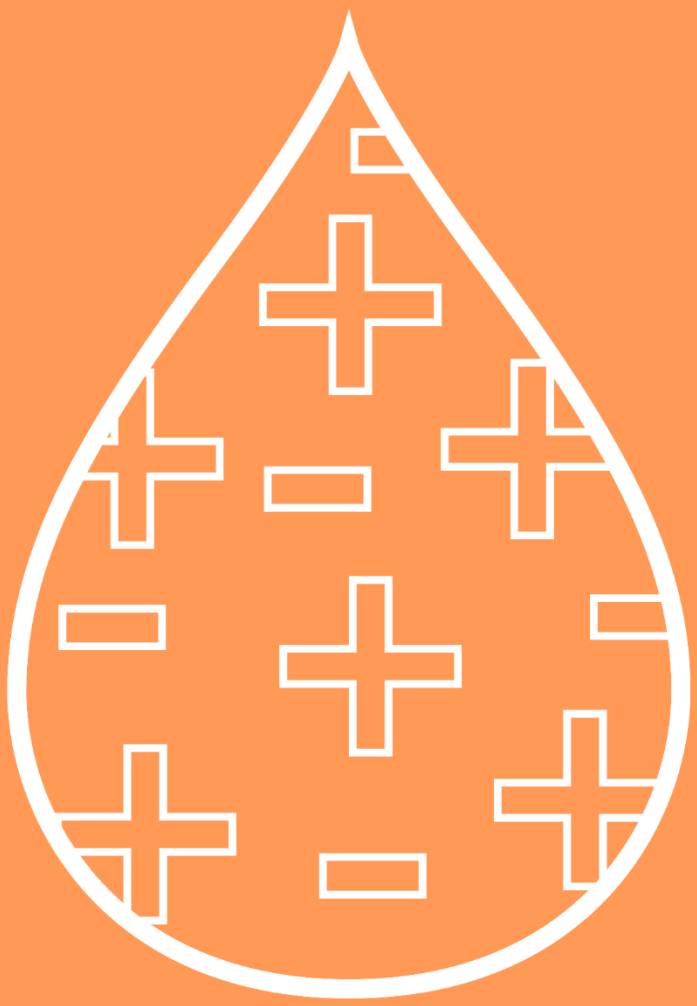

2026 EUCHEMSIL

30th EUChemS Conference on Molten Salts and Ionic Liquids

26th - 31st July 2026
Cambridge, UK

RSC DISCUSSION GROUP
MOLTEN SALTS
AND IONIC LIQUIDS

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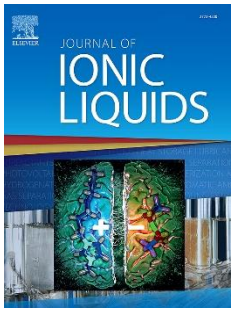

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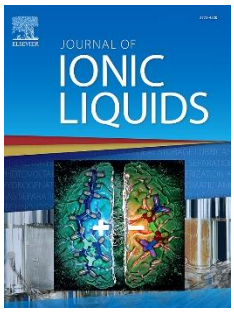

This meeting was organised by the Royal Society of Chemistry Molten Salts and Ionic Liquids Discussion Group (MSILDG) with support from the Royal Society of Chemistry. For more information visit www.msildg.org.

Welcome

Dear Colleagues and Friends,

It is our great pleasure to welcome you to **30th EUCHEMSIL 2026** in Cambridge. We are delighted to bring together around **150 participants from 31 countries**, reflecting the truly international and collaborative nature of the molten salts, ionic liquids, deep eutectic solvents, and related liquids community. Over the coming week, we look forward to vibrant scientific discussions, the exchange of new ideas, the forging of new collaborations, and the strengthening of existing friendships.

Whether you are attending EUCHEMSIL for the first time or are a regular participant in this historic conference series, we hope you find the programme stimulating, inspiring, and enjoyable. We thank you for joining us and wish you a productive and memorable stay in Cambridge.

Dr Agi Brandt-Talbot
Imperial College London
Co-Chair, EUCHEMSIL 2026

Dr Ian McPherson
Loughborough University
Co-Chair, EUCHEMSIL 2026

History of the Conference

Welcome to Cambridge for the EUCHEMSIL 2026 conference. This series conference has arrived at its 30th edition, whilst I still remember the 17th edition in Porquerolles, France,1998 when my poster on carbon nanotubes and nano-eggs from molten salts won the first poster prize. (A senior asked me where the nano-chicken was in front of the poster!).

By then, the conference name was the 17th EUCHEM Conference on Molten Salts 1998, shortened as EUCHEM 1998, although there were quite many talks and posters on ionic liquids. I do not remember anyone talking about the inclusion of ionic liquids into the conference name until 2006 when the conference name was edited as the 21st EUCHEM Conference on Molten Salts and Ionic Liquids, Tunisia, 2006.

It was in this edition when a quite interesting discussion proceeded on new names that can merge molten salts, ionic liquids and other ionic media. Several suggestions were discussed whilst, to my knowledge, only “liquid salts” and “Columbic fluids” are still in use in the literature. In the past decade or so, particularly since the name change of the group from MSDG to MSILDG in 2019, efforts have been ongoing to define the scope of the group. It comes gradually to a consensus that “any liquid containing more than 50% of ions by mass falls in the scope”. Then, what name could best describe such liquid media? As the organiser of the EUCHEMSIL 2026, the MSILDG has used “liquid salts” in the official conference webpages of EUCHEMSIL 2026. Fluid is not selected because it covers both liquids and gases.

The aim is mainly to make the conference as inclusive as possible in terms of topics and areas. In other words, the EUCHEMSIL 2026 covers research in and beyond molten salts and ionic liquids, such as deep eutectic solvents and water (solvent)-in-salts. I believe the use of liquid salts can help bridge research efforts and developments in different ionic media for fundamental and applied purposes. I hope you will agree with the MSILDG on promoting the use of liquid salts as a collective name for all ionic media, and enjoy the EUCHEMSIL 2026 in the beautiful English summer in Cambridge.

Prof. George Chen

Chair of MSILDG and EUCHEM 2026 Scientific Committee

Organising Committee

EUCHEMSIL 2026 is organised by the Royal Society of Chemistry's Molten Salts and Ionic Liquids Discussion Group (MSILDG). The group has been active for over 5 decades and has a long history with the EUCHEMS meetings, having organised meetings previously in 1972 and 1988. The group exists for the advancement of work on molten salts, ionic liquids and related materials, and to foster and encourage the dissemination of chemical information by holding scientific meetings.

The organising committee consists of:

Prof. George Chen (MSILDG Chair, Scientific Committee chair)

University of Nottingham

Dr Ian McPherson (MSILDG Secretary, EUCHEMSIL co-chair)

Loughborough University

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(Imperial College London, UK)

Program

26th Jul 2026 – Wolfson Hall

16:00 - 18:00	**Registration**
18:00 - 19:30	**Welcome Reception** Prof Agi Brandt-Talbot, Dr Ian McPherson

27th Jul 2026 - Wolfson Hall

08:30 - 09:00	**Tea and Coffee**
09:00 - 09:15	**Welcome**
09:15 - 10:00	**Plenary** **[01] Ionic liquids in nano-confinement: layers, bilayers, packing and interference** Susan Perkin
10:05 - 11:05	**Session 1** **[03] Porous Silicon Anodes Derived from Molten Salt Dealloying of $CaSi_2$for Lithium-Ion Batteries** Bing Li **[04] Proton Transfer Mechanisms in Protic Ionic Liquids: A Machine-Learning Force Field Study** Miguel A. Boado, Martín Otero-Lema, Ángel Míguez-Roel, Trinidad Méndez-Morales, Hadrián Montes-Campos, Luis M. Varela **[02] Realising the transition towards fluorine-free ionic liquids using functionalised cations.** Frederik Philippi, Margarida Costa Gomes, Daniel Rauber
11:05 - 11:35	**Coffee Break**
11:35 - 12:40	**Session 2** **[06] Electrolysis of regolith for simultaneous oxygen and metal production** Mathieu Gibilaro, Laurent Massot, Pierre Chamelot, Christelle Chrion **[07] Bridging Data and Prediction: Machine Learning for Ionic Liquid Properties and Sigma-Profile Viscosity Modeling** Pawan Chhipa, Dinis O. Abranches, Oliver Järvik **[05] Exploring Halogen Bonding in Ionic Liquids** Patricia Hunt, Muhammad Hashmi

12:40 - 12:50	**Sponsor Talks**
12:50 - 13:00	**Conference Photograph**
13:00 - 14:15	**Lunch**
14:20 - 14:50	**Keynote** **[08] The Applications of Molten Salts for Electrochemical Energy Storage** Kai Jiang
14:55 - 16:15	**Session 3** **[09] Theoretical and experimental approaches to reducing the melting point of new lithium salt-based systems** Alexis Colly, Pierre Chamelot, Mathieu Gibilaro, Gaëtan Buvat, Laurent Massot **[10] The influence of solutal convection on the cycling behaviour of liquid metal batteries featuring Pb-cathodes** Faezeh Nirousham, William Nash, Paolo Personnettaz, Norbert Weber, Tom Weier **[12] Oxide Chemistry in Molten Fluorides for Molten Salt Reactor Applications** Miao Shen, Yuan Qian
16:15 - 16:45	**Coffee Break**
16:45 - 18:00	**Session 4** **[13] Unlocking the Full Potential of Deep Eutectic Solvents in Synthesis** Raul Alberto Pacheco-Muiño, Vivienne Cadogan, John Stockton, Sarah Hunter, Matt Foulkes, Silvia Díez-González **[14] Thermal properties of triazolium based protic ionic liquids for thermal energy storage application.** Iqbaal Abdurrokhman, Oliver Järvik **[15] Structural and Dynamic Features of Diastereomeric (Deep) Eutectic Systems of Homochiral Components (DIADES)** Margherita Teresa Barbero, Maria Enrica Di Pietro, Maria Nicole Franchini, Grazia Isa Carla Righetti, Alessandro Mariani, Sara Rozas Azcona, Santiago Aparicio, Sahar Nasrallah, Mirjana Minceva, Andrea Mele **[16] Poly(Ionic Liquid)–Mediated Colloidal Stabilization in Low-Dielectric Media: Interplay of Ion Pairing, Steric Confinement, and Depletion Forces** Nik Nur Azreen Nik Fauzi, Jit Kang Lim, Mohamad Danial Shafiq

28th Jul 2026 - Wolfson Hall *or* Club Room

08:30 - 09:00	**Tea and Coffee**
09:00 - 09:45	**Plenary** **[17] Electrodeposition of Difficult-to-Plate Elements from High-Temperature Molten Salts** Toshiyuki Nohira, Yutaro Norikawa
09:50 - 11:10 **Wolfson Hall**	**Session 5** **[18] Ioncell® Technology: Manufacturing High-Strength Fibers for Versatile Applications** Inge Schlapp-Hackl, Herbert Sixta, Michael Hummel **[19] Composition-Controlled Ionic Liquid Biorefining of Softwood for Microfibrillated Cellulose Production** Ruihua Luo, Jason Hallett **[20] Catalytic Binary and Ternary Ionic Liquid Mixtures as reaction media for the Xylose to Furfural conversion** Salvatore Marullo, Giovanna Raia, Francesca D'Anna **[21] A sustainable and effective ethanol-free IonoSolv process for high-purity cellulose pulp production** Cariny Polesca, Jason Hallett
09:50 - 11:10 **Club Room**	**Session 6** **[22] Electrochemical Study of Salt-Metal Interactions in LiCl-KCl at 400 °C: Implications for the Corrosion of Alloys in Molten Salt Reactors** Zineb Benbraik, Marie Colmont, Sylvie Daviero-Minaud, Caroline Pirovano **[23] The Dual Role of MgCl2 on Structure–Transport Coupling in Molten Chloride Fast Reactor Fuels** Woei Jer Ng, Kateryna Goloviznina, Vincent Sarou-Kanian, Mathieu Salanne, Aydar Rakhmatullin **[24] Evaluating Cesium / Iodine Effluent Production in Pyrochemical Reprocessing Systems for Advanced Reactor Fuel Cycles** Jacob Brookhart, Guy Fredrickson, Michael Glaser, Alonzo Martinez, John Olson, Rachael Roenfeldt, Darin Snyder **[25] Plutonium(III) simulant for molten chloride salt nuclear fuel** Kateryna Goloviznina, Mathieu Salanne
11:10 - 11:40	**Coffee Break**

11:40 - 13:00 **Wolfson Hall**	**Session 7** **[26] Nature of electrodeposition Al-Mn from molten salts** Sreesvarna Bhaskaramohan, M. J. N. V. Prasad, G. V. D. Jonnalagadda, Sankara Sarma V Tatiparti **[27] Recovery of Rhenium from Spent Ni-based Superalloy through Molten Salt Processing** Kaixin Liu, Xiao Yang **[29] Behaviour of oxidizing elements in the molten salt NaCl-CaCl2 (600°C) using SmCl3/SmCl2 system** Marc Cabrières, Céline Cannes, David Rodrigue, Charly Carrière, Sylvie Delpech **[28] Synthesis of cerium oxide nanoparticles by thermal decomposition of cerium oxalate in molten salts** Raphaëlla Pedreira, Caroline Pirovano, Elisa Capelli, Marie Colmont, Murielle Rivenet
11:40 - 13:00 **Club Room**	**Session 8** **[30] Simulation of energy storage materials: Applications to solid electrolytes interfaces and proton transfer** Luis M. Varela, Martín Otero-Lema, Trinidad Méndez-Morales, Hadrian Montes-Campos **[31] Graphene oxide–Ionic Liquid Composites : From Molecular Design to 3D Electrode Architectures** Alexandre Piton, Alexandros Ploumistos, Tharuneesan Thangavelu, Francisco Fernandes, Ana-Gabriela Porras-Guttierrez, Laurent Michot, Laurent Gaillon, Cécile Rizzi **[32] Salt–Salt Induced TFSI Biphasic Electrolytes for Membrane-Free Redox Flow Batteries** Gabriel L. Camilo, Murilo L. Alcântara, Ana M. Ferreira, João A. P. Coutinho **[33] Water-Modulated Interfacial Structure and Electrochemical Response of Ionic Liquid–Lithium Electrolytes: A Molecular Dynamics Study** Ángel Míguez-Roel, Martín Otero-Lema, Miguel Á. Boado, Raúl Lois-Cuns, Trinidad Méndez-Morales, Hadrián Montes-Campos, Luis M. Varela
13:00 - 14:15	**Lunch**
14:20 - 14:50	**Keynote** **[34] Advanced electrolytes for energy storage applications** Mega Kar

14:55 - 16:15 **Wolfson Hall**	**Session 9** **[35] Towards Fluorine-Free Electrolytes: Physicochemical Properties and Ionic Interactions in Acesulfame-Based Ionic Electrolytes** Wern Huay Mah, Jhonatan Soto Puelles, Julius Tiongson, Luke O'Dell, Fangfang Chen, Jenny Pringle **[36] Ionic liquids for electrochemical applications: Correlation between molecular structure and electrochemical stability window** Christian Silvio Pomelli, Erik Piatti, Lorenzo Guazzelli, Andrea Mezzetta, Felicia D'Andrea, Stefano Roddaro, Giorgio Tofani **[37] On the road to large scale electrolyte production for Aluminum-Ion Batteries** Samuel Lorenz, Thomas Schubert, Felix Pippert **[38] Probing electrical double layer structure in ionic liquids with the electrochemical Surface Force Balance (e-SFB)** Neave Taylor, Susan Perkin
14:55 - 16:15 **Club Room**	**Session 10** **[39] The FFC-Cambridge Electro-deoxidation Process: Synthesis of Materials and Aspects of Sustainability** Carsten Schwandt **[40] Molten salts versus organometallics for electrodeposition of Al-Mg alloys** Sankara Sarma Tatiparti, Sreesvarna Bhaskaramohan, Fereshteh Ebrahimi **[41] Technological and Industrial Progress of Recycling Secondary Tungsten Resources by Molten Salt Electrolysis** Liwen Zhang **[42] Corrosion Resistant Nickel-Chromium Alloy Generation From Dense Ionic Fluid Electrolytes** David Sconyers, Daniel Curran, Noah Cooper, Joshua Maurer
16:15 - 16:45	**Coffee Break**
16:45 - 18:45	**Poster Session**

29th Jul 2026 – Wolfson Hall

08:30 - 09:00	**Tea and Coffee**
09:00 - 09:45	**Plenary** **[43] The role(s) of deep eutectic systems towards greener technologies in life sciences** Ana Rita Duarte

09:50 - 11:10	**Session 11** **[45] Modulating Protein Folding Landscapes: The Role of Ionic Liquids in Controlling Metastable States and Kinetic Traps** Angelo M Figueiredo, Eurico J Cabrita **[46] Piperonylic acid-based ionic liquids (PAILs) as synergists for insecticide formulations** Ramana Pydi, Jennifer Bernard, Christoph Zutz, Patrick-Julian Mikuni-Mester **[44] Old Drugs, New Tricks: A New Approach to Drug Detection using Functional Ionic Liquids** Anthony Fitzpatrick **[47] Methylimidazolium ionic liquids – a new class of forever chemicals?** Matthew Wright
11:10 - 11:30	**Coffee Break**
11:30 - 11:50	**Keynote** **[48] Water-in-salts, a new family of electrolytes** Mathieu Salanne
11:50 - 13:20	**Session 12** **[49] Molecular Structure, Dynamics, and Thermodynamics of Water-in-Salt Mixtures** Ilan Shumilin, Susan Perkin **[51] Ionic liquid crystals as superior solid-state electrolytes** Shuai Tan **[52] Ion pairing restructures the electric double layer in water-in-salt electrolytes on graphite and alters capacitance** Hannah Wood, Fulu Zhou, Jan Dočkal, Martin Lísal, Filip Moučka, Sittipong Kaewmorakot, Robert Dryfe, Paola Carbone **[50] Thermoresponsive ionic liqulds endowing reversible overheating protection for lithium metal batteries** Caihong Wang
13:20 - 14:20	**Lunch**
14:20 - 17:00	**Sightseeing**

30th Jul 2026 - Wolfson Hall *or* Club Room

	Wolfson Hall
08:30 - 09:00	**Tea and Coffee**
09:00 - 09:45	**Plenary** **[53] Molten salt electrolysis of carbon dioxide** Dihua Wang
09:50 - 11:10 **Wolfson Hall**	**Session 13** **[54] Resource Recovery of Sulfate-bearing Solid Waste in Molten CaCl2** Bin Yang, Xiao Yang **[55] Removal of Rare Earth Element Impurities from LiCl-KCl Molten Salt via Oxidative Precipitation Using Gaseous and Solid Oxidants** Yalan Liu, Ziyu Liu **[56] Research progress in the separation of tungsten and cobalt by molten salt electrolysis of cemented carbide** Xiaoli Xi **[57] Electrochemical Reduction of MnO to Metallic Mn in Molten Salt: Mechanism and Oxygen Transport** Muhammad Abdullah, Zepeng Lv, Shaolong Li, Jianxun Song
09:50 - 11:10 **Club Room**	**Session 14** **[58] Compositional Control of Electrochemical Carbon Formation in Carbonate–Chloride** Haiyan Zhao, Riley Masters **[59] Probing the Effects of Current on Electrochemical Carbon Nanotube Synthesis in Molten Salt Electrolytes** Prashant Acharya, Zhixu Zhu, Anna Hankin **[60] Ionic liquids as additives and electrolytes for hydrogen generation and transport** Thomas Schubert, Boyan Iliev **[61] Molten salt-promoted Ni-Fe/Al2O3 catalyst for methane pyrolysis** Qian Xu
11:10 - 11:40	**Coffee Break**

11:40 - 13:00 **Wolfson Hall**	**Session 15** **[63] Decoupling network mechanics from ion transport in ionogels through preferential interactions** Coby J. Clarke, Richard P. Matthews, Matthew J. Palmer, kevin Butler, Claudia Almuzara Romero, Alex Brogan, Peter Licence **[62] Multifunctional Conjugated Polymers: Integrating Molecular Engineering and Ionic Liquid Processing for Next-Generation Organic Electronics** Mohammed Al-Hashimi **[64] Hydrophobic Eutectic-based Soft Materials: a Green Strategy for the Removal of Emerging Water Contaminants** Maria Enrica Di Pietro, Chiara Carotti, Gloria Nicastro, Laura Riva, Grazia Isa Carla Righetti, Arianna Rossetti, Alberto Mannu, Francesco Briatico Vangosa, Carlo Punta, Andrea Mele **[65] Low-Melting Ionic Solids for Energy and Optoelectronics: A Structural and Optical Correlation** Biswajit Bhattacharyya, Andreas Taubert
11:40 - 13:00 **Club Room**	**Session 16** **[67] Development of electrochemical sensors for in-situ free oxygen monitoring in molten chloride media for pyrochemical fuel cycle applications** Narcís Gay Villaret, Tom Breugelmans, Bart Geboes **[68] Study of a molten carbonate salt for trapping gaseous fission products from a molten salt nuclear reactor** Robin Delaire, Sylvie Delpech, Céline Cannes, David Rodrigues **[69] Machine Learning-Based Molecular Dynamics Study of f-Block Element-Containing Molten Salt Systems** Jianhui Lan **[66] Beyond Robeson, Beyond Downhill Diffusion: Molten-Salt Membranes for CO2 Capture** Greg Mutch
13:00 - 14:20	**Lunch**
14:20 - 14:50	**Keynote** **[70] Structural Heterogeneity in Ionic Liquids and Its Role in Transport** Adilson Freitas, Mariana Ramos Pereira, Miguel Alexandre Martins Nunes, José Nuno Canongia Lopes, Karina Shimizu

14:50 - 16:10 **Wolfson Hall**	**Session 17** **[71] Phosphate removal from high-phosphorus iron ore in molten CaCl2** Xiao Yang **[73] Dual chemical and physical study on the reaction between rare earths elements and molten sulfates** Mustapha Grib, Anne-Laure Rollet, Ana Gabriela Porras Gutierrez, Christian Simon, Vincent Sarou-Kanian, Sandra Ory, Delphine Talbot **[74] Microplasma electrochemical method for the extraction of critical metals from molten salts** Yuexiang Lu, Zhe Wang, Jing Chen **[72] Corrosion-Resistant Microplasma Anode Array for High-Temperature Molten Salt Electrolysis and In-Situ Analysis** Zhe Wang, Junhan Luo, Yuexiang Lu, Jing Chen
14:50 - 16:10 **Club Room**	**Session 18** **[77] AI-Screening of Ionic Liquids for Task-Specific applications** Murilo Alcantara, João Fabian, Filipe Sosa, João Coutinho **[78] Ionic liquid and solvent design for chemical recycling of plastic-containing packaging** Giacomo Damilano, Harriet Judah, Shanshan Li, Jake Nicholson, Ryan M O'Shea, Jason Hallett, Alex Brogan, Agi Brandt-Talbot **[75] How Many Neighbors? Alkali cation solvation in [BMIm][NTf_2] revealed by Raman spectroscopy** Cedric Malherbe, Aurelie Rensonnet, Gauthier Eppe **[76] Modification of ionic transport in *N*-alkyl-4-cyanopyridinium ionic liquids through formation of charge-transfer complexes with polyaromatic hydrocarbons** Aloisia King, Josh Bailey, Małgorzata Swadźba-Kwaśny, John Holbrey
16:10 - 16:40	**Coffee Break**
18:00 - 23:59	**Gala Dinner**

31st Jul 2026 – Wolfson Hall

08:30 - 09:00	**Tea and Coffee**
09:00 - 09:45	**Plenary** **[79] Charge and proton transfer in ionic liquids** Christian Schröder
09:50 - 10:30	**Session 19** **[80] The fate of the proton in protic and aprotic ionic liquids: acidity and ion transfer studied by Raman spectroscopy** Aurelie Rensonnet, Irelie Ebardo, Alyna Lange, Patricia Hunt, Andreas Taubert, Cedric Malherbe **[81] Resolving Oligomeric Anions in Carboxylic Acid–Carboxylate Systems: Proton Dynamics in Choline–Geranate** Elixabete Rezabal
10:30 - 11:00	**Keynote** **[82] TBC** Santiago Aparicio
11:00 - 11:20	**Coffee Break**
11:20 - 12:00	**Session 20** **[83] Ionic Liquid-Based Extraction of Chromium from Ferrous Alloys and Ores** Joshua Maurer, Daniel Curran, Musashi Briem, David Sconyers **[84] Chemical and Thermal Stability of Ionic Liquids for High-Temperature applications** João Vitor Fabian, Murilo Alcantara, Filipe Sosa, João Coutinho
12:00 - 12:15	**Closing Remarks**
12:15 - 13:15	**Lunch**

Abstracts

01

Ionic liquids in nano-confinement: layers, bilayers, packing and interference

Susan Perkin

Oxford University, Oxford, United Kingdom

Abstract

Ionic liquids at charged interfaces and in confined geometries are found to display a range of structural and dynamic features beyond mean-field or bulk fluidic predictions. Strong ion correlations, high density and asymmetric ionic structures combine and compete to allow for diverse possibilities.

In my laboratory we perform high-resolution measurements using a Surface Force Balance (SFB) to interrogate the optical, mechanical and (statistical-)thermodynamic properties of confined fluids. In this lecture I will overview a range of phenomena uncovered over the last decade or so of measurements with ionic liquids confined to nano-scale films. These include oscillatory charge density, self-assembled structures, structural transitions with added solvent, and 'interference' effects in mixtures of ionic liquids of differing preferred lengthscales.

Realising the transition towards fluorine-free ionic liquids using functionalised cations.

Frederik Philippi[1], Margarida Costa Gomes[1], Daniel Rauber[2]

[1]ENS de Lyon, Lyon, France. [2]Saarland University, Saarbrücken, Germany

Abstract

Fluorinated anions have become the gold standard in the ionic liquid community. However, many of these anions are now recognised as persistent environmental pollutants, leading to increasing societal and regulatory pressure to develop non-fluorinated alternatives. This transition requires significant effort from the community to catch up with the existing work on fluorinated anions. Here, we outline the key challenges that must be addressed to leave the fluorinated comfort zone and present examples of fluorine-free ionic liquids that we have developed with this goal in mind. Specifically, we have identified ether-functionalised cations as a key design element to overcome the high melting points and viscosities often observed in ionic liquids with fluorine-free anions.

Porous Silicon Anodes Derived from Molten Salt Dealloying of $CaSi_2$for Lithium-Ion Batteries

Bing Li

East China University of Science and Technology, Shanghai, China

Abstract

$CaSi_2$ serves as a key precursor for the preparation of layered silicon-based materials. However, the conventional process of calcium removal via etching in HCl solution often leads to excessive oxygen and hydroxyl group incorporation, which adversely affects the performance of silicon-based materials as anodes for lithium-ion batteries. In this study, calcium stripping from $CaSi_2$ was systematically investigated under two conditions: in a $CaCl_2$-KCl molten salt at 700 °C, and without molten salt at 900 °C, with a focus on the influence of holding time on the efficiency of calcium extraction and the resulting products. The results indicate that both elevated temperature and chloride-based molten salts facilitate the calcium stripping process. Further experiments conducted in $CaCl_2$ molten salt at 900 °C achieved complete single-step calcium removal after a 24 h holding period, leading to the formation of a microporous silicon-based material (designated as MC-3). Comprehensive characterization by XRD and XPS confirmed the high crystallinity of the product, with only trace surface oxidation. A silicon-carbon composite (MC-3@C) was subsequently prepared via dopamine coating followed by carbonization. Electrochemical evaluation revealed that the MC-3@C anode delivers a specific capacity of 647.5 mAh g^{-1} after 700 cycles at a current density of 1 A g^{-1}, along with excellent rate capability. This study demonstrates that high-temperature molten salt treatment significantly accelerates the calcium stripping process, enabling the synthesis of crystalline silicon with a microporous structure while effectively suppressing oxygen incorporation.

Proton Transfer Mechanisms in Protic Ionic Liquids: A Machine-Learning Force Field Study

Miguel A. Boado[1,2], Martín Otero-Lema[1,2], Ángel Míguez-Roel[1,2], Trinidad Méndez-Morales[1,2], Hadrián Montes-Campos[1,2], Luis M. Varela[1,2]

[1]Grupo de Nanomateriais, Fotónica e Materia Branda, Departamento de Física de Partículas, Universidade de Santiago de Compostela, Campus Vida s/n, E-15782, Santiago de Compostela, Spain. [2]Instituto de Materiais (iMATUS), Universidade de Santiago de Compostela, Avenida do Mestre Mateo 25, E-15782, Santiago de Compostela, Spain

Abstract

Proton conduction is a central process in proton-exchange membrane fuel cells, water electrolysers and the emerging class of rechargeable proton batteries. Beyond traditional aqueous electrolytes, protic or pseudo-protic ionic liquids (PILs and pPILs) have emerged as promising proton-conducting systems [1]. However, proton transport in these materials lacks a thorough understanding and requires improved theoretical frameworks.

In this work, we study the proton transfer mechanism in 1-ethylimidazolium bis(trifluoromethanesulfonyl)imide ([HEIM][TFSI]) ionic liquid and in mixtures containing varying fractions of the corresponding neutral species ([EIM] and [HTFSI]) using molecular dynamics simulations. Classical force fields are inadequate for this purpose, as they cannot capture bond breaking or charge transfer, and *ab initio* methods impose limitations on accessible system sizes and simulation timescales. To address this, we employ machine-learning force fields [2], which combine the accuracy of quantum-mechanical descriptions with the computational efficiency required for statistically meaningful simulations. We trace how proton transfer evolves with composition and predict the concentration-dependent conductivity behaviour of these PIL-based systems.

References

[1] Otero-Lema, Martín, et al. "Modelling proton transfer in [HEIM][TFSI] ionic liquid." *Materials today energy* (2025): 102018.

[2] Musaelian, Albert, et al. "Learning local equivariant representations for large-scale atomistic dynamics." *Nature Communications* 14.1 (2023): 579.

Acknowledgements

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Exploring Halogen Bonding in Ionic Liquids

Patricia Hunt, Muhammad Hashmi

Victoria University of Wellington, Wellington, New Zealand

Abstract

Halogen bonding (X-bonding) is emerging as a versatile bonding mode across diverse fields including: materials chemistry, crystal engineering, anion sensing, and catalysis.[1–4] X-Bonding is a highly directional noncovalent interaction that has not yet been fully explored in ionic liquids (ILs).

Electron density within a C-X (X=Br or I) σ-bond can be highly polarised forming an electron-deficient area (δ+) or σ-hole on the X atom opposite the C-X bond, **Fig. 1a**. At the same time an area of increased electron density (δ-) forms in a torus around the bond which is Lewis basic. The cation of an IL can be functionalized with Br or I atoms, leading to polarisation of the electron density and formation of a σ-hole which interacts with an anion forming an X-bond, **Fig. 1b**.

We have investigated the potential for forming X-bonds for n-iodo-1-ethyl-3-methyl-imidazolium [n-iodo-C_2C_1im]$^+$ (*n*=2, 4, 5, 6, 7, 8) with different anions. Calculations have been carried out at the B3LYP/6-311G(d,p)/ECP46MWB_VTZ-PP level, with charge, electrostatic potential, density, molecular orbital and non-covalent interaction analysis to characterise the X-bond interaction.

A key finding is that the σ-hole is largest on the C^2-iodo substituted cation enabling a robust X-bond to form. Other positional isomers show smaller σ-holes and tend to favour H-bond conformers. The strongest X-bonds exhibit both electrostatic and partial covalent character, while the weaker X-bonds exhibit predominantly dispersive interactions. We find that the rotational profile of the ethyl group is sensitive to the position of iodine, with implications for entropic contributions and the kinetic stability of any X-bond formed. Comparative charge transfer studies between [C_2C_1im]$^+$ and the iodo-functionalized cations emphasise the electronic effects of halogenation, offering insights into the nature and strength of X-bonding interactions. These results provide valuable design principles for tailoring ILs with specific noncovalent interactions for advanced functional applications.

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Electrolysis of regolith for simultaneous oxygen and metal production

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Abstract

Worldwide, spatial agencies agree that the future missions of exploration on the Moon will require longer stay time for activities on the lunar surface, imposing to settle down with permanent lunar bases. Incorporation of In-Situ Resources Utilization (ISRU) to produce life support consumables and everyday life objects will greatly reduce the mass, the cost and the risk of missions. The ISRU concept considers the resources at the exploration site with the use of lunar regolith as raw material.

In this context, the behaviour of a lunar soil analog was investigated in LiF-NaF at 800 °C for in situ production by electrolysis of metals (cathode) and O_2 gas (anode) as a part of In Situ Resource Utilization (ISRU) research.

The 1st step was to compare the individual solubility of the main oxides composing the lunar soil (SiO_2, Al_2O_3, Fe_2O_3, $FeTiO_3$ and MgO) with the solubility of the crystalline analog using Inductively Coupled Plasma – Atomic Emission Spectroscopy.

The 2nd step was to verify by cyclic voltammetry the electroactivity of all oxide species in LiF-NaF. Electrolyses on different cathodic substrates were performed at different conditions and analysed with a scanning electron microscope (SEM-EDS). Then, the electrochemical behaviour of the crystalline lunar simulant was compared with a mixed powder made of the different oxides.

The last step is the oxygen extraction from the lunar soil, where the need of resistant materials used under severe conditions is essential. Electrochemical studies and oxygen gas analyser were used to demonstrate and quantify the amount of produced O_2.

Bridging Data and Prediction: Machine Learning for Ionic Liquid Properties and Sigma-Profile Viscosity Modeling

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Abstract

The rapid growth of data-driven methods in chemistry has created new opportunities for predicting the properties of ionic liquids (ILs), yet the practical effectiveness of machine learning (ML) in this domain remains constrained by data availability and chemical space coverage. This work critically addresses the current landscape of ML applications for IL property prediction, focusing on key thermophysical properties including thermal conductivity, heat capacity, density, viscosity, surface tension, melting point, enthalpy, CO_2 solubility, and toxicity. Particular emphasis is placed on dataset size, chemical space coverage, biases, and practical limitations.

We compare modeling approaches spanning from conventional QSPR/QSAR and group-contribution methods to contemporary ML approaches including kernel models, ensemble methods, graph neural networks, and deep learning architectures. The impact of molecular representations and descriptor choices, and validation strategies in determining model robustness and transferability is examined. Beyond methodological performance, we analyze how these models are being applied to practical challenges. Throughout, the focus remains on what works in practice rather than theoretical possibilities alone.

Alongside, we present our ongoing work on ML-based viscosity prediction, where the wide dynamic range, and strong dependence on molecular structure, and temperature and vast chemical diversity of ILs pose particular modeling challenges. We use COSMO-RS-derived sigma profiles as molecular descriptors that capture charge density distributions of cations and anions, paired with Gaussian process. This approach provides improved generalization with highly promising predictive accuracy across structurally diverse ILs compared to purely fingerprint-based representations.

Finally, we propose recommendations for dataset standardization, open sharing of data and code, and the establishment of benchmark validation protocols to improve reproducibility and accelerate ML-based viscosity prediction for task-specific ILs.

The Applications of Molten Salts for Electrochemical Energy Storage

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Abstract

Large-scale electric energy storage is the key for integration of renewable energy, which highlights the urgent demand for safe, low-cost, long-cycle batteries. Herein, we report some studies on molten salt electrochemistry applied to energy storage batteries, due to the intrinsic non-flammability, wide temperature operation window, abundant raw materials and eco-friendly characteristics of molten salts.

Firstly, molten salt electrochemical synthesis strategy was proposed to prepare high-performance electrode materials including titanium-, niobium- and molybdenum-based oxides. By regulating electric fields and molten salt cation-anion environments, pure-phase, sub-valence functional materials with superior lithium/sodium storage capacity were controllably synthesized. Secondly, molten salt medium modification was developed to address the sluggish ion transport at solid-state electrolyte-electrode interfaces. An $AgNO_3$ molten salt infiltration strategy constructs gradient porous LLZTO ion-conductive networks, significantly boosting lithium migration depth, critical current density and full-cell cycling stability. Thirdly, molten salt-based liquid metal batteries (LMBs) were thoroughly investigated. Novel Sb/Bi/Te alloy positive electrodes and multi-cation low-melting molten salt electrolytes were designed, lowering operating temperature to 350°C and achieving a Coulombic efficiency of 99.96%. Key bottlenecks including liquid-liquid interfacial instability, multi-physical field coupling aging and pack inconsistency were resolved. In summary, molten salt electrochemistry was successfully applied to electrode materials preparation, electrode interface modification and novel battery construction, accelerating the development of high-performance electrochemical energy storage technologies.

Theoretical and experimental approaches to reducing the melting point of new lithium salt-based systems

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Abstract

Today, lithium (Li) is a key element in electrochemical energy storage technologies, notably through its use in lithium-ion batteries (LIBs) and lithium-metal batteries (LMBs). It also plays a crucial role in thermal batteries, where molten lithium salts serve as electrolyte. The current industrial sector remains constrained by limited production volumes and high costs, primarily resulting from challenging operating conditions. The main technological bottleneck concerns the high temperatures required for molten-salts electrolysis baths, such as the LiCl-KCleut, which has a melting point of 353 °C. This imposes limitations on both the production processes of metallic lithium and the operation of thermal batteries.

This study aligns with this objective of exploring new salts formulations combining various alkali metals to reduce the phase transition temperature of the salts (< 350 °C) while maintaining electrochemical properties compatible with the intended applications, as well as a high lithium content (> 60 mol %).

To address this challenge, a combined computational and experimental approach was implemented. First, a predictive exploration of the thermal properties of binary compositions was performed using thermodynamic calculations based on the FactSage thermochemical database. This step enabled the identification of eutectic compositions in binary salts and subsequently allowed simulation of the effect of various additives on lowering the melting point of lithium-based systems. Second, candidate formulations, primarily composed of iodide and bromide salts were synthesized. Thermal properties were characterized using Differential Scanning Calorimetry (DSC), allowing precise validation of phase transition temperatures and measurement of fusion enthalpies.

The influence of solutal convection on the cycling behaviour of liquid metal batteries featuring Pb-cathodes

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Abstract

Liquid metal batteries (LMBs) are discussed as potential large-scale storage options for energy systems dominated by volatile renewable sources such as photovoltaics and wind power. A characteristic feature of these devices is a horizontal interface between a molten salt electrolyte (top) and a molten metallic cathode (bottom). Discharge entails alloying of the latter with an alkali or earth-alkali metal, which is transported in ionic form through the electrolyte to this interface. This itinerant metal is supplied by a molten metallic anode, which is contained in a foam made of an iron group metal that is immersed in the salt.

We will address the role of the salt mixture used as the electrolyte. To keep the operating temperature within a manageable range, molten salt eutectics must be used. For cells with Li anodes, mixtures containing Li^+ ions and various anions (e.g., LiF-LiCl-LiI) exhibit sufficiently low melting points. However, for cells with Na-anodes, Na-salt eutectics that merely combine different anions (e.g., NaF-NaCl-NaI) offer more modest reductions in melting temperature. Therefore, using mixtures containing multiple cations (e.g., LiCl-KCl-NaCl) has become popular recently. However, this might influence the cathode-alloy properties.

The main focus of our contribution will be on solutal convection and stable stratification in the cathode, specifically its influence on the cycling behaviour of cells employing Pb-alloy cathodes and Li- or Na-anodes. During charge, depletion of the low density anode metals (Li or Na) at the top of the cathode - just beneath its interface with the overlying electrolyte - lead to a local increase in its density. Such a density distribution is subject to an instability mechanism similar to the Rayleigh-Taylor instability with the exception of a well-defined interface that possesses interfacial tension. After a short phase characterised by purely diffusional Na or Li mass transport, instability prevails and quickly leads to intense solutal convection, mixing the cathode alloy well. Convection onset is in most cases independent of cell geometry and can be universally described using inner scaling and properly defined non-dimensional variables. The scaling is clearly confirmed by numerically and experimentally obtained values as shown in the figure.

Discharge, however, is characterised by stable stratification within the cathode, which leads to high mass transport overvoltages. This situation can be mitigated by various stirring methods, some of which we will discuss.

Oxide Chemistry in Molten Fluorides for Molten Salt Reactor Applications

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Abstract

The chemistry of oxide species in molten fluoride salts is a critical factor affecting the performance and safety of molten salt reactors (MSRs). Because fluoride salts are highly hygroscopic, any residual moisture present in raw materials or within the operating environment can trigger pyrohydrolysis, leading to the formation of oxide impurities in the melt. These oxides can induce undesirable precipitation of solid phases, such as UO_2 in fuels containing UF_4, and accelerate corrosion of structural materials. Therefore, a comprehensive understanding and effective control of oxide behavior are essential for reliable reactor operation. Recent studies have employed electrochemical techniques, nuclear magnetic resonance (NMR) spectroscopy and inert gas fusion method to detect and quantify oxide species in fluoride melts. It has been shown that maintaining oxide levels below ~200 ppm, achievable through pre-purification with H_2/HF treatment, can prevent oxide-induced precipitation and mitigates associated corrosion. Alternatively, chemical stabilization by the addition of ZrF_4 can convert reactive O^{2-} into stable oxy-fluoride complexes, thereby alleviating their adverse effects. This study offers practical strategies for oxide control in fluoride-salt systems, which is essential for ensuring material stability in related high-temperature applications.

Unlocking the Full Potential of Deep Eutectic Solvents in Synthesis

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Abstract

Solvents are essential components of most chemical process, yet they constitute the highest contributors to the environmental impact of reactions, simply on account of them being used in the highest quantities. Further aggravating this is the fact that most solvents employed in synthesis are the so-called volatile organic compounds (VOCs), which tend to be toxic, flammable, and, as their name indicates, volatile.[1] A promising alternative to traditional VOCs are Deep Eutectic Solvents, or DESs for short. They are formed by mixing two or more components at fixed molar rations, with the resulting mixture having a lower melting point than the consituents components due to the formation of a hydrogen bond network. There are numerous advantages to the use of DESs, but particularly exciting for synthetic purposes is their potential to outperform VOCs for certain applications, or to allow transformations that otherwise would not occur.[2] Yet the potential of DESs for synthesis remains underdeveloped, with the interplay between the physical properties of the DESs and reaction outcomes reamining understudied.

We aim to cover this gap by carrying out case reactions in a DES, followed by the study of reaction outcomes when the hydrogen bond donor and acceptor components are systematically changed. Statistical methods have been used to elucidate the correlations between the physical properties and reaction outcomes. The communication will highlight work in this area on three case studies: the oxidation of aldehydes to carboxylic acids, 1,3-azide alkene dipolar cycloadditions, and S_NAr reactions. Clear solvent effects can be appreciated in all cases, not only impacting the yield observed, but also product distribution and the identity of side products in certain cases.

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Thermal properties of triazolium based protic ionic liquids for thermal energy storage application.

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Abstract

The low-grade waste heat below 100 °C, generated in processing industries, urban infrastructures, as well as datacenters are not fully utilized yet [1]. Thus, the development of a phase change materials capable of capturing low-grade waste heat and storing it as thermal energy, which subsequently can be released when it is in high demand, has attracting more interest. Ionic liquids (ILs) have been sought as potential alternatives because they offer a wide range of cation-anion combinations and tunable properties that could be beneficial for thermal energy storage applications, e.g. nonflammability, high chemical and thermal stability [2].

The current work focuses on protic ILs (PILs), a sub of ILs containing a labile proton, which are considered promising materials for thermal energy storage due to their ease of synthesis. In this study, halogen-free anions, such as bis(2-ethylhexyl)phosphate, acetate, hydrogen oxalate and benzenesulfonate, were investigated in combination with 1-methyl-1,2,4-triazolium and 1-ethyl-1,2,4-triazolium cations. The influence of different anions to key thermal properties such as thermal stability, phase behavior and the enthalpy of fusion of PILs, was thoroughly studied. Moreover, the temperature dependent physicochemical properties of the PILs were studied to elucidate the effect of cation and anions structures on the structure-property relationship, thereby providing valuable insights for the development of PIL-based thermal energy storage materials.

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Structural and Dynamic Features of Diastereomeric (Deep) Eutectic Systems of Homochiral Components (DIADES)

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Abstract

Chirality is a fundamental property of biological systems and of essential chemical compounds, which often exist in one single enantiomeric form. Chiral compounds are highly valuable in pharmaceuticals and materials because of their distinct stereostructures. Recently, Deep Eutectic Solvents (DES) have been prepared combining homochiral components, often available from the chiral pool of natural compounds.[1,2,3]

Using only enantiopure substances as DES components leads to the formation of diastereomeric deep eutectic solvents (DIADES). Although DES have emerged as versatile green media, the chemical space arising from the combination of chiral components remains largely unexplored.

In this presentation we investigate four DIADES prepared through the combination of (+)-menthol, (–)-menthol, (+)-camphor, and (–)-camphor (Figure 1).

A preliminary mapping of the chiral environment is carried out through NMR spectroscopy, DFT and MD simulations, whilst the mesoscopic structural heterogeneity is investigated by SAXS.

Further information will be obtained by dissolving chiral solutes in these new media and investigating the molecular interactions and transport properties as a function of the absolute configuration of the components. Our findings provide a rational framework for understanding the solvation behaviour in these novel systems directly connected to the individual stereochemical configurations. This work establishes a foundation for the strategic design of enantioselective media in advanced chemical applications.

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Poly(Ionic Liquid)–Mediated Colloidal Stabilization in Low-Dielectric Media: Interplay of Ion Pairing, Steric Confinement, and Depletion Forces

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Abstract

Colloidal stabilization in low-dielectric media presents a fundamental challenge due to suppressed charge dissociation and long-range Coulombic interactions arising from the enlarged Bjerrum length. In hydrocarbon oils, weak electrostatic screening and negligible surface charging promote carbonaceous particle aggregation, limiting the effectiveness of conventional dispersants. Here, we investigate imidazolium- and phosphonium-based polyisobutylene ionic liquids (PILs) as model amphiphilic ionomers to elucidate ion-mediated stabilization mechanisms in nonpolar fluids. These PILs combine oil-soluble polyisobutylene backbones with tethered ionic headgroups, enabling simultaneous steric confinement and localized electrostatic structuring. Surface-tension measurements reveal concentration-dependent self-assembly and early-stage interfacial aggregation, indicating ion-driven organization even under low-permittivity conditions. UV–Vis adsorption isotherms, analyzed using Langmuir and Freundlich models, demonstrate strong surface affinity and mixed monolayer/heterogeneous adsorption, reflecting cooperative interactions between ionic moieties and carbon surfaces. Small-angle neutron scattering (SANS) and small-angle X-ray scattering (SAXS) resolve the nanoscale organization of PILs in bulk oil and at particle interfaces. Model fitting reveals a concentration-dependent transition in stabilization mechanism: at low PIL loading, extended electrostatic repulsion emerges from partially dissociated ion pairs and correlated ionic domains, whereas at intermediate concentrations steric stabilization dominates via excluded-volume effects of the polyisobutylene corona. At high concentrations, reaggregation is observed and interpreted through depletion-induced attractions consistent with Asakura–Oosawa-type osmotic imbalance, highlighting the delicate interplay between ionic correlations and polymer-mediated entropic forces. Tribological measurements under boundary-lubrication conditions establish a direct structure–function relationship, where nanoscale interfacial ordering and adsorption thermodynamics govern macroscopic friction and wear reduction. Collectively, this work provides a mechanistic framework for understanding how ionic liquids operate in low-polarity environments, extending classical colloid and polyelectrolyte theory to hydrocarbon media. The results elucidate how ion pairing, dielectric confinement, and amphiphilic architecture cooperatively dictate stabilization, offering molecular-level insight into ionic-liquid-enabled lubrication in nonpolar systems.

Electrodeposition of Difficult-to-Plate Elements from High-Temperature Molten Salts

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Abstract

High-temperature molten salts are expected to be utilized in the production and recycling of various valuable materials due to their wide electrochemical window and ability to dissolve a wide range of substances. In particular, elements that are difficult to deposit in aqueous solutions or at room temperature can be obtained using high-temperature molten salts. In our study, we focused on silicon (Si), titanium (Ti), and tungsten (W) as difficult-to-deposit elements. We developed KF–KCl and CsF–CsCl molten salts as novel systems for the electroplating of Si, Ti, and W [1]. These molten salts not only yield high-quality deposits but also feature high solubility in water, making it easy to remove residual salts by water washing.

Silicon is a key element used for solar cells and as a negative electrode in lithium-ion batteries (LIBs). We successfully deposited n-type and p-type photoconductive silicon [2] and fabricated solar cells. We also found that using deposited silicon as a negative electrode in LIBs improves charge-discharge performance [3].

Titanium is a functional material with high corrosion resistance and biocompatibility. We have succeeded in electroplating Ti that is free of cracks and voids and exhibits corrosion resistance against seawater [4].

Tungsten is used in many fields due to its high heat resistance and hardness, and recently, it is particularly expected to be used as a material for reactor walls in nuclear fusion reactors. Depending on the experimental conditions, we succeeded in selectively electroplating α-W with a body-centered cubic structure and β-W with an A15-type cubic structure [5]. In particular, we succeeded in obtaining a β-W film with an extremely smooth, mirror-like surface [6]. We also confirmed that this plating method shows promise as a new repair method for nuclear fusion reactor walls.

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Ioncell® Technology: Manufacturing High-Strength Fibers for Versatile Applications

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Abstract

The emerging Ioncell® process has been employed to investigate various lignocellulosic materials, including pulps and textile waste, for the production of high-quality fibers suitable for diverse applications utilizing ionic liquids as solvents.

Driven by the growing world population and the rising global purchasing power, the textile and fashion industry consumes resources at an alarming pace. To tackle the problems of the textile industry, the European Commission stated a strategy to create sustainable and circular textiles. The strategy follows the motto #ReFashionNow, which aims on the improvement of textile quality, durability, longer use, repair and reuse. A common industrial technology roadmap on circularity is developed promoting fiber-to-fiber recycling research and innovations.

Ioncell® is a technology designed for the eco-friendly manufacturing of man-made cellulose fibres (MMCFs), enabling the production of sustainable, high-strength fibers with dry tenacities reaching up to 60 cN/tex. Additionally, it facilitates resource recovery from various lignocellulosic waste materials, such as cardboard boxes, newspapers, cotton, hemp, and more, through fiber-to-fiber recycling to promote a circular economy.

In this presentation, we explore the potential of the Ioncell® process in creating fibers for a wide range of impressive uses. This includes staple fibers for textiles, continuous fibers for composite materials, and even investigations into carbon fibers.

Composition-Controlled Ionic Liquid Biorefining of Softwood for Microfibrillated Cellulose Production

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Abstract

Microfibrillated cellulose (MFC) production from lignocellulosic biomass is conventionally based on kraft pulping followed by strong acid hydrolysis or intensive mechanical processing. Such routes typically involve high chemical severity, limited compositional tunability, and restricted control over fibre chemistry. In contrast, **ionic liquid (IL) pretreatment provides a greener and highly tuneable alternative**, enabling controlled biomass fractionation under comparatively mild conditions.

Here, we present a **composition-controlled IL pretreatment strategy** in which the **acidity, temperature, residence time, and water content** of a mild IL, **triethanolammonium methanesulfonate (TEA $MeSO_3$)**, are systematically adjusted to induce **quantifiable and reproducible variations in pulp composition**, particularly in hemicellulose and lignin content. Taken together with subsequent fibre activation and fibrillation results, these findings indicate that **IL pretreatment acts as the primary upstream control**, defining the pulp compositional and chemical landscape that governs nanofibrillation behaviour.

To further facilitate fibrillation from these compositionally preconditioned pulps, a **subsequent electrochemical pulp bleaching step**, operated under **near-neutral to mildly alkaline conditions**, is employed primarily as a **fibre activation process rather than exhaustive delignification**. Precise oxidant dose control enables the selective oxidation of residual hydroxyl and other surface functional groups on pulp fibres, promoting fibre swelling and defibrillation while minimising chemical severity.

Following ultrasonic fibrillation, the resulting MFC suspensions exhibit clear composition-dependent behaviour, as characterised by scanning electron microscopy, viscosity, optical transmittance, and zeta potential measurements. Compared with conventional kraft-based and sulfuric acid-hydrolysed MFC routes, this approach offers **enhanced sustainability, improved chemical tunability, and superior control over structure–property relationships** in MFC production.

Catalytic Binary and Ternary Ionic Liquid Mixtures as reaction media for the Xylose to Furfural conversion

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Abstract

The conversion of lignocellulosic biomass into industrially relevant products, and in particular of carbohydrates into furanic compounds, is a cornerstone of current research efforts in sustainable chemistry.[1] In addition, it is desirable to find catalytic systems, able to promote the conversion of more challenging carbohydrates, which despite being less reactive, make up more abundant biomass fractions. In this context, the conversion of xylose raises interest, since it is remarkably abundant in hemicellulose, allowing the valorization of such fraction of lignocellulosic biomass.[2] Based on these considerations, herein we present an investigation of the dehydration reaction of xylose to furfural, in binary and ternary ionic liquids mixtures, in which one component is a SO_3H-functionalized cation, acting as catalyst.

We optimized the reactions in terms of temperature, catalyst loading, reaction time and composition of the mixtures, investigating the effects of the nature of the cation and the anion. In this regard, both aromatic and aromatic ionic liquids cations were considered. Subsequently, we measured the viscosity of the solvent media to elucidate the effect of this parameter on the reaction outcome. Recyclability of the catalytic ionic liquid mixture was also investigated.

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A sustainable and effective ethanol-free IonoSolv process for high-purity cellulose pulp production

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Abstract

The continued reliance on fossil feedstocks to produce chemicals, energy and materials is associated with negative environmental impacts, reinforcing the transition toward renewable feedstocks and sustainable processes. Cellulose, the most abundant biopolymer in nature, represents a key pillar for this transition. In this context, our research group has developed the IonoSolv process, based on Protic Ionic Liquids (PILs) for the selective extraction of lignin and hemicellulose from lignocellulosic biomass, while preserving a cellulose-rich pulp. This process has demonstrated cost-effectiveness across diverse biomass feedstocks, including grasses, softwoods and hardwoods, delivering high-purity cellulose pulps and lignin, alongside high IL recovery and reuse rates. Despite these advances, ethanol is still employed at laboratory scale during pulp washing, emphasising the need for the development of an effective washing without using a volatile and flammable solvent, while further reducing residual lignin content in the cellulose pulp [1,2]. Here, we report the development of an ethanol-free IonoSolv process using the low-cost PIL N,N,N-dimethylbutylammonium hydrogen sulphate ([DMBA][HSO_4], 80 wt% in water, a:b ratio 1:1). A statistical design of experiments was applied to optimise the pulp washing step, evaluating the effects of IL concentration, pulp: IL ratio, and temperature. The resulting pulps were characterised by compositional analysis and Kappa number determination, while an enzymatic saccharification assay was used to assess glucan accessibility. Cellulose pulps containing up to 92% glucan were obtained. Commercial cellulose and cotton were analysed as standards, confirming both the high purity of the cellulose pulps obtained in this study and the challenges associated with soluble lignin quantification during compositional analysis due to the formation of secondary products during the acid hydrolysis. Overall, this study demonstrates that a single and cost-effective PIL can effectively enable both biomass fractionation and cellulose purification, offering a more sustainable pathway for lignocellulosic biomass valorisation. The authors acknowledge support from the UKRI Bio-derived and Bio-inspired Advanced Materials for Sustainable Industries (VALUED) programme (EP/W031019/1).

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Electrochemical Study of Salt-Metal Interactions in LiCl-KCl at 400 °C: Implications for the Corrosion of Alloys in Molten Salt Reactors

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Abstract

Molten salt reactors (MSRs) based on chloride salts represent a promising technology for fast neutron reactors. However, corrosion of structural materials—primarily Ni-, Fe-, or Cu-based alloys—by the molten salt itself, exacerbated by the presence of fission products, remains a major barrier to their development. To investigate these phenomena in the laboratory without handling radioactive materials, neodymium (Nd) and cerium (Ce) were employed as non-radioactive simulants for plutonium, owing to their similar redox properties, thermodynamics, and complexation behavior [1].

An electrochemical study was conducted in a model LiCl–KCl eutectic melt at 400 °C using cyclic voltammetry, in the presence of one or more transition metal elements added either as metals or as chloride species, in order to characterize redox behavior and metal–salt interactions in the molten medium. Complementary differential scanning calorimetry (DSC) analyses were performed on selected systems to assess the thermal properties of the bath (melting point, phase transitions, thermodynamic data, etc.) in the presence of the added metallic species.

The evolution of the bath composition following these reactions was also monitored by X-ray diffraction (XRD) to identify the phases formed through redox processes. The presence of metal salts in their +II/+III ionic forms shift the redox potential of the bath and promotes the oxidative dissolution of metals. The phases formed during these redox reactions in the molten salt bath were identified, and their thermal stability was investigated.

The thermodynamic values derived from these studies will contribute to populating databases used for the calculation of associated binary and ternary phase diagrams. These data help guide the selection of structural materials to achieve improved control of corrosion processes between molten salt fuel baths and reactor vessels.

Keywords: molten salt reactor, cyclic voltammetry, DSC, corrosion, eutectic, electrochemistry

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The Dual Role of $MgCl_2$ on Structure–Transport Coupling in Molten Chloride Fast Reactor Fuels

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Abstract

France is currently exploring $NaCl–MgCl_2–PuCl_3–AmCl_3$ as a molten chloride fast reactor (MCFR) fuel to reduce the actinide inventory in spent nuclear fuel [1]. In previous work, we employed $NaCl–MgCl_2–LaCl_3$ as a non-radioactive surrogate MCFR fuel, combining high-temperature nuclear magnetic resonance (HT NMR), classical molecular dynamics (MD) simulations, and first-principles NMR calculations to probe the local La–Cl–La network structure and coordination environments [2]. At fixed $LaCl_3$ concentrations, we found that increasing the $MgCl_2$ content raises the average La–Cl coordination number while disrupting continuous La–Cl–La networks, suggesting that $MgCl_2$ may reduce melt viscosity in MCFR fuels. However, subsequent MD simulations of transport properties reveal that $MgCl_2$ does not affect $LaCl_3$-poor and $LaCl_3$-rich melts equivalently. In $LaCl_3$-rich regimes, $MgCl_2$ lowers viscosity by suppressing the formation of extended, interdigitated $[La_xCl_y]^{3x-y}$ complexes. In contrast, at low $LaCl_3$ concentrations, $MgCl_2$ slightly increases viscosity through the formation of $[Mg_xCl_y]^{2x-y}$ complexes [3]. This previously unrecognised dual role of $MgCl_2$ highlights the importance of composition-dependent effects in molten chloride systems and may guide experimental efforts to improve the transport properties of related high-temperature ionic melts for energy and industrial applications.

Acknowledgement: This work was carried out as part of the ISAC project funded by the France 2030 government program.

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Evaluating Cesium / Iodine Effluent Production in Pyrochemical Reprocessing Systems for Advanced Reactor Fuel Cycles

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Abstract

Evaluating Cesium / Iodine Effluent Production in Pyrochemical Reprocessing Systems for Advanced Reactor Fuel Cycles

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With the increasing energy demand expected for an AI-powered future, renewed interest in nuclear power is motivating a reassessment of regulatory guidance for commercial facility licensing. Many newly proposed reactor designs rely on High-Assay Low-Enriched Uranium (HALEU) as fuel, for which current domestic production cannot meet projected demand. Idaho National Laboratory is a partner in the HALEU supply chain, downblending used highly enriched Experimental Breeder Reactor II (EBR-II) fast metallic fuel through pyrochemical reprocessing.

Pyrochemical reprocessing has inherent safeguards advantages over aqueous PUREX processes and is thought to minimize or eliminate portions of gaseous waste streams that pose environmental concerns. Current facility models assert that fission-product iodine is quantitatively captured in the LiCl-KCl eutectic molten salt during anodic dissolution of the fuel. However, recent thermodynamic modeling of these salt systems by Ngelale and Bruffey[1,2] calls this assertion into question, identifying Cs_2I_2 as a probable electrorefiner off-gas species.

This work seeks to provide experimental validation of this refutation by analyzing both testbed electrorefiner effluents and samples from INL's Fuel Conditioning Facility using high-sensitivity Accelerator Mass Spectrometry (AMS) and Thermal Ionization Mass Spectrometry (TIMS). Comparing $^{137}Cs/^{135}Cs/^{133}Cs$ and $^{129}I/^{127}I$ ratios to local background levels and modeled data will help inform discussions on the environmental impacts of commercial facility licensing by the Nuclear Regulatory Commission (NRC).

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Plutonium(III) simulant for molten chloride salt nuclear fuel

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Abstract

Molten salts are a promising fuel candidate for fourth-generation nuclear reactors, such as molten chloride fast reactors. [1] Composed primarily of actinide chlorides combined with alkali and alkaline earth metal salts, they offer distinct advantages over traditional solid oxide fuels, including a liquid state and near-atmospheric operating pressures. [2] However, the physicochemical properties of these fuels are difficult to study experimentally due to the artificial nature and high radioactivity of actinides like plutonium. While simulants such as cerium(IV) or thorium(IV) are commonly used for metal(IV) oxide fuels, their suitability for molten chloride salts—where plutonium exists in the +III oxidation state—has not been systematically evaluated.

In the present work, we aimed to identify the most accurate simulant for plutonium(III) in chloride melts using quantum chemistry calculations and polarizable molecular dynamics (MD) simulations. [3] Using density functional theory, we demonstrated that, among the lanthanide series, the neodymium(III) cation exhibits the closest interactions with chloride anions when compared to the ones involving plutonium(III). Then, using MD simulations, we predicted the physical and thermodynamic properties, and the local structure of the eutectic NaCl–$NdCl_3$, NaCl–$CeCl_3$, and NaCl–$PuCl_3$ mixtures. Our findings confirm that neodymium(III) is the best choice to simulate plutonium(III) properties with the greatest accuracy. Additionally, the error introduced when considering cerium(III) as an alternative is quantified.

Acknowledgement: This work was performed as part of the ISAC (Innovative System for Actinide Conversion) project funded by the France 2030 government program. The simulations were performed on the SACADO MeSU platform at Sorbonne Université.

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Nature of electrodeposition Al-Mn from molten salts

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Abstract

Aluminium (Al) alloys are promising in aerospace and automotive applications due to their high strength-to-weight ratio. Al-Manganese (Mn) alloys can offer desired corrosion resistance, strength and formability for such applications. Al-Mn alloys with such properties can be electrodeposited – a bottom-up approach. However, Al cannot be electrodeposited using aqueous electrolytes owing to its standard reduction potential ($Al^{3+}|Al$: −1.676 vs NHE) being more negative to water splitting [1]. Chloride-based molten salts are explored in the literature for Al-Mn electrodeposition due to their accessibility and ease of handling.

In the present work on Al-Mn electrodeposition, all electrochemical experiments were done at 180 °C using fresh electrolytes comprising $AlCl_3$, NaCl, KCl and $MnCl_2$ employing CHI660E electrochemical workstation. The chemicals were handled in a glove box (with O_2 and H_2O <0.1 ppm) as they are hygroscopic and/or moisture sensitive. Commercial copper strip was used as the working electrode, a pure Al (99.99% Al) rod and strip as the counter and reference electrodes, respectively. Cyclic Voltammetry was conducted from Open Circuit Potential to −1.0 and +2.5 V vs Al(III)|Al to select the potentials for deposition. Electrodeposition was conducted at overpotentials of −0.60, −0.65, −0.70, −0.75, −0.80, −0.85, and −0.90 V. Mn content in the deposit increases from 22.3 to 32.77 wt.% with increasing overpotentials. Contrarily, it is expected that Al content should increase with overpotential as it is the less noble metal than Mn. Further, the Mn content does not change drastically after reaching a threshold value (~32 wt.%). The reasons for the encouraged deposition of Mn and its threshold value in the deposits are not yet investigated in the literature.

Electrodeposition of every binary metallic system can be assigned a 'Nature'. Brenner [1], upon extensive investigation on electrodeposition, categorised the natures as 'regular', 'irregular', 'equilibrium', 'anomalous', and 'induced' – based on the trends in metal contents in deposits and electrolytes. It is essential to understand the trends of deposit compositions versus those of the spent electrolytes, overpotentials (or current densities), temperature, and agitation to reveal the nature of the electrodeposition of a binary system. Analysis of such trends reveals the nature of Al-Mn electrodeposition as 'induced'. The reasons for such induced deposition of Al-Mn are explored here. Understanding these reasons will be of both fundamental and practical importance.

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Recovery of Rhenium from Spent Ni-based Superalloy through Molten Salt Processing

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Abstract

Rhenium (Re), a rare and high-value element, is added in considerable amounts (up to 6 wt.%) to Ni-based superalloys, which are primarily used in the manufacture of turbine blades for aircraft engines. In addition to its economic importance, the limited availability of Re, coupled with the increasing demand for superalloys, has raised concerns about a potential supply-demand imbalance. Consequently, considerable research efforts have been directed toward developing effective recovery techniques for Re from Ni-based superalloy scrap.

This work proposes a novel process for recycling Re from spent superalloy in molten $CaCl_2$–NaCl–KCl–CaO. A separation strategy integrating electrolysis and precipitation was employed. By leveraging the distinct electrochemical behaviors of the constituent metals in the superalloy and the dissolution behaviors of their oxides in the melt, Re within the Ni matrix can be effectively recovered in various forms, including metallic Re, and ReO_2. Further details will be provided during the presentation.

Synthesis of cerium oxide nanoparticles by thermal decomposition of cerium oxalate in molten salts

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Abstract

The excellent redox reactivity of cerium, combined with oxygen vacancies at the surface of the oxide CeO_2, makes it widely used in many applications such as catalysis [1] and photocatalysis [2]. Nowadays, these applications are being extended to nanotechnologies, which implies to synthesize CeO_2 nanoparticles (CeO_2-NP) with enhanced properties owing to their great specific surface area.

Among the various routes allowing to synthesize CeO_2-NP [3], the thermal decomposition of the cerium oxalate $Ce_2(C_2O_4)_3{\cdot}10H_2O$ in hydrothermal conditions leads to CeO_2-NP at lower temperatures (160-250°C) [4-5] compared to the thermal decomposition of cerium oxalate in air which occurs between 270 and 450°C [6]. However, the hydrothermal decomposition of $Ce_2(C_2O_4)_3{\cdot}10H_2O$ takes at least 24 hours. In order to minimize the reaction time and to synthesize CeO_2-NP this work was focused on the thermal decomposition of cerium oxalate in molten salts.

To determine the influence of experimental conditions for the synthesis of CeO_2-NP in molten salts, several salts were studied (hydroxides, carbonates, etc.) knowing that the various systems also had an input on the reaction temperature based on their eutectics. After the reaction, the soluble phases were dissolved in deionized water then X-Ray Diffraction, Infrared spectroscopy and Energy-Dispersive X-Ray spectroscopy were used in order to identify the phases formed during the synthesis in molten salts. The morphology of the ceria particles was determined by Scanning Electron Microscopy.

It results from our work that the nature of the salt is of great importance regarding the size and morphology of CeO_2 particles formed, as seen in figure 1 which compares the CeO_2 (nano)particles obtained in nitrates and chlorides salts after three hours of reaction. The morphology of nanoparticles is also influenced by the atmosphere and varies from spherical to multi-facetted with respect the oxidizing or reducing atmosphere. The reaction temperature also has an influence on the morphology of the particles: in hydroxides, at 300°C, there is the presence of aggregated nanoparticles while at to 200°C, the results showed needle-like CeO_2 particles with micrometric length and nanometric width (figure 2).

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Behaviour of oxidizing elements in the molten salt NaCl-$CaCl_2$ (600°C) using $SmCl_3/SmCl_2$ system

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Abstract

Corrosion towards metallic alloy elements in molten chloride salts present a significant challenge. In chloride molten salt systems, protective oxide layers do not provide the same level of protection as in aqueous systems [1]. Consequently, metallic alloys are directly exposed to the molten salt and to the oxidizing elements that may form. Under certain conditions, $H_2O(g)$ et $O_2(g)$ react with chloride salts, creating oxidizing species such as HCl(g) and $Cl_2(g)$ [2,3]. These species act as oxidants towards metallic elements including chromium, iron and nickel.

This work presents a method, using the $SmCl_3/SmCl_2$ soluble-soluble redox couple, to quantify and detect the formation of oxidative species in the molten salt. The apparent standard potential of the samarium couple, experimentally determined at -1.84V vs $Cl_2(g)/Cl^-$, is well situated to detect the oxidizing species of the metallic alloy elements (Figure 1). Electrochemistry, spectroscopy (ICP-OES) and gas chromatography are used to monitor the evolution of the samarium system and to follow the introduction of oxidizing species in the molten salt according to the chosen experimental device.

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Simulation of energy storage materials: Applications to solid electrolytes interfaces and proton transfer

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Abstract

Electron and proton transfer processes are fundamental to the operation of electrochemical devices such as batteries, fuel cells, and electrolyzers. A proper understanding and optimizing electron and proton transport is essential for advancing sustainable energy technologies, which usually demands computer simulations to circumvent highly sophisticated and even impossible experimental observations. In this talk we review several frontier applications performed in our research group of different simulation techniques (molecular dynamic simulations, specifically those based on neural network potentials, and DFT-based methods to the simulations of electron and proton transfer processes through electrolytes (water-in-salt, ionic liquids) and at the electrochemical interface with relevant electrode materials to mimic redox reactions such as the formation and growth of the solid electrolyte interface (SEI), and hydrogen or oxygen evolution reaction mechanisms in electrolyzers and fuel cells.

Acknowledgements

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Graphene oxide–Ionic Liquid Composites : From Molecular Design to 3D Electrode Architectures

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Abstract

The theoretical capacity of tin (~993 mAh/g) is nearly three times that of graphite (372 mAh/g). However, tin anodes experience a volume expansion of around 300% during lithiation, which often leads to rapid structural degradation. In the long term, our goal is to develop a ternary composite that combines tin, a functionalized imidazolium ionic liquid (IL), and graphene-based materials (GO). In such a system, the IL is expected to stabilize interfaces and enhance electrochemical performance [1]. As an initial step, the present work focuses on a simpler binary system-graphene oxide and ionic liquid (GO–IL) to understand how ILs chemically interact with the graphene matrix and influence its structure.

To explore structure–property relationships, we synthesized three imidazolium-based ILs with alkyl amine chains of different lengths, all sharing the same imidazolium core and $TFSI^-$ counterion. This design enables a systematic investigation of the impact of chain length. These ILs were intended to be covalently grafted onto GO via notably via epoxide ring-opening, following a method inspired by previous work [2]. For comparison, non-covalent GO–IL mixtures were also prepared relying on physical adsorption.

To evaluate the chemical integration of the ionic liquids within the graphene oxide framework, a set of characterization techniques were employed, such as NMR, EDX and FTIR to detect features of the imidazolium moieties and provide insight into their interaction with the GO matrix and TGA to assess the thermal stability of the composites. DSC could offer complementary information on possible transitions linked to the IL incorporation. Finally, XPS was carried out to examine the surface chemistry, particularly the potential formation of C–N bonds and the disappearance of epoxide signals, which would suggest covalent grafting.

A subsequent process of the GO–IL suspensions into porous 3D monoliths using freeze-casting allow fine structuration of the composite materials in open porous structure. At last, thermal annealing step partially reduced GO into rGO, restoring electrical conductivity and yielding lightweight, binder-free, self-supporting foams. These materials were tested in lithium-ion half-cell configurations to assess their electrochemical behaviour and explore the influence the IL chain length. This composite GO–IL platform, with a tunable surface chemistry and scalable architecture, serves as a foundation for integrating active materials like tin.

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Salt–Salt Induced TFSI Biphasic Electrolytes for Membrane-Free Redox Flow Batteries

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Abstract

Membrane-free aqueous redox flow batteries (RFBs) based on biphasic aqueous electrolytes represent a promising strategy to overcome the cost and durability limitations associated with ion-exchange membranes. In this study, a series of salt-induced aqueous biphasic systems (ABS) composed of LiTFSI or NaTFSI combined with LiCl or $(NH_4)_2SO_4$ were developed and characterized to obtain stable and selective immiscible liquid phases suitable for membrane-free electrochemical applications. The systems display a well-defined TFSI-rich lower phase and a hydrophilic upper phase, whose polarity contrast enables confinement of redox-active species.

Partition experiments demonstrated high phase selectivity for all investigated redox mediators. Potassium and sodium ferrocyanide were completely retained in the hydrophilic top phase, whereas methyl viologen and its ethyl and benzyl derivatives preferentially partitioned into the TFSI-rich phase. Partition coefficients (K) close to or higher than 100 confirm efficient thermodynamic separation and limited crossover between phases.

Electrochemical characterization by cyclic voltammetry (CV) revealed highly reversible redox behavior for both ferrocyanide and viologen species, with narrow peak separations and stable current responses. Repetitive cycling over 100 consecutive scans confirmed electrochemical stability, with no significant signal decay or potential drift. Based on the formal potentials determined in each phase, theoretical open-circuit voltages (OCV) exceeding 1.0 V were estimated, confirming favorable energetic alignment of the redox couples.

These results demonstrate that salt–salt induced TFSI-based ABS provide a robust biphasic electrolyte platform for membrane-free energy storage.

Acknowledgments

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Water-Modulated Interfacial Structure and Electrochemical Response of Ionic Liquid–Lithium Electrolytes: A Molecular Dynamics Study

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Abstract

This work investigates the interfacial structure and electrochemical behavior of a ternary ionic liquid/water/Li-salt electrolyte using polarizable molecular dynamics (OpenMM[1]) with the CL&Pol forcefield.[2] Electrodes were modeled as constant-potential graphene layers[3] to characterize charge and polarization effects.

Results show that while low water concentrations minimally impact interfacial organization, higher water content and voltages lead to preferential water accumulation at the negative electrode, enhancing lithium transport but destabilizing the interface. Notably, we observe a progressive loss of short-range surface charge correlations at the negative electrode with increasing voltage and hydration. We characterize this behavior theoretically, decomposing the contributions of individual ionic species. This phenomenon serves as a useful indicator of interfacial disruption in aqueous ionic liquid electrolytes.

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Advanced electrolytes for energy storage applications

Mega Kar

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Abstract

There is a critical need to design inexpensive, non-flammable and stable materials for the next generation of rechargeable batteries to overcome the variability of renewable energy in Australia. Metal have come a long way since the 1920's since the progression in non-aqueous electrolytes have been employed to overcome safety concerns with moisture and air-sensitive metals, i.e. Li. Recently, advanced electrolytes based on liquid salts have garnered enormous interest in the field of electrochemistry for energy storage technologies. Herein the design of a series of weakly-coordinating borate-based anions and ionic liquids as battery electrolytes[1-3], with low-volatility and high oxidative stability, is reported. Such materials make them immensely attractive for high-voltage cathodes. Moreover, their electrochemical compatibility with a number of various metals including lithium (Li), sodium (Na) and magnesium (Mg) is demonstrated, making them highly appealing for a number of emerging rechargeable metal battery technologies such as high-energy density batteries based on Li as well as affordable, safer alternatives such as sodium and magnesium.

Towards Fluorine-Free Electrolytes: Physicochemical Properties and Ionic Interactions in Acesulfame-Based Ionic Electrolytes

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Abstract

Ionic liquids and salts containing fluorine-free anions are generating interest as safer and more sustainable electrolytes for Li-ion batteries, addressing the flammability of conventional carbonate-based electrolytes and the environmental persistence of fluorinated anions. This motivates the use of the non-fluorinated acesulfame (ACE^-) anion, derived from potassium acesulfame, a toxicologically evaluated tabletop sweetener. Further, ether-functionalised cations may facilitate lithium-ion transport by promoting favourable lithium coordination environments. Here, two ionic electrolytes were prepared by combining the ACE^- anion with two oxygen-containing cations, N-ethyl-N-methyloxazolidinium (C_2moxa^+) and N-methoxy-N,N,N-trimethylammonium ($N_{111(1O1)}^+$), together with lithium acesulfame (Li-ACE), to evaluate the suitability of these mixtures as battery electrolytes. The thermal and transport properties and the ion dynamics of these electrolytes were probed to understand the effect of anion structure. At 10 mol % Li-ACE, the $[N_{111(1O1)}][ACE]$ electrolyte exhibited the highest ionic conductivity (5.4×10^{-4} S cm^{-1}) and total ion diffusivity (1.0×10^{-11} m^2 s^{-1}) at 50 °C. However, $[C_2moxa][ACE]$ electrolytes exhibit greater Li^+ diffusivity ratio at 20 and 50 mol% Li-ACE content, indicating greater Li^+ mobility. Importantly, the solvation of Li^+ in acesulfame-based electrolytes were investigated experimentally for the first time and complemented with molecular dynamics simulations. In both electrolytes, Li^+ coordinates strongly to the nitrogen atom on the ACE^- anion, followed by the sulfonyl and carbonyl oxygens. Additionally, smaller Li clusters were observed in the oxazolidinium-based electrolytes than the ammonium-based electrolytes, which may be a reason for the enhanced Li^+ mobility in $[C_2moxa][ACE]$ electrolytes at higher lithium content (20 and 50 mol %). This highlights the influence of the position of ether functionality in the cation on the Li^+ solvation structure and ion transport.

Ionic liquids for electrochemical applications: Correlation between molecular structure and electrochemical stability window

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Abstract

Ionic liquids have many properties that are useful in various fields of science and technology. Ionic gating is an effective and versatile tool for the tuning of charge-carrier density of materials and for control its electronic ground state. Low-temperature devices like electrochemical transistors can be developed also.

The high thermal stability and electrochemical stability of ionic liquids make them a promising gating agent.

An ionic liquid to be a good gating agent must have a Tg < −50 °C and a wide electrochemical window at low temperatures.

A series of 23 ionic liquids where the anion is keep fixed (Tf_2N) and the cations are quaternary ammonium salts with three short alkyl chains and a long one has been studied. Anodic and cationic limits at −33 °C via linear-sweep voltammetry.

Electrochemical windows between 2.9 and 5.7 V have been measured.

Some significant empirical correlations have been found:

1. The variation of the cation structure affects both cathodic and anodic limits.
2. Asymmetric cations are more electrochemically stable than symmetric ones.
3. The length of the cation alkyl long chain is inversely proportional to electrochemical stability.
4. Alkyl long chains show a larger anodic limit, but smaller cathodic limit than ether long chains having the same length.
5. The ether chain with largest electrochemical stability comprises three carbon atoms and one oxygen.

Some computational studies are also presented in order to rationalize the role of the structure of the ions and of the anion-cation interactions on their electrochemical properties.

On the road to large scale electrolyte production for Aluminum-Ion Batteries

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Abstract

For many reasons the development of cheap, safe and highly efficient batteries is today one of the major technical challenges. Li-Ion batteries, although today well-established, have their limitations, especially regarding long-term resource availability with Lithium having been added to the Critical Raw Material list in 2020.

Aluminum-Ion Batteries offer a very interesting alternative to Li-Ion batteries in many applications due to a very high cycle life and high power densities. Furthermore, the avoidance of any critical raw materials and PFAS components make AIBs very attractive from an ecological impact and resource availability viewpoint.

However, there are still several challenges to be addressed on the way towards an industrial-scale production of AIBs one of which is the scale-up of the ionic liquid electrolyte.

In our contribution we will address some of the challenges we face as electrolyte manufacturer in the transition from lab-scale and what steps have already been taken.

While on lab-scale battery cell tests a single bottle of electrolyte will suffice for extensive testing the move to larger pouch cells and battery modules necessitates a more comprehensive analytic and a deeper understanding of the effect of electrolyte impurities on battery performance. We will show recent improvements to our analytical process and reproducibility of electrolyte performance.

The second important challenge is the scale-up of the synthesis itself as well as the starting material purification. We will show what methods for the scale-up of the synthesis we have developed and how purification processes can be scaled or facilitated.

In the outlook of our contribution, we'll give an overview of our roadmap to prepare for large-scale electrolyte production.

Probing electrical double layer structure in ionic liquids with the electrochemical Surface Force Balance (e-SFB)

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Abstract

New measurements of ionic liquids using an electrochemical surface force balance (e-SFB) will be presented. Across multiple ionic liquid measurements, experimental distance resolution is sufficiently high that the 'squeezing out' of ion pair layers at a gold surface can be resolved. The gold surface was held at a variety of different potentials, and the stiffness of the ion pair layers was found to vary with potential whilst long-range forces were largely unchanged and remained repulsive at every potential.

This work helps resolve long-standing disagreement between AFM[1, 2] and SFB[3] force measurements of ionic liquids at potential controlled interfaces. A comparison of these results with prior measurements and existing models for understanding ionic liquids will be discussed in detail.

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The FFC-Cambridge Electro-deoxidation Process: Synthesis of Materials and Aspects of Sustainability

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Abstract

The FFC-Cambridge process is a generic molten salt electrolytic method that was invented at the Department of Materials Science and Metallurgy of the University of Cambridge around the turn of the millennium. It makes possible the direct conversion of metal oxides into the corresponding metals through the cathodic polarisation of the oxide in a molten salt electrolyte based on calcium chloride. The process is rather universal in its applicability, and numerous studies on metals, alloys and intermetallics have since been performed at the place of its invention and worldwide.

This presentation features some recent and ongoing research lines. The overarching theme is the harnessing of the FFC process for the synthesis of multinary materials that are difficult to achieve via conventional metallurgical methods. Systems of interest include high-entropy and other complex alloys and carbides for refractory applications, porous beta-titanium alloys for biomedical applications, and nanostructured silicon carbide for use as the lithium-ion battery negative electrode. Finally, the question is raised how the process needs to be operated to become sustainable.

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Molten salts versus organometallics for electrodeposition of Al-Mg alloys

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Abstract

Electrodeposition of industrially, fundamentally important Al-Mg alloys has been attempted with chloride-molten-salts and organometallics in literature. The organometallics can offer Mg-rich deposits; whereas the chloride-molten-salts offer Al-rich deposits. There has never been a study in literature that compares and understands the compositional trends between deposits and electrolytes in these systems. Such a comparison is the purpose of this work.

In the present work Al-Mg alloys are deposited using an organometallic-electrolyte and a chloride-molten-salt in an inert atmosphere. Using $Na[AlEt_4]+2Na[Et_3Al\text{-}H\text{-}AlEt_3]+2.5AlEt_3$+ 6toluene (where Et:–($C_2H_5$)) organometallic-electrolyte, they are galvanostatically deposited between 60-150 $mAcm^{-2}$ at 60, 90 °C using Mg anode and rotating Cu cathode employing a PAR 263 workstation [1]. However, using $62AlCl_3+17NaCl+15KCl+6MgCl_2$ (all concentrations in mol%) molten salt, Al-Mg alloys are potentiostatically deposited at 180 °C using Pt anode and Cu-strip cathode [2] between overpotentials of -1.05 and -1.30 V employing a CHI660E workstation.

The Al-Mg deposits from organometallic-electrolyte exhibit vast range of compositions between 5-55 atom% Mg with fcc Al(+Mg), hcp Mg(+Al) phases and $Al_{12}Mg_{17}$ intermetallic (minority). The deposits from chloride-molten-salt possess a maximum of 13.7 atom% Mg with Al(+Mg) and $Al_{12}Mg_{17}$. The results show that the phases possess strong dependency on the corresponding deposit compositions. This facilitates the construction of 'composition curves' – plots between the composition (and their ratios) of deposits versus those of the corresponding spent electrolytes. Such curves can provide several insights into these electrodeposition systems.

The Al-Mg deposits from organometallic lie in the Mg (less noble) preferential regime; whereas those from chloride-molten-salt transit from Al (more noble) preferential regime to the Mg preferential regime. This is because Al-Mg deposition from the organometallic requires extraction of Al^{3+} from $[Et_3Al\text{-}H\text{-}AlEt_3]^-$ which is sluggish. However, the chloride-molten-salt does not suffer from such as limitation rendering the transition of Al-to-Mg preferential regime possible in its composition curve. The present work shows that a subtle change in the electrolyte composition can yield wide deposit compositions with hcp Mg(+Al) phase from the organometallic system and with fcc Al(+Mg) phase from the chloride-molten-salt. This offers flexibility in choosing the electrolyte system based on the requirement for Al-Mg deposition.

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Technological and Industrial Progress of Recycling Secondary Tungsten Resources by Molten Salt Electrolysis

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Abstract

Addressing the shortcomings of existing recycling methods for cemented carbide, a novel approach utilising molten salt electrolysis for treating waste cemented carbide has been proposed. This achieves short-process recycling of the refractory metal tungsten as a secondary resource. Employing cemented carbide as a soluble anode, molten salt electrolysis enables the dissolution of tungsten and cobalt in ionic form, which are then deposited at the cathode, thereby realising short-process recycling of secondary resources. Initial research utilised the potential difference system between tungsten and cobalt dissolution/deposition to investigate their separation, proposing stepwise electrolytic separation. However, during scaled-up experiments, low cobalt concentrations and inadequate control of electrolytic conditions resulted in excessively prolonged cobalt separation times, hindering industrialisation. Consequently, a strategy was proposed involving rapid anodic dissolution, followed by co-deposition of tungsten and carbon at the cathode to form tungsten carbide and cobalt, thereby achieving phase separation. To better align with industrial production realities, molten salt electrolysis technology under air atmosphere was developed. The molten salt system was subsequently replaced with a multi-component molten salt system incorporating tungstate salts and sintered materials containing cemented carbide additives. This modification enhanced the universality and scalability of the system, apparatus, and process.

Corrosion Resistant Nickel-Chromium Alloy Generation From Dense Ionic Fluid Electrolytes

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Abstract

Nickel-Chromium (NiCr) alloy coatings have the potential to combine the corrosion resistance of traditional nickel coatings with the durability and wear characteristics of hard chrome coatings. However, electrodeposition of these coatings has traditionally, been difficult to achieve using aqueous hexavalent chromium based solutions due to the strong oxidative nature of hexavalent chromium and its unique electrodeposition conditions. Additionally, the use of hexavalent chromium in surface finishing is highly undesirable due to its extreme toxicity and the associated environmental impacts. Some attempts have previously been made to deposit these coatings from trivalent chromium-nickel salt solutions, but these attempts have largely resulted in oxide and hydroxide-rich deposits or exhibit limited Cr content. Using dense ionic fluid (DIF)-based electrolyte solutions containing trivalent chromium salts, nickel salts, and water, we have developed a novel method of depositing metallic NiCr coatings. The composition of these coatings can be tuned based on the current density used for electrodeposition and/or the composition of the electrolyte. These tuning methods allow for the rapid generation of coatings tailored for specific applications. Here, we show the electrochemical analysis of the deposition, deposit structure and properties, and assess corrosion behavior of these coatings.

The role(s) of deep eutectic systems towards greener technologies in life sciences

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Abstract

The concept of green solvents was introduced by John Warner and Paul Anastas, in 1998, when they listed the 12 principles of green chemistry. One of these principles assumes that the use of solvents, should be as an auxiliary substances, in the synthesis and preparation processes, and emphasises that they should be made unnecessary wherever possible, and if used they should be innocuous.[1] The sustainability of a process or a product is, hence, a result of the complex interaction between the product or process implemented and environment, technology and economy factors.[2] In the current scenario of a worldwide quest for sustainable and "greener" alternatives for current applications, in the past two decades the number of reports on NADES/DES applicability in various situations has rapidly grown. The tailor-made versatility of these eutectics, meaning in practical terms a wide range of chemical and physical properties, has resulted in promising studies applied in industry, biotechnology, cosmetics, pharmaceuticals, food, and health.[3]

In life science applications, several challenges arise. In particular, the formulation of therapeutic deep eutectic systems (THEDES) revealed to be very promising to enhance the characteristics of existing drugs and optimize new formulations that could be easily administrated and more effective, providing higher dissolution rates of the API, enhancement of solubility, permeability and absorption through tissues, or they can be incorporated in suitable polymer to potentiate the efficiency of biomedical devices. The use of DES as stabilizing agents has also paved its way in the biomedical field, as additives for blood preservation and in the cryopreservation of cells. In this communication, these different examples will be presented and discussed.

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Old Drugs, New Tricks: A New Approach to Drug Detection using Functional Ionic Liquids

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Abstract

Presumptive tests are ubiquitous in clinical and forensic laboratory settings. They usually have excellent sensitivity and good to very good specificity.[1] For many commonly used tests, a metal complex or organic molecule act as a catalyst for redox reactions or coordinates to the target drug molecule. These microchemical reactions have undergone rigorous validation[2] to ensure that they can produce reliable results among different illicit materials and doping agents, but they have seen little in the way of chemical development or innovation. Many presumptive tests also use concentrated acids such as sulphuric acid as the carrier solvent which present challenges in handling, preparation, safety and shelf life. Here we present a new class of presumptive tests combing similar microchemical reactions combined with intrinsic ionic liquids properties to increase promising properties for testing such as, solubilising power and shelf stability. Thus far, we have developed ionic liquid-based tests for numerous illicit materials, fig. 1, based on known tests such as the Scott's test for cocaine, Mandelin and Froehde tests which are multipurpose tests, Simons tests for primary and secondary amines, and the Chen-Kao test for phenylalkylamines. Investigation of their chemical, physical and reaction properties have been undertaken to compare to traditional presumptive tests current used in the sector.

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Modulating Protein Folding Landscapes: The Role of Ionic Liquids in Controlling Metastable States and Kinetic Traps

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Abstract

The therapeutic and industrial utility of proteins is frequently constrained by their escape from the native folding funnel into off-pathway aggregation landscapes. Traditional aqueous buffers provide limited control over these early misfolding events. Here we show that specially chosen ionic liquids (ILs) in aqueous solutions act as tunable physicochemical matrices that both reshape protein free-energy surfaces and kinetically regulate conformational search. We investigated how the “glassy” nature of some ILs - produced by high viscosity, strong ion pairing and altered dielectric screening - dramatically slows folding and unfolding trajectories, increasing solvent friction and reducing conformational diffusion. This kinetic deceleration reveals transient, partially unfolded intermediates otherwise too short-lived to detect, and promotes the formation of localized, structured “metastable kernels” that serve as precursors to oligomerization.

Using two model proteins systems extensively used in the protein folding community, SH3 domain and protein G B1 domain, combined with residue-resolved NMR spectroscopy, we demonstrate that ILs can stabilise these kernels via protective, ion-mediated solvation shells that mask hydrophobic patches and reorganize local solvent structure. By tuning ion identity, concentration and ion-pairing propensity we can trap kernels reversibly, preventing their maturation into irreversible amyloid-like fibrils or disordered aggregates. Crucially, the same IL properties that enable stabilization can be dialed to either minimize aggregation for biopharmaceutical formulations or to promote controlled, reversible assembly for materials applications. These results position ILs as programmable “molecular brakes” for the earliest stages of protein misfolding, offering both a platform to study nascent aggregation mechanisms with high temporal resolution and practical design rules for IL-enabled stabilisation or assembly.

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Piperonylic acid-based ionic liquids (PAILs) as synergists for insecticide formulations

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Abstract

In this work, we employed the Active Pharmaceutical Ingredient-Ionic Liquid (API-IL) concept for developing next-generation synergists that are both effective and environmentally safe. Herein, we synthesized 32 piperonylic acid-based ionic liquids (PAILs) through a clean, one-pot reaction using green methods and evaluated the ecotoxicity and synergistic activity of PAILs. We report 4 piperonylic acid derivatives, as innovative and eco-friendly synergists to attain more effective insecticide formulations. Notably, increased alkyl chain length of the cation in PAILs correlated with higher ecotoxicity. The applied computational methods indicated that imidazolium cations are less biodegradable and should be avoided, whereas quaternary ammonium ILs suggested greater biodegradability. Our in vitro assays revealed that piperonylic acid derivatives and PAILs displayed significant inhibitory activity on detoxification enzymes of Blattella germanica (German cockroach) connected to insecticide resistance. In vivo evaluation revealed synergistic efficacy of 4 piperonylic acid derivatives and three PAILs, comparable to a commercial synergist. In this work, we propose a novel approach to ecofriendly synergists through a combination of experimental and computational methods to evaluate the relationship between chemical structure and their properties such as ecotoxicity, biodegradability and biological activity.

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Methylimidazolium ionic liquids – a new class of forever chemicals?

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Abstract

Soil samples around a poorly-managed landfill waste site were examined for the presence of toxic chemicals using analytic screening (for known chemicals) and effect-based methods (for unknown chemicals). Extracts from some sample sites were toxic to mammalian cells in culture and the toxicity was traced to an 8C methylimidazolium cation (C8mim). Using the Cl^- salt of this ionic liquid (M8OI), it was shown that M8OI is concentrated into mitochondria and likely inhibits complex I of the electron transport chain – leading to cell death.

The toxicity of methylimidazolium ion liquids was also examined since shorter chain variants (C2 and C) are likely more useful industrially. These variants were less toxic to mammalian cells with toxicity related to chain length (longer chain, greater toxicity).

However, studies with fresh river water indicated that the short chain variants (C2, C4) were resistant to breakdown (over 7 weeks) although longer chain variants C8 and C10, whilst resistant, appear to be oxidised and mineralised to some extent.

Risk assessment of chemicals is a process strongly influenced by manufacturing levels. The development and change in use levels of new chemicals may be too fast for the assessment process to provide protection to the environment and human health. An assessment of environmental stability may be a good place to start for any new chemical that is expected to be used at high use levels.

Water-in-salts, a new family of electrolytes

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Abstract

Water-in-salt electrolytes (WISE) are solutions in which amount of dissolved salt by weight or volume is larger than the amount of water that these salts are dissolved in. In recent years they have sparked a lot of interest in energy community thanks to the extended stability voltage window (>3 V) that these aqueous systems can provide, thus enabling energy density approaching those of non-aqueous batteries. In order to understand their peculiar properties, molecular simulations offer very complementary information to spectroscopy and electrochemistry studies since they allow to study the dynamics and the reactivity of the systems and to link them to atomic-scale structural features. In particular, we have established that transport quantities such as diffusion coefficients or the electrical conductivity variation with increasing temperatures are largely due to the formation of large heterodomains consisting of lithium dissolved in water-rich regions on the one hand and fluorinated anions on the other hand.[1] The nanostructure of the liquid extends to the interface with electrodes, which can explain the changes of reactivity of the water molecules.[2] By using ab initio molecular dynamics simulations accelerated with enhanced sampling techniques, we have investigated the reactivity of the anion, providing a lead towards the first steps occurring upon formation of a solid electrolyte interphase at the surface of the electrodes.[3] More recently, we have extended this work to the case of non-fluorinated WISE, that provide an interesting alternative for catalysis applications.[4,5] Future work should leverage the use of machine-learning potentials to enable a more precise descriptions of the interactions at play while keeping reasonable computational costs.

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Molecular Structure, Dynamics, and Thermodynamics of Water-in-Salt Mixtures

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Abstract

A major limitation of ionic liquids (ILs) and deep eutectic solvents (DESs) in electrochemical devices is their inherently high viscosity. The addition of small amounts of water can significantly reduce viscosity, but at the cost of a diminished electrochemical stability window. Introducing inorganic salts into such mixtures can partially restore electrochemical stability, counteracting the adverse effects of water. The concept of deliberately engineering ternary, highly concentrated electrolytes for electrochemical devices is relatively recent, and many of their fundamental physicochemical properties remain poorly characterized. Here we systematically characterize the bulk properties of these mixtures, including phase behavior (solubility), thermal stability, viscosity, activity coefficients, and electrochemical performance. Using a surface force balance, we further reveal the emergence of well-defined nanostructures under confinement near charged interfaces, and correlate these confined (surface) structures with changes in bulk properties. Together, these results provide a mechanistic framework for designing low-viscosity yet electrochemically robust electrolytes, highlighting the promise of water-in-salt–type mixtures for next-generation electrochemical devices.

Thermoresponsive ionic liqulds endowing reversible overheating protection for lithium metal batteries

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Abstract

Ionic liquid electrolytes are intrinsically thermally safe and have excellent electrochemical properties. However, fabricating intrinsic safe batteries remains challenging. The lower critical solution temperature (LCST) electrolytes as a temperature sensitive matter have been reported to endow the thermoresponsive overheating protection for energy devices[1]. We have fabricated a thermoresponsive ion gel electrolyte enabling a gradually inhibited electrochemical reaction process from 80 °C to 110 °C, thereby, reducing the heat generation of the lithium metal batteries. When it comes to room temperature, the cell is reversible to work. The present LCST gel electrolytes could exhibit an in-situ ion blocking at 160 ºC within seconds, but it is reversible within 10 mins at room temperature. Notably, it is the first time to achieve ion transfer blocking in bulk phase electrolytes. The in-situ ion blocking mechanism is based on microphase separation in the bulk phase. It is different from the reported ones, which are relied on the thermoresponsive aggregates deposition on electrodes determining the ion transfer blocking in cells. Furthermore, the LCST system could regulate the thermoresponsive temperatures to be well matched with the characteristic temperatures during the thermal runaway process of batteries.[2] This has established an intrinsic overheat management capability for lithium-ion batteries in research. The aforementioned research provides a theoretical foundation for the various applications of ionic liquids in energy devices.

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Ionic liquid crystals as superior solid-state electrolytes

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Abstract

Developing electrolytes combining solid-like instinct stability and liquid-like conducting performance would be satisfactory for efficient and durable Li-ion batteries. However, the rational design of satisfactory electrolytes is still daunting challenge for efficient and sustainable energy devices, as ideal platforms for high-performance electrolytes remain to be explored. Herein lamellar lyotropic ionic liquid crystals (LLCs) demonstrate high-voltage windows, efficient charge transport, and inherent thermal safety as solid-state electrolytes in lithium-ion batteries. Lamellar LLCs are simply prepared by nanosegregation of $[C_{16}Mim][BF_4]$ and $LiBF_4$/PC liquid solutions, which induce lamellar assembly of the liquids as dynamic conducting pathways. Broadened liquid conducting pathways would boost the conducting performance of the LLC electrolytes. The lyotropic lamellar nanostructures enable liquid-like ion conductivity of the LLC electrolytes at ambient temperatures, as well as provide solid-like stability for the electrolytes to resist high voltage and flammability overwhelming to $LiBF_4$/PC liquid electrolytes. Despite minor consumption of PC solvents (34.5% wt.), the lamellar electrolytes show energy conversion efficiency comparable to the liquid electrolytes (PC wt. 92.8%) in Li/$LiFePO_4$ batteries under ambient temperatures even at a 2 C current density, and exhibit attractively robust stability after 200^{th} cyclic charge/discharge even under 60 ℃. The work demonstrate LLC electrolytes have a great potential to supersede traditional liquid electrolytes for efficient and durable Li-ion batteries.

Ion pairing restructures the electric double layer in water-in-salt electrolytes on graphite and alters capacitance

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Abstract

The structure and thickness of the electrical double layer (EDL) at carbon electrodes strongly influence electrochemical performance, yet remain poorly understood in concentrated aqueous electrolytes. Here we combine classical and quantum-mechanical molecular dynamics simulations with experimental analyses to resolve the interfacial organisation of aqueous LiCl from dilute to water-in-salt (WiS) (1-20 mol kg^{-1}) concentrations at graphitic electrodes, and compare with electrochemical differential-capacitance measurements from which the potential of zero charge (PZC) is obtained. We uncover a concentration-driven restructuring of the EDL: below 6 mol kg^{-1}, solvated Li^+ dominates the outer Helmholtz plane (OHP), but at higher concentrations co-adsorption of Cl^- through solvent-separated ion pairs enforces a near 1:1 Li:Cl ratio at the interface. This transition expands the effective EDL thickness, redistributes the interfacial potential drop, and drives a decrease in the PZC, matching the trend inferred from differential-capacitance measurements on electrolyte-graphite interfaces. Capacitance calculations reveal that while both EDL and quantum contributions vary strongly with concentration, their opposing trends make the total capacitance appear nearly constant for pristine few-layer graphite; for electrodes with smaller quantum capacitance, however, the concentration dependence of the EDL capacitance would be directly reflected in the total capacitance. Solvent-separated ion pairing is identified as the key driver of non-monotonic EDL behaviour in LiCl WiS electrolytes, establishing design considerations for tuning interfacial capacitance and stability in next-generation carbon-based aqueous energy storage systems.

Molten salt electrolysis of carbon dioxide

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Abstract

Molten salt is a unique electrolyte for CO_2 capture and utilization driven by green electricity. It has not only wide potential window and high ionic conductivity but also has adjustable CO_2 absorption capability, it is the only electrolyte to produce carbon materials directly from CO_2. In recent decades, the so-called MSCC-ET (molten salt CO_2 capture and electrochemical transformation) technology is developing in Wuhan University and where else. In this talk, the fundamentals and engineering aspects will be introduced base on our research in WHU. Firstly, the cathodic kinetics of CO_2 reduction in molten carbonates was identified and several pathways of accelerating reaction kinetics were proposed. Secondly, the anodic processes of different materials in the molten salts were discussed and a stable anode for oxygen evolution was determined. It was found that the concentration of oxygen anion in the electrolyte is crucial for the processes involved, i.e., CO_2. Capture, reduction kinetics and products, stability of inert anode, therefore, a basicity meter was designed. Based on the fundamental findings, a 10KA CO_2 electrolysis cell was constructed. The potential of its industrial application was further confirmed.

Acknowledgement

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Keywords

Molten salt electrolysis, Carbon dioxide capture and utilization, Electrolyte basicity, Inert anode

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Resource Recovery of Sulfate-bearing Solid Waste in Molten $CaCl_2$

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Abstract

The generation and accumulation of $CaSO_4$-bearing solid waste has become a pressing environmental challenge. Current treatment routes are often limited by high energy costs and the risks of secondary environmental pollution. Molten-salt processing offers a promising alternative because it can enhance reaction kinetics and lower energy consumption. Here, we develop a molten-salt-based approach for resource recover from $CaSO_4$-bearing solid waste, using molten $CaCl_2$ as the reaction medium due to its low melting point, high thermal stability, strong ionic conductivity, and excellent solubility for various Ca-based oxyanion salts.

To demonstrate the technical concept, we first quantified the solubility of $CaSO_4$ in molten $CaCl_2$, established phase relationship in the $CaCl_2$–$CaSO_4$ binary system, and elucidated the dissolution mechanism to provide a theoretical foundation for subsequent reaction studies. We then performed the carbothermal reduction of $CaSO_4$ dissolved in molten $CaCl_2$ and analyzed the reaction products. The results confirm that elemental sulfur (S) and SO_2 can be produced, which can be further utilized for sulfuric acid manufacture. Overall, this molten-salt-based approach provides a potential pathway for the mitigation and resource recovery of sulfate-based solid waste.

Removal of Rare Earth Element Impurities from LiCl-KCl Molten Salt via Oxidative Precipitation Using Gaseous and Solid Oxidants

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Abstract

During the electrolytic refining process of spent nuclear fuel, lanthanide fission products continuously accumulate in LiCl-KCl molten salt. This study employs oxidative precipitation technology to remove Ln(III) (La, Ce, Nd). Firstly, the combined use of air and H_2O(g) oxidation achieved effective purification of the molten salt at 773 K. Comparing different gas sparging conditions revealed that sparging can suppress the formation of a precipitate film at the interface. At a gas flow rate of 0.2 L/min, the removal efficiency of Ln(III) exceeded 99% within 18 hours. Mechanistic studies indicated that Ln(III) reacts with O_2 and H_2O(g) to form LaOCl, CeO_2, and NdOCl, respectively. Characterization showed that under natural oxidation, LnOCl grows with preferred orientation along specific crystal planes. Synchrotron radiation micro-CT provided the first in-situ visualization of product formation at the micron scale, elucidating the gas–liquid reaction mechanism. In a 500 g scale test, after 116.5 hours, the conversion rates for La, Ce, and Nd were 90.31%, 33.33%, and 18.30%, respectively. Subsequently, solid lithium oxide was used as an oxidizing agent for precipitation studies at 773 K. Increasing the O^{2-} concentration in the melt accelerated the reaction. When the Ln:O ratio was 1:1.5, the conversion rate of Ln(III) exceeded 99.9%. For a 500 g molten salt system containing 10% Ln(III), the addition of 1.5 times the stoichiometric amount of Li_2O achieved 99% removal within 1 hour. The precipitate accumulated at the bottom of the crucible and could be separated from the salt via high-temperature filtration. This technology has now been successfully applied to the removal of Ln ions from molten salt in batches of 20 kg, providing key experimental support for its engineering application.

Research progress in the separation of tungsten and cobalt by molten salt electrolysis of cemented carbide

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Abstract

To address the limitations of current cemented carbide recycling methods, molten salt electrolysis has been developed as a promising short-process technique for reclaiming tungsten and cobalt. This method leverages the difference in dissolution/deposition potentials of tungsten and cobalt to achieve separation, yielding nano-sized tungsten (less than 200 nm) and cobalt (less than 100 nm) powders. However, its large-scale application was initially hindered by low current efficiency.

To improve efficiency, active substances like Na_2WO_4 were added to the molten salt to increase tungsten ion concentration. For industrialization, calcined waste materials ($CoWO_4/WO_3$) were used as active substances, enabling electrolysis in an air atmosphere and enhancing anode dissolution. A challenge arose from the formation of Co_3W alloy impurities during deposition, which affected product purity. This was mitigated by adding carbonates to the molten salt, which provides a carbon source to promote the in-situ formation of tungsten carbide (WC), thereby preventing the alloying reaction and resulting in a composite of WC and cobalt powder.

Furthermore, the difficulty of collecting electrolytic powders from the molten salt was addressed by adopting liquid zinc as a fluid cathode, utilizing its fluidity and de-alloying effect to facilitate product recovery. The integration of these technologies has enabled the kilogram-scale regeneration of waste cemented carbide into reusable WC-Co composite powders.

Electrochemical Reduction of MnO to Metallic Mn in Molten Salt: Mechanism and Oxygen Transport

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Abstract

The sustainable production of metallic manganese (Mn) is important for advanced alloys, energy storage systems, and functional materials, yet conventional carbothermic processes are energy intensive and CO_2 emitting. Direct electrochemical reduction of $MnCO_3$ in molten salts is challenging due to multistep decomposition and gas evolution. Here, we present a controlled electrochemical pathway for Mn production in a NaCl-$CaCl_2$ molten salt at 750 °C, employing $MnCO_3$ as the starting material for the first time, via a MnO intermediate. $MnCO_3$ was first converted to phase-pure MnO through reductive calcination under H_2/Ar, confirmed by X-ray diffraction (XRD). Thermodynamic predictions using HSC Chemistry software indicated that MnO reduction occurs within the electrochemical stability window of the chloride melt. Electrochemical characterization of the blank electrolyte using cyclic voltammetry (CV) in a three-electrode configuration revealed a cathodic limit near -1.8 V (vs. Pt quasi-reference electrode), attributed to Ca^{2+} reduction. Further, the reduction of Ca^{2+} at -1.9 V produced calcium deposits on the Mo electrode. The physical stability of MnO pellets was evaluated by prolonged immersion (2-8 h) in the molten salt, showing minimal chemical dissolution and confirming their suitability for electrodeoxidation. To examine oxygen transport, CaO (2 wt %) was introduced into the melt; X-ray photoelectron spectroscopy (XPS) indicated dissolution of oxide species, demonstrating the electrolyte's ability to accommodate and transport oxygen ions during reduction. CV of MnO-containing melts exhibited a single cathodic peak at approximately -0.68 V and a corresponding anodic peak near -0.48 V, suggesting a direct Mn(II) → Mn(0) reduction pathway. Square wave voltammetry (SWV) was employed to enhance peak resolution and confirm the electrochemical process. Galvanostatic electrolysis was then performed in a two-electrode configuration at cell voltages of 2.8-3.0 V for 4-8 h, enabling progressive reduction of MnO to metallic Mn. Phase and compositional analyses using XRD, XPS, scanning electron microscopy (SEM), and energy-dispersive X-ray spectroscopy (EDS) confirmed the progressive formation of metallic Mn. These findings establish a viable molten salt electrochemical route for producing Mn from $MnCO_3$-derived MnO and provide mechanistic insight into oxygen ion transport and reduction behavior in chloride melts. The approach contributes to the development of lower-carbon electrometallurgical pathways for Mn and related transition metals.

Keywords: Molten salt electrolysis; MnO preparation; Oxygen ion transport; MnO electroreduction; Mn production

Compositional Control of Electrochemical Carbon Formation in Carbonate–Chloride

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Abstract

Carbonate–chloride molten salts provide a versatile liquid electrolyte platform for high-temperature electrochemical conversion of carbonates and CO_2 into solid carbon materials. Their electrochemical performance is strongly governed by salt composition, yet the influence of carbonate concentration and cation chemistry within chloride matrices remains insufficiently understood. This work examines how systematic variation of carbonate species and loading alters electrochemical behavior in mixed carbonate–chloride molten salts. Electrochemical properties are investigated using cyclic voltammetry and controlled electrolysis to evaluate carbonate reduction behavior, current response, and the onset of carbon formation. Differences in electrochemical activity are correlated with carbonate content and the nature of the alkali or alkaline-earth cation, revealing composition-dependent trends in reaction kinetics and reduction pathways. The role of carbonate dilution in chloride matrices is examined as a strategy to modulate carbonate availability while maintaining high ionic conductivity.

Probing the Effects of Current on Electrochemical Carbon Nanotube Synthesis in Molten Salt Electrolytes

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Abstract

Carbon nanotubes (CNTs) are hollow cylinders formed from one or more layers of graphene and have exceptional mechanical strength, electrical conductivity, and thermal conductivity. CNTs are utilized in a variety of applications ranging from energy storage to electronics and water purification. Electrochemical CO_2 reduction offers a pathway to the synthesis of CNTs as well as an avenue towards CO_2 capture, conversion, and utilization. A molten Li_2O electrolyte can capture CO_2 exothermically to produce Li_2CO_3, which can subsequently be converted to carbon species including CNTs via electrochemical reduction at high temperature (750 – 800 °C).

In this study, we investigated the impact of the magnitudes of constant current and pulsed current on the properties of CNTs synthesized in molten salt electrolytes. Constant current electrolysis was conducted at values corresponding to current densities of 100, 200, 500, 750, and 1000 mA/cm_2, while pulsed current electrolysis was carried out by alternating between a lower current density value of 5 mA/cm_2 and higher current densities (100, 200, 500, 750, and 1000 mA/cm_2). All the experiments were conducted in Li_2CO_3 molten salt electrolyte at 770 °C. The anode and cathode materials were nickel and iron, respectively. The synthesized products were studied by using a suite of characterization tools: Raman spectroscopy, X-ray diffraction (XRD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM). The results offer a key insight into the kinetics and reaction mechanisms of CNT nucleation which are critical in our next phase of reactor design and scaling up of the synthesis.

Ionic liquids as additives and electrolytes for hydrogen generation and transport

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Abstract

Steam methane reforming (SMR) is a well-established process and as the main method for industrial hydrogen production.

A viable alternative to that process is water electrolysis, which although still less energy-efficient, has major advantages: it produces no direct emissions, uses abundant and inexpensive materials and has been used on smaller scale for decades. In order to tackle these problems, we have engaged in a multidisciplinary European research project, named ENDURION.

ENDURION aims to develop an efficient, durable, and cost-effective pressurized electrolyser through the use of novel cell-stack design, utilizing CRM-free materials and up-scalable processing methods to achieve energy consumption of below 50 kWh/kg H_2 with degradation as low as <0.7%/1000 h.

Ionic liquids are attractive electrolytes and electrolyte additives for the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) in such electrolysers because they provide unique control over the electrochemical interface and reaction environment. In HER, certain ionic liquids facilitate proton transfer and stabilize adsorbed hydrogen, while in OER they can strengthen catalyst stability by suppressing metal dissolution and surface corrosion at high potentials. Furthermore their relatively high gas solubility and viscosity can reduce bubble accumulation at electrode surfaces, improving active site utilization.

Another way to produce green hydrogen with help of ionic liquids is through reduction of aqueous solutions of CO_2. The ILs help to regulate the overpotential on the electrodes and thus modify the selectivity of the reaction; depending on the IL mixture used we can produce from almost pure hydrogen over syngas to almost pure CO.

In order for the so produced hydrogen to be transported and stored it needs to be compressed. And this is a further point where ionic liquids come into play. Since they have high thermal stability, very low vapor pressure and compressibility, some ILs that have low hydrogen solubility are well suited for this application. A liquid piston hydrogen compressor has the advantage of having considerably less moving parts (500 *vs* 10), a longer service life, and energy costs can be reduced up to 20% compared with standard reciprocating compressor. This technology has been already brought to the market by the company Linde.

In our presentation we will present the view and research results of a company, specialized in the synthesis and technology development in the field of ionic liquids, which has been on the market for almost 20 years on its way to future technologies.

Molten salt-promoted Ni-Fe/Al2O3 catalyst for methane pyrolysis

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Abstract

Bimetallic Ni-Fe/Al_2O_3 catalysts were prepared by the molten salt method, and the catalytic performance of the Ni-Fe/Al_2O_3 catalysts with KCl-$NiCl_2$ melt for methane pyrolysis was evaluated at 800 °C. The catalysts and carbon products were characterized by XRD, SEM/EDS, XRF and Raman spectroscopy techniques. The results show that molten salt-promoted Ni-Fe/Al_2O_3 catalysts exhibit high activity and long-term stability up to 1000 min on stream without any deactivation. The carbon products over the molten salt-promoted Ni-Fe/Al_2O_3 catalysts are in the form of small granular particles instead of filamentous carbon for the catalyst without molten salt. The promotional effect of the molten salt may attribute to the higher wettability of the Ni-Fe alloy by molten salt, which can prevent the catalysts from deactivation due to carbon encapsulation.

Multifunctional Conjugated Polymers: Integrating Molecular Engineering and Ionic Liquid Processing for Next-Generation Organic Electronics

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Abstract

Plastic electronics has experienced remarkable commercial and scientific progress over the past decade, driven by emerging applications including organic field-effect transistors for flexible backplanes and e-paper displays, as well as organic photovoltaics for lightweight and large-area energy harvesting. A key enabler of this progress has been advances in processing strategies, including solution processing in unconventional media such as ionic liquids and deep eutectic solvents, which offer tunable solvation environments, reduced volatility, and improved control over polymer assembly and film formation. The field of π-conjugated organic semiconductors has advanced significantly due to extensive efforts toward developing cost-effective, solution-processable, and mechanically flexible electronic materials. Among these materials, alternating donor–acceptor (D–A) conjugated polymers have attracted considerable attention owing to their tunable optoelectronic properties and compatibility with scalable printing technologies. Through careful modification of donor and acceptor building blocks, it is possible to systematically tune frontier molecular orbital energy levels, broaden absorption profiles, enhance backbone coplanarity, and improve interchain connectivity, ultimately leading to superior charge transport characteristics and enhanced photovoltaic power conversion efficiencies.

In this work, we report the design and synthesis of a new generation of conjugated polymers incorporating highly electron-deficient building blocks, including thiazole-functionalized rylene imides and benzothiadiazole derivatives, for advanced organic electronic applications. Molecular engineering strategies were employed to optimize polymer planarity, intermolecular interactions, and solution processability while maintaining excellent thermal and electrochemical stability. Computational studies revealed that incorporation of thiazole moieties increases the electron-deficient nature of the conjugated backbone and promotes favorable molecular packing, enabling efficient electron transport in all-acceptor and donor–acceptor polymer systems.

Beyond molecular design, this work also systematically investigates the role of ionic liquid-inspired processing media in conjugated polymer synthesis and thin-film formation. These unconventional solvent systems provide highly tunable ionic environments that can influence polymerization kinetics, aggregation pathways, crystallinity, and nanoscale morphology, while also enabling more sustainable processing by replacing volatile organic solvents. The strong ion–dipole and π–ionic interactions inherent to these media facilitate improved polymer organization and enhanced charge transport pathways within the resulting semiconducting films.

The developed conjugated polymers exhibit excellent solution processability and promising electronic performance for applications in OFETs, OPVs, energy storage, and emerging flexible electronic technologies. This work highlights the synergistic combination of advanced conjugated polymer design with ionic liquid-inspired processing strategies as a powerful route toward sustainable, high-performance organic electronic materials.

Decoupling network mechanics from ion transport in ionogels through preferential interactions

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Abstract

In the past few decades, there has been a revolution in soft matter that has given us new materials with outstanding properties such as shape memory, self-healing behaviour, and ultra tough tensile strength. Many of these properties arise from the collective power of dynamic, molecular-scale interactions. This talk focuses on soft gel materials prepared from highly cross-linked polymers and ionic liquids. These materials are named ionogels and their properties are very different to traditional gels such as hydrogels or organogels because they are highly conductive and not susceptible to evaporation. Hence, they are excellent candidates for flexible electronics such as ionic skins, actuators, and sensors. In this work, we show how to decouple two properties—network mechanics and ion transport—that are intrinsically linked because they originate from solvent-polymer interactions pre- and post- polymerisation. The decoupling arises from preferential interactions from solvent mixtures, which can be exploited to access new property combinations that would not otherwise exist with single solvents. We use a range of analytical methods to pry apart the complex molecular interactions in ionogels (e.g., cation-anion, ion-polymer, polymer-polymer)[3] to help understand how they influence structure, transport properties, and surface composition. This talk gives a comprehensive overview of ionogel properties and rationalises them in terms of molecular scale interactions, which is important for the design of emerging soft materials or gel polymer electrolytes for energy applications.

Hydrophobic Eutectic-based Soft Materials: a Green Strategy for the Removal of Emerging Water Contaminants

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Abstract

Water is indispensable for life, yet only 40% of surface water bodies currently achieve a "good ecological status," emphasizing the pressing need for more effective pollution monitoring and remediation strategies.[1] Conventional methods for the removal of emerging industrial contaminants often rely on toxic solvents and poorly sustainable sorbents with limited capacity.

In this work, hydrophobic (deep) non-ionic eutectic solvents (HES) are proposed as greener alternatives. Readily prepared from mostly renewable precursors, HES are characterized by 100% atom economy, high sustainability and remarkable dissolution abilities. To expand their practical use, two HES-based materials were developed: hydrophobic supramolecular eutectogels (HEG), obtained through the self-assembly of a low-molecular weight gelator,[2] and HES-loaded cellulose nanosponges (HECS), which integrate HES within environmentally benign nanostructured cellulose aerogels.[3] Both pristine and hybrid materials were thoroughly characterized and evaluated for the extraction of phthalates (DEP) and phenols (BPA) from model aqueous samples. The systems exhibited encouraging performance, enabling efficient contaminant removal while minimizing solvent leaching.[4]

The development of HES-based hydrophobic eutectogels and cellulose nanosponges represent a significant advancement in sustainable water treatment technologies. By addressing key limitations of current extraction methods, this study introduces safer, more efficient, and eco-friendly materials for the removal of hazardous pollutants. These platforms hold strong potential for contributing to global clean water goals and for further progress in the field of green chemistry.

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Low-Melting Ionic Solids for Energy and Optoelectronics: A Structural and Optical Correlation

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Abstract

Low-melting metal halides templated in ionic liquids are a tunable class of organic-inorganic hybrid compounds. These halometallates combine the structural flexibility and non-volatility of ionic liquids with the functional chemistry of metal halides, enabling interesting optical and ionic transport properties. These materials also provide easy access for dissolving and processing them, enabling promising applications in optoelectronics, catalysis, metal deposition, and energy systems.

In this presentation, I will discuss the structure–property relationships of two halometallate compounds probed by different optical spectroscopies (steady-state and time-resolved) with X-ray absorption, complemented by structural and thermal analysis. The studies reveal how local coordination geometry, halide composition, and cation identity govern lattice dynamics and electronic coupling. Finally, I will show some applications of these flexible functional solids in the development of next-generation optoelectronic materials.

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Beyond Robeson, Beyond Downhill Diffusion: Molten-Salt Membranes for CO2 Capture

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Abstract

This talk will describe our work on supported molten-salt membranes, which we have established as high-temperature carbon dioxide separation media capable of overcoming the permeability–selectivity (Robeson) upper bound and meeting the performance metrics required for economically viable post-combustion carbon dioxide capture. By tuning membrane composition, wettability, and pore geometry, and coupling these with transport modelling, our research elucidates coupled ionic–molecular transport, interfacial resistances, and self-healing phenomena arising from capillary retention and dynamic wetting. The membranes demonstrate stable CO_2/N_2 separation at process-relevant temperatures with suppressed degradation pathways. Our recent work introduced a new paradigm for dilute CO_2 capture, i.e., directly from air: the humidity-driven membrane, in which ambient energy in the form of a humidity gradient is exploited to drive CO_2 "uphill", against its concentration difference. Our current research focuses on reducing operating temperature while maintaining performance, by tuning molten-salt composition.

Development of electrochemical sensors for in-situ free oxygen monitoring in molten chloride media for pyrochemical fuel cycle applications

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Abstract

Nuclear energy is experiencing renewed interest, including advanced reactor concepts targeting improved fuel utilization and reduced waste inventory. As novel fuels emerge, alternative reprocessing strategies beyond aqueous PUREX become increasingly relevant. Pyrochemical processing in molten salts is considered a promising approach due to its tolerance to complex fuel compositions, reduced criticality constraints, and compatibility with high heat load fuels. The two principal pyrochemical processes, electroreduction and electrorefining, rely on controlled electrochemical transformations in high-temperature molten chloride media.

Concentration of dissolved oxygen species and oxygen-containing impurities play a critical role in both processes. In electroreduction, oxygen ion activity is needed, directly influencing process efficiency, while in electrorefining it needs to be avoided as it reacts with actinide salts. Despite this importance, reliable in-situ quantification of free oxygen ions under operating conditions remains a major challenge.

Electrochemical sensing has proven to be among the most reliable techniques. However, the uncertainties associated with determining the working electrode (WE) area are a considerable restriction. This study focuses on the development of a sensor for LiCl-KCl, at low oxygen concentrations. Experiments aimed at obtaining a constant active area by plating the sensor material into a substrate that responds to dissolved O^{2-} on a different potential region. The electrochemical response on W, Mo, Ni, Au and glassy carbon (GC) was studied. The clear peak separation between Au and GC led to the development of a Au plated glassy carbon (AupGC) WE. This sensor exhibited a proportional and distinguishable response to O^{2-} ion content from 50 to 750 ppm both in cyclic voltammetry (CV) and square wave voltammetry (SWV), with the Au response remaining independent from the immersion depth (Figure 1).

The AupGC sensor concept could prove to be an advantage for pyrochemical applications, as well as molten salt reactor systems, which could benefit from an active surface independent from salt level. However, further studies into optimization of the plating conditions, stability and applicability to different salt types would be required to enable reliable operational use.

Study of a molten carbonate salt for trapping gaseous fission products from a molten salt nuclear reactor

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Abstract

One distinctive feature of molten salt reactors is the use of a liquid fuel consisting of molten salt. This allows elevated temperatures to be reached at atmospheric pressure. In this design, gaseous fission products are continuously extracted by bubbling a neutral helium gas through the salt. This inert atmosphere is essential for the proper functioning of a molten salt reactor. Helium is typically employed as a sparging and cover gas because of its chemical inertness and extremely low neutron absorption cross-section.

The inert gas used becomes progressively loaded with radioactive gaseous fission products and the decay products of these aerosols as well as volatile chlorinated compounds such as Xe(g), $ZrCl_4$(g) and Cd(g). To ensure stable operation, the inert gas must be regularly purified before being reinjected into the reactor core. This is achieved through a dedicated gas management system comprising several purification stages.

This research focuses on a specific stage of the purification process involving a high-temperature scrubber. This involves bringing the contaminated cover gas into contact with a reactive liquid medium that can chemically trap volatile species. Helium is bubbled through this medium to encourage the transfer of matter between the gas and liquid phases, and to facilitate the chemical reactions that convert volatile contaminants into stable, non-gaseous forms which are then either dissolved in the liquid or precipitated as solids. However, given the low boiling point of water and the high temperatures generated by the radioactive decay of fission products, aqueous solutions cannot be used. This is why the use of molten salts is being considered.

The concept of molten salt scrubber was previously explored in MSBR using molten hydroxides [1]. However, these are unstable at high temperatures above 550 °C and undergo strong thermal decomposition producing water. They are also highly corrosive and prone to radiolysis. This is why the focus of this research is on the binary eutectic carbonate mixture Li_2CO_3 – Na_2CO_3 (52 – 48 %mol) used at 600 °C. The ternary $(LiNaK)_2CO_3$ mixture was also studied but was not chosen due to the presence of potassium, which cannot be handled by current methods of treating high-level nuclear waste.

Thus, the behavior and trapping capacity of several elements originating from gaseous fission products such as Cs, Rb, Ba, Sr, La, Mo, Sn and Se in this carbonate molten salt were examined through thermodynamic calculations, electrochemical measurements, ICP-OES spectroscopy and XRD crystalline phase characterization.

Machine Learning-Based Molecular Dynamics Study of f-Block Element-Containing Molten Salt Systems

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Abstract

Among dry reprocessing technologies, molten salt electrorefining is considered as a particularly promising approach for separation of nuclides like uranium and plutonium from strongly radioactive spent fuels like oxides and metals. To improve the separation efficiency of actinides, there is an urgent need to explore the coordination chemistry of f-block elements and their potential impact on the microstructure and macroscopic properties of molten salts. The high computational cost of ab initio molecular dynamics (AIMD) poses a major challenge for large-scale molten salt simulations, especially for predicting macroscopic properties. Moreover, simulating actinide-containing molten salts requires consideration of relativistic and strong electron correlation effects. Machine learning (ML) based MD simulation represents a new paradigm in computational chemistry and materials science. By training models like neural network with high-precision AIMD data, ML potential (MLP) that combine AIMD accuracy with classical force field efficiency can be constructed [1-3]. With reliable MLPs, it becomes feasible to simulate complex molten salt systems at large spatial and temporal scales, aiding in uncovering microscopic structures and dynamic behaviors that are difficult to capture using traditional theoretical methods. In recent years, ML based MD simulations have been increasingly applied to lanthanide and actinide-bearing molten salt systems [4-6].

Our research has developed a series of accurate ML potentials capable of describing molten salt systems such as LiCl-KCl-$CsCl_3$-MCl_3 (M = La, Nd) and LiCl-KCl-MCl_3 (M = U, Np, Pu) [4-7]. Based on large-scale MD simulations with MLPs, we investigated the coordination structures and species distribution of actinide and lanthanide ions as well as their time dependence in molten salts. The macroscopic properties such as density, viscosity and diffusion coefficients of actinide and lanthanide ions have also been simulated. As to LiCl-KCl-MCl_3 (M = U, Np, Pu), U^{3+} ions were found to possess average coordination numbers ranging from 6.20~6.33, and those for Np^{4+} ions range from 6.07~6.24. These two ions both prefer to form 6-coordination structures from 723 to 923 K; However, for Pu^{3+} ions, the 7-coordination structure becomes dominant within a temperature range of 773 K ~ 1073 K, and the average coordination numbers reach about 6.11~6.62. Increasing temperature primarily drives the transformation of the higher-coordinated $[PuCl_7]^{4-}$ into the lower-coordinated $[PuCl_6]^{3-}$.

Structural Heterogeneity in Ionic Liquids and Its Role in Transport

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Abstract

Several molecular simulation studies have consistently reported the presence of medium-range ordering in ionic liquids (ILs), indicating the existence of persistent microscopic domains within the liquid phase. In addition, the sluggish dynamics and long-lived local environments observed in these systems resemble features typically associated with glassy states. A range of experimental observations, including thermophysical properties such as viscosity, diffusion, and electrical conductivity, further support this picture of structural and dynamic heterogeneity.

These observations raise the question of how such heterogeneous organisation can be described in a consistent way, and to what extent it is relevant for macroscopic behaviour.

In this keynote, atomistic molecular dynamics simulations will be used to characterise the structure of ionic liquids in different environments, including the pure liquid and systems containing small molecular solutes. Particular attention will be given to medium-range ordering, the persistence of local environments, and their representation through structural descriptors.

Rather than assuming direct structure–property relationships, the discussion will focus on how these descriptors can be used to analyse trends in transport properties such as diffusion and viscosity. This approach is relevant for systems where transport plays a central role, including electrolytes for lithium- and sodium-based applications and the interaction of ILs with small molecules such as CO_2.

Clarifying the role of structural heterogeneity remains an open question and a necessary step towards a more consistent understanding of ionic liquids.

Phosphate removal from high-phosphorus iron ore in molten $CaCl_2$

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Abstract

High-phosphorus iron ore is abundant in many countries but underutilized because phosphate is tightly associated with iron minerals and must be strictly limited in steelmaking. Existing phosphate removal routes are often complex and energy-intensive, limiting their suitability for sustainable metallurgy. This study proposes a process integrating molten $CaCl_2$ leaching with carbothermal reduction to achieve efficient dephosphorization and enable phosphorus recovery. In the first stage, molten $CaCl_2$ selectively leaches phosphate-bearing phases from iron ore, concentrating phosphate in the molten-salt phase. In the second stage, carbon-based reductants remove phosphate from the melt via carbothermal reduction. The proposed route offers a cleaner, potentially resource-recovering strategy for utilizing high-phosphorus iron ore.

Corrosion-Resistant Microplasma Anode Array for High-Temperature Molten Salt Electrolysis and In-Situ Analysis

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Abstract

Nuclear energy offers high energy output with minimal CO_2 emissions and its sustainable development highly relies on the reprocessing of spent fuel to recycle uranium sources. Molten salt electrolysis is a promising process for uranium separation and recovery, especially for the uranium oxide and metallic fuel of fast reactors. The electrolytic reduction of spent nuclear fuels faces two major challenges: the lack of corrosion-resistant anode materials and the difficulty in monitoring molten salt composition. This work introduces a gaseous microplasma anode for the electrochemical reduction of UO_2 in LiCl-Li_2O molten salt, achieving a high reduction degree. Compared to traditional anodes (Pt, C, Mo, W), the microplasma anode demonstrates superior corrosion resistance, maintaining stability for over 150 hours, while Pt electrode with a diameter of 1 mm could only work for less than 1.2 hours. Cost analysis indicates that replacing Pt with the microplasma anode reduces the anode cost by more than 90% for processing 1 kg of UO_2. Crucially, it enables *in situ* monitoring of salt composition via atomic emission spectroscopy collected from the plasma. To address industrial-scale needs, a microplasma array was designed, successfully amplifying the electrolysis current from 25 mA to 100 mA while allowing multi-point regional monitoring. This study presents the microplasma anode as a promising, cost-effective solution that simultaneously ensures long-term operational stability and enables real-time compositional analysis in high-temperature molten salt electrolysis.

Dual chemical and physical study on the reaction between rare earths elements and molten sulfates

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Abstract

Recycling rare earth elements (REEs) from urban waste streams is becoming increasingly critical in the context of resource sustainability and supply security. Molten salt processes have emerged as promising routes for REE recovery. In particular, molten salts have been used for the recycling of REEs from NdFeB permanent magnets[1,2].

Oxygen-containing molten salts, such a molten hydroxydes, carbonates or sulfates offer a promising solution for the recycling of devices present in urban mines as they are capable of degrading organic matter into graphite[3] which could enable the treatment of complex materials found in urban mines.

Among these systems, molten sulfates have shown strong potential for REE extraction from complex matrices[4,5]. However, the degradation of organic components may lead to the formation of graphite coatings on REE-containing particles, which may significantly modify their chemical reactivity in the molten salt environment. A detailed understanding of the chemical and physical interactions between REEs and molten salts, as well as the influence of graphite coatings on these interactions, is therefore required to assess the viability of these processes.

In this work, we investigate the reaction pathways between rare earth oxides (REOs), with a focus on CeO_2, and oxygen-containing molten salts, combining chemical and morphological analyses to understand the reaction mechanisms, and evaluate the impact of graphite coatings.

In this presentation, we will show the results obtained by using molten sulphates ($KHSO_4/K_2S_2O_7$), that reveal a rapid, multistep reaction sequence leading to the formation of cerium sulfate phases (Fig 1)[6].

In contrast, graphite-coated CeO_2 nanoparticles exhibit strongly different reactivity in the same molten sulfate medium offering insights into the viability of this method for a recycling process. Ongoing studies aim to elucidate the detailed mechanisms governing these reactions and to correlate chemical reactivity with particle morphology and surface evolution. A combination of complementary characterisation techniques, including X-ray diffraction (XRD), small-angle X-ray scattering (SAXS), scanning electron microscopy (SEM), electrochemical measurements, differential scanning calorimetry (DSC), and thermogravimetric analysis (TGA), is used to achieve a comprehensive understanding of the studied systems.

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Microplasma electrochemical method for the extraction of critical metals from molten salts

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Abstract

A novel gaseous electrode utilizing microplasma based on glow discharge has recently emerged as a focus of significant research interest. Characterized by its compact size, this electrode can operate efficiently at room temperature and atmospheric pressure, offering key advantages such as low cost, operational simplicity, and stable performance. Distinct from conventional solid electrodes, it employs a plasma gas jet for charge transfer, eliminating the need for direct contact with the electrolyte. This unique non-contact discharge mechanism minimizes electrode-electrolyte interaction, thereby granting exceptional corrosion resistance and positioning it as a highly promising anode for molten salt electrolysis. When applied as cathodes, metals can be electro reduced to form nanoparticles in the molten salt instead of on the solid electrodes. Furthermore, the microplasma also functions as an effective excitation source for conducting atomic emission spectroscopy on metal ions within molten salts. Based on these advantages, we have applied the microplasma electrode in the reduction of uranium ions, uranyl ions and uranium oxides.

How Many Neighbors? Alkali cation solvation in [BMIm][NTf_2] revealed by Raman spectroscopy

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Abstract

Room-temperature ionic liquids (RTILs) have emerged over the last decades as attractive alternatives to conventional molecular solvents due to their negligible vapor pressure, wide electrochemical windows and tuneable physico-chemical properties[1]. Among them, imidazolium-based ionic liquids built from weakly coordinating anions such as bis(trifluoromethane)sulfonimide (NTf_2^-) are of particular interest for applications involving strong acidity and highly reactive ionic species. In such media, the nature and extent of ionic solvation play a key role in controlling reactivity, yet remain difficult to quantify[2]. In contrast to molecular solvents like water, where small ions are strongly solvated by extended hydrogen-bond networks, ionic liquids provide a highly structured but weakly coordinating environment. As a result, the solvation of small cations, including protons and alkali metal ions, is expected to differ markedly from aqueous behaviour, with important consequences for acidity, ion pairing and transport properties[3,4]. For the proton, we demonstrated that a unitary solvation number is obtained in the ionic liquid [BMIm][NTf_2], indicating coordination to a single NTf_2^- anion[5]. This weak solvation contrasts sharply with aqueous systems and provides a direct spectroscopic explanation for the super-acidity commonly experienced in NTf_2^--based imidazolium ionic liquids. In this communication, we report a systematic investigation of the solvation numbers of monovalent cations (H^+, Li^+, Na^+, K^+, Rb^+ and Cs^+) in [BMIm][NTf_2] derived from *in situ* far-field Raman spectroscopy. Extension of our experimental approach to alkali cations beyond proton reveals systematic trends in coordination numbers across the series, reflecting the balance between ion size, charge density and anion affinity in low-solvating medium, providing direct, non-invasive and fundamental insight into ion–solvent interactions in [BMIm][NTf_2].

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Modification of ionic transport in *N*-alkyl-4-cyanopyridinium ionic liquids through formation of charge-transfer complexes with polyaromatic hydrocarbons

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Abstract

Previously work has shown that ionic liquids with *N*-alkyl-4-cyanopyridinium cations form charge-transfer complexes on the addition of polyaromatic hydrocarbons such as 1-methylnaphthalene.[1,2] Here, we explore the impact of supramolecular aggregation as a modifier for viscosity and conductivity across a series of *N*-alkyl-4-cyanopyridinium bis(trifluoromethylsulfonyl)imide ($[C_n{}^4CNPy][NTf_2]$)/1-methynaphthalene charge transfer complex liquids as a function of the *N*-alkyl chain from methyl to butyl).

Strikingly, neat $[C_2{}^4CNPy][NTf_2]$ has anomalously high viscosity *and* conductivity compared to the other members of the series. However, formation of charge transfer complexes with 1-methylnaphthalene suppresses the variations in viscosity and conductivity across the series of ionic liquids leading to convergent transport profiles (see Fig. 1) that reveal how π-π interactions reshape nanoscale structure and dynamics.

Figure 1: Variation in viscosity between neat $[C_n{}^4CNPy][NTf_2]$ (open symbols) and $[C_n{}^4CNPy][NTf_2]$)/1-methynaphthalene mixtures (filled symbols) showing the convergence in viscosities in the CTC mixtures.

The impacts of cation-aromatic aggreggation in the liquid CTC formation on thermophysical and electrochemical behaviour will be described, drawing on results from electrochemical impedance spectroscopy and $^1H/^{19}F$ DOSY NMR to explore the ion dynamics that suggest a role of ionic liquids cations with high π-electron affinities as surface modifiers for graphitic materials, for example electrodes.

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AI-Screening of Ionic Liquids for Task-Specific applications

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Abstract

Ionic liquid applications such as reactive separations, gas capture, catalysis, biomass processing, and electrochemical systems require solvents that simultaneously satisfy multiple performance and feasibility criteria. These typically include high decomposition temperature (Td), low melting point (Tm), manageable viscosity (η), acceptable cytotoxicity (Cy), and favorable solute–solvent interactions expressed through infinite-dilution activity coefficients (γ∞). Although ionic liquids (ILs) offer exceptional tunability and properties for a wide range of applications, their vast chemical design space makes it difficult to identify and rank suitable candidates, particularly when multiple constraints must be satisfied simultaneously.

In this work, we apply two complementary artificial intelligence models to enable large-scale screening of ionic liquids and extract structure–property insights from the screened chemical space. First, ILBERT, a BERT-based chemical language model, is used to predict key physicochemical properties of ILs. ILBERT leverages pre-training on more than 31 million unlabeled IL-like structures and data augmentation strategies to address the scarcity of labeled IL datasets, and has been benchmarked to outperform alternative machine learning approaches across twelve IL property prediction tasks [1]. Second, a temperature-dependent graph neural network (GNN-T) is used to predict infinite-dilution activity coefficients (γ∞) of solutes in ILs. GNN models are particularly suitable for mixture screening because they learn molecular graph–property relationships and can generalize to ILs and solutes not seen during training, while remaining competitive with state-of-the-art recommender systems and outperforming classical activity-coefficient models [2].

A combinatorial library containing approximately 20 million IL candidates was constructed to screen solvents for CO_2 hydrogenation to methanol. The ILBERT and GNN-T models were used to predict IL properties under application-relevant conditions and predefined feasibility constraints. A weighted multi-criteria ranking framework was implemented to account for application-specific requirements, allowing constraints and property weights to be adjusted depending on the target technology.

This workflow reduced the initial library of 20 million candidates to the top 100 ILs for methanol synthesis within minutes. In addition, statistical analysis of the screened library was used to quantify how ion families and functional groups influence individual predicted properties and overall ranking performance. These trends provide actionable insights into which chemistries are most likely to satisfy multiple constraints simultaneously, improving interpretability of screening outcomes and supporting rational IL design. Overall, this study demonstrates how a machine-learning-based framework can compress a vast IL design space into a small, interpretable shortlist, accelerating solvent discovery for diverse chemical technologies.

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Ionic liquid and solvent design for chemical recycling of plastic-containing packaging

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Abstract

Plastic is a pressing global challenge of today's society. Global plastics production doubled from 234 to 460 million tonnes between 2000 and 2019, while plastic waste increased from 156 to 353 million tonnes over the same period.[1] UNEP estimates that less than 10% of plastic waste is ultimately recycled, leaving most plastic waste landfilled, incinerated, mismanaged or leaked to the environment.[1,2] Packaging is central to this challenge, accounting for around 40% of global plastic waste and spanning formats from rigid containers to flexible pouches.[1]

Mechanical recycling by melt reprocessing remains the main established method for plastic waste recycling, but its effectiveness is limited by polymer degradation, mixed feedstocks, contamination, additives, colour build-up and inconsistent recyclate quality. These limitations are particularly acute for plastic-containing packaging, which is a heterogeneous and deliberately engineered feedstock. Packaging materials combine polymers, additives, adhesives, coatings, barrier layers, inks and contaminants within formats designed for performance rather than end-of-life recovery. This complexity demands recycling strategies that are matched to both polymer chemistry and packaging architecture.

This requires clear strategies that decouple plastic production from plastic pollution and fossil-resource extraction. To meet growing pressure for higher plastic recycling rates, chemical recycling technologies must be developed as part of an integrated system, rather than as isolated solutions.[3] In this context, ionic liquids and related solvent systems can play an important role as tunable media for chemical recycling, separation and delamination.

In this contribution, we present recent work on ionic-liquid and solvent design for plastic recycling. Solvent screening was used to identify effective, low-cost ionic-liquid systems for the depolymerisation of PET into terephthalic acid and ethylene glycol, with a waste-minimised approach based on low-cost ionic-liquids.[4] In addition, the design and use of alkylphosphonium ionic liquids to stabilise and enhance enzymes for the depolymerisation of PET and polyurethane at temperatures up to 90 °C will be showcased. Finally, we extend the discussion to solvent design for delaminating and recycling plastic-containing multilayer packaging, including general considerations on how constraints influence technology development.

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Charge and proton transfer in ionic liquids

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Abstract

Understanding why protic ionic liquids behave as they do remains a central challenge for both experiment and theory. Their conductivity, viscosity, and structural organization are governed by a subtle balance of hydrogen bonding, ion pairing, solvation, and proton exchange, phenomena that are strongly coupled and highly dynamic. Experiments probe the consequences of this complexity with increasing precision, but translating these observables into a molecular-level picture is far from straightforward.

Recent advances in molecular simulation help bridge this gap. While classical fixed-charge molecular dynamics simulations provided valuable structural insight, it often gives a poor description of dynamics because electrostatic interactions are too strong, leading to overly rigid local structures and overestimated viscosity. Polarizable force fields overcome this limitation by allowing the electronic structure to respond to the local environment. This greatly improves the description of transport and structure, and it also leads to effectively reduced Coulomb interactions, an effect that may resemble charge transfer, although it originates from explicit polarization.

For protic ionic liquids, however, polarization alone is not enough. Their conductivity is often shaped by proton transfer through hydrogen-bond networks, that is, by Grotthuss-like hopping in addition to ordinary vehicular motion. I will therefore discuss how polarizable force fields can be combined with the PROTEX reactive molecular dynamics framework, in which protonation states and molecular topologies are updated based on quantum-chemically derived reaction probabilities. This makes it possible to simulate complex reactive networks on length and time scales relevant to experiment.

Applications to systems such as 1-methylimidazolium acetate show that this combined approach can reproduce experimental conductivity and reveal the microscopic origin of efficient charge transport: proton hopping and the associated transient rearrangement of solvation structures. The overall message is that only by combining polarization and reactivity can simulations fully capture the physics of protic ionic liquids and thereby become a predictive partner for experiment and materials design.

The fate of the proton in protic and aprotic ionic liquids: acidity and ion transfer studied by Raman spectroscopy

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Abstract

Ionic liquids (ILs), interesting for their tunable solvation behavior and ability to reach high acidities, are commonly classified as protic (PILs) and aprotic (AILs). PILs result from proton transfer between a Brønsted acid and a Brønsted base, yielding a protonated cation. However, acidity is not restricted to PILs, as both PILs and AILs can be acidic depending on whether the proton is associated with the cation or with an acidic anion, respectively.[1] Moreover, high acidity can also be achieved by dissolving Brønsted acids in ILs, owing to the weakly coordinating nature of their anions, leading to high proton activity.

Acidity in ILs is commonly evaluated using Hammett acidity functions, based on the protonation of weakly basic indicators. Protonation is traditionally monitored by UV-Visible spectroscopy, but Raman spectroscopy has been recently implemented in AILs, which allowed us to reveal the influence of the indicator concentration on acidity determination, an effect previously unexplored.[2,3] These results, and the comparison with those obtained with UV-Vis, highlighted the presence of ion pairing in ILs, and how the latter differently influences the UV and Raman spectra, leading to differences in the measured acidity. This hypothesis was further investigated by measuring acidity functions in dissociating and non-dissociating solvents, in which ion pairing is present or minimized.

Raman spectroscopy is also a valuable tool for probing proton transfer in PILs. Studies were performed on a sulfonic acid-functionalized ammonium IL paired with a methanesulfonate anion with and without the presence of methanesulfonic acid. The analysis of Raman specific bands of the IL, coupled with computational modeling using SMD-GIL solvation model, enabled molecular-level insight into the state of the proton. This combined approach revealed that the proton is not permanently localized but can reversibly shuttle between the ammonium group of the cation and the methanesulfonate anion. Furthermore, it allowed us to follow the evolution of the proton environment upon acid addition, highlighting changes in cation–anion interactions and in the hydrogen-bonding network.

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Resolving Oligomeric Anions in Carboxylic Acid–Carboxylate Systems: Proton Dynamics in Choline–Geranate

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Abstract

Carboxylic acid/carboxylate mixtures in ionic liquids are frequently proposed to form oligomeric anionic species stabilized by hydrogen bonding, although the protonation state within these aggregates—ranging from localized to dynamically exchanging or symmetrically shared protons—often remains difficult to determine experimentally[1]. One prominent example is choline–geranic acid at a 1:2 ratio (CAGE12), which has attracted considerable attention due to its outstanding therapeutic performance in drug delivery and activation, particularly in transdermal and anticancer applications [2-4]. In this system, NMR observations indicating proton mobility have led to suggestions that oligomeric anionic motifs may be present; however, whether these correspond to long-lived complex anions or to dynamically fluctuating acid–carboxylate pairs remains unresolved.

Here we combine ATR–FTIR spectroscopy with ab initio and machine-learned force-field molecular dynamics simulations to elucidate the structure and proton dynamics of CAGE12. The simulations reveal a highly fluctuating hydrogen-bond network and provide key dynamical insight: although geranic acid (AGE) and geranate (GE) frequently form hydrogen-bonded contacts, these associations are short-lived and do not stabilize oligomeric anions. Proton transfer between AGE and GE occurs intermittently through a dynamically exchanging (“rattling”) proton, consistent with available NMR observations, and requires comparatively sustained hydrogen-bond configurations that are only occasionally achieved.

The proton is thus not symmetrically shared but shuttles between distinct molecular species while preserving carboxylic and carboxylate chemical identities. In agreement with this picture, experimental and theoretical vibrational spectra display coexisting carboxylate and carboxylic acid signatures, with no spectral features characteristic of proton-shared oligomeric anions.

These results reconcile apparently conflicting spectroscopic interpretations and demonstrate that CAGE12 is governed by transient carboxylic/carboxylate pairing rather than long-lived complex anions. More broadly, this work shows how combining vibrational spectroscopy with machine-learned molecular dynamics enables direct resolution of proton dynamics and ion-pairing motifs in complex ionic liquids relevant to functional and biomedical applications.

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TBC

Santiago Aparicio

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Abstract

TBC

Ionic Liquid-Based Extraction of Chromium from Ferrous Alloys and Ores

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Abstract

Hexavalent chromium (Cr(VI)) is a pervasive, toxic and environmentally impactful component of numerous manufacturing processes, including electroplating, conversion coatings, and paint primers. Alternative chemistries for many of these applications are presently in development and are often based on formulations containing more benign trivalent chromium (Cr(III)) complexes. However, a major environmental deficiency in the implementation of Cr(III) chemistries is that nearly all Cr(III) materials commercially available arise from Cr(VI) intermediates or as secondary byproducts thereof during their synthesis. To address these health & safety challenges, here we have developed robust, Cr(VI)-free chemical preparations of Cr(III) chlorides and the ionic liquid (IL)-based separation science to isolate them. By carrying out chemical leaching with chromite ore directly or widely available ferrous alloys, e.g. ferrochromium, a ubiquitous material used globally in the production of stainless steels, we generate complex mixtures of cationic metal species. To isolate chromium, we harness the uniquely suitable reactivity and physicochemical properties of imidazolium chloride-based ILs in mixtures with water to produce biphasic solutions, where we have studied the dependence of alkyl chain length and solution composition on the resultant extraction efficacy. Leveraging the hydrophobic properties of halometallate anions generated in these extractions, we have further applied the system as a framework toward separation of other binary metal systems.

Chemical and Thermal Stability of Ionic Liquids for High-Temperature applications

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Abstract

High-temperature processes such as CO_2 hydrogenation to methanol and gas dehydration can benefit significantly from the use of task-specific solvents. Ionic liquids (ILs), in particular, have shown strong potential to intensify these processes. For example, selecting ILs with affinity for methanol and water can shift the reaction equilibrium in CO_2 hydrogenation, increasing methanol yields from about 25% to nearly 67% at 250 °C. Similarly, highly stable ILs could enable intensified reactor concepts such as trickle-bed systems operating under harsh conditions.

However, the practical implementation of these approaches critically depends on the thermal and chemical stability of the selected ILs. Above 150 °C, very few solvents remain stable over the prolonged exposure times required in industrial operation. A major challenge is that the stability metrics most commonly reported for ILs, particularly onset decomposition temperatures (Tonset)

obtained from short, non-isothermal thermogravimetric analysis (TGA), often overestimate real operational stability. Long-term studies indicate that these short-term indicators can deviate by 100–300 °C from the temperatures at which slow degradation occurs, which is the relevant regime for continuous high-temperature processes.

In this work, we investigate the long-term thermal stability of several ILs using the temperature that produces 1% mass loss after 10 h of exposure ($T_{0.01/10h}$) as a practical stability metric. While previous studies suggest that 5–7 TGA experiments are required to estimate this parameter, we demonstrate that reliable predictions can be obtained using only 3–4 experiments through an optimized combination of temperature ramps, isothermal measurements, and evaluation of alternative kinetic degradation models.

Beyond thermal resistance, ILs must also remain chemically stable in the presence of catalysts, reactor materials, and reaction components. Therefore, the chemical stability of selected ILs was evaluated under realistic conditions for CO_2 hydrogenation to methanol at 240 °C. Degradation signatures and extents were analyzed using ^{1}H and ^{13}C NMR.

Together, these results provide practical stability benchmarks and an accelerated experimental workflow to screen IL candidates for durable, high-temperature CO_2 hydrogenation to methanol.

This work was developed within the scope of the project CICECO Aveiro Institute of Materia ls, UIDB/50011/2020, UIDP/50011/2020 & LA/P/0006/2020, financed by national funds throug h the FCT/MCTES (PIDDAC). This study also received financial support from Illimited project, financed by Horizon Europe agreement n° 101192964.

Extraction of vanadium from industrial by-products with the minimal generation of secondary waste using ionic liquids

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Abstract

A sustainable method for the extraction of vanadium(V) from industrial and environmental secondary resources is presented, with particular focus on complex feedstocks such as gasifier ash and metallurgical residues. The process utilises aqueous quaternary ammonium hydroxide-based solutions as selective leaching agents, optionally in the presence of oxidising agents, to solubilise vanadium into the liquid phase under moderate operating conditions. Compared with conventional vanadium recovery routes involving roasting, acidic leaching, and solvent extraction, this approach reduces process complexity and minimises secondary waste generation.

Following leaching, the dissolved vanadium(V) can be separated from residual solids and subsequently recovered through a combination of electrochemical processing and selective precipitation. Electrochemical treatment in a membrane-divided reactor enables purification of vanadium(V) while simultaneously regenerating the leaching medium, supporting closed-loop operation. Precipitation using ammonium salts produces ammonium metavanadate, which can be thermally decomposed to yield high-purity vanadium(V) oxide (>99 wt%). The formation of organo-vanadium intermediates during electrochemical processing was also observed, and these phases were characterised using X-ray diffraction.

The method is particularly effective for low-grade and heterogeneous feedstocks containing approximately 10–25 wt% vanadium, such as gasifier ash, while demonstrating limited co-extraction of common impurity metals. The combination of mild operating conditions, reagent recyclability, and high product purity highlights the potential of this approach as a viable route for vanadium recovery aligned with circular economy principles and growing demand from applications such as vanadium redox flow batteries.

Synthesis of imidazolium-based ionic phosphines for Ir-catalyzed hydroformylation of olefins

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Abstract

The stereo-electronic properties of a ligand play pivotal role in tuning the catalytic performance of transition metal complexes in homogeneous catalysis. Herein, we pay our great effort on synthesis of imidazolium-based ionic phosphines with different steric and electronic effects, with aim to enhance the performance of Ir-catalysts rather than Rh-ones for hydroformylation of olefins[1].

The two novel ionic phosphines (**L1** and **L2**) which was implanted with electron-rich and steric-bulky P^{t}Bu$_2$-fragment for the challenging $IrCl_3 \cdot 3H_2O$ catalysis for hydroformylation [2]. It was found that L**1** and **L2** were featured with excellent air/moisture insensitivity in contrast to the notorious P(^{t}Bu)$_3$, due to the strong electron-withdrawing effect of the neighbored imidazolium cation to delocalize the electron density of phosphorus-atom. Additionally, **L1** became a decent electron-deficient ligand with good tolerance against oxidation-degradation (i.e. poor reducibility). As a result, **L1** tailed with piperidyl-group enables $IrCl_3.3H_2O$ to effectively catalyze olefin-hydroformylation that provides the corresponding aldehydes in significant yields while completely suppressing the side-reactions like hydrogenation and isomerization. And the redox reaction between **L1** and $IrCl_3 \cdot 3H_2O$ is suppressed and the expected coordination-complexation between them became dominant, giving rise to the activity, selectivity, and good catalyst-stability subjected to more than 9-run recycling use.

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Research Progress on Efficient Recycling of Secondary Resources of Refractory Metals

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Abstract

The development of the high-precision industry has led to a significant increase in the demand for refractory metals, and the world's mineral reserves of refractory metals are currently in a critical situation. The secondary resources of refractory metals is high quality and simple in composition. The recovery of secondary resources can not only reduce the pollution caused by primary mining and smelting, but also improve the efficiency of resource utilisation. Conventional hydrometallurgical recovery methods use large amounts of chemical reagents and place a high load on the environment. We have developed a short process recycling method using molten salt electrolysis, which enables the recovery of W, Mo, Ti, Ta and Nb wastes without pollution in the process. Complex feedstocks including tungsten carbide (WC-Co), waste photovoltaic tungsten wires (W-La_2O_3) and other secondary resource alloys (TC4, TaNb etc.) were studied in detail, including separation principles, molten salt ion migration processes and electrochemical reduction processes. And one-step regeneration from waste to product (W, WC, WC-Co, Mo, Ti, Ta, Nb etc.) is realised. Cemented carbide recycling process has been scaled up on an industrial scale, where kilograms of W powder or W coating can be obtained in a single molten salt electrolysis. On the basis of the research on ‘Recovery Cemented Carbide Scrap by Molten Salt Electrolysis, we are continuously expanding research. We will also continue to promote the industrialization of secondary resources of refractory metals, and ultimately build an ecology for the recycling and efficient use of secondary resources of refractory metals.

Research on Molten Salt Oxidation Technology for Treatment of Radioactive Organic Waste Liquids

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Abstract

Organic waste liquids, such as spent tributyl phosphate (TBP) and waste vacuum pump oil, generated during the operation of the nuclear industry are difficult-to-treat radioactive organic wastes. Traditional disposal methods like cement solidification significantly increase the volume, while incineration tends to cause secondary pollution. There is an urgent need to develop efficient and safe treatment technologies. Molten Salt Oxidation (MSO) offers an innovative pathway for treating organic radioactive waste liquids due to its unique reaction mechanism and environmental compatibility. The core of MSO technology lies in utilizing high-temperature molten salt as the reaction medium. For radioactive organic waste liquids primarily containing TBP, MSO demonstrates excellent treatment capability. While TBP tends to produce toxic and harmful P_2O_5 during pyrolysis, in the molten salt environment, the phosphorus from its decomposition products rapidly reacts with the molten salt to form stable phosphate compounds as the TBP molecules undergo oxidative decomposition. This effectively prevents the release of harmful gases, and the radionuclides are retained within the molten salt. Similarly, high degradation efficiency and effective nuclide retention are achieved for waste vacuum pump oil. With advantages such as high volume reduction efficiency, minimal secondary waste generation, and reliable nuclide immobilization, molten salt oxidation technology provides an effective solution for the clean treatment of radioactive organic waste liquids, making it suitable for organic waste liquid management in nuclear power plants and reprocessing facilities.

Glow With the Flow: Defining the Properties for Luminescent Ionic Liquids for Anti-Counterfeiting

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Abstract

Counterfeiting represents a major global challenge, affecting world economies. Current technologies used in security are easy to forge, common fluorophores used has broad emission spectrum and lack complexity. Thus arises the need for novel security inks that are spectrally complex. Utilising ionic liquids for anticounterfeiting addresses the challenges in the synthesis and formulation of security inks, such as complexity, solubility, miscibility, and tuneability. Here, we explore ionic liquids of different alkyl phosphonium cations with anionic lanthanide coordination complexes. Lanthanide centers are sensitised with an organic ligand to enhance emission; the resultant coordination complexes are subjected to anion exchange to obtain luminescent colourless ionic liquids.[1] Physicochemical properties of ionic liquids, such as melting point, glass transition temperature, crystallisation point, and phase behaviour, are investigated using Differential Scanning Calorimetry with respect to different alkyl phosphonium with varying size and symmetry. Thermogravimetric assay reveals high temperature stability with water loss. Viscosity trends are analysed to decide the best candidates for inks. Photophysical properties are investigated and characteristic emission peaks are observed corresponding to the energy level transitions of the lanthanide present in the ionic liquid.[2] Physicochemical properties are dependent on cation structure and do not affect photophysical properties. Further studies investigate the usability of mixtures in developing complex barcodes and developing polymer composites.

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An Ionic Liquid Frustrated Lewis Pair

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Abstract

Frustrated Lewis acid/base pairs (FLPs) are catalytically active combinations of LA/LB that have the potential to replace platinum group metals for small molecule activation. They are most commonly used in homogeneous dilute solutions. The objective here was to investigate whether IL design principles can be applied to produce a concentrated 'solvent-free' FLP system in which the potential number of encounter complex active sites is magnified enabling enhanced reactivity. One such, purely organic, example that emerged with the potential to be adapted to an IL FLP system is the pairing of heterocyclic *N*-alkylacridinium salts with heterocyclic bases such as 2,6-lutidine.[1]

We have previously demonstrated that IL environments can extend the life-times of FLP encounter complexes to the NMR timescale[2] and reasoned that, using IL design principles – *viz* variation of cation *N*-alkyl substitution and selection of appropriate anions –the *N*-alkylacridinium/lutidine FLP could be transformed into an IL system. Here we report the first studies on the *N*-alkylacridinium bistrifylimide/lutidine IL-FLP system as a solvent-free FLP catalyst (Fig. 1).

This system, albeit slow ca. 6 days, has been shown to activate H_2 (1 bar) and deactivate H_2. The liquid structure of the FLP system has been studied via neutron scattering, in which the dominant features within the liquid are π-π interactions.

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Atomistic Modelling of Fluoride Salts in Molten Salt Reactors

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Abstract

Molten Salt Reactors (MSRs) are a Generation IV technology with the potential to deliver modular, scalable, carbon-neutral power. During operation, many fission products form in the fuel salt, and their solubility and chemical form can change salt properties and affect reactor performance. In this work, we present an approach to map fission product influence in molten fluoride salts using the Polarizable Ion Model (PIM) for classical MD simulations and a DFT-based force-fitting method to determine the unknown classical interaction parameters. The PIM parameters are fitted by matching to DFT-calculated forces, enabling a consistent description of both salt-salt and salt-impurity interactions for relevant species in the fuel salt.

Based on MD simulations, we calculate thermophysical properties (e.g. density, heat capacity, viscosity) of the fresh fuel salt as well as during burn-up, and map how these properties are altered when additives used for corrosion control or impurities such as fission products are present in the salt. We focus on certain groups of elements that are expected to behave differently in the salt, including species that remain dissolved, species that tend to form complexes, and species that may precipitate or accumulate at interfaces. The main application is the NaF-KF-UF_4 eutectic (FUNaK) fuel salt used in the Saltfoss Energy MSR concept, where the pure salt properties are increasingly well known but fission-product effects are not. The method is tested against experimental data for the pure fuel salt, and preliminary results for FUNaK containing impurities are presented.

Microextraction of Emerging Contaminants from Wastewater using Hydrophobic Eutectic Solvent loaded onto Cellulose Hydrogel

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Abstract

Hydrophobic eutectic solvents (HES), prepared from natural components are attracting interest as an eco-sustainable alternative to organic solvents in liquid-liquid extraction technique for the removal of emerging water pollutants [1]. However, the challenging phase separation and partial cross-contamination limit their applicability. The post modification of polymeric adsorbents loaded with HES has undergone intense investigation in recent times addressing these challenges [2]. Nevertheless, the use of fossil-based polymeric materials is not economically sustainable and environmentally friendly. Thus, the purpose of this research study was to explore HES-loaded cellulose hydrogels for the extraction of dyes and pesticides from water samples.

In this study, malachite green chloride was used as a model dye, and imidacloprid was used as a model pesticide. Cellulose hydrogels were prepared via phase inversion technique by co-dissolving microcrystalline cellulose (MCC) into a mixture of the ionic liquid 1-ethyl-3-methylimidazolium acetate ([EMIm][OAc] and cosolvent DMSO. HES were preliminarily screened in liquid-liquid extraction, and the most promising HES were loaded into cellulose hydrogels and further tested in solid-liquid extraction. The morphology of HES–loaded hydrogel was observed by using scanning electron microscopy and leaching of HES was determined by using ^{1}H NMR spectroscopy. The results showed that EE (extraction efficiency) of HES–loaded cellulose hydrogels increased compared to neat cellulose hydrogel. When HES based on (C8:C10) fatty acid was loaded into cellulose hydrogel, the extraction of malachite green chloride increased from 44.07% to 84.32%. Similarly, when cellulose hydrogel loaded with HES composed of thymol and octanoic acid an increased extraction of imidacloprid from 8.16% to 74.28% was reported.

Keywords: Hydrophobic eutectic solvent (HES), Cellulose, and Emerging contaminants

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STM Characterization of Bismuth (111) | 1-Butyl-1-methylpyrrolidinium Bis(fluorosulfonyl)imide Interface

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Abstract

1-Butyl-1-methylpyrrolidinium bis(fluorosulfonyl)imide (BMPyrFSI) is an ionic liquid with low viscosity that has been investigated as a possible electrolyte for ionic liquid based lithium-ion batteries[1].

The Bi(111) surface was selected for this study because no surface reconstruction processes occur within the ideal polarizability range[2]. The Bi(111) | BMPyrFSI interface has been previously characterized electrochemically[3]. In earlier in-situ STM studies, BMPyrFSI was investigated on HOPG and Au(111) electrodes, where surface processes were found to depend strongly on the electrode material[4]. On Au(111), trace amounts of water and oxygen were shown to form a film-like structure. The wide electrochemical window shown in previous work may therefore be attributed to a similar film-like structure forming on Bi(111) surface.

This work provides insight into the structure of Bi(111) | ionic liquid interface with scanning tunneling microscopy measurements. On the Bi(111) surface, the measured ideal polarizability range in BMPyrFSI is $-1.1\ V < E < 0.4\ V$. The 1.5 V potential window is limited at positive potentials by bismuth oxidation and at negative potentials by the reduction of trace water[3]. The potential window is wider than that of $EMImBF_4$ (1 V) and EMImFSI (0.9 V)[3]. Future studies will investigate this interface in the presence of metalloporphyrin additives. These additives are known to adsorb at the surface; however, their adsorption structure remains unknown.

Acknowledgements

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From Waste to Wealth: Selective Palladium and Platinum Recovery from Automotive Catalysts via [TOA][P204] Ionic Liquid

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Abstract

Automotive catalytic converters represent an important secondary source of platinum group metals (PGMs), including palladium (Pd), platinum (Pt), and rhodium (Rh). Due to their limited natural availability, high economic value, and classification as critical raw materials by the European Union, the recovery of PGMs from spent catalysts is essential for sustainable resource management and circular economy strategies. A major challenge in PGM recycling arises from the complex composition of catalyst leachates, which contain high concentrations of base metals that hinder selective metal separation.

In this study, a task-specific ionic liquid (IL), tri-n-octylammonium bis(2-ethylhexyl) phosphate ([TOA][P204]), was synthesized via an acid-base neutralization reaction between tri-n-octylamine and bis(2-ethylhexyl) phosphoric acid and applied for the selective recovery of Pd and Pt from hydrochloric acid leachates of spent automotive catalysts. The chemical structure of the synthesized IL was confirmed using Fourier transform infrared spectroscopy and nuclear magnetic resonance. The pregnant leach solution contained 241 mg/L Pd, 36.7 mg/L Pt, and 8 mg/L Rh in the presence of aluminum (3173 mg/L) and iron (726 mg/L), representing a challenging separation system.

The influence of key extraction parameters, including IL concentration (10–50%), temperature (25-65 °C), organic-to-aqueous phase ratio (O/A: 0.5-2), contact time (1-45 min), diluent type, chloride ion concentration, and stripping conditions, was systematically investigated. Increasing the IL concentration significantly enhanced Pd extraction efficiency from 39.7% to 80% and Pt from 13% to 90.7%. Increasing the O/A ratio further improved Pd recovery from 59.3% to 91% and Pt recovery from 86.4% to 97.8%, while the effect on iron extraction was negligible. Temperature exhibited only a moderate influence, and an optimal contact time of 20 minutes was sufficient to reach equilibrium. Among the tested diluents, butyl acetate achieved the highest Pd extraction efficiency (81%), whereas kerosene provided the highest Pt extraction efficiency (86.4%). Chloride ions were found to adversely affect extraction, emphasizing the importance of controlling leachate chemistry.

Among the evaluated stripping systems, a mixed NaOH-NaCl solution demonstrated the most effective and selective stripping performance. Under optimized operating conditions, recovery efficiencies of up to 92% for Pd and 98% for Pt were achieved. Rhodium and aluminum were not extracted, and iron was effectively remained in the organic phase during the selective stripping stage.

A Study on Domain-Adversarial Neural Network on GAF-Encoded Cyclic Voltammogram to Predict Ion Concentrations in Molten Salt Thermal Convection Loop (MSTCL)

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Abstract

The type and concentration of ions dissolved in molten salts are crucial for predicting corrosion behavior in molten salts. Cyclic voltammograms (CV) contain signals from multiple ions and exhibit overlapping patterns, limiting the ability to decompose and extract valuable information. To address this issue, we propose method using the domain-adversarial neural network (DANN) that compares CVs of individual ions (source domain where experimental conditions are known) with CVs measured in molten salt thermal convection loop (MSTCL) during corrosion test (target domain). Each CV from both domains is encoded into image with Gramian angular field (GAF) method. Features of GAF-encoded images, which are extracted with convolution neutral network (CNN) are combined with metadata of temperature and scan rate to build input feature vector for DANN algorithm. A multi-input hybrid model based on CNN and DANN has been built to address domain shift between both domains. The training dataset comprised 648 GAF images from the source domain and 120 from the target domain for ions of Cr, Fe, Mn, Mo and Ni. Model evaluation using 5-fold cross-validation on data from the target domain yielded a mean absolute error of 846.5 ± 28.5 mg/kg. This result demonstrates that despite differing experimental environments and measurement conditions, the DANN-based pipeline achieved a certain level of generalization performance. Linear calibration partially reduced the error, but residuals remained, especially for Fe and Ni. Therefore, further improvement in prediction accuracy requires addressing training data imbalance, sample size limitations, and the specificity of deep learning architectures for electrochemical signals. This study represents one of the first attempts to apply a domain-adaptive deep learning model to the prediction of metal ion concentration prediction with cyclic voltammetry in real systems. It empirically identified both practical limitations and directions for future improvement. The results of this study can serve as novel method for future real-time diagnosis with transient electrochemical methods and automated measurement system implementation based on linking laboratory and field data.

Ionic Liquid Extraction of W and V from SCR Catalysts

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Abstract

Selective catalytic reduction (SCR) catalysts are extensively employed for the abatement of nitrogen oxides emissions and represent an important secondary resource due to their significant contents of vanadium, tungsten, and titanium, which are classified as critical raw materials. The recovery of these metals from spent SCR catalysts is essential for sustainable resource management and circular economy strategies; however, it remains challenging due to the catalyst matrix's complex composition.

An integrated hydrothermal leaching-ionic liquid extraction approach was developed to selectively recover vanadium and tungsten from spent SCR catalysts, while titanium remained largely unaffected during alkaline leaching with 5 M NaOH at 280 °C. The resulting pregnant leach solution (PLS) contained approximately 1400 mg/L V, 2600 mg/L W, 1230 mg/L Al, along with high sodium concentrations (~100 g/L) originating from the alkaline leaching medium.

Subsequently, solvent extraction using the ionic liquid Aliquat 336 was investigated for the preferential recovery of tungsten over vanadium from the alkaline PLS. Key extraction parameters, including ionic liquid concentration (10–50 vol%), temperature (25-65 °C), organic-to-aqueous phase ratio (O/A = 0.5–2), contact time (5–60 min), diluent type, pH (2-14.8), and stripping agents, were systematically evaluated. Among these parameters, pH adjustment was identified as the most influential factor governing extraction efficiency. Reducing the pH from strongly alkaline conditions (pH 14.8) to 2 significantly enhanced tungsten recovery from 37.8% to 96.8%, while also increasing vanadium recovery from approximately 1% to 56.5%. Increasing the ionic liquid concentration from 10 to 50% moderately improved tungsten extraction (from 23.1% to 38.7%), whereas its effect on vanadium extraction remained negligible (1-2%). Temperature, contact time, and O/A ratio showed only moderate effects, with equilibrium reached within 10 minutes. Aliquat 336 did not extract aluminum or sodium under any of the investigated conditions, confirming its high selectivity toward tungsten.

The results further demonstrated that diluent choice strongly affected extraction performance, with chloroform outperforming kerosene, toluene, and butyl acetate, achieving extraction efficiencies of 99.5% for vanadium and 95.8% for tungsten. This behavior was attributed to chloroform's higher polarity and its enhanced extraction of anionic vanadate (VO_3^-) and tungstate (WO_4^{2-}) species. Among the stripping agents, NH_4Cl enabled effective and selective stripping of tungsten from the loaded organic phase.

Developing a waste-free process for PET chemical recycling using ionic liquid-water mixtures

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Abstract

Poly(ethylene terephthalate) (PET) is one of the most widely used non-degradable plastics and needs to be efficiently recycled to reduce leakage into the environment and retain its value. Chemical recycling is a promising approach to achieve a closed-loop plastics economy as it recovers purified monomers and allows the production of high-quality recycled polymer. Here, work on the hydrolytic depolymerisation of PET into terephthalic acid (TPA) and ethylene glycol (EG) using low-cost ionic liquid-water mixtures is showcased. While ionic liquids have been reported for catalysing PET depolymerisation, many examples involve ionic liquids with complex chemical structures that are associated with high production cost. In this work, a series of pseudo-protic ionic liquids (PPILs) were investigated as both catalysts and co-solvents for PET hydrolysis. These PPILs were prepared by combining 1-butylimidazole or tributylamine with acetic acid, hexanoic acid, or octanoic acid. They were selected due to their low cost, easy synthesis, and high boiling points, which may facilitate separation of the products from the solvent and enable ionic liquid recycling to allow a waste-free process in the future. All PPILs demonstrated effective depolymerisation of PET into the monomers TPA and EG under the screening condition. These findings show the potential of PPILs as effective catalytic solvents for PET chemical recycling with prospects for industrial application.

Bimetallic Ionic Liquids: A Sustainable Approach to Fuel Desulfurization

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Abstract

A series of dicationic ionic liquids (DcILs) with varying alkyl chain lengths and $[FeCl_3Br]^-$ as the counter anion were synthesized and thoroughly characterized using FT-IR, Raman spectroscopy, mass spectrometry, and single-crystal X-ray analysis. Their thermal stability, chemical structure, and elemental composition were further examined through thermogravimetric analysis (TGA) and X-ray photoelectron spectroscopy (XPS). These DcILs were investigated as both extractants and catalysts for oxidative desulfurization (ODS) of liquid fuels, utilizing H_2O_2 as the oxidant. The effects of reaction time, temperature, catalyst loading, oxidant-to-sulfur ratio, and sulfur substrate reactivity were systematically assessed. The DcILs exhibited high extraction and catalytic efficiency under mild conditions, achieving rapid equilibrium and substantial sulfur removal at room temperature with minimal catalyst and oxidant usage. With their low solubility in liquid fuels and high recyclability, these DcILs offer a green and sustainable approach to desulfurization, effectively minimizing fuel contamination while promoting environmental sustainability.

Imidazolium-Based Ionic Liquids as Efficient Corrosion Inhibitors for Mild Steel in Acidic Medium: Experimental and Theoretical Insights

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Abstract

Novel imidazolium-based ionic liquid derivatives with different alkyl chain lengths (IL-1, IL-2, and IL-3) were investigated as corrosion inhibitors for mild steel in 1 M HCl solution. Electrochemical Impedance Spectroscopy (EIS) and potentiodynamic polarization (PDP) measurements were employed to evaluate their inhibition performance. The electrochemical results revealed high inhibition efficiencies exceeding 90%, indicating that the studied ionic liquids act as mixed-type inhibitors. Adsorption of the inhibitors on the steel surface followed the Langmuir adsorption isotherm. Surface characterization using SEM and EDX confirmed the formation of a protective adsorbed film on the mild steel surface. In addition, density functional theory (DFT) calculations at the B3LYP/6-311G(d,p) level were performed to analyze the electronic properties and reactivity of the molecules. Monte Carlo simulations on the Fe(110) surface were further carried out to gain deeper insight into the adsorption behavior and interaction mechanisms responsible for the corrosion inhibition process.

NaSCN-Induced Expansion of Chemical Space and Selectivity in Aqueous Biphasic Systems for Membrane-Free RFBs

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Abstract

Membrane-free redox flow batteries (RFBs) offer a cost-effective alternative to conventional architectures by eliminating ion-selective membranes, thereby reducing both capital cost and internal resistance. Their implementation relies on aqueous biphasic systems (ABS) that ensure stable liquid–liquid separation and high selectivity toward redox-active species. Sodium thiocyanate (NaSCN) has been reported as an effective modulator of redox-species partitioning in biphasic systems [1]. In this work, NaSCN was investigated as an additive to modify ionic liquid (IL)-based ABS and enlarge the biphasic region. Ternary systems composed of $(NH_4)_2SO_4$ + IL + H_2O were evaluated using four chloride-based ILs: $[C_2mim]Cl$, $[C_4mim]Cl$, $[N_{2222}]Cl$, and $[N_{3333}]Cl$.

The addition of 5 wt% NaSCN promotes partial anion exchange ($Cl^- \rightarrow SCN^-$), inducing a transition from solid–liquid to stable liquid–liquid equilibria and significantly enlarging the biphasic region. Ammonium-based ILs generated broader biphasic domains than imidazolium analogues, highlighting the influence of cation structure on phase behavior. Liquid–liquid–solid equilibria further delineated the NaSCN-induced expansion of accessible compositions.

Partition coefficients determined for viologens, TEMPO derivatives and ferro/ferricyanide species showed increased selectivity upon NaSCN addition. Benzyl and ethyl viologen were identified as suitable anolytes, while $K_4[Fe(CN)_6]$ proved suitable as catholyte. Cyclic voltammetry revealed reversible redox behavior and stable electrochemical responses. Partial IL substitution by NaSCN enables a 21–24% reduction in electrolyte cost without compromising separation performance.

Acknowledgments

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Solubility of Terephthalic Acid in Acetate Ionic Liquids and Ionic Liquid–Water Mixtures: Quantification by ^{1}H NMR and Phase-Equilibrium Modeling

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Abstract

Aprotic and pseudoprotic acetate-based ionic liquids (ILs) have been shown to effectively promote the depolymerization of poly(ethylene terephthalate) (PET) in the presence of water.(Suleman, Judah et al. 2025) To enable waste-free recovery of terephthalic acid (TPA) via crystallization, reliable solubility data in ILs—particularly in IL–water mixtures—are needed, yet remain scarce, limiting downstream separation design for IL-catalyzed PET depolymerization. Here, we determined the solubility of TPA in two acetate ILs, 1-ethyl-3-methylimidazolium acetate ([Emim][OAc]) and 1-methylimidazolium acetate ([Hmim][OAc]), as well as in their binary mixtures with water. After evaluating several analytical approaches, we employed quantitative ^{1}H NMR spectroscopy to measure TPA solubility rapidly and reproducibly; compared with conventional HPLC workflows, this approach substantially increases throughput while maintaining accuracy verified for the present systems. The resulting dataset was used to correlate and model solubility and phase equilibrium in the TPA–IL and TPA–IL–water systems, providing thermodynamic inputs for designing crystallization-based product recovery and integrating depolymerization with separation.

Designing Ionic Liquid/Salt Biphasic Systems for Membrane-Free Batteries

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Abstract

Aqueous biphasic systems (ABS) have emerged as versatile liquid–liquid platforms for separations, reaction engineering, and electrochemical processes due to their high water content, tunable polarity, and low interfacial resistance. Designing task-specific ABS requires balancing several competing factors, including phase stability, viscosity, solute partition, and chemical compatibility with target molecules. Expanding the compositional space of viable ABS while preserving these properties is thus a central challenge for the development of new biphasic technologies.

This work investigates strategies to expand the chemical space of ionic liquid (IL) and salt-based ABS through systematic electrolyte design. First, salt–salt ABS based on TFSI-containing electrolytes were developed as a platform for low-viscosity biphasic systems. Two complementary modifications were explored: replacing Li^+ with Na^+ to obtain more sustainable and cost-effective NaTFSI-based systems, and replacing ammonium sulfate with highly soluble LiCl to suppress salt precipitation and widen the liquid–liquid composition region. These modifications generate stable biphasic electrolytes composed of a TFSI-rich phase and a hydrophilic salt-rich phase; resulting in high partition coefficients frequently exceeding $|K| \approx 100$ for selected redox-active molecules.

In parallel, the chemical space of IL-based ABS was expanded through the use of sodium thiocyanate (NaSCN) as a formulation additive. The chaotropic SCN^- anion modifies ion–water interactions and promotes anion exchange in chloride-based ionic liquids, converting systems that originally display only solid–liquid equilibria into stable liquid–liquid biphasic systems. In addition to enabling phase separation, NaSCN allows control over solute partitioning and partially replaces expensive ionic liquids in the formulation, improving the economic feasibility of the resulting ABS.

These ABS were developed for membrane-free redox flow batteries (RFBs) applications. In this architecture, two immiscible aqueous electrolytes spatially confine redox-active species, enabling battery operation without ion-exchange membranes. Partition experiments were used to identify suitable catholyte–anolyte combinations, with ferrocyanide and viologen derivatives showing favorable separation in ABS formed with imidazolium and quaternary ammonium ionic liquids. Appropriate NaSCN concentrations expand the accessible chemical space and operational window of these systems while reducing cross-contamination between phases. Electrochemical measurements further confirm the stability of the selected redox couples in the proposed electrolytes, with estimated open-circuit voltages exceeding 1 V. This study demonstrates that targeted IL/salt electrolyte design can significantly expand the accessible chemical space of ABS for specific applications capable of balancing phase stability, selectivity, and cost.

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Distillable and Recyclable Liquid Salts for Herbaceous Biomass Delignification

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Abstract

Lignocellulosic biomass is widely abundant across Europe, with forests in Slovenia covering more than 58% of the country's land area, which is nearly 20% higher than the EU average. This places the country among the leading ones in terms of lignocellulosic biomass availability, ranking third after Finland and Sweden. As such, Slovenia holds significant potential for the expansion and further development of bio-based industries.

Conventional wood-processing industries predominantly utilize Kraft pulping for cellulose production, treating lignin merely as a by-product in the form of a liquid side stream. In contrast, smaller-scale biorefineries offer distinct advantages due to their robustness and flexibility in processing a broad range of feedstocks, including forestry and agricultural residues. For example, the lignin-first approach employed in organosolv processes offers a significant advantage over Kraft pulping by enabling the recovery of a high-purity lignin fraction without compromising the integrity of the cellulose. While ethanol-based biorefineries have already been demonstrated at the pilot scale, the distillable ionic liquid (DIL) biorefinery route remains relatively underexplored. Nevertheless, it represents a highly promising alternative to the organosolv process for the efficient and selective valorization of lignocellulosic biomass.

In this study, we investigate the use of various distillable ionic liquids (DILs) for the selective extraction of lignin from grass-derived waste biomass. The process enables the extraction of organosolv-like lignin with low molecular weight and controlled dispersity under milder (lower temperature and pressure) and less acidic (no sulphuric acid catalyst required) conditions than in organosolv biorefineries. Using the most promising DIL identified, the resulting yellowish cellulose-rich pulp exhibits an α-cellulose content exceeding 90% and both the cellulose and DIL remain chemically stable during pulping. Furthermore, the extracted lignin serves as an ideal intermediate for subsequent conversion into high-value green chemicals such as phenolic monomers and oligomers, or for processing into biomaterials including biopolymers and bioadhesives. Similar to ethanol recovery in organosolv processes, the DIL can be efficiently recovered through distillation, and its high thermal and chemical stability allows for repeated reuse within the same process.

Electric Double Layer Structure of Lithium Salts in Ethylammonium Nitrate using a Mercury as a Metal Model Electrode

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Abstract

Binary mixtures of ionic liquids (ILs) and inorganic salts have attracted increasing attention as advanced electrolytes for electrochemical energy-storage devices because of their improved ionic conductivity and enhanced electrochemical and thermal stability. However, the rational optimization of these systems requires a systematic understanding of how added salts modify the electrolyte/electrode interfacial structure.

In this work, mercury (Hg) was employed as a well-defined metallic model electrode to investigate the electrical double layer (EDL) in mixtures of ethylammonium nitrate (EAN) and lithium nitrate ($LiNO_3$). Owing to its smooth, reproducible, and non-structured surface, Hg provides an ideal interface for resolving the interfacial effects induced by lithium salts in EAN. Differential capacitance, potential of zero charge, and charge density curves were measured over a wide range of $LiNO_3$ molal concentrations to characterize the interfacial organization and charging behavior of the system.

The results establish a robust framework for proposing the EDL structure of neat EAN, which serves as a reference for identifying the specific roles of lithium and nitrate ions in the binary mixtures at electrified interfaces. The interfacial properties of the EAN layer adjacent to the electrode were interpreted using the Helmholtz model. Although simple, this approach yielded EDL thickness estimates that were independently validated, supporting its reliability for the present system. This study aims to provide a fundamental methodology for assessing ion adsorbability and the structural contributions of inorganic salts in IL-based electrolytes, offering a valuable insight into the design of next-generation electrified interfaces for electrochemical energy-storage applications.

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Engineering aqueous deep eutectic solvents (ADES) for enhanced enzymatic reaction

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Abstract

Engineering aqueous deep eutectic solvents (ADES) for enhanced enzymatic reaction

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Deep eutectic solvents (DESs) are a class of sustainable, low-toxic, and biodegradable solvent systems formed by hydrogen bond donors and acceptors, offering tunable physicochemical properties for biomolecular applications. However, their inherently high viscosity can limit enzymatic efficiency. This limitation can be overcome by introducing water to form aqueous deep eutectic solvents (ADES)**,** which reduce viscosity while maintaining a favorable environment for enzymatic function.[1-4]In this study, the catalytic activity and thermodynamic stability of horseradish peroxidase (HRP) were investigated in a ADES systems composed of [choline-chloride: ethylene-glycol: sorbitol: water] (CESW), using spectroscopy and molecular dynamics simulations. The microscopic structure of the ADES was systematically analyzed by varying water content from 5% to 95% to understand hydration behavior, hydrogen-bonding networks, intermolecular interactions, and peroxidase activity of HRP. Under optimized condition, 5-10% CESW exhibited a significant enhancement in reaction velocity (~120 $nM \cdot s^{-1}$) compared to conventional phosphate buffer saline (PBS) (~40 $nM \cdot s^{-1}$), corresponding to an overall increase in HRP activity of approximately 350%. These findings demonstrate that ADES provide tunable and efficient microenvironments that significantly enhance enzymatic performance, highlighting their potential for advancing sustainable biocatalytic applications.

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Corrosion Process for the Reprocessing of Solid Oxide Electrode-Supported Cells, Using Oxidizing Acidic Salt Media

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Abstract

Solid Oxide Fuel Cells (SOFCs) are promising electrochemical systems but offering new challenges for the recycling industry. Widely used in automotive and heating sectors, SOFCs are multilayer ceramics systems composed of a solid electrolyte (mainly YSZ-yttria-stabilized zirconia) and multi oxides components electrodes like LSCF (lanthanum-cobalt rich phase) as cathode and Ni-YSZ cermet as anode. Within this framework, the studied FESC-type models (fuel electrode-supported cells) use the Ni-YSZ cermet as a support, which accounts for half of the cell mass where Ni representing nearly 65% molar of the cermet composition, is a challenging element to reprocess. [1,2]

This research work takes a part in the "Life Cycle Analysis and Recycling" workpackage of the CLUED-O Interreg European project. The objective is to propose a robust and innovant recycling process enabling the recovery of strategic metals (Mn, Co, Sr…) and rare earth elements (Y, La, Ce, Gd…) operating under soft conditions (i.e. below 500–600°C) without resorting to conventional mechanical methods. To date, literature only reports hydrochemical reprocessing routes assorted with numerous mechanical steps (scratching, crushing, grinding…) leading to processes difficult to implement on an industrial scale and energy consuming. [3] For innovation purpose, our plan aims to combine pyrometallurgy via reactions in oxidizing molten salts media and hydrometallurgy. The latest leveraged to separate and identify soluble phases dissolved in aqueous media. In order to predict optimal dissolution and reaction conditions in the molten salt media a thermodynamic approach is considered using FactSage software, including phase diagram creation and thermodynamic equilibrium studies. X-ray diffraction is used as a routine analytical technique to identify phases formed after chemical dissolution. In addition, EDX analyses coupled with SEM enable a qualitative evaluation of surface state modification. Several salts have been tested, depending on their acido-basicity and redox potential to isolate the most promising one. Due to the complex geometry and composition of the SOFCs, several schemes are foreseen. First results related to the recycling of the anode part will be discussed in the presentation. [4]

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DES Electrolytes in MXene Supercapacitors

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Abstract

Deep eutectic solvents (DES) have gained prominence as sustainable alternatives to conventional electrolytes. Formed via hydrogen-bond donor–acceptor pairs, DES offer favorable features: biodegradability, low volatility, straightforward synthesis, and broad electrochemical stability windows, offering a cost-effective and environmentally friendly option for energy storage applications.[1] MXenes, a class of two-dimensional (2D) transition metal carbides or nitrides, have emerged as exceptional electrode materials for energy storage devices.[2] Despite progress in both materials, the interfacial structure and dynamics between MXenes and DES remain underexplored. The intricate behavior governed by hydrogen-bond networks in DES, combined with the complex surface terminations of MXenes, warrants a detailed atomistic understanding to optimize charge storage and overall device performance.[2] Molecular dynamics (MD) simulations, particularly those employing constant-potential methods, are powerful tools to probe such interfacial structures and processes with atomic precision. In this work, we perform comprehensive constant-potential MD simulations to analyze the behavior of DES confined between MXene electrodes. Our approach includes: (i) structural examination of interfacial layering and hydrogen-bond networks, (ii) dynamical analysis of solvent orientation, and (iii) evaluation of charge accumulation and differential capacitance modulation by surface functional groups. From our study, we figure out how DES interacts with MXene surface terminations and the interplay with electrochemical performance. Aspiring to bridge theoretical predictions with practical applications, our findings contribute foundational insights and design guidelines for the development of high-performance, sustainable supercapacitors leveraging MXene–DES architectures.

Thermal storage capacity of tarpenes and fatty acid-based eutectic mixtures

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Abstract

Deep eutectic solvents (DESs) have emerged as promising soft materials whose phase behavior can be tailored through molecular pairing and hydrogen-bond organization. Despite this tunability, their potential as phase change materials for thermal energy storage (TES) remains insufficiently developed. In this study, a series of fatty acid-based DESs was prepared and examined as sustainable TES candidates using differential scanning calorimetry to determine melting behavior, fusion enthalpy, specific heat capacity, and resistance to repeated thermal cycling.

The investigated systems displayed composition-dependent thermal transitions and appreciable latent heat storage, demonstrating that subtle changes in intermolecular organization can strongly influence energy storage performance. The results show that eutectic formulation provides a practical route to adjust transition temperatures while maintaining favorable thermal reversibility. Analysis of the thermal response further indicates that hydrogen-bonding networks and component ratio play decisive roles in defining the balance between phase stability and storage capacity.

These findings position fatty acid-based DESs as attractive alternatives to conventional TES media, combining low cost, renewable feedstock origin, and adaptable thermal properties. More broadly, the work supports the use of molecular-level design strategies to develop next-generation DES-based materials for sustainable heat storage technologies.

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Bifunctional Pyrrolidine–Thiazolium Chiral Ionic Liquids for Asymmetric Michael and Stetter Reactions

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Abstract

We have developed chiral ionic liquid catalysts based on the natural amino acid proline and investigated their application in asymmetric Michael addition reactions. Meanwhile, thiazolium salts are known to form *N*-heterocyclic carbenes upon deprotonation in the presence of a base, thereby catalyzing the Stetter reaction. In this study, we synthesized a pyrrolidine–thiazolium conjugated chiral ionic liquid catalyst (Fig. 1). This catalyst integrates a pyrrolidine moiety responsible for asymmetric Michael addition with a thiazolium moiety active in the Stetter reaction. This bifunctional catalyst is expected to enable cascade reactions in which both transformations proceed sequentially using a single catalyst.

In an asymmetric Michael addition reaction, a chiral catalyst bearing a thiazole moiety exhibited catalytic activity towards both aldehydes and ketones. In contrast, the chiral ionic liquid catalyst bearing a thiazolium moiety showed substrate selectivity, being active only towards aldehydes.

Table 1 summarizes the results of the Stetter reaction using furfural and ethyl acrylate as substrates. The maximum yield was 68% using a thiazolium-only catalyst (Entry 1), whereas a comparable yield of 71% was obtained with the pyrrolidine–thiazolium conjugated catalyst (Entry 2). These results indicate that incorporation of the pyrrolidine moiety has a negligible impact on Stetter reaction catalysis and does not hinder its application in cascade reactions. Furthermore, replacing the anion with a halide rendered the ionic liquid catalyst hydrophilic, affording a remarkably high yield of 88% (Entry 3). The applicability of this catalyst was examined across a variety of substrates. While effective for a wide range of substrates, no reaction was observed with benzaldehyde or *p*-nitrobenzaldehyde, likely due to competing side reactions and substituent effects.

Imidazopyridine-based Ionic Liquids: Synthesis, Properties, and Optical Behavior

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Abstract

We synthesized imidazopyridine-based ionic liquids and evaluated their physicochemical properties. [$C_n$impy][Br] (n = 4, 6, 8, 10), bearing an alkyl group at the N_1 position of imidazo[1,2-*a*]pyridine, were all solids at room temperature. Anion exchange of [$C_n$impy][Br] with $N(CN)_2^-$ and FSI^- afforded the corresponding ionic liquids, [$C_n$impy][$N(CN)_2$] and [$C_n$impy][FSI], which were liquid at room temperature. In particular, the DSC thermogram of [C_{10}impy][FSI] exhibited a clear melting point at 22 °C.

In the case of [$C_n$impy][TFSI], ionic liquids with shorter alkyl chains (n = 4, 6) were solids at room temperature, whereas those with longer alkyl chains (n = 8, 10) were liquids. Among the ionic liquids that are liquid at room temperature, [$C_n$impy][FSI] showed lower viscosity than those containing other anions. In particular, [C_4impy][FSI], with its relatively short alkyl chain, exhibited a viscosity of 101 mPa·s at 25 °C, indicating its suitability for practical applications. A 50 µM acetonitrile solution of [C_4impy][FSI] exhibited fluorescence with a maximum emission at 336 nm. Its emission wavelength was shorter than that of imidazo[1,2-*a*]pyridine, while its fluorescence quantum yield (Φ_F = 0.39) was higher (Table 1). These results suggest its potential application as a component in composite materials utilizing FRET with fluorophores emitting in the visible region.

Table1. Optical spectroscopy data for imidazo[1, 2-*a*]pyridine and [C_4impy][FSI][a]

Compound	λ_{abs} / nm	$\lambda_{em}(\lambda_{ex})$ / nm	Φ_F[b]
imidazo[1, 2-*a*]pyridine	221, 302	373 (302)	0.22
[C_4impy][FSI]	213, 384	336 (384)	0.39

[a] All spectra were recorded in acetonitrile solution (7.0 X 10^{-6} M) at 25°C. [b]Fluorescence quantum yield determined relative to naphthalene in 7.0 X 10^{-5} M (Φ_F = 0.23) as standard.

On the molecular origins of Stokes-Einstein breakdown in choline chloride based deep eutectic solevents

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Abstract

Deep eutectic solvents (DESs) have attracted significant interest as sustainable alternatives to conventional ionic liquids, owing to their low cost, low toxicity, and tunable physicochemical properties.[1] However, their relatively high viscosities and low ionic conductivities remain key barriers to widespread application. While macroscopic transport behavior in these systems has been extensively characterized, its molecular-scale underpinnings remain largely unexplored. In this work, we investigate the microscopic diffusion dynamics of three choline chloride (ChCl)-based DESs formed with urea, glycerol, and ethylene glycol as hydrogen bond donors (HBDs), using quasielastic neutron scattering (QENS). By systematically comparing the nanoscale diffusion mechanisms of cholinium ions across these systems, we elucidate how the chemical nature and molecular structure of the HBD modulate transport at molecular length scales.

The molecular-scale dynamics of cholinium ions were resolved into two distinct components: long-range translational diffusion and localized motions.[2] The spatial and temporal characteristics governing translational diffusion exhibit a systematic dependence on the nature of the HBD. Although cholinium ions undergo larger molecular displacements in reline, the stronger hydrogen-bond network significantly slows the associated relaxation timescale, resulting in the slowest translational diffusion among the three systems. In contrast, ethaline exhibits the fastest translational dynamics, as cholinium ions disrupts the hydrogen-bond network between ethylene glycol molecules, thereby facilitating comparatively faster diffusion at molecular length scales.

The interplay between these parameters becomes particularly evident in the context of Stokes-Einstein (SE) relation. While all three DESs exhibit a pronounced breakdown of the SE relation in translational diffusivity, the physical origin of this breakdown is found to be system dependent. In ethaline and glyceline, the deviation is governed predominantly by the geometry of diffusion, arising from finite, non-local displacements in particle dynamics. In contrast, reline represents a limiting case where both geometric constraints and relaxation timescales contribute cooperatively to the observed breakdown. Overall, this study highlights the fundamentally scale-dependent nature of transport in DESs and provides new insights into the microscopic origins of Stokes–Einstein breakdown.

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Controlled growth of in-situ carbide layers on refractory metals by salt-bath carburization in molten $CaCl_2$–CaC_2

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Abstract

The conventional construction of carbide layers on refractory metals usually relies on high-temperature vacuum processing or multistep gas–solid reactions, making it difficult to balance process simplicity, solid–liquid interfacial wettability, and microstructural control. Here we report an in-situ salt-bath carburization method based on molten $CaCl_2$–CaC_2, in which CaC_2 acts as the active carbon source and establishes a unified thermodynamic basis for the conversion of Ti, Nb, Ta, and Mo, together with their oxides, into the corresponding carbides. Thermodynamic and kinetic analyses show that layer growth is governed not by independent metal-specific mechanisms, but by a shared carbon-potential gradient established through the coupling of interfacial carbon supply and inward carbon diffusion within the preformed carbide layer, leading to an overall parabolic growth behavior. Under $CaCl_2$–2 wt.% CaC_2 at 900 °C for 8 h, the carbide-layer thickness follows the order Ti (105 μm) > Mo (2.8 μm) ≈ Nb (2.6 μm) > Ta (1.5 μm), indicating that intrinsic substrate reactivity and carbon diffusivity within the carbide layer strongly modulate growth scale under the same diffusion-controlled framework. More importantly, this difference in growth scale gives rise to distinct structural outcomes: a thick, flat, and dense TiC layer at higher growth flux, and a single-phase porous coral-like Mo_2C layer at lower growth flux. The latter also follows parabolic kinetics, with an apparent activation energy of 174.2 kJ mol^{-1} and a pronounced surface-leveling effect. These results show that salt-bath carburization in molten $CaCl_2$–CaC_2 is not only a practical method for carbide-layer preparation, but also a controllable route for regulating layer thickness, compactness, and porosity.

Integrated Valorisation of Lignocellulosic Biomass into Biomaterials Using Biocompatible Ionic Liquids

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Abstract

Lignocellulosic biomass is the most abundant renewable source of materials in the world; however, its efficient valorisation remains challenging due to its recalcitrant structure. In this work, we present a sustainable and efficient strategy for lignocellulosic biomass valorisation and subsequent lignin processing into advanced biomaterials using biocompatible ionic liquids (ILs). While cellulose is currently the primary value-added fraction, lignin remains underutilised, representing both a challenge and an opportunity for the development of biorefineries and sustainable biomaterials. Here, lignin is selectively recovered and processed into biomaterials, while the cellulose-rich pulp is simultaneously valorised into biomaterials. The resulting formulations and biomaterials were comprehensively characterised, with particular emphasis on their rheological and mechanical properties. Overall, this work highlights an integrated valorisation of lignocellulosic biomass, enabling the development of advanced biomaterials with promising potential in the biomedical field. The authors acknowledge support from the UKRI Bio-derived and Bio-inspired Advanced Materials for Sustainable Industries (VALUED) programme (EP/W031019/1).

A Vibrational Spectroscopy Study of Non-Stoichiometric Protic Ionic Liquids Based on DBN and DBU Superbases

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Abstract

Protic ionic liquids (PILs) are formed by proton transfer between a Brønsted acid and base. Unlike aprotic ILs, PILs exhibit an intrinsic acid-base equilibrium that leads to the coexistence of ionic and neutral species in the liquid phase.[1] The extent of proton transfer depends on the relative strength of the acid and base, making these systems structurally complex and tunable. Consequently, PILs may form non-stoichiometric mixtures containing neutral molecules and ion pairs.[2] Previous studies on PILs based on superbases 1,5-diazabicyclo(4.3.0)non-5-ene (DBN) and 1,8-diazabicycloundec-7-ene (DBU) combined with carboxylic acids have shown azeotropic compositions enriched in acid.[2] This behavior has been attributed to hydrogen-bonded complexes where neutral acid molecules interact with ion pairs, forming supramolecular structures in the liquid phase.[2]

In this work, the liquid structure of PILs formed by DBN and DBU with acetic acid (HAc) and octanoic acid (HOct) was investigated using vibrational spectroscopy (infrared (IR) and Raman), supported by quantum-chemical calculations and *ab initio* molecular dynamics (AIMD) simulations. To probe the role of composition and the acid-base equilibrium, IR and Raman spectra were collected for mixtures with different base:acid ratios (10:1 to 1:10). Figure 1 illustrates the results for DBN:HAc mixtures. Characteristic bands of the neutral bases (1653 cm^{-1} for DBN) progressively decrease in intensity with increasing acid concentration, however, a small fraction of neutral base remains even at the equimolar composition corresponding to the PIL. Cooling the PIL decreases the neutral base band intensity, consistent with a temperature-dependent acid-base equilibrium. The stretching mode ν(C=O) of the acids appears in the same spectral region and presents multiple components, reflecting the coexistence of cyclic dimers, linear chains, and "free" molecules. In acid-rich mixtures, ion pairs and hydrogen-bonded structures $[DBNH]^{+}\cdots[Ac]^{-}\cdots[HAc]$ disrupt the original acid network and reduce the population of cyclic dimers. Further insights arise from the high-frequency IR region (1800–3600 cm^{-1}) where AIMD simulations reproduce the spectral evolution and indicate increasingly mobile protons. Analysis of N-H and O-H distances suggests proton exchange between $[DBNH]^{+}\cdots[Ac]^{-}$ in equimolar clusters and between $[Ac]^{-}\cdots[HAc]$ in acid-rich systems.

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Liquid Metal Electrochemistry

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Abstract

Most metals are produced in the liquid form such as iron, steels, aluminum, magnesium, copper, and rare earth metals. Since metal extraction is a big CO_2 emitter, the low-carbon metal extraction methods are much needed to resolve the climate change associated with the tradition metal extraction. In this context, the transition from fossil fuels-driven extraction processes to renewable energy-driven processes has been considered as an effective way to achieve the zero-carbon metal extraction. Thus, the road to carbon neutrality is paved with electrochemical technology. In this regard, molten salt electrochemistry plays an important role in enabling the electrification of clean metal extraction (e.g., desulfurization of liquid sulfide cathodes, sulfide anode electrolysis) and liquid metal batteries. Both electrochemical metal extraction and liquid metal batteries are dictated by the principle of so-called liquid metal electrochemistry. The first approach is using renewable electricity to driven metal extraction, and later one is to storage renewable energy in the liquid metals. The same goal is to integrate renewable energy to our current industries and daily lives, aiming to achieving a low-carbon or zero-carbon society. In addition to laboratory research, the industrial application of liquid metal electrolysis has been applied in the lead-acid battery field, by which the M-Pb master alloys are produced and used for grid alloy production.

Recovery of Silver and Silicon from Spent Solar Cells by Direct Separation Driven by Galvanic and Chemical Etching in Molten Chloride

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Abstract

The rapid expansion of photovoltaic deployment underscores the critical need for sustainable recycling of silver (Ag) and silicon (Si) from retired modules. However, alkaline etching methods inevitably attack both SiO_2 and Si. Herein, the Ag/Si interface and SiN_x layer are removed in molten NaCl-$CaCl_2$ within 1 min by galvanic and chemical etching. The galvanic etching happens between the Al back layer as the anode and the SiO_2 at Ag/Si interface as the cathode within the molten NaCl-$CaCl_2$ as the electrolyte. During galvanic etching, Al is oxidized to Al_2O_3 and SiO_2 is reduced to Si with volume shrinkage, leading to the separation of Ag from Si. Simultaneously, the chemical etching is enabled by the reaction of $CaCO_3$/CaO with SiO_2 and SiN_x, resulting in removing Ag and SiN_x. This method achieves a 99.0% Ag and Si recovery efficiency because Si is almost inert to the etching agent. Furthermore, life cycle assessment (LCA) and life cycle costing (LCC) confirm a reduction of 11.0 kg CO_2-eq and a benefit of $14.04 per kg of cells recycled. Overall, the molten salt provides a selective medium to allow both galvanic and chemical etching with lower materials consumption, offering a technically viable circular pathway for photovoltaics.

Upcycling of waste sodium sulfate to sodium carbonate and sulfur

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Abstract

Over 20 million tons of waste sodium sulfate (Na_2SO_4) are generated annually[1-3], yet current recycling strategies are hindered by prohibitive capital costs or a reliance on toxic ammonia (NH_3)[4-6]. Herein, we propose a novel, NH_3-free thermochemical pathway to upcycle waste Na_2SO_4 into high-value sodium carbonate (Na_2CO_3) and elemental sulfur. This process comprises two stages: (1) a carbothermal reduction at 750–850 °C that converts molten Na_2SO_4 into Na_2S without toxic SO_x emissions, utilizing a carbon matrix to prevent sintering; and (2) a low-temperature carbonation at 300 °C, where Na_2S reacts with CO_2 (**Figs. 1a-b**). Scale-up experiments utilizing 50 g of waste salt achieved a 95.35% carbonate yield with a purity of 99.53%. Crucially, this method exhibits robust tolerance to chloride impurities (**Fig. 1c**), overcoming a major limitation of conventional processes. Comprehensive life-cycle assessment (LCA) and cost analyses validate its superiority: compared to traditional methods, this anhydrous route reduces water consumption by over 55.7% and lowers the global warming potential (GWP) by >0.43 kg CO_2-eq per kilogram of product (**Figs. 1d-f**). By valorizing hazardous byproducts into essential feedstocks while simultaneously utilizing CO_2, this scalable, low-carbon strategy offers a transformative and highly profitable solution for industrial waste management (**Fig. 1g**).

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The Effect of Tertiary Amine Alkyl Chain Length on Ionic Liquid Properties and Biomass Fractionation in the Ionosolv Process

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Abstract

The push toward sustainable biorefineries has driven significant interest in the fractionation of lignocellulosic biomass into its constituent polymers - cellulose, hemicellulose, and lignin. The ionosolv process offers a promising route to achieve this separation using low-cost ionic liquids, typically formed from sulfuric acid and a tertiary amine. While both the cation and anion influence fractionation efficiency, the role of amine structure remains incompletely understood. This study systematically investigates how alkyl chain length in the amine cation affects ionic liquid properties and, ultimately, biomass fractionation performance.

Four tertiary asymmetric amines paired with a bisulfate ($[HSO_4]^-$) anion were synthesised and evaluated using *Miscanthus giganteus* as the biomass feedstock. Building on the established use of N, N-dimethyl butylamine (DMBA) as the standard ionosolv cation, the series was designed to probe the effect of increasing alkyl chain length on both the physicochemical properties of the ionic liquid and the quality of the resulting fractions.

All four ionic liquids were characterised for viscosity, conductivity, and acidity. A clear trend emerged with increasing chain length: longer chain amines produced ionic liquids with progressively higher viscosity and conductivity. However, higher viscosity did not translate to better fractionation outcomes. The cellulose-rich pulps were assessed by enzymatic saccharification to determine glucose yield and pulp purity as well as the NREL method for compositional analysis to determine the component percentages, while isolated lignin fractions were analysed by HSQC NMR spectroscopy. Additionally, microscopy and particle size analysis were employed to characterise the physical properties of the pulps and relate them to the ionic liquid used.

DMBA, bearing a four-carbon alkyl chain, outperformed all other amines tested, delivering the highest cellulose purity and the best cellulose recovery. The longest chain amine, by contrast, despite its more pronounced physical properties, ended up not following the previously held pattern, showing peak performance with [DMBA][HSO_4]. We propose that this reflects an optimal balance in polymer coordination: a four-carbon chain is sufficient for the amine to interact effectively with the biomass polymers and facilitate their separation, whereas excessively long chains begin to disrupt the polymers themselves, reducing overall recovery and purity.

These findings suggest that amine chain length is a critical design parameter in ionic liquid optimisation for the ionosolv process, and that moderate chain lengths strike the most effective balance between ionic liquid character and biomass interactions. This has practical implications for the rational design of low-cost ionic liquids for scalable biorefinery applications.

High-Temperature Gas Diffusion Electrode Enables Energy-Efficient Electroreduction of Flue Gas to Syngas at Ampere-Level Current Density

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Abstract

The capture and electrochemical conversion of CO_2, especially from industrial flue gas, offers a promising route to mitigate greenhouse gas emissions. However, the low CO_2 concentration in practical flue gas (typically 10–14 vol%) poses major challenges for developing CO_2 electroreduction technologies that are cost-effective, energy-efficient, selective, and capable of operating at high current density. Here, we report a high-temperature co-electrolysis strategy for humid CO_2 at 750 °C, where both CO_2 and H_2O vapor—two major components of power plant flue gas—are simultaneously converted into syngas. At this temperature, hydrogen evolution from steam and CO generation from CO_2 are both thermodynamically and kinetically favorable. To exploit the advantages of this high-temperature reaction environment, we developed a cost-effective high-temperature gas diffusion electrode (HT-GDE) based on commercial Cu foam, paired with a molten salt electrolyte. This system enables the direct conversion of humid CO_2 into syngas at ampere-level current densities, with an H_2/CO ratio well suited for Fischer–Tropsch synthesis. Notably, H_2O/CO_2 co-electrolysis also unexpectedly reduces anodic polarization, delivering an energy efficiency of up to 60.0% even at current densities above 1 A cm^{-2}, together with stable operation for at least 100 h. In addition, a kinetic overlap between H_2 and CO production was observed, and the system showed broad adaptability to flue gases from different types of power plants. This HT-GDE-assisted molten salt co-electrolysis technology provides a versatile and efficient platform for direct flue gas utilization.

Online Electrochemical Detection of O^{2-} in Molten Carbonates

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Abstract

Oxide ions (O^{2-}) govern the reaction kinetics, mass transport, and corrosion behavior in high-temperature molten salt electrolysis, yet their real-time activity during operation has never been directly measurable. Here, we present a potentiometric YSZ-Pt oxide ion-sensing electrode (YSE) that enables online monitoring of O^{2-} activity in molten carbonates.

The YSE shows excellent Nernstian response ($R^2 > 0.9998$) to controlled changes in O^{2-} activity via CO_2 partial pressure. Deployed during CO_2 electrolysis, the sensor reveals a clear and previously unseen phenomenon: O^{2-} accumulates near the cathode while being depleted near the anode. These direct measurements provide the first experimental evidence of local basification and acidification caused by transport limitations in molten salt electrolysis.

Our work establishes a reliable, real-time alkalinity meter for high-temperature molten salts, offering a powerful new tool to understand concentration polarization, optimize electrode design, and improve efficiency in processes ranging from CO_2 conversion to aluminum electrolysis and nuclear fuel recycling.

Recycling alloy scraps and CO_2 by paired electrolysis in $CaCl_2$-based molten salts

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Abstract

Nickel-based superalloy scrap is one of the most difficult wastes to recycle owing to its excellent corrosion resistance, oxidation resistance, and high-temperature resistance. Studies on the stability of nickel-based metal anodes in molten carbonates have been reported. These studies have shown that the anodic oxide film formed in electrolytes containing Cl^- exhibits higher porosity, and the pores in these oxide films may serve as channels for electrolyte penetration into the metal matrix, thereby accelerating the corrosion of the metal anode. Herein, we designed a molten salt electrolyzer using alloy scrap as the anode and a metallic Ni plate as the cathode to achieve paired electrolysis recycling of alloy scrap and CO_2. Under a cell voltage of 2.4 V at 700 °C for 7.5 h, oxidation efficiency of the alloy scrap is 97.43%, and the oxidation rate of the alloy anode exhibited a linear relationship with time. Moreover, the anode corrosion demonstrated a "temperature effect", with active corrosion at lower temperatures and passivation oxygen evolution at higher temperatures (≥ 750 °C). Meanwhile, CO_2 was indirectly reduced at the cathode in the form of CO_3^{2-} to C/CO, while releasing O^{2-} to absorb CO_2 and replenish the continuously consumed CO_3^{2-} in the electrolyte.

Unravelling the role of aqueous choline chloride-polyol based deep eutectic solvents in protein stability

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Abstract

Protein stability is crucial for their effective usage in drug delivery, biotherapeutics, and industrial applications etc,. The instability of proteins often leads to degradation and loss of biological activity. In this context, NADES have been employed as a promising alternative solvents to improve protein stability. Initially, we performed molecular dynamics simulations of aqueous DES (ADES) composed of choline chloride and three polyols - erythritol, xylitol and sorbitol, at 0, 25, 50 and 75 wt% of water to investigate structural reorganization of DES components by water. Radial distribution function (RDF) and cluster size analyses revealed that alcohol-alcohol clustering decreases with increasing water content, whereas water-water clustering shows a non-monotonic dependence, indicating the emergence of bulk like water behavior at higher hydration levels. These results highlighted the importance of tuning DES composition to control water-mediated structuring for their chemical and biological applications. Subsequently, MD simulations of lysozyme in NADES were carried out to examine the structural and dynamical properties of the system. The stable Rg, RMSD, RMSF reveals the enhanced protein compactness and stability, which was further supported by secondary structure analysis. Further, the RDFs and hydrogen bond analysis of the solvent reveal the preservation of bulk structure of the ADES components even in the presence of lysozyme. Together, these results suggest that choline chloride-polyol based NADES, particularly in the presence of water provide a stabilizing environment for proteins, making them promising solvents for biotechnological and therapeutic applications.

Molecular Dynamics Insights into Ionic Conduction in Cyclopropenium-Based State-Independent Electrolytes

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Abstract

Ion conductivity is one of the most important characteristics of batteries and fuel cells and is highly dependent on the thermodynamic state in conventional electrolytes. At the liquid-to-solid phase transition, a pronounced decrease in ion mobility is typically observed, accompanied by a shift from linear Arrhenius behavior to the non-linear Vogel-Tammann-Fulcher relationship [1]. Recently, a family of ionic liquids (ILs) based on the tris(trialkoxyphenyl) cyclopropenium cation paired with a halide counterion was synthesized and shown to exhibit Arrhenius-like ionic conductivity across transitions from an isotropic liquid to a liquid crystalline state, and then to a crystalline solid [2]. In this study, we conducted molecular dynamics simulations in the 298-400 K temperature range to elucidate the molecular origins of this behavior in these novel compounds (Figure 1). The results reveal that the self-assembled cation columns formed upon cooling remain sufficiently flexible to permit chloride ion mobility, which governs charge transport in these ILs.

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High-Temperature In Situ Spectroscopic Study on the Coordination Structure of Zr-Containing Fluoride Molten Salts

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Abstract

Molten salt reactors use molten fluoride salts as media, in which UF_4 is dissolved to form a liquid fuel. To suppress the reaction between UF_4 and water/oxygen species in the molten salt that produces UO_2 precipitates, ZrF_4 is typically introduced into the system as an oxygen scavenger. However, Zr^{4+} also exhibits strong coordination capability toward F^-, forming structures such as $[ZrF_6]^{2-}$, $[ZrF_7]^{3-}$, $[ZrF_8]^{4-}$, and $[ZrF_9]^{5-}$. Meanwhile, the presence of Zr^{4+} competes with Be^{2+} for F^- coordination, thereby altering the chemical environment of F^- ions in the molten salt and consequently changing the corrosiveness of the molten salt and the solubility of nuclear fuel. To address this issue, in situ characterization of FLiBeZr was carried out using high-temperature NMR and high-temperature XAFS. The chemical environments of molten salt at different ZrF_4 contents were investigated. The results show that the addition of ZrF_4 promotes the formation of network environment, accompanied by a decrease in the average Zr-F coordination number.

Investigation of Structure and Thermophysical Properties of Zirconium-Containing Molten Salts for Reactor Applications via Machine Learning Molecular Dynamics

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Abstract

Fluoride molten salts are widely used in molten salt reactors as nuclear fuel carriers and coolants, in which thorium- and uranium-based fuels are dissolved to form liquid fuel salts during reactor operation. To suppress the reaction between UF_4 and oxygen/moisture impurities in molten salts that leads to UO_2 precipitation, ZrF_4 is commonly introduced as an oxygen scavenger. As a high ionic-potential cation, Zr^{4+} readily coordinates with F^- ions; therefore, the incorporation of ZrF_4 modifies the original coordination environment of the molten salt and consequently affects its thermophysical properties.

In this work, the FNaBeZr molten salt system was systematically investigated using machine learning potential molecular dynamics simulations to elucidate the evolution of microscopic structures and thermophysical properties under different temperatures and ZrF_4 concentrations. The results reveal that Zr^{4+} exhibits stronger coordination capability than Be^{2+}. The partially covalent nature of Be-F bonds together with the strong solvation effect of Zr-F interactions jointly promote the formation of network structures in the molten salt, which exhibit excellent stability against thermal perturbations. With increasing ZrF_4 concentration, $[BeF_4]^{2-}$ and $[ZrF_6]^{2-}$ polyhedra progressively connect through bridging F^- ions, leading to the formation of a more compact Be-F-Zr network structure. This enhanced network connectivity suppresses ionic mobility, resulting in increased viscosity and reduced thermal conductivity of the molten salt.

This work systematically clarifies the relationship between structure evolution and thermophysical properties in FNaBeZr molten salts, providing theoretical insights and supporting data for thermal-hydraulic design and safety assessment of molten salt reactors.

[DMBA][HSO_4]-Based ionoSolv Fractionation of Miscanthus for Cellulose Fibre Formation

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Abstract

Lignocellulosic biomass offers a renewable route towards sustainable materials, but its naturally recalcitrant structure makes selective cellulose recovery challenging. Miscanthus is a promising non-food biomass feedstock because it can be cultivated on marginal land and can support circular biorefinery systems. In this work, Miscanthus biomass was fractionated using the ionoSolv process with the ionic liquid [DMBA][HSO_4], which enabled the disruption of the lignocellulosic matrix and recovery of a cellulose-rich pulp for subsequent fibre formation.

The processing route involved ionoSolv oven treatment, washing, followed by bleaching, sonication, freeze-drying, and characterisation. The conventional Soxhlet extraction step after ionoSolv pretreatment was omitted, simplifying the downstream processing route. Response surface methodology was also used to optimise sonication conditions, aiming to promote fibrillation and cellulose network formation. The resulting materials were analysed using compositional analysis, FTIR, SEM, XRD, TGA, and film formation assessment.

Compositional analysis showed that direct bleaching and sonication after ionoSolv pretreatment produced a cellulose-rich pulp with around 90% cellulose content. FTIR supported this result, with the disappearance of the carbonyl-associated peak around 1700 cm^{-1} and increased intensity in the cellulose fingerprint region. SEM images showed a transition from compact raw biomass to exposed cellulose bundles after ionoSolv treatment, followed by an interconnected fibre network after bleaching and sonication. XRD confirmed the presence of characteristic cellulose peaks, while TGA showed a more cellulose-like degradation profile in the bleached and sonicated pulp. The processed cellulose-rich pulp was also able to form free-standing films, suggesting sufficient fibre-fibre interaction and network cohesion.

Overall, this work demonstrates that [DMBA][HSO_4] ionic liquid plays an important role in the IonoSolv fractionation of Miscanthus by disrupting the biomass structure and enabling selective recovery of cellulose-rich pulp through a simplified downstream route. Subsequent bleaching and sonication further refined the pulp into a fibrillated cellulose network capable of forming free-standing films. These results support the use of ionic-liquid-based biorefineries to convert non-food lignocellulosic biomass into higher-value cellulose materials, contributing to circular and sustainable material development. Future studies will focus on optimising film properties for packaging applications.

Thermally Responsive Selective Fractionation of Birch Wood Biomass Using Hydrophilic-Hydrophobic DES Systems

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Abstract

Selective physicochemical fractionation, integrated with low-energy separation of wood biomass, remains a major limitation to scalability in biorefineries. Deep eutectic solvents (DES) have been reported as greener neoteric solvents for biomass processing in single-phase systems. Herein, we report a thermally responsive biphasic DES platform that combines hydrophilic and hydrophobic DES for birch biomass deconstruction to perform a one-pot fractionation process, with in situ component partitioning. The system combines cost-effective hydrophilic DESs based on Hydrogen bond acceptors (HBA), (choline chloride and betaine), with acidic hydrogen-bond donors (HBD), alongside a hydrophobic DES composed of thymol and a long-chain fatty acid. Upon pretreatment of birch under mild conditions, the system forms a homogeneous phase at high temperature that exhibits lower critical solution temperature (LCST) behavior during cooling, enabling phase-directed fractionation with uniform penetration. Preferentially, lignin partitions into the hydrophobic phase due to π-π stacking, while other components remain in the solid or liquid phase. Varying the HBD and HBA in the rational design of DES significantly affects lignin and hemicellulose recovery and cellulose purity. Remarkably, this work establishes a design principle for switchable, multiphase DES systems that integrate reaction and separation within a single solvent architecture. The concept offers a scalable and adaptable route toward next-generation biomass valorization, where solvent chemistry directly dictates both deconstruction and downstream separation.

Ionic Liquid-Assisted Extraction and Stabilisation of Bioactive Cannabinoids from Medicinal Cannabis

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Abstract

Medicinal cannabis has gained considerable scientific and pharmaceutical interest considering the wide scope of application of cannabinoids and terpenoids for chronic pain, inflammation, epilepsy, anxiety and neurodegenerative diseases. Conventional extraction methods for cannabinoids use the application of volatile organic solvents, high energy requirements and less selectivity. More recently ionic liquids and deep eutectic solvents have been introduced as sustainable means for the extraction and stabilisation of bioactives from natural products. This research explores a solvent system in the form of ionic liquids for the optimized extraction, purification and stabilization of cannabinoids from medicinal cannabis biomass. Ionic liquid solutions were screened as to their extractability and selectivity for cannabidiol and tetrahydrocannabinol as well as their effect on terpene retention. Physical and chemical properties of the ionic liquids like viscosity conductivity polarity and thermal stability were linked to cannabinoid extractability and stability.

The compounds obtained were characterised using chromatography and spectroscopic techniques and comparison made with traditional ethanol extraction procedures. Initial results show ionic liquids were potentially able to increase cannabinoid recovery, improve the retention of the plant derived terpenes as well as decrease volatile nature and environmental impact. The efficacies of certain ionic liquids systems in improving cannabinoid rich extract solubilisation and formulation stability was also explored.

The findings highlight the potential of ionic liquids and analogous molten salts as environmentally friendly media in the processing and formulation of medicinal cannabis. These results are one component of a rapidly expanding system that employs sustainable green solvent systems in natural product chemistry and medicinal plant studies.

Keywords: Medicinal cannabis; ionic liquids; eutectic solvents; cannabinoid extraction; CBD; THC; green chemistry; terpene preservation.

Deep Eutectic Solvents for Biocatalysis: Advanced Materials and Enzymatic Modulation

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Abstract

Deep eutectic solvents (DESs) are formed through the association of hydrogen-bond acceptors (HBAs) and hydrogen-bond donors (HBDs), generating eutectic mixtures with melting temperatures lower than those of their individual components. Their tunable composition and hydrogen-bonding interactions enable the design of microenvironments of interest for biocatalytic applications.

An example of DES-based advanced materials is eutectozymes, enzyme-loaded eutectogels designed to enhance enzyme stability, catalytic efficiency, and operational reusability [1]. These soft hybrid materials address the need for sustainable and robust biocatalytic platforms and provide an improvement in enzymatic immobilization [2]. Compared to conventional systems, their gel-like consistency, biocompatible matrix and resilience under operational conditions opens new avenues in biotechnology, bioelectronics, and environmental technologies.

In this talk, we will present computational research on such DES-based biocatalytic systems, by focusing on two areas: understanding the basis of euctectogel stability, and the modulation of enzymatic activity in DES environments. A combined computational and experimental approach is used to uncover structure–property relationship of DES-based materials, supporting their rational design for targeted functions.

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Chiral Imine-linked Porous Organic Frameworks as Catalysts for Asymmetric Reactions in Deep Eutectics Solvents

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Abstract

Chiral compounds are important in pharmaceutics, agriculture and in chemical industries.[1,2] For the above reason, asymmetric catalysis is recognized as one of the most important topics in the area of the synthesis of optically active compounds.[3] Porous organic frameworks (POFs) represent an emerging class of materials, frequently used as catalysts. In particular, chiral POFs combines the unique properties of these materials, such as highly regular porous structures and well-ordered catalytic sites, making them enantioselective materials able of effectively catalyzing asymmetric reactions.[3] In this study, we considered the prolinate anion as catalyst for aldol reaction in different deep eutectics solvents.[4] Therefore, we designed and synthesized a prolinate-based chiral POF to perform the aldol reaction. We employed DESs based on choline chloride and different glycols to investigate the influence of HBD on yield and enantioselectivity. Furthermore, we investigated the influence of HBA, employing betaine as HBA with TEG, which proved to be the best HBD.

It worth noting that yields and enantioselectivities were significantly affected by the DES nature and this result suggested that different effects, such as solvation or chelation effects could play a crucial role. The synergic use of DESs and POF to perform aldol reaction represents a new approach that combines new and modulable materials with green and sustainable solvents.

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Ion Transport and Solvation Structure in Bisolvent-in-Salt Electrolytes for Lithium-Ion Batteries

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Abstract

Lithium-ion batteries (LIBs) remain the dominant electrochemical energy storage technology and their applications are ranging from portable electronics to large scale grid storage. [1] Optimization of LIBs to achieve higher energy density requires refinement of electrolyte properties including conductivity, electrochemical stability window, thermal stability, and a stable anode solid electrolyte interphase (SEI). Solvent-in-salt (SiS) electrolytes have emerged as promising candidates for LIBs owing to their distinctive ion solvation environments and enhanced electrochemical stability. [2] Nevertheless, strong ion–ion interactions in such highly concentrated electrolytes lead to non-ideal transport behavior. To address this, we employ a bisolvent strategy, in which strongly and weakly coordinating solvents are combined to systematically modulate liquid structure and Li^+ coordination. [3,4]

Equimolar binary mixtures were prepared by combining lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) with strongly coordinating solvents, monoglyme (G1) and diglyme (G2), and weakly coordinating solvents, tetrahydrofuran (THF) and 1,3-dioxolane (DOL). Ion–solvent and ion–ion interactions were characterized by Raman spectroscopy, complemented by spectral deconvolution analysis. In addition, ion transport was investigated using pulsed field gradient (PFG) NMR diffusion, electrochemical impedance spectroscopy (EIS), and electrophoretic NMR (eNMR). Key physicochemical properties including self-diffusion coefficients (D_i), ionic conductivity (σ), electrophoretic mobilities (μ_i), effective charges (ε_i), and transference numbers (t^+_i) were determined. The results reveal a pronounced inhomogeneous solvation structure, which directly influences ion transport properties. Among the five bisolvent systems investigated (G1/DOL, G1/THF, G2/DOL, G2/THF, and DOL/THF) significant differences in self-diffusion, ionic conductivity, and Li-$TFSI^-$ coordination are observed. A key finding is the fact that the neutral solvents migrate in the electric field, and the electrophoretic mobility of the stronger coordinating solvent generally exceeds that of Li^+, reflecting the heterogeneous nature of the Li^+ coordination environment.

In conclusion, our findings provide fundamental insight into how liquid structure and ion correlations govern transport in highly concentrated electrolyte solutions, demonstrating that solvent pairing could be a reasonable approach for tuning ionic mobilities and transference numbers in the solvent-in-salt regime.

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Ionic Correlations and Transport Dynamics in Localized High-Concentration Electrolytes

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Abstract

Localized high-concentration electrolytes (LHCEs) are electrolyte systems that combine highly concentrated salt environments with non-solvating diluents to preserve local ion coordination while improving transport properties. Charge transport and salt transport in concentrated electrolytes are generally governed by strong ionic correlations and persistent lithium–anion coordination structures, leading to significant deviations from ideal dilute solution behaviour. Understanding these correlated transport processes is essential for the rational design of advanced electrolyte systems with improved electrochemical stability and transport properties.[1]

In this work, ion dynamics and correlated ion transport in LHCEs were systematically investigated using lithium bis(fluorosulfonyl)imide (LiFSI) and lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) salts dissolved in dimethyl carbonate (DMC). Salt concentrations were selected near the solubility limit for the high-concentration electrolyte (HCE). A small amount of non-solvating diluent, i.e., 1,1,2,2-tetrafluoroethyl-2,2,3,3-tetrafluoropropyl ether (TTE) has been added to study the impact of dilution.

To characterize ionic transport, pulsed-field gradient NMR (PFG-NMR) diffusion measurements were performed to determine self-diffusion coefficients, while electrophoretic NMR (eNMR), electrochemical impedance spectroscopy (EIS), and concentration cell measurements provided the experimental observables required for transport analysis. Five experimental quantities were derived which are to extract the Onsager transport coefficients (σ_{++}, σ_{--}, and σ_{+-}) and the thermodynamic factor. To this end, an overdetermination approach introduced earlier was employed, [2] resulting in respective quantities and their associated uncertainties by a Reverse Monte Carlo analysis.[3] Distinct differences between LiFSI- and LiTFSI-based systems highlight the influence of anion chemistry on ion pairing and transport dynamics.

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Activity coefficients at infinite dilution for diverse solutes in 1-ethyl-3-methylimidazolium and 1-(2-hydroxyethyl)-3-methylimidazolium 1,2,4-triazolide ionic liquids: Effect of cation hydroxyl functionalization

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Abstract

Ionic liquids (ILs) are known for their broad tunability for separation, catalytic and material design. With over one million possible ion combinations, new experimental data on structurally distinct, underexplored ILs are valuable for rational design. Activity coefficients at infinite dilution (IDAC) are valuable for understanding the solute–solvent interactions and act as an initial metric for solvent design in extraction applications.

To broaden understanding of solute–solvent interactions beyond well-studied IL families, we measured IDAC for protic solutes (ethanol, methanol and water) in imidazolium 1,2,4-triazolides (Figure 1) that combine underexplored anion with and without cation hydroxyl (-OH) functionalization ([Emim][Tz] and [HOEmim][Tz]) using a gas-liquid chromatography method. Results were modeled and interpreted with the quantum-chemistry-based solvation model (COSMO-RS), which reproduced experimental trends.

These triazolide-based ILs showed high solute–solvent interactions with polar protic solutes (especially with water). Interestingly, -OH functionalization weakens the solute–solvent interactions with polar protic solutes. COSMO-RS analysis suggests that introducing an -OH group increases the cation–anion interactions via hydrogen bonding. This makes it more difficult for solutes to disrupt these interactions, thereby weakening solute–solvent interactions.

By combining new IDAC data with COSMO-RS interpretation, we not only provide new experimental data for imidazolium triazolides but also establish a link between cation hydroxyl functionalization and IDAC. These results provide a structure-informed basis for the rational design of ionic liquids for separation applications.

Porous Organic Frameworks and Deep Eutectic Solvents in biomass valorization: conversion of fructose to 5-hydroxymethylfurfural.

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Abstract

Valorization of lignocellulosic biomass is currently a topic of great interest to reduce dependence of the modern society on fossil fuels, as biomass is a zero-emissions source of materials, renewable and available.[1] Among the chemicals derived from lignocellulosic biomass, 5-hydroxymethylfurfural (5-HMF) stands out due to its versatility as chemical platform.[2] In this work, we explored the use of deep eutectic solvents and porous organic frameworks for the synthesis of 5-hydromethylfurfural from fructose, using choliniun choride-based DES combined with an imine-linked POF, synthetized from 1,3,5-triformylfloroglucinol and 2,5-diaminobenzensulfonic acid.

The reaction conditions were optimized in terms of reaction temperature and time, catalyst, and substrate loading. Using DES and POF a 60% of 5-HMF yield was achieved at 120 °C in 60 minutes. The solvent-catalyst system can be reused for at least four cycles, without significant loss in performance. In addition, 5-HMF can be easily recovered with high purity by a liquid-liquid extraction, using safe ethyl acetate. Green metrics analysis indicates that the process is scalable and applicable.

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Electrochemical Behavior of Multivalent Uranium Ions in LiCl-KCl Eutectic Melt

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Abstract

The valence state transformation and electrochemical behavior of uranium ions in molten chloride systems constitute an important research area in the dry reprocessing of spent nuclear fuel. They are essential for understanding the reaction characteristics of actinides in high-temperature ionic media. In the LiCl-KCl eutectic melt, uranium can exist in several valence states, yet the interconversion among these species and their influence on the electrode processes remain insufficiently understood.

In this work, an environment in which uranium ions of multiple valence states coexist was established using LiCl-KCl eutectic melt as the medium. A combination of electrochemical techniques, including cyclic voltammetry, square wave voltammetry, chronoamperometry and potentiostatic electrolysis, was employed to systematically investigate the redox behavior, mass transport properties and deposition processes of uranium ions. The morphology and microstructure of the electrodeposits were further characterized to examine the nucleation and growth behavior of uranium during electrodeposition under different conditions. Preliminary results indicated that the reduction of U(III) to uranium metal proceeded via a single-step electron transfer exhibiting quasi-reversible electrochemical characteristics. The uranyl ion, in contrast, underwent a two-step consecutive reduction with strongly irreversible electrode reactions. Distinct differences were observed in the reduction potential distributions of the different uranium species. Notably, the reduction of uranyl ions occurred at more positive potentials than that of U(III) ions. Chronoamperometric analysis revealed that the electrodeposition of uranium metal followed a three-dimensional instantaneous nucleation and growth mechanism, and the deposition proceeded through typical stages of nucleation, growth and coalescence. These findings advance the understanding of the electrochemical behavior of multivalent uranium ions in molten chloride systems and provide an experimental basis for investigating the reaction mechanisms of actinides in high-temperature molten salts.

Thermodynamic interactions of L-serine in aqueous 1-butyl-3-methylimidazolium bromide solutions at T = (288.15-318.15) K

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Abstract

Ionic liquids gained more interest in recent years due to their wide applications in the field of chemical synthesis as well as in technology development such as solubilize protein, increase the protein activity, refolding for biocatalysis and also preserve the enzyme's stability. In this context, researchers are trying to develop the ionic liquids, which are of biological origin so that they can be used safely and can have applications in the field of medicine and protein chemistry. In view of above, densities, ρ of L-serine in water and in aqueous 1-butyl-3-methylimidazolium bromide, [BMIm][Br] solutions of various molalities, (0.1-1.0) mol·kg^{-1} over the temperature range T = (288.15-318.15) K and at atmospheric pressure have been determined using vibrating-tube digital density meter (DMA 4500M, Anton Paar, Austria). The density data have been used to calculate the apparent molar volume, partial molar volume and partial molar volumes of transfer. The partial molar volume values of L-serine in aqueous solutions are higher than those in water and thus exhibit positive partial molar volumes of transfer, which are indicative of strong interactions between L-serine and [BMIm][Br]. The volumetric interaction parameters and hydration numbers have also been calculated to discuss in context of hydration of L-serine.

Sustainable Recovery of REEs and Critical Materials from Secondary Industrial Resources via an Eco-Friendly Oxidative Leaching System

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Abstract

The depletion of traditional strategic deposits necessitates the development of efficient hydrometallurgical approaches to reclaim critical materials from secondary industrial resources. This study focuses on the sustainable recovery of rare earth elements (REEs), vanadium, and selenium from depleted core samples obtained from subterranean in-situ leaching (ISL) operations after the extraction of the primary target metals. Traditional sulfuric acid systems often face limitations in mobilizing these co-existing elements due to complex mineralogical occurrences and stringent redox-controlled migration pathways. To overcome these constraints, an innovative eco-friendly chlorine-containing oxidative leaching system ($HCl/Cl^-/OCl^-$) was investigated. This system leverages high oxidation-reduction potential and advanced complexation mechanisms to target refractory mineral phases, including phosphate matrices, where REEs are firmly bound within the host sandstone core samples.

Comprehensive chemical and mineralogical characterization identified specific occurrence forms of by-product components within the complex geomatrix. A systematic series of agitated and filtration-mode leaching tests were executed to define optimal hydrodynamic and chemical parameters without disclosing confidential operational formulations. The multi-component oxidative system demonstrated superior efficiency, destabilizing resistant host mineral lattices and stabilizing highly soluble chloride complex forms. The results indicate significant mobilization potential, achieving robust extraction yields for total critical components (average recoveries reaching approximately 80% for REEs, 75% for vanadium, and 60% for selenium).

Integrating this oxidative methodology into existing subterranean leaching lifecycles provides a highly viable, economically sound path for secondary processing. This approach transforms depleted operational blocks into alternative, environmentally sustainable feedstocks essential for modern clean energy technologies.

Keywords: Rare earth elements, Critical materials, Secondary resources, Oxidative leaching, In-situ leaching, Chlorine-containing system.

Nutraceutical-Ionic Liquids (NILs): Synergists for Insecticide Formulations

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Abstract

Background: Synergists in insecticide formulations requiring safer, eco-friendly to enhance insecticide efficacy while reducing health risks and environmental impact. This study explores vanillic acid-based nutraceutical ionic liquids (NILs) as sustainable synergists using the Active Pharmaceutical Ingredient-Ionic Liquid (API-IL) concept.[1]

Methods: 10 novel ILs were synthesized in one pot reaction and evaluated for ecotoxicity against bacteria and fungi. Their synergistic potential was assessed through *in vitro* enzyme inhibition of Glutathione-S-Transferase (GST) and Esterase (EST). *In vivo* synergism and efficacy against tolerant *Blattella germanica*, was compared to a commercial synergist.

Results: 9 NILs (Out of 10 NILs) were harmless to bacteria and fungi.[2] *In silico* analysis using the AquaBoxIL[3] tool predicted quaternary ammonium ILs are more biodegradable. Our *in vitro* assays revealed significant inhibitory activity of detoxification enzymes (GST, EST), both in its native form and as NILs. On these insights, *in vivo* evaluations of 4 NILs and vanillic acid in *Blattella germanica* revealed efficacy of 4 NILs (Out of 10 NILs) comparable to a commercially available synergist.

Conclusion: NILs enhance insecticide efficacy, reduce ecological risks, and enable novel ionic liquids as synergists for insecticide formulations.

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Development of Ionic Liquid Composites for Acidic Gas Contaminants Mitigation

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Abstract

The mitigation of acidic gases (e.g. sulfur oxides, hydrogen sulfide and nitrogen oxides) is essential for various applications, including in the purification of air used in fuel cells, data centers and semiconductor fabrication. This talk will focus on our research efforts in the design, synthesis, characterization, and 3D printing efforts of ionic liquid-based composites for acidic gas mitigation. Emphasis will be given to work on metal-based ionic liquids/salts of type $M_x[R]_y[C_2mim]_z$, where R is an acetate or citrate anion, for sulfur dioxide mitigation. The results of computational modeling, 3D printing processes, and gas sorption testing, including the sorption performance (breakthrough times, selectivity, and sorption capacity), will be discussed.

Catalyst-Free Deep Eutectic Solvent–DMSO Biphasic Conversion of Agro-Industrial Wastewater into 5-Hydroxymethylfurfural for Circular Biorefinery

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Abstract

Carbohydrate-rich agro-industrial wastewater represents an underutilized renewable carbon source, but its direct conversion into platform chemicals remains challenging due to dilution, complex composition, and product degradation in aqueous acidic media. This study developed a catalyst-free deep eutectic solvent (DES)–DMSO biphasic system for the direct conversion of food-processing wastewater into 5-hydroxymethylfurfural (5-HMF), an important bio-based precursor for fuels, polymers, and furan-derived chemicals. Pineapple peel waste liquid (PPWL) and sweet potato waste liquid (SPWL) were selected as representative real wastewater feedstocks without prior purification or pretreatment. Fifteen choline chloride-based DES formulations were screened using different hydrogen bond donors and molar ratios. For PPWL, ChCl acid (1:2) showed the highest catalytic performance, achieving a 5-HMF yield of 83.64 ± 1.68%, while further optimization of the waste liquid/DMSO ratio increased the yield to 85.51 ± 2.76%. For SPWL, response surface methodology identified optimal reaction conditions of 150 °C for 135 min, producing 20.93 g/L 5-HMF. The DMSO-rich biphasic system improved product stabilization and reduced side reactions, while NH_4Cl-assisted salting-out followed by THF extraction enabled near-quantitative 5-HMF recovery, with extraction efficiencies of 99.99% and 99.94% for PPWL and SPWL, respectively. Preliminary two-fold scale-up experiments showed no significant decrease in 5-HMF production, suggesting good process robustness. Recovered DES maintained stable catalytic performance over three consecutive cycles in a fructose model system, although lower recyclability was observed in complex wastewater matrices. Overall, this work demonstrates a metal-free, catalyst-free, and recyclable DES-based strategy for transforming food-processing wastewater into high-value platform chemicals. The proposed process provides a practical route for integrating liquid salt chemistry, biomass valorization, and circular biorefinery design.

Pyrochemical recycling of rare earth elements: a study of material degradation and metal transformation mechanisms

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Abstract

The recycling of rare earth elements (REEs) from urban mines is becoming increasingly important in the context of resource sustainability and supply security. Molten salt processes offer interesting advantages for recovering these elements.Indeed, oxygen-containing molten salts, such as hydroxides, carbonates, or sulfates, are capable of degrading organic matter into graphite, which could enable the processing of complex devices found in urban mines. However, this degradation could lead to the formation of graphite coatings over REEs, altering their reactivity in molten salts. A detailed understanding of the chemical and physical interactions between REEs and molten salts, as well as the influence of graphite coatings on these interactions, is therefore necessary to assess the viability of these processes.

In this poster, our results on the behaviour of CeO_2 with or without graphite coating in various molten salts will be presented.

Phosphine-Modified [FeFe]-Hydrogenase Mimics with Various –S(CH_2)nS– Linker Lengths (n = 4, 5, 7, 8): Impact of PPh_3 Ligand on Structure, Redox Properties and Catalytic Activity

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Abstract

In this study, we synthesized a series of PPh_3-substituted diiron complexes with the general formula [$Fe_2(CO)_5PPh_3\{\mu$-$S(CH_2)_nS\}$] (n = 4 (**1**), 5 (**2**), 7 (**3**), 8 (**4**)), bearing structural similarities to the active site of [FeFe]-hydrogenase. These complexes were derived from their parent analogues, [$Fe_2(CO)_6\{\mu$-$S(CH_2)_nS\}$] (n = 4, 5, 7, 8), through ligand substitution. Their formation was verified through a combination of spectroscopic methods, elemental analysis, and X-ray crystallography, confirming their structural integrity and composition. Moreover, we examined how the PPh_3 ligand and the varying lengths of the dithiolato linker in complexes **1**-**4** affect their redox properties and catalytic performance. Using cyclic voltammetry, we evaluated their electrochemical behavior and proton reduction activity in the presence of acetic acid (AcOH). Consequently, the reduction potential shifts of complexes **1**-**4**, in comparison to their precursors, followed the sequence: **3** > **2** > **1** > **4**. Furthermore, at the highest AcOH concentration established, complex **3** demonstrates the most significant current enhancement (i_{cat}/i_p = 26.2). In comparison, complexes **1**, **2**, and **4** exhibit relatively similar i_{cat}/i_p values of 13.6, 13.0, and 11.9, respectively.

Evolution of cellulose nanofibril gels during sequential solvent exchange: a comparative study of ionogels, hydrogels and eutectogels

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Abstract

Cellulose nanofibrils (CNFs) derived from lignocellulosic biomass, combined with advanced fluid media offer a versatile platform for designing sustainable, high-performance functional gels. This work investigates the structural, thermal, and mechanical evolution of CNF-based networks as they transition through three distinct gel states (ionogel, hydrogel, and eutectogel) via a sequential solvent exchange strategy.

CNFs were dissolved in the ionic liquid 1-ethyl-3-methylimidazolium acetate ([EMIM][Ac]) to form a highly entangled, transparent ionogel. Subsequent solvent exchange with water regenerated the cellulose matrix, yielding a hydrogel. A secondary exchange then replaced the aqueous phase with a choline chloride:glycerol (ChCl:Gly) natural deep eutectic solvent (NADES), producing the target eutectogel.

To elucidate the influence of the embedding fluid on the nanocellulose network, all three gel types were systematically characterized. Fourier-transform infrared spectroscopy (FTIR) tracked structural modifications and specific interactions between CNF functional groups and each solvent system. Thermogravimetric analysis (TGA) revealed distinct thermal degradation profiles across states. Compression testing demonstrated how mechanical resilience and elasticity evolve under load, while contact angle measurements confirmed a tailored transition in surface wettability. Electrochemical impedance spectroscopy further highlighted significant variations in ionic conductivity among the three systems.

This comprehensive comparative study underscores how sequential solvent exchange enables tuning of the physicochemical properties of CNF-based gels.

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