المؤتمر الدولي التاسع والثلاثون حول كيمياء المحاليل

39th INTERNATIONAL CONFERENCE ON SOLUTION CHEMISRY

ICSC 2025

TUNISIAN CHEMICAL SOCIETY
الجمعية الكيميائية التونسية

ICSC
39 I C S C

IUPAC
INTERNATIONAL UNION OF
PURE AND APPLIED CHEMISTRY

14-17 September 2025

Rosa Beach Hotel
Skanès-Monastir, Tunisia

Abstracts of Lectures and Communications
List of Participants

Foreword

Dear Fellow Chemists and Physical Chemists,

It is our great pleasure an honor to organize and chair the 39th International Conference on Solution Chemistry in Monastir town, Tunisia, at Rosa Beach Hotel, from 14-17 September 2025 under the joint auspices of International Steering Committee of the ICSC, International Union of Pure and Applied Chemistry (IUPAC), Tunisian Chemical Society (TCS) as co-organizer, and the University of Monastir.

ICSC is a traditional conference founded in 1967 in Hamilton, Canada. It is organized every two years in different countries over the world, but this is the first time it has taken place in Africa.

Following on the successful and productive previous meetings during the last ten years: in Kyoto (2013, Japan), Prague (2015, Czech Republic), Szeged (2018, Hungary), Xining (2019, China), Cartagena, (2021 Colombia), Belgrade (2023 Serbia), the 39th ICSC2025 aims to continue the tradition by promoting scientific and cultural interaction between the different research communities worldwide, in particular between North and South countries, in order to share their most recent findings, both fundamental and practical, to spread knowledge and guide the new generations and to develop technology and innovation towards the wellbeing of the society and environmental protection.

Solution chemistry is a broad and interdisciplinary field of chemistry, physics and biology, as well as pharmaceutical and medical sciences. In particular, the expansion of solution chemistry to interface chemistry, polymer chemistry and supramolecular chemistry has made it possible to bring important innovations to analytical chemistry, coordination chemistry and nanocomposites.

On the other hand, the development of molecular dynamics calculations combined with quantum calculations and their confrontation with the most recent spectroscopic techniques at different scales, has made it possible to better describe qualitatively and quantitatively the structures and dynamics in solution, especially in complex solutions, and Deep Eutectic Solvents.

The 39th ICSC2025 will cover fundamental aspects, applied research and various applications of solutions, divided into 14 topics. Over 148 researchers from all continents and 37 countries will participate over 4 days.

The 39th ICSC2025 will provide 5 Plenary lectures and 11 Key Note lectures given by world renowned professors, 53 Oral presentations in three parallel sessions covering the conference themes, and 61 Posters in three sessions.

Welcome to Monastir (Ruspina), which is a university City, and one of the foremost lovely coastal touristic region of Tunisia.

We hope that our social and Cultural activities will be of pleasure for all participants and their companions at the event. Welcome and we appreciate and value your kind participation.

Jalel MHALLA (Chair)
FSM - Monastir, University of Monastir

Adel MEGRICHE (Co-chair)
FST - Tunis, University of Tunis El Manar

INTERNATIONAL STEERING COMMITTEE

Professor Toshio YAMAGUCHI	*Fukuoka University, Japan*
Professor Ivo NEZBEDA	*Czech Academy of Sciences, Prague, Czech*
Professor Yongquan ZHOU	*Qinghai Institute of Salt Lakes, Chinese Academy of Sciences, China*
Professor Marija BEŠTER ROGAČ	*University of Ljubljana, Slovenia*
Professor Jalel MHALLA	*University of Monastir, Tunisia*
Professor Glenn HEFTER	*Murdoch University, Perth, Australia*
Professor Pál SIPOS	*University of Szeged, Hungary*
Professor Edgar MOSQUERA VARGAS	*University of Valle, Cali, Colombia*
Professor Slobodan GADŽURIĆ	*University of Novi Sad, Serbia*
Professor Paola D’ANGELO	*Sapienza University of Rome, Italy*

SCIENTIFIC COMMITTEE

Prof. Robert GUILLAUMONT (Honorius member) Member of the Academy of Sciences of France	*Academy of Sciences, Paris, France*
Prof. Mourad AMARA	*Sidi Abdellah Technological Hub, Algiers, Algeria*
Prof. Mikhail KISELEV	*Krestov Institute of Solution Chemistry of the RAS, Ivanovo, Russia*
Prof. Jean-François DUFRECHE	*University of Montpellier, France*
Prof. Abdenacer IDRISSI	*University of Lille, France*
Prof. Winfield Earle WAGHORNE	*University College Dublin, Ireland*
Prof. Hatem MAJDOUB	*University of Monastir, Tunisia*
Prof. Taieb Ben DHIA	*University of Tunis El Manar, Tunisia*
Prof. Sondes BOUGHAMMOURA	*University of Monastir, Tunisia*
Prof. Latifa LATROUS	*University of Tunis El Manar, Tunisia*
Prof. Jalel MHALLA	*University of Monastir, Tunisia*

ORGANIZING COMMITTEE

Jalel MHALLA (Chair)	*FSM - Monastir, University of Monastir, Tunisia*
Adel MEGRICHE (Co-chair)	*FST - Tunis, University of Tunis El Manar, Tunisia*
Robert GUILLAUMONT (Honorius member)	*Member of the Academy of Sciences of France*
Mohamed Lotfi EFRIT	*FST - Tunis, University of Tunis El Manar, Tunisia*
Mourad AMARA	*National School of Nanoscience and Nanotechnology, Algiers, Algeria*
Amine MNIF	*FST - Tunis, University of Tunis El Manar, Tunisia*
Mikhail KISELEV	*Institute of Solution Chemistry RAS, Ivanovo, Russia*
Hatem MAJDOUB	*FSM - Monastir, University of Monastir, Tunisia*
Jean-François DUFRECHE	*Université de Montpellier, France*
Mohamed Taieb BEN DHIA	*FST - Tunis, University of Tunis El Manar, Tunisia*
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Abdenacer IDRISSI	*Université de Lille, France*
Latifa LATROUS	*IPEIEM - Tunis, University of Tunis El Manar, Tunisia*
Winfield Earle WAGHORNE	*University College, Dublin, Ireland*
Imed LAAJIMI	*Tunisian Chemical Society, Tunisia*

ICSC 2025 Program

	Sunday 14 September 2025
14.00 - 17.00	**Welcoming participants, Distribution of Documents and Check in**
14.00 – 19.00	**Room B** **Subcommittee on Solubility and Equilibrium Data (SSED) Annual Meeting**
17.00 - 17.30	**Opening Ceremony**
17.30 - 18.20 **Room A**	**Topic C. Plenary Lecture 1** **DENG Tianlong** **Chair**: W. E. Waghorne *Tianjin University of Science & Technology, Tianjin, China* **Prediction System for Phase Equilibria in Salt Lake Brine Systems and Its Applications**
18.20 - 19.10 **Room A**	**Topic M. Plenary Lecture 2** **KISELEV Mikhail** **Chair**: Y. Zhou *Krestov Institute of Solution Chemistry of the RAS, Ivanovo, Russia* **Screening of Polymorphism in Pharmaceutical Compounds Under Supercritical State Parameters**
19.10 - 20.00	**Welcome Ceremony**
20.00	***Dinner***

<table>
<tr><th></th><th colspan="6"><i>Monday 15 September 2025 (Morning)</i></th></tr>
<tr><td>09.00 - 09.50
Room A</td><td colspan="6">Topic D. Plenary Lecture 3 TERAZIMA Masahide Chair: S. Gadžurić
<i>University of Kyoto, Japan</i>
Dynamics of conformation changes and biological functions of proteins by time-resolved diffusion techniques</td></tr>
<tr><td>09.50- 10.30</td><td colspan="2">Room A
Topic B. Keynote 1 - Naceur IDRISSI
<i>“Structural and Dynamic Characteristics of Liquid-Vapor Interfaces in Aqueous Solutions, Ionic Liquids, and Supercritical Fluids”</i>
Chair: M. Kiselev</td><td colspan="2">Room B
Topic I. Keynote 2 - Valentine ANANIKOV
<i>"Solution state organometallic chemistry of Pd, Pt, Ni, Cu and Au complexes and clusters - the key to high performance catalysis"</i>
Chair: Z. Yu</td><td colspan="2">Room C
Topic D. Keynote 3 - Virginie MARRY
<i>“Understanding clay/water systems from the compacted to the colloidal state: Coupling modelling and experiments”</i>
Chair: M. Terazima</td></tr>
<tr><td>10.30- 11.30</td><td colspan="6">Poster Session 1 (P 1 - P 20) Alphabetical Order</td></tr>
<tr><td></td><td colspan="6">Oral Communications - Session 1</td></tr>
<tr><td></td><td colspan="2">Room A - Chair: M. Kiselev
Topic: A</td><td colspan="2">Room B - Chair: M.T. Ben Dhia - V. Ananikov
Topic: H</td><td colspan="2">Room C - Chair: M. Virginie
Topic: D</td></tr>
<tr><td></td><td><i>Com.</i></td><td><i>Communicating</i></td><td><i>Com.</i></td><td><i>Communicating</i></td><td><i>Com.</i></td><td><i>Communicating</i></td></tr>
<tr><td>11.30 - 11.45</td><td>OC-01A</td><td>HEFTER Glenn Australia</td><td>OC-01B</td><td>BERGAOUI Souad TUN</td><td>OC-01C</td><td>BOHINC Klemen Slovenia</td></tr>
<tr><td>11.45- 12.00</td><td>OC-02A</td><td>CERAR Janez Slovenia</td><td>OC-02B</td><td>BOUBAKRI Saber TUN</td><td>OC-02C</td><td>BOUZAIENE Roua TUN</td></tr>
<tr><td>12.00 - 12.15</td><td>OC-03A</td><td>EL HADI Djamel ALG</td><td>OC-03B</td><td>BOUKERROUI Abdelhamid ALG</td><td>OC-03C</td><td>CHANG Chien-Hsiang Taiwan</td></tr>
<tr><td>12.15 - 12.30</td><td>OC-04A</td><td>GALINDRES JIMÉNEZ Diana Madelen Spain</td><td>OC-04B</td><td>ZHOU Yongquan China</td><td>OC-04C</td><td>CHORĄŻEWSKI Mirosław Poland</td></tr>
<tr><td>13.00</td><td colspan="6"><i>Lunch</i></td></tr>
</table>

	Monday 15 September 2025 (Afternoon)					
14.45 - 15.35 **Room A**	**Topic K. Plenary Lecture 4 LEBLANC Roger** Chair: G. Hefter *University of Miami, Coral Gables, Florida, USA* **Physicochemical Characterization of a Novel Carbon Nanomaterial: Carbon Dots**					
15.35 - 16.15	**Room A** **Topic B. Keynote 4- D'ANGELO Paola** *Deep Eutectic solvents: The relationship between structure and properties* **Chair**: Y. Zhao		**Room B** **Topic H. Keynote 5 - DUFRECHE Jean-François** *"Modelling complex solutions: separation chemistry and recycling of strategic metals"* **Chair**: A. Amine		**Room C** **Topic L. Keynote 6- MATUBAYASI Nobuyuki** *Cosolvent effects on aggregation of bio-related molecules studied with all-atom MD and a solvation theory* **Chair**: A. Idrissi	
	Oral Communications - Session 2					
	Room A - Chair: G. Hefter **Topic: A**		**Room B - Chair**: Z. Yu **Topics: G, H, I**		**Room C - Chairs**: S. Boughammoura - P. D'Angelo **Topics: D, E, N**	
	Com.	*Communicating*	*Com.*	*Communicating*	*Com.*	*Communicating*
16.15 - 16.30	**OC-05A**	SOHR Julia **Germany**	**OC-05B**	TABASSUM Salma **Türkiye** H	**OC-05C**	GIACOMELLI Fernando C. **Brazil** D
16.30 - 16.45	**OC-06A**	MAJLESI Kavosh **Iran**	**OC-06B**	SALIH Kifah S.M. **Qatar** G	**OC-06C**	GÓMEZ ESTÉVEZ Juan Luis **Spain** D
16.45 - 17.00	**OC-07A**	POSTNIKOV Eugene **Russia**	**OC-07B**	MANNUCCI Giorgia **Italy** I	**OC-07C**	WANG Huiyong **China**
17.00 - 17.15	**OC-08A**	ŠARAC Bojan **Slovenia**	**OC-08B**	MRABET Molka **TUN** I	**OC-08C**	TÖRÖK Péter **Hungary** N
17.15- 18.00	**Coffee break + Poster Session 2 (P 21 - P 40) Alphabetical Order**					
	Oral Communications - Session 3					
	***Room A* - Chair**: W. E. Waghorne **Topic: G**		***Room B* - Chair**: T. Deng **Topics: L, N**		***Room C* - Chairs**: Y. Zhao - S. Gadžurić **Topic: E**	
	Com.	*Communicating*	*Com.*	*Communicating*	*Com.*	*Communicating*
18.00 - 18.15	**OC-09A**	RODRIK Geoffroy **France**	**OC-09B**	COSTENOBLE Sandrine **France** N	**OC-09C**	DOMAŃSKA-ŻELAZNA Urszula **Poland**
18.15 - 18.30	**OC-10A**	BRUDAR Sandi **Slovenia**	**OC-10B**	IBRAHIM Issaad **TUN** L	**OC-10C**	KHAN Imran **Oman**
18.30 - 18.45	**OC-11A**	ISHII Yoshiki **JPN**	**OC-11B**	SYCHEV Alexander **Russia** L	**OC-11C**	LI Zhiyong **China**
18.45 - 19.00	**OC-12A**	LIU Ruirui **China**	**OC-12B**	PAPP Judit **Hungary** N	**OC-12C**	ALMASY Laszlo **Hungary** E
19.30	***Dinner***					

	Tuesday 16 September 2025 (Morning)					
09.00 - 09.50 **Room A**	**Topic G. Plenary Lecture 5** **WAGHORNE Winfield Earle** Chair: P. D'Angelo *University College Dublin, Ireland* **Empirical solvent parameters, computational chemistry and the real world**					
09.50 - 10.40	**Room A** **Topic H. Keynote 8- AMINE Aziz** *"Recent advances in molecular imprinting polymers for analytical chemistry"* **Chair**: M. Amara		**Room B** **Topic E. Keynote 7 - GADŽURIĆ Slobodan** *"Carboxylic ionic liquids: Synthesis, properties, acidic constants and application"* **Chair**: T. Deng			
10.40 - 11.30	**Poster Session 3 (P 41 - P 65) Alphabetical Order**					
	Oral Communications - Session 4					
	Room A - Chair: N. Matubayasi **Topic: G**		**Room B - Chair**: J-F. Dufreche **Topics: D, N**		**Room C - Chair**: A. Amine **Topics: K**	
	Com.	*Communicating*	*Com.*	*Communicating*	*Com.*	*Communicating*
11.30 - 11.45	**OC-13A**	LUKŠIČ Miha **Slovenia**	**OC-13B**	KOVÁCS Izabella **Hungary** N	**OC-13C**	BAOUEB Mohamed Hassen **TUN**
11.45 - 12.00	**OC-14A**	OKAZAKI Susumu **JPN**	**OC-14B**	KUTUS Bence **Hungary** N	**OC-14C**	BEN MANAA Marwa **TUN**
12.00 - 12.15	**OC-15A**	PIETROPAOLI Eva **Italy**	**OC-15B**	DAMMAK Ilyes **TUN** D	**OC-15C**	KHATTAK Rozina **PAK**
12.30	***Lunch***					

	Tuesday 16 September 2025 (Afternoon)
14.00	**Cultural Activities: The Amphitheater of El Djem or Kairouan City**
19.30	**Conference Dinner (Banquet)**

<table>
<tr><td></td><td colspan="6"><i>Wednesday 17 September 2025 (Morning)</i></td></tr>
<tr><td>09.00 - 09.40</td><td colspan="2">Room A
Topics N. D. Keynote 9 - AMARA Mourad
<i>From Polyelectrolyte Conformation to Species Selectivity: A PEI Chelation-Based Approach to Membrane Transport</i>
Chair: J.-F. Dufreche</td><td colspan="2">Room B
Topic H. Keynote 10 - YU Zhiwu
<i>"Excess Spectroscopy: Theoretical Considerations and Recent Applications"</i>
Chair: V. Ananikov</td><td colspan="2">Room C
Topic E. Keynote 11 - ZHAO Yang
<i>"Imidazolium - Based Ionic Liquids for CO_2 Capture and Electroreduction"</i>
Chair: L. Latrous</td></tr>
<tr><td></td><td colspan="6">Oral Communications - Session 5</td></tr>
<tr><td></td><td colspan="3">Room A - Chair: A. Idrissi
Topic: B</td><td colspan="3">Room B - Chair: M. Amara
Topics: F, J</td></tr>
<tr><td></td><td><i>Com.</i></td><td colspan="2"><i>Communicating</i></td><td><i>Com.</i></td><td colspan="2"><i>Communicating</i></td></tr>
<tr><td>09.45 - 10.00</td><td>OC-16A</td><td colspan="2">BUSATO Matteo Italy</td><td>OC-16B</td><td colspan="2">AROUS Omar ALG F</td></tr>
<tr><td>10.00 - 10.15</td><td>OC-17A</td><td colspan="2">HAN Jihae Korea</td><td>OC-17B</td><td colspan="2">VANINA Anastasia Russia F</td></tr>
<tr><td>10.15 - 10.30</td><td>OC-18A</td><td colspan="2">JING Zhuanfang China</td><td>OC-18B</td><td colspan="2">ZOGHLAMI Nada TUN F</td></tr>
<tr><td>10.30 - 10.45</td><td>OC-19A</td><td colspan="2">SATO Hina JPN</td><td>OC-19B</td><td colspan="2">KALLEL Jihene TUN J</td></tr>
<tr><td>11.00</td><td colspan="6">Closing Ceremony
Remarks and Best Posters Awards</td></tr>
<tr><td>13.00</td><td colspan="6"><i>Lunch</i></td></tr>
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Topics of ICSC 2025
A. Solution thermodynamics
B. Solution structure and dynamics
C. Solubility phenomena
D. Electrolytes, Polyelectrolytes, Colloids and interfaces
E. Ionic liquids
F. Polymers in Solution, Soft matter
G. Computational solution chemistry
H. Analytical Chemistry
I. Coordination Chemistry
J. Supra molecular chemistry
K. Surface and Interfaces, Nano sensors
L. Biochemical effects in solutions
M. Supercritical fluids and solutions under extreme conditions
N. Industrial applications of solutions

Speakers' Abstracts

Tianlong
DENG

Professor Deng was promoted to Full Professor in 2001 and joined the PhD programme as a supervisor in 2025. He currently serves as Dean of the School of Ocean and Environment, Director of the Key Laboratory of Marine Resource Chemistry and Food Technology (Ministry of Education), and Head of both the ‘One Belt and Road’ Joint Laboratory (Tianjin Government) and the national first-class course *Phase Diagram of Water and Salt System*.

He has been recognized as an innovative team leader by the Ministry of Education and honored through multiple national and provincial distinctions, including the ‘Hundred Talent Plan’ (Chinese Academy of Sciences), Special Professor of Tianjin, and inclusion in Stanford University’s ‘Influential Scholars’ and ‘Lifetime Scientific Influence Ranking’ lists (2023 & 2024).

Professor Deng has led major national and provincial research projects, including one under the National Key R&D Program and multiple NSFC-funded initiatives. He has authored and edited several monographs and textbooks on salt lake chemistry and phase diagrams, and published over 350 SCI papers - more than 50 in top-tier journals (impact factor >10). His work has earned 3 international patents and 34 national invention patents. He has mentored 4 postdoctoral fellows and over 30 doctoral students.

Research Interests

- Comprehensive utilization of salt lake brine and geothermal water resources;
- Phase equilibrium and phase diagram;
- Thermodynamic and thermal analysis; Marine chemistry.

Prediction System for Phase Equilibria in Salt Lake Brine Systems and Its Applications

Linxue YAN, Long LI, Kaiyu ZHAO, Yafei GUO*, Shiqian WANG,
Xiaoping YU and Tianlong DENG*

State Key Laboratory of Bio-based Fiber Materials
Key Laboratory of Marine Resource Chemistry and Food Technology (TUST) in Ministry of Education
College of Chemical Engineering and Materials Science, Tianjin University of Science and Technology,
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The salt lakes of the Qinghai-Tibet Plateau are famous around the world for their rich deposits of lithium, boron, and potassium. The Tibet region, with its unique geographical conditions, the rare elements such as lithium, rubidium, and cesium are rich in geothermal brine resources. Conducting fundamental research on the phase chemistry and thermochemistry of brine systems, studying key technologies for the high-value utilization of brine chemical resources, and exploring prospective research on integrated production of salt lakes and salt chemical industries are of great significance for elucidating the formation and evolution of brine resources and promoting the green and efficient utilization of these valuable resources.

This report presents the progress made by the team in recent years in fundamental research on the phase chemistry and thermochemistry of brine systems, key technologies for the high-value utilization of brine chemical resources, and forward-looking research on integrated production of salt lakes and salt chemical industries, with a particular focus on thermodynamic properties such as phase equilibrium and phase diagrams, dissolution heat, dilution heat, and mixing heat, as well as phase equilibrium dynamic prediction systems and their applications.

Acknowledgment: The authors gratefully acknowledge the funds supported by the key project program of the National Natural Science Foundation of China (U21A20299), the Innovation Project of Excellent Doctoral Dissertation of Tianjin University of Science and Technology (YB2023002), the Tianjin International Joint Laboratory on Belt and Road (24PTLYHZ00270) and the Innovative Research Team of the Chinese University (grant number IRT17R81).

Mikhail G. KISELEV

153045 Ivanovo, Kalinzeva, 55, Russia , mgk@isc-ras.ru
Director of the Institute of Solution Chemistry of the RAS, Ivanovo, Russia
Head of Laboratory of Spectroscopy and Computer simulation

Main research fields

Computer Simulation, Quantum chemistry calculations, Statistical mechanics ,Theory of liquids and supercritical fluids, Critical phenomena

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WOS Researcher ID O-2056-2015

Scopus Author ID 7005285779

Education

Master Degree, Ivanovo State University, (1977-1982)

PhD courses:

The study of hexamethylphosphortriamide hydration using MD simulation, supervisor: Prof. Y.M. Kessler, Institiute of Solution Chemistry of the RAS

Institute of Solution Chemistry of the RAS (1984-1987)

Dr. Sc. In Chemistry 2003, Institute of Solution Chemistry of the RAS

Teaching/supervising experience

Professor, University for Chemistry and Technology, Ivanovo, Russia, (2006-present)

Supervising master degree dissertations

Professor, Institute of Solution Chemistry of the RAS, Ivanovo, Russia, 2012-present

Statistical mechanics courses for PhD students

Guest Professor, Mahidol University, Bangkok, Thailand 2001-2004

Guest Professor, Lille University for technology, Lille, France, 2007-2012

Screening of Polymorphism in Pharmaceutical Compounds under Supercritical State Parameters

Kiselev M.G., Oparin R.D., Ivlev D.V., Dyshin A.A., Khodov I.A.

G. A. Krestov Institute of Solution Chemistry of the RAS, Akademicheskaya st. 1, Ivanovo, Russia

The technologies of supercritical fluids (SCF) are increasingly being utilized for the synthesis and targeted modification of materials and composites. In the pharmaceutical field, these materials are widely applied to enhance the bioavailability of drugs, control their release, and obtain multi-component crystals, among other applications. One of the promising SCF technologies in pharmaceuticals is the formation of micronized particles for use in inhalers. The main advantages of SCF technologies for producing suspensions for inhalation include the following:

- Obtaining micronized forms of the target substance with the ability to control the particle size of the resulting crystals across a wide range of state parameters.
- Achieving a high degree of purity for the target product using both rapid expansion of supercritical solution (RESS) methods and those based on the anti-solvent effect (SAS).
- Controlling the polymorphism of the obtained target product by adjusting the thermodynamic parameters of the supercritical fluid during crystallization, thereby enabling the production of samples with the desired polymorphic purity.

Screening for polymorphism is usually a completely empirical procedure. This report presents a new methodology for screening conformational polymorphism, based on the correlation identified in the authors' previous works between the distribution of conformers of a drug compound dissolved in a supercritical solvent and the polymorph that forms under the studied state parameters. By altering the distribution of conformers based on these state parameters, it becomes possible to screen for polymorphism and, consequently, to predict the formation of polymorphs during micronization. To facilitate this prediction, a methodology was developed that combines experimental approaches (such as IR and NMR spectroscopy) with computational methods (including quantum-chemical calculations, molecular dynamics simulation, and density functional theory).

Key words: supercritical fluids, polymorphism, IR spectroscopy, NMR spectroscopy,
MD simulation

*** This work was supported by the Russian Science Foundation (project 22-13-00257-P).

Roger M. LEBLANC

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Dr. Roger M. Leblanc received his B.S. in chemistry in 1964 from Université Laval, Canada, and Ph.D. in physical chemistry in 1968 from the same university. He was appointed as professor in 1994 and chair of Department of Chemistry at University of Miami from 1994 to 2002 and again from 2013 to 2021. He was also one of the three editors of Colloids and Surfaces B: Biointerfaces from 1998 to 2013. He has published 540 scientific articles in peer-reviewed journals. As a professor, he has supervised more than 100 M.S. and Ph.D. students.

Physicochemical Characterization of a Novel Carbon Nanomaterial: Carbon Dots

Roger M. Leblanc

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Carbon dots (CDs) are a group of novel carbon-based spherical nanoparticles (NPs) with diameters less than 10 nm. They are widely present in the nature and can be also synthesized using various carbon-based substances as precursors by either top-down or bottom-up approaches. They are well characterized for tunable surface functionality, excellent photoluminescence (PL), high photostability and water dispersity, good biocompatibility, and nontoxicity. Also, they display different sizes and surface chemistry depending on the preparation methods and precursors applied. Applications of CDs in drug delivery, bioimaging, sensing, and other nanotechnology fields are rapidly rising due to their aforementioned unique properties. In addition, various spectroscopic and microscopic measurements have been performed on diverse CD preparations, which revealed some typical physicochemical features of CDs. For example, UV/vis absorption spectra of CDs usually display two peaks at 250 and 350 nm, which corresponds to C=C and C=O conjugate structures, respectively. Most fluorescence emission spectra have shown an excitation-dependent PL emission of CDs, which arouses a debate regarding the PL mechanism of CDs. The spherical morphologies of different CDs are studied through a combination of atomic force microscopy (AFM) and transmission electron microscopy (TEM) to obtain the three-dimensional data. As for the structural analysis of CDs, Fouriertransform infrared spectroscopy (FTIR), X-ray photoelectron spectroscopy (XPS), Raman spectroscopy, X-ray diffraction (XRD), small-angle X-ray scattering (SAXS), and thermogravimetric analysis (TGA) have all been utilized to investigate the surface functionalities and core structures. Considering the abundant functionalities such as COOH and -NH2, distinct CDs were conjugated via an amidation reaction mediated by EDC and NHS to explore the construction of large multifunctional carbon-based nanostructures. Also, zeta potential studies show most CDs carry negative charge on the surface, which inspires numerous researches on the electrical or dielectric properties of CDs.

Keywords: Carbon Dots, Physicochemical Characterization, Structure, Conjugation, Dielectric properties.

Abdenacer
IDRISSI

Personal data

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E-mail:	nacer.idrissi@univ-lille.fr
Date of Birth:	1962-10-19
Language	- French - English (everyday and technical speaking, reading, writing) - German (basic)
Qualification	M.Sc. in Physics (1990) Ph.D. in Physical Chemistry (1994)
Working places	
1990-1992	Teacher of physics and Chemistry at different high schools of the Nord French Region
1992-1994	University of Sciences and Technologies, Department of Chemistry, researcher
1996-2012	University of Sciences and Technologies, Associate Professor
2012-	University of Sciences and Technologies, professor

Research areas

My research interest is focused on the understanding of the structure and dynamics of fluids including ionic liquids and supercritical fluids. The main problematics are the understanding of the cellulose dissolution, the control of the polymorphic forms of the bioactive molecules and the characterization of the short time dynamics of the dyes used in solar cells. These research are carried out using a combination of an array of spectroscopic technics (IR, Raman, neutron scattering, time resolved spectroscopy) with molecular dynamics simulation.

Structural and Dynamic Characteristics of Liquid-Vapor Interfaces in Aqueous Solutions, Ionic Liquids, and Supercritical Fluids

Abdenacer Idrissi

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In this work, I will present our findings from molecular simulations and intrinsic surface analysis, which explore the structural and dynamic properties of liquid-vapor interfaces across a range of systems, including ionic liquids [1], organic solvent-water mixtures [2], and gas-liquid equilibria [3]. Our research on imidazolium-based ionic liquids reveals how the spatial organization of ions at the free surface is influenced by anion type and cation alkyl chain length, impacting interfacial charge distribution and mobility. Studies on organic solvent-water mixtures, such as N,N-dimethylformamide-water and DMSO-water, emphasize the role of hydrogen bonding and molecular interactions in shaping interface structure and dynamics. Investigations into aqueous ionic and surfactant solutions provide valuable insights into charge segregation and amphiphilic behavior at the surface. Additionally, analyses of acetone-CO_2 and acetone-methanol mixtures focus on vapor-liquid equilibrium, phase separation, and critical point behavior. Collectively, these studies enhance our fundamental understanding of interfacial phenomena, with broad implications for energy storage, separation technologies, and materials science.

Key words: Interface, Ionic Liquids, Liquids Mixtures, Supercritical fluids

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PROFESSIONAL EXPERIENCE

2024: Honorary Academician of National Academy of Sciences of Bashkortostan Republic
2022: Head of Chemistry Section of the Division of Chemistry and Materials Sciences of Russian Academy of Sciences
2019: Academician of Russian Academy of Sciences
2012: Professor, Chemistry Department, Moscow State University
2009: Head, Division of Structural Studies, Zelinsky Institute of Organic Chemistry
2008: Elected Member of Russian Academy of Sciences
2005: Head, Laboratory of Transition Metal and Nanoparticle Catalysis, Zelinsky Institute of Organic Chemistry
2004 - 2005: Leading Scientist
2000 - 2003: Researcher of Zelinsky Institute of Organic Chemistry
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Solution state organometallic chemistry of Pd, Pt, Ni, Cu and Au complexes and clusters – the key to high performance catalysis

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This presentation will highlight the crucial role of solution-state organometallic chemistry in the design and performance of advanced homogeneous catalysts based on Pd, Pt, Ni, Cu, and Au. In contrast to solid-state systems, the molecular precision and tunability of organometallic species in solution enable detailed control over reaction pathways, selectivity, and catalyst dynamics. Recent advances have revealed that molecular catalysts often undergo reversible transformations in solution - such as ligand exchange, redox processes, and aggregation into reactive clusters - which directly influence catalytic efficiency and stability.

The emerging concept of 4D catalysis [1], originally applied to single-atom and nanoparticle systems, finds a powerful analogue in solution-state chemistry. Time-resolved spectroscopic and computational methods [2] now allow the observation of dynamic speciation and intermediate evolution under catalytic conditions. These insights have led to dramatic improvements in catalyst performance, including reductions in metal loading by up to two orders of magnitude without compromising turnover or selectivity [3,4].

By mapping the full catalytic cycle in solution, including the formation and decomposition of active species, one can optimize reactivity, avoid catalyst deactivation, and design new cooperative multinuclear systems. This presentation will discuss examples ranging from classical Pd-mediated cross-coupling [1-4] to emerging Ni- and Cu-based photocatalysts [5], emphasizing how molecular-level understanding in solution unlocks new frontiers in green and efficient catalysis.

Acknowledgement: The study was supported by Russian Science Foundation (grant 25-13-00387).

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Virginie
MARRY

Virginie Marry holds a PhD from Ecole Normale Supérieure de Lyon in Chemistry. She is specialist in molecular modelling of porous media and in particular of clay materials.

She was recruited as Associate Professor in 2004 by the Pierre et Marie Curie University and became full Professor in 2011.

She conducts her R&D work at the PHENIX Lab. dealing with the physical-chemistry of interfacial nanosystems and electrolytes. She is also in charge of a Master degree in “Physics, Theory and Analytical Chemistry” at the Sorbonne University.

Virginie Marry is co-author of about fifty papers publications in international peer-reviewed journals.

She received the Verdaguer award from the France Institute in 2011 and an award from La Recherche magazine in 2007 (in the category dealing with the research in the energy sector).

She is member since 2019 of the Modelling and Simulation Advisory Board Committee of the Chemical French Society.

Understanding clay/water systems from the compacted to the colloidal state: Coupling modeling and experiments

Marry Virginie

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Clays are multilayered, multiporous materials that exhibit very diverse behaviors in the presence of water: some clays, classified as hydrophilic, swell in the presence of water, while others, rather hydrophobic, do not swell, or only swell moderately. This diversity arises, among other things, from the crystalline structure of the clay, particularly its (negative) charge and its location in the cell, the nature of the counter-ions present between the clay layers, as well as the presence or absence of fluorine in the layer.

At the scale of the clay layer, the interfacial phenomena between clays and aqueous solutions and the origin of the differences between clays can be probed using molecular simulations. Structural, thermodynamic and dynamic results can be compared with experiments, where available, thus challenging the force fields used to assess interactions between species during simulations.

At a more macroscopic scale, clay/water suspensions can be simulated using more or less coarse-grained models. We will show an example of such a model, which finely takes into account the electrostatics and flexibility of clay sheets to describe the isotropic/nematic transition of colloidal clay suspensions.

Key words: clays, modelling, molecular dynamics, colloidal suspensions, swelling

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Education and degrees

1978.April-1982.March, Department of Chemistry, Faculty of Science, Kyoto University, Degree Awarded: B. Sc.

1982.April-1984.March, Department of Chemistry, Graduate School of Science, Kyoto University, Degree Awarded: M. Sc.

1984.April-1986.August, Department of Chemistry, Graduate School of Science, Ph.D. course, Kyoto University

(1985.Oct.-1986.August., Research Associate, Wayne State University, USA)
Degree: Ph.D from Kyoto University

Positions

1986.August-1990.June, Research Associate, Department of Chemistry, Faculty of Science, Tohoku University

1990.July-1993.June, Lecturer, Dept of Chemistry, Faculty of Science, Kyoto University

(1991.July-1992.Feb., Research Associate, Stanford University, USA)

1993.July-1995.April, Associate Professor, Department of Chemistry, Faculty of Science, Kyoto University

1995.April-2001.July, Associate Professor, Graduate School of Science, Kyoto University

2001.July- present, full Professor, Department of Chemistry, Graduate School of Science, Kyoto University

Awards:

1999, Award of Japanese Photochemistry Association

2002, Japanese IBM award of Science

2003, The Chemical Society of Japan Award for Creative Work

2003, BCSJ Award

2009, Inoue Prize

2012, Awards of the Japan Society for Molecular Science

2022, The photobiology Association of Japan award

Dynamics of conformation changes and biological functions of proteins by time-resolved diffusion techniques

Masahide Terazima

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Kyoto, 606-8502, Japan

The translational diffusion coefficient (*D*) in solution is an important physical property that reflects not only a molecular size but also conformation and intermolecular interactions of a macromolecule. Many techniques, e.g., dynamic light scattering, Taylor dispersion, capillary method, NMR spectroscopy, have been developed to monitor molecular diffusion so far. However, molecular diffusion has never been considered to be a time dependent property by these methods, because it usually takes a long time (e.g., several minutes or hours) to measure *D*. This difficulty, the slow time resolution, was overcome by using the pulsed-laser induced transient grating (TG) technique. Now, one can use *D* as a powerful probe to investigate chemical reactions in particular, proteins. Here, we present some applications to protein reactions in time domain.

One of examples is studies on the signalling route and reaction dynamics of Photoactivated adenylate cyclases (PAC) from Oscillatoria acuminata (OaPAC), which consists of a light sensor BLUF domain, an adenylate cyclase domain, and a connector helix. Although the circular dichroism and small-angle X-ray scattering measurements did not show significant changes upon light illumination, the TG method successfully detected light-induced changes in the diffusion coefficient (diffusion-sensitive conformational change (DSCC)) of full-length OaPAC (FL-PAC) and the BLUF domain with the linker-helix. DSCC of FL-PAC was observed only when both protomers in a dimer were photoexcited. This light intensity dependence suggests that OaPAC is a cyclase with a nonlinear light intensity response. The enzymatic activity indeed nonlinearly depends on light intensity, that is, OaPAC is activated under strong light conditions. Based on these findings, a reaction scheme was proposed together with the reaction dynamics.

Key words: protein reaction, diffusion, dynamics, protein-water interaction

Paola
D'ANGELO

Paola D’Angelo is full Professor at the University of Rome “La Sapienza”.

She is the President of the Italian Society of Synchrotron Light (SILS), ex-officio chair of the International X-ray Absorption Society (IXAS), Senior Research Fellow of the Sapienza School for Advanced Studies (SSAS), Coordinator of the PhD Program in Chemical Science at the Sapienza University of Rome

She earned an award from Enimont for her degree curriculum, her Ph.D thesis won an award for the best Italian thesis from Federchimica and she won the “Young Scientist Award” of the International XAFS Society.

She published more than 200 publications in international journals, cited more than 7000 times. Her current h-index is 50 (Scopus) or 52 (Google Scholar).

She is currently the head of the XAMD group that is involved in the structural characterization of disordered and biological systems. She developed advanced methods that combine XAS spectroscopy and computational methods to shed light on the structure and dynamics of disordered or ill defined systems that cannot be characterized through conventional methods.

Deep Eutectic solvents: The relationship between structure and properties

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Deep eutectic solvents (DESs) are currently ruling the research topic about advanced processing media as a more sustainable alternative to traditional solvents owing to their simple preparation, versatility, and environmentally benign pedigree. DESs also belong to the "designer" solvents category, meaning that their chemical-physical properties can be tuned to meet specific requirements through a judicious choice of the precursors and their relative composition. Aside from practical significance, the scientific debate about the fundamental definition of these systems is still going on. At present, DESs are defined as mixtures of two or more compounds showing a melting point depression that is deeper than the ideally predicted one for a defined composition. This unusual thermal behavior seems to rely on the hydrogen-bond (H-bond) network established between the parent compounds. However, alternative interactions concurring as a driving force for the melting point depression have been also demonstrated, and thus this definition seems to start crackling. On the other hand, the achievement of a clearer predictive understanding of the structure–property relationship necessary to design new task-specific DESs is a legitimate goal.

In this contribution, I will show you the results from our work where we tackled some of these unanswered questions through an in-depth structural investigation of different types of DESs. This includes both salt-based DESs belonging to the so-called type "I – IV" categories, and the more recently developed "type V" ones, which are formed by neutral molecular species like terpenes and phenolic compounds.[1,2] Attention will be given also to the structural modification induced by the addition of a co-solvent (*e.g.*, water, methanol, ethanol) to the DES phase.[3] To this purpose, we resorted to a combined approach among different techniques, including synchrotron radiation X-ray absorption and scattering, Raman/IR spectroscopies, differential scanning calorimetry, and molecular dynamics simulations. The combined experimental and theoretical outcome was able to elucidate the complex nature of interactions able to shape the structural arrangement of these H-bonded systems.

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Education and Academic Career:

since 2009:	professor Univ. Montpellier - Institute for Separation Chemistry in Marcoulee (ICSM)
2003-2009:	Chargé de Recherche CNRS laboratory PECSA (Université Paris 6-UPMC))
2001-2003:	Post-Doc University of Cambridge (UK) Department of Chemistry (Jean-Pierre Hansen group) about phase separation in colloids
1999-2001:	PhD Université Paris 6-UPMC Laboratory Ionic Liquids and charged interfaces about dynamics in electrolyte solutions
1998-1999:	CEA/DAM Department of theoretical physics and applications about dense hydrogen
1994-1999:	Undergraduate studies, École Normale Supérieure de Lyon

Research interests (keywords)

Separation chemistry, Multi-scale descriptions, Electrolyte solutions, Charged suspensions. Confined media. Structural and Dynamical properties in Soft Matter systems, Coarse-Graining. Statistical thermodynamics. Theoretical Chemistry. Molecular dynamics, Monte-Carlo simulations.

Teaching activities

- Supervision of 25 PhD students
- Around 200 hours /year of teaching in physical chemistry at any level of the university (from 1 year Batchelor to PhD lectures through master courses: general chemistry, modelling, soft matter, etc. since 2009
- Teaching administration: master “enseignement des sciences en lycée professional”, master “CAPLP math/sciences”, DEA matière condense, cours ecole doctorale.
- Member of commission “finance” and commission “pédagogie” of the Dpt of Chemistry

Evaluation, Awards & Fellowships:

- h-factor = 38 (Scholar), total number of citations = 3703, 350 citations/year the last 5 years
- Group leader of Modelling and Theoretical Chemistry lab (9 scientists: 3 permanent, 3 PhD and 3 post docs).
- AERES evaluation : A+ and A in 2010, 2015 and 2020
- Prize of the French Magazine “La Recherche” (section energy, co-winner, 10 000 €)
- Professeur de classe exceptionnelle in 2024
- ERC senior project REE-CYCLE (sup. Th. Zemb) 2013
- 19 international invited conferences – 17 national invited conferences
- Organization of IUPAC Solution chemistry in La Grande Motte in 2011 (with Pierre Turq)

Publications

- 130 articles (in peer-reviewed international journals)
- 20 international invited conferences, 58 oral communications in international conferences
- H index: 38 Citations 3703 (Google Scholar)

Five representative publications:

1. *Deciphering Second Harmonic Generation Signals* Y. Foucaud, B. Siboulet, M. Duvail, A. Jonchère, O. Diat, R. Vuilleumier, J.-F. Dufrêche *Chem. Sci.* **12**, 15134 – 15142 (2021) (IF = 9,83)
2. *Theory of Ternary Fluids under Centrifugal Fields* S. Stemplinger, S. Prévost, Th. Zemb, D. Horinek, J.-F. Dufrêche *J. Phys. Chem. B* **125** (43), 12054 – 12062 (2021) (IF = 2,99)
3. *How Adsorption of Pheromones on Aerosols Controls Their Transport* L. Jami, Th. Zemb, J. Casas, J.-F. Dufrêche *ACS Cent. Sci.* **6** (9), 1628 – 1638 (2020) (IF = 14,55)
4. *Synergistic Solvent Extraction Is Driven by Entropy* M. Špadina, K. Bohinc, Th. Zemb, J.-F. Dufrêche *ACS Nano* **13** 13745 – 13758 (2019) (IF = 15,88)
5. *Selective layer-free blood serum ionogram based on ion-specific interactions with a nanotransistor* R. Sivakumarasamy, R. Hartkamp, B. Siboulet, J.-F. Dufrêche, K. Nishiguchi, A. Fujiwara, N. Clément *Nature Materials* **17**, 464 – 470 (2018) (IF = 43,84)

Modelling complex solutions:
Separation chemistry and recycling of strategic metals

J.-F. Dufrêche, B. Siboulet, M. Duvail, M. Vatin, E. Guillam, G. Szczepan, Th. Zemb, A. Coste

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Separation chemistry, which aims to separate elements from natural resources or waste for recycling, requires sophisticated methods such as flotation or liquid-liquid extraction. These industrial processes involve complex solutions in which the element, usually in ionic form, is solubilized through specific interactions involving structures at multiple scales. Here we present our results in the case of rare earth extraction. Using a multiscale theoretical approach, implementing molecular simulation methods and mesoscopic descriptions based on soft matter theory, we show how to understand these complex systems. Separation is thus achieved through a subtle balance between short-range forces such as complexation, which enables extraction, and other larger-scale interactions, often of an entropic nature, which play an important role in selectivity. The description of these phenomena therefore requires going beyond the usual elementary chemistry described in terms of first-sphere interactions to take into account collective effects, linked for example to surface properties, molecular curvature, or the formation of larger aggregates.

Key words: Separation chemistry, Rare earth extraction, Multiscale modelling

Slobodan GADŽURIĆ

Slobodan Gadžurić graduated in Chemistry at the Faculty of Sciences, University of Novi Sad, Serbia. PhD degree he obtained in 2006 at the University of Provence in Marseille, France. He has expertise in analytical and physical chemistry of high and low -temperature processes, green chemistry and ionic liquids, chemical equilibria, and association in non-aqueous media. Slobodan Gadžurić is a Chair of the IUPAC Analytical Chemistry Division - Subcommittee on Solubility and Equilibrium Data and a member of the Serbian Chemical Society. He is a Full professor at the Faculty of Science in Novi Sad, Serbia, and head of the Analytical Chemistry Chair, where he is teaching several courses in the field of Analytical Chemistry. For his scientific achievements, he obtained the IUPAC Franzosini Award in 2014.

Carboxylic Ionic Liquids: Synthesis, Properties, Acidic Constants and Application

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Carboxylic ionic liquids (CILs) represent a unique subclass of ionic liquids that incorporate carboxyl functional groups, offering a versatile platform for tunable physicochemical properties and a wide range of applications. This work presents an overview of the synthesis strategies for CILs, focusing on the selection of carboxyl-containing anions and compatible cationic counterparts to ensure stability and desired acidity. The fundamental properties of CILs, including thermal behavior, viscosity, electrical conductivity, and density, are discussed in terms of their molecular structure. Special attention is given to the determination of acidic dissociation constants (pK_a values), which are crucial for understanding the proton-donating ability of these ionic liquids and their behavior in various chemical environments. The influence of structure on acidity is examined, providing insight into structure-property relationships. Finally, the potential applications of CILs are explored, ranging from green solvents in organic synthesis to catalysts, CO_2 capture agents, and functional additives in materials science and pharmaceuticals. Through their tunable acidity, low volatility, and structural diversity, carboxylic ionic liquids offer significant promise in developing sustainable and efficient chemical processes.

Key words: ionic liquids, acidic constants, physico-chemical properties, thermal properties

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Education
1973, Ph.D., Australian National University, Canberra, Australia
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Professional

2011 – Emeritus Professor
2009 – Joint Editor in Chief, Journal of Solution Chemistry
2008 – 2024 Secretary, IUPAC Subcommittee on Solubility and Equilibrium Data
2008 – 2011 Head of School, UCD School of Chemistry and Chemical Biology (UCD-SCCB)
2006 – 2009 Institute of Chemistry of Ireland representative on the Ownership Board of the journal Physical Chemistry Chemical Physics
2003 – 2008 Head of Teaching and Learning and Deputy Head of School, UCD-SCCB
2000 – Associate Professor UCD-SCCB
2000 – 2009 Member of the Editorial Board, Journal of Solution Chemistry
1998 – 2003 Member, Management Committee, UCD-SCCB
1995 – 2000 Director, UCD Soft Matter and Biomaterials Research Centre
1988 – 2000 Senior Lecturer, UCD-SCCB
1975 – 1990 Lecturer UCD-SCCB
1973 – 1975 Department of Education Post doctoral Fellow, UCD-SCCB

Research Interests

The study of the interactions of solute molecules with the surrounding medium is one of the classic problems of physical chemistry. It has long been known that solvents exert a profound influence on chemical systems; recently the role of solvation in biological systems has been recognised, for example, the importance of hydrophobic interactions in processes such as protein folding. Our interests in solution chemistry have included the study of the solvation of both electrolytes and non-electrolytes in aqueous, non-aqueous and mixed solvents. Our approach involves the application of a range of experimental techniques, in combination with solvation theories.

Empirical Solvent Parameters, Computational Chemistry and the Real World

W. Earle Waghorne

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The use of empirical solvent parameters in the analysis and prediction of solvent effects on chemical properties and processes is well established and a range of empirical parameters that are designed to reflect individual interactions have been developed. Correlation of solvent parameters with molecular properties determined using computational chemistry shows that there is marked consistency, such that, for example, the Gutmann's donor number, Kamlet and Taft's β and Catalan's *SB*, all measures of solvent basicity, are strongly corelated with the partial charge on the most negative atom and the energy of the donor orbital [1]. Similar correlations are found for solvent acidity and polarity/polarizability parameters [2]. The correlations also highlight a number of interesting features of the empirical parameters.

Application of linear free energy relationships, LFER, to solubility data, using empirical parameters and using calculated molecular properties, show that the empirical parameters give the better correlations but also highlight some interesting complexities in the LFER approach.

Key words: empirical solvent parameters, computational chemistry, data correlation

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AMINE

- Engineer and PhD from the Free University of Brussels (Belgium,1993)
- Lecturer in Chemical Engineering at the Faculty of Science and Technology, Hassan II University, Casablanca since 1995.
- Director of the environmental and process engineering research laboratory for more than 20 years.
- Supervisor of more than 20 PhD theses.
- Over 200 scientific articles with more than **13,000 citations** and an **H-index of 63**, according to Google Scholar.
- Chairman of the International Workshop on Biosensors (www.biocap.ma)
- Chairman of the International Congress on Analytical Sciences (www.jpfsa.com)
- Editor of a Section of the international journal 'Biosensors & Bioelectronics' published by Elsevier (FI 10.7).
- Associate Editor of Chemistry Africa (Springer)
- Coordinated several national and international projects.
- Member of the national committee for the selection and evaluation of research projects.
- Cited for the fourth year running by Stanford University as one of the 2% most cited researchers in the world.
- GoogleScholar :https://scholar.google.com/citations?user=yycHU3UAAAAJ&hl=en&oi=ao
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Recent advances in molecular imprinting polymers for analytical chemistry

Aziz Amine

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This abstract presents advanced strategies for improving analyte detection in complex matrices. Innovative approaches in the bio-inspired design and application of molecularly imprinted polymers (MIPs) are explored to address challenges in selective separation. MIPs were prepared and subsequently integrated into paper-based platforms or applied in solid-phase extraction protocols for the rapid extraction and detection of analytes such as antibiotics, pesticides, toxins, phenols, flavonoids, metals, and metabolites. Smartphones were successfully employed for colorimetric, fluorescent, and luminescent detection.

The conventional synthesis of MIPs faces several challenges, including lengthy reaction times, high energy consumption, the use of toxic and costly reagents, and low polymer efficiency. To overcome these limitations, our approach utilizes readily available biopolymers, such as chitosan and alginate, as functional materials for the preparation of molecularly imprinted membranes (MIMs). Furthermore, biopolymers with diverse functional groups were tested, offering a versatile strategy for imprinting a wide range of templates and thereby broadening the scope of MIM applications.

Non-specific adsorption was effectively minimized either through post-synthetic modification of the MIPs or by selecting appropriate cross-linkers in the case of MIMs.

This study paves the way for the development of sustainable, cost-effective, and highly selective affinity polymers for next-generation imprinting technologies.

Key words: molecularly imprinted polymers, molecularly imprinted membranes, biopolymer, non-specific adsorption, cross-linking, improved selectivity

Noboyuki MATUBAYASI

Nobuyuki MATUBAYASI received his PhD degree in chemistry from Rutgers University, New Brunswick, New Jersey in 1995 and is a Professor in Division of Chemical Engineering, Graduate School of Engineering Science, Osaka University since 2014. Through combination with state-of-art molecular simulation, he has been developing statistical-mechanical theories of solvation and transport properties, with molecular-level analysis of solvent effects on protein, binding functions of such molecular aggregates as micelle, lipid membrane, and polymer, and electric conduction and diffusion in ionic liquids.

46 h-index

Disciplines

- Theoretical Chemistry
- Physical Chemistry
- Molecular Physics
- Computational Physics
- Biophysics

Cosolvent effects on aggregation of bio-related molecules studied with all-atom MD and a solvation theory

Nobuyuki Matubayasi

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ATP (adenosine triphosphate) is present in cells at concentrations much higher than required for its biological reactions as the energy source, and it has been shown experimentally that ATP acts as a cosolvent to inhibit the aggregation of proteins and peptides [1]. This work addresses the molecular mechanism of the ATP's effects on peptide aggregation from the energetic standpoint by combining all-atom MD simulation and a solvation theory [2,3]. The aggregation core of amyloid β was employed as a model peptide, and the changes in the equilibria between the dissociated and aggregate states of the peptide induced by addition of ATP as a cosolvent was examined in comparison to the case of urea cosolvent. It is shown that with addition of ATP or urea as a cosolvent, the dissociated state of the peptide is more strongly stabilized than aggregates. This means that the cosolvents act to inhibit the aggregation, and ATP is more effective by two orders of magnitude compared with urea at similar concentrations. Through the decomposition of free energy, it is revealed that the van der Waals interaction leads to the inhibition of aggregation both for ATP and urea. Although the electrostatic interaction with the highly charged ATP is strong, it is essentially cancelled by the loss of interactions with water. The observed features of energetics are common between ATP and urea, indictive of the non-specificity of the ATP's (and urea's) effects of aggregate inhibition.

Keywords: cosolvent, ATP, free energy, MD simulation, solvation theory

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He has been an invited speaker at numerous international conferences and serves as an expert advisor in electrolysis, water treatment, chemical speciation, and solution chemistry.

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From Polyelectrolyte Conformation to Species Selectivity: A PEI Chelation-Based Approach to Membrane Transport

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The primary function of membrane materials lies in their ability to selectively transport and separate chemical species. Their performance depends on key surface properties such as charge, hydrophilic/hydrophobic balance, morphology, and chemical reactivity, all of which are influenced by the surrounding medium. Developing selective membranes therefore requires going beyond simple size exclusion, toward mechanisms involving molecular recognition and coordination. One promising strategy involves the formation of reversible complexes within the membrane structure, particularly during chelation-assisted transport. This mechanism enhances the membrane's selectivity, even in complex and heterogeneous environments.

Polymer Inclusion Membranes (PIMs) offer an effective platform for such transport processes, relying on complexation–decomplexation cycles across the membrane interface. Polyethylenimine (PEI), a water-soluble polymer with strong chelating capabilities, has been extensively studied in this context. In aqueous media, its behavior as a polyelectrolyte is highly dependent on pH and ionic strength, which influence its viscosity, degree of protonation, and molecular conformation. In acidic environments, particularly in hydrochloric acid solutions, PEI can reach protonation levels of up to 70%, greatly enhancing its interaction with ionic species. At a pH close to its pKa (8.8), PEI contains both amine and ammonium groups, which impart surface polarity to the membrane. Under alkaline conditions, non-protonated amine groups predominate, enabling metal complexation through lone electron pairs rather than classical ion exchange. At higher pH, negatively charged metal–ligand complexes can be transported through the membrane bulk via ion -pair mechanisms.

In addition to their use in polymer inclusion membranes, PEI has also been explored as a surface modifier for ion exchange and ultrafiltration membranes. This strategy aims to improve membrane selectivity and stability by introducing functional groups that promote selective ion binding and facilitated transport. The structural and chemical effects of this modification have been confirmed through physicochemical characterization techniques such as Scanning Electron Microscopy (SEM) and Fourier-Transform Infrared Spectroscopy (FTIR), which reveal both morphological changes and the appearance of new functional groups. These PEI-functionalized membranes open promising pathways for the reuse of aged or end-of-life membranes, particularly from desalination facilities. Instead of being discarded, these materials can be repurposed for new separation applications, including water purification and selective metal recovery. This approach contributes to the development of more sustainable, circular membrane technologies.

Keywords : Membrane modification, Polyethyleneimine complexation, selectivity, separation process

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尉志武

Prof. Zhiwu Yu received his B.Sc. and Ph.D. degrees from Tsinghua University and King’s College London, respectively. He is now a full professor at the Department of Chemistry, Tsinghua University. His main research fields are chemical thermodynamics and molecular spectroscopy; the main interests are in solution structures and self-assemblies of amphiphilic molecules.

Prof. Yu has published more than 150 research papers on peer reviewed journals. He has been a member of the Chinese Chemical Society since 2002 and now serves as the director of the Committee of Chemical Thermodynamics and Thermal Analysis. He also serves now in the Education Committee (Chair), previously in the Scientific Awards Committee (member for two terms), of the International Confederation of Calorimetry and Thermal Analysis (ICTAC). He is now an editor of Journal of Molecular Liquids and a member and guest editor in the editorial board of Molecules.

Excess Spectroscopy: Theoretical Considerations and Recent Applications

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The physicochemical properties of matters are mainly determined by their structures. This is also true to liquids and liquid mixtures. Unfortunately, our present knowledge on the structures of liquids is very limited. It is widely accepted that microheterogeneity exists in liquids and terms like associates/aggregates/clusters are thus frequently seen in literatures. Due to the dynamic nature of liquids, however, in situ identification of them has been a challenging task.

Among various efforts from different laboratories, we proposed the method of excess spectroscopy, initially applied to FTIR. Then after, it was extended to other types of spectroscopies including Raman spectroscopy. Different formulations to calculate excess spectra and different applications were also reported. The ideal spectra can be constructed either from the wavenumber-dependent absorptivity or absorbance, with some restrict conditions. Excess spectroscopy can be used to enhance apparent spectral resolution, judge the non-ideality of mixtures, determine the selectivity of molecular interactions, and provide specific information on molecular interactions.

When used to identify clusters in liquids, excess spectroscopy can be regarded as a perturbation method. By adding a guest component, the populations of clusters, as well as the types of clusters, in the initial solutions would be perturbated, exposing the structural details. Deriving positive and negative excess peaks is the first and important step of the method. The assignments of the peaks and their analysis are the next key steps. Density functional theory has been used to accomplish the task, while molecular dynamics simulation has been tried recently to provide an alternative.

After addressing the above issues, recent applications of excess spectroscopy in unveiling the heterogeneous acid strength in liquids and the clusters in electrolytes will be presented.

Key words: Excess spectroscopy, Microheterogeneity of liquids, Local acidity, Electrolytes

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Yang Zhao, professor from School of Chemistry and Chemical Engineering, Henan Normal University, Xinxiang, China. She is serving as the Deputy Director of the Chemical Thermodynamics and Thermal Analysis Professional Committee of the Chemical Society of China. Her research interest focus on the functional solution chemisty, green chemisty based on ionic liquids. She has presided over and completed more than 10 national natural science foundation projects and provincial-level projects, winning two first prizes in scientific and technological progress Henan Province, 2 National Teaching Achievement Awards.

Imidazolium - based ionic liquids for CO_2 capture and Electroreduction

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CO_2 is a major greenhouse gas and an important C1 resource[1]. The combination of CO_2 capture and electrochemical CO_2 reduction reaction (CO_2RR) is of great significance for the resource utilization of CO_2. It can not only convert CO_2 into high-value-added chemicals, but also provide an effective method for the storage of renewable energy [2]. Ionic liquids (ILs), due to their advantages such as low saturated vapor pressure, wide electrochemical window and configurable structure, playing a significant role in regulating CO_2 capture and electroreduction processes[3]. However, figuring out the regulatory mechanism of ILs on CO_2 capture and electroreduction performance remains a challenging task. Herein, this study designed and synthesized a series of imidazole-based IL and applied them to the process of CO_2 capture and electrochemical reduction for the preparation of syngas. The main conclusions are as follows.

1. As an example, 1-butyl-3-methylimidazol-1,2,4-triazolium ([C_4mim][4-Triaz]) was used to investigate the regulatory mechanism of the absorption performance of synthesized 12 kinds of basic imidazolium ILs for humid CO_2. The results show that the basic anion activates the C2 site of the imidazolium cation, leading to the reaction of the C2 site with CO_2 to form imidazole-2-carboxylate (NHC-CO_2). The inhalation of water molecules in moist CO_2 can disrupt the structure of NHC-CO_2, resulting in the formation of $[HCO_3]^-$ and thereby increasing the final absorption capacity.

2. A quantitative method was established to estimate the absorption capacity of different absorption sites for CO_2 by using 1-ethyl-3-methylimidazolium glycinate ([C_2mim][Gly]) to absorb humid CO_2. It is found that the absorption capacity of CO_2 is as high as 0.91 mol CO_2 per mol IL in the wet environment, which is nearly double that of dry CO_2 by neat IL. Quantitative studies using various spectral techniques and quantitative calculations have shown that the inhaled H_2O leads to the generation of $[HCO_3]^-$ in the system and the activation of the C2 site of the imidazolium cation. It is precisely this active site that reacts with CO_2 to form NHC-CO_2, significantly enhancing the absorption capacity of CO_2.

3. CO_2RR-to-syngas in the1-butyl-3-methylimidazolium hexafluorophosphate-acetonitrile ([C_4mim][PF_6]-MeCN) electrolyte, and the molar ratio of CO/ H_2 in the syngas was modulated within the range of 1/5 to 26/1. In flow-cell, when the molar ratio of CO/ H_2 was 1/1, 1/2 and 1/3, the corresponding current densities reached 363.6, 458.2 and 644.7 mA cm^{-2} respectively. The C2-H with methyl-substituted imidazolium cation can achieve the switching of CO_2RR products from syngas to CO, and the corresponding current density is as high as 528.3 mA cm^{-2}. The results of the mechanism study show that the C2-H of [C_4mim][PF_6] is mainly responsible for generating H_2, while the C4/5-H co-catalyst to stabilize the intermediate *COO- to generate CO is the key to improving the performance of the final CO_2RR-to-syngas.

Key words: Ionic liquid, CO_2 capture, electroreduction, syngas, regulatory mechanism

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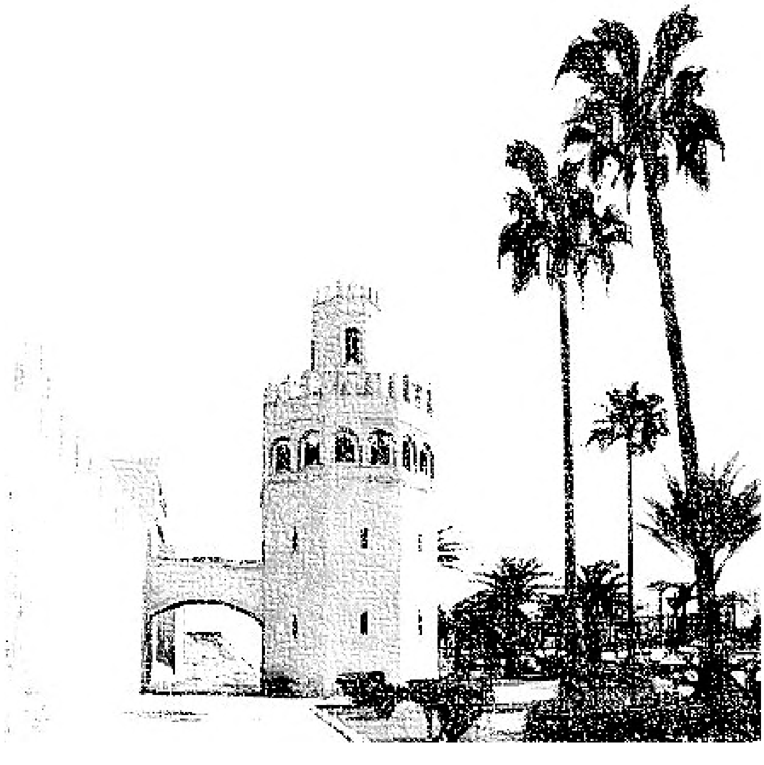
List of Oral Communications

Communicatings' Names	**Ref**
L. Almasy, F. Matroodi, B. Rossi, M. Avdeev, M. Paolantoni, A. Mele *HUN-REN | Centre for Energy Research, Budapest, Hungary* Solvation behavior of BMIM ionic liquids by small-angle Neutron scattering and UV Raman spectroscopy	**OC 12C**
O. Arous, F. Bougheriou *University of Science and Technology Houari Boumediene, Algiers, Algeria* Synthesis and characterization of modified polymer inclusion membranes for water purification	**OC 16B**
M.H. Baoueb, L. Hedhili *IPEIM - Monastir* Nanocellulose: The material of the future for biological applications and specific sensors	**OC 13C**
M. Ben Manaa, A. Ben Lamine *FSM - Monastir* Investigation of adsorption isotherms of Paprika oleoresin dye on TiO_2 mesoporous for dye sensitized solar cells using statistical physics modeling	**OC 14C**
S. Bergaoui, C. Macherki *FSM - Monastir* Electrochemical synthesis of a functional semi-conducting oligomer	**OC 01B**
K. Bohinc *FHS - University of Ljubljana, Slovenia* Incorporation of ion, macroion and solvent structure into modeling of the electric double layer	**OC 01C**
S. Boubakri, R. Iafi, N. Saidi, W. Mabrouk *CERTE - Borj Cédria* Simultaneous adsorptive removal of cationic dyes using an eco-friendly composite: Bentonite-few-layer graphene	**OC 02B**
A. Boukerroui, N.E.H. Laouar, C. Meziti, S. Azoug, A. Zoukel *Abderrahmane Mira University, Bejaia, Algeria* Removal of methylene blue dye using leucaena leucocephala pods: Kinetic and thermodynamic study	**OC 03B**
R. Bouzaiene, B. Šarac, S. Boughammoura, J. Mhalla *FSM - Monastir* Physicochemical characterization of TTAB, SDS, and mixed (SDS-TTAB) surfactant systems in aqueous solutions	**OC 02C**
S. Brudar, K. A. Dill, B. Hribar-Lee *University of Ljubljana, Slovenia* Sticky antibodies: Modeling clusters and viscosity of antibody solutions	**OC 10A**
M. Busato, A. Tofoni, I. Rigacci, M. Giustini, P. D'angelo *Sapienza University of Rome, Italy* Impact of cosolvent on Co^{2+} ion speciation in 'Reline' deep eutectic solvent	**OC 16A**
J. Cerar *FCCT - University of Ljubljana, Slovenia* Real meaning of activity coefficients in electrolyte solutions and thermodynamics behind them: The case of the Debye-Hückel equation	**OC 02A**
C-H. Chang, L. Wei-Lin *National Cheng Kung University, Tainan, Taiwan* Development of catanionic vesicle/hyaluronate complexes for drug delivery applications	**OC 03C**

Communicatings' Names	**Ref**
M. Chorążewski, A. R Lowe *University of Silesia, Poland* Scanning transitiometry for determining the mechanical and thermal energy of lyophobic materials	**OC 04C**
S. Costenoble, L. Lacombe, R. Caprani, B. Arab-Chapelet, C. Quenault, N. Golles *CEA - University of Montpellier, Marcoule, France* Zirconium molybdate inhibition strategy: experimental validation under chemical conditions representative of the industrial nuclear fuel recycling process	**OC 09B**
I. Dammak, S. Cherif, P.J. do Amaral Sobral *ENIS - Sfax* Natural emulsifier-based nanoemulsions for co-encapsulation of β-carotene and (−)-α-bisabolol: Toward stable lipid-based drug delivery systems	**OC 15B**
U. Domańska-Żelazna, A. Wiśniewska, Z. Dąbrowski *ŁUKASIEWICZ Research Network - Industrial Chemistry Institute, Poland* Separation of valuable metals in the recycling of waste Li-ion batteries with solvent extraction and chemical precipitation	**OC 09C**
D. El Hadi, D. Tair, M. Kalla *Blida 1 University, Algeria* New correlations for chemical composition determination of aqueous solutions	**OC 03A**
D.M. Galindres Jiménez, N. Espitia-Galindo , A. Crespo, E. F. Vargas , A. C. F. Ribeiro , M. A. Esteso *Universidad Católica de Ávila, España* Thermodynamic and diffusional analysis of the complexation of sodium salicylate with β-cyclodextrin and anionic resorcin[4]arene	**OC 04A**
F.C. Giacomelli, C. A. S. Ribeiro, G. B. Mondo, I. C. Bellettini *Universidade Federal do ABC, Santo André, Brasil* Polyethylenimine as a versatile simultaneous reducing and stabilizing agent enabling One-Pot synthesis of transition-metal nanoparticles: Fundamental aspects and practical implications	**OC 05C**
J-L. Gómez Estévez, - *Universitat de Barcelona, Espanya* Enthalpies of electrolyte solutions within the context of the McMillan-Mayer theory of solutions in the grand canonical ensemble	**OC 06C**
J. Han, E. Otani, H. Watanabe, Y. Umebayashi *Niigata University, Japan* Speciation and dielectric relaxation study of glass-forming liquid electrolyte consisting of Li[N(SO$_2$CF$_3$)$_2$] and 1,3-propanesultone	**OC 17A**
G. Hefter, L. Hnedkovsky, X. Xiao, T. Vielma, N. Espitia-Galindo, P. A. Martínez-Montoya, L. Ruiz-Virgen *Murdoch University, Perth, Australia* Volumes and heat capacities of nitrate solutions to elevated temperatures	**OC 01A**
I. Ibrahim, A. Naifar, C. Bouraoui, Y. Ben Torkia *FSM - Monastir* Olive mill waste water	**OC 10B**
Y. Ishii, H. Torii, Y. Ikemoto, H. Washizu *Kitasato University, Japan* Molecular Insights on the spatially-dependent properties of hydrogen bonds and infrared vibrational bands on polymer-water interfaces revealed by all-atom MD simulation	**OC 11A**
Z. Jing, T. Yamaguchi, S. Machda, T. Hattori, T. Yamada, H. Tamatsukuri, M. Matsuura, Y. Zhou *Qinghai Institute of Salt Lakes, Chinese Academy of Sciences, China* Ion solvation under gigapascal pressure	**OC 18A**

Communicatings' Names	**Ref**
J. Kallel, N. Jaoued, E. Riahi, C. Bordes, Y. Chevalier, S. Hbaieb *FST - Tunis* NMR study of hydroxypropyl-cyclodextrin inclusion complexes with active molecules of plant mother tinctures	**OC 19B**
I. Khan, Z. Al Mamari, N. Rohman *Sultan Qaboos University, Al Khod, Oman* Modulating SDS surfactant micellization behavior using choline salicylate-derived ionic liquids	**OC 10C**
R. Khattak, - *Shaheed Benazir Bhutto Women University, Peshawar, Pakistan* Sustainable innovations in hazardous dye degradation with ternary metal oxides	**OC 15C**
I. Kovács, P. Sipos, B. Kutus *University of Szeged, Hungary* Hydrolysis and neutralization processes of hydroxy sodalite	**OC 13B**
B. Kutus, P. Sipos, R. Zahorán *University of Szeged, Hungary* Neutralization reactions of katoite, an important reactive component in bauxite residue	**OC 14B**
Z. Li, W. Li, H. Zhao, L. Niu, Y. Zhao *Henan Normal University, China* Spiropyran-based ionic liquid microemulsions: From phase behavior modulation to CO_2 light-triggered release	**OC 11C**
R. Liu, F. Zhu, X. Zhao, Y. Du, Y. Zhou, C. Wang, Y. Zhang *Qinghai Institute of Salt Lakes, Chinese Academy of Sciences, China* A Study on the aggregation and dehydration behavior of aqueous boric acid solutions confined in carbon	**OC 12A**
M. Lukšič *University of Ljubljana, Slovenia* Polymerizing hard-spheres: A resummed thermodynamic perturbation theory for double square-well potential model	**OC 13A**
K. Majlesi, C. De Stefano, F. Crea, C. Bretti *Islamic Azad University, Science & Research Branch, Tehran, Iran* Simulation of the pregabalin behaviour in seawater and urine	**OC 06A**
G. Mannucci, M. Busato, A. Tofoni, M. Giustini, P. D'angelo *Sapienza University of Rome, Italy* Investigating metal speciation in metal-based deep eutectic solvents via combined spectroscopic and computational methods	**OC 07B**
M. Mrabet, F. Ayari *FSM - Monastir* Mo-oxo complexes as active sites for vanillin oxidation under microwave irradiation	**OC 08B**
S. Okazaki, M. Kitabata, A. Yamada, T. Kaneko *Yokohama City University, Japan* A new MD calculation method	**OC 14A**
J. Papp, M. Szabados, P. Sipos, B. Kutus *University of Szeged, Hungary* Synthesis and neutralization behavior of Al-substituted Fe-(oxy)-hydroxide phases	**OC 12B**
E. Pietropaoli, G. Mannucci, M. Palluzzi, M.Busato, P. D'angelo *Sapienza University of Rome, Italy* Exploring π-π stacking in deep eutectic solvents	**OC 15A**

Communicatings' Names	**Ref**
E. Postnikov, A. S. Vanina, A. V. Sychev *Kursk State University, Russia* Phase diagram of sugar-cytric acid-water natural deep eutectic solvents: A predictive approach	**OC 07A**
G. Rodrik, Y. Foucaud, B. Siboulet, J.-F. Dufrêche *University of Montpellier / CEA, France* Hydration and surface chemistry of UO_2: Insights from first-principles molecular dynamics	**OC 09A**
K.S.M. Salih, - *Qatar University, Doha, Qatar* Hydrogen bond influence on tautomeric equilibria of bisimines: Experimental and DFT investigations	**OC 06B**
B. Šarac, Ž. Medoš, M. Bešter-Rogač *FCCT - University of Ljubljana, Slovenia* Revisiting micellization thermodynamics of dodecyltrimethylammonium cations in the presence of salicylate anions	**OC 08A**
H. Sato, K. Banda, S. Nagamine, J. Han, K. Dokko, Y. Umebayashi *Niigata University, Japan* Ion transport properties and Raman spectroscopic analysis of the speciation of $Li[N(FSO_2)_2]$-fluoroethylene carbonate	**OC 19A**
J. Sohr *TU Bergakademie Freiberg, Germany* Properties of solutions of the oceanic salt system calculated with the THEREDA database	**OC 05A**
A. Sychev, A. S. Vanina, E. B. Postnikov *Kursk State University, Russia* Spectral and colorimetric characterisation of resazurin and resorufin solutions with a wide range of varying acidity	**OC 11B**
S. Tabassum, J. Li, H. Altundag *Sakarya University, Serdivan, Türkiye* Nitrate and atrazine-contaminated groundwater remediation: Unveiling the power of mass bio system and solid organic carbon sources	**OC 05B**
P. Török, B. Kutus *University of Szeged, Hungary* Conversion of lithium chloride to lithium hydroxide using tricalcium aluminate	**OC 08C**
A. Vanina, A. V. Sychev, E. B. Postnikov *Kursk State University, Russia* The use of natural deep eutectic solvents for the production of biomolecular components from fish raw materials	**OC 17B**
H. Wang , Y. Guo, T. Song, C. Pang, J. Wang *Henan Normal University, China* The liquid phase exfoliation of two-dimensional materials in ionic liquid	**OC 07C**
Y. Zhou, Z. Jing, D. Pang, H. Wang, M. Ikram *Qinghai Institute of Salt Lakes, Chinese Academy of Sciences, China* Salt Lake cesium resource identification adsorption separation	**OC 04B**
N. Zoghlami, H. El Ayeb, T. Soltani, Y. Chevalier, S. Hbaieb *FST - Tunis* Development of pickering emulsions of Lentisk essential oil stabilized by β-cyclodextrin-modified silica nanoparticles	**OC 18B**



Abstracts of Oral Communications

Program of
Monday 15
September 2025

Volumes and Heat Capacities of Nitrate Solutions to Elevated Temperatures

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Aqueous solutions of nitric acid, nitrate salts, and their mixtures have wide applications in areas as diverse as agriculture, hydrometallurgy, explosives and so on. Because of their widespread application such solutions are also of concern as environmental pollutants in the hydrosphere and atmosphere. From a purely scientific perspective, metal nitrate solutions are of special interest as more-or-less fully dissociated electrolytes, even with higher-valent cations. While the behaviour of nitrate solutions is generally well known at near-ambient temperatures (ca. 25 ^{o}C) and modest concentrations (<1 mol·kg^{-1}), typically few data are available at higher temperatures and concentrations. Of the various physicochemical properties of electrolyte solutions, densities (volumes) and heat capacities are regarded as particularly important. This is because such quantities are required for process engineering calculations involving mass transfer (densities) and heat transfer (heat capacities). This presentation will describe some recent improvements in our techniques and apparatus, which have enabled us to determine the densities and heat capacities of several divalent-metal nitrate solutions and nitric acid to 200 ^{o}C. Measurements on some ternary mixtures (two solutes + solvent) will also be presented and discussed by comparison with results obtained from ideal mixing (Young's) rules.

Real Meaning of Activity Coefficients in Electrolyte Solutions and Thermodynamics Behind Them: The Case of the Debye-Hückel Equation

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Despite the widespread use of the Poisson-Boltzmann equation, the thermodynamic foundations of the Debye-Hückel equation [1] - arguably the most significant and widely applied result derived from Poisson-Boltzmann theory - remain poorly understood. Departing from conventional approaches, we propose a novel perspective by conceptualizing the process of inserting an ion into a Debye-Hückel-model electrolyte solution. This framework enables the distinct calculation of contributions from attractive and repulsive interactions to the total excess electrostatic energy (ΔE) of the system. Crucially, the expression for ΔE derived when accounting for both interaction types differs from that obtained when considering only attractive interactions. For solutions containing finite-sized ions, the absolute ratio of attractive-to-repulsive interaction strengths asymptotically approaches four in the infinite-dilution limit. From ΔE, we further derive the excess Helmholtz free energy (ΔA) and entropy (ΔS) [2]. Notably, the derived expression for ΔA aligns precisely with the classical result of Debye and Hückel [1], validating our approach while offering fresh mechanistic insights.

By partitioning thermodynamics into attractive and repulsive contributions, our analysis provides a clearer physical interpretation of the Debye-Hückel model. Furthermore, it permits quantitative evaluation of how these competing interactions influence macroscopic properties such as the activity coefficient.

Key words: attractive forces, repulsive forces, internal energy, entropy

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New Correlations for Chemical Composition Determination of Aqueous Solutions

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From a thermodynamics point of view, an ideal solution is a class of solution yielded of Raoult's law; where no change in the volume $(\Delta V = 0)$ as well as a thermal effect is however registered $(\Delta H = 0)$ during its formation. Although, most real solutions deviate from Raoult's law and tile now, the structure of these solutions is only known in broad outline, and no general theory of the liquid state has been yet established. Hence, predicting and calculating the various properties of liquid solutions seem a hard task due to the toolless, relatively to the gas and the solid state. However, tables contain the density values of aqueous solutions of commonly used acids, bases, or salts as a function of the mass content for different temperatures. Where in some cases, these properties are unknown, and correlations have to be used in this case. For an ideal solution at a given temperature, the mass percentage C of an aqueous solution varies as a function of the density ρ according to a model type « $C = a + b\rho^{-1}$ ». Whereas, in the case of real solutions, we propose more general empirical model in the form of « $C = a + b\rho^{-1} + c\rho + d\rho^{2}$ ». Based on a database, giving the mass percentage C and the density ρ at $20°C$, the use of the proposed model for a number of aqueous solutions $(HNO_3,\ NH_3,\ HCOOH,\ KCl,...)$ allowed us to carry out the characteristic constants (a, b, c and d) for each type of solution. And the comparison between the calculated and experimental values C shows thus, the proposed models are characterized by very high precision, with an average absolute error of $(eamoy \approx 0.422\%)$ and a correlation coefficient $(0.998 < \mathrm{R} < 1.000)$.

Key words: Solution, Aqueous, Composition, Density, Modeling

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Thermodynamic and diffusional analysis of the complexation of sodium salicylate with *β*-cyclodextrin and anionic resorcin[4]arene

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The interaction of sodium salicylate (NaSal) with both *β*-cyclodextrin (*β*-CD) and the anionic macrocycle Na_4EtRA was studied by mutual diffusion, Job plot analysis, NMR spectroscopy, and computational modeling. Diffusion experiments revealed significant differences in transport between the two systems. For NaSal–Na_4EtRA, D_{12} showed positive values, while D_{21} was close to zero, indicating co-transport of NaSal with Na_4EtRA. These results, together with those of NMR and computational calculations (which displayed unfavorable conditions for NaSal inclusion), are consistent with an outer-side complexation mechanism [1].

In contrast, the NaSal–*β*-CD system exhibited negative D_{12} values, denoting counter-current flows indicative of inclusion complex formation. ^{1}H-NMR data as well as computational analyses (which identified a stable inclusion with $\Delta E = –36.26$ kcal/mol) supported this hypothesis. Thermodynamic analysis confirmed the formation of the NaSal–*β*-CD complex ($\Delta G = –17.72$ kcal/mol) [1]. Finally, the agreement between the experimental and simulated UV-Vis spectra reinforced the possibility of the formation of complex structures.

Key words: β-cyclodextrin; sodium sulfonated-resorcinarenes; sodium salicylate; diffusion by Taylor technique; transport properties; computational calculations

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Properties of solutions of the oceanic salt system calculated with the THEREDA database

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The Thermodynamic Reference Database (THEREDA) is designed for geochemical modelling in the context of radioactive waste repositories. It especially addresses high-salinity aqueous solutions and supports the Pitzer ion-interaction approach. While the database's primary focus is on the correct calculation of solubilities, this study investigates THEREDA's capabilities in calculating caloric properties of salt solutions.

Enthalpies of solution and crystallisation of binary and ternary systems of oceanic salts are calculated and compared with available experimental data from the literature.

Key words: Solution thermodynamics, thermodynamic modelling, THEREDA database, oceanic salts

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Simulation of the pregabalin behaviour in seawater and urine

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Pregabalin has been identified as an emerging contaminant in aquatic environments, primarily due to its widespread use in treating anxiety and neuropathic pain. Evidence suggests that a significant amount of pregabalin is eliminated from the body without undergoing degradation or chemical modification. In studies of biologically and environmentally significant ligands, it is often crucial to understand their behaviour in real systems, such as biological fluids or natural water. Understanding the protonation constants of environmentally relevant pharmaceuticals is essential for accurately assessing their presence, behaviour, and impact.

The acid-base properties of pregabalin were investigated under various ionic media (NaCl, $(C_2H_5)_4NI$ and $NaClO_4$), ionic strengths ($0.1 \leq I/\text{mol kg}^{-1}(H_2O) \leq 1$), and temperatures ($288.15 \leq T/\text{K} \leq 310.15$). The thermodynamic formation parameters were modeled in relation to variations in temperature and ionic strength, using both the Specific Ion Interaction Theory (SIT) and an extended Debye-Hückel type equation. Simulations were carried out in a multicomponent solution that mimicked seawater with a salinity of 35%, considering all internal interactions between the primary components, as well as their interactions with metals (Zn^{2+} and Cu^{2+}) and pregabalin. The results suggest that at the pH level of seawater (pH = 8.2), approximately 58% of pregabalin is bound to Cu^{2+}, while about 41% exists as the LH^0 species. In the Zn^{2+}/pregabalin system, only about 28% of ligand is complexed, with roughly 70% existing in a protonated form [1].

Key words: Simulation, Pregabalin, Emerging contaminants

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Phase diagram of sugar-cytric acid-water natural deep eutectic solvents: A predictive approach

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We consider aqueous ternary mixtures of either fructose or glucose with citric acid, which are argued in literature for some fixed sugar:acid ratios as forming natural deep eutectic solvents. To analyse this feature in-depth, a wide range of sugar-acid molar rations is explored experimentally, and the water activity diagram, which plays the role of eutonic counterpart to the eutectic diagram, is analysed theoretically. Here we discuss that the diagram's branches, formed by the saturated aqueous solution of one component with sequentially added another one, can be accurately predicted, except the vicinity of eutonic point, by the Norrish-Ross model as well as the dependence for amounts of substances giving a fixed total molar content. This leads to the conclusion that Fru:Cit:Water and Glu:Cit:Water systems behave like a quasi-ideal mixture of two non-ideal solutions everywhere outside of the vicinity of the eutonic point, where they exhibit properties resembling deep eutectic solvents. In addition, using the viscosity data from work by Troter et al., and our original method of fast quenching of solutions, we considered the predictability of the glass transition for the system of considered monosaccharides and citric acid in 1:1 molar ratio comparably using the fractional generalization of the Vogel-Fulcher-Tammann equation and Mauro-Allan-Potuzak's model.

Key words: NADES, ternary mixtures, water activity, phase diagram, glass transition

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Revisiting Micellization Thermodynamics of Dodecyltrimethylammonium Cations in the Presence of Salicylate Anions

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The salicylate ion (Sal$^-$) is a well-known hydrotrope that promotes the formation of worm-like micelles from the quaternary ammonium surfactant dodecyltrimethylammonium chloride (DTAC). This self-assembly process is strongly influenced by the molar ratio between DTA$^+$ and Sal$^-$ ions, with Sal$^-$ – alongside Cl$^-$ – acting as counterions to DTA$^+$ during micellization [1].

Using isothermal titration calorimetry (ITC), supported by viscosity, particle size, ζ-potential, and UV-Vis spectroscopy measurements, we systematically examined the self-assembly behavior of DTAC across a broad concentration range and at different temperatures. This comprehensive approach allowed us to refine the understanding of the micellization process in the presence of salicylate. A series of unique ITC experiments was conducted to investigate the micellization of DTA$^+$ ions in the presence of Sal$^-$ anions. The resulting thermograms were analyzed using a novel thermodynamic model, which provided a detailed insight into the aggregation behavior of the surfactant system.

The experiments revealed a strong interaction between Sal$^-$ and DTA$^+$ ions during aggregation process. Initially, small aggregates form, which rapidly grow into worm-like micelles at a molar ratio of NaSal/DTAC = 0.5, reaching maximum micellar length at ratio 2. These structural transitions, along with the redistribution of Sal$^-$ ions, are clearly reflected in the thermodynamic profiles and corroborated by changes in viscosity, particle size, and spectroscopic responses.

Key words: Isothermal titration calorimetry, DTAC, salicylate, worm-like micelles

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Hydration and Surface Chemistry of UO_2: Insights from First-Principles Molecular Dynamics

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Uranium dioxide (UO_2) is the primary nuclear fuel, and its surface chemistry—especially water adsorption—is key to fuel reprocessing and disposal. However, the molecular-scale mechanisms remain elusive, and current computational studies rely on static models[1], despite the inherently dynamic nature of the process.

Building on this knowledge, we therefore employed first-principles molecular dynamics (DFT-MD) to investigate the hydration of UO_2 surfaces, focusing on the three most stable terminations: (111), (110), and (100)[2]. By coupling DFT with molecular dynamics, we analyzed how water adsorption evolves with increasing coverage, how hydration layers form and structure themselves over time, and how surface charge emerges at equilibrium. The simulations reveal distinct behaviors: while (111) and (110) favor molecular adsorption with partial dissociation and develop positive surface charges, the more reactive (100) surface undergoes full hydroxylation and remains nearly neutral. Water structuring was also surface-dependent, with up to three ordered layers on (111), fewer on (110), and a rapid transition to bulk behavior on (100).

Key words: Uranium dioxide (UO_2), Surface chemistry, Nuclear fuel reprocessing, *Ab initio* molecular dynamics, Water adsorption and dissociation, Hydration of minerals

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Sticky Antibodies: Modeling Clusters and Viscosity of Antibody solutions

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High-concentration monoclonal antibody (mAb) formulations often suffer from elevated viscosities, hindering their therapeutic use. To uncover the molecular origins of this behavior, we combined experimental data (viscosity, G_{22}, B_{22}, and cluster distributions) with Wertheim's thermodynamic perturbation theory. By modeling antibodies as Y-shaped 7-bead structures (Fig. 1), we derived cluster-size distributions and linked them to viscosities across protein concentrations. Our results show that viscosity is mainly governed by mAb clustering dynamics, with weakly interacting mAbs limited by nucleation and strongly interacting ones by propagation. Viscosity correlated well with the experimentally determined G_{22} values, but not with B_{22}. Theoretical predictions using a single Wertheim energetic parameter for mAb stickiness capture these effects, providing a quantitative framework for optimizing antibody formulations by modulating self-association—ultimately enhancing therapeutic delivery.

Key words: mAb, Wertheim perturbation theory, protein aggregation, G_{22}, B_{22}

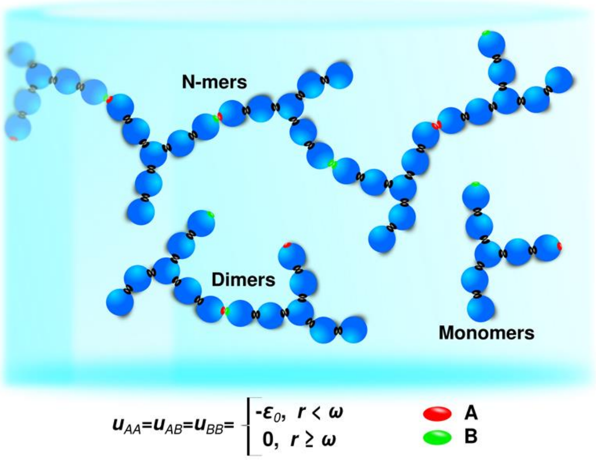

Figure 1: 7-bead mAb model with its interacting sites A and B in monomeric, dimeric and multimeric form.

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Molecular Insights on the Spatially-Dependent Properties of Hydrogen Bonds and Infrared Vibrational Bands on Polymer-Water Interfaces Revealed by All-Atom MD simulation

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Understanding the hydrogen-bonding properties of water molecules in the vicinity of soft materials plays a key role in preventing the adsorption of biomolecules, and also in controlling the degradation of material properties.[1] To elucidate the hydrogen-bonding structures and nanoscopic functions of water molecules at soft material interface, experimental measurements of infrared (IR) spectroscopy and its theoretical analysis based on molecular dynamics (MD) simulation have been widely reported for various polymer-water interfaces.[2] Here we recently developed a spatially-decomposed approach for analyzing the IR band of OH stretching vibrational mode for water molecules on the basis of quantum-chemical calculations,[3] which can be adopted to nanoscopic regions on the polymer-water interface.[4] With this theoretical approach in the framework of all-atom MD simulation, we found that displacements of water molecules away from the polymer interface can induce a low-frequency shift of the OH stretching mode of water by the formation of hydrogen bonds with other water molecules included in the polymer and water phases. Furthermore, the modulation of OH stretching mode for water can be also revealed to occur within a nanometer-scale region near the polymer interface.

Key words: molecular dynamics, infrared band, water, polymer, hydrogen bonds.

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A Study on the Aggregation and Dehydration Behavior of Aqueous Boric Acid Solutions Confined in Carbon

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The properties and structure of boric acid aqueous solutions confined in different carbon nanotubes (CNTs) with pore sizes are investigated using multi-scale simulations. The study shows that a CNTs pore size of 2.56 nm is a critical value for the properties and structure of confined boric acid solutions. When the pore size of CNT is less than 2.56 nm, the properties of boric acid solutions show a noticeable confinement effect, which gradually decreases with increasing pore size, and approaches those of a bulk solution. In small-sized CNTs (0.82 and 0.96 nm), boric acid molecules do not polymerize with each other. With further increasing pore size, polymerization occurs between boric acid molecules in a bidentate manner. In small CNTs (0.82 and 0.96 nm), boric acid molecules undergo dehydration and transform into metaboric acid molecules. This study provides a theoretical basis for green enrichment, separation, and high-value utilization of boron resources.

Key words: Boric acid; Carbon nanotubes; Molecular dynamics simulation

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Electrochemical Synthesis of a functional semi-conducting oligomer

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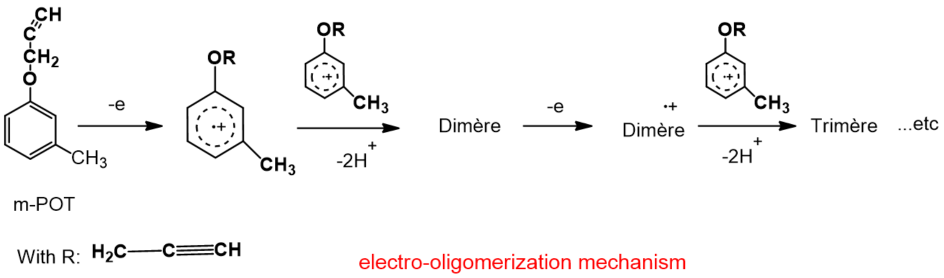

electro-oligomerization mechanism

An electrochemical oxidation of m-propargyloxytoluene (m-POT) was performed in acetonitrile on a platinum electrode. Voltammetric analysis of this product showed that it is electroactive and exhibits a single irreversible peak. At concentrations exceeding 10^{-2} mol·L^{-1}, surface phenomena were observed, leading to the formation of a film on the electrode surface during successive potential sweeps.

Intentiostatic preparative electrolysis resulted in the deposition of a solid film on the electrode, along with the formation of a chloroform-soluble product. IR and NMR spectroscopic analyses confirmed the formation of oligomers derived from m-POT. The electro-oligomerization proceeds via coupling of radical cation intermediates.

Preliminary physico-chemical studies showed that the resulting new functional material is thermally stable up to 254°C and a semiconductor. In addition, the chloroform-soluble oligomer is photoluminescent. Its maximum emission is located in the green spectrum. This property highlights its potential application in the development of organic light-emitting diodes (OLEDs).

Key words: functional oligophenylene, electropolymerization, Electron transfer, green photoluminescence

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Simultaneous Adsorptive Removal of Cationic Dyes Using an Eco-Friendly Composite: Bentonite–Few-Layer Graphene

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In this study, a bentonite–few-layer graphene (BFLG) composite was synthesized and thoroughly characterized using Fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), Brunauer–Emmett–Teller (BET) surface area analysis, X-ray photoelectron spectroscopy (XPS), and thermogravimetric analysis (TGA). The BFLG exhibited a high specific surface area along with well-developed structural and physicochemical properties. It was employed as an efficient adsorbent for the rapid and simultaneous removal of two cationic dyes, auramine O (AO) and rhodamine B (RB), adsorption was predominantly influenced by electrostatic forces and π–π stacking. Key operational parameters such as pH, adsorbent dosage, contact time, and initial dye concentration were systematically investigated and optimized to enhance dye removal efficiency. Under optimal conditions (pH 9), the composite achieved maximum adsorption capacities of 288 mg/g for AO and 294 mg/g for RB. Adsorption equilibrium data were best described by the Langmuir isotherm model, indicating homogeneous monolayer adsorption, while kinetic data fitted the pseudo-second-order model, suggesting chemisorption as the dominant mechanism. Thermodynamic analyses confirmed the adsorption process to be spontaneous and endothermic. Moreover, the composite demonstrated good reusability, highlighting its potential as a cost-effective and eco-friendly adsorbent for treating dye-contaminated wastewater.

Keywords: Bentonite–few-layer graphene, Cationic dyes, Adsorption, Langmuir isotherm, Wastewater treatment.

Removal of methylene blue dye using leucaena leucocephala pods: Kinetic and thermodynamic study

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Leucaena Leucocephala Pods (LLP) were handpicked under their trees situated from the campus area garden of Bejaia university (Algeria), and were used as an effective bioadsorbant to eliminate Methylene Blue (MB) dye. The pods were first washed, dried, crushed and sieved through an 250 µm standard sieve. Findings of FTIR characterisation method suggest that the most common functional groups present on the surface of LLP waste are the O-H group, C-O group, C-H group, C-C and C=N or C=C groups, that enhance the adsorption performance of cationic MB dye [1]. The adsorption studies were performed under batch mode and focused on the effects of adsorbent dosage (1.5 g.L^{-1}), initial MB concentrations (40 mg.L^{-1}), and contact time (60 min). Kinetic analyses showed adsorption following a pseudo-second-order model, with a maximum adsorption capacity (q_{max}) of 144.92 mg.g^{-1} according to the Langmuir model. The comparison of q_{max} value of other biomaterials, it could be concluded that q_{max} value of LLP is comparable to other efficient bioadsorbents; such as Papaya seeds (120.48 mg.g^{-1}) [1], Bagasse Fly Ash (15.5 mg.g^{-1}) [2] and Bamboobiomass AC (83.3 mg.g^{-1} [3]. Thermodynamic parameters indicated that MB adsorption process onto LLP biomaterial is spontaneous and endothermic (ΔH>0).

Key words: Adsorption, Methylene Blue, Isotherm, Kinetic, Leucaena Leucocephala .

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Salt Lake Cesium Resource Identification Adsorption Separation

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Cesium (Cs) are important and expensive alkali metals widely used in fields such as national defense, catalysis, night vision imaging, and solar cells etc. Rb and Cs are extensively present in salt lake brines, but their concentrations are extremely low compared to other ions such as Na^+, K^+, Mg^{2+}, Cl^-, and SO_4^{2-}. During the evaporation process of salt lakes, they often "disappeared" from the brines due to the formation of solid solutions like (K, Rb, Cs)$MgCl_3 \cdot 6H_2O$ [1], making effective enrich during salt ponder process challenging. The hydration and competitive complexation under high ionic strength further exacerbate the difficulty of selective separation. Selectivity adsorption or ion exchange is one of the most important methods for selectively recovering Cs resource from salt lake brines.

We developed a process for selectively extracting cesium through pre-saponified *t*-BAMBP, and revealed that, in addition to the traditional electrostatic attraction between the phenolic hydroxyl group (-OR) and Cs^+, ion-π interactions play a significant role in the selective extraction of cesium by *t*-BAMBP[2] also. Based on the excellent alkali metal recognition properties of crown ethers, a magnetic separation adsorbent for Cs^+ was prepared by amidating 18-crown-6 ether functional groups onto carboxylated Fe_3O_4 magnetic nanoparticles (Fe_3O_4@R−COOH)[3], and its high-selectivity mechanism was discussed[4]. Furthermore, in order to develop inorganic adsorbents which are more suitable for salt lake brine systems and address issues such as poor hydraulic performance and dissolution losses, we designed and synthesized cobalt hexacyanoferrate double-hollow nano-bubble prisms (Co-PBA DHNPs) with controllable morphology via a self-templating method[5]. Recently, we also prepared a potassium-ion-supported layered metal sulfide Cs^+ recognition adsorbent, achieving selective extraction of Cs^+ from brines through ion size sieving and the hard-soft acid-base (HSAB) theory. These adsorbents are expected to enable highly efficient separation and recovery of Cs^+ from salt lake brines.

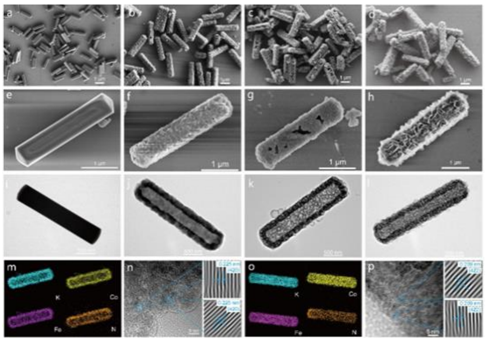

Figure 1. Potassium cobalt ferrocyanide double-hollow nano-bubble prisms (Co-PBA DHNP) adsorbent

Key words: Salt lake brine, Cs^+ adsorption separation, Ion exchange, Ion hydration

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Nitrate and Atrazine-Contaminated Groundwater Remediation: Unveiling the Power of Mass Bio System and Solid Organic Carbon Sources

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Nitrate has become one of the world's most common groundwater (GW) contaminants.[1] Nitrate exists in the form of NO_3^- ions in water and can exist stably for a long time without forming precipitation. Nitrate forms nitrite after entering the organism, causing significant harm to the health of humans and other organisms. One of the most popular herbicides in the world, atrazine (ATZ), poses a serious risk to agricultural safety and groundwater use. ATZ's aqueous solubility, slow hydrolysis, non-volatility, and non-biodegradability have led to its frequent detection in surface and groundwater[2]. In the current study, we combine and extend the recent work of our lab[3]. Using solid organic matter, rice straw and paper plates as carbon sources, inoculated with activated sludge and mixed with the novel Mass Bio System (MBS) as the medium to remove nitrate from groundwater is feasible. The effectiveness of solid-state denitrification for the simultaneous removal of nitrate and atrazine from groundwater was investigated using rice straw as a carbon source, using a self-designed plexiglass reaction column in this current study. Increasing the nitrate content in water, atrazine load and changing the hydraulic retention time, the effects of nitrate concentration, atrazine concentration and hydraulic retention time on the solid-phase denitrification system were investigated. When initial nitrate concentrations were 50 and 100 mg/L, respectively, the effluent nitrate concentrations reached high removal efficiency within 5 days. When the initial nitrate concentration was increased to 150 mg/L, the nitrate removal efficiency decreased to 82.3%. The system demonstrated stable denitrification and a certain degree of resistance to shock loads. The study also found that removal efficiency decreased from 80% to 30% as atrazine concentrations increased. The removal of atrazine primarily relies on the adsorption of rice straw. Nitrate removal efficiency remained above 80% throughout the experiment. Rice straw reached saturation adsorption for atrazine, with a maximum removal efficiency of 78.64%. Overall, this technology appears cost-effective, cleaner, more denitrification-efficient, and non-toxic to deal with nitrate and atrazine-contaminated water for application in actual engineering.

Key words: Groundwater, Biological denitrification, Solid organic carbon source, Nitrate, Atrazine, Mass Bio System

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Hydrogen Bond Influence on Tautomeric Equilibria of Bisimines: Experimental and DFT Investigations

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A key focus for researchers in the field of synthetic chemistry is to develop new structures with extensive functional groups for diverse applications. Bisimine-functionalized compounds play a significant role in tuning the physicochemical properties.[1] These derivatives exhibit notable uses and are widely utilized as dyes, pigments, polymer stabilizers, and intermediates in organic synthesis. [2] A series of bisimines was synthesized through typical condensation of hydroxydiamine and 2-thienylcarboxaldehyde precursors. After characterization, variable-temperature ^{1}H-NMR was employed to study the influence of solvent polarity. The solvent's ability to form hydrogen bond was found to significantly influence the tautomerization of the synthesized structures. Thermochemical parameters calculated using DFT and MP2 methods indicated that the target compound exists in equilibrium between two tautomers. Additional DFT approaches (TD-DFT) were employed to explore the basis of electronic absorptions, while surface analysis was conducted to identify electrophilic and nucleophilic regions. The effect of solvent polarity on absorption spectra was also examined. A solvation relationship was established between Gutmann's donicity numbers and the experimental λ_{max}. [3-4]

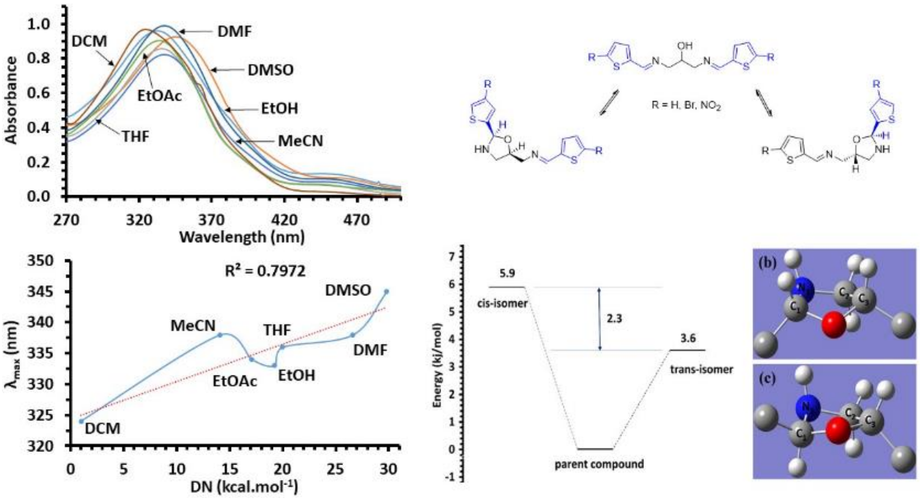

Figure 1: Solvent influence on Absorption Spectra and Tautomerism.

Key words: solvent polarity, tautomerism, hydrogen bond, MP2, TD-DFT

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Investigating Metal Speciation in Metal-Based Deep Eutectic Solvents via Combined Spectroscopic and Computational Methods

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Deep eutectic solvents (DESs) are an emerging class of green solvents that have attracted significant attention due to their distinctive physicochemical properties. A growing area of interest involves metal-based deep eutectic solvents (MDESs), a subclass incorporating metal salts. Owing to their high polarity and conductivity, MDESs are promising for applications such as electrolytes, electrodeposition, and catalysis [1,2]. Understanding metal ion speciation in MDESs is essential to realizing their full potential in these domains.

Here, we demonstrate the value of an integrated experimental and computational strategy for probing metal speciation in MDESs, illustrated through two case studies. First, a $NiCl_2 \cdot 6H_2O$:urea (1:3.5) MDES is analyzed using molecular dynamics, UV-Vis, SAXS/WAXS, and X-ray absorption spectroscopy. The results reveal that Ni^{2+} forms chloride- and water-bridged oligomers in the neat MDES, which dissociate into fully solvated species upon water addition, indicating a shift to aqueous coordination. Second, a ChCl:$CoCl_2 \cdot 6H_2O$ (1:2) MDES is studied via UV–Vis, XAS, and multivariate curve resolution (MCR), revealing tetrahedral and octahedral Co^{2+} species, with water favoring the latter. EXAFS and XANES confirm the structural assignments.

Together, these studies showcase how a synergistic methodology offers detailed insights into metal coordination in MDESs and provides a generalizable framework for understanding speciation in complex solvent systems-advancing the design of sustainable and functional chemical media.

Key words: DES, X-ray absorption spectroscopy, MCR, UV/Vis spectroscopy.

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Mo-oxo complexes as active sites for vanillin oxidation under microwave irradiation

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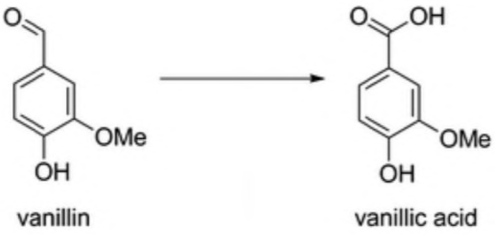
Vanillic acid is an important phenolic compound with several therapeutic properties, *e.g*. anti-cancer, anti-obesity, antibacterial, and anti-inflammation [1]. Few studies have focused on the oxidation of vanillin into vanillic acid (Scheme 1).



Scheme 1: Vanillin oxidation into vanillic acid

The reaction in Scheme 1 was catalyzed by $_{79}Au$ nanoparticles supported on Al_2O_3 with a yield of 100 % obtained after 30 minutes at 80 °C under 5 bar of oxygen [2]. In the present study, vanillin was oxidized into vanillic acid under microwaves in the presence of few amounts of H_2O_2 and molybdenum based catalysts.

The catalysts were prepared by solid state exchange of different Mo precursors and several zeolitic materials. Using a specific MFI zeolite at 9 *wt*. % of Mo, 100 % of acid yield was obtained after 10 minutes of irradiation. According to the characterization results, tetraoxomolybdate(2–) and/or μ-oxo-hexaoxomolybdate(2-) complexe(s) are (is) the active site(s). Hydrogen peroxide and (Mo=O) bond in the catalyst are required for the reaction since the catalytic runs performed with pure zeolite, with distilled H_2O (instead of H_2O_2) and without catalyst led to poor catalytic activities as revealed by HPLC.

Key words: Vanillin, Vanillic acid, oxo-species, HPLC, Microwave

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Zirconium molybdate inhibition strategy: Experimental validation under chemical conditions representative of the industrial nuclear fuel recycling process

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Every day, the dissolution stage of irradiated nuclear fuel is carried out in semi-continuous mode in a dissolver-wheel reactor at the La Hague plant (France). It is an essential phase in the spent fuel treatment-recycling (PUREX) process, which determines the efficiency of subsequent separation of recoverable materials (uranium and plutonium), with the aim of completely dissolving the spent fuel in using concentrated nitric acid heated to 92°C [1]. However, this operation is hampered by the undesirable precipitation of zirconium molybdate (ZM), which occurs when local zirconium and molybdenum concentrations reach a critical threshold. This phenomenon, which causes solid deposits that can trap actinides or clog equipment, represents a major challenge in terms of safety, performance and industrial availability.

In order to develop robust inhibition strategies, an innovative experimental set-up has been designed by CEA. This dedicated system is easily implanted into a nuclear glovebox, and is capable of reproducing, under continuous conditions, the ZM formation mechanisms observed in industrial environments. This original set-up is based on a tailor-made quartz reactor simulating the hydrodynamic behavior of a wheel dissolver, coupled with a regulated feed system (pumps and flowmeters) compatible with glovebox in the presence of actinides (U, Pu). Compared with studies using batch reactors, this represents a significant advance in terms of representativeness of industrial conditions.

Two experimental campaigns were carried out in active media to evaluate the effectiveness of a precipitation inhibitor. The first was carried out under reference conditions (Mo, Zr, U, Pu), while the second incorporated the inhibitor. Comparative analysis of the precipitates obtained - in terms of mass, morphology and structure - provides critical data for assessing the potential of this inhibition strategy, and paves the way for industrial transposition.

Keywords: zirconium molybdate, precipitation, inhibition, industrial dissolver, actinides

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Olive Mill Wastewater Treatment through a Combined Experimental and Kinetics Studies

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This current paper presents a novel approach for the treatment of Olive Mill Wastewater (OMW) integrating Quartz Crystal Microbalance (QCM) experiments with statistical physics modeling. The exploration aims to enhance the adsorption efficiency of OMW by optimizing clay-based adsorbent through the incorporation of Thyme. Correlating experimental data with validated models enables the construction of a realistic microscopic framework for the retention process. The kinetic modeling revealed that the adhesion reaction adheres to the Brouers-Sotolongo model at T= 30°C and 40°C. Our regression analysis revealed that, at the optimal temperature of 30°C, the maximum adsorbed amount is equal to 2.41 μg/cm^2.

Keywords: Quartz Cristal Microbalance, Olive Mill Wastewater, Statistical physics.

Spectral and colorimetric characterisation of resazurin and resorufin solutions with a wide range of varying acidity

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Recently, the blue-coloured aqueous solution of resazurin sodium salt has been widely applied for testing bacterial culture viability and drug response due to its response to the cellular respiratory processes leading to its reduction to pink resorufin. This process is not only a qualitative indicator; it can be characterized quantitatively [1] but only under conditions of a neutral medium. At the same time, there are multiple processes of interest which take place in an acidic medium resulting in non-trivial colourimetric behaviour. In this work, we present the results of a systematic study of the interplay between molecular properties of solvents and spectral and colourimetric responses of resazurin/resorufin systems in solutions with pH varying in the range of 0.1–10. Investigations of full spectra in the range of visible light, spectral shifts of maxima induced by the protonation of particular groups and its quantitative adjustment with the trajectories in special CIE-based colourimetric spaces were carried out. The latter leads to an efficient decoupling of principal components conditioned by a solvent's properties and the indicator's response to chemical and biochemical reactions within the frames of analytical chemical colourimetry. From the practical point of view, the results of the study open perspectives for the application of new easily implementable colourimetric tests for the monitoring of biochemical status (freshness, microbial contamination) of coloured liquid food products, which can be coloured themselves (e.g. apple, grape, pineapple juices, etc.) with pH values different from neutral.

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Synthesis and neutralization behavior of Al-substituted Fe-(oxy)-hydroxide phases

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Red mud or bauxite residue is undoubtedly the most significant by-product of the alumina industry, with well-known environmental impacts: in addition to its heavy metal content, its high pH (11.3 on average [1]) is the main obstacle for further recovery and utilisation. One of the simplest and most cost-effective way to reduce the alkali content of bauxite residue is to neutralize it with strong acids, such as hydrochloric acid. In turn, effective neutralization requires detailed knowledge on the neutralization of solid phase which could potentially contribute to the alkalinity of bauxite residue.

Thus, our aim was to investigate the acid-base reactions of the two most abundant phases, i.e. partially aluminium-substituted goethite (iron oxy-hydroxides, $Fe_{1-x}Al_xOOH$) and hematite (iron oxides, $Fe_{2-y}Al_yO_3$). For the production of goethite [2], we used a modified synthesis route based on the co-precipitation of iron and aluminium salts. Two types of synthesis were applied for low Al- and high Al-substituted samples. $NaAl(OH)_4$ and Fe(III) nitrate salt were used for low Al-substituted samples, whereas Fe(II) chloride and Al(III) chloride were used for high Al-ones. The thus obtained goethite phases underwent low-temperature calcination yielding the respective hematite phases.

After optimization of the experimental conditions, extensive structural characterizations of the products were performed before and after the reaction with HCl.

Key words: bauxite residue, aluminium-substituted goethite, aluminium-substituted hematite

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Incorporation of ion, macroion and solvent structure into modeling of the electric double layer

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Electrostatic interactions between charged macromolecules in electrolyte solutions are of fundamental importance in colloid and surface chemistry [1,2]. Mobile ions in the electrolyte interact with charged macroions and an electric double layer is formed. In this work, we focus on structural details of the ions, solvent structure and the structure of charged surfaces [3-5]. The structural details include beside steric effects also the presence of charge distributions on individual ions, spatially extended ions/molecules, and internal ionic degrees of freedom[3]. The solvent structure is included via Langevin dipoles. The charge regulation of macroions surfaces and the charge structure of lipid head group is included as well [4]. We discuss how various theoretical models predict structural properties of diffusive electric double layer and compare theoretical predictions with computer simulations.We showed that the multivalent ions/molecules with spatially distributed charge can induce attraction between like-charged objects. The attraction results from inter-ionic correlations [5].

Key words: solvent structure, macroions, ions, electric double layer

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Physicochemical Characterization of TTAB, SDS, and mixed (SDS-TTAB) surfactant systems in aqueous solutions

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This study focuses on the physicochemical characterization of three surfactant systems: the cationic system (water-TTAB), the anionic system (water-SDS), and their mixed system (water-SDS-TTAB). A combination of analytical techniques was employed, including fluorescence quenching, light (TDSLS), neutron (SANS) scattering methods, zeta potential measurements, and isothermal titration calorimetry (ITC) [1-3]. However, their reported data concerning the parameters of micellisation (with different CMC concentrations), hydration and ionic condensation, scatter markedly. The conductivity method combined to the ion-selective electrode (ISE) method appears as one of the most appropriate techniques because of their high sensitivity even at high dilution, and because of their well-established theory [4,5].

The individual systems were first analyzed to determine their intrinsic micellar properties, followed by a systematic investigation of the mixed surfactant system to evaluate the synergistic or antagonistic interactions between SDS and TTAB. Conductivity and ISE measurements provided insight into well-defined CMC values and counter-ion binding, while zeta potential analysis highlighted changes in surface charge associated with mixed micelles. ITC offered thermodynamic parameters, including enthalpy and entropy changes, demonstrating the energy profiles of micellization and surfactant interactions. DLS measurements supported the characterization of micelle size and aggregation number variations in the presence of mixed surfactants.

The results confirmed that SDS and TTAB exhibit significant interaction in mixed micelle formation, with low CMC, indicating an expected strong synergistic effect due to electrostatic and hydrophobic forces at play [6-8].

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Development of catanionic vesicle/hyaluronate complexes for drug delivery applications

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In this study, positively charged catanionic vesicles were prepared by a forced formation process using hexadecyltrimethylammonium:dodecylsulfate, dihexadecyldimethylammonium bromide, and cholesterol. Then, negatively charged sodium hyaluronate (HA) was added to form catanionic vesicle/HA complexes through electrostatic attraction. The binding behavior of the catanionic vesicles and HA and the influence of the environment on the catanionic vesicle/HA complexes were investigated. It was found that HAs of different molecular weights had similar binding behavior with the catanionic vesicles. Dynamic light scattering and fluorescence polarization analyses showed that the physical properties of the complexes could be modulated by the HA molecular weight and content. When a sufficient amount of HA was adsorbed on the vesicle surfaces, the complexes became negatively charged. As the environment became more acidic, the absolute value of the zeta potential was decreased. Under relatively alkaline conditions, especially at pH 7.4, the complexes could maintain stable. Furthermore, the complexes remained intact in the temperature range of 25-70℃. Increasing the ionic strength of the environment would decrease the size of the complexes. However, the complex structures still remained stable when the ionic strength was comparable to that of human body fluids. Finally, the feasibility of the catanionic vesicle/HA complexes as drug delivery carriers was demonstrated by the high encapsulation efficiency for vitamin E acetate.

Key words: catanionic vesicle, ion pair amphiphile, sodium hyaluronate, vesicle/hyaluronate complex

Scanning Transitiometry for determining the mechanical and thermal energy of lyophobic materials

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The scanning transitiometry technique is applied to determine the heat of liquid water intruding into and from hydrophobic porous media. The experimental technique and the challenges around the experimental design will be presented, to overcome losing the valuable thermodynamic data in the calorimetric signal. The results of these experiments demonstrate that the intrusion process is exothermic and extrusion process is endothermic at 25°C. At higher temperature becomes endothermic.[1–3] During the same process mechanical energy is stored under pressure. For hydrophobic systems the amount of energy stored and release can be adjusted by using solutes, which are either too large in size to enter into the porous media or small enough to enter into the porous media. These thermophysical properties are important for designing new types of shock absorbers, bumpers, energy dissipaters and molecular springs which are made of liquid-solid interfacial systems. Using water as the solvent different aqueous solutions are used to change the physical properties of intrusion/extrusion pressure and the heat of intrusion/extrusion values.[4] These are the external properties which control the total amount of energy stored within a system.

Key words: calorimetry, heat of solution, aqueous solutions, nanomaterials, high-pressure

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Polyethylenimine as a Versatile Simultaneous Reducing and Stabilizing Agent Enabling One-Pot Synthesis of Transition-Metal Nanoparticles: Fundamental Aspects and Practical Implications

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The large surface area of metallic nanoparticles provides them with particular optical, chemical, and biological properties, accordingly enabling their use in a wide array of applications. In this regard, facile and fast synthetic approaches are desirable for ready-to-use functional materials. Following investigations focused on the direct synthesis of polymer-coated gold nanoparticles,[1] we demonstrate that such a strategy can be also used to manufacture different types of d-block transition-metal nanoparticles via a one-pot method in aqueous media and mild temperature conditions. Palladium (Pd^{2+}) and silver (Ag^{+}) ions could be reduced using only polyethylenimine (PEI) or PEI derivatives acting simultaneously as a reducing and stabilizing agent and without the aid of any other external agent.[3] The process gave rise, for instance, to Pd raspberry-like nanostructures with large surface area and outstanding catalytic performance. The polymer-stabilized AgNPs were demonstrated to be biocide against a variety of microorganisms, whereas AuNPs with enhanced cellular uptake could be also produced.[3] These findings provide significant advances toward the practical, facile, and ready-to-use manufacturing of transition-metal nanoparticles for a myriad of applications.

Key words: metallic nanoparticles, nitrogen-containing polymers, one-pot synthesis, catalytic activity, antimicrobial properties, cellular uptake

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Enthalpies of electrolyte solutions within the context of the McMillan-Mayer theory of solutions in the grand canonical ensemble

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The McMillan-Mayer (MM) theory of solutions is a very general theory that was formulated in the grand canonical ensemble [1]. The natural variables are the temperature, the volume of the system and the chemical potentials of the solution components. This theory allows to treat the solution as a system where the solvent does not appear in an explicit way. The thermodynamic properties obtained are the apparent molar properties as defined in thermodynamics [2].

In this work a general expression for the solution's apparent molar enthalpy is obtained in terms of the pair correlation functions for the solute and the pair potential of mean force at infinite dilution. Experimental dilution enthalpies can be analysed in terms of a given model after correcting the differences between the grand canonical variables and the usual experimental variables (temperature, pressure and concentration of solutes in the solution). As an example, the limiting law for the enthalpy of dilution is obtained for the Debye-Hückel theory [2].

This general treatment will be compared with that of Friedman [3], Ramanathan and Friedman [4], Krienke and Faigl [5] and the more recent work of Simonin [6)].

Key words: McMillan-Mayer, Grand canonical ensemble, Electrolyte solutions, Apparent molar enthalpies, Heats of dilution.

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The liquid phase exfoliation of two-dimensional materials in ionic liquid

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Two-dimensional layered materials, with their advantages such as low density, high mechanical strength, low friction coefficient, and good thermal conductivity, have found widespread applications in energy, environment, electronics, biology, and other fields. These materials include graphene, black phosphorus, hexagonal boron nitride, transition metal chalcogenides, metal-organic frameworks, and covalent organic frameworks (COFs), among others. Among the existing methods, liquid-phase exfoliation stands out as one of the feasible approaches suitable for large-scale production of two-dimensional layered materials [1-3]. However, the current liquid-phase exfoliation of two-dimensional layered materials generally faces challenges such as low yield and the use of mostly toxic solvents. Ionic liquids, with extremely low vapor pressure, excellent solubility, and good thermal stability, provide a new opportunity for the liquid-phase exfoliation of two-dimensional layered materials. Therefore, we systematically investigated the structure-activity relationship between ionic liquids and the liquid-phase exfoliation performance of COFs and MX_2 (M= Ti, Zr, Hf, Mo, X=S, Se, Te) and obtained an efficient liquid-phase exfoliation system. The research results indicate that ionic liquids should possess suitable molecular size, surface energy matching that of two-dimensional materials, compatible Hansen solubility parameters, and strong interactions. Only ionic liquids meeting these conditions have the potential for efficient and layer-controlled liquid-phase exfoliation of COFs and MX_2 (M= Ti, Zr, Hf, Mo, X=S, Se, Te).

Key words: Two-dimensional materials, Liquid-phase exfoliation, Ionic liquid, Mechanism

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Conversion of lithium chloride to lithium hydroxide using tricalcium aluminate

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Recently, $LiOH \cdot H_2O$ is becoming the main precursor for lithium-ion battery cathodes [1]. One of the most important source of LiOH production is LiCl, since ca. two-thirds of lithium reserves are found in the form of dilute brines [2]. Current synthesis methods are based on the precipitation of Li_2CO_3 and its conversion with $Ca(OH)_2$. Since the last step is characterized by low yields, it would be advantageous to produce LiOH bypassing the carbonate intermediate. To this end, we studied the one-step conversion of LiCl using tricalcium aluminate, $Ca_3Al_2O_6$, via the formation of Friedel's salt, $[Ca_2(Al(OH)_6)]_2Cl_2 \cdot 4H_2O$ [3].

We conducted conversion experiments using LiCl solutions with an initial Li^+ concentration of 10 g L^{-1} in temperature range of 5–75°C; the LiCl:$Ca_3Al_2O_6$ molar ratio was 2:1. Upon increasing the reaction time from 1 hours to 1 week, the conversion yield increased gradually from 57% to 74%, exhibiting a plateau after 6 hours at 25°C. Varying the reaction temperature, the yield changed in the order 40% (5°C), 65% (25°C), 66% (50°C), and 57% (75°C), applying 2 hours of reaction time. The XRD patterns of the obtained solids clearly showed that Friedel's salt is the dominant product with no discernible traces of $Ca_3Al_2O_6$ or its hydrated from, $Ca_3Al_2(OH)_{12}$.

In summary, we find that concentrated LiCl solutions can be converted to LiOH with fair yields already under ambient conditions. Further optimization including initial Li^+ concentration and LiCl:$Ca_3Al_2O_6$ molar ratio is in progress.

Keywords: lithium chloride, lithium hydroxide, Friedel's salt, tricalcium aluminate

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Separation of valuable metals in the recycling of waste Li-ion batteries with solvent extraction and chemical precipitation

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The leaching liquid composed of DES (choline chloride and malonic acid (1:1) with glycine, hydrogen peroxide, H_2O_2 and didecyldimethyl ammonium chloride surfactant, DDACl - two-stages extraction and double stripping) was used for the extraction of valuable elements from the black mass (BM) of the Lithium-ion batteries (LiBs). The study was carried out to investigate the extraction and separation of Co(II), Ni(II), Cu(II), Li(I) and Mn(II) from the solid powder BM. Leaching from the solid phase was proposed with DES with different additives. The separation of metal ions was proposed with, D2EHPA, two ionic liquids (ILs) showing synergistic effect for the separation of Co/Ni, different solvents and acids for the stripping and chemical precipitations. The synergistic effect of two ionic liquids (ILs), trihexyltetradecylphosphonium chloride, $[P_{6,6,6,14}][Cl]$ and trihexyltetradecyl bis(2,4,4-trimethylpentyl) phosphinate, $[P_{6,6,6,14}]$[CYANEX 272]/naphtha revealed high separation selectivity of Co/Ni. The dimethylglyoxime, DMG was used for the precipitation of Ni. The probe of precipitation of Li with sodium phosphate, Na_3PO_4 or sodium carbonate, Na_2CO_3 were tested. For all the systems, the solvent concentration, the amount of additivities, temperature of the extraction, pH and liquid/solid as well as organic/water ratios and the selectivity and distribution ratios were described. The utilization of new DESs /ILs with additives can serve as a potential alternative leaching solvents [1]. The metal ions content in aqueous and stripped organic solutions was determined by the ICP-MS or ICP-OES method. All these results show that the solvent extraction could successfully replace traditional hydrometallurgical and pyrometallurgical methods in new technologies for the assess of metals from the black mass (BM), obtained from LiPBs.

Key words: Li-ion battery recycling, Process optimization, Flowsheet proposal

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Modulating SDS Surfactant Micellization Behavior Using Choline Salicylate-Derived Ionic Liquids

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Modifying the behavior of surfactants in aqueous solutions is essential for enhancing their performance, particularly through the incorporation of biocompatible ionic liquids (ILs) into the solvent system [1,2]. This study explores the thermodynamic behavior of the anionic surfactant sodium dodecyl sulfate (SDS) in the presence of novel choline salicylate-based ILs: choline salicylate ([Ch][SA]), choline *para*-methyl salicylate ([Ch][p-MSA]), choline *para*-amino salicylate ([Ch][p-ASA]), choline *para*-nitro salicylate ([Ch][p-NSA]), choline *para*-chloro salicylate ([Ch][p-ClSA]), choline *para*-hydroxy salicylate ([Ch][p-HSA]), and choline acetyl salicylate ([Ch][AcSA]).

Given the wide industrial relevance of surfactant systems, understanding the impact of IL additives on SDS solutions is of significant interest. The aggregation behavior of SDS was investigated in both the absence and presence of 5 mM ILs across three temperatures: 288.15 K, 298.15 K, and 308.15 K. Critical micelle concentration (CMC) values were determined using electrical conductivity and surface tension measurements. The results reveal that all ILs reduce the CMC of SDS, following the trend: [Ch][p-ClSA] > [Ch][p-NSA] > [Ch][p-ASA] > [Ch][p-HSA] > [Ch][SA] > water. These CMC values were further used to calculate the standard thermodynamic parameters of micellization – free energy (ΔG_m°), enthalpy (ΔH_m°), and entropy (ΔS_m°). The negative ΔG_m° values confirm the spontaneous nature of micelle formation in all systems. It is observed that an endothermic micellization at lower temperatures, turning exothermic as temperature rises due to weakened hydrogen bonds and increased London-dispersion forces. Additional interfacial parameters, including maximum surface excess concentration ($\Gamma_{\max}$), minimum area per molecule (A_{min}), surface pressure at CMC (π_{CMC}), adsorption efficiency, and molecular packing parameters, were evaluated to provide insight into how IL anions influence surfactant efficiency. These findings contribute to a deeper understanding of IL-assisted optimization of surfactant behavior in aqueous environments.

Key words: Surfactant, Ionic Liquids, Micellization, Surface Properties

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Spiropyran-based ionic liquid microemulsions: From phase behavior modulation to CO_2 light-triggered release

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Spiropyran is a classical photochromic group that exhibits high photoisomerization efficiency and excellent reversibility. The equilibrium between its closed-ring (SP) and open-ring (MC) structures is highly dependent on the polarity of the solvent. [1-2] Based on a systematic understanding of the solvation behavior of spiropyran-based ionic liquids, a series of light-responsive spiropyran-based ionic liquid microemulsions were developed. In the microemulsion system, the spiropyran functional groups undergo a transition from the open-ring [MC(H)] structure to the closed-ring (SP) structure upon visible light irradiation. This isomerization process involves the release and uptake of protons (H^+), leading to notable changes in the pH of the local microenvironment. Utilizing this property, we employed these microemulsions as adsorbents to regulate the solubility and pH of the target ionic liquid by designing the structure of the photoacid, thereby enabling light-controlled pH variation for CO_2 capture and subsequent light-triggered release.

Key words: microemulsion, ionic liquids, light responsiveness, CO_2 capture

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Solvation behavior of ionic liquids by small-angle neutron scattering and Raman spectroscopy

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Solvation behavior of small organic molecules in aqueous solutions is closely related to their structural organization and eventual self-assembly. In this study, we investigated series of aqueous solutions of methyl-imidazolium - based ionic liquids by UV Raman spectroscopy and small-angle neutron scattering. Selected Raman signals in different wavenumber ranges provide insights into the local organization of cation-anion pairs as a function of the increasing amount of water in a wide range of concentrations. The high-frequency range of the Raman spectra is analyzed by a differential method to extract from the OH stretching profile of water the solute-correlated (SC) spectra, which emphasize the molecular structuring of the interfacial water in the hydration shells around the selected anions.

The neutron scattering data reveal the water – IL segregation at nanoscale, whereas the Raman data indicate that the organization of the interfacial water differs markedly for different solutions, being affected by specific anion–water interactions. In particular, in the case of [BMIM][BF_4], which forms weaker hydrogen bonds with water, the aggregation propensity depends strongly on the concentration, as reflected by local changes in the spectra of the interfacial water, and seen also in the neutron scattering patterns. On the other hand, stronger water–anion hydrogen bonds and more persistent hydration layers were observed for [BMIM][TfO], which likely suppress the formation of IL aggregates.

Key words: ionic liquid, Raman scattering, small-angle scattering, microheterogeneity

Program of
Tuesday 16
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Polymerizing hard-spheres: A resummed thermodynamic perturbation theory for double square-well potential model

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We studied a primitive model of polymerizing hard spheres, characterized by hard-sphere repulsive interaction and short-ranged double square-well attractive interaction. The system consisted of an equimolar two-component mixture of hard spheres with identical diameter (σ), where particles of different species interacted *via* a double square-well potential with two distinct binding minima at distances $0 < L_s < L_l < \sigma$.

The resulting aggregate structures depend on the bonding distances L_s and L_l. (i) When both L_s and L_l are less than σ/2, only dimers with two bonding lengths can form. (ii) If $L_s < \sigma/2$ and $\sigma/2 < L_l < \sigma/\sqrt{3}$ particles may form either a single bond of length L_s or two bonds of length L_l, leading to a mixture of dimers (with L_s) and linear chains (with L_l). (iii) For larger L_s values (i.e., $\sigma/2 < L_s < \sigma/\sqrt{3}$), chains with alternating bond lengths L_s and L_l emerge. Further increases in bonding distances produces more complex aggregate topologies, not studied in this work.

The model qualitatively reproduces the most important features of associating fluids and is simple enough to be treated theoretically. The theoretical framework employs an extension of the resummed thermodynamic perturbation theory for associating fluids with central-force interactions [1,2]. We computed thermodynamic and aggregation properties of the model, depending on density, temperature and potential parameters. Comparing theory with Monte Carlo simulation results, we observed good agreement. We showed that the model exhibits nontrivial aggregation behaviour, driven by competition between bonding at L_s and L_l. By tuning potential parameters (well depths and widths), we identified two distinct temperature-dependent scenarios: (1) Upon cooling, dimers (with L_s) initially form but then dissociate into linear chains (with L_l) at lower temperatures. (2) Linear chains appear first but break apart into dimers upon further cooling. This counterintuitive behaviour allows external control over cluster formation, enabling transitions between different ordered states, including liquid crystal-like structures.

Key words: hard-spheres, association, polymerization, resumed TPT

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A new MD calculation method of free energy of mixing for binary systems with very different molecular sizes and interactions

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Free energy of mixing is one of the most fundamental thermodynamic quantities, which can describe miscibility or affinity of the two component liquids. It has been obtained experimentally for many liquid pairs based on the vapor pressure measurements. It has been investigated, too, by molecular simulations for near half century from the old [1] to the latest [2-3]. Recently, thermodynamic integration method has been mostly used, which gives satisfactory prediction for the free energy of small molecules once the force fields were given [2-3]. However, when molecular size is very different between two component molecules, the calculation often becomes unstable particularly at $\lambda \approx 0$. Further, if the difference in the intermolecular interaction between the two becomes great during the change in the thermodynamic state, the system shows phase separation. This makes the integration incorrect.

In the present study, a new integration path is proposed related to the molecular size and interaction, following which we can avoid divergence and discontinuity of the integration. We demonstrate satisfactory calculations of free energy of mixing of polymers into small solvents.

Key words: free energy of mixing, MD calculation, thermodynamic integration method,

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Exploring π-π Stacking in Deep Eutectic Solvents

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Deep eutectic solvents (DESs) have emerged as a promising and eco-friendly alternative to conventional organic solvents, thanks to their excellent biocompatibility and sustainable nature.[1] These solvents are easily obtained by combining two compounds, leading to a significant depression of the mixture's melting point (MP).[2] Among recent developments, type V DESs have attracted growing interest. Their precursors can generally be classified into two types: hydrogen bond acceptors (HBAs) and hydrogen bond donors (HBDs). However, despite their increasing popularity, the detailed interactions responsible for DES formation are still not fully understood. This study aims to better define the "deep" eutectic behavior exhibited by DESs by performing a detailed structural analysis of selected precursors to reveal the molecular interactions involved. While hydrogen bonding is widely accepted as a key factor, other interactions, such as π-π stacking, are also likely to play a role.[3] Therefore, this research focuses on exploring all relevant interactions, with special attention to the potential impact of π-π stacking in DES formation. To investigate this, we selected two different sets of molecules with distinct hydrogen bonding capabilities. Specifically, the study examines systems composed of 1,3,5-trimethoxybenzene (TMB) and 1,3-diacetylbenzene (13DAB), as well as combinations of 3,5-dimethoxyphenol (DMP) and 13DAB.[4] Through a multidisciplinary approach combining theoretical modeling and experimental analysis, we aim to gain a deeper understanding of the processes driving DES formation. Eutectic behavior is predicted using the conductor-like screening model (COSMO). Thermal properties are assessed through differential scanning calorimetry (DSC), while molecular dynamics (MD) simulations provide insights into interactions at the molecular level.

Key words: Deep eutectic solvent, π-π stacking, COSMO, hydrogen bond.

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Hydrolysis and neutralization processes of hydroxy sodalite

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The Bayer process generates over 150 million tonnes of bauxite residue (BxR) annually [1]. Its alkalinity (average pH 11.3) makes acidic treatment essential for safe storage and use; however, neutralization is complicated by the dissolution of solid-phase components acting as buffers [2]. Hydroxy sodalite (HXS) is one of the most important reactive components in BxR; yet, little is known about its behaviour in aqueous medium. Therefore, our research focused on the synthesis, hydrolysis, and neutralization behaviour of HXS.

First, we synthesized HXS by digesting kaolinite in a concentrated (~19 M) NaOH solution, the average composition of the thus obtain solids was $Na_8[AlSiO_4]_6(OH)_{1.5}(CO_3)_{0.25}\cdot 2.8H_2O$.

The time and concentration dependence of HXS suspensions with $c_{\mathrm{HXS}} = 0.01–100\ \mathrm{g\ L^{-1}}$ at room temperature was monitored using pH-metry. We found that approximately 20 to 30 days were required to reach a constant pH. Additionally, the dissolution of HXS involves phase transformation. Three solid phases may be in equilibrium: HXS (dominant above pH ≈ 10.5) and two hydrosodalite phases (HS1, HS2; dominant below pH ≈10.5) without OH^-/CO_3^{2-} ions in the β-cages, characteristic of sodalites.

Next, HCl solutions were added to HXS suspension to neutralize the cage OH^- and CO_3^{2-} ions. Initially, a rapid neutralization was observed, followed by a gradual increase in pH, caused by the slow dissolution of the forming HS phases. Steady-state experiments showed that reaching a stable pH of 8 requires the use of 4 moles of HCl per mole of HXS.

In summary, our results suggest that the slow dissolution of HXS and that of hydrosodalite phases formed during neutralization contribute significantly to the alkaline pH of BxR.

Keywords: hydroxy sodalite, bauxite residue, solubility, neutralization

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Neutralization reactions of katoite, an important reactive component in bauxite residue

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Katoites, $[Ca_3Al_2(SiO_4)_x(OH)_{12-4x}$, $x \leq 1.5$ (KAT), belong the hydrogarnet family of minerals [1] which are formed during the Bayer process [1,2]. These solids are discharged with bauxite residue, the by-product of the Bayer process, and their hydrolysis rises solution pH. Since bauxite residue is classified as hazardous material due to its alkaline nature (pH = 9.2–12.8 [2]), neutralization of KATs is pivotal to BxR processing and safe disposal. In this work, we synthesized KAT phases with different silica content and studied its reactions with HCl.

First, we prepared KAT phases by digesting CaO and kaolinite in hot $NaAl(OH)_4/NaOH$ solutions. We obtained virtually phase-pure products for KATs with $x \leq 0.4$. As for solids with $x > 0.4$, KATs still formed but hydroxy-sodalite, $Na_8[AlSiO_4]_6(OH)_2\cdot 2H_2O$ (HXS), appeared in increasing amounts, correlating to the enhancement of initial silica concentration.

Next, we carried out neutralization experiments, which showed that phase-pure KAT requires six equivalents of acid to bring the pH down to ~7. This is in line with the same acid consumption found for silica-free tricalcium aluminate hexahydrate, $Ca_3Al_2(OH)_{12}$ (TCA) [3], and can be attributed to the strong proton binding of both OH^- and SiO_4^{4-} ions. Furthermore, the presence of silica prevents KAT to transform to Friedel's salt, $Ca_2[Al(OH)_6]_2Cl_2\cdot 4H_2O$, a layered double hydroxide, as opposed to TCA.

In summary, silica content does not alter the acid consumption KAT but gives rise to a neutralization mechanism fundamentally different from that of TCA.

Keywords: katoite, tricalcium aluminate, bauxite residue, neutralization, Friedel's salt

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Natural Emulsifier-Based Nanoemulsions for Co-Encapsulation of β-Carotene and (−)-α-Bisabolol: Toward Stable Lipid-Based Drug Delivery Systems

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The design of lipid-based drug delivery systems (LBDDS) increasingly integrates co-encapsulation of poorly water-soluble bioactives with natural emulsifiers to enhance both physicochemical stability and functional performance. Building on our prior study [1], which reported successful co-encapsulation of β-carotene and (−)-α-bisabolol using soy lecithin and sodium caseinate, the present work extends the investigation by evaluating the influence of extraction purity, emulsifier ratios, and antioxidant synergy mechanisms in O/W nanoemulsions. We introduce a refined formulation design using varying lecithin:caseinate ratios and antioxidant assays under oxidative stress conditions, alongside extended shelf-life stability monitoring under light and temperature fluctuations. Dynamic light scattering and zeta potential analysis reveal optimal interfacial arrangement at a 2:1 lecithin-to-caseinate ratio, yielding droplet sizes below 150 nm and ζ-potentials around -45 mV. Antioxidant assays (DPPH, ABTS, FRAP) highlight a significant synergistic enhancement compared to single-bioactive systems (IC_{50} reduced by 35%), attributed to co-localization within the dispersed phase. This study provides new insights into the role of emulsifier composition in modulating interfacial architecture and enhancing functional properties, reinforcing the potential of clean-label nanoemulsions for nutraceutical and functional food applications.

Key words: Interfacial stability, Emulsifiers, Nanoemulsion, Lipid-based drug delivery.

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Nanocellulose: The Material of the Future for Biological Applications, and Specific Sensors.

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This oral presentation aims to demonstrate the feasibility of converting microcrystalline cellulose (MCC) into nanocellulose (NC), as well as the preparation of 2,3-dialdehyde nanocellulose (DANC). The latter is subsequently modified via a Schiff base reaction, leading to various imine-functionalized derivatives. The resulting fluorescent materials are characterized using a range of analytical techniques, including Fourier-transform infrared spectroscopy (FT-IR), scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy (SEM-EDX), X-ray diffraction (XRD), and photoluminescence spectroscopy, among others.

Subsequently, their fluorescent properties, as well as their magnetic behavior after incorporation of magnetite nanoparticles ($Fe3O4$, NPs), are investigated. The highly sensitive fluorescent probes obtained are capable of selectively detecting heavy metals in aqueous media, as monitored by photoluminescence spectroscopy.

Two potential application pathways are considered:

1. The use of one of the developed materials for the selective detection of Fe (III) in seawater.
2. The employment of a blue, fluorescent sensor for the specific detection of Fe (II) and Fe (III), as well as for the identification of hemoglobin and methemoglobin through the detection of Fe (II) and Fe (III) metal cations present in these biostructures, via a fluorescence quenching mechanism in a biological matrix such as human serum.

This presentation highlights the conversion of microcrystalline cellulose into dialdehyde nanocellulose functionalized via Schiff bases, yielding fluorescent materials. Upon incorporation of magnetite nanoparticles, their optical and magnetic properties are examined for selective heavy metal detection. Two applications are explored: Fe(III) detection in seawater and hemoglobin identification using a fluorescent probe in biological media

Key words: Functionalized nanocellulose, Fluorescent probe, Heavy metal detection, Schiff base reaction

Investigation of adsorption isotherms of Paprika oleoresin dye on TiO_2 mesoporous for dye sensitized solar cells using statistical physics modeling

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In this paper, three adsorption isotherms of Paprika oleoresin dye (*Capsicum annuum L*) on TiO_2 mesoporous, at three different temperatures, were fitted by models established through statistical physics treatment. A monolayer model with four energies is able to give good fitting of these experimental data. This model contained theoretical parameters that can be utilized to understand the dye adsorption mechanism. Steric and energetic parameters are involved in the fitting of the experimental adsorption isotherms such as the number of adsorbed dye molecules per site ni, the densities of receptor sites Nmi and the four energetic parameters C_1, C_2, C_3, and C_4. The steric investigation shows that the dye molecules can be anchored on the TiO_2 mesoporous with the two parallel and nonparallel configurations. From the energetic viewpoint, the calculated adsorption energies values revealed that the dye is adsorbed physically and chemically on the TiO_2 surface.

Key words: Paprika Oleoresin dye, statistical physics, adsorption isotherms, modeling, dye sensitized solar cells

Sustainable Innovations in Hazardous Dye Degradation with Ternary Metal Oxides

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The study focused on synthesizing and applying an economical photocatalyst utilizing a blend of ternary metal oxides, including barium oxide, zinc oxide, and ceric oxide, to degrade the hazardous malachite green (MG) dye. While malachite green is extensively used and inexpensive across various industries, it carries significant dangers due to its high toxicity, potential carcinogenic properties, and durability in aquatic ecosystems. A range of advanced techniques, such as Fourier transform infrared (FTIR) spectroscopy, X-ray diffraction (XRD) analysis, scanning electron microscopy (SEM), energy dispersive X-ray (EDX) analysis, diffuse reflectance spectroscopy (DRS) and ultraviolet-visible (UV-visible) spectrophotometry, were used to examine and characterize the composite material. The resulting composite displayed porous and semi-crystalline structure, along with a decreased optical band gap that enhanced its conductivity. The degradation products of the MG dye were analyzed using gas chromatography-mass spectrometry (GC-MS). The research evaluated the impact of several factors, including the presence of oxidant, pH levels, initial dye concentration, amount of catalyst, temperature, and interfering ions, on the degradation reaction of MG. The composite demonstrated remarkable photocatalytic performance under natural sunlight, accomplishing nearly complete degradation of MG within 11, 20, and 23 minutes using a catalyst dosage of 0.5 mg at pH levels of 1, 10, and neutral (7) respectively, along with a synergistic contribution from 10.8 mg of potassium peroxodisulfate (oxidant). The photocatalyst retained its efficiency over five successive cycles for the MG dye. Tests on the photocatalytic degradation of a textile wastewater sample showed remarkable outcomes under optimized conditions, highlighting the practical applications of the composite.

Key words: ternary composite, malachite green, photocatalysis, degradation

Program of
Wednesday 17
September 2025

Impact of Cosolvent on Co^{2+} Ion Speciation in 'Reline' Deep Eutectic Solvent

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A key feature of deep eutectic solvents (DESs) is their ability to solubilize metal salts and oxides, making them attractive for metal leaching from both primary and secondary resources as a greener alternative to conventional acid-based methods. However, their high viscosity can limit their use in separation processes. The addition of cosolvents like water or alcohols is a promising strategy to mitigate this issue, yet it can significantly alter metal speciation in solution, depending on the cosolvent's binding affinity and concentration.[1,2] Understanding metal speciation in DESs is thus critical for optimizing metal extraction and recovery mechanisms.

In this study, we investigate the coordination environment of the Co^{2+} ion in the archetypal DES "reline" (choline chloride:urea 1:2) upon the addition of water, methanol, and ethanol at varying concentrations. Cobalt is a critical component in the cathodes of lithium-ion batteries (LIBs), including the widely used NMC (Nickel Manganese Cobalt Oxide) and NCA (Nickel Cobalt Aluminum Oxide). Given its limited availability, high cost, and environmental concerns, efficient cobalt recovery from spent LIBs is of paramount importance. To unravel the structural effects of cosolvent addition, we employ a multi-technique approach combining UV-Vis absorption, X-ray absorption spectroscopy (XAS), and advanced data analysis methods, including EXAFS and XANES analysis, as well as a chemometric strategy based on multivariate curve resolution–principal component analysis (MCR-PCA). Our findings provide a detailed structural picture of the Co^{2+} ion coordination environment in different DES-cosolvent mixtures, revealing how speciation evolves with cosolvent type and concentration.

These insights pave the way for a more rational design of DESs as advanced receiving phases for metal ion recovery, with promising implications for sustainable cobalt recycling from spent LIBs.

Key words: deep eutectic solvents, cobalt, coordination, EXAFS, XANES, UV-Vis

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Speciation and Dielectric Relaxation Study of Glass-forming Liquid Electrolyte Consisting of $Li[N(SO_2CF_3)_2]$ and 1,3-propanesultone

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As a polysulfides insoluble electrolyte for Lithium-sulfur (Li-S) batteries, Watanabe *et al.*, proposed a solvated ionic liquid (SIL) composed of an equimolar mixture of LiTFSA (TFSA: $(CF_3SO_2)_2N^-$) and glyme, tough the Li ion transference number of glyme-based SILs remained relatively low. Dokko et al. reported a superconcentrated electrolyte solution (SCES) consisting of LiTFSA and sulfolane (SL: tetrahydrothiophene-1,1-dioxide), which showed Li ion transference number higher than 0.5 [2]. This high Li ion transference number was attributed to the formation of aggregates, where Li ions were bridged by both solvent molecules and anions. To further promote aggregate formation for enhanced Li ion conduction, we investigated mixtures of LiTFSA and 1,3-propanesultone (PS), a solvent with weaker solvation ability, and found that the Li ion transference number was comparable to that of SL-based systems. In addition, the LiTFSA-PS mixtures exhibited a glass transition over a broad range of compositions and temperatures, without any signs of melting or crystallization. Thus, we believe that these mixtures represent a new of liquids, termed glass-forming liquid electrolytes. In this study, we investigated the speciation and dipole reorientation dynamics using Raman and dielectric relaxation spectroscopy to elucidate the distinctive Li^+ conduction mechanism in the PS system, in comparison with the SL system. Two-dimensional correlation analysis of Raman and dielectric relaxation spectra attributed the observed relaxation below 0.1 GHz to aggregates. These results suggest that large-scale aggregates formed at high lithium salt concentrations play a crucial role in enhancing specific lithium-ion conduction.

Key words: Glass-forming liquid electrolyte, Speciation, Reorientation dynamics

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Ion solvation under gigapascal pressure

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Ion solvation in a gigapascal (GPa) pressure range is of great significance for high-pressure chemical synthesis and the circulation of matter within the Earth's interior[1]. We adopted neutron scattering (NS) and molecular dynamics (MD) simulations of a series of alkali metal chloride aqueous solutions to reveal the changes of ion solvation structure and dynamics induced by compression. Upon compression to 0.7 GPa, the outer water molecules enter the nearest neighbor of ions, and the solvated ion clusters become denser, which reflects the peak and minimum positions of $M^+\cdots Ow$ and $M^+\cdots Dw$ pair distribution functions (pdfs), and the ion-water dipole orientation. When considering the orientation distribution of the water dipole in the first solvation shell, both the hydration factor (f_h) and hydration number (n_{hyd}) indicate from a microscopic perspective that the compression weakens the hydration ability of the ions. Moreover, compression hinders the diffusion of ions, which is closely related to the changes in ion solvation structure. The compression effect is more significant for the structure-breaking ions, Rb^+ and Cs^+.

Key words: Structure and dynamics, Ion solvation, Pressure effect, Structure-making and structure-breaking

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Ion transport properties and Raman spectroscopic analysis of the speciation of Li[N(FSO$_2$)$_2$]-fluoroethylene carbonate

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Lithium-sulfur (Li-S) batteries are expected to have five to six times the energy density of current lithium-ion batteries. However, polysulfide (PS) leaching and dendrite formation in the lithium anode remain significant problems. Recently, Ishikawa et al. demonstrated that Li[N(CF$_3$SO$_2$)$_2$] (LiTFSA), when dissolved in a mixture of fluoroethylene carbonate (FEC) and 1,1,2,2-tetrafluoroethyl-2,2,3,3-tetrafluoropropyl ether (HFE), forms a stable solid electrolyte interphase (SEI) at the cathode. Li[N(FSO$_2$)$_2$] (LiFSA), an analog of LiTFSA, is known for its low viscosity, high ionic conductivity, and fast electrode response.

In this study, the ion transport properties of LiFSA-FEC solutions were investigated and the speciation of lithium ions was analyzed by Raman spectroscopy. When the lithium salt mole fraction (xLi) of the LiFSA-FEC solutions was $0.1 < xLi < 0.3$, no melting or freezing point peaks were observed; instead, only a glass transition point was detected, indicating that the LiFSA-FEC solution behaves as a glass-forming liquid electrolyte [4]. Raman spectroscopy revealed the average stoichiometric ratios of the dissolved species, indicating less contact ion pairing and aggregation in the FSA system than in the TFSA system. Although the Li$^+$ transport rate was lower in the FSA system, the ionic conductivity resulting from solvated lithium ions was higher. These results suggest that contact ion pairing and aggregation contribute to higher Li$^+$ transport rates and that the static heterogeneous structure of these species leads to dynamic heterogeneity and glass formation.

Key words: Lithium sulfur battery, Raman spectroscopy, Dynamic heterogeneity

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Synthesis and characterization of modified polymer inclusion membranes for water purification

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Water pollution, which affects rivers, seas, groundwater and lakes, is the result of the discharge of wastewater without treatment or at an insufficient level of treatment, which causes degradation of the ecosystem. In this work, we have developed a novel class of ions exchange membranes for heavy metals elimination. All synthesized polymeric inclusion membranes (PIMs) are made up of nontoxic polymers like cellulose triacetate (CTA) or polycaprolactone (PCL) modified by polyelectrolytes (polyvinyl alcohol) or polyanetholsulfonic acid sodium salt to improve the interfacial charges (SO_3^- or COO^-) and trioctyle phosphine oxide (TOPO) incorporated into the polymer as a selective carrier. The elaborated membranes were plasticized by dioctyle phtalate (DOP) to ameliorate their elasticity, hydrophobicity and fooling resistance. The synthesized PIMs were characterized using Fourier transform infrared (FTIR), X-ray diffraction (XRD), thermogravimetric analysis (TGA) and scanning electron microscopy (SEM). The influence of the membrane nature is studied using supports with different physical characteristics (porosity, thickness, hydrophobia) **[1, 2]**. As application, a study of heavy metals retention using the synthesized membranes was realized. Dialysis experiments of Pb^{2+} and Cd^{2+} transfer across the synthesized polymer inclusion membranes have proved their good performance. FTIR spectroscopy confirmed the coexistence of all the compounds used for the development of the membranes. The obtained TGA results showed that all the elaborated membranes have good thermal stability and resist up to a temperature of 160°C. As application, quality parameters including turbidity, total dissolved solutes (TDS), electric conductivity (EC), nitrates, chlorides, sodium, carbonates, bicarbonates, heavy metals (Cd, Pb) and other trace elements, were determined before and after treatment of real wastewater.

The results obtained clearly showed that the water treatment by the developed polymeric membranes is very satisfactory, with an elimination of 39.09% of carbonates, a strong reduction in hardness (39.32%), an appreciable reduction in chloride ions (20%) and a very good elimination of bicarbonate ions (75%). We found also significant reductions in turbidity (96.89%), nitrates (68.57%), lead (52.17%), cadmium (39.64%), total dissolved solutes (TDS) (37.83%),

The synthesized membranes demonstrated significant potential for heavy metal removal, offering a sustainable approach to wastewater treatment. Overall, this research emphasizes the value of natural materials in developing efficient filtration technologies.

Key words: Biopolymers, Membranes, Water purification, Heavy metals elimination.

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The use of natural deep eutectic solvents for the production of biomolecular components from fish raw materials

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Natural deep eutectic solvents (NADES) are a novel type of solvents with unique properties, which make them promising for a wide range of applications. In particular, it is assumed that NADES based on sugars and organic acids can increase the efficiency of the extraction of functional biological polymers from organic raw materials keeping the manufacturing process green and sustainable. In the present work, we explored the processing of the dermal integuments of scaleless fish to extract native collagen using NADES based on fructose–citric acid mixtures with a small amount of water added. This approach is considered an alternative to the conventional method involving weak solutions of organic acids. The results indicate not only an acceleration of the chemical treatment of raw materials but also an effective separation of lipid and protein components and preventing, simultaneously, unwanted hydrolysis of collagen. These features were confirmed by the comparative analysis of samples treated by both methods using colour optical microscopy (by staining with a fat-soluble dye Sudan III, which demonstrated colourless areas of the protein part with a few easily separable coagulated lipid droplets) and electron scanning microscopy (for the analysis of fibrillary structures). A discussion of the specificity of intermolecular interactions in the investigated NADES/protein/lipid system leading to the revealed features will be provided.

Key words: NADES, green biotechnology, extracting of collagen, green chemistry.

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Postnikov E.B., Vanina A.S., Wasiak M. Sychev A.V., Chorążewski M. Thermodynamic properties of natural deep eutectic solvents and their aqueous solutions exemplified by fructose-citric acid-water mixtures. In: *Molecular thermodynamics of aqueous systems: Binary and ternary solutions/mixtures* (submitted).

Development of Pickering Emulsions of Lentisk Essential Oil Stabilized by β-Cyclodextrin-Modified Silica Nanoparticles

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Emulsions are fundamental in the cosmetics industry, where they enable the formulation of stable mixtures of immiscible liquids while enhancing sensory appeal. Their composition is carefully optimized, as each component influences the final product's quality. Among emerging stabilizers, β-cyclodextrin-modified silica nanoparticles have attracted significant attention due to their unique properties. β-Cyclodextrins, with their truncated cone-shaped structure, possess a highly hydrophilic exterior, making them effective in stabilizing emulsions (Figure 1). Pickering emulsions, stabilized by solid particles rather than surfactants, offer enhanced stability and environmentally friendly formulations, making them particularly promising for pharmaceutical and cosmetic applications.

This study investigates the stabilization of Pickering emulsions using β-cyclodextrin-modified silica nanoparticles, with lentisk essential oil as the dispersed phase. Key emulsification parameters were analyzed, followed by the evaluation of different oil compositions to determine optimal silica, water, and oil ratios for long-term stability. The emulsions were characterized through stability assessments, particle size distribution analysis, and rheological measurements. Droplet size analysis and zeta potential measurements confirmed the effective stabilization provided by β-CD-modified silica. These findings highlight the potential of combining lentisk essential oil with β-CD-modified silica nanoparticles to develop stable and sustainable Pickering emulsions for cosmetic and pharmaceutical applications.

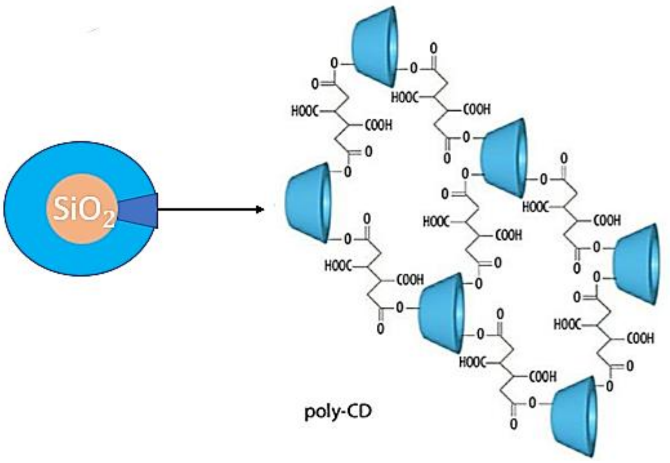

Figure 1: Schematic representation of poly (β-cyclodextrin) grafted onto a silica particle.

Keyswords: Cosmetics industry, Immiscible liquids, β-Cyclodextrin-modified silica nanoparticles, Pickering emulsions, environmentally friendly formulations, pharmaceutical applications, Cosmetic applications, Lentisk essential oil.

Topic: This study focuses on the use of β-cyclodextrin-modified silica nanoparticles to stabilize Pickering emulsions containing lentisk essential oil, highlighting their potential applications in cosmetic and pharmaceutical formulations.

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NMR study of hydroxypropyl-cyclodextrin inclusion complexes with active molecules of plant mother tinctures

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This study explores the formation of inclusion complexes between hydroxypropylated cyclodextrins (HP-β-CD and HP-γ-CD) and selected bioactive molecules (BAMs) known for their potential to mask the unpleasant taste of herbal extracts, such as horehound, eucalyptus, plantain, and thyme. The BAMs studied : thymol, carvacrol, and eucalyptol were complexed with HP-cyclodextrins and analyzed using ^{1}H NMR spectroscopy. The complexes exhibited a 1:1 stoichiometry (BAM:HP-CD). Changes in the ^{1}H NMR chemical shifts of the guest molecules enabled the calculation of binding constants, revealing stronger and more stable inclusion with HP-γ-CD, likely due to its larger cavity and greater conformational flexibility. Two-dimensional ROESY and NOESY experiments provided further insight into the spatial orientation of the host–guest interactions. A simplified thermodynamic model underscored the role of hydrogen bonding in stabilizing the complexes. Additionally, when carvacrol and eucalyptol were mixed, carvacrol consistently formed the most stable complex with HP-CD, even in combination.

Keywords: HP-cyclodextrin, bioactive molecules, inclusion complex, taste masking,
^{1}H NMR spectroscopy

List of Poster Communications

Communicatings' Names	**Ref**
H. Abid, A. Mechria *FSG - Gabès* Synthesis and crystal structure of a novel Schiff base ligand with potential for transition metal coordination	**PC 1**
A. Ayad, J. Kilele, A. Negadi, L. Negadi *University of Tlemcen, Algeria* Thermodynamic Properties of N, N-dimethylacetamide with 1-butanol, 1-pentanol, furfural or furfuryl alcohol at temperatures from (293.15 to 323.15) K	**PC 2**
A. Ayad, M. Ebrahiminejadhasanabadi, W.M. Nelson, L. Negadi, P. Naidoo *University of Tlemcen, Algeria* Experimental determination and modelling of high-pressure phase equilibrium for carbon dioxide solubility with biofuels	**PC 3**
A. Belabbaci, K.N. Abdellaoui, A. Ayad, A. Negadi, L. Negadi *University of Tlemcen, Algeria* Thermodynamic, ultrasonic, and transport study of binary mixtures containing 1-hexene and alcohols at (293.15 - 303.15) K	**PC 4**
A. Belabbaci, Z. Boudellal, A. Ayad, L. Negadi, A. Negadi *University of Tlemcen, Algeria* Physicochemical properties of binary mixtures of furfural or furfuryl alcohol with 1-propanol or 2-propanol at temperatures from (293.15 to 323.15) K	**PC 5**
S. Bergaoui, C. Macherki *FSM - Monastir* Click reaction modification of a new anodic-synthesized oligophenylene material	**PC 6**
S. Boughammoura, A. Belaid, J. Mhalla *FSM - Monastir* Potentiometric and conductometric study of the speciation of zirconocene dichloride Cp_2ZrCl_2 in aqueous solution.	**PC 7**
M. Chehaibi, I. Kamoun, M. Oudni-M'rad, S. M'rad, F. Ayari *FSM - Monastir* Activity of terpenes-doped oxides against Echinococcus granulosus protoscoleces	**PC 8**
I. Dammak, S. Cherif, A. Aloulou *ENIS - Sfax* Natural extracts from Acacia tortilis subsp. raddiana as bio-based emulsifiers: Influence of solvent extraction on antioxidant and interfacial properties in colloidal systems	**PC 9**
M. Dendeni, M. Ferhi *Centre de Biotechnologie - Borj Cédria* Eco-Friendly and cost-effective bioadsorbent for efficient dye removal: Structural characterization and kinetic modeling	**PC 10**
M. Djama, Y. Larbah, B. Idir, B. Rahal, H. Mezazigh, L. Benhaddad *CRTI - Echahid Mohamed Abbassi, Algiers, Algeria* Structural and morphological characterization of Sol-Gel derived ZnO thin films on Fe-10Cr alloy	**PC 11**
I. Essid, H. Abdelkafi, M. Jeanty *Novalix - Sidi Thabet* Selective $C(sp^3)$–$C(sp^2)$ bond formation via homogeneous electrochemical cross-coupling in solution	**PC 12**
M-A. Esteso, M. Maldonado, D.M. Galindres-Jimenez, A. Crespo, E. Sanabria, C. Maria Romero *Universidad Católica de Ávila, España* The use of cyclodextrins for the complexation of hydrocortisone	**PC 13**
M-A. Esteso, A. Crespo, D.M. Galindres-Jiménez, A.C.F. Ribeiro *Universidad Católica de Ávila, España* The use of cyclodextrins for the removal of sodium sulfadiazine from hospital wastewater	**PC 14**
D.M. Galindres Jiménez, N.S. Bernal, A.T. Castillo, N. Espitia-Galindo, E.F. Vargas, Miguel A. Esteso *Universidad Católica de Ávila, España* Supramolecular interactions of an anionic resorcinarene with transition metal ions: Combined experimental and theoretical study	**PC 15**

Communicatings' Names	Ref
I. Gotlib, A. Koneva, P. Korchak, E. Safonova, A. Victorov *Saint Petersburg State University, Russia* Glycine and sodium glycinate in water: Molecular dynamics simulations and experiment	**PC 16**
Z. Graba, Y. Tiliouine *FSE, A. MIRA University of Béjaia, Algeria* Removal of a dye, Bezacryl Yellow (BY), by crushed cardoon leaves	**PC 17**
J. Han, S. Nagamine, R. Kanzaki, H. Maki, A. Kita, K. Murase, Y. Umebayashi *Niigata University, Japan* Thermal properties of AlCl3 mixtures with amides and carbamides	**PC 18**
L. Hedhili, N. Bouharb, S. Agren, A. Mehri, M.H. Bouab, E. Ben Salem *IPEIM - Monastir* Sustainable purification and deoxygenation of olive pomace oil using low-cost catalytic solutions for biofuel applications	**PC 19**
N. Hosni, W. Selmi, H. Maghraoui-Meherzi *FST - Tunis* Enhanced electrocatalytic performance of $NiFe_2O_4$-graphene oxide composites: Role of interfacial charge transfer	**PC 20**
B. Idir, M. Djama, D. Addadj, L. Benhaddad, A. Kouache *CRTI - Cheraga, Algiers, Algeria* Eco-friendly corrosion inhibitor system based on expired pharmaceuticals and iodide ions for aluminum alloys	**PC 21**
D. Ingrachen, S. Azoug *Abderrahmane Mira University, Bejaia, Algeria* Adsorption of methylene blue and the regeneration of MCM-41 mesoporous silica	**PC 22**
Y. Ito, Y. Yasuda, Y. Konishi, K. Dokko, K. Fujimoto *Kansai University, Japan* Insights into the structure and dynamics of a lithium sulfur battery electrolyte using molecular dynamics simulations	**PC 23**
N. Janković, A. Rilak Simović, E. Milović, L. Milović *Institute for Information Technologies Kragujevac* Synthesis and antioxidative activity of self-assembled tetrahydropyrimidines-based organogels	**PC 24**
N. Jaouadi, N.E.H. Ben Fatma, N. Jegham, S. Mahfoudhi, R. Kechaou, M. Laribi *Toxicology Lab, Fattouma Bourguiba Hospital, Monastir* In silico evaluation of the affinity of quinoline derivatives for the AChE receptor through molecular docking	**PC 25**
N. Jaouadi, N. Jegham, N.E.H. Ben Fatma, S. Mahfoudhi, R. Kechaou, M. Laribi *Toxicology Lab, Fattouma Bourguiba Hospital, Monastir* In silico evaluation of the affinity of quinoline derivatives for the NMDA receptor through molecular docking	**PC 26**
S. Jebri, W. Mabrouk, H. Elfil, M. Hichri *CERTE - Borj Cédria* Calcium phosphate–supported nanocomposites for enhanced visible-light photodegradation of methylene blue	**PC 27**
N. Jegham, S. Mahfoudhi, R. Rassas, A. Trabelsi, N. Kalboussi, B. Kacem *Faculty of Pharmacy and Sahloul Hospital* Study of the physicochemical and microbiological stability of dexamethasone-based mouthwashes	**PC 28**
N. Jegham, S. Gabsi, N.E.H. Ben Fatma, F. Hfaeidh, S. Mahfoudhi, M.A. El Kaibi, M. Laribi *Faculty of Pharmacy and Sahloul Hospital* Castor oil and laxative activity: Virtual screening of ricinoleic acid analogues	**PC 29**
J. Kallel, C. Bordes, Y. Chevalier, N. Jaffrezic-Renault, S. Hbaieb *FST - Tunis* Taste-masking of caffeic acid via inclusion complexation with hydroxypropyl-β-cyclodextrin: Evidence from NMR and conductometric sensing	**PC 30**
T. Kamiyama, A. Aoki *Kindai University, Japan* Thermodynamic study of inclusion of ionic liquid by cyclodextrin in water	**PC 31**

Communicatings' Names	Ref
H. Khireddine, D. Sidane *University of Bejaia, Algeria* Effect of TiO_2 on the adhesion and bioactivity of a sol-gel-derived hydroxyapatite coating on 316L stainless steel surface: Biomedical application	**PC 32**
K. Kikuchi, K. Fujimoto, A. Shimizu, K. Kaneko, T. Matsuyama, J. Ida *GSSE - Soka University, Japan* All-atom molecular dynamics study on cellulose dissolution in ionic liquids under high pressure: Prediction and mechanistic insights	**PC 33**
E. Kirilova, A. Maleckis, M. Kirjusina, R. Fridmans, E. Romanovska-Dzalbe, T. Grigorjeva, I. Mihailova *Daugavpils University, Latvia* Spectroscopic study of the coordination of metal ions with anthrone derivatives	**PC 34**
M. Kirjusina, E. Romanovska-Dzalbe, A. Maleckis, L. Mezaraupe, I. Rubenina, S. Kecko, M. Savicka, J. Kirilova *Daugavpils University, Latvia* Photophysical properties and potential application of substituted benzanthrones	**PC 35**
T. Kitagawa, Y. Yasuda, T. Nagai, K. Fujimoto *Kansai University, Japan* Molecular dynamics investigation of hydronium ion transport mechanisms in Nafion® membranes	**PC 36**
R. Lafi, W. Mabrouk, D. Ghorbel, N. Saidi *CERTE - Borj Cédria* Adsorption of Rhodamine B onto few layer graphene: Experiments, statistical physics and artificial neural network modeling	**PC 37**
B.W. Lee, B. Kwang-Hyun *Korea Maritime & Ocean University, Busan, Korea* Influence of inorganic and organic additives on the properties of sodium silicate solutions	**PC 38**
T. Lee, B. Woo Lee *Keoyang Linkers, Seoul, Korea* Manufacturing of hydrogel composition for extinguishing metal fires in electric vehicles	**PC 39**
J. Ma, Z. Yu *Tsinghua University, China* Sodium ion electrolyte solution structures by excess spectroscopy	**PC 40**
S. Mahfoudhi, N. Zitouni, F. Ouaer, Y. Mokni, K. Zribi *Faculty of Pharmacy - Monastir* Quality control of vitamin C in dietary supplements using HPLC-UV analysis	**PC 41**
S. Mahfoudhi, N. Zitouni, Y. Mokni, K. Zribi, F. Safta *Faculty of Pharmacy - Monastir* Development and validation of two methods for the determination of magnesium and calcium ions by UV-visible spectrophotometry in dietary supplements	**PC 42**
N. Makhlouf, A. Hajjem, F. Zouari, M. Ziadi, K. Mnekbi, M.R. Louhaichi *Faculty of Pharmacy - Monastir* Development and validation of a glassware cleaning protocol in a pharmaceutical quality control laboratory	**PC 43**
A. Mars, A. Mejri, A. Midouni, A.H. Hamzaoui *CERTE - Borj Cédria* Efficient green hydrogen generation via catalytic hydrazine-assisted water splitting using PEDOT:PSS-stabilized lithium ferrite porous nanostructures decorated with MoS_2 quantum dots	**PC 44**
A. Mejri, A. Midouni, A.H. Hamzaoui, A. Mars *INSAT - Tunis / CERTE* CeO_2 quantum dot-decorated PEDOT:PSS-lithium ferrite porous nanostructures for high-sensitivity electrocatalytic detection of pesticides	**PC 45**
I. Mihailova, V. Gerbreders, M. Krasovska, E. Sledevskis, V. Mizers, J. Keviss, J. Kirilova *Daugavpils University, Daugavpils, Latvia* Electrochemical CuO sensor for H_2O_2 detection and MgO nanoparticle remediation in drought-stressed oat	**PC 46**
T. Miyamoto, S. Waida, T. Kamiyama *FSE - Kindai University, Japan* Effect of cyclodextrin on acidic and thermal denaturation of Cytochrome c	**PC 47**

Communicatings' Names	**Ref**
Y. Okazaki , T. Kamiyama *FSE - Kindai University, Japan* Preferential solvation of lysozyme in aqueous DES solutions	**PC 48**
M. Saidani, A. Fkiri, A. Mezni *FSB - Bizerte* Synthesis of multifunctional ternary $Au@ZnO/\alpha\text{-}Fe_2O_3$ nanocomposite for organic pollutant removal	**PC 49**
C. Saoudi, S. Jebri, H. Elfil, M. Hichri *CERTE - Borj Cédria* Magnetic ferrite nanoparticles for the removal of textile dyes	**PC 50**
Á. Serfőző, P. Sipos, M. Szabados *University of Szeged, Hungary* Stabilization study of sodium metamizole in aqueous medium by intercalation into layered double hydroxides	**PC 51**
Y. Shimono, T. Kamiyama *Kindai University, Japan* Thermodynamic investigation of the interaction between lipid bilayers and βLG using ITC	**PC 52**
T. Sun, Z. Yu *Tsinghua University, China* Identifying species in imidazolium chloride-based ionic liquid with ε-caprolactone via excess infrared spectroscopy	**PC 53**
L. Taouri, M. Bourouina, S. Bourouina, D. Hauchard *University of Bejaia, Algeria* An innovative nanoparticle modified carbon paste micro-sensor for ultrasensitive and selective detection of ciprofloxacin in environmental	**PC 54**
S. Waida, M. Noma,T. Kamiyama *Kindai University, Japan* Dependence of alkyl chain length of ionic liquids on the thermal stability of cytochrome c	**PC 55**
F. Wang, P. Lin, X. Zhuang *Nanjing Normal University, China* Effects of ionic liquid types on the structure and thermal properties of different silk fibroin	**PC 56**
S. Xu, Z. Yu *Tsinghua University, China* A hybrid computational framework for excess infrared spectral decomposition in tert-butanol-carbon tetrachloride solutions	**PC 57**
C. Yoshida, T. Kamiyama *FSE - Kindai University, Japan* Thermodynamic study of cyclodextrin-protein interaction by titration calorimetry	**PC 58**
N. Zitouni, Y. Mokni, S. Mahfoudhi, K. Zribi *Faculty of Pharmacy - Monastir* Control of iron-based dietary supplements using flame atomic absorption spectrophotometry	**PC 59**
N. Zitouni, Y. Mokni, S. Mahfoudhi, K. Zribi *Faculty of Pharmacy - Monastir* Control of zinc-based dietary supplements using flame atomic absorption spectrophotometry (FAAS)	**PC 60**
S. Zrafi, M.A. Lassoued, F. Ayari *FSM - Monastir* Efficient Beer-Lamber law for analyzing hybrid materials in sunscreen creams	**PC 61**

Abstracts of Poster Communications

Synthesis and Crystal Structure of a Novel Schiff Base Ligand with Potential for Transition Metal Coordination

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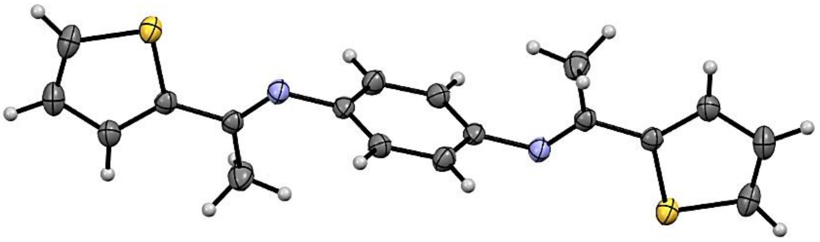
A new Schiff base ligand was synthesized via the condensation of 2-acetylthiophene with p-phenylenediamine in methanol under reflux conditions. The structure and purity of the ligand were confirmed using infrared (IR) spectroscopy, proton and carbon nuclear magnetic resonance (^{1}H and ^{13}C NMR), ultraviolet-visible (UV-Vis) spectroscopy, and mass spectrometry (MS). Single-crystal X-ray diffraction (SCXRD) analysis unambiguously established the molecular structure, confirming the formation of the expected diimine moiety and revealing a well-defined geometry. This new ligand exhibits promising coordination sites, making it a suitable candidate for future complexation with transition metals, particularly palladium (II) and nickel (II), for potential applications in catalysis and materials science.



Key words: Spectroscopic characterization; NMR; UV-Vis; Mass spectrometry;
X-ray crystallography; Molecular structure.

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Thermodynamic Properties of N, N-dimethylacetamide with 1-butanol, 1-pentanol, furfural or furfuryl alcohol at temperatures from (293.15 to 323.15) K

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N,N-Dimethylacetamide (DMA) is frequently utilized in many industrial processes due to its special characteristics, which include a high boiling point, strong thermal stability, low toxicity, and its miscibility in the majority of organic solvents. Understanding thermophysical properties is essential in the chemical industry for optimizing processes such as mass transfer, heat transfer, chemical separations, and fluid flow [1].

In this work, density, speed of sound and refractive index of four binary mixtures containing N,N-Dimethylacetamide with 1-butanol, 1-pentanol, furfural or furfuryl alcohol were measured over the entire composition range and at temperature from T= 293.15 K to 323.15 K. From the experimental results, excess molar volume, isentropic compressibility, excess isentropic compressibility and excess refractive index properties were calculated [2]. The excess properties were successfully fitted to the Redlich-Kister polynomial equation. The obtained results were discussed in terms of the nature of intermolecular interactions. Perturbed chain statistical associating fluid theory equation of state (PC-SAFT EoS) [3] was used for modeling the density of the pure fluids and binary mixtures.

Key words: density, speed of sound, refractive index, excess properties, equation of state.

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Experimental determination and modelling of high-pressure phase equilibrium for carbon dioxide solubility with biofuels

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The phase behavior of carbon dioxide-containing systems is crucial for the development of supercritical solvent applications and procedures for reducing carbon emissions [1]. Biomass resources are getting more attention for their potential as fuels or as raw materials for chemical products.

In this work, the solubility of carbon dioxide in two solvents, 2,5-dimethylfuran and methyl levulinate, were measured using both the isothermal synthetic technique and the variable volume synthetic method. Experimental vapor–liquid equilibrium data were obtained for the binary systems at different temperatures (283.15, 303.15 and 323.15) K and high pressure up to 9.1 MPa. The study examines how CO_2 interacts with either 2,5-dimethylfuran, a furan compound, or methyl levulinate, an ester. The experimental data were modeled using the Peng-Robinson Equation of State with the Wong-Sandler mixing rule [3,4] Positive deviations from ideality were observed in both systems.

Key words: density, speed of sound, refractive index, excess properties, equation of state.

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Thermodynamic, Ultrasonic, and Transport Study of Binary Mixtures Containing 1-hexene and Alcohols at (293.15 - 303.15) K

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Alcohol fuels can be an alternative source of environmentally friendly fuels to reduce exhaust emissions by using renewable energy in different countries of the world, they can be employed as oxygenated fuel additives with fossil fuels for diesel engines [1]. Furthermore hydrocarbons/alcohols mixtures constitute crucial products in the industry and remarkable systems from the thermodynamic point of view. Within this framework, light alcohols are frequently used as blending agent in the formulation new gasoline, taking into account environmental constraints, to both partly replace for hydrocarbon car fuels and augment their octane number while enhancing vehicle emissions [2]. Thermodynamic and transport properties of binary mixtures containing Hydrocarbons and alcohols are essential in the fundamental understanding, for various engineering and industrial applications. In this work, densities, speeds of sound and refractive indices of binary mixtures1-hexene with methanol, 1-propanol or 1-pentanol were measured in the temperature range from (293.15 to 303.15)K over the whole composition range and atmospheric pressure [3]. From this data, excess molar volumes,V_m^E, deviation in speed of sound,Δu and deviation in refractive indices, Δn_D, for all studied mixtures were calculated and correlated as function of temperature using Redlich-Kister polynomial equation. The density of binary mixtures of 1-hexene with alcohols was predicted using the Perturbed Chain Statistical Associating Fluid Theory (PC-SAFT) equation of state. Schaaff's Collision Factor Theory (SCFT) and Nomoto's Relation (NR) were also applied to model the experimental speed of sound data for these mixtures. The density of the binary mixtures has been correctly modeled with PC-SAFT. On the other hand, the 4 mixing rules used in the refractive index computation showed good quantitative agreement with the experimental data, and both SCFT and NR showed low deviations and good quantitative agreement with the experimental speed of sound.

Key words: excess properties, density, Redlich-Kister equation, refractive index, speed of sound.

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Physicochemical properties of binary mixtures of Furfural or Furfuryl alcohol with 1-propanol or 2-propanolat temperatures from (293.15 to 323.15) K

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The thermodynamic properties of binary mixtures with a self-associated component deviate significantly from ideality due to variations in the hydrogen bonding between similar and unlike molecules as well as variations in molecular size. Furfural has received much attention due to its unique physical and chemical properties [1].

In this work, densities, speeds of sound, and refractive indices, for binary mixtures of furfural and furfuryl alcohol with 1–propanol or 2–propanol at temperature from T= 293.1 5 K to 323.15 K and at atmospheric pressure over the entire range of composition were measured [2]. Experimental data were used to calculate the isentropic compressibility, κ_s. From this data, excess molar volumes, V_m^{E}, deviation in isentropic compressibilities, $\Delta\kappa_s$, and deviation in refractive indices, Δn_D, for all studied mixtures were calculated and correlated as function of temperature using Redlich-Kister polynomial equation [3]. The results were interpreted in terms of molecular interactions and molecular structures occurring in the binary mixtures.

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Click reaction modification of a new anodic-synthesized oligophenylene material

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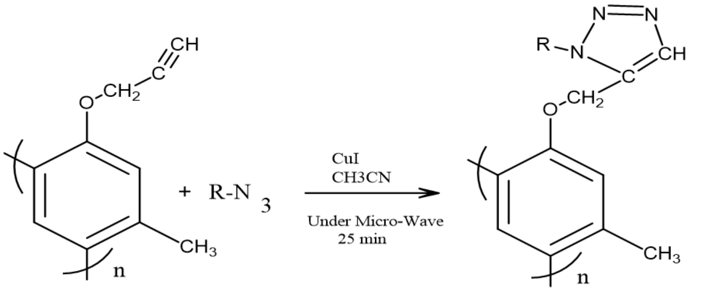

Oligo m-POT synthesized
by anodic oxidation

Oligo m-POT modified by
Click Reaction

A fast modification by copper (CuI)-catalyzed click reaction was performed under microwave on an oligophenylene. It was synthesized by anodic oxidation of the m-propargyloxytoluene (m-POT). This oxydation leads to two oligomers ; one soluble and the other insoluble, deposited on the platinum surface. The soluble modified oligomer was characterized by various spectroscopic techniques: 1H NMR, FTIR and UV. The insoluble oligomer, which develops in the form of a compact and homogeneous film during the potential scan, was also modified. Electrochemical and optical study revealed a change in the forbidden gap from modified Oligomer to unmodified one. The development of this type of material allows the design of smart and supramolecular polymers, opening the way to numerous applications in optoelectronics.

Key words: Click reaction, oligophenylene, m-propargyloxytoluene, Conjugated polymers

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Potentiometric and Conductometric Study of the Speciation of Zirconocene Dichloride Cp_2ZrCl_2 in Aqueous Solution

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Zirconocene dichloride Cp_2ZrCl_2 is known for its role as a catalyst for aqueous emulsion Nano-polymerization of styrene within SDS (sodium dodecyl sulfate) micelles. However, according to the bibliographic references [1, 2] the effective catalyst agent for this polymerization is rather the hydrolyzed form: $Cp_2Zr(OH)^+$ in acidic medium, which is absorbed with the styrene molecules in the organic nano-phase of SDS. The study of this Nanopolymerization process requires a preliminary quantitative potentiometric and conductimetric study of the hydrolysis of Zirconocene Cp_2ZrCl_2 at 25°C and 1 atm, in order to determine the thermodynamic hydrolysis constant K_h and the variation of the concentration of $Cp_2Zr(OH)^+$ as a function of the initial total concentration of Zirconocene and the measured pH, as well as the ionic conductivity at infinite dilution $\lambda°_{CP2Zr(OH)^+}$. Theoretical modeling is based on the following complete reaction and the following equilibria:

$CP_2ZrCl_2 + H_20 \rightarrow CP_2Zr(OH)^+ + H^+ + 2Cl^-$ (1)

$CP_2Zr(OH)^+ + H_20 \rightleftharpoons CP_2Zr(OH)_2 + H^+ \quad (K_h)$ (2)

$H_2CO_3 \rightleftharpoons HCO_3^- + H^+ \quad (K_a); \quad H_2O \rightleftharpoons OH^- + H^+ \quad (K_e)$ (3-4)

The use of the conditions of conservation of atoms and the principle of electro-neutrality, results in a system of equations allowing the calculation of the concentrations of the different species involved as a function of the measured pH, and thus leads to the determination of the hydrolysis constant $K_h \approx 6.2\ 10^{-4}$, taking into account the activity coefficients calculated according to the Debye-MSA theory as a function of the ionic strength I. On the other hand, the adjustment of the measured conductivity $\chi^m{}_{CP2ZrCl2}$ to its theoretical expression according to the formula:

$\chi^m{}_{CP2ZrCl2} = 10^{-3}\,(C_{CP2Zr(OH)^+}\,\lambda_{CP2Zr(OH)^+} + C_{H+}\,\lambda_{H+} + C_{Cl-}\,\lambda_{Cl-} + C_{HCO3-}\,\lambda_{HCO3-} + C'_{OH-}\,\lambda_{OH-})$,

in which the conductivities λ_i are calculated via the Onsager-Kim-MSA theory for mixed electrolytes, resulted in a value of $\lambda°_{CP2Zr(OH)^+} \approx 104.8\ \Omega^{-1}$ cm2 equiv^{-1}.

Key words: Zirconocene, hydrolysis, conductivity, Onsager-Kim-MSA

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Activity of terpenes-doped oxides against *Echinococcus granulosus* protoscoleces

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Cystic echinococcosis (CE) is a globally prevalent zoonotic parasitic infection affecting humans and various animal hosts [1]. The disease is caused by the larval stage of *Echinococcus granulosus*, following accidental ingestion of parasite eggs excreted by infected dogs. In general, the treatment modalities are associated with considerable risks, including hepatotoxicity and cyst rupture. This study aimed to evaluate the *in-vitro* eradication of protoscoleces using terpenes-doped metal oxides. The oxides were prepared by sol-gel method and then characterized by different techniques. The terpenes were deposited at the surface of oxide using a particular method. The results obtained with selected samples are compiled Table 1.

Table 1. Mortality rates of *E. granulosus* protoscoleces treated with terpenes-doped metal oxides.

Oxide	Amount of retained terpenes	Protoscoleces mortality (%)
Al_2O_3	160 mg g^{-1}	100
TiO_2	100 mg g^{-1}	80
Al_2O_3-TiO_2	140 mg g^{-1}	73
Al_2O_3	No terpenes	43
TiO_2	No terpenes	0
-	Unsupported terpenes	21

The results revealed the efficiency of the pure and modified Al_2O_3 in the eradication of *Echinococcus granulosus* protoscoleces after a contact time ranging from 2 to 5 minutes. According to dynamic light scattering (DLS) and zetametry analyses, there is a synergetic effect between the terpene's molecules and the protoscoleces in solution. These results encourage the use of these samples for *in*-vivo assays since very low concentrations were employed (2 and 4 mg mL^{-1}).

Key words: *Echinococcus granulosus*, metal oxides, sol-gel, DLS

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Natural Extracts from *Acacia tortilis* subsp. *raddiana* as Bio-Based Emulsifiers: Influence of Solvent Extraction on Antioxidant and Interfacial Properties in Colloidal Systems

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This study investigates the solution-phase extraction and functional characterization of bioactive compounds from various parts of *Acacia tortilis* subsp. *raddiana* (seeds, pods, leaves, and gum). Different aqueous–ethanolic solvent systems (20:80, 50:50, and 80:20 water:ethanol, as well as pure solvents) were evaluated to optimize the selective solubility and extraction of total polyphenols, flavonoids, saponins, proteins, and total sugars.

The gum extracts obtained with a 50:50 water:ethanol mixture exhibited the highest concentrations of total polyphenols (1096 µg/mL) and flavonoids (240 µg/mL), along with significant saponin content, indicating enhanced solubility under moderately aqueous conditions. The antioxidant potential of the extracts was assessed via DPPH assay, where the leaf extract prepared with 20:80 water:ethanol displayed the highest activity (IC_{50} = 1.2 µg/mL), suggesting the presence of stable, soluble antioxidant compounds.

The interfacial properties of these extracts were further examined through their ability to reduce oil–water surface tension and stabilize oil-in-water emulsions. Gum-based emulsions demonstrated excellent colloidal stability over 21 days, with average droplet sizes near 600 nm and high negative zeta potentials (-40 to -50 mV), promoting electrostatic repulsion. In contrast, leaf-based emulsions showed pronounced instability, with droplet size increasing from 900 nm to over 1100 nm during storage.

These findings highlight the critical role of solvent polarity in modulating both the compositional profile and interfacial behavior of plant extracts. Future work will explore extract combinations to enhance emulsion functionality and broaden the scope of biological activity assessments.

Key words: Interfacial stability, Emulsifiers, Nanoemulsion, Lipid-based drug delivery.

Eco-Friendly and Cost-Effective Bioadsorbent for Efficient Dye Removal: Structural Characterization and Kinetic Modeling

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Nowadays, ecosystems continue to suffer from the severe impacts of dye pollutants. This study investigates the efficiency of an eco-friendly and zero-cost adsorbent prepared from prickly pear seeds. The objective of this work is to evaluate the adsorption properties of Methylene Blue (MB) using prickly pear seeds as a biomass-based adsorbent.

The prepared adsorbent was characterized using X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), and thermogravimetric analysis (TGA). Adsorption kinetics were studied using UV-visible (UV/Vis) spectroscopy. Several factors affecting dye adsorption were examined, including pH, stirring rate, contact time, temperature, and both adsorbate and adsorbent dosage.

The adsorption capacity of prickly pear seeds for MB was found to be 144 $mg\cdot g^{-1}$ under optimal experimental conditions. A detailed investigation into isotherm models, kinetic models, and thermodynamic parameters was also conducted. The adsorption dynamics were best described by the pseudo-second-order kinetic model, and the process was found to be endothermic. Furthermore, the isotherm data showed good correlation with both the Langmuir and Temkin models, as revealed through analysis of the experimental data using various adsorption models.

Keywords: Adsorption, Methylene Blue, kinetics models, isotherms models

Structural and Morphological Characterization of Sol-Gel Derived ZnO Thin Films on Fe-10Cr Alloy

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In this study, ZnO thin films were deposited on Fe-10Cr alloy substrates using the sol-gel method combined with spin-coating. Each coating cycle was followed by a drying step, and the final films were annealed at high temperature to enhance crystallinity. Structural and morphological analyses were carried out using X-ray diffraction (XRD), scanning electron microscopy (SEM), and energy-dispersive spectroscopy (EDS). XRD confirmed the formation of the hexagonal wurtzite ZnO phase. SEM images showed smooth, uniform, and well-adherent surfaces, while EDS mapping verified the expected elemental composition. These results highlight the efficiency of the sol-gel technique in producing high-quality ZnO coatings, with promising potential for the surface protection of Fe-based alloys.

Keywords: ZnO thin films, Sol-gel method, Spin-coating, Fe-10Cr alloy,
Surface morphology, Structural characterization.

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Selective C(sp³)–C(sp²) Bond Formation via Homogeneous Electrochemical Cross-Coupling in Solution

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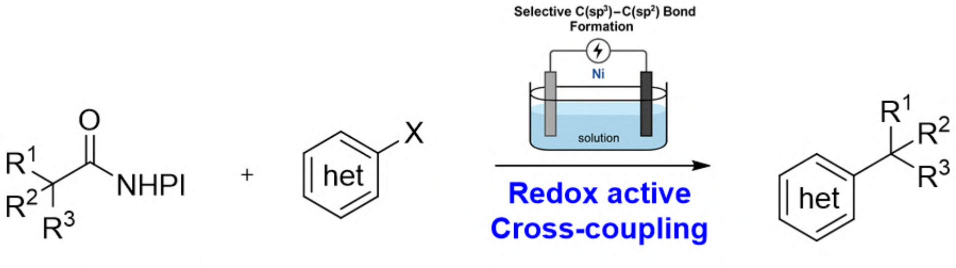
We report a homogeneous electrochemical strategy for the selective formation of C(sp³)-C(sp²) bonds through decarboxylative cross-coupling of redox-active esters catalyzed by nickel under mild conditions. Precise control of nickel oxidation states at the electrode–solution interface, combined with systematic optimization of solution parameters-solvent, supporting electrolyte, and reagent concentrations-enables excellent chemoselectivity and broad functional group tolerance [1,2].

This method is effective across a wide range of alkyl esters, including complex substrates, offering a sustainable platform for late-stage diversification of bioactive molecules. Solvent choice (NMP, ACN, DMF, tBuCN) and electrode materials (magnesium, RVC) significantly impact intermediate formation and overall reaction efficiency. Control over solution homogeneity and deposition phenomena ensures reproducibility and high performance.



Key words: Electrocatalysis, electrode–solution, Nikel Oxidation, chemoselectivity

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The use of cyclodextrins for the complexation of hydrocortisone

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The complex formation of hydrocortisone (HC) with cyclodextrins (2-HP-α-CD, 2-HP-β-CD and 2-HP-γ-CD) was investigated by NMR and volumetric techniques [1]. Furthermore, diffusion coefficients for the system {HC+2-HP-β-CD+water} were also determined [2]. The results showed that (2-HP-β- and γ-CD) form stable complexes with HC, whereas (2-HP-α-CD) does not, probably due to its smaller cavity size [2]. ^{1}H NMR studies suggested the entry of HC into the cavity of the β- and γ-CDs. Volumetric data confirmed the formation of host-guest type complexes between HC and cyclodextrins (2-HP-β and γ-CD) [1], which is consistent with what was observed in diffusion studies in media containing (2-HP-β-CD) [2].
The present study suggests that the use of 2-HP-β-CD and 2-HP-γ-CD could improve the solubility, stability, and bioavailability of hydrocortisone, making these systems promising candidates for pharmaceutical applications focused on controlled drug release.

Key words: 2-Hydroxypropyl-cyclodextrins, Hydrocortisone, Host–guest complexes.

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The use of cyclodextrins for the removal of sodium sulfadiazine from hospital wastewater

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Antibiotics are widely used in the treatment of a variety of hospital-treated illnesses. They are generally prescribed in higher doses than therapeutic due to their typically low bioavailability. This means that a significant portion of them goes unused and excreted, through urine and faeces, into the hospital's wastewater. If this wastewater is not properly treated, these antibiotics end up in aquifers, contaminating the environment.

In this communication, we present a procedure, based on complexation with cyclodextrins, to reduce the presence of sodium sulfadiazine in hospital wastewater. The formation of these complex species has been monitored by studying the volumetric properties of this antibiotic in aqueous solution.

Key words: Sodium sulfadiazine, cyclodextrins, volumetric properties, host-guest complexes.

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Supramolecular Interactions of an Anionic Resorcinarene with Transition Metal Ions: Combined Experimental and Theoretical Study

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The interaction between the anionic macrocycle sodium C-tetra(ethyl)resorcin[4]arene sulfonate (Na_4EtRA) and five transition metal ions (Pb^{2+}, Cu^{2+}, Zn^{2+}, Fe^{3+}, and Cr^{3+}) was investigated in aqueous solution using UV-Vis and fluorescence spectroscopy, complemented by computational studies. The experimental results revealed the formation of 1:1 complexes for Cu^{2+}, Zn^{2+}, Cr^{3+}, and Fe^{3+}, and a 1:2 stoichiometry for Pb^{2+}. All metals induced a marked decrease in the fluorescence intensity of Na_4EtRA, indicating a turn-off effect associated with charge transfer interactions. Stern–Volmer and Benesi–Hildebrand analyses confirmed static quenching and allowed for the determination of binding and quenching constants[1]. The highest sensitivity was observed for Cu^{2+} and Pb^{2+}, supported by low detection and quantification limits.

Key words: Transition metal ions; sodium sulfonated-resorcinarenes; transport properties; computational calculations

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Glycine and sodium glycinate in water: Molecular dynamics simulations and experiment

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In recent years, aqueous solutions of amino acid salts have attracted attention as promising carbon dioxide absorbents, in addition to the fundamental role in processes of life played by amino acids in general. To understand physicochemical properties of amino acids and their salts in solutions, computer simulations, particularly molecular dynamics (MD), are quite helpful when their results are matched to the experimental data. One problem here is adjusting the model potential parameters, typically within the framework of an existing force field, to reproduce the behavior of the system as observed in experiment. While the simplest amino acid, glycine, was extensively studied by MD before, this is not the case for its anionic salts.

In the present work, we performed MD simulations of glycine (Gly) and sodium glycinate (NaGly) aqueous solutions, using the OPLS-AA force field for short-range interactions, testing two water models (SPC/E and TIP4P/2005), different atomic charge sets for the glycine zwitterion and the glycinate anion, and different model potentials for Na^+. The MD results were compared with our measurements of diffusion in those solutions by the PGSE NMR method and with experimental data on densities and transport characteristics from other authors.

We have found that in MD, to obtain a reasonable agreement with the experiment, one should assume relatively low charges on N and H in amino groups. MD using the TIP4P/2005 water model (that predicts the diffusion coefficient and viscosity of pure H_2O better than SPC/E), the Joung – Cheatham potential for Na^+, and CNDO atomic charges for glycine and glycinate gives a quite satisfactory agreement with the experimental data for both Gly and NaGly solutions.

Acknowledgements: PGSE NMR measurements were performed at the Research Park of Saint Petersburg State University (“Center for Magnetic Resonance”). The work was supported by Russian Science Foundation (project 20-13-00038).

Key words: glycine, sodium glycinate, molecular dynamics, diffusion, NMR diffusometry

Removal of a dye, Bezacryl Yellow (BY), by crushed cardoon leaves

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The objective of our study is to recover an agricultural residue (crushed cardoon leaves) for the elimination of an organic pollutant, Bezacryl Yellow (BY), which plays a harmful role on the environment. The study of the influence of several physicochemical parameters on the adsorption capacity of Bezacryl Yellow on agricultural residue showed that: The maximum amount of Bezacryl Yellow adsorbed (34.12 mg/g) and the highest removal rate (80.32%) were obtained for a BY concentration of 200 mg/L, an agricultural residue concentration of 8 g/L with a particle size of < 100 µm, at pH 10, at a stirring speed of 500 rpm, and at a temperature of 50°C. The thermodynamic study revealed that JB adsorption is endothermic ($\Delta H° > 0$), physical in nature, and non-spontaneous. The adsorption isotherm of JB by the agricultural residue is L-type, indicating that JB dye molecules adsorb horizontally (flat) on the adsorbent surface. Application of the Langmuir, Freundlich, and Temkin models to the experimental results showed that JB adsorption on crushed cardoon leaves is closer to the Temkin model. Processing the experimental values with the various kinetic models yielded a highly significant correlation coefficient for the second-order model.

Keywords : adsorption, agricultural waste, dyes.

Thermal properties of $AlCl_3$ mixtures with amides and carbamides

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Binary mixtures of acetamide (AA) or urea (Ur) with excess $AlCl_3$ exist as liquids at room temperature, enabling aluminum electrodeposition under ambient conditions for next-generation room-temperature aluminum (Al) deposition processes [1]. These mixtures have been referred to as solvated ionic liquids (SILs) or deep eutectic solvents (DESs); however, their physicochemical properties, particularly their phase behavior and the Al ion speciation, remain insufficiently understood. In this study, we investigated the phase behavior of $AlCl_3$-amide and $AlCl_3$-carbamide mixtures, along with ^{27}Al NMR speciation analysis, to elucidate the molecular origin of their liquid state at room temperature and room-temperature aluminum deposition. The $AlCl_3$-amide and $AlCl_3$-carbamide mixtures exhibited glass transition behavior without crystallization over specific compositional ranges. The maximum difference (ΔT) between the glass transition temperature and the ideal melting temperature was found to be over 200 °C for both amide and carbamide systems, exceeding those (ΔT = 172°C) of typical choline chloride-urea DESs. This indicates strong resistance to crystallization, suggesting that these mixtures may be categorized as a new class of liquids, termed glass-forming liquid electrolytes (GLEs). The freezing point depression behavior was analyzed using an extended equation applicable to concentrated solutions. We are currently measuring the heat capacity (C_p) and the activity coefficient (f) of solvent. We expect that these parameters will serve as valuable indicators for the discovery of new DESs and GLEs.

Key words: Glass-forming liquid electrolyte, Phase diagram, Freezing-point depression

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Sustainable purification and deoxygenation of Olive Pomace Oil using low-cost catalytic solutions for biofuel applications

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Olive pomace oil, a by-product of the olive oil industry, contains a high level of oxygenated impurities that limit its industrial valorization [1]. This study presents a low-cost, eco-friendly solution chemistry approach for the purification and catalytic deoxygenation of this waste oil using easily accessible materials [2]. The purification process involves successive steps of solid-liquid separation, dehydration, acid neutralization, and pigment removal, using natural clays, charcoal, and edible acids [3]. The purified oil is then subjected to a mild catalytic reduction using heterogeneous catalysts such as Fe/Al_2O_3 and biochar, combined with hydrogen donors like formic acid or isopropanol, under moderate heating (80–120°C) and atmospheric or low pressure [4]. Analytical evaluation using acidity index, peroxide value, turbidity, and spectrophotometry confirms significant reduction of free fatty acids, peroxides, and pigments, with improved thermal stability [5]. These results demonstrate the viability of this accessible protocol as a green pathway to produce stable biofuel precursors, contributing to circular economy and sustainable energy goals in developing regions [6].

Key words: Olive pomace oil, purification, catalytic reduction, biofuel

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Enhanced Electrocatalytic Performance of $NiFe_2O_4$-Graphene Oxide Composites: Role of Interfacial Charge Transfer

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The electrochemical splitting of water has emerged as a critical process for clean energy technologies, driving research into efficient, non-precious electrocatalysts. In this study, we developed a $NiFe_2O_4$-graphene oxide (GO) composite supported on stainless steel ($NiFe_2O_4$-GO/SS) with enhanced electrocatalytic properties. Structural characterization by X-ray diffraction (XRD) and Fourier-transform infrared (FTIR) spectroscopy confirmed the spinel formation and successful GO incorporation, while scanning electron microscopy (SEM) revealed an optimized porous morphology. Electrochemical measurements demonstrated superior performance, with the composite exhibiting a Tafel slope of 39.4 $mV \cdot dec^{-1}$ (vs. 105.6 $mV \cdot dec^{-1}$ for bare $NiFe_2O_4$) and reduced charge transfer resistance (10 Ω vs. 20 Ω). These improvements are attributed to GO's dual role in enhancing electrical conductivity and facilitating interfacial charge transfer. Our findings present a promising approach for designing transition metal oxide-carbon hybrid materials with tailored electrocatalytic activity.

Key words: $NiFe_2O_4$, Graphene oxide, Electrocatalysis, Oxygen evolution reaction

Eco-friendly corrosion inhibitor system based on expired pharmaceuticals and iodide ions for aluminum alloys

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This study explores the synergistic corrosion inhibition effect of iodide ions and the expired drug Nifuroxazide (NFZ) on aluminum alloy 2024 in 1 M HCl solution. A combination of electrochemical techniques, surface analysis, and theoretical modeling was employed. Electrochemical results revealed that iodide ions significantly enhance NFZ's inhibition performance, reaching a maximum efficiency of 98% at the optimal NFZ–KI concentration. The results indicate that both NFZ and its mixture with iodide ions predominantly protect the cathodic sites of the aluminum surface.

Adsorption studies showed that NFZ follows the Freundlich isotherm, and thermodynamic analysis confirmed a physical adsorption mechanism. Surface characterization via optical microscopy and depth profilometry further validated the protective effect, showing minimal corrosion damage in the presence of inhibitors. FT-IR (ATR) analysis confirmed interactions between the inhibitors and the aluminum surface.

Theoretical calculations supported the experimental findings, highlighting the physical nature of adsorption and clarifying the synergistic interaction between NFZ and iodide ions. Overall, the study demonstrates that expired pharmaceutical compounds, when combined with iodide ions, offer an effective, sustainable, and low-cost strategy for protecting aluminum in acidic environments [1, 2].

Key words: Corrosion inhibition, Aluminum alloys, Nifuroxazide, Iodide ions, Electrochemical analysis, DFT.

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Adsorption of methylene blue and the regeneration of MCM-41 mesoporous silica

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The adsorption of methylene blue (MB) was conducted using calcined MCM-41. The influence of various parameters, particularly pH, was examined. The study also assessed the reusability of MCM-41 and explored the adsorption mechanism of MB. MCM-41 was synthesized, then calcined, and its structural properties were confirmed through characterization techniques including X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), and thermogravimetric analysis (TGA). These analyses validated the successful formation of the mesoporous MCM-41 structure. MB adsorption experiments revealed high dye removal efficiencies and fast adsorption kinetics, especially under acidic conditions. Kinetic modeling was performed using both pseudo-first-order and pseudo-second-order models. While the pseudo-first-order model provided a good fit, the pseudo-second-order model better described the adsorption behavior for the calcined material. Regeneration tests demonstrated that calcined MCM-41 retained approximately 90% of its initial adsorption capacity after three reuse cycles. These findings highlight the potential of calcined MCM-41 as a cost-effective and environmentally friendly material for wastewater treatment applications.

Key words: Adsorption, Methylene blue, MCM-41, Regeneration

Insights into the Structure and Dynamics of a Lithium Sulfur Battery Electrolyte using Molecular Dynamics Simulations

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This study investigates the Li ion transport mechanisms in lithium-sulfur (Li-S) batteries. Currently, the structure of their electrolytes and the dynamics of Li ion transport are not well understood, so we employed classical all-atom molecular dynamics simulations exceeding 100 ns to explore long-time Li ion transport, structural changes, and multiphase dynamics.

Results indicate the electrolyte structure is separated into a LiTFSA-rich microphase and an HFE-rich phase, with many LiTFSA clusters present (Fig. 1). Consequently, the presence of these clusters increases the Li ion diffusion coefficient. These result clearly that the electrolyte achieves highly efficient charge transfer by utilizing the HFE-rich phase as an electrical conduction pathway. In addition, in the LiTFSA-rich microphase, Li ions exhibited oscillatory motion and hopping to different TFSA.

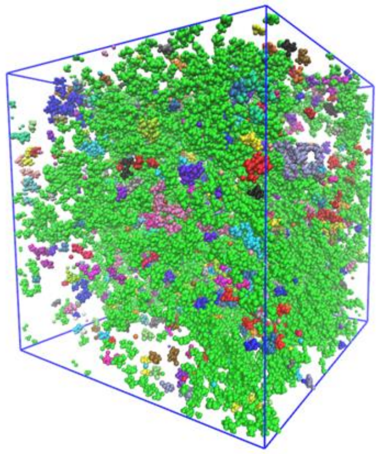

Fig. 1 Snapshot of the LiTFSA-rich microphase and LiTFSA clusters.

Key words: Lithium-sulfur batteries, Molecular dynamics simulation, Phase separation, Region-dependent dynamics

Synthesis and antioxidative activity of self-assembled tetrahydropyrimidines-based organogels

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In the past few years, tetrahydropyrimidines (THPMs) have been increasingly used in polymer chemistry as a monomer in the biobased polymers with the wide biological activities.[1,2] Here, THPMs synthesized *via* the Biginelli reaction utilizing *O,O'-bis*-vanillin as a bio-based starting material, have been explored as low-molecular-weight organogelators (LMOGs).[3] Synthetized THPMs have been evaluated for their gelation properties in various solvents, and it has been found that the critical gelation concentrations were between 4% and 7% (*w*/*v*) in DMSO as solvent. The added SiO_2 (2 wt%, average size ~7 nm) enabled fine-tuning of the organogels' rheological properties, enhancing their mechanical performance. Scanning electron microscopy (SEM) revealed highly porous 3D networks, while rheological analysis demonstrated shear-thinning and thixotropic behaviour, indicating potential for biomedical applications. Despite low antioxidant activity observed in optical assays, electron paramagnetic resonance (EPR) measurements confirmed the organogels' ability to scavenge free radicals effectively. In summary, these findings highlight the potential of THPM-based organogels for skin protection and wound healing by combating oxidative stress.

Key words: Biginelli reaction, vanillin, organogels, antioxidants

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In silico evaluation of the affinity of quinoline derivatives for the AChE receptor through molecular docking

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Introduction: Acetylcholinesterase (AChE) is a key enzyme responsible for the hydrolysis of acetylcholine, and its inhibition is a well-established therapeutic strategy in the treatment of Alzheimer's disease. In light of the cholinergic deficit observed in neurodegenerative conditions, identifying novel AChE inhibitors remains a priority in drug discovery. This study aimed to evaluate the inhibitory potential of eight novel quinoline derivatives against AChE through molecular docking simulations. **Materials and Methods:** The *in-silico* analysis focused on predicting the anticholinesterase activity of eight quinoline-based derivatives for the AChE receptor, utilizing AutoDock Vina®. Rivastigmine, the reference compound, was included for comparison. The physicochemical and pharmacokinetic properties (ADMET) and drug-likeness predictions were evaluated using SwissADME® and pkCSM®. **Results and Discussion:** Molecular docking studies revealed that Compound 3 showed the highest affinity for AChE, scoring a lower binding energy (-9.5 kcal/mol) than that of Rivastigmine (-7.5 kcal/mol) and an RMSD of less than 2.5 Å. Both molecules interacted with the AChE receptor through the same types of bonds, including π–alkyl, π–π stacking, π–σ, and hydrogen bonds, which contributed to ligand stabilization within the binding pocket. Compound 3 was assessed as drug-like, with a pharmacokinetic profile showing good gastrointestinal absorption and a high volume of distribution (VDss). The toxicity prediction revealed negative Ames's test results, classifying this compound as non-genotoxic. **Conclusion:** This study highlights the potential of the quinoline analogue, particularly Compound 3, as an AChE receptor antagonist with promising ADMET properties, although further safety optimization is required.

Keywords: in silico Model, Nicotinic Receptors, quinolines

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In silico evaluation of the affinity of quinoline derivatives for the NMDA receptor through molecular docking

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Introduction: The N-methyl-D-aspartate (NMDA) receptor is crucial for synaptic plasticity and cognition, with its dysregulation linked to excitotoxicity and neurodegeneration, particularly in Alzheimer's disease. This study aims to explore the binding affinity of novel quinoline derivatives toward the NMDA receptor via structure-based molecular docking. **Materials and methods:** *In silico* analysis was performed to predict the affinity of eight quinoline-based derivatives for the NMDA receptor using AutoDock Vina®. Ifenprodil, a non-competitive antagonist specific to the GluN 2 B subunit, was the reference. Physicochemical and pharmacokinetic properties (ADMET), and drug-likeness were assessed using SwissADME® and pkCSM®. **Results and discussion:** Molecular docking analysis revealed compound 2 had the most favorable binding, with a binding energy of –9.1 kcal/mol and an RMSD below 2.5 Å, indicating a well-aligned pose relative to the reference ligand. Both molecules formed comparable non-covalent interactions with the NMDA receptor, including π–alkyl, π–π stacking, π–sigma, and hydrogen bonds. This similarity in interaction profiles accounts for the comparable docking scores observed. The pharmacokinetics profile prediction results of analogue 2 showed good gastrointestinal absorption, high Caco-2 cell permeability, and a large volume of distribution (VDss). Despite, compound 2 meeting all major drug-likeness criteria, predicted hepatotoxicity and hERG II inhibition raise safety considerations for further optimization. **Conclusion:** This study highlights the potential of quinoline analogues, especially compound 2, as NMDA receptor antagonists with promising ADMET properties, though safety optimization is required.

Keywords: in silico Model, NMDA receptor, quinolines

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Calcium phosphate–supported nanocomposites for enhanced visible-light photodegradation of methylene blue

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In this study, calcium phosphate–supported nanocomposites were developed and investigated for the enhanced photocatalytic degradation of methylene blue (MB) dye under visible light irradiation. The nanocomposites were synthesized by incorporating metal oxide nanoparticles into a hydroxyapatite (HAp) matrix via a wet chemical route. Comprehensive characterization was conducted using Fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), transmission electron microscopy (TEM), and UV–Vis diffuse reflectance spectroscopy to confirm the successful integration of the photocatalyst, the preservation of the crystalline structure, and the improvement of optical absorption in the visible region.

The photocatalytic activity of the synthesized materials was evaluated through the degradation of methylene blue, taking into account various operating parameters.

The photocatalytic performance was assessed through MB degradation under various conditions, with a focus on pH and irradiation time. Enhanced efficiency was observed in mildly alkaline media and the optimized nanocomposite outperformed other formulations. Furthermore, the degradation followed pseudo-first-order kinetics, confirming both efficiency and reproducibility. These findings highlight the potential of the developed nanocomposites for application in wastewater treatment, particularly for dye-contaminated effluents with alkaline characteristics.

Key words: Photocatalysis, Calcium phosphate nanocomposites, MB degradation

Study of the physicochemical and microbiological stability of dexamethasone-based mouthwashes

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Introduction: Oral mucositis is a common and painful side effect of chemotherapy and radiotherapy in cancer patients, significantly impairing their quality of life and adherence to treatment. Although dexamethasone is recognized for its anti-inflammatory properties, no commercial mouthwash formulation exists at a concentration of 0.1 mg/mL. This study aimed to formulate and evaluate the physicochemical and microbiological stability of hospital-prepared dexamethasone-based mouthwashes. **Materials and Methods:** Nine different formulations were developed by varying the humectants, cosolvents, and surfactants. Stability was assessed over 28 days by monitoring pH, viscosity, density, zeta potential, and dexamethasone concentration using HPLC. Microbiological quality was also evaluated. Statistical analyses were conducted using Student's t-test and ANOVA. **Results and Discussion:** Formula F9, composed of sorbitol as humectant and propylene glycol as cosolvent, demonstrated optimal physicochemical stability, with non-significant variation in viscosity and acceptable pH levels. The dexamethasone content remained within 98.48% after 52 days. Microbiological analyses showed no contamination at Day 28. **Conclusion:** The F9 formulation appears to be a stable and safe candidate for clinical use as a dexamethasone-based mouthwash. Further clinical studies are warranted to confirm its therapeutic benefits in the management of oral mucositis.

Keywords: Mouthwash, Dexamethasone, Formulation

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Castor oil and laxative activity: Virtual screening of ricinoleic acid analogues

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Introduction: Castor oil has long been recognized for its laxative activity, used in traditional and conventional medicines for the treatment of constipation The objective of this study was to identify potential candidates for future drug development. **Materials and Methods:** The molecules related to ricinoleic acid that we investigated were obtained from the" Related compounds" section in PubChem. This section gathers all parent compounds, mixtures, salt forms, as well as similar compounds and conformers with structural similarities to the compound of interest in terms of 2D or 3D chemical structure. We utilized the Python library Dockstring to conduct virtual screening on 100 randomly selected molecules. Their SMILES codes were loaded from a CSV file, along with the target file and the configuration file containing grid box coordinates. Subsequently, 3D conformations were generated, followed by molecular docking using Autodock Vina. The resulting data was then recorded for analysis. **Results and Discussion:**The virtual screening results of the 100 molecules related to RA showed that some molecules outperformed RA in terms of affinity score. Among these molecules, certain ones exhibited more negative interaction scores, suggesting a potential to establish stronger, more stable, and more specific interactions with the target molecule. The top 10 molecules with the highest scores were selected. The difference in the affinity scores of the RA-related molecules studied compared to that of RA can be explained by the presence of additional bonds established by related molecules such as salt bridges, Pi-Sigma type hydrophobic bonds as well as the number of connections established. This may explain this affinity improvement. Further analysis of these molecules highlighted four candidates (26, 28, 38, and 4) with favorable physicochemical, pharmacokinetic, and toxicological properties, suggesting their potential for therapeutic development. **Conclusion:** Through molecular modeling and virtual screening, we identified several promising compounds with potential enhanced efficacy compared to ricinoleic acid. However, to translate these findings into clinical practice, rigorous experimental validation, including molecular dynamics studies and in vitro and in vivo experiments, is crucial.

Keywords: *in silico, castor oil, laxative*

Taste-Masking of Caffeic Acid via Inclusion Complexation with Hydroxypropyl-β-Cyclodextrin: Evidence from NMR and Conductometric Sensing

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Caffeic acid (CA), or 3,4-dihydroxycinnamic acid, is a bioactive polyphenol belonging to the hydroxycinnamic acid family. Despite its recognized therapeutic potential, its application in pharmaceutical and nutraceutical formulations is limited by its intense bitterness, which negatively impacts consumer compliance. To address this challenge, we investigated the encapsulation of CA using hydroxypropyl-β-cyclodextrin (HP-β-CD), aiming to mask its unpleasant taste while preserving its bioactivity. The inclusion complex between CA and HP-β-CD was first characterized using ^{1}H NMR spectroscopy, which confirmed the formation of a 1:1 host–guest complex. The association constant (K) was calculated to be 240, indicating a stable interaction. To evaluate the sensory masking effect, a microconductometric sensor was designed and implemented. The sensor demonstrated high sensitivity, with a detection limit reaching 10^{-5} M and a response time ranging from 10 to 50 seconds. The reduced interaction of free CA with the sensor upon complexation further confirmed the effective taste-masking by HP-β-CD. These findings support the potential of cyclodextrin-based encapsulation as an effective strategy for enhancing the palatability of bitter bioactive compounds like caffeic acid, paving the way for broader acceptance in oral therapeutic products.

Key words: Caffeic acid, hydroxypropyl-β-cyclodextrin, taste masking, inclusion complex, ^{1}H NMR, conductometric sensor, encapsulation, host–guest chemistry.

Thermodynamic study of inclusion of ionic liquid by cyclodextrin in water

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Cyclodextrins (CDs) have hydrophobic cavities that enable the inclusion of hydrophobic guest molecules in aqueous environments, serving as useful models for enzyme–ligand interactions. Ionic liquids (ILs), especially the 1-alkyl-3-methylimidazolium series ($[\mathrm{C}_n\mathrm{mim}][\mathrm{Cl}]$) with varying alkyl chain lengths and high water solubility, are ideal for studying the contributions of electrostatic and hydrophobic interactions to CD inclusion mechanisms. In this study, thermodynamic parameters for the inclusion of α-CD, β-CD, Me-β-CD, and γ-CD with $[\mathrm{C}_n\mathrm{mim}][\mathrm{Cl}]$ (n = 4, 6, 8, 10, 12, and 14) were determined by isothermal titration calorimetry (ITC) at 298.15 K.

The host–guest interactions were evaluated using 1:1 and 1:2 models. For $[\mathrm{C}_6\mathrm{mim}][\mathrm{Cl}]$, α-CD and β-CD showed exothermic inclusion, while Me-β-CD and γ-CD exhibited endothermic behavior. α-CD inclusion was enthalpy-driven (ΔH_{inc} = –15.6 kJ mol^{-1}, $T\Delta S_{\mathrm{inc}}$ = –5.2 kJ mol^{-1}), indicating strong hydrophobic interaction and restricted guest mobility within the narrow cavity. In contrast, Me-β-CD inclusion was entropy-driven, suggesting a dominant dehydration effect due to methylation of hydroxyl groups. For longer-chain ILs such as $[\mathrm{C}_{12}\mathrm{mim}][\mathrm{Cl}]$, γ-CD showed significant inclusion when $n > 10$, with a 2:1 stoichiometry (CD:IL). β-CD and γ-CD exhibited two-step inclusion processes, with initial enthalpy-driven binding followed by entropy-driven binding. Additionally, ILs with $n > 10$ displayed sigmoidal dilution curves, indicative of micelle formation. Across all α-CD complexes, inclusion enthalpy remained negative, although stoichiometry shifted with chain length. These results demonstrate that CD inclusion behavior is strongly influenced by cavity size, chemical modifications, and IL alkyl chain length, suggesting the potential to control molecular recognition through appropriate host selection.

Key words: Ionic liquid, Cyclodextrin, Inclusion, Titration calorimetry

Effect of TiO_2 on the adhesion and bioactivity of a sol-gel-derived hydroxyapatite coating on 316L stainless steel surface: Biomedical application

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Hydroxyapatite (Ca10(PO4)6(OH)2, HAP) is widely used for hard tissues repair due to its chemical and structural similarities with the mineral phase of bone and teeth [1] . In this study we investigated the effect of the addition of TiO2 inner-layer on the morphological and mechanical properties of hydroxyapatite (HAP) bioceramic coatings on 316L stainless steel by sol-gel method in order to improve the properties of hydroxyapatite and expand its clinical application [2]. We have noticed that thin films of HAP/TiO2 on 316L SS possess combined advantages of bioactivity and corrosion-resistant properties [3]. We recall that the indentation hardness is often used as an initial guideline for the qualification of a coating for any application requiring wear resistance. Intrinsic film hardness can be directly measured when the penetration depth of the indenter is lower than 10% of the coating thickness. In our study, The deposition of the inner-layer have provided the formation of new types of hydroxyapatite coatings. Classical hardness measurements conducted on the coated systems under the same indentation load (10g) indicates that the microhardness of the HAP coating is improved by the addition of TiO2 inner-layer on the 316L stainless steel substrate, the adhesion to the steel is also improved. We notice that the hardness is comparable with those of natural teeth.

By referring to the literature this can be explained by the solution containing Ca^{2+} and PO_4^{3-} ions serving to form the HAP phase. This reacted with TiO2 during sintering, forming the CaTiO3 and $Ca_3(PO_4)_2$ phases at the HAP-316 L interface. The presence of Ti in the HAP coating significantly improved its mechanical strength. This was due to the reaction bonds (and consequently the increase in chemical bonds between the coating particles). Thus, the amount of energy required to separate the HAP-TiO2 from the 316 L steel increased considerably compared to HAP coating on the 316 L steel. The corrosion resistance of the 316L stainless steel in simulated body fluid (SBF) was found to increase after the deposition of the HAP and HAP/TiO2 coatings as confirmed by the cyclic voltammetry test.

Biological tests confirmed that the HAP-TiO2 coating on 316L stainless steel is highly bioactive and promotes cellular activity. We observed Ca-P growth in simulated body fluid (SBF) solution after 2 to 4 week(s). In addition, the concentration of calcium and phosphorus in the SBF solution showed that Ca-P growth was effective. This means that PO_4^{3-} and Ca^{2+} ions from the SBF solution were deposited on the pretreated surface to form a thick Ca-P layer, as in the case of bone growth.

Key words: Sol gel, Hydroxyapatite, TiO_2, Characterization, indentation, corrosion, bioactivity.

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All-Atom Molecular Dynamics Study on Cellulose Dissolution in Ionic Liquids Under High Pressure: Prediction and Mechanistic Insights

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Key words: Cellulose dissolution, Ionic liquid, High pressure, AA-MD simulation

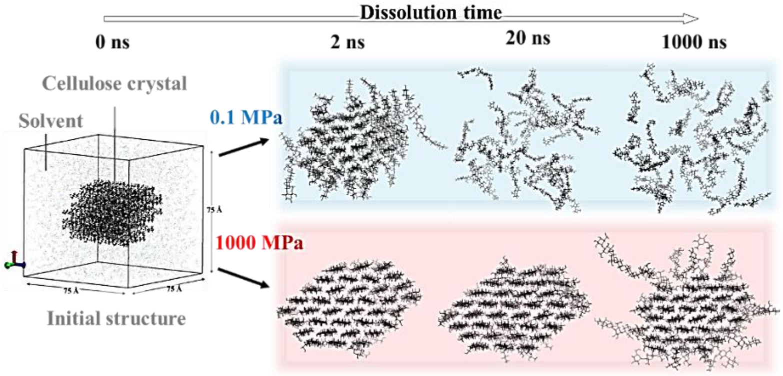

Fig. 1 Dissolution process under *P* = 0.1 and 1000 MPa

Cellulose has broad potential in eco-friendly and health-related applications, but its use requires dissolution in solvents like ionic liquids(1). Pressure is a promising tool to enhance solubility without breaking covalent bonds or consuming much energy, yet experimental studies are limited. Here, we used all-atom molecular dynamics simulations to explore how high pressure affects cellulose dissolution in ionic liquid/DMSO mixtures. Our results suggest that pressure can improve solubility but may slow the dissolution rate.

To assess how pressure influences cellulose solubility, we calculated the dissolution free energy $\Delta G_{Dissolution}$ using the Umbrella Sampling Method. As a result, $\Delta G_{Dissolution}$ decreases consistently across the pressure range of 0.1 to 1000 MPa, indicating that elevated pressure promotes cellulose solubility.

To evaluate how pressure affects the cellulose dissolution rate, we simulated the dissolution of a cellulose crystal under pressures ranging from 0.1 to 1000 MPa. Fig. 1 compares the dissolution behavior at 0.1 MPa and 1000 MPa. At 0.1 MPa, cellulose chains fully dissolved within 1000 ns. In contrast, under 1000 MPa, the crystal structure remained largely intact, with only limited disruption after the same time period. These results suggest that higher pressure slows down the dissolution process.

We used MD simulations to study how high pressure affects cellulose dissolution and found that pressure enhances solubility but slows dissolution, indicating a trade-off. Details of the molecular mechanism will be presented in the session.

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Spectroscopic study of the coordination of metal ions with anthrone derivatives

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Many metal ions demonstrate a great ability to coordinate with organic ligands. These properties help to shed light on the physicochemical nature of molecular interactions. Coordination is widely used to construct supramolecular systems and hybrid materials [1,2].

In our previous studies, a systematic study of the coordination between metal ions and the amidine group of benzanthrone derivatives was carried out. Crystallographic and spectroscopic studies had been performed of structures, coordination and chemical bonding for series of metal ions.

The present work describes the synthesis and characterization of a various metal complex with novel amidine derivatives of anthrone. Within this investigation, obtained complexes were meticulously examined using spectroscopic techniques. Fourier transform infrared, UV-Vis absorption and fluorescence spectroscopic techniques were used to investigate the coordination. The structure of these complexes was deduced according to the mole ratio method obtained as a result of spectroscopic studies of complex solutions of the ions under study. FTIR spectroscopy provides information on the vibrational modes involving coordinating sites. On complex formation several changes in FTIR spectra were observed.

The absorption spectra of the solutions of the obtained complexes in the UV-visible region showed a bathochromic shift in the visible region compared to the initial amidines. The emission spectra of these complexes also showed significant changes in the position and intensity of the fluorescence bands.

Key words: Anthrone, amidines, metal complex, spectroscopy

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Photophysical properties and potential application of substituted benzanthrones

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Fluorescent compounds play a key role in the development of modern materials and methods for scientific research and industrial applications. Among the wide range of fluorescent dyes currently in use, benzanthrone dyes are of particular interest due to their excellent spectral properties [1,2].

The present work describes the synthesis and characterization of new fluorophores based on benzanthrone with an extended conjugation chain. The solvatochromic behavior of obtained compounds with electron donating and accepting group was investigated in nonpolar, polar aprotic and protic solvents experimentally. The photophysical behavior of these dyes in various solvent was attributed to the intramolecular charge transfer of the compound along with specific and nonspecific interaction with organic solvents.

In our previous studies, the synthesized dyes were found to be useful for detailed and rapid biovisualization of trematodes and nematodes using confocal laser scanning microscopy and visualization of their digestive, reproductive and excretory systems [2,3].

In continuation of our research, we studied the suitability of the newly developed luminescent dyes with the selection of the most promising of them for staining various biological objects. In this way, benzanthrone derivatives with nitrogen-containing substituents in the molecule were selected and studied.

Key words: Benzanthrone, fluorescent dyes, spectroscopy, microscopy

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Molecular Dynamics Investigation of Hydronium Ion Transport Mechanisms in Nafion® Membranes

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To clarify the long-timescale transport mechanisms of hydronium ions (H_3O^+) in Nafion®, a polymer electrolyte membrane used in Polymer electrolyte fuel cells (PEFCs), we conducted 300 ns all-atom molecular dynamics simulations at hydration levels of λ = 6, 10, 14, employing modified DREIDING force fields[1] for Nafion® and F3C for water model. Spatial mesh-based analysis, free energy mapping, percolation analysis, and mean square displacement were performed to characterize ion transport pathways. Our results showed that H_3O^+ ion diffusion was spatially heterogeneous and proceeds via multiple transport mechanism, some of which impedes H_3O^+ mobility. This reduced mobility was caused by Nafion® morophorogy and by electorostatic interactions of H_3O^+ with the negative charged SO_3^- groups.

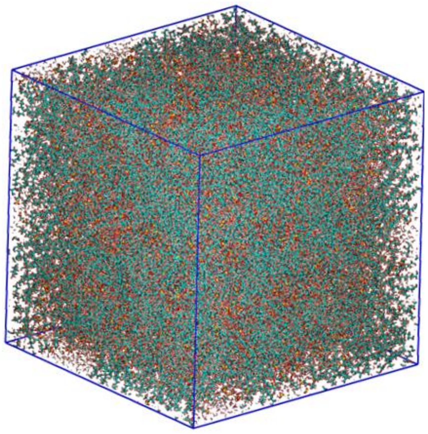

Fig.1 Snapshots of the Nafion® model at λ =10

Key words: Fuel Cell, Nafion®, Molecular dynamics simulation, dynamics

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Adsorption of Rhodamine B onto Few Layer Graphene: Experiments, statistical physics and artificial neural network modeling

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Few Layer Graphene (FLG) is an adsorbent for the removal of Rhodamine B (Rh B) in water treatment. The impact of operating parameters and the thermodynamics of Rh B adsorption on FLG was studied to identify the best removal conditions. The Rh B adsorption mechanism was analyzed via physicochemical characterization including SEM, BET, Raman and X-ray. Results showed that a maximum Rh B adsorption of 380.22 mg/g was obtained at a solution pH of the 4.75 and at 20 °C. The Rh B adsorption performance of FLG was highly dependent on temperature and solution pH. For a deeper insight into the Rh B adsorption mechanism, a monolayer model formulated via statistical physics was adopted to describe the adsorption geometry of this relevant water pollutant and also to further characterize the interactions between Rh B and FLG. Finally, a multi-layer feed-forward neural network (ANN), comprising 6 input parameters, a hidden layer, and an output parameter, was employed to predict Rh B removal efficiency. The mean absolute error was found to be 0.2418; the mean squared error was 0.6524; and the coefficient of determination (R^2) was 0.9896, suggesting a high prediction accuracy of the model and the great promise it carries.

Key words: Few Layer Graphene, Rhodamine B, Adsorption,

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Influence of inorganic and organic additives on the properties of sodium silicate solutions

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Sodium silicate solutions (waterglass) have become one of the most widely used industrial chemicals. The most interesting and characteristic property of silicate solutions is their ability to form gels having various viscosities with various activators. Moreover, the structure and distribution of these species are highly dependent on activators of various inorganic and/or organic components. The ability of sodium silicate solutions to form gels through chemical reactions with strong or weak acids has resulted in impressive binding capabilities with some water insoluble products [1]. The acid-treated silicate solutions tend to become very viscous, polymerized semi-solid gels that are difficult to handle, so the rate and process of gelation of silicate solutions must be rheologically controlled to reduce their viscosity to keep them easy to apply. Some organic (polymer) additives can also lead to viscous gels in silicate solutions. The polymer molecules can form intermolecular interactions, entangling between water molecules in silicate solutions to provide a polymer interpenetrating network gel system that exhibits enhanced viscosity in the gel state. Both acid and polymer-added silicate solutions showed controllable rheological properties. In this study, the rheological control on the properties of sodium silicate solutions by introducing some inorganic and organic additives has been elucidated. Some samples modified with weak or strong acids were also treated with Na-polyacrylate and PVA (polyvinyl alcohol). Various functional additives including TEOS (Tetraethoxysilane) and SDS (sodium dodecyl sulfate) were used to form stable homogeneous solutions. This study will provide a fundamental understanding of the gelation mechanism and kinetics for the silicate solutions.

Key words: Na-silicate solution, viscous gel, gelation additives, crosslink.

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Manufacturing of Hydrogel Composition for Extinguishing Metal Fires in Electric Vehicles

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This study is about a hydrogel composition for extinguishing metal fires, and more specifically, It is about manufacturing a hydrogel composition for extinguishing metal fires that can simultaneously act as a metal-silicate agent that suffocates the fire source and water agent that induces cooling, that is, induces a strong chemical bond between the two components so that they are not easily separated, and thus can be applied simultaneously to various metal fires. Metal fires mainly refer to fires that occur in highly reactive combustible metals such as lithium, sodium, potassium, cesium, magnesium, zirconium, and aluminum powders. Such combustible metal powders can spontaneously combust (dust explosion) without an external fire source, and can also cause fires by contact with moisture or air moisture, in which case hydrogen gas is generated along with heat, leading to an explosion. Except for metal fires, the most effective substance for other fires is liquid water (H_2O), which is superior to other powder fire extinguishing agents in terms of storage and field application, has a low vaporization temperature, and has a high heat capacity, making it an excellent extinguishing agent with a cooling effect. However, when extinguishing high-temperature metal fires with water, explosive hydrogen may be generated through a chemical reaction or a vapor explosion may occur, so its use is limited.

To solve this problem, Korean Patent Publication No. 10-2022-0083140 proposes a fire extinguishing powder for metal fires that includes a first fire extinguishing powder composed of ammonium phosphate, a second fire extinguishing powder composed of expanded vermiculite, expanded glass, and expanded pearlite. However, this pre-published patent uses only a suffocating agent, and although initial extinguishment is possible, it has the disadvantage that its cooling performance is low, so it takes a long time to cool to room temperature, and there is a risk of re-ignition. Therefore, in order to reduce damage caused by such metal fires, the development of a new concept fire extinguishing agent composition that can simultaneously apply a suffocating agent and a cooling agent is required.

Therefore, the purpose of this study is to provide a hydrogel composition for extinguishing metal fires that can extinguish fires in a short time by simultaneously performing suffocation and cooling actions without generating hydrogen gas or explosive vapor when applied to fires occurring in various metals including Li, and can reduce the risk of re-ignition due to the cooling action. Another purpose of this study is to provide a hydrogel composition for extinguishing metal fires that is non-toxic to the environment and generates almost no toxic gases, so that it can be used safely.

Key words: Hydrogel, extinguishing metal fires, Electric Vehicles

Sodium ion electrolyte solution structures by excess spectroscopy

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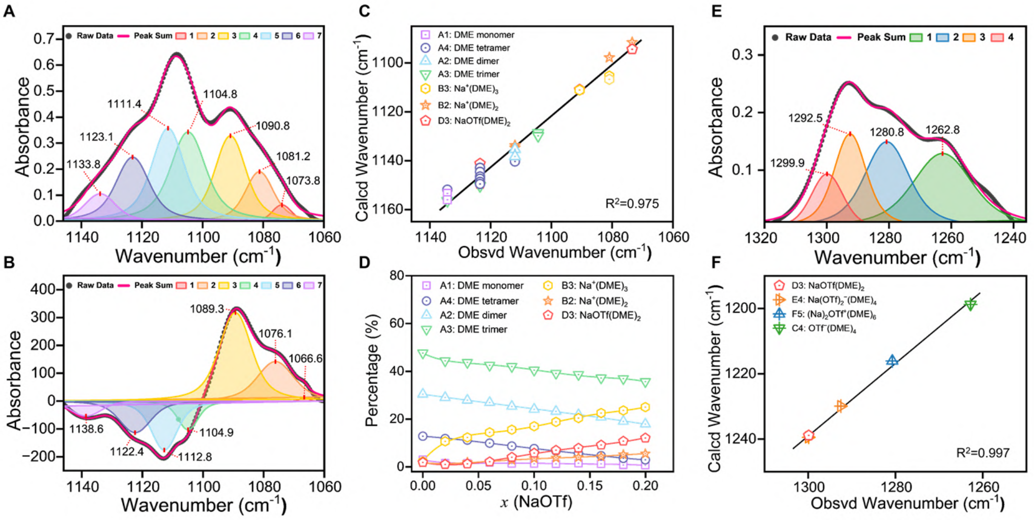
Sodium-ion batteries have attracted increasing attention in the field of energy storage due to their theoretically high energy density, long cycle life, and excellent safety. As a key component, the electrolyte governs ion transport and significantly influences battery performance. Excess infrared spectroscopy has been progressively developed over the years and is now widely applied to the study of solution structures and intermolecular interactions.[1-3] In this study, we employed excess infrared spectroscopy as the primary tool, supported by quantum chemical calculations, NMR spectroscopy, to investigate the solution structure and intermolecular interactions in a model electrolyte composed of sodium trifluoromethanesulfonate (NaOTf) and 1,2-dimethoxyethane (DME).



Ten electrolyte species were identified, including charged complexes such as $[Na^+(DME)_3]$, $[Na(OTf)_2^-(DME)_4]$, and $[(Na)_2OTf^+(DME)_6]$, as well as neutral species like $[NaOTf(DME)_2]$ and $(DME)_n$ (n=1~4). Na^+ exhibits a typical solvation number of ~ 6. With increasing salt concentration, the species distribution transforms from individually solvated ions to contact ion pairs. Interaction analysis shows that DME interacts most strongly with Na^+, less strongly with OTf^-, and the least with itself. This suggests that Na^+ transports mainly via a solvation-carriage mechanism, while OTf^- likely follows a hopping pathway. These findings offer molecular-level insights into ion transport and would assist the electrolyte design for sodium-ion batteries.

Key words: excess infrared spectroscopy, sodium-ion battery, solution structure

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Quality Control of Vitamin C in Dietary Supplements Using HPLC-UV Analysis

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Introduction: Vitamin C is widely used in dietary supplements for its health benefits, particularly in preventing fatigue and infections. However, discrepancies between declared and actual contents have been reported. This study aimed to validate a high-performance liquid chromatography (HPLC) coupled with ultraviolet (UV) detection method for quantifying vitamin C and to assess the consistency between labeled and measured concentrations in commercial supplements.

Materials and Methods: An HPLC-UV analytical method was developed and optimized by adjusting key parameters, including the mobile phase composition, stationary phase, and detection wavelength. The method was validated according to ICH and SFSTP guidelines, evaluating specificity, linearity, precision, and accuracy. Once validated, the method was applied to five commercial vitamin C supplements marketed in Tunisia. **Results:** The validated method showed excellent specificity, linearity ($R^2 = 0.9987$), precision (repeatability CVr = 0.21%), and accuracy (mean recovery between 98.58% and 100.07%). Uniformity of mass testing showed that three products (S3, S4, and S5) complied with pharmacopeial standards, while S1 and S2 did not. Quantitative analysis revealed significant discrepancies between labeled and measured vitamin C contents: S1 and S4 were compliant (106.24% and 98.96%), while S2, S3, and S5 showed non-conformities, with measured values ranging from 61.97% to 129.8% of the declared amounts.

Conclusion: This study highlights notable inconsistencies in the quality of vitamin C supplements available on the Tunisian market. Strengthening regulatory oversight and ensuring better transparency are essential to guarantee the safety and efficacy of dietary supplements.

Key words: vitamin C, HPLC, analytical validation, control quality

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Development and validation of two methods for the determination of magnesium and calcium ions by UV-visible spectrophotometry in dietary supplements

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Introduction: The increasing consumption of dietary supplements worldwide, including in Tunisia, highlights the importance of verifying their quality and label accuracy, especially given the limited local regulatory framework. Magnesium and calcium, widely used minerals in supplements, were selected for this study to assess the compliance of marketed products with their declared contents.

Materials and Methods: Five magnesium-based and five calcium-based dietary supplements were analyzed. Quantification of magnesium and calcium was performed using UV-visible spectrophotometry after complexation with Eriochrome Black T at pH 10. Two analytical approaches, external calibration and standard addition, were optimized and applied. Method validation assessed specificity, linearity, precision, and accuracy according to standard criteria

Results: The method demonstrated satisfactory linearity with correlation coefficients exceeding 0.99, as well as acceptable precision and accuracy. Quantitative analysis revealed that three out of five magnesium supplements complied with their declared content, whereas for calcium, only two out of five products met the specifications. Significant discrepancies were observed between labeled and measured values, with some products deviating markedly from the acceptable ranges, indicating inconsistencies in formulation quality. **Conclusion:** This study confirms the relevance of UV-visible spectrophotometry for the quality control of magnesium and calcium in dietary supplements. The findings emphasize the need for stricter regulatory measures to ensure the safety, transparency, and reliability of supplements marketed in Tunisia.

Key words: Magnesium, Calcium, Dietary supplements, UV-Visible spectrophotometry, Quality control

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Development and Validation of a Glassware Cleaning Protocol in a Pharmaceutical Quality Control Laboratory

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Introduction: In a pharmaceutical quality control laboratory, achieving precision is crucial to ensure reliable results. The validation of the cleaning methods ensures that analysis methods are implemented with clean glassware to mitigate cross-contamination(1). In this context, the aim of this study is to develop and validate a glassware cleaning protocol.

Materials and Methods: This study was conducted in the quality control laboratory. It involved the development of a glassware cleaning protocol followed by its validation. Initially, worst-case scenarios were identified, including defining the "worst case" molecule (in this case, trihexyphenidyle) and selecting difficult-to-clean glassware, such as a 100 ml flask, a 5 ml flask, a 5 ml test tube, a 2 ml pipette, and a mortar. Validation criteria included fidelity, linearity, limit of detection, and limit of quantification. After cleaning various types of glassware, rinse waters were sampled for trihexyphenidyle quantification via liquid chromatography.

Results: Among the validation criteria for the trihexyphenidyle trace dosage method after glassware cleaning, linearity was assessed by measuring the areas of five test solutions at concentrations of 0.2 ppm, 1 ppm, 10 ppm, 50 ppm, and 100 ppm. A linear curve was obtained with a correlation coefficient of 0.998. The precision of the study was conducted by modifying the operator witch revealed a coefficient of variation (RSD) of 0.83%. The method's detection and quantification limits were established at 0.984 µg/ml and 2.896 µg/ml, respectively. By varying the detergent concentration during the washing process, a non-detectable concentration of trihexyphenidyle was achieved for all tested glassware.

Conclusion: The results of this study confirm that the glassware cleaning method, as described in the established protocol, meets the defined acceptance criteria. The cleaning protocol confirms its effectiveness, thus ensuring the integrity of future analyses.

Keywords: *Glassware Cleaning; method validation; Analytical Control.*

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Efficient Green Hydrogen generation via Catalytic Hydrazine-Assisted Water Splitting Using PEDOT:PSS-Stabilized Lithium Ferrite Porous Nanostructures Decorated with MoS_2 Quantum Dots

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Green hydrogen production through sustainable water splitting is a promising strategy for clean energy generation [1]. In this study, we demonstrate an efficient hydrazine-assisted water splitting system using a novel porous lithium ferrite ($LiFeO_2$) nanostructure stabilized with poly(3,4-ethylenedioxythiophene):polystyrene sulfonate (PEDOT:PSS) and decorated with molybdenum disulfide (MoS_2) quantum dots (QDs) as a high-performance catalyst. The PEDOT:PSS matrix enhances structural stability and charge transport, while the MoS_2 QDs provide abundant active sites for hydrogen evolution. The synergistic effects between the conductive polymer, lithium ferrite, and quantum dots result in significantly improved catalytic activity and durability [2]. The electrcatalyst was characterized through microscopic (SEM), spectroscopic (Raman, IR), and structural (XRD) analyses, alongside electrochemical impedance spectroscopy, confirming its optimized morphology, chemical stability, and charge-transfer properties. Electrochemical studies revealed exceptional bifunctional activity, with low overpotentials for both the hydrogen evolution reaction (HER) and hydrazine oxidation reaction (HzOR).

Key words: Green hydrogen, electrocatalytic platform, hydrazine-assisted water splitting, synergetic nanocomposites.

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CeO_2 Quantum Dot-Decorated PEDOT:PSS-Lithium Ferrite Porous Nanostructures for High-Sensitivity Electrocatalytic Detection of Pesticides

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The escalating need for pesticide monitoring in environmental and agricultural systems demands advanced electrocatalytic sensing platforms [1]. In this work, we present a high-performance electrochemical sensor based on *CeO_2 quantum dot-decorated PEDOT:PSS-stabilized lithium ferrite ($LiFeO_2$) porous nanostructures* for the ultrasensitive detection of imidacloprid and methyl parathion pesticides. The synergistic interplay between the conductive PEDOT:PSS matrix, redox-active $LiFeO_2$, and catalytically efficient CeO_2 quantum dots enables enhanced electron transfer and pesticide reduction [2]. Comprehensive characterization (SEM, XRD, Raman, EIS) confirms the nanohybrid's porous morphology, structural stability, and tailored electronic properties. Electrochemical studies reveal exceptional sensitivity, a low detection limit (9.7 nM), and robust anti-interference capability for target pesticides. The platform's reproducibility (RSD < 3.6%) and recovery rates (~97.3–103.8% in real samples) underscore its viability for on-field environmental monitoring.

Key words: electrocatalysis, electrochemical sensing, pesticide, synergetic nanocomposites.

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Electrochemical CuO Sensor for H_2O_2 Detection and MgO Nanoparticle Remediation in Drought-Stressed Oat

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Drought stress is a major abiotic factor limiting plant growth, development, and yield, with one of its earliest physiological effects being the accumulation of reactive oxygen species (ROS), particularly hydrogen peroxide (H_2O_2). Elevated H_2O_2 levels can trigger oxidative damage but also act as signaling molecules in stress responses. This study presents a dual approach for monitoring and mitigation of drought-induced oxidative stress in oat (*Avena sativa*). A nanostructured copper oxide (CuO) electrode was fabricated via hydrothermal synthesis for sensitive electrochemical detection of H_2O_2. The morphology and crystallinity of the CuO nanostructures were characterized by scanning electron microscopy (SEM) and X-ray diffraction (XRD), while cyclic voltammetry (CV) and differential pulse voltammetry (DPV) confirmed their favorable electrochemical properties. In parallel, magnesium oxide (MgO) nanoparticles (NPs) were applied to drought-stressed oat plants to evaluate their potential in oxidative stress alleviation. Results demonstrated that MgO NP treatment significantly reduced H_2O_2 accumulation, likely through ROS modulation and magnesium-mediated enhancement of chlorophyll biosynthesis and photosynthetic performance. The developed CuO-based sensor exhibited high sensitivity, a nanomolar detection limit, and a wide linear range, effectively distinguishing between treated and untreated samples. This work underscores the synergistic potential of CuO nanostructure-based electrochemical sensing and MgO nanoparticle treatment for precision plant stress diagnostics and management.

Acknowledgement: Activity 1.1.1.9 "Post-doctoral Research" of the Specific Objective 1.1.1 "Strengthening research and innovative capacities and introduction of advanced technologies in the common R&D system" of the European Union's Cohesion Policy Programme for 2021-2027 research application No 1.1.1.9/LZP/1/24/185 *"Development of Electrochemical Multisensor System for Biomarker Detection (EMS-Bio)"*

Key words: electrochemical sensor, H_2O_2, nanostructures, oxidative stress

Effect of cyclodextrin on acidic and thermal denaturation of Cytochrome *c*

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This study investigates the effects of cyclodextrin (CyD), particularly Methyl-β-CyD, on the structural stability of cytochrome *c* (cyt *c*) as model protein. CyD is known to include hydrophobic molecules and can disrupt hydrophobic interactions vital for protein folding. Using circular dichroism (CD) spectroscopy, the thermal and acidic denaturation of cyt *c* in the presence of various concentrations of Methyl-β-CyD wave measured. Thermal midpoint temperature (T_m), binding constants, the difference in number of bound CyD (Δn), and secondary structure changes were analyzed. The CyD concentration increased, *T*m shifted to lower temperatures, indicating destabilization of the native state. CD spectra also showed a transition from α-helical structures to random coils with temperature increase. Nonlinear least-squares fitting revealed K values of 15~18 M^{-1} and $\Delta n = 4.3$ at 0.5 mM HCl, while at 1.0 mM HCl, K increased to 35~52 M^{-1} and Δn decreased to 1.8. These results suggest stronger binding of CyD to the native state at lower pH. Acid denaturation also showed decreased midpoint concentration with increasing CyD, indicating similar destabilizing effects. The Gibbs free energy change (ΔG_0°) indicated a destabilization of 43.5 kJ mol^{-1} at 20% CyD. The findings suggest CyD significantly destabilizes both thermally and acid-induced unfolded states of cyt c, depending on concentration and pH.

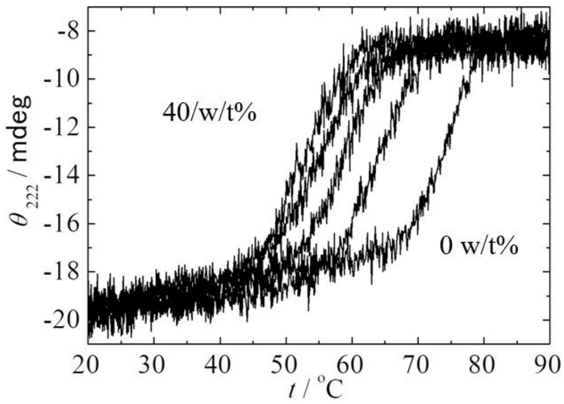

Fig. 1 Temperature dependence of θ_{222} of cyt *c* in Me-β-CyD solutions.

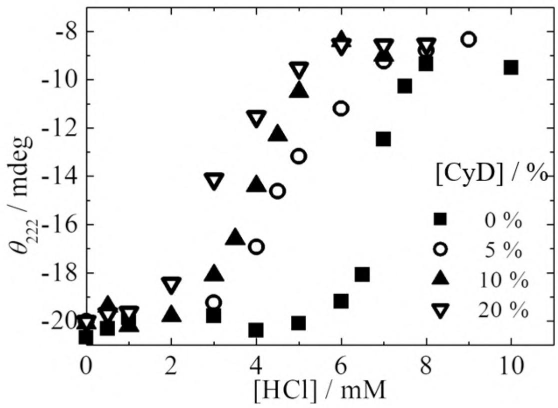

Fig. 2 Dependence of HCl concentration on the $\boldsymbol{\theta}_{222}$ of cyt *c* in Me-β-CyD solutions.

Key words: Cytochrome *c*, Cyclodextrin, Acidic denaturation,

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Preferential solvation of lysozyme in aqueous Deep eutectic solvent solutions

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In aqueous solutions containing additives, the local concentrations of components around the protein are unevenly distributed according to their affinities for the protein, a phenomenon known as preferential solvation. In the case of proteins, such selective distribution of additives around the protein surface is closely related to their effects on protein stability, often by altering the local solvation environment and influencing protein–solvent interactions. In this study, the preferential solvation number was calculated based on the concentration dependence of the protein in ternary systems, and the effect of additives on protein stability was investigated.

Lysozyme was used at concentrations ranging from 0.3% to 0.8%, and the density and viscosity of mixed aqueous solutions of water and DES (1 M and 2 M) were measured to calculate the partial specific volume. The results showed that the partial specific volume was larger in DES solutions, indicating a smaller volume decrease due to hydration. Preferential solvation was observed in the 2 M DES aqueous solution, with a preferential solvation number of +0.724 mol/mol. Furthermore, circular dichroism (CD) spectroscopy confirmed that lysozyme retained its native structure even in the presence of DES. Further investigations at higher DES concentrations are planned.

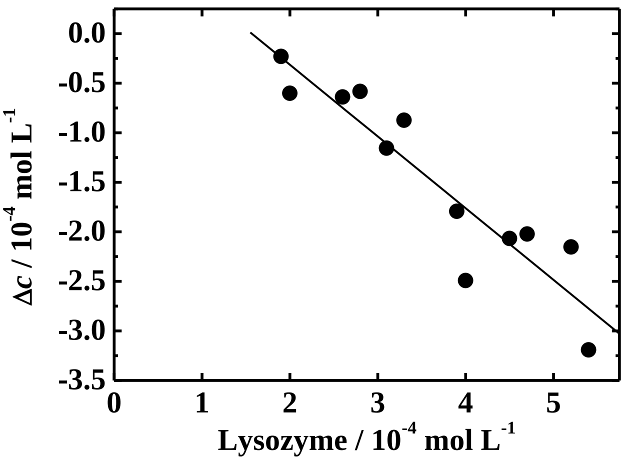

Fig. 1 Relationship between Lysozyme concentration and bulk concentration

Key words: Lysozyme, DES, partial specific volume, preferential solvation number

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Synthesis of Multifunctional Ternary Au@ZnO/α-Fe_2O_3 Nanocomposite for Organic Pollutant Removal

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This study presents the synthesis of multifunctional Au@ZnO/α-Fe_2O_3 ternary nanocomposites via a rapid and straightforward solvothermal method. The developed approach enables the formation of well-dispersed Au@ZnO/α-Fe_2O_3 heterojunctions without the use of ligands, bases, or surfactants. Dimethyl sulfoxide (DMSO) is believed to play a key role in directing nanostructure growth during the synthesis. Structural and optical characterizations were conducted using XRD, TEM, UV–Vis spectroscopy, photoluminescence (PL), BET surface area analysis, and XPS. The photocatalytic activity of the synthesized nanocomposites was evaluated under optimized UV irradiation conditions, focusing on the degradation of methylene blue and diuron pesticide. The results demonstrated excellent photocatalytic performance, with rate constants (k) of 28.35×10^{-3} min^{-1} for MB and 17.48×10^{-3} min^{-1} for diuron. These findings underline the strong potential of the Au@ZnO/α-Fe_2O_3 nanocomposite for environmental applications, particularly in wastewater treatment and organic pollutant removal.

Key words: Au@ZnO/α-Fe_2O_3, Photocatalysis, Methylene blue, Diuron, Environmental applications

Magnetic ferrite nanoparticles for the removal of textile dyes

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Magnetic ferrite nanoparticles were successfully synthesized and evaluated as efficient photocatalysts for the degradation of textile dyes under UV-irradiation. The structural integrity and phase composition of the synthesized materials were confirmed by X-ray diffraction (XRD), while Fourier-transform infrared spectroscopy (FTIR) provided insight into the chemical bonding and surface functionalities. The optical properties, including light absorption behavior, were investigated through UV–Vis diffuse reflectance spectroscopy, revealing suitable band gap values for photocatalytic applications.

The photocatalytic activity was assessed using methylene blue (MB) as a representative dye pollutant. The influence of key operational parameters such as pH and irradiation time was systematically studied. Notably, under neutral pH conditions, more than 90% of the dye was degraded within just a few minutes of exposure, highlighting the rapid and effective performance of the catalyst. These results underline the potential of the synthesized magnetic ferrite nanoparticles as a promising material for practical wastewater treatment, particularly for the rapid removal of dye contaminants under UV light.

Key words: Magnetic ferrite nanoparticles, Photocatalysis, Textile dye degradation.

Stabilization study of sodium metamizole in aqueous medium by intercalation into layered double hydroxides

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Sodium metamizole is a well-known oral non-steroidal anti-inflammatory drug, yet it is little known that it is not stable in aqueous media. Under the influence of water and dissolved oxygen, the C-S bond is hydrolysed (and oxidized) and $NaSO_3$ units are broken off from the molecule [1], which does not reduce the drug content, but significantly impairs the water solubility and thus the bioavailability.

Layered double hydroxides (LDHs) known as anionic, lamellar solids composed of positively charged layers and anions hydrated between them. They can be represented by the $[M(II)_{1-x}M(III)_x(OH)_2]^{x+}[A^{m-}_{x/m}\bullet nH_2O)]^{x-}$ formula, where M(II) and M(III) are di- and trivalent metal ions, x= M(III)/[M(II)+M(III)] and A^{m-} stands for the interlayer anions [2]. The incorporation (intercalation) of drug molecules into the interlayer space of LDHs has several advantages, such as controlled and highly dispersed release, increased water solubility and thus bioavailability of drug molecules, economical production and safe handling.

In this work, we investigated the intercalation of metamizole anions into highly biocompatible MgFe and CaFe LDHs. To this end, several synthesis techniques were utilized, such as co-precipitation, direct anion exchange, dehydration-rehydration and even a specific mechanochemically-assisted route. The results showed that the inhibition of hydrolysis of metamizole was key to obtaining by-product-free LDH systems. However, other aspects (molecule size, parameters of the technique used) also influenced the success of intercalation.

Key words: metamizol, layered double hydroxide, intercalation, stabilization

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Thermodynamic investigation of the interaction between lipid bilayers and βLG using ITC

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Phospholipids are amphiphilic molecules with both hydrophilic and hydrophobic groups, assembling into lipid bilayers (vesicles) in water. [1] Previous studies have reported that the structure of certain proteins changes from β-sheet to α-helix upon binding to the lipid bilayer. In this study, we use isothermal titration calorimetry (ITC) to measure the heat of mixing between lipid bilayers and proteins.

The solutions were prepared by dissolving 1,2-dimyristoyl-sn-glycero-3-phosphocholine (DMPC) and β-lactoglobulin with water, respectively. Calorimetry was performed using MCS-ITC (Malvern) with β-lactoglobulin solution in the syringe side and DMPC solution in the sample cell, titrating 10.021 μL 15 times each at 30°C.

ITC measurements were performed using a DMPC solution concentration of 1.017 mM and a β-lactoglobulin solution concentration of 0.611 mM to obtain a final molar ratio of [DMPC]:[β-lactoglobulin]=200:1. Fig. 1 shows the heat of mixing per mol of β-lactoglobulin in one titration. ΔH initially shows endothermic behavior, but as the molar ratio increases, it changes to exothermic.

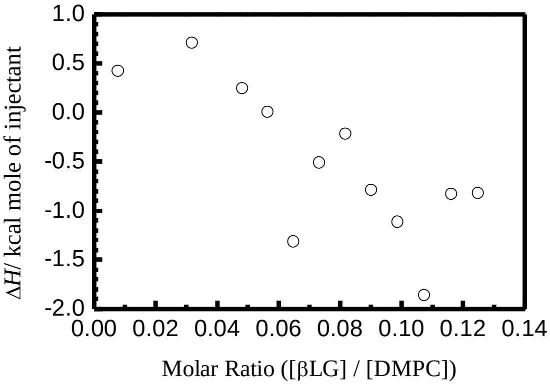

Fig. 1 Heat of mixing DMPC and βLG for each molar ratio of βLG in the heat of mixing DMPC and βLG

Key words: Lipid bilayer, ITC, β-lactoglobulin , DMPC

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Identifying Species in Imidazolium Chloride-Based Ionic Liquid with ε-Caprolactone via Excess Infrared Spectroscopy

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Studying the molecular interactions and solution microstructure of IL-ester binary systems is helpful to understand the activation mechanism of C=O/C-O and the catalytic reaction mechanisms. In this work, we selected ε-caprolactone (ε-CL) as the monomer model molecule for polyester, and we chose 1-ethyl-3-methylimidazolium chloride (EMImCl) ionic liquid. Using excess infrared spectroscopy and quantum chemical calculations, we systematically investigated the intermolecular interactions and microheterogeneity in the binary system and identified six aggregate structures in the solutions. For the identified species [$Cl^-(CL)_4$, $EMImCl(CL)_3$, $EMIm^+(CL)_2$ and $(EMIm)_2(Cl)_2CL$], the alkoxy bond lengths of ε-CL are all longer than that of ε-CL monomer, while the acyl C–O bond lengths are all shorter. At the same time, the alkoxy C and the carbonyl C in ionic liquid-ester clusters exhibit higher positive charge density than those in the pure ester, suggesting their preferential susceptibility to halide anion attack in the catalytic hydrolysis process. This is consistent with the experimental results of the cleavage of the polyester alkoxy bond. [标文献] Our findings would provide deeper insights into the reaction mechanism of this class of polyester catalytic process.

Key words: Excess spectroscopy, Solution structure, Ionic liquids, Polyester hydrolysis

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An innovative nanoparticle modified carbon paste micro-sensor for ultrasensitive and selective detection of ciprofloxacin in environmental

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Ciprofloxacin (CIP) is a fluoroquinolone synthetic antibiotic, it is the top five generic antibiotic manufactured worldwide, and the most prescribed drug for humans and animals [1]. CIP is widely used to treat infectious diseases in livestock, poultry, urinary tract infections, pneumonia, gastrointestinal, skin infections and sexually transmitted diseases in humans [2, 3]. However, higher consumption of CIP can lead to various and serious side effects. Furthermore, the presence of CIP in the environment is of great concern due to the potential emergence of antibiotic-resistant bacteria [4]. Therefore, the development of fast, sensitive, and efficient techniques to monitor CIP levels in is necessary to ensure the protection of the human health.

In this context, we present a simple, economical, selective and sensitive electrochemical sensor for the quantification of ciprofloxacin in water samples without any pretreatment step of real samples, using of a micro-cavity electrode integrated nanostructured material. The analysis was performed and validated after optimization of operating conditions in environmental water samples and the results showed a good accuracy (less than 3 %) with a satisfactory recovery (less than 7 %), indicating the absence of interference effects of the water matrix. Therefore, the proposed electrochemical sensor is a potential candidate for the determination of ciprofloxacin in water matrices.

Key words: ciprofloxacin, microsensor, electrochemical detection, water

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Dependence of alkyl chain length of ionic liquids on the thermal stability of Cytochrome *c*

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Ionic liquids have both hydrophobic and ionic parts and are effective model co-solvents for clarifying the effects of hydrophobic and electrostatic interactions on the mechanism of protein conformation. We have systematically shown that the thermal stability of Lysozyme is decreased by the ionic liquid addition and the effects of each alkyl chain and ionic part [1]. In this study, we systematically clarify the thermal unstable effect on bovine Cytochrome *c* by changing the alkyl chain length of 1-alkyl-3-methylimidazolium Chloride ($[C_nMIM][Cl]$). VP-DSC (Malvern) was used to determine the denaturation midpoint temperature T_m, the enthalpy change of denaturation ΔH_m, and the width at half maximum $T_{1/2}$ of Cytochrome *c* (0.1 w/v %) in aqueous ionic liquid solutions at a temperature increase rate of 1 °C/min.

Fig. 1 shows the DSC results of Cytochrome *c* in aqueous solutions (mole fractions $x = 0$, 0.0015, 0.003, 0.005, 0.007) of ionic liquids $n = 6$, 8, 10. As the alkyl chain length increases, T_m and ΔH_m show a decreasing trend, while $T_{1/2}$ shows an increasing trend, indicating that the unstable effect increases with increasing alkyl chain length. The dependence on alkyl chain length of binding constant and difference of ionic liquids and Cytochrome *c* will be determined by the dependent mole fraction at each chain length, then discuss the role of hydrophobic interactions on the stability of the protein.

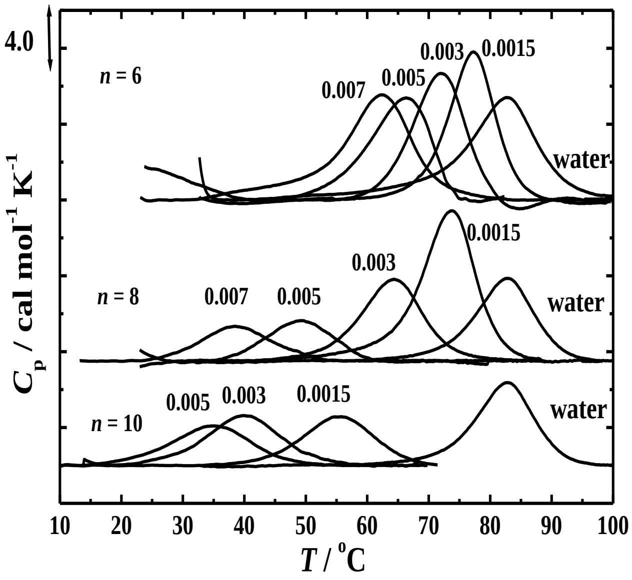

Fig 1. DSC curve for each alkyl chain length for mole fractions 0 ~ 0.007

Key words: Ionic liquids, Cytochrome *c*, hydrophobic interaction

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Effects of Ionic Liquid Types on the Structure and Thermal Properties of Different Silk Fibroin

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Ionic liquids, distinguished by their commendable environmental sustainability, tailorability, and versatile properties, open up considerable prospects in the realms of advanced biotissue engineering, pharmaceuticals, and energy-related materials. Employing ionic liquids as solvents for silk fibroin has emerged as an efficacious approach, offering substantial improvements over traditional preparation methods by streamlining the process, curtailing time expenditure, and mitigating environmental impact, while concurrently augmenting the biomaterial's physicochemical traits. This investigation assesses the viability of fabricating regenerated silk fibroin membranes with an array of imidazole-based ionic liquids. In-depth solubility analysis of silk fibroin within these solvents was conducted via solution microcalorimetry, complemented by quantitative assessments of protein-ionic liquid interactions utilizing thermodynamic metrics and Fourier transform infrared spectroscopy. The findings indicate that the dissolution of silk fibroin in ionic liquids is characterized as an exothermic and orderly process, which is emphatically shaped by the constituent anions and cations of the employed ionic liquids. These ions are pivotal in dictating the β-sheet content and influencing the regenerative film's physical attributes. Notably, ionic liquids enriched with $[EMIM]^+$ cations bolster the tensile resilience and thermal stability of silk fibroin films due to their enhanced molecular interactions. Moreover, ionic liquids containing acetic anions (Ac^-) demonstrated exemplary cell compatibility. These pivotal insights contribute valuable knowledge for the development of innovative biomaterials and the fabrication of high-performance regenerated silk fibroin membranes, thereby facilitating progress in the field of biomedical material applications.

Keywords: Ionic liquid, fibroin protein, solution calorimetry, β-sheet, interaction

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A Hybrid Computational Framework for Excess Infrared Spectral Decomposition in Tert-Butanol - Carbon Tetrachloride Solutions

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Excess infrared spectroscopy [1] provides molecular-level insights into solution structure by identifying various interacting species [2-3]. Assigning peaks in excess infrared spectra is a challenging task in practical solution studies. This work proposes a method that combines molecular dynamics (MD) simulations with large-scale quantum chemical calculations to identify excess infrared spectra. The proposed approach assigns each peak in the excess spectrum of the tert-butanol-carbon tetrachloride (TBA-CCl_4) binary solution It interprets the significance of positive and negative peaks in terms of changes in aggregate proportions. Analysis of the spectral contributions from different clusters indicates that the monomer fraction increases significantly with rising X_{CCl4}. The fractions of dimers and trimers decrease more slowly, while larger clusters gradually diminish. Further calculations based on the theoretical formula of excess spectroscopy reveal that monomers, dimers, and trimers contribute positive excess peaks across the entire concentration range, whereas larger oligomers give rise to negative peaks. This finding validates the experimental observation that the excess signals arise from the growing presence of smaller clusters and the reduction of larger clusters upon dilution. The study also highlights the complexity of excess spectral features: each sub-peak results from overlapping infrared absorptions of multiple clusters, rather than being attributed to a single species. These results provide a robust theoretical framework for analysing species distributions in solution. They enhance the accuracy of excess peak assignment and establish a solid scientific foundation for applying excess spectroscopy in a wide range of solution systems.

Key words: Excess infrared spectroscopy, Molecular dynamic simulation

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Thermodynamic study of cyclodextrin-protein interaction by titration calorimetry

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Cyclodextrin (CD) is a cyclic oligosaccharide that forms inclusion complexes by incorporating hydrophobic substances into its intramolecular cavity. When CD was added to proteins in solution, the midpoint temperature (T_m) for the thermal denaturation of protein decreased in a CD concentration.[1] This effect is considered to result from the preferential inclusion of hydrophobic side chains, which become exposed during protein denaturation, by CD. As a consequence, CD is believed to exhibit a higher binding affinity for the denatured state of the protein than for the native state; however, this preferential binding mechanism has not been directly measured. In this study, we aim to directly elucidate the thermal destabilization of proteins by using isothermal titration calorimetry (ITC).

We used the displacement method, which is used to determine thermodynamic parameters for weakly bound systems, because the obtained inclusion enthalpy was too small. In this method, a guest molecule (e.g., pentanol) that binds more strongly to CD is added to a system in which a weak complex (CD + lysozyme) has already formed. The thermodynamic parameters related to the weak interaction are then derived from the apparent changes in the thermodynamic quantities of the stronger interaction (guest molecule + CD). The measurements were conducted at six different temperatures, and the thermodynamic parameters was evaluated to investigate the effect of CD inclusion on the thermal stability of lysozyme.

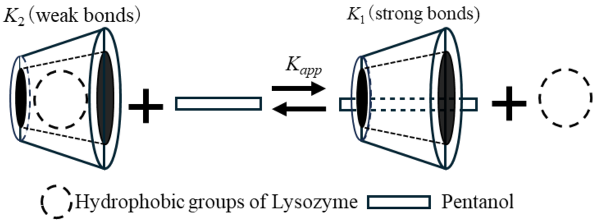

Fig.1 Model of displacement method.

Key words: Lysozyme, Cyclodextrin, ITC, Displacement method, Protein Stability

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Control of Iron-Based Dietary Supplements Using Flame Atomic Absorption Spectrophotometry

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Introduction: Iron is an essential trace element frequently consumed as a dietary supplement, often without medical supervision. This study aims to assess the quality of iron-containing dietary supplements using flame atomic absorption spectrophotometry (FAAS), following the development and validation of an analytical method.

Methods: Three dietary supplement samples were analyzed. After an optimized mineralization process based on a one-variable-at-a-time approach, the method was validated according to SFSTP standards (specificity, linearity, accuracy, precision). Quality controls included mass uniformity testing, global dosage determination, and individual unit dosage by FAAS.

Results: The optimized mineralization yielded over 90% efficiency under more environmentally friendly conditions. The method showed satisfactory linearity between 2.4 and 5.6 ppm ($r = 0.995$), high precision ($CV < 2\%$), and good accuracy (recovery rate between 98.2% and 104%). All three supplements complied with pharmacopeial standards for mass uniformity, iron content (90%-125% of labeled claim), and individual unit dosage. **Conclusion:** The tested supplements met quality criteria for iron content. Broader studies are needed to assess market-wide compliance.

Key words: Iron supplements, Quality control, Flame atomic absorption spectrophotometry, Method validation

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Control of Zinc-Based Dietary Supplements Using Flame Atomic Absorption Spectrophotometry (FAAS)

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Introduction: The growing use of zinc by consumers to improve well-being has raised concerns regarding the quality of such products. This study aims to assess the quality of zinc-containing dietary supplements using flame atomic absorption spectrophotometry (FAAS), following the development and validation of a dedicated analytical method. **Materials and Methods:** Nine zinc-containing dietary supplements were collected for analysis. Samples underwent a mineralization process. Method validation was performed according to SFSTP standards, evaluating specificity, linearity, accuracy, and precision. Subsequently, the supplements were subjected to thorough quality controls, including mass uniformity, global dosage determination by FAAS, and individual unit dosage.

Results and Discussion:

Optimal mineralization parameters were established (10 mL HNO_3, 4 mL HCl, agitation for 1 hour at controlled temperature). The FAAS method demonstrated good linearity between 0.6 and 1.4 ppm ($r = 0.992$), satisfactory precision ($CV < 2\%$), and recovery rates between 97.7% and 102.4%. However, the majority of locally manufactured samples (5 out of 7) failed quality control tests, raising concerns about product reliability. Significant variability in zinc content was observed.

Conclusion: This study highlights the need to implement systematic quality control measures for dietary supplements marketed in Tunisia. Strengthening regulatory oversight is essential to ensure product safety and reinforce confidence in the national health sector.

Key words: Zinc supplements, Quality control, Flame atomic absorption spectrophotometry, Method validation

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Efficient Beer-Lamber law for analyzing hybrid materials in sunscreen creams

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Prolonged exposure to solar ultraviolet (UV) radiation is a major factor in skin aging, erythema, and skin cancers whose mortality rate continues to rise [1]. In response to these challenges, solution chemistry is increasingly focused on the design of innovative UV hybrid filters. Normally, the transmittance of sunscreens and/or hybrid filters is quantified with diffuse reflectance spectroscopy in the solid-state [2]. In this study, the photoprotective potential of different oxides doped with benzanilide (BZ) against UV-A and UV-B radiations were evaluated in aqueous solution.

Table 1: Transmittance of commercial and prepared sunscreens. Cream concentration: 0.66 g L^{-1}

Sunscreen	**Transmittance at 400 nm (UV-A)**	**Transmittance at 320 nm (UV-A)**
Commercial sunscreen	38 %	29 %
Our formulated sunscreen: 0.2 *wt.* % of BZ/kaolin	60 %	57 %
Our formulated sunscreen: 0.2 *wt.* % of BZ/zeolite	30 %	24 %
Our formulated sunscreen: 0.2 *wt.* % of BZ/Al_2O_3	55 %	52 %
Placebo (No UV filter)	69 %	55 %

The results compiled in Table 1 indicate that the sunscreen containing 0.2 *wt.* % of zeolite doped with BZ is efficient against UV radiations. The affinity of BZ towards kaolin and alumina is low, due to their textural properties. In this study, we realized that the photoprotective properties of sunscreens could be elucidated by UV/Vis spectrophotometry instead of experiences involving animals (mouse, rats, *etc*.). In this context, (*i*) choosing the appropriate dilution factor and (*ii*) dispersing the hybrid filter (or sunscreen) in the appropriate (and inert) solvent before transmittance measurement are crucial steps.

Keywords: Sunscreen, hybrid filter, UV/Vis spectrophotometry, Transmittance

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