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X-ray-based technologies in emerging fuel cell research

Vivian Stojanoff[a]* and Narayanasami Sukumar[b]*

[a]Center of Biomolecular Structure, NSLS-II, Building 745, Brookhaven National Laboratory, Upton, NY 11973, USA, and [b]NECAT, Department of Chemistry and Chemical Biology, Cornell University, Building 436E, Argonne National Laboratory, Argonne, IL 60439, USA. *Correspondence e-mail: stojanof@bnl.gov, sukumar@cornell.edu

The workshop titled 'X-ray-based technologies in emerging fuel cell research', organized by Vivian Stojanoff from Brookhaven National Laboratory (BNL) and Narayanasami Sukumar from Cornell University/Advanced Photon Source-Northeastern Collaborative Access Team, was a notable segment of the National Synchrotron Light Source II and Center for Functional Nanomaterials Users' Meeting held 13–17 May 2024. This one-day event, on 13 May 2024, at BNL in New York, aimed to bring together researchers, beamline scientists, management and developers to propel fuel cell technology forward using model systems inspired by natural photosynthesis and redox enzymes. This summary encapsulates the key discussions, advancements and future implications of the workshop.

1. Overview

Fuel cells are pivotal for developing sustainable energy solutions, converting energy-poor molecules into energy-rich ones using sunlight. Artificial photosynthesis, which emulates natural photosynthesis, is a significant research area. Plants naturally split water into oxygen and hydrogen, generating electrons through photosynthesis. Similarly, many researchers strive to thoroughly understand the redox enzyme mechanism to potentially replace or enhance the design of inefficient and costly catalysts (*e.g.* platinum) in fuel cells. A workshop titled 'X-ray-based technologies in emerging fuel cell research' was held on 13 May 2024 at Brookhaven National Laboratory (BNL) in New York as part of the National Synchrotron Light Source II (NSLS-II) and Center for Functional Nanomaterials (CFN) Users' Meeting. This workshop aimed to unite fuel cell researchers with various expertise, employing both X-ray- and non-X-ray-based techniques, to foster collaborative exchanges, ultimately leading to efficient fuel cells. Additionally, insights from researchers at the National Renewable Energy Laboratory (NREL) and the Joint BioEnergy Institute (JBEI), who are at the forefront of renewable energy research, were sought. This convergence of researchers who typically do not interface due to differing approaches and procedures, along with beamline developers and management, was intended to discuss the current status, limitations and future directions in the field. The ultimate goal was to create highly efficient and durable fuel cells that utilize abundant natural resources and consume less energy, thereby reducing dependency on fossil fuels and mitigating CO_2 emissions.

The workshop attracted approximately 130 registrants, including beamline scientists and management from various US national laboratories (Brookhaven National Laboratory, Argonne National Laboratory, Lawrence Berkeley National

Laboratory and Stanford-Linac Coherent Light Source) and several eminent scientists from the USA and Germany. The participants discussed the current status and recent advances in photosynthesis and redox enzyme research, focusing on both X-ray and non-X-ray techniques to characterize these systems. Researchers from NREL and JBEI, exclusive Department of Energy (DOE) research institutes for non-fossil fuel research, shared their current research status.

The workshop began with a welcome address from the organizers and a talk by Sean McSweeney (BNL), the Biological, Environmental and Planetary Sciences Division Director at National Synchrotron Light Source II (NSLS-II). He discussed the advanced tools available at NSLS-II for fuel cell research, highlighting various imaging, spectroscopic and crystallographic techniques and their applications in studying biological and non-biological materials. This was followed by a series of talks on natural and artificial photosynthesis, redox enzymes and advances in renewable energy.

2. Natural and artificial photosynthesis

The goal of this session was to emphasize how advancements in photosynthesis research could propel fuel cell technology forward. Masakazu Iwai (Lawrence Berkeley National Laboratory) focused on the role of evolution in photosynthetic light harvesting, presenting examples from prokaryotic and eukaryotic systems. He discussed how plants dissipate excess light energy and how fine-tuning photoprotection mechanisms can improve crop yields. His research utilizes both X-ray and non-X-ray techniques, including 2D electronic vibrational spectroscopy and X-ray free-electron lasers (XFELs). Francesca Toma (Helmholtz-Zentrum Hereon, Germany) introduced a multimodal approach (multiple techniques that capture the same spot on the same samples) to artificial photosynthesis, comparing it with the correlative approach (multiple techniques with multiple users/sample sites). She discussed the current status and limitations of photoelectrodes for solar fuel generation and how interface engineering can improve their stability and efficiency. Techniques such as ambient pressure X-ray photoelectron spectroscopy, computational electrochemical atomic force microscopy, photoconductive atomic force microscopy and scanning transmission X-ray microscopy have been used to characterize material properties. Matthias Kling [Linac Coherent Light Source (LCLS)] described the unique capabilities of the LCLSII, including its latest source, Linac Coherent Light Source II-High Energy (LCLSII-HE), and their relevance to studying fast dynamics in picoseconds, contrasting it with synchrotron sources that capture only millisecond dynamics. He presented research highlights based on projects brought by users to his facility, particularly in photosystem II dynamics and redox enzyme systems for sustainable fuel production. Gabriela Schlau-Cohen (Massachusetts Institute of Technology) explored how plants dissipate excess light energy as heat, identifying chlorophyll-to-carotenoid energy transfer as a dissipative pathway. Her work, based on non-X-ray techniques, provides insights into the parameters responsible for plant photoprotection mechanisms. Petra Fromme (Arizona State University) concluded the session with a talk on her experiments at LCLS on time-resolved studies of photosystem II. She described how short pulses of <10 fs helped to collect undamaged data to differentiate Mn oxidative states in the Mn_4CaO_5 catalytic center of photosystem II. She also spoke of building a compact XFEL source at her institution.

3. Redox enzymes as model systems

The afternoon session focused on redox enzymes and their potential in fuel cell research. Kara Bren (University of Rochester) discussed 'Engineered biocatalysts for light-driven fuel formation', emphasizing the use of cytochromes with covalently attached polypeptides to generate hydrogen in the laboratory. Her research aims at creating robust, sustainable systems that function in water using both metal and metal-free systems. Yi Lu (University of Texas Austin) highlighted the inefficiencies of oxygen reduction reactions (ORR) catalyzed by precious metals and proposed artificial metalloenzymes as efficient alternatives. His work demonstrates how increasing hydrophobicity in type-I copper proteins could vary their reduction potential, a useful feature for fuel cell technology. Both X-ray and non-X-ray techniques were employed in his research. Narayanasami Sukumar (Cornell University/Advanced Photon Source-Northeastern Collaborative Access Team), one of the organizers, presented the application of charge density methods in X-ray crystallography to study the type-I copper protein amicyanin. He discussed the importance of understanding electron transfer and redox processes and their impact on fuel cell research, and also how technology limitations can affect research outcomes. He proposed adding features to beamlines to improve data collection for metalloenzymes.

4. Advances in renewable energy

The final session addressed recent advancements in renewable energy. Smaranda Marinescu (University of Southern California) discussed biologically inspired catalytic systems for solar-to-fuel technologies, focusing on hydrogen evolution reaction activity using metal–organic frameworks (MOFs). Her research utilizes X-ray, mechanistic and computational studies to understand MOF properties. Todd Deutsch (NREL) spoke about photo-electrolysis and identifying degradation mechanisms in solar fuel systems. He has used both X-ray (using various synchrotron sources) and non-X-ray techniques to study photoelectrochemical water splitting. Jose Henrique Pereira (JBEI) highlighted the role of structural biology in bioenergy research, discussing enzymes like galactan synthase I and decarboxylase, which play significant roles in biofuel production.

5. Conclusion and future directions

The workshop concluded with a brainstorming session titled 'Looking forward', chaired by one of the organizers, Vivian

Stojanoff (BNL), involving graduate and post-doctoral researchers whose participation was made possible by generous funding from the DOE. The discussions centered on the current status and future developments in fuel cell research. Invited speakers answered numerous questions, fostering a collaborative environment. The workshop also featured a poster session and a flash talk from a graduate student.

The workshop successfully highlighted the importance of X-ray-based technologies in advancing environmentally friendly fuel cell research alongside non-X-ray techniques, emphasizing the need for collaboration between academic researchers and centers/facilities at government-funded laboratories. The insights gained from natural and artificial photosynthesis, redox enzymes and renewable energy technologies showcased the potential of these systems in creating sustainable energy solutions. The event underscored the value of integrating various techniques and fostering interdisciplinary collaborations to drive progress in the field.

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