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Introduction to Frontiers in Electrocatalysis for Clean Energy

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Electrochemical reactions are of immense interest for their potential to help reduce emissions in fuel generation and its use. Electrocatalytic reactions involve electron transfer, and the presence of ions results in an electric field, yielding differences in reaction mechanism compared catalytic reactions without explicit control over the electrochemical potential (sometimes described as "conventional" or "thermal"). Such reactions are employed even now to generate "green" hydrogen *via* electrolysis, producing almost 4% global hydrogen. However, the US Department of Energy (DOE), has recently revised its green hydrogen targets to decarbonize the steel industry, ammonia production, and other major industrial sectors and set new estimates of $1 per kg by 2030.[1] Due to the renewable energy technology advancement, photovoltaic (PV) cost has reduced since 2009 from 0.5$ per kW h to 0.09$ per kW h 2022.[2] Like PV technology, the cost reduction in wind power has been significant over the past decade, driven by improvements in technology and increased efficiency. This cost reduction in renewable energy sources brings tremendous potential for electrified chemical transformations.

In electrocatalytic reactions, there are three major components which impact

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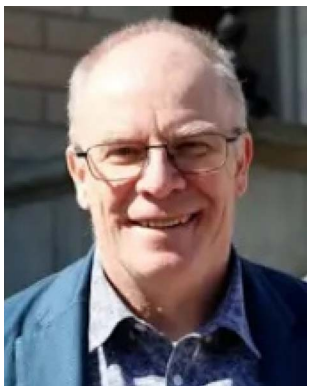

Anders Hagfeldt

Anders Hagfeldt has been a vice-chancellor at Uppsala University since 2021 and professor of physical chemistry. He obtained his PhD at Uppsala University in 1993. His research has focused on the fields of dye-sensitized solar cells, perovskite solar cells and solar fuels. He has published more than 660 scientific papers that have received over 113 000 citations. 2014–2020 he was a professor at The Swiss Federal Institute of Technology in Lausanne (EPFL). 2013–2019 he chaired the Committee for Development Research at the Swedish Research Council. He is co-founder and board member of the company Dyenamo AB and Chief Editor of Journal of Materials Chemistry A.

the performance. Firstly, the nature of the electrocatalyst, with requirements including but not limited to, good electrical conductivity, durability under the electrochemical micro-environment, proficient electrochemical kinetics, and reasonable cost.[3] Secondly, methods of electrocatalyst deposition as an active material on the conducting support and its nature. Thirdly, the nature and role of electrolytes that help in ion transport and affect the efficiency, reaction kinetics, and overall electrochemical device performance. All these are interrelated to evaluate the candidate as an ideal electrocatalyst.

This theme "Frontiers in Electrocatalysis for Clean Energy" is timely and focused on the interplay between active materials, the electrochemical microenvironment, durable and high-performing electrocatalysts, single-atom catalysts (SACs), the role of the conducting support, electrocatalyst structural transformations, benchmarking CO_2 conversion to C_2 products and other electrochemical clean energy reactions. In the recent past, electrocatalysis has seen advancements *via* the conjunction of nanotechnology, materials science, and improvement in electrochemical engineering. The convergence of these interdisciplinary approaches has enabled the development of highly efficient, durable, cost-effective electrocatalytic materials which ameliorated the performance of major electrifying chemical transformations.[4] To effectively reduce the cost of conventional electrolysis and fuel cell devices requires effective use of noble metals (platinum, ruthenium, iridium *etc.*). Alternatively, huge efforts have been devoted to exploring new electrocatalytic systems based on transition metal catalysts, such as nickel, cobalt, molybdenum and iron *etc.* as alternative substitutes.[5] Significant efforts are underway to selectively reduce carbon dioxide into C_2 products through effective copper-based catalysts.

Despite huge progress, several major challenges hinder the upscaling of electrocatalysis technology for industrially important clean energy processes. This includes catalyst durability, sustaining real-time harsh environments, high temperatures, corrosive environments, and changeable loads. These features can result in electrocatalyst degradation, compromised durability, low activity, and declining long-term feasibility of this electrochemical technology.[6] To address these major challenges that impede commercialization and the technology readiness level (TRL) of electrocatalysis for clean energy reactions, it's important to explore interdisciplinary approaches to develop highly stable, efficient, protective electrocatalyst materials for upscaling to replace the noble metal-based systems. It is important to note that while various promising electrocatalytic systems have been investigated, their potential to advance the TRL remains unfulfilled, likely due to the absence of interdisciplinary approaches integrating materials science and engineering.

This themed issue also covered various potential clean energy reactions ranging from improved electrolysis, corrosion-resistant electrode materials, urea synthesis, and selective CO_2 reduction, to theoretical investigations of electrocatalysis *etc.* Zhao *et al.* explored a density functional theory (DFT) tool to investigate (**https://doi.org/10.1039/d4ta01719f**) single-atom transition metals on conducting support (carbon nanotubes with small curvature) and developed volcanic curves amongst the adsorption free energy of H* (ΔG_{H^*}) and current density for the hydrogen evolution reaction (HER), and obtained RhN_4 at the peak of the volcano, suggesting current density higher than commercial Pt when CNT curvature is lower than (10,10). They observed a linear relationship between the d-band center and CNT curvature. Thangamuthu *et al.* (**https://**

Kelsey A. Stoerzinger

Kelsey A. Stoerzinger is an associate professor in chemical engineering and materials science at the University of Minnesota. The Stoerzinger research group works to develop and understand electrocatalysts enabling the storage of renewable electricity and their use in reactions integral to sustainable chemical production. Their design approach stems from a fundamental understanding of material surfaces and the electrode/electrolyte interface, often employing model catalysts and in situ spectroscopies. Stoerzinger started her career in 2018 at Oregon State University with a joint appointment at Pacific Northwest National Laboratory, where she was a Linus Pauling Distinguished Postdoctoral Fellow. She completed her doctoral studies in materials science and engineering in 2016 from the Massachusetts Institute of Technology.

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doi.org/10.1039/d4ta00711e) transformed metal waste into an electrochemically active catalyst for hydrogen production through surface modification. The catalyst surface is transformed through atomically ultrathin deposition of Pt for HER and Co as co-catalysts for oxygen evolution reactions (OER) with enhanced performance. Through this sustainable approach, cheap metal waste can be modified and explored for large-scale electrochemical systems. Herrán *et al.* (**https://doi.org/10.1039/d4ta02904f**) explored a hybrid approach to develop organic–inorganic materials such as cuprous oxide/polycarbazole (a conducting polymer) for electrochemical reduction of molecular nitrogen and nitrogen oxoanions. These hybrid electrode materials showed improved performance. Guo *et al.* (**https://doi.org/10.1039/d4ta02903h**) demonstrated that imidazolium cations can accelerate the CO_2 reduction in nonaqueous electrolytes. In this work, they proposed different reaction mechanisms as how imidazolium cations promote CO_2 reduction. It's important to understand the CO_2 electrochemical reduction mechanism as this reaction is complex and results in more than 25 reaction products. In general, *operando* techniques are critical for clean energy based electrochemical reactions, to understand their process which gives insight and can lead to the development of high-performance electrode materials. Similarly, artificial intelligence (AI) and machine learning (ML) tools are important for designing better electrocatalysis, improved processes, and eventually electrochemical technology.

This themed issue presents a snapshot of critical and focused research work on electrocatalysis, to electrochemistry and materials chemistry readers. In the last 15 years, electrocatalysis research has advanced enormously and it's difficult to cover all the aspects of the fast-evolving subject in a theme. This small collection of articles published in *Journal of Materials Chemistry A*, will provide insight and an overview of recent progress made in electrocatalysts and their future development. Advancing ML tools may potentially enable the discovery of next-generation materials for renewably electrified chemical reactions, understanding their mechanistic pathways, establishing structure–property relationships and the interplay of advanced materials for improved industrial processes. We hope readers will enjoy this themed issue which covers a range of sub-topics and pushes the electrocatalysis field further in terms of fundamental understanding and practical industrial applications.

Finally, we thank all the contributing authors and the journal team.

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