

EEWS 2016: Progress and Perspectives of Energy Science and Technology

▼ stablished in 2009, the Graduate School of EEWS (Energy, Environment, Water, and Sustainability) at the ■ Korea Advanced Institute of Science and Technology (KAIST) is the first of its kind, an interdisciplinary department at KAIST collectively addressing with interdisciplinary approaches for the emerging and urgent issues in energy, environment, water, and natural resources of the twenty-first century for sustainable society through science, technology, and education (http://eewseng.kaist.ac.kr). Currently housing 12 research groups with diverse backgrounds in chemistry; physics; chemical, electrical, mechanical, and environmental engineering; and materials science, the EEWS is the culmination of unprecedented collaboration under the same roof with close interaction of students and faculty from unlikely backgrounds (Figure 1). The output in a relatively short period of time is

Research Subjects of EEWS

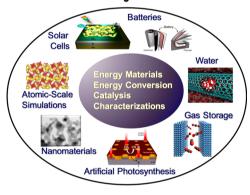


Figure 1. Primary areas of research interest at the Graduate School of EEWS of KAIST.

remarkable; the collaborative research combining basic and applied disciplines of seemingly different subjects have produced many novel concepts and approaches in various energy science and technology fields that are otherwise difficult to conceive in a traditional way. In an effort to critically assess the current status of the energy research, identify major challenges, and further stimulate active interactions among the disciplines to solve the challenges, we held the first EEWS forum, "EEWS 2016: Progress and Perspectives of Energy Science and Technology", in the KI Fusion Hall of KAIST on October 20, 2016. The meeting featured eight internationally recognized energy experts from around the world introducing their cutting-edge research covering a wide range of topics in energy materials, advanced characterization tools, and catalysis, from both experimental and theoretical viewpoints (Figure 2).

The forum started with an affirmation that the destructive impact of fossil fuels on human civilization mandates energy research and technology to be a necessity, calling for every effort in finding solutions. In the first of two talks on energy



Figure 2. Photograph of 8 invited speakers and over 200 participants at EEWS 2016: Progress and Perspectives of Energy Science and Technology. (Photo courtesy of Sangpil Yoon).

materials, Prof. Yi Cui (Stanford University, United States) identified energy storage into Li-ion batteries to be at the forefront for energy research because alternative energy sources are not able to compete with the high energy storage density of fossil fuels. He particularly emphasized the high-capacity electrode designs for metallic lithium anodes that adopt three-dimensional (3D) frameworks for the accommodation of metallic lithium without dendrite growth. His approaches largely resolve longstanding difficulties in battery research, such as in binders and grain expansion control, and are expected to deliver a considerable impact to the battery research community as a viable solution for moving beyond graphite electrodes.

In the second talk on energy materials, Prof. Yang-Kook Sun (Hanyang University, Korea) discussed the cathode in lithium rechargeable batteries. Particularly, he introduced high-nickel layered cathode materials that overcome the challenging capacity fading problem by a gradient composition.² In simple terms, Ni content gradually decreases from the core to the surface. This gradient composition also avoids crack formation, another well-known drawback of previous high-nickel cases. Impressively, these cathode materials reached 3000 cycles without noticeable degradation, which corresponds to an approximately 10 year service life when adapted to electric vehicles.

In conventional energy-intensive chemical technologies, suitable design of a catalyst could alleviate energy losses by energy conservation. Because many catalysts work heterogeneously, atomic and molecular level characterization of a

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surface under reaction conditions is critical for designing advanced catalyst materials. However, many techniques used in surface science often rely on ultrahigh vacuum (UHV) environments, whereas practical catalyst surfaces are surrounded by gases at ambient pressure and liquids. Dr. Miguel Salmeron (Lawrence Berkeley National Laboratory and University of California at Berkeley, United States) highlighted the current studies on surface science techniques operated in operando conditions, such as ambient pressure X-ray photoelectron spectroscopy (XPS), ambient pressure scanning tunneling microscopy (STM) and X-ray absorption spectroscopy (XAS), which can unravel the physics and chemistry of a surface in equilibrium with the gas or liquid phases. 4 He further demonstrated that the XAS technique can be extended to investigate the solid-liquid interface during electrochemical reactions by measuring electron yield current collection at the same electrode under study.5

A finer look on the crystal construction could also assist in designing better energy conservation through energy materials. For example, grain boundaries (GBs) in polycrystalline materials are solid-phase interfaces between two adjacent grains having an identical composition and crystal structure in different crystallographic orientations. As a result, they often exhibit notable properties relevant to ionic diffusion and mass transport for efficient energy conversion. Prof. Yuichi Ikuhara (The University of Tokyo, Japan) highlighted the importance of understanding and controlling atomic structures and the chemistry of GBs in energy materials through atom-resolved characterization techniques and first-principles calculations. Prof. Ikuhara demonstrated that additional oxygen vacancies are introduced in GBs to relax GB structural distortion and different dopants segregation behaviors depending on GB character in various oxide materials such as CeO₂ and ZrO₂.

The petrochemical industry is at the heart of the energy conundrum, and small optimizations in any steps of chemical refining and catalysis often yield major energy savings in the downstream processes. Particularly in the amidation of hydrocarbons, Prof. Sukbok Chang (KAIST, Korea) showed how difficult but rewarding C-H activations could be. Nitrogen-containing commodities are usually synthesized by high-temperature reactions or multiple steps with poor atom economy. He showed that amidation could be carried out at ambient conditions by readily available azide building blocks and a recyclable noble metal catalyst. He also highlighted that unconventional substrates, such as azidoformates, could install protected amine functionalities to unactivated hydrocarbons by using a suitably designed catalyst. These developments point to a more energy efficient chemical industry through the use of powerful new catalysts and substrates.

A significant fraction of current subjects in energy research deal with electrochemistry and electrochemical interfaces; however, their theoretical treatments to gain insights are far from trivial. Advances in theory and methods of quantum mechanical (QM) calculations are thus essential to address theoretically key questions in energy fields, such as to understand the mechanisms of electrochemical catalytic reactions and design new materials for efficient energy conversion applications. Prof. William A. Goddard III (Caltech, United States) presented new methods including QM metadynamics calculations for energetics of electrocatalysts at operational temperatures and potentials. With this method, he identified the reaction mechanism for the electrocatalytic oxygen reduction reaction on Pt(111) and Pt alloys and critical

potentials for CO₂ reduction on (100) and (111) Cu surfaces to form hydrocarbon fuels at various pH from 0 to 14. Atomistic understanding and insights obtained from these novel quantum chemical calculations offered a few new design concepts.

Hydrocarbon separations are immensely energy intensive operations that bring significant energy penalties for both the energy sector and the production of chemical commodities that rely on petroleum. 11 Prof. Mohamed Eddaoudi (KAUST, Saudi Arabia) showed that a precisely engineered porous crystalline material could remove a hydrocarbon from another by a simple molecular sieving procedure. The approach is unique, as conventional separations rely almost exclusively on distillations. In particular, his team was able to separate propylene from propane (olefin-paraffin separations account for 3% of total energy used by separations industry) by tuning the pore opening of a H₂S stable metal-organic framework (KAUST-7) to 4.75 Å. 12 This was all due to a ubiquitous building block approach, in which a theoretical design of a 3D framework could later be realized in the laboratory. 13 He demonstrated that one could design and synthesize MOFs for any molecular separations where sizes or shapes differ slightly, enabling a vast toolbox for scientists that develop energy-efficient petrochemical separations.

In a complete alternative and promising energy path, solardriven chemical reactions at a semiconductor/electrolyte interface could lead to solar fuel production and solar-powered water treatment applications. Although common semiconductors such as TiO2, WO3, and Fe2O3 are used in photocatalysis, their poor charge separation in metal oxide semiconductors limits conversion efficiency and their use in practical applications. Prof. Wonyong Choi (POSTECH, Korea) presented various approaches to boost photocatalytic efficiency of earth-abundant semiconductors. 14 He demonstrated that surface modifications at TiO₂ by metal nanoparticles, thin layers of TaO_xN_v, and graphenes significantly reduce the charge recombination and enhance the interfacial charge transfer. These advances, ultimately, could increase photoelectrochemical and photocatalytic conversion efficiencies for water splitting and water treatments.

In this one-day forum, attendees witnessed advances, challenges, and opportunities in energy science and technology for EEWS problems. The challenges are vast, but energy research is moving steadily forward to tackle them by understanding and controlling energy materials from atomic scale to bulk materials through interdisciplinary collaboration across the fields of science and engineering. The EEWS international forum will continue to address new challenges in energy research and technology in the coming years.

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Notes

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