formed complexes were determined using dynamic light scattering (DLS) and electrophoretic light scattering (ELS), respectively. The results demonstrate the formation of stable aggregates, several of which exhibit nanoscale dimensions.

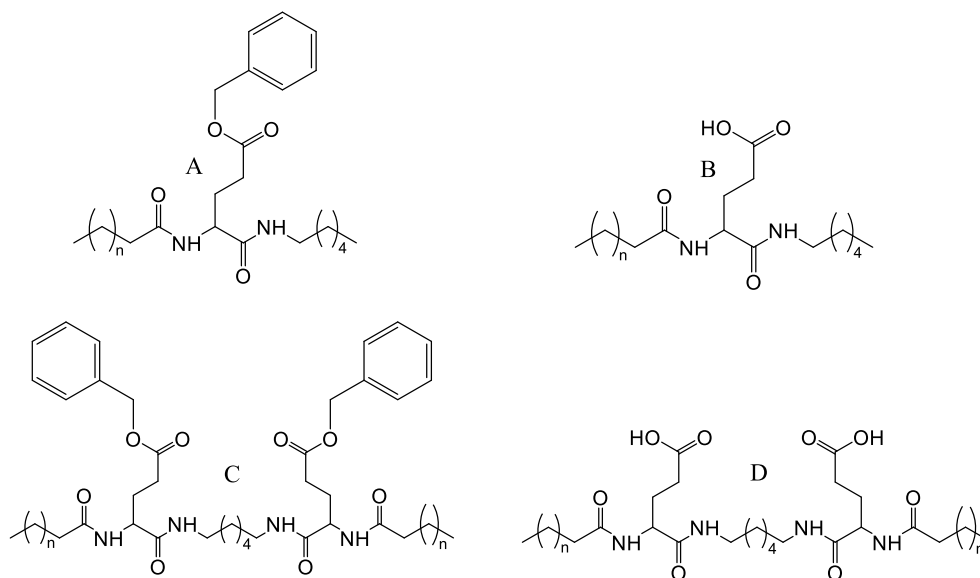


Figure 1. Chemical structures of the newly-synthesized compounds (n=3, 5, 6, 7, 8, 11).

Acknowledgements: This study is funded by the European Union, programme "Research, Innovation and Digitalization for Smart Transformation" 2021–2027, project BG16RFPR002-1.009-0003, "ABC-BIO-CAR. The authors thank the Bulgarian Ministry of Education and Science for the support provided via the "National Center for Biomedical Photonics" (DO1-101/2025), part of Bulgarian National Roadmap for Scientific Infrastructures 2020-2027.

Sonochemically prepared high-entropy spinel oxides (CoMnFeNiX₃)₄, where X=Cr, Zn, Al, for methanol decomposition

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Keywords: High-entropy spinel oxide, sonochemical method, methanol decomposition

High-entropy spinel oxides have emerged as a promising class of catalytic materials due to their tunable composition, structural stability, and unique electronic properties. In particular, their multi-cationic nature enables fine control over catalytic activity and selectivity in complex reactions such as methanol decomposition.

In this study, nanosized high-entropy spinel oxides with a general formula (CoMnFeNiX)₃O₄ (X = Cr, Zn, Al) were synthesized via the sonochemical method. The obtained materials were thermally treated at 400°C for 1 h and characterized by X-ray diffraction (XRD), nitrogen physisorption, and transmission electron microscopy (TEM), confirming the formation of single-phase spinel structures with nanoscale morphology.

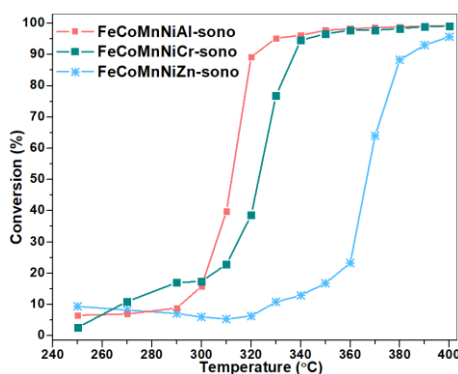


Fig.1 Conversion of methanol as a function of the temperature

The catalytic performance of the synthesized oxides was evaluated in methanol decomposition to hydrogen-rich products. The (CoMnFeNiAl)₃O₄ and (CoMnFeNiCr)₃O₄ samples exhibited superior activity, reaching 50% methanol conversion at approx. 310°C and 320°C, respectively, and exceeding 90% conversion at 340°C. In contrast, the (CoMnFeNiZn)₃O₄ sample showed significantly lower activity, with a delayed onset of conversion and 50% conversion achieved only at around 370°C. These findings demonstrate the potential of sonochemically synthesized high-entropy spinel oxides as efficient catalysts for methanol decomposition and provide insights into composition–activity relationships in multi-component oxide systems.

Acknowledgments: The authors are thankful to Project KP-06-M89/3 "Synthesis and characterization of High-entropy spinel oxides with applications in catalysis".

Influence of Crystal Structure and Cu Substitution on Sodium Storage in NaFeO₂-based Electrodes

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Keywords: NaFeO₂, sodium-ion battery

Sodium-ion batteries (SIBs) are emerging as a highly promising, sustainable alternative to lithium-ion technologies, given the abundance and low cost of sodium resources. A key requirement for SIB electrode materials is to achieve an optimal balance between electrochemical performance and chemical simplicity. In this context, sodium iron oxides (NaFeO₂) are an attractive option as they use earth-abundant, non-toxic and inexpensive iron.¹ Depending on the synthesis route, NaFeO₂ can crystallize in two distinct structural forms: α -NaFeO₂, which is a layered O3-type phase comprising octahedral FeO₆ sheets; and β -NaFeO₂, which is an orthorhombic wurtzite-derived phase consisting of tetrahedral moieties. Despite their potential, these polymorphs remain poorly studied, and their sodium storage behavior is not well understood.

This studies aim is twofold: (i) to develop fast and easy synthetic methods for preparation of two structural modifications, α -NaFeO₂ and β -NaFeO₂, and (ii) to evaluate their sodium-storage capabilities in model sodium-ion cells. Additionally, the electrochemical performance of NaFeO₂ is optimized through targeted copper substitution. We found that β -NaFeO₂ stored sodium below 2.0 V via a conversion mechanism, whereas α -NaFeO₂ reversibly intercalated sodium above 2.0 V, delivering a capacity of approximately 85 mAh g⁻¹. Remarkably, Cu substitution dramatically enhances sodium-storage performance, increasing capacity to around 150 mAh g⁻¹ and improving cycling stability and rate capability. By establishing synthesis-structure-property relationships, this work provides essential insights for designing high-performance cobalt- and nickel-free cathode materials, supporting the advancement of grid-scale sodium-ion energy storage.

Acknowledgements: The authors thank to project EcoCapatery (IC-RS/04/2026-2028) for collaboration with Serbian team.

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Tribocatalytic Degradation of Antibiotics in Waters with Varying Hardness Using Nanoflowers

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Keywords: Tribocatalysis, Antibiotics, Water Hardness, Nanoflowers

The persistence of antibiotic contaminants in aquatic systems represents a critical environmental challenge, particularly under realistic water conditions where dissolved ions can significantly affect catalytic performance. In this work, we propose a tribocatalytic approach for antibiotic degradation based on ZnO and ZnO/Gd₂O₃ nanoflower structures, specifically designed to operate under non-ideal aqueous conditions.

The study focuses on evaluating the role of water matrix composition by systematically comparing distilled water with model systems of increasing hardness, containing representative concentrations of Ca²⁺ and Mg²⁺ ions. ZnO-based nanoflowers are selected due to their high surface area, defect-rich structure, and ability to generate reactive oxygen species under mechanical stimulation, while Gd₂O₃ modification is expected to promote interfacial charge separation and enhance catalytic efficiency.

Particular emphasis is placed on understanding how water hardness influences tribocatalytic activity through surface interactions, active site accessibility, and radical scavenging effects. The proposed framework aims to bridge the gap between ideal laboratory conditions and real-world water treatment scenarios, where ionic composition plays a decisive role in process efficiency.

This work provides a systematic platform for investigating tribocatalysis in complex aqueous environments and highlights the potential of engineered ZnO-based nanostructures for sustainable antibiotic removal. The insights gained are expected to contribute to the rational design of next-generation tribocatalysts capable of operating under realistic environmental conditions.

Acknowledgements: The authors are grateful to financially supported by the Bulgarian NSF project KP-06-N89/07 (КП-06-H89/07).

Phase Transitions Inducing Changes in the Luminescent Properties of Manganese(II) Coordination Complexes

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Keywords: coordination complexes; luminescent; materials

Manganese(II) coordination complexes have attracted considerable attention as low-cost and environmentally benign alternatives to lanthanide- and platinum-based luminescent materials. Their narrow-band green emission and high photoluminescence efficiency make them promising candidates for optoelectronic applications. In this work, the influence of structural phase transitions on the luminescent properties of bis(triphenylphosphine oxide)dichloridomanganese(II) is investigated. The complex was characterized by UV–Vis absorption spectroscopy, powder X-ray diffraction (PXRD), single-crystal X-ray diffraction (SCXRD), electron paramagnetic resonance (EPR) spectroscopy, and differential thermal analysis (DTA). A spontaneous transformation from a metastable, non-luminescent polymorph to a thermodynamically more stable, highly luminescent polymorph was observed.

These findings demonstrate a direct correlation between polymorphic phase transitions and the optical response of the complex, highlighting the decisive role of crystal structure in governing its luminescent properties.

Li/Na competition in naphthalimide electrochemical matrix

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Keywords: Organic electrode materials, Li/Na ion batteries, ionic liquid based electrolytes

Organic electrode materials (OEMs) have recently emerged as promising redox-active materials for application in both lithium- and sodium-ion batteries. Their growing interest stems from several intrinsic advantages, including structural tunability, environmental sustainability, and the ability to reversibly accommodate both cations and anions within a single molecular framework. Owing to their structural flexibility, OEMs are considerably less affected by the size of the charge carrier than conventional inorganic intercalation compounds. This characteristic makes them particularly attractive for sodium-ion batteries, where the relatively large Na⁺ ion often leads to sluggish diffusion kinetics and structural degradation in inorganic hosts.

In this work, the bipolar redox behaviour of naphthalimide (NI) derivatives was investigated as cathode materials for lithium and sodium half-cells employing ionic liquid electrolytes. To overcome the intrinsically low electronic conductivity of the organic compounds, the NI derivatives were combined with reduced graphene oxide (rGO) to form conductive composites.

Electrochemical performance was evaluated using both cyclic voltammetry and galvanostatic charge–discharge measurements over a potential window of 1.0–4.6 V. Cyclic voltammetry confirmed the bipolar redox activity of the investigated NI derivatives. In addition, cycling stability studies were carried out to assess the influence of the substituents attached to the imide nitrogen as well as the halogen atom incorporated into the naphthalimide core. The lithium half-cells reached stable specific capacities after approximately 20 cycles, whereas the sodium half-cells achieved stable performance after only five cycles, regardless of the nature of the halogen substituent. Long-term galvanostatic cycling at elevated current densities further demonstrated the excellent rate capability of the sodium cells. At a current density of 500 mA g⁻¹, the specific capacity decreased only slightly, from approximately 45 to 35 mAh g⁻¹, indicating good electrochemical stability and sustained high-rate performance of the cathode material.

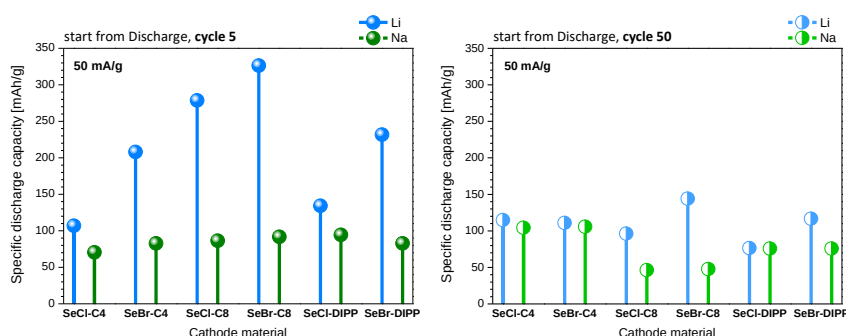


Figure 1. Discharge capacity of NIs cycled in lithium half-cells (blue bars) and sodium half-cells (orange bars) for the 10th and 50th cycle, starting from a discharging mode at current load 50 mA/g.

Acknowledgements: The Bulgarian National Science Fund funded this research by grant number KP-06-H69/1 (8.12.2022). Research equipment of the project № BG16RFPR002-1.014-0006 "National Centre of Excellence Mechatronics and Clean Technologies" was used for experimental work financially supported by European Regional Development Fund "Research, Innovation and Digitization for Smart Transformation" program 2021-2027.

Hydrothermal Synthesis of Sodium Titanates as High-Capacity Electrodes in Sodium-Ion Batteries

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Keywords: sodium-ion batteries, sodium titanates, synthesis

In recent years, sodium-ion batteries (NIBs) have become an attractive energy storage technology. A barrier to their implementation is the lack of anode materials with the desired charge rate and cycling stability. The performance of sodium-ion batteries critically depends on the correct choice of composition, structure and morphology of the electrode materials. Among them, sodium titanates are the most intriguing, as they exhibit a variety of compositions, flexible structure and interact reversibly with a large amount of Na⁺ at low potentials. Here we focused on the preparation of disodium hexatitanates, Na₂Ti₆O₁₃, with a tunnel-hybrid structure and nanowire morphology as anode materials for Na-ion batteries. The preparation of Na₂Ti₆O₁₃ consists of hydrothermal treatment of a suspension of TiO₂ in concentrated NaOH at 150 °C at different pressures. At low pressure (i.e. up to 2 bar) nanowires with a length of ~ 2 µm and a diameter of 0.1 µm are formed. By increasing the pressure from 2 to 30 bar, the length of the nanowires increases slightly compared to the diameter: the dimensions of the nanowires obtained under 30 bar are 3.0 µm long and 0.2 µm in diameter. The phase composition contains Na₂Ti₆O₁₃ and impurities Na₂Ti₃O₇ (less than 10 wt%). The Na₂Ti₆O₁₃ nanowire were tested as anodes in half-Na cells. The results show that the nanowire titanates obtained at a pressure of 5 bar show a higher Na storage capacity: about 136 mAh/g for a C/2 rate, respectively. The best cycling stability is achieved for Na₂Ti₆O₁₃ obtained at a pressure of 2 bar: at a rate of 5 C, this oxide provides a capacity of 55 mAh/g in a Na-cell. When the titanates are prepared at 30 bar, the performance (in terms of capacity and rate capability) becomes worse. The cycling stability appears to be insensitive to the hydrothermal pressure used for synthesis. The phase composition is preserved after cycling in a Na-ion cell. Post-mortem TEM analysis reveals that the nanowires undergo a reduction in length upon prolonged cycling, while the diameter remains unchanged. These results demonstrate the advantages of hydrothermal synthesis for obtaining electrode materials with controlled morphology, storage capacity, and rate.

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Company *presentations*



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Keywords: Aurubis Bulgaria, sustainable growth, metal production, copper smelting, metal recycling, carbon neutrality

The Aurubis group is one of the leading multi-metal producers active in more than 20 countries with production sites in Europe and the USA. It is the largest copper producer in Europe and the largest copper recycler in the world, focused on closing the circular economy loop. The company owns the most sustainable and environmentally friendly network of smelters with a carbon neutrality target before 2050. Its divisions of multimetal recycling and custom smelting & products use mining concentrates, scrap, and other recycling materials to produce copper cathodes, base metals, precious metals, sulphuric acid, as well as rods, shapes, and other products.

Aurubis' integrated business model is “closing the loop” of metal production by recycling and further processing of primary and secondary materials. Aurubis Bulgaria is a leading European producer of cathode copper (Pirdop brand), anodes, and co-products (H₂SO₄ and iron silicate). It is the country's main international trader: 7.3% of exports, 4.4% of imports (2023); the main employer and social partner in the region of Srednogorie. Aurubis Bulgaria is in the top 3 largest companies of Bulgaria by annual revenues: EUR 3.56 B (2023, second place), EUR 4.01 B (2022, first place).

Within its 68-year history, the company has established world-class technological know-how combined with strong local copper production traditions. Located in an EU member state, it serves as a gateway to Asia and Africa with close links to Aurubis Group's smelter network. Our plans for growth in Bulgaria are a key focus in Aurubis Group's investment strategy.

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Keywords: Laboratory equipment, Pharmaceutical products, Service

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- In 2004, a fruitful cooperation with **VWR** in the field of laboratory equipment and consumables started;

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I S S P 22

**22nd International Symposium on
Solubility Phenomena
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31 Aug – 3 Sep 2026



Sofia, Bulgaria

SATELLITE WORKSHOP

**Tailored Properties of
Ionic Liquid Electrolytes
for Sustainable
Energy Storage Applications**



PROGRAM - WORKSHOP

03.09.2026, Thursday

Tailored Properties of Ionic Liquid Electrolytes for Sustainable Energy Storage Applications”

IUPAC project Ref: Proposal 2025-032-1

Session 9 Chairperson: Assoc. Prof. Simão Pinho	
9:00 - 9:45	PL W1 Gero Frisch Measuring What Matters? Speciation and Chemical Behaviour of Ionic Liquids and Deep Eutectic Solvents in Energy Storage Applications.
9:45 - 10:00	OP W1 Şefik Süzer Şefik Süzer, Tapping into Electrical-Double Layer Formation in Ionic Liquid/Carbon Interfaces using DC/AC/Pulsed X-Ray Photoelectron Spectroscopy
10:00 - 10:15	OP W2 Snežana Papović S. Papović, T.T. Borović, M. Vraneš, M.E. di Pietro, A. Rossetti, A. Roganović: Improving the thermal stability of lithium-ion battery electrolytes safety
10:15 - 10:45	Coffee break
Session 10 Chairperson: Prof. Earle Waghorne	
10:45 - 11:30	PL W2 Xinpei Gao Xinpei Gao, Heterogeneous Colloid Electrolytes: Ionic Liquids, Plastic Crystals, and Liquid Crystals
11:30 - 11:45	OP W3 Pedro Carvalho Beatriz F. Esteves, Rita Nunes, Bruna R. M. Ferreira, Pedro J. Carvalho, Ionic Liquid-based Composite Membranes for Efficient Greenhouse Gases Separation
11:45 – 12:00	OP W4 Slobodan Gadžurić S. Gadžurić, N. Cakó Bagány, S. Belić, T. T. Borović, M. Vraneš, S. Papović, F. Dian, B. Šarac, D. Goste, A. Melchior, Tailoring the Properties of Ionic Liquids for Targeted Applications
12:00 – 12:30	Closing remarks
14:00 – 15:00 Round table - IUPAC project Ref: Proposal 2025-032-1 Working Group on Standardized Measurement and Properties of Ionic Liquid Electrolytes for Sustainable Energy Storage Applications	

*Legend: PL – plenary lecture; IL – invited lecture; OP – oral presentation



Acknowledgement

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Measuring What Matters? Speciation and Chemical Behaviour of Ionic Liquids and Deep Eutectic Solvents in Energy Storage Applications.

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Keywords: ionic liquids; deep eutectic solvents; speciation; electrochemistry; energy storage

Ionic liquids, deep eutectic solvents and related ionic liquid analogues are chemically active electrolyte formulations for which apparent tunability rests on controllable equilibria and reaction kinetics rather than on the solvent composition alone. Their composition can, in principle, tailor solubility, phase behaviour, transport, redox potentials and interfacial reactions. The operative electrolyte, however, is defined by the actual species present and properties such as solubilities, activities, Lewis acidity, viscosity and conductivity, water or other impurities, temperature, and electrochemical history.

A useful foundation for energy-storage applications therefore begins with speciation and property measurement. Structural studies show that the first coordination shell of a dissolved metal is defined by the medium: ligand exchange, Lewis acidity and basicity, and competing donor sites alter both thermodynamics and electrode kinetics. At the same time, knowledge of bulk speciation is necessary but not sufficient, because double-layer structure, diffusion-related concentration gradients, nucleation, passivation and degradation reactions can dominate the observed electrochemical behaviour. Examples from metal complexes in ionic liquids and deep eutectic solvents, redox metrology from electroplating applications and chloroaluminate/amide electrolytes for batteries illustrate how nominal composition connects to metal deposition and stripping, graphite intercalation, self-discharge and stability only through validated analytical and electrochemical context.

Rational electrolyte design therefore requires more than new formulations. Progress in tailored electrolytes depends as much on measuring the right quantities reproducibly and comparably as on inventing new recipes. Claims about electrolyte chemistry, performance, stability windows, potentials and transport properties are only as reliable as the methodology, metadata and reference procedures that accompany them. Possible areas for future IUPAC activity include harmonised protocols for assessing key parameters such as solubility, phase behaviour, redox potentials and electrochemical windows as well as their critical evaluation under operating conditions.

Heterogeneous Colloid Electrolytes: Ionic Liquids, Plastic Crystals, and Liquid Crystals

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Keywords: colloid electrolytes; ionic liquids; liquid crystals; ion cluster; ion aggregation

The electrolyte, filling the space between the positive and negative electrodes, serves as both an ion transport carrier and a charge transfer medium. Its physicochemical properties and interfacial behavior fundamentally determine the ultimate performance limits of energy storage systems. In recent years, with the deepening understanding of electrolyte systems and the expansion of research scopes, the scientific community has gradually recognized that electrolytes are not simply disordered salt solutions. Ions and solvent molecules in electrolytes can self-assemble into multi-scale ordered aggregation structures, including supramolecular structures represented by ion clusters and ordered aggregates represented by micelle-like structures. At this point, electrolyte systems exhibit typical characteristics of colloidal dispersion systems. Therefore, following the classical theories in colloid and interface chemistry, we systematically studied the ion clusters' aggregation behaviors in typical heterogeneous electrolytes, including ionic liquid electrolytes, plastic crystals-based electrolytes, and liquid crystal electrolytes, as well as their impacts on the electrolytes' ion transport mechanisms and electrolytes' electrochemical performance.

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Tapping into Electrical-Double Layer Formation in Ionic Liquid/Carbon Interfaces using DC/AC/Pulsed X-Ray Photoelectron Spectroscopy

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Keywords:

Electrochemical devices are based on the ion migration and accumulation on surfaces. Complex molecular properties of ions and device dimensions control the entire process and define the overall dynamics. For ionic liquid-based electrolytes it is often not clear which property and to what extent contributes to the overall performance of the device. Herein we use X-ray photoelectron spectroscopy (XPS), while the device is under electrical bias. Such a procedure reveals localized electrical potential developments, through binding energy shifts of the atomic core levels, in a chemically specific fashion. Combining it with Square-Wave AC Modulation, the information can also be extended to time domain, and investigate devices configured as a coplanar capacitor, having an ionic liquid as the electrolyte, in macro-dimensions. Our analysis reveals that nonlinear voltage profile across the device emerges from spatially nonuniform electrical double layer formation on electrode surfaces. The present results propose a new experimental approach and provide new insights into the dynamics of ions across electrochemical devices. [1, 2]

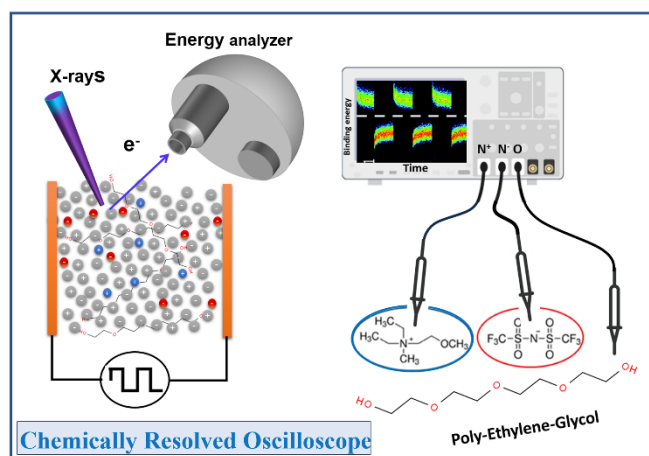


Figure 1. Schematics of the Experimental Set-up.

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Improving the thermal stability of lithium-ion battery electrolytes safety

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Keywords: Lithium-ion batteries, electrolyte, zwitterion additives

The development of high-energy density, safe, affordable energy storage devices is crucial for the energy transition. Lithium-ion batteries (LIBs) currently dominate the global energy storage market, but their safety, cost, and environmental impact are significant concerns. The highly flammable and toxic state-of-the-art electrolytes used in LIBs are a major concern, as they can pose a risk to both people and environment. Electrolyte additives, though typically used in small concentrations, have a disproportionate impact on battery performance by influencing interfacial chemistry, thermal stability, electrochemical stability, and overall battery lifespan [1].

To address this challenge, we are developing electrolytes that can perform multiple functions simultaneously, including stabilizing electrode materials. In this context, we conducted a comprehensive study involving physicochemical, thermal, and electrochemical testing to evaluate the stability of an electrolyte containing newly synthesized zwitterionic compounds as additives. The use of electrolyte additives could be a cost-effective and efficient approach to improve the safety of LIBs. In this work we synthesized a series of zwitterion analogs: 1-propylsulfonate-3-alkylimidazole and 1-butylsulfonate-3-alkylimidazole (where alkyl stands for methyl, ethyl or vinyl).

Our study utilized 1.0 M LiPF₆ in a 50/50 mixture of ethylene carbonate and dimethyl carbonate (EC/DMC) as our battery-grade electrolyte solution. We compared physico-chemical, thermochemical as well electrochemical performances of the electrolyte with 1% additives in the electrolyte and commercially used electrolytes, to assess their effectiveness. The growing complexity of modern LIB chemistries, including high-voltage cathodes and graphite-based anodes, has necessitated the development of next-generation additives capable of meeting more demanding electrochemical environments.

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Ionic Liquid-based Composite Membranes for Efficient Greenhouse Gases Separation

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Keywords:

Greenhouse gas (GHG) emissions have grown rapidly in recent decades, increasing their atmospheric concentrations and amplifying the natural greenhouse effect. Annual global emissions reach about 50 billion tons of CO₂ equivalents, comprising CO₂, CH₄, N₂O and fluorinated gases. Various mitigation technologies, including absorption, adsorption and electrochemical reduction, have been explored, but they often suffer from major drawbacks such as high energy demands, limited efficiency and solvent toxicity.¹ These limitations underscore the need for more efficient and sustainable GHG mitigation approaches. Non-volatile solvents, particularly Ionic Liquids (ILs), have emerged as promising alternatives to conventional solvents, due to their negligible vapor pressure, high thermal stability and tuneable properties. However, direct implementation in traditional separation units is limited by the large separation units and high energy demands for solvent recovery.² To address these challenges, we proposed a membrane contactor using hollow-fiber polyetherimide membranes coated with a thin Pebax® layer functionalized with ILs, combining the high sorption capacity and selectivity of ILs with the modularity and scalability of membrane technology.

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Tailoring the Properties of Ionic Liquids for Targeted Applications

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Keywords: ionic liquids, extraction, rare earths, volumetric properties, thermodynamics

Ionic liquids (ILs) have emerged as a versatile class of designer solvents whose physicochemical properties can be systematically tuned through judicious selection of cation and anion combinations. The central challenge in this field lies in establishing reliable structure-property relationships that enable rational design of ILs with predefined characteristics for specific applications. This presentation summarizes our systematic investigations into how anion structure – particularly the presence and position of functional groups – governs the macroscopic behavior of ILs in both pure form and aqueous solutions.

Our research strategy combines comprehensive experimental characterization with computational modeling to elucidate the molecular origins of IL properties. Density, viscosity, electrical conductivity, and thermal stability measurements are integrated with density functional theory (DFT) calculations and molecular dynamics (MD) simulations to provide a complete picture of ion-ion and ion-solvent interactions. This combined approach has proven essential for understanding the delicate balance of forces that determine IL behavior. A key finding is the profound influence of the anion's functional groups on critical properties. Our investigations extend beyond fundamental properties to demonstrate practical applications enabled by this molecular-level understanding. The structure–property relationships established through this work provide a rational framework for designing ILs with tailored properties. Whether the target application requires enhanced thermal stability, specific aggregation behavior, selective extraction capability, or antimicrobial activity, our findings demonstrate that careful anion functionalization offers a powerful strategy for achieving desired performance characteristics. This molecular design approach positions ILs as truly tunable materials capable of addressing challenges across separation science, environmental monitoring, and industrial-scale applications.