02

THE STUDY OF NEXT-GENERATION MATERIALS FOR GREEN ENERGY SYSTEMS AND ENVIRONMENTAL MONITORING

The growing global population, rapid industrialization of developing economies, and increased pressure on governments and industry to reduce carbon emissions and tackle climate change have put an unprecedented strain on the energy industry.

A transformation in the way we produce, transport and store energy is required if these demands are to be met. Central to this transformation is the study of materials for next-generation devices in green energy systems and environmental monitoring.

Advancements in battery and fuel cell technology and the role of analytical chemistry in the development of such devices is a crucial topic. This chapter will explore the implications of such devices on the environment and techniques used to monitor their impact, as well as the future of energy in the digital era.

Energy sources and storaget

The growing demand for renewable energy, sophisticated portable electronics, and electric vehicles requires innovative material solutions in which analytical chemistry plays a central role. Advances in fuel cells and rechargeable batteries would help usher in a new age of energy storage and conservation by supplementing intermittent renewable sources such as solar and wind and by providing faster charging, high capacity batteries for electric vehicles.

Both fuel cells and batteries produce energy via the oxidation of atoms and subsequent flow of electrons and ions through an external circuit and electrolyte, respectively. However, unlike batteries, fuel cells require a constant supply of fuel, typically a hydrogen or a hydrogen-rich substance.

Batteries and fuel cells play a central role in green transport, mobile electronics, energy management systems, and mass-energy storage. Current research centers around improving the performance, safety, and cost of energy storage devices.

A detailed understanding of the underlying chemistry and structure is required to implement new materials in commercial devices. Advanced characterization techniques such as x-ray diffraction (XRD), x-ray

absorption spectroscopy (XAS), and tunneling electron microscopy (TEM) help reveal essential properties, such as degradation mechanisms, that could influence the battery's performance.

Advancements in battery technology

With their lightweight, high energy density, low self-discharge rate, and rechargeability, lithium-ion (Li-ion) batteries have become the leading energy storage technology used today.

To improve the capacity and safety of new Li-ion devices, current Li-ion battery research centers around possible new electrode materials, electrolyte components, and understanding dendrite formation. Advanced characterization methods are necessary to shed light on the behavior of novel battery materials or configurations, ideally under operating conditions.

NMR spectroscopy is one such method, providing a means to characterize local structures by detecting characteristic electromagnetic signals induced by a combination of constant and oscillating magnetic fields, even in highly disordered and reactive systems such as Li-ion electrolytes.

MRI is a non-destructive imaging technique that operates by the same principles as NMR spectroscopy. In contrast, it takes time-resolved measurements, providing valuable information to complement NMR inferences.

Li-ion batteries have raised cost concerns as the need for large-scale energy storage intensifies. Sodium has been championed as a possible solution due to its low cost, abundance on Earth, and similar electrochemical mechanisms to lithium. Sodium-ion (Na-ion) batteries are configured in much the same way to their lithium counterparts, but with a sodium-containing mineral as the cathode. The similarities between Li-ion and Na-ion batteries means that their manufacturing processes are also similar and fully adaptable to produce Na-ion devices.

The impact of energy on the environment

The growing population and continued industrialization and urbanization of society are putting an increasing strain on our planet. Humanmade issues, such as pollution, global warming, overpopulation, waste disposal, and deforestation, all of which are largely the product of unsustainable consumption of natural resources, cause changes in the environment.

Our dependence on Li-ion technology has not come without cost to the environment. There is a growing battery waste problem worldwide, which has led many regions, such as the EU, California, and New York, to ban the disposal of rechargeable batteries in landfills, necessitating the development of alternative waste management strategies. However, lithium from Li-ion cells is not the only polluting element infiltrating our soil, air, and water.

The introduction of foreign chemical species into an aquatic ecosystem can be detrimental to ecosystems and public health. Water chemical analysis is crucial when water is reintroduced to the environment following an industrial process or used for drinking to ensure there will be no harm to people or ecosystems. Standard methods used to identify natural elements and chemical species in water are gas chromatography and mass spectroscopy.

Looking to the Future

The advancement of human society and the new societal demands that come with it drives progression and innovation in analytical chemistry. Analytical science is increasingly called on to provide solutions to problems such as unexpected environmental contamination events and the emergence of new, unregulated pollutants. It is under scrutiny like never before due to the increased connectivity of modern society. The development of new analytical methodologies and instruments to tackle such issues has focused on areas such as miniaturization, automation, cost reduction, and sustainability.

As the world's population grows, the impact of human activity on the environment intensifies, and demands for green energy solutions and new environmental monitoring techniques increases.

The demands placed on the analytical chemistry community will not diminish as efforts to reduce our impact on the environment progress. However, they will continue to change as the need for new energy sources and monitoring solutions arise.

> The development of new materials and characterization instruments will be essential in the coming decades as governments and industries continue to tackle climate change.

2.1 HOW ANALYTICAL CHEMISTRY CAN HELP ENERGY SOLUTIONS AND THE ENVIRONMENT

In 2018, 85% of the world's primary energy consumption came from fossil fuels (oil, gas, and coal), and the US saw a 3.1% rise in carbon emissions. Due to rising populations and energy demand, especially in developing countries such as China and India, it is forecast that oil demand will increase by 70% and carbon emissions by 130% by 2050 without significant policy changes, corresponding to a 6 °C rise in global average temperature. Such a scenario would result in a devastating and irreversible change to our natural environment. It is of paramount importance that new solutions are found for more reliable, inexpensive clean energy if climate change is to be abated.

The challenges faced due to the current, unsustainable consumption of the planet's natural resources are not limited to greenhouse gas emissions. Pollution of other kinds, such as water contamination caused by drilling and mining, pose concerns for public health and the conservation of ecosystems.

Advancements in battery and fuel cell technology, central to both renewable energy storage facilities and electric vehicles, and the role of analytical chemistry in the development of such devices will be discussed, with particular focus on next-generation Li-ion batteries. The environmental implications of such devices and techniques to monitor their impact will also be explored, as will the future of energy in the digital era.

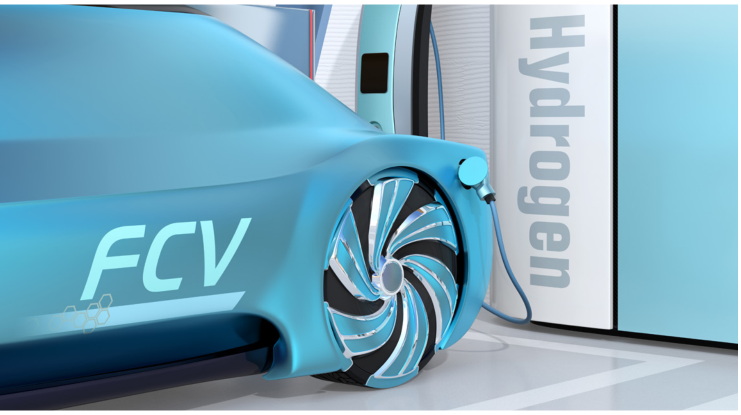
References

- BP (2019) BP Statistical Review of World Energy. (68th edition) https://www.bp.com/content/dam/bp/business-sites/en/global/corporate/pdfs/energy-economics/statistical-review/bp-stats-review-2019-full-report.pdf
- Enerdata (2020) Global Energy Statistical Yearbook 2020. https://yearbook.enerdata.net/
- GreenFacts. Introduction: What challenges is the energy sector facing? https://www.greenfacts.org/en/energy-technologies/l-2/1-energy-sector-challenges.htm
- BBVA Open Mind. Current Challenges in Energy. https://www.bbvaopenmind.com/en/articles/current-challenges-in-energy/
- Joi Scientific (2018) Three Energy Challenges for 2018. https://www.joiscientific.com/three-energy-challenges-for-2018/
- BBC (2017) The biggest energy challenges facing humanity. https://www.bbc.com/future/article/20170313-the-biggest-energy-challenges-facing-humanity

2.1a NEW MATERIALS AND METHODS IN ENERGY

The growing demand for renewable energy, sophisticated portable electronics, and electric vehicles requires innovative material solutions in which analytical chemistry plays a central role. Understanding the structure, chemistry, and dynamic processes that exist within novel materials for energy generation and storage is crucial if new, efficient, high-performance devices are to become a commercial reality.

Advances in fuel cells and rechargeable batteries would help usher in a new age of energy storage and conservation by supplementing intermittent renewable sources such as solar and wind and by providing faster charging, high capacity batteries for electric vehicles.



Fuel cells

Fuel cells produce electricity by converting chemical energy into electrical energy, similar to a conventional battery. However, unlike batteries, they require a constant supply of fuel, typically hydrogen or a hydrogen-rich substance.

Sir William Grove developed the first fuel cells in 1838. However, it took another 100 years before they first began to be used commercially when English engineer Francis Thomas Bacon produced the first alkaline fuel cell in 1932. NASA went on to use this form of fuel cell as a means of supplying electricity and water to astronauts on space missions from the mid-60s.

There are many different fuel cell configurations, but most consist of two electrodes, a negative anode, and a positive cathode, sandwiching an electrolyte. Fuel is oxidized by passing it through a catalyst at the anode, removing electrons to leave positively charged ions. The ions diffuse across the electrolyte towards the cathode, and the electrons pass through an external circuit. This produces a direct current, before meeting the ions at the cathode where, with the introduction of oxygen, they recombine to form water.

Fuel cells currently operate at a 40% to 60% efficiency, which is superior to combustion engines that first convert chemical energy to heat, before producing kinetic work, losing energy in the process.

Another positive is that there are no harmful byproducts from the process, only water and heat, and fuel cell production is far more environmentally friendly than obtaining fossil fuels for conventional engines. The lack of moving parts in a fuel cell also makes them more reliable and quieter than their fossil fuel counterparts.

The versatility of fuel cells makes them particularly attractive to industry, with uses ranging from clean transportation to portable electronics with superior battery life.

Hydrogen fuel cells

Fuel cells commonly use hydrogen that can be produced via electrolysis, the splitting of water into its constituent hydrogen and oxygen gases. If powered by renewable means, the whole process can be made carbon neutral.

The fueling infrastructure for hydrogen-powered electric vehicles is available and continuously improving. For example, Nel Hydrogen's new H2Station can refuel three times faster than current fueling stations while taking up a third of the space.

Polymer electrolyte membrane fuel cells

The most common fuel cell configuration is the Polymer Electrolyte Membrane (PEMFC), which utilizes a solid, organic polymer membrane as the ion-conducting electrolyte. These devices have a lower weight and volume than most fuel cells, making them ideal for electric vehicles due to their impressive power-to-weight ratio. However, the use of platinum as a catalyst is necessary, which increases their cost and also makes the fuel cell susceptible to carbon monoxide poisoning.

For delegates interested in PEMFCs, Johna Leddy and Joshua Coduto gave a presentation entitled 'Magnetic Effects on Hydrogen Evolution Reaction', where they discussed work being conducted on relatively inexpensive carbon electrodes modified with films containing magnetoelectrocatalysts for next-generation PEMFCs.

Proton conducting fuel cell

Fuel cells are beginning to be employed in tandem with other renewables such as wind turbines and solar panels, where intermittent power generation necessitates the storage of energy during downtime. Some of the electricity generated is used to produce hydrogen and oxygen gas from water via electrolysis, which is then used to run fuel cells during periods of low energy production.

Proton conducting fuel cells (PCFCs) take this reversible idea a step further, employing a single catalyst that can produce and use hydrogen fuel.

In current devices, steam and electricity are fed into a ceramic catalyst anode, which both splits the water molecules into their constituent oxygen and hydrogen particles and oxidizes them, generating power through the flow of stripped electrons as in a regular cell. The hydrogen and oxygen ions, together with the stripped electrons, are then reduced back into the water at the nickel-based catalyst cathode.

Researchers are currently studying how to improve the 70% electric-to-hydrogen energy conversion efficiency of ceramic catalysts. In a recent paper published in Nature Energy, Ryan O'Hare, a chemist at the Colorado School of Mines, reported an efficiency of 98% from a ceramic catalyst made up of five elements.

Fuel cells of the future

Research is currently being conducted on microbe catalysts where microorganisms such as bacteria are used to oxidize hydrogen. Microbial fuel cells have been demonstrated to be energy positive systems with potential applications in low power electronics.

Battery materials

Batteries play a central role in green transport, mobile electronics, energy management systems, and mass-energy storage. The search for materials that can provide high energy density, high storage capacity, mobility, and supplement intermittent renewable energy sources is vital in the fight to reduce global carbon emissions. Current research into battery materials centers around improving the performance, safety, and cost of energy storage devices.

Techniques and methods for lithium-ion and lithium-selenium batteries

Li-ion batteries are the most common energy storage devices used in portable electronic devices and electric vehicles today.

Similar to fuel cells, they consist of an anode and cathode, generally made of graphite and lithium cobalt oxide, respectively, sandwiching an electrolyte. During the discharge process, lithium atoms at the anode are oxidized, and the resulting lithium ions discharge towards the cathode. At the same time, the stripped electrons flow through an external circuit, producing an electric current.

Li-ion batteries have the highest energy density of any current commercial battery and are capable of delivering large currents for high-power applications. However, their conventional electrode materials limit their maximum energy density, which is not significant enough to satisfy the growing demand for high-capacity energy storage, especially in modern electric vehicles (EVs).

Another major issue with Li-ion batteries is safety, with devices often overheating and occasionally, as in the case of the Samsung Galaxy Note 7, combusting. The cost of Li-ion batteries is also around 40% higher than Ni-Cd.

An emerging alternative to Li-ion is lithium-selenium (Li-Se), which promises higher energy density at a lower cost. Lithium metal is viewed as the most promising anode material for next-generation batteries due to its high specific capacity. Lithium anodes have previously been twinned with sulfur cathodes in Li-S batteries due to sulfur's impressive capacity. However, the insulating nature of sulfur, together with its poor cycle life and power density, has led many researchers to investigate selenium as an alternative cathode material.

Selenium has a similar electron structure and chemical properties to sulfur but importantly is also highly conductive. However, selenium cathodes still have issues, including low utilization and poor cycling stability. Research into alternative selenium cathode configurations is necessary if Li-Se devices are to become commercially viable.

Characterization techniques for batteries

To implement new materials in commercial devices, a detailed understanding of their underlying chemistry and structure is required.

> Advanced characterization techniques such as x-ray diffraction (XRD), x-ray absorption spectroscopy (XAS), and tunneling electron microscopy (TEM) help reveal essential properties, such as degradation mechanisms, that could influence the battery's performance.

XRD is the most commonly used technique to determine the structure of potential electrode materials. Determining the ionic distribution and crystal structure of materials is paramount if the performance of the material under operating conditions is to be fully understood.

XRD utilizes the elastic scattering of x-rays by a periodic crystal lattice to reveal the electron density of a material and disclosing information on the atomic structure and chemical bonds present in a sample. This is especially useful when investigating novel materials for battery electrodes, where the response to electrochemical reactions is not well known.

One of the leading manufacturers in this field is Bruker, whose XRD instruments enable a detailed analysis of any material from fundamental research to industrial quality control.

XAS is another characterization technique particularly suited to the study of battery materials. XAS operates by using tunable, monochromatic x-rays, usually generated by a synchrotron, to excite core electrons in a material. Structural and electronic information is obtained from the resulting absorption spectrum, such as specific oxidation states and atomic symmetry.

XAS is particularly suited to the characterization of materials that are not crystalline and, therefore, cannot be studied using XRD. Due to the elemental specificity and high penetration depth of XAS x-rays, it is possible to perform operando measurements of battery materials using specially developed in situ electrochemical cells.

TEM is of interest in battery material analysis due to its ability to provide in situ, time-resolved analysis of dynamic processes within batteries. TEM works by directing a beam of electrons at a sample with a thickness of less than 100 nm. It then measures the subsequent electron diffraction pattern to form an image of features down to the atomic scale.

The impressive resolution of TEM makes it particularly suited to the study of charge/discharge mechanisms and solid electrolyte interphase formation. TEM is a destructive imaging technique, meaning it is necessary to optimize the beam conditions to minimize the damage caused to the sample. However, recent studies have shown that beam damage can reveal useful information on the breakdown of electrolytes, potentially opening up an entirely new field of battery research.

The techniques mentioned above are typically used in tandem with other characterization methods to build a bigger picture of the structural form and electrochemical processes present within batteries and battery materials.

For more on all the topics discussed in this chapter, delegates were urged to attend Hector Abruna's presentation on 'Energy Conversion and Storage: Novel Materials and Operando Methods', in which the development of new materials and operando methods for energy conversion and storage with emphasis on fuel cells and battery materials and technologies was discussed.

Advances in fuel cell and battery technology will play a significant part in the development of the world's green infrastructure in years to come, be it in mass energy storage facilities or next-generation electric vehicles. However, Li-ion batteries remain one of the leading energy storage technologies used today, and we will explore advancements in these devices and the fundamental techniques analysis used to characterize them.

References

- Liu, C. et al. (2010) Advanced Materials for Energy Storage. Advanced Materials. https://www.researchgate.net/deref/http%3A%2F%2Fdx.doi.org%2F10.1002%2Fadma.200903328

- Nel Hydrogen. Hydrogen fueling equipment. https://nelhydrogen.com/hydrogen-fueling-equipment/

- Service, R. (2019) New fuel cell could help fix the renewable energy storage problem. Science Mag. https://www.sciencemag.org/news/2019/03/new-fuel-cell-could-help-fix-renewable-energy-storage-problem

- Duan, C. et al. (2019) Highly efficient reversible protonic ceramic electrochemical cells for power generation and fuel production. Nature Energy. https://www.nature.com/articles/s41560-019-0333-2

- Walter, A. X. et al. (2020) Microbial fuel cells directly powering a microcomputer. Journal of Power Sources. https://www.sciencedirect.com/science/article/pii/S0378775319313217

- M. Ruscalleda Beylier (2011) Environmental Biotechnology and Safety. Comprehensive Biotechnology (Second Edition). https://www.sciencedirect.com/topics/biochemistry-genetics-and-molecular-biology/microbial-fuel-cell

- Malvern Panalytical. Battery and energy. https://www.malvernpanalytical.com/en/industries/advanced-materials/batteries

- Xia, Y. et al. (2019) Freestanding layer-structure selenium cathodes with ultrahigh Se loading for high areal capacity Li-Se batteries. Electrochemistry Communications. https://www.sciencedirect.com/science/article/pii/S1388248118303369

- Jin, Y. et al. (2020) High-Energy-Density Solid-Electrolyte-Based Liquid Li-S and Li-Se Batteries. Joule. https://www.sciencedirect.com/science/article/abs/pii/S2542435119304313

- Zhou, J. et al. (2017) A high performance lithium–selenium battery using a microporous carbon confined selenium cathode and a compatible electrolyte. Journal of Materials Chemistry A. https://pubs.rsc.org/en/content/articlelanding/2017/ta/c7ta01564j#!divAbstract

- Bruker. X-ray Diffraction (XRD) and Scattering. https://www.bruker.com/products/x-ray-diffraction-and-elemental-analysis/x-ray-diffraction.html

- Giorgetti, M. & Stievano, L. (2017) X-Ray Absorption Spectroscopy Study of Battery Materials. https://www.intechopen.com/books/x-ray-characterization-of-nanostructured-energy-materials-by-synchrotron-radiation/x-ray-absorption-spectroscopy-study-of-battery-materials

- Wheatcroft, L. (2018) Towards in-situ TEM for Li-ion Battery Research. Energy Procedia. https://www.sciencedirect.com/science/article/pii/S1876610218305861

- SIGMA-ALDRICH. (2013) Materials for Energy Storage and Efficiency. Material Matters. https://www.sigmaaldrich.com/content/dam/sigma-aldrich/docs/Aldrich/Brochure/1/material-matters-v8-n4.pdf

- Knorr, F. et al. (2019) Methanol as antifreeze agent for cold start of automotive polymer electrolyte membrane fuel cells. Applied Energy. https://www.sciencedirect.com/science/article/pii/S0306261919300364

- Yezerska, K. et al. (2020) Analysis of the regeneration behavior of high temperature polymer electrolyte membrane fuel cells after hydrogen starvation. Journal of Power Sources. https://www.sciencedirect.com/science/article/pii/S0378775319315551

- Nelson, J. et al. (2012) In Operando X-ray Diffraction and Transmission X-ray Microscopy of Lithium Sulfur Batteries. Journal of the American Chemical Society. https://pubs.acs.org/doi/10.1021/ja2121926

2.1b ADVANCEMENTS IN LITHIUM-ION

With their lightweight, high energy density, low self-discharge rate, and rechargeability, Li-ion batteries have become the leading energy storage technology used today.

These useful properties have seen Li-ion batteries adopted across a variety of industries, from portable electronics where Li-ion is the dominant battery technology to green transport where their small size and lightweight have seen Li-ion batteries widely incorporated into hybrid and electric car design.

Current Li-ion battery research is centered on possible new electrode materials, electrolyte components, and understanding dendrite formation to improve the capacity and safety of new Li-ion devices.

NMR in Li-Ion batteries

The application of new electrode or electrolyte materials is necessary for the advancement of Li-ion battery technology. Critical to the success of new devices is an understanding of the underlying chemistry of these materials. Advanced characterization methods are necessary to shed light on the behavior of novel battery materials or configurations, ideally under operating conditions.

NMR spectroscopy is one such method, providing a means to characterize local structures, even in highly disordered and reactive systems such as in Li-ion electrolytes. NMR reveals the molecular structure, dynamic processes, and chemical reactions occurring within a material by detecting characteristic electromagnetic signals induced by a combination of constant and oscillating magnetic fields.

A key advantage of NMR over most other characterization techniques is that all species present in a material can be detected simultaneously, regardless of their phase, making it a valuable tool for in situ observation of electrochemical reactions within a working cell.

Another aspect of NMR that lends itself to in situ detection is that it is non-destructive, enabling non-invasive observation of reactions and ensuring the preservation of the material to mimic actual operating conditions, unlike techniques such as electron microscopy.

Many Li-ion battery electrolytes, such as LiPF6, and their degradation products contain spin ½ atoms with significant gyromagnetic ratios, which are ideally suited for study using NMR spectroscopy.

Bruker provides an extensive range of NMR equipment and tools to complement other analytical techniques in the characterization of battery materials.

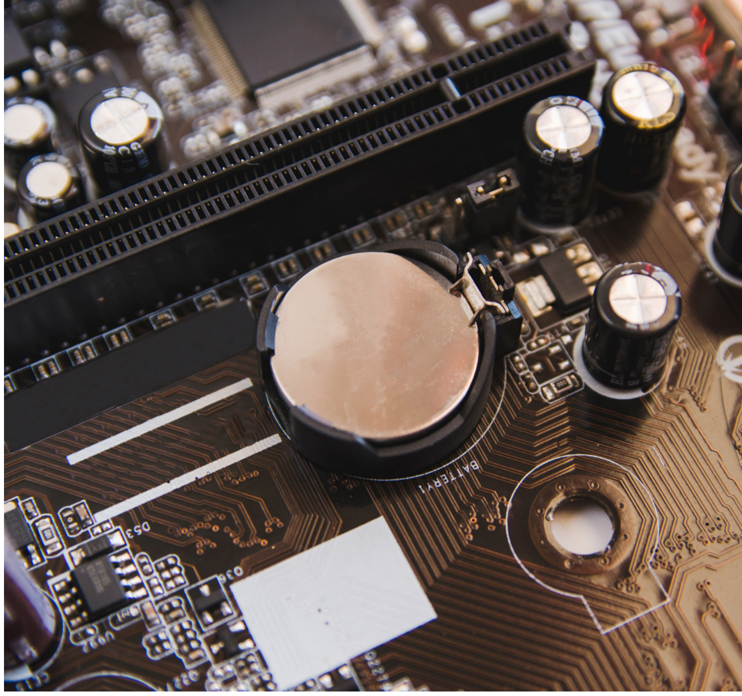
MRI in Li-ion batteries

MRI is a non-destructive imaging technique that operates by the same principles as NMR spectroscopy but differs by taking time-resolved measurements, providing valuable information to complement NMR inferences.

MRI is particularly beneficial to the study of Li-ion batteries as it is sensitive to dendrite growth and is capable of resolving different lithium microstructure morphologies. It is possible to localize these structural changes and create a series of in situ, time-resolved 3D images of a functioning cell.

NMR and MRI have proven invaluable analytical techniques for the study of battery materials due to their non-destructive nature and their ability to perform in situ measurements and image bulk components (as opposed to exclusively surface-sensitive electron and optical microscopies).

'Advanced NMR and MRI Studies of Lithium-Ion Batteries' gave delegates at Pittcon the opportunity to learn more about NMR and MRI's role in unveiling the essential structural characteristics of new materials critical to next-generation Li-ion battery performance.



Sodium-ion battery chemistry by MRI

Concerns have been raised over the cost of Li-ion batteries as the need for large-scale energy storage intensifies. Sodium has been championed as a possible solution due to its abundance on Earth and similar electrochemical mechanisms to lithium.

Sodium-ion batteries (Na-ion) are configured in much the same way as their lithium counterparts, but with a sodium-containing mineral as the cathode. This substitution further reduces the cost of such devices by enabling the use of an aluminum (which does not alloy with sodium) current collector at the anode, rather than the copper used in Li-ion batteries, and removing the need for cobalt in the electrodes. The similarities between Li-ion and Na-ion batteries means that their manufacturing processes are also similar and fully adaptable to produce Na-ion devices.

Storage of surplus renewable energy is seen as a critical application of Na-ion batteries that would be a cheaper backup for intermittent energy sources than the current lithium-based storage facilities.

However, current Na-ion battery anodes have limited capacity, unstable performance, and are susceptible to sodium dendrite growth, further reducing energy efficiency. Existing solid-electrolyte interface materials also show poor stability. NMR spectroscopy and MRI can help solve these issues by enabling the visualization of electroactive species in both the electrolyte and electrode environments.

Melanie Britton discussed the role of NMR and MRI in Na-ion battery development and reported on experimental results in her Pittcon talk, 'In Operando Visualization of Sodium-Ion Battery Chemistry by Magnetic Resonance Imaging'.

As the world moves away from fossil fuels in favor of renewable energy and electric vehicles, the need for efficient, low-cost energy storage solutions is intensifying. The optimization of Li-ion batteries and the discovery of new battery materials for next-generation devices are crucial to meet the demand for energy storage.

Alexej Jerschow gave a talk at Pittcon on 'Battery Diagnostics with Inside-out MRI and Magnetometry', in which new battery assessment technology based on MRI and magnetometry techniques was discussed.

While such advances are crucial to meeting the growing de mand for green energy, it is essential to understand the impact such technology has on the environment. In the following sections, we will discuss the influence of emerging energy solutions on the environment, and how this can be monitored and reduced.

References

- *Office of Energy Efficiency & Renewable Energy (2017) How Does a Lithium-ion Battery Work? https://www.energy.gov/eere/articles/how-does-lithium-ion-battery-work*
- *Clean Energy Institute. LITHIUM-ION BATTERY. https://www.cei.washington.edu/education/science-of-solar/battery-technology/*
- *Pecher, O. et al. (2017) Materials' Methods: NMR in Battery Research. Chemistry of Materials. https://pubs.acs.org/doi/abs/10.1021/acs.chemmater.6b03183*
- *Bruker. Nuclear Magnetic Resonance Spectroscopy. https://www.bruker.com/products/mr/nmr.html*
- *Llott, A. J. et al. (2018) Rechargeable lithium-ion cell state of charge and defect detection by in-situ inside-out magnetic resonance imaging. Nature Communications. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC5934497/*
- *IOP Science. ESC Meeting Abstracts. http://ma.ecsdl.org/content/MA2017-01/1/96.abstract*
- *Llott, A. J. et al. (2016) Real-time 3D imaging of microstructure growth in battery cells using indirect MRI. PNAS. https://www.pnas.org/content/113/39/10779*
- *Anklin, C. (2019) Investigating lithium ion batteries with magnetic resonance techniques. Spectroscopy Europe Asia. https://www.spectroscopyeurope.com/article/investigating-lithium-ion-batteries-magnetic-resonance-techniques*
- *Zhang, W. et al. (2019) Sodium-ion battery anodes: Status and future trends. EnergyChem. https://www.sciencedirect.com/science/article/pii/S2589778019300156*
- *Notman, N. (2019) A battery technology worth its salt. Royal Society of Chemistry. https://www.chemistryworld.com/features/a-battery-technology-worth-its-salt/3010966.article*

2.1c THE COST TO OUR ENVIRONMENT

Our growing population and the continued industrialization and urbanization of society is putting an increasing strain on our planet. Many changes in the environment are caused by human-made issues, such as pollution, global warming, overpopulation, waste disposal, and deforestation, all of which are largely the product of unsustainable consumption of natural resources.

Carbon dioxide and other greenhouse gas emissions is an incredibly damaging example of unsustainable consumption and a key factor behind the increase in extreme weather events in recent years.

The impact on health cannot be ignored, with almost 10% of death and disease worldwide attributed to unsafe water, air pollution, poor sanitation, and climate change.

With 79% of the total US energy consumption in 2018 coming from fossil fuels, there is a clear need for further scientific research and development in renewable energy sources.

Many renewable energy sources are used around the world today, including solar, wind, hydroelectric, and geothermal power. However, issues such as power availability, cost, and location have prevented renewables from displacing fossil fuels as the world's leading energy source.

The detrimental effect burning fossil fuels has on the environment extends far beyond greenhouse gas emissions. Mining and drilling results in the contamination of water with substances harmful to both humans and the environment, such as heavy solids hydrocarbons and radioactive materials, and the release of natural gas, the main component of which is methane (a greenhouse gas far more damaging to global temperature than carbon dioxide). Fuel transportation is harmful due to the obvious vehicle emissions, but also through pipeline leaks or oil spills that cause water, air, and soil pollution.

The impact of Li-ion batteries on the environment

As discussed, the need for new energy sources and storage solutions and the central role of the Li-ion battery in current technology has been discussed. However, our dependence on Li-ion technology has not come without cost to the environment.

There is a growing battery waste problem worldwide, which has led many regions, such as the EU, California, and New York, to ban the disposal of rechargeable batteries in landfills, necessitating the development of alternative waste management strategies.

Infrastructure for recycling valuable metals contained within batteries is currently in place. However, the variety of battery configurations and continuously evolving technology makes the recovery of low-volume materials, such as lithium and electrolyte, difficult to justify from an economic standpoint, with many recycling facilities solely focused on the extraction of cobalt, nickel, and copper.

The development of less polluting, more efficient, and cost-effective recycling procedures for Li-ion batteries is not only essential due to the scarcity of natural resources and pollution associated with mining, but also to stem the increase in toxic lithium contamination of our water supply, soil, and air. In a recent study published in Nature Communications, a correlation between the significant population increase in Seoul, South Korea, and levels of aqueous lithium was reported.

However, lithium from Li-ion batteries is not the only polluting element infiltrating our soil, air, and water.

Water pollution

Water pollution is the contamination of water bodies, such as rivers, oceans, or groundwater, with pollutants usually caused by human activity. The introduction of foreign chemical species into an aquatic ecosystem can be detrimental to ecosystems and public health.

The origins of water pollution are numerous and include industrial waste containing toxic chemicals such as lead and sulfur, sewage and wastewater containing harmful bacteria and pathogens, fertilizers and pesticides used for farming, acid rain caused by the burning of fossil fuels, and toxic elements introduced by mining activity and oil leakages.

Water chemical analysis is crucial when water is reintroduced to the environment following an industrial process or used for drinking to ensure there will be no harm to people or ecosystems. Water analysis includes the determination of pH value, the alkalinity, and the total water hardness.

Standard methods to identify natural elements and chemical species in water are gas chromatography and mass spectroscopy. Both OI Analytical and Metrohm provide water instrumentation for laboratory and in-process analysis, enabling high-precision industrial and environmental monitoring.

For more on cutting-edge water analysis techniques, delegates were recommended to attend 'Recent Advances in On-line, On-site Monitoring for Process Control of Haloacetic Acids in Drinking Water Distribution Systems', during which recent improvements to the post-column reaction ion chromatography (PCR-IC) analyzer with nicotinamide fluorescence enabling on-line and on-site analysis of HAAs were discussed.

Water contamination is not the only form of pollution impacting the planet. Air pollution contributes to smog and can lead to respiratory problems. Airborne nitrogen and sulfur oxides contribute to acid rain, which, in turn, worsens water pollution. Soil pollution, caused by improper disposal of toxic industrial substances such as lead or pesticides, adds to the corruption of ecosystems and poses a threat to public health due to the risk of water contamination.

With the advancement of human civilization comes a demand for new energy sources to meet growing technological and environmental demands. However, such advancements can come at a cost, and it is important to understand the influence of new technology on the environment if its impact is to be minimized.

References

- *Singh, R. L. & Singh, P. K. (2016) Global Environmental Problems. Springer Link. https://link.springer.com/chapter/10.1007/978-981-10-1866-4_2*
- *U.S. Energy Information Administration. Energy and the environment explained: Where greenhouse gases come from. https://www.eia.gov/energyexplained/energy-and-the-environment/where-greenhouse-gases-come-from.php*
- *Moradiya, M. A. (2019) The Challenges Renewable Energy Sources Face. https://www.azocleantech.com/article.aspx?ArticleID=836*
- *Zeng, X. & Li, J. (2014) Spent rechargeable lithium batteries in e-waste: composition and its implications. Frontiers of Environmental Science & Engineering. https://link.springer.com/article/10.1007/s11783-014-0705-6*
- *Wang, X. et al. (2014) Economic and environmental characterization of an evolving Li-ion battery waste stream. Journal of Environmental Management. https://www.sciencedirect.com/science/article/pii/S030147971400036X*
- *Choi, H. et al. (2019) The impact of anthropogenic inputs on lithium content in river and tap water. Nature Communications. https://www.nature.com/articles/s41467-019-13376-y*
- *Li, H. et al. (2019) Recycling and Treatment of Waste Batteries. IOP Conference Series: Materials Science and Engineering. https://iopscience.iop.org/article/10.1088/1757-899X/612/5/052020/meta*
- *O.I. Corporation. Drinking Water. https://www.oico.com/industries/drinking-water*

1.2d ADDRESSING THE FUTURE OF THE ENVIRONMENT IN THE DIGITAL ERA

As discussed previously, due to the planets increasing population and the global move away from fossil fuels in favor of renewables and green transport, the role of the modern-day analytical scientist is to provide energy sources and energy storage solutions to meet the needs of ever-advancing sustainable technologies.

The advancement of human society, and the new societal demands that come with it, drives progression and innovation in analytical chemistry. Analytical science is increasingly called on to provide solutions to problems such as unexpected environmental contamination events and the emergence of new, unregulated pollutants. It is under scrutiny never before experienced by the field due to the increased connectivity of modern society. The development of new analytical methodologies and instruments to tackle such issues has focused on miniaturization, automation, cost reduction, and sustainability.

The increasing demand for benchtop and portable analytical devices for field applications has driven the miniaturization of characterization instruments. Rapid advances in microelectromechanical systems (MEMS) have enabled previously cumbersome instruments, such as spectrometers, to be used outside the laboratory. This is of great benefit to environmental monitoring and geological survey research where fieldwork is crucial.

The benefits of miniaturization are extensive. Smaller devices reduce manufacturing costs, require less energy and space, and are easier to operate.

Companies at the cutting edge of analyzer development include Shimadzu, whose state-of-the-art total organic carbon analyzers maximize both sensitivity and productivity, making them ideally suited to water monitoring.

Automation is of particular importance in an industry where automatic emission detectors and flow analysis is required due to largescale operations. Automation also aids the modern laboratory scientist due to the vast amounts of data produced by ever-improving instruments. Software for data sorting and analysis, as well as automated laboratory processes, enables scientists to maximize the impact of their research.

Sustainability has become a significant issue for scientific laboratories in society. The key goals for sustainable chemistry are to reduce the use of toxic substances, such as reagents and solvents, and minimize adverse effects of research on people and the environment.

Efforts are made to mitigate toxic solvent use through recycling or non-toxic alternatives. On-line treatment of waste is commonly implemented to reduce the impact of research on the environment, and the development of energy-saving instruments helps reduce the carbon footprint of laboratories.

At Pittcon, the topic of the future of analytical science included 'Addressing Water Quality and Environmental Chemistry Challenges in the Digital Era', during which presenters from a commercial laboratory, water utility, public laboratory, research institution, and instrumentation vendor presented how they are employing existing and novel analytical instrumentation to respond to the latest challenges in the water quality and environmental chemistry fields.

'Challenges for Commercial Laboratories in Adopting New Technology for Environmental Testing' was presented by William Lipps. This talk outlined the problems faced by scientists analyzing new compounds of environmental concern.

For delegates interested in how the Internet of Things is being incorporated into modern environmental laboratories, Ruth Marfil-Vega gave a presentation on 'Adding Value to the Analytical Workflows in the Digital Era'. Examples of the latest hardware developments for incorporating Internet of Things into labs were shared, as well as options for maximizing the value of acquired data.

Analytical chemistry will play a central role in the future of energy, and the advancement of human society will require the field to continuously adapt to meet the demands of new technology. Change will also be required to reduce the impact of laboratory activity on the environment as the field comes under increasing scrutiny.

References

- *Trojanowicz, M. (2013) Challenges of Modern Analytical Chemistry. Modern Chemistry & Applications. https://www.longdom.org/open-access/challenges-of-modern-analytical-chemistry-2329-6798.1000e113.pdf*
- *Zolotov, Y. A. (2017) Some Trends in Modern Analytical Chemistry. Journal of Chromatography. https://www.omicsonline.org/open-access/some-trends-in-modern-analytical-chemistry-2157-7064-1000355.php?aid=87304*
- *SHIMADZU. Total Organic Carbon (TOC) Analyzers. https://www.ssi.shimadzu.com/products/toc-analyzers/index.html*

CONCLUSION

As the world's population grows, the impact of human activity on the environment intensifies, as do demands for green energy solutions and new environmental monitoring techniques.

Advances in technologies such as fuel cells and batteries are essential if we are to meet the increasing calls for renewable energy and efficient green transport, as are the efforts of companies such as Bruker and Nel Hydrogen in providing the analytical equipment and fueling infrastructure to make these advancements a reality.

Environmental monitoring is also crucial to help understand the impact of current and new technology on ecosystems and public health. Water characterization instruments provided by manufacturers such as OI Analytical and Metrohm are central in reducing pollution from industrial processes and laboratory activity.

The demands placed on the analytical chemistry community will not diminish as efforts to reduce our impact on the environment progress but will continue to change as the need for new energy sources and monitoring solutions arise. The development of new materials and characterization instruments will be essential in the coming decades as governments and industries continue to tackle climate change.

2.2 SUSTAINABLE AND ECONOMICAL CASCADE-BASED ELECTROCATALYSIS

An interview with Shelley Minteer, Professor of Chemistry at the University of Utah, discussing how sustainable and economical cascade-based electrocatalysis could lead to a brighter future across research and industry.

How are electrocatalysts used in research and industry?

Electrocatalysts are abundant across the industry and are used for water splitting and producing hydrogen and oxygen in fuel cells for electric vehicles. They are also used in a variety of electrical chemical and industrial processes, such as the chloralkali process to produce chlorine gas.

Most of the electrocatalytic systems that have been developed over the past two decades have been single electrocatalysts. Why is this?

When thinking about developing a catalyst, it is usually easier to initially create a catalyst that does a single transformation. This could be a one-electron, two-electron, or maybe a four-electron process, but essentially it is a small step to the overall process.

As we begin to think about doing more complex transformations, it becomes more complicated. This is because we now need more than one catalyst to be on our electrode surface, and we need to design the materials so that we can have those multiple catalysts.

Why do scientists want to develop alternatives to single electrocatalysts?

The single electrocatalysts are very effective at carrying out a single electron, two-electron, or even four-electron transformation. That is somewhat limiting because it allows you to make hydrogen from protons or chlorine gas from chloride ions, but it does not enable you to carry out complex transformations that require maybe 10, 12, or even 15 electrons to do the complete process.

What are enzymatic bioelectrocatalysts and how can they be used to overcome the issues with single electrocatalysts?

Most biocatalysts are for redox reactions. Therefore, catalyzing redox reactions that you would think of from an electric chemical perspective, are oxidoreductase enzymes and can catalyze a variety of redox reactions. Interestingly, there are thousands of different oxidoreductase enzymes in living cells. Therefore, living cells give us the model by which we can think about doing very complex redox chemistry.

If you think about food, take a normal lunch, you are going to have some sugars, a few carbohydrates, a little bit of fat, oil, and protein, and your body essentially has oxidoreductase enzymes within it to catalyze the oxidation of all of those complex molecules.

These are all fuel so that you can do the energy conversion that you need for your everyday life. Therefore, we are using biology as the inspiration to carry out interesting chemistry because biology gives us such a wide variety of chemistry applications.

How are these catalysts developed and how do you mediate electron transfer?

These catalysts from an initial generation perspective are naturally occurring. They are isolated and purified from their natural sources (microorganisms). Then, as we end up with catalysts that we are interested in using electrochemically, we will carry out enzyme engineering on them to make them more appropriate for electrochemical applications versus in vivo applications.

In one study, you made the sustainable biosynthesis of polyhydroxybutyrate economical. Please can you tell us about this research?

One of the things that we are interested in is whether or not we can use electrocatalysis to produce products more sustainably. Plastics are a product that we are interested in creating, especially sustainable polymers.

We developed a system where we took microorganisms that could produce plastics and removed the part of the microorganism that was responsible for that chemistry. We then immobilized it on electrode surfaces to be able to electrically and chemically generate plastics.

In another study, you focused on selectively producing chiral amines using bioelectrocatalysis. How did you achieve this?

As we become more interested in sustainable chemistry and using electric chemistry as a tool to produce products, we began to realize that there are several products that the pharmaceutical industry is interested in, including chiral amines. If you look at drugs, a lot of pharmaceuticals are chiral amines themselves. We were interested in whether or not we could design and use a series of enzymes to be able to make these drug candidates and drug intermediates.

Why did you choose to present this research at Pittcon?

Pittcon is the place to present your new work, and I have been attending for 20 years. For the last year and a half, this is a new research area in my lab. It was an excellent opportunity to show the community the new work that is happening in our research lab.

What does the future hold for enzymatic cascades and your research?

I think the future is going to focus on safer and cleaner ways to produce chemicals, whether those are pharmaceuticals or commodity chemicals or fine chemicals. We are going to have to focus on greener, safer, more sustainable production processes, and this gives us an excellent opportunity to use electric chemistry to essentially use renewable energy to produce molecules more safely and in a greener way.

Why do you think events such as Pittcon are important for the analytical chemistry / scientific industry?

Pittcon is, first and foremost, a trade show. It is an excellent opportunity to attend every year and discover new instrumentation being developed and what new equipment is out there in analytical chemistry and sciences.

It is a great opportunity to see the latest and greatest in terms of technology. However, it is also a chance to see where the field is going at the talks. The talks are usually presenting things that are going to take several years to become commercial products, but it gives you a chance to see where the science is going so that you can make better choices in terms of where your research is going to focus.

2.3 GAS CHROMATOGRAPHY-MASS SPECTROMETRY (GC-MS) IN ENVIRONMENTAL ANALYSIS

Gas chromatography-mass spectrometry (GC-MS) brings several advantages for studying environmental samples, such as soils, sediments, groundwater, and air. These include high throughput, accuracy, and sensitivity.

GC-MS measures target compounds at very low levels (parts per trillion) and is used to identify and measure unknown compounds. It can also quantify several kinds of different compounds in a single run, such as polychlorinated biphenyls (PCBs), or over one hundred different organic compounds.

In the environmental industry, GC is the preferred analyzing technique for a variety of pollutants, including mineral oils (MOs), volatile organic compounds (VOCs), organochlorine pesticides (OCPs), endocrine-disrupting chemicals (EDCs), polychlorinated biphenyls (PCBs), and polyaromatic hydrocarbons (PAHs).

MOs are a class of petroleum products that include white, lubricating, and fuel oils such as liquid paraffin. They enter the environment from industrial discharges, leaks, or spillages, contaminating soil and groundwater that passes into nearby streams and rivers. MOs pose a concern as various toxic components of MOs do not biodegrade and persist in the environment, posing dangers to aquatic and human life.

Often emitted from industrial sites, VOCs are organic compounds, such as toluene and benzene, which can be vaporized. Amid mounting concerns about health and air pollution, strict regulations are now in place governing the emissions of and testing for VOCs. They can also be found in drinking and tap water, in surface and groundwater, as well in wastewater.

OCPs, such as DDT, were used widely from the 1940s through to the 1960s but have been linked to a range of serious health issues. They persist and accumulate in the environment and biological tissues, even though their use has been banned or restricted in the past several decades.

Concerns have grown as EDCs, such as natural and synthetic steroidal estrogens, enter rivers and streams, mainly as a result of discharges from municipal and industrial sewage treatment plants. These steroidal hormones can affect aquatic life, for example, by feminizing male fish, and have been detected in drinking water sources. A further concern is that these compounds are active at very low-level concentrations.

PCBs and PAHs are semi-volatile organic compounds that can contaminate soils, air, sediments, and water. They present a host of dangers to the environment and people as they are not biodegradable, carry over long distances, and accumulate in the food chain. Regulations in the US and EU require companies and countries to monitor their presence as they are toxic even at very low concentrations.

In a presentation entitled ‘Increased Laboratory Productivity with a Consolidated GC-MS Approach for Soil Contaminants Testing’, Mark Belmont from Thermo Scientific discusses the significant challenges for the analysis of PAHs and PCBs. These include lengthy manual sample preparation, long chromatographic separations, low sample throughput, and high cost of analysis. Research often involves using several methods for both sample preparation and GC-MS analysis. He reported on a consolidated automated process that speeds up analysis and reduces costs when studying PAHs and PCBs in solid environmental samples. The study used the company’s ISQ 7000™ GC-MS technology and demonstrates how an analyst can control and automate sample preparation, data acquisition, processing, and reporting using the company’s Chromeleon Chromatography Data System™.

At Pittcon, Ramkumar Dhandapani of Phenomenex also discussed how to improve GC-MS for analysis of PAHs, such as naphthalene and chrysene. In his talk entitled 'Fast Analysis of Regulated PAH by GC-MS', he explained how accurate analysis of these PAHs (with fewer false positives) is critical for both food and environmental regulations. In this study, he reported on various column sensitivities to achieve the best accuracy, sensitivity, and speed.

Shimadzu was among manufacturers that exhibited at Pittcon. Its GCMS-QP2010 SE with an EST Purge and Trap has been validated for all US EPA tests for volatile organic compounds. The device is affordable and can be coupled to an HS-20 headspace sampler for the analysis of volatiles. The Shimadzu GCMS-QP2020 has been validated for all US EPA tests for semi-volatile organic compounds methods. With improved sensitivity and fast scanning speeds, the user can extract fewer samples and reduce run times without compromising on performance.

In summary, GC-MS is the analytical instrument of choice for environmental analysis, allowing the detection of a range of pollutants and contaminants to help protect the environment.

References

- *Environmental Technology (2013) GC(GCMS), the Multi Tool for Environmental Analyses https://www.envirotech-online.com/article/environmental-laboratory/7/unassigned-independant-article/gcgcms-the-multi-toolnbspfor-environmental-analyses/1348*
- *Aluyor, E. & Ori-jesu, M. (2009) Biodegradation of mineral oils – A review, African Journal of Biotechnology https://www.ajol.info/index.php/ajb/article/viewFile/59986/48255*
- *Barlow, S. et al. (2015) Drugs During Pregnancy and Lactation (Third Edition) https://www.sciencedirect.com/topics/medicine-and-dentistry/organochlorine-pesticide*
- *AWE International (2009) Chromatography in Environmental Analysis https://www.aweimagazine.com/article/chromatography-in-environmental-analysis-333/*
- *Zacs, D. et al. (2016) Determination of steroidal oestrogens in tap water samples using solid-phase extraction on a molecularly imprinted polymer sorbent and quantification with gas chromatography-mass spectrometry (GC-MS), Environmental Monitoring and Assessment. https://doi.org/10.1007/s10661-016-5435-8*
- *Pittcon 2020, Increased Laboratory Productivity with a Consolidated GC-MS Approach for Soil Contaminants Testing https://s23.a2zinc.net/clients/pittcon/pit20/Public/SessionDetails.aspx?FromPage=Sessions.aspx&SessionID=1571&SessionDateID=5*
- *Pittcon 2020, Fast Analysis of Regulated PAH by GC-MS https://s23.a2zinc.net/clients/pittcon/pit20/Public/SessionDetails.aspx?FromPage=Sessions.aspx&SessionID=1034&SessionDateID=4*
- *SHIMADZU, Gas Chromatography Mass Spectrometry (GCMS) https://www.ssi.shimadzu.com/industry/environmental/gas-chromatography-mass-spectrometry.html*