# NGenE 2021: Electrochemistry is Everywhere

In 2016, an Editorial in ACS Nano, entitled "The Rising and Receding Fortunes of Electrochemists",1 reflected the growing scientific consensus that existing initiatives in fundamental research were undermatched to the fact that electrochemistry was becoming ubiquitous in applications in energy, thus handicapping progress toward social impact. That same year, Next Generation Electrochemistry (NGenE) hosted its first edition at the University of Illinois at Chicago (UIC). NGenE is an annual Summer workshop focused on describing emerging challenges at the frontiers of research in electrochemistry, and the application of innovative strategies to address them. The original premise behind NGenE was also that, despite its reach and importance, fundamental electrochemistry had gone through a rather slow period of activity in the early 21st century compared to many companion fields. Back in 2016, one of the causes was ascribed to a deficit in electrochemistry training at the graduate level, 2,3 leading to calls for increased emphasis in research in this area.<sup>4</sup> Since 2016, NGenE has tackled these deficiencies by broadening the knowledge and perspective of senior graduate students and postdoctoral researchers. A series of worldrenowned experts in various walks of electrochemistry examine fundamental phenomena at an advanced level, identifying critical gaps in our understanding and innovative strategies to address them. The program assumes baseline knowledge and prior experience in electrochemistry. NGenE does not ask, "What is electrochemistry?" but instead "What will electrochemistry become?". As such, it tackles the very same issues raised in the aforementioned Editorial.

Fast-forwarding five years, support and activities in fundamental electrochemical research have undergone very significant growth. Furthermore, new applications of electrochemistry that were not on our radar in 2016 have emerged, especially among organic chemists.<sup>5</sup> It is an exciting time to be an electrochemist and new generations of leaders in research are increasingly pursuing this path. Simultaneously, NGenE has evolved from a program with a focus in rather specific topics, such as batteries, to expose the major diversity of fields interested in electrochemistry and finding common elements between their challenges. In 2020, the world ground to a halt with the onset of the COVID-19 pandemic and NGenE had to adapt to the reality that meetings in person were not possible. The program migrated from a format of interactive lectures led by individual researchers to panel discussions involving multiple researchers talking to each other and with the attendees, who were provided the virtual floor to ask questions. The outcome was a series of highly dynamic discussions that are now free to watch on demand by anyone in the world.<sup>6</sup>

NGenE 2021 was divided into a series of panels dedicated to a specific topic at the frontiers of electrochemical research. In this status report, we summarize the key messages emerging from the discussions. While some panels covered aspects not limited to energy technology, the commonality of lessons and challenges highlight the many opportunities ahead for cross-pollination to establish electrochemistry as central to our current transition away from the fossil-fuel paradigm. By sharing them here, we strive to motivate the community to pursue directions that move us beyond the current frontiers. This summary is divided in themes that map out of the specific panel topics.

### Can Electrochemistry Replace Thermochemistry?

In thermochemistry, temperature and pressure are major driving forces for chemical transformations. Existing high-temperature thermochemical processes rely on burning fossil fuels to achieve high temperatures in the furnace, reactor, or kiln. By burning fossil fuels to achieve the desired chemical transformation, CO<sub>2</sub> is emitted, which adds to its toll as a major greenhouse gas. Steel and cement

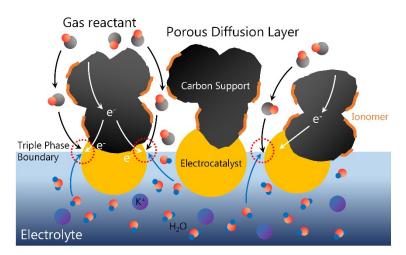
manufacturing, steam-methane reforming, and the Haber-Bosch process are some of the examples of thermochemical processes at high temperature that are challenging to decarbonize. These industries rely on mature technologies that have evolved over decades and have not changed significantly in the last decade. With the sustained declines in the cost of installing and using renewable sources of energy, electricity continues its transition to becoming a sustainable energy carrier free of emissions of greenhouse gases. All the major sources of renewable and carbon-neutral energy (solar, wind, nuclear) generate electricity ensuring that a renewably powered society will be electrified. Shifting from thermochemistry to electrochemistry in industrial production could accelerate this transition by relying on electricity free of emissions.

Electrifying the generation of heat is one way that could enable an electrified thermochemical industry. However, estimates suggest that if all thermal needs were electrified, doubling the electricity running through the distribution system would be needed. This transition will be challenging without a tremendous increase in electrical transmission and distribution infrastructure. Thus, as a potential alternative, it is valuable to explore new processes where electricity can substitute for heat, which would be particularly compelling if requiring low temperature and/or pressure to be inherently more efficient. Most likely, electrochemical processes will not serve as a drop-in replacement for existing thermochemical technologies but instead will reinvent these and become clean alternatives. Because these are GW-scale industries, technologies with potential for scale-up should be prioritized. Fortunately, there are several examples of electrochemical processes at large scale in industry today, such as the production of Al or the chlor-alkali process, where Cl<sub>2</sub> and NaOH are formed in an electrolyzer. These examples can serve as templates when seeking to transform thermochemical technologies, and they hint at the possibility that new processes will be enabled that are simply prohibitive thermochemically.

Creative solutions could transform industries that are difficult to decarbonize. Recently, a low-temperature method was introduced to use electrolysis to produce precursors of cement. In steel manufacturing, the initial production of iron could be induced through reduction of the ore by electrogeneration of both CO and H<sub>2</sub>, rather than the current use of carbothermal reduction, which consumes vast amounts of energy and is a major contributor to CO<sub>2</sub> in the atmosphere. This outcome relies on transforming the production of H<sub>2</sub> first, 99% of which, in the US, currently relies on steam-methane reforming. To transition away from such "grey H<sub>2</sub>", "green H<sub>2</sub>", whose carbon intensity is low, could be produced by electrolysis of H<sub>2</sub>O. Electrolysis has made major strides in recent decades, to the point where it is becoming feasible at low temperature, without greenhouse gas emissions and with only H<sub>2</sub>O and electricity as input. Further developments in performance metrics would not only bring this possible scenario into fruition, but also unlock opportunities in other sectors that are difficult to decarbonize, such as shipping, aviation or heavy-duty transportation, which can use "green H<sub>2</sub>" through fuel cells. 12

Opportunities for using electricity from renewables to transition away from thermal processes powered by fossil fuels are not limited to "green H<sub>2</sub>", as electrochemical routes are now within reach to compete with the Haber-Bosch reaction to produce NH<sub>3</sub>,<sup>13</sup> technologies for negative emissions (i.e., CO<sub>2</sub> valorization),<sup>14</sup> and even the alternative production of precursors used by the plastic industry.<sup>15</sup> In all cases, a central barrier toward technological disruption is the need for electrocatalysts that promote the desired reactions at high yield, efficiency and durability. A secondary challenge exists around reactor engineering, as most thermocatalytic reactors use volumetric packed-bed reactors, whereas electrocatalytic cell use planar reactors. As an added benefit compared to traditional thermal catalysis, many electrocatalytic processes operate near ambient conditions, which allows access to non-thermal product distributions that unlock new applications. However, all the processes listed so far have yet to meaningfully replace

incumbents in many cases because current yields and efficiency are not high enough. In our NGenE discussions, emphasis was placed on classical questions in electrocatalysis, such as defining its operating mechanisms, integrating computational approaches and experimental methods, and conducting any such studies simultaneous to the reaction. However, our knowledge today clearly points to the need to move "beyond the catalytic site" toward interrogating whether secondary interactions with the local environment, such as ions in the electrolyte, the support architecture or even ionomer membranes (Figure 1), could offer control knobs that were heretofore not considered. This holistic approach to the design of electrocatalytic reactions was identified as a focal point for future research. The ensuing complexity of these interactions opens the door to the application of new machine learning and computational tools to help accelerate discovery of permutations with transformative properties.



**Figure 1:** Schematic depicting the complexity of a typical electrode-electrolyte interface in a gas-fed flow reactor. Electrocatalyst particles are mixed with ionomers (for charge conductivity), and then sprayed onto a porous gas diffusion layer (for gas diffusion and electron conductivity) to form a typical gas diffusion electrode.

### Solvation science applied to electrochemistry

Understanding the nature and behavior of ions in solution can amplify our control of electrocatalytic processes. Achieving this control motivates the study of the science of solvation. Solvation phenomena play a key role in many applications in energy storage. Most future projections to support increasing use of sustainable, intermittent energy resources, point towards a rapidly increasing demand for electrification; towards multiple TWh of production per year. While Li-ion is currently the world-leading technology and likely to remain such for many years, it is prudent to research and develop alternatives; to diversify resource demands and meet different use cases.

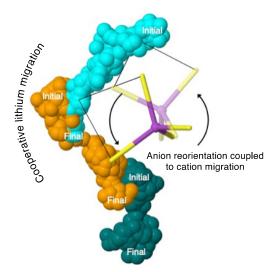
Development of novel concepts of energy storage come with many challenges to our current theories that describe solvation. For example, moving from monovalent to multivalent charge carriers introduces changes in solvation and interfacial reactions; which require a completely new understanding to enable control. Researchers have recently established that multivalent ions have a much higher tendency to form clusters and aggregates in organic electrolytes, <sup>16</sup> which can be further manipulated by pushing into "solvent-in-salt" spaces. The formation of such clusters and aggregates affects the transport properties of the bulk electrolyte. Less intuitively, it also determines the stability of the electrolyte at the electrified interface. Coupling solvation phenomena such as ion-pair formation to electrolyte stability under charge-transfer is a

crucial piece of that understanding, and now enables computational screening of salts and solvents with improved stability.

Interfacial stability also includes the formation of electrode surface layers, such as the surface-electrolyte interface (SEI) on the graphite anode in modern Li-ion batteries. These surface layers form from spontaneous, out-of-equilibrium reactions between the electrode and the electrolyte during the first cycles. In the best-case scenario, the result is a thin film that passivates against electron flow while conducting the active ion. The entire Li-ion industry would not exist without the serendipitous discovery of the beneficial role of ethylene carbonate in the formation of an SEI on graphite. Yet despite decades of study, we still do not know how to design these interfaces. Future work to accelerate development of novel concepts for energy storage needs to meet this challenge by developing predictive theories and frameworks for SEI growth and surface passivation.

While "solvation" tends to evoke more or less free molecules surrounding an ion, it is actually defined by IUPAC as "any stabilizing interaction of a solute (or solute moiety) and the solvent, or a similar interaction of solvent with groups of an insoluble material[...]". Within the solvation panel, discussions fully exploited this definition to venture toward concept of solvation in solid electrolytes. Solid electrolytes – and the solid-state batteries they might enable – have become a very popular topic in electrochemistry R&D. Ramples of solid electrolytes include organic materials such as polymers, and inorganic systems such as crystalline solids (oxides, sulfides, etc.) and their amorphous analogues, glasses. In contrast to solvation in liquids, where the solvating shell can transport with the working ion, in solids the solvation shell does not translate. Given their stationary nature, solvating shells in solids might be best described as *cages*.

The role of cages in solid-state ion transport has not received as much attention as have the role of shells in liquid systems. Typically, ions that migrate through a solid must navigate the free energy surface (and barriers) generated by the largely static cages. The static nature of the cages might lead one to believe that ion migration is a simple process whose features are influenced primary by the structure of the cage. However, recent studies have challenged this simplistic viewpoint. For example, in inorganic glasses or crystals containing complex anions the rotational motion of the anions has been shown to facilitate ion motion by lowering energy barriers for ion hopping. One example of this transport mechanism is shown in Figure 2. Here, large, quasi-permanent reorientations of PS<sub>4</sub> anions in the glass Li<sub>3</sub>PS<sub>4</sub> strongly correlate (in space and in time) with the migration of Li-ions, <sup>19</sup> an effect often referred to as the 'paddlewheel' mechanism. Hence, even in materials where the solvating component (the cage) is translationally stationary, the (rotational) dynamics of that entity can still play an important role in influencing ionic conductivity.<sup>20</sup>



**Figure 2:** Relationship between cage dynamics and ion transport in a glassy Li<sub>3</sub>PS<sub>4</sub>. Li-ion migration event involving the displacement of three Li-ions and a neighboring PS<sub>4</sub> anion. The position of the anion is shown before and after migration using transparent and opaque shading. Adapted with permission from reference 21. Copyright 2021 Cell Press.

Finally, the panel discussed whether it could be possible to develop a theory that unifies the concept of solvation across all classes of electrolytes: liquids, polymers, and inorganic solids. In such a scheme the behavior of shells in liquids and that of shells and cages in crystals would represent the endpoints of a continuum, with polymers and inorganic glasses somewhere in between. Defining order parameters that describe the translational and rotational features of the solvating entities might be a useful for developing such a theory. A recent publication by some of the panelists describes some early steps in this direction.<sup>21</sup>

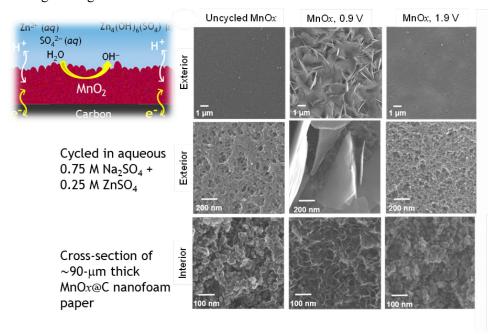
## There is also plenty of room at the bottom in electrochemistry

Based on the descriptions above, it is clear that electrocatalysis and solvation science display limiting phenomena at characteristic lengths at the nanoscale. These nanoscale length scales highlight the importance of designing electrodes as architectures in which the entire volume is wired continuously in three dimensions for electron, ion, and molecular transport so as to expand the reactive electrochemical turf beyond the limited footprint imposed by a two-dimensional cross-section. Amplifying the electron-wired interfacial area by hundreds of square centimeters per cross-sectional square centimeter converts redox reactions that lose morphological control at high local current density into more uniformly reactive events that experience low local current density. Aperiodic architectures such as foams and sponges effectively distribute the available electrified interface while maintaining a co-continuous mapping of the ions and molecules necessary to sustain the redox reaction.

Using batteries as a motivating application, electrode architectures show the power of controlling energy-storage reactions locally by distributing them within electron-wired high-surface interiors. The arrangement ensures that per area current remains low throughout the volume of the electrode, yet the electrified area sums to provide device-relevant current. A relevant example is how formulating Zn into a monolithic sponge form factor suppresses formation of separator-piercing metallic dendrites upon charge–discharge cycling in alkaline cells.<sup>22</sup> In the sponge anode, the complex chemistry/electrochemistry initiated on discharge as Zn oxidizes distributes uniformly at the interior walls, thus circumventing the critical

current density necessary to form dendrites. Armed with this control, aqueous, safer zinc-based rechargeable batteries can now compete with lithium-based batteries at the system level,<sup>23</sup> and do so using low supply-risk elements.<sup>24</sup>

In Zn-ion cells in which protons inserting into a layered metal oxide in the cathode balances zinc oxidation, formulating lamellar birnessite-like MnOx as a nanometric coating throughout a high surface-area carbon nanofoam distributes the accompanying electro-precipitated zinc salt along the interior walls of the macroscale 3D electron/ion/molecule-wired nanofoam (Figure 3). The microns-thick salt layer that carpets macroscopic surfaces at the powder-composite cathodes of Zn-ion cells is absent at the MnOx-painted carbon nanofoam, thus improving rate performance.<sup>25</sup> The architected cathode even delivers electrochemical capacitor function in mixed Na<sup>+</sup>/Zn<sup>2+</sup> aqueous electrolytes, as verified using a 3D Bode analysis of capacitance–frequency–potential to distinguish double-layer capacitance, pseudocapacitance, and insertion charge storage.<sup>25,26</sup>



**Figure 3:** Schematic depicting  $H^+$  insertion into  $MnO_x$  from mild aqueous electrolyte containing  $Zn^{2^+}$ ; ex situ scanning electron microscopy survey of an architected cathode prepared by "painting" the walls of carbon nanofoam with nanometric  $MnO_x$  to create a cathode that distributes the pH-driven precipitation of salt (zinc hydroxy sulfate) not just at the exterior but throughout the interior of the macroscale thick carbon nanofoam upon changes in interfacial pH upon proton insertion (at 0.9 V vs. Zn) and deinsertion at 1.9 V. Adapted with permission from reference 26. Copyright 2018 Springer-Nature.

### Electrochemistry down to single entities... borrowing from bioelectrochemistry

Broadly, nanoscale electrochemistry can help us to learn about the fundamentals of electrochemistry without the concerns for overlapping side effects and scale-averaging issues. If proper tools and expertise are utilized, one can learn much about interfacial interactions, charge transport, and chemical reactions selectively controlled by kinetics and thermodynamics. Our panel discussions highlighted the many potential contributions that remain to be fulfilled by developing novel and pushing existing methods based on local probes of electrochemistry. Prominent examples are in situ transmission electron microscopy

(TEM) and cryogenic TEM (cryo-TEM), powerful techniques for understanding electrochemical reactions at scales not seen before. Examples of phenomena that in situ and cryo-TEM can probe are phase transformations due to reactions of electrodes with alkali metals, ion-transport mechanisms within the electrodes, solid electrolyte interfaces, chemistry and structure of electrode-electrolyte interphases, and role of microstructural defects.<sup>27</sup> In light of new image detectors and cameras that can now capture images under low electron dose and below millisecond time resolutions,<sup>28</sup> new probing tools located within the TEM chamber,<sup>29,30</sup> improved TEM specimen holders,<sup>31</sup> and integrating artificial intelligence and data science to analyze TEM data,<sup>32</sup> the ensuing scientific breakthroughs will likely transform the field of modern electrochemistry.

Coupling observations of electrochemistry at the nanoscale in real time was identified as central to the most important challenges discussed in our panels. An attractive proposition is to double up our probing tools as electrochemical cells using micro and nanoscale electrodes. The variety of such probes is now immense, with scanning electrochemical and atomic force microscopies being two prominent examples.<sup>33</sup> Opportunities for cross-pollination across disciplines are brought forth by considering equivalent experiments that have growing interest in neuroscience: in vivo electrochemistry. Such experiments have been pursued using carbon-fiber electrodes for about four decades, and they have unlocked many of the secrets of rapid dopamine signaling underlying behavior.<sup>34</sup> However, there are still many outstanding challenges for this class of electrochemical tool. One of these challenges is designing electrodes specific to a variety of compounds of interest. Many new electrodes have been designed from an exquisite variety of carbon nanomaterials (nanotubes, nanospikes, nanohorns and new forms of graphene), but their chemical specificity remains to be wholly assessed. Further, new materials and strategies are needed to extend these materials to detect other classes of chemicals. Materials such as diamond and nanodiamond may also be useful for designing electrodes with less fouling. Completely new ways of building electrodes may also be useful as well. For example, 3D printing of polymer photoresists, which are then pyrolyzed into carbon. The shape and geometry of 3D printed electrodes can be customized to the application, and electrodes can be fabricated reproducibly. This strategy is used at a lab scale today, but as printers are optimized and become more available, it may become commercially viable to make electrodes with 3D printing.

While electrochemistry using carbon electrodes has revolutionized our understanding of electrochemical processes, alternative methods are still needed. These methods can fully exploit the spectrum of experimental conditions. A novel example is an electrode based on the Interface Between Two Immiscible Electrolyte Solutions (ITIES). ITIES technology relies on a liquid/liquid junction between an aqueous phase and an oil phase, located inside and outside a pipette. Thus, an external potential is applied, ion transfer is driven through the ITIES liquid/liquid junction, generating a current. Thus, analytes can be qualitatively and quantitatively detected. Electrochemistry at ITIES electrodes measures both faradaic and non-faradaic processes, analogous to the interface between metal/carbon and electrolyte solutions. Analytes that are detected at ITIES electrodes are electro-active while not redox-active. Nanoscale ITIES electrodes have already contributed to bioelectrochemistry by detecting and quantifying neurotransmitters from living neuronal structures (single synaptic cleft and single cell). While ITIES has evolved as a powerful electrochemical method over the past 40 years, applications remain to be exploited in many growing areas including electrocatalysis, metal-ion detection, or the study of ionic and electron-transfer mechanisms. The small size of ITIES electrodes make them amenable to rastering, so that the distribution of products can be mapped on an area of interest at the nanoscale.

Several critical challenges and limitations must be overcome to maximize the analytical power of electrochemistry to detect local phenomena, even down to a single entity. The first challenge lies in

detecting non-electroactive species, a common problem when the window of available potentials is limited by the electrolyte, which biochemistry encounters frequently due to the need to study aqueous systems with sensitive biological components. In the electroanalytical context, examples exist where researchers have modified electrode surfaces with enzymes that produce electroactive species upon interaction with a target, 36-38 yet, so far, at the expense of temporal resolution. The second challenge lies in quantitative characterization of electroactive species that are produced at slow and gradual levels, such as tonic release in biological systems. Traditional background-subtracted techniques will not work for these studies due to challenges of detection. The third challenge lies in electrode design. Specifically, electrode materials that have an affinity for the species one wants to detect tend to promote more sensitive detection, but also significantly more fouling. Researchers are always struggling to quantitatively track changes in electrode sensitivity and knowing when an electrode needs to be cleaned or replaced. The fourth challenge lies in the need to simplify systems of measurement to facilitate electrochemical measurements. This problem is often confronted by bioelectrochemists because most biological cells, for example, are not sitting in stagnant fluid conditions, which is how most electrochemical measurements are done to avoid significant background noise. Overall, it is important for electrochemists to figure out how to add complexity (like moving fluid or complex mixtures) to draw conclusions relevant to device design or biological application from tractable in vitro measurements. These challenges are worth taking on because the quantitative power of electrochemical measurements would give critical insight.

#### New twists to a classical problem: corrosion

Despite being one of the most studied processes in electrochemistry, the prevention of corrosion remains a challenge<sup>39</sup> to the design of efficient and durable aircraft<sup>40</sup> or nuclear reactors.<sup>41</sup> Electrochemical methods are an invaluable tool to diagnose corrosion in situ, from mild environments, such 0.1M H<sub>2</sub>SO<sub>4</sub> at room temperature, to extreme ones, such as molten salts at temperatures as high as 850°C. In the latter, it is for instance emphasized that in-situ electrochemistry is the *only* in-situ method largely used in the literature capable of measuring corrosion kinetics with some confidence. During the panel discussion, it became clear that the lack of standardization in corrosion testing is highly detrimental to the field. Well-detailed experimental procedures are necessary since the volume of electrolyte, surface area of the working electrode, and materials used for containment, for instance, play a significant role in the observed properties. It was suggested to draw inspiration from other fields in electrochemistry, such as energy storage, where similar concerns applied to battery performance have led journals such as *ACS Energy Letters* to articulate checklists that enable standardization.<sup>42</sup> With similar guidelines, comparison of reports of corrosion testing and electrochemical methods would gain new value and allow meta-analyses of the literature towards materials code qualification.

Qualification is another topic attracting urgency in corrosion science, since it can take decades, a timescale that is incompatible with the need for advanced technology deployment to fight climate change, such as in the case of nuclear reactors. Thus, corrosion testing of materials must be accelerated in addition to being standardized. High-throughput corrosion testing of materials is at its infancy, but electrochemical methods are deemed extremely valuable because they can provide a large amount of data (e.g., oxide growth, dissolution, analyte diffusion coefficients) as a function of time. This approach is a significant departure from the "cook and look" approach. In that sense, electrochemical methods are compatible with a high-throughput approach towards the development of materials that resist corrosion. Further development of these approaches would greatly benefit this area of research.

### The emerging frontier of large data sets in electrochemistry

Research centered on data science was identified in several discussions as crucial to advancing electrochemical science. A typical experiment of *in vivo*, *in situ* or *operando* electrochemistry may only require a few hours of collection, but it might result in tens of thousands of data points in the form of complex outputs such as cyclic voltammograms, spectra or analytical profiles. High-throughput electrochemical characterization methods targeted at mapping corrosion conditions not only generate similarly daunting datasets, but they also cannot alone accelerate discovery of solutions. Other aspects of materials design, such as the exploration of molecular or electrocatalytic spaces with large compositional permutations, remain to be efficiently accelerated as well. The field of electrochemistry at large is ramping up automated methods for data analysis, but they are far from perfect.

Over the past 10 years, artificial intelligence and machine (AI/ML) learning have been increasingly incorporated into the scientific workflow, including in electrochemical applications.<sup>44</sup> AI/ML is often thought as a means to provide new insights into what materials could be interesting, but AI has potential use as a tool throughout the entire scientific process. AI is often used to automate data analysis for instance using clustering to reduce the overall number of diffraction patterns needed to analyze via Rietveld refinement or using image analysis tools to identify and count defects in electron micrographs.<sup>32</sup> Similarly, AI can be used as a method of circumventing expensive atomistic calculations, for instance using physically informed neural networks to generate interatomic potentials to facilitate molecular dynamics calculations.

In using AI for discovery, it is important to consider both the featurization of materials (the attributes that represent the composition, processing, and microstructure) and, in supervised AI techniques, the source of the data used for training. Attributes should, to the extent possible, contain physiochemical theories or heuristics relating composition/microstructure to more fundamental properties of the elements or microstructure. These theories, if incomplete or resource extensive to compute, can be approximated with a proxy ML model, although the results should be treated critically. The trained model can then be used to explore broader composition space to search for new interesting materials. It is important to keep in mind that most AI models do not extrapolate well, but also that extrapolation does not necessarily mean looking at new elements not inside the training data set provided the attributes capture the underlying physics. Rather, extrapolation can be thought of as choosing locations in a featured space where the underlying mechanism behind the emergent properties changes in a way that is not captured by the training set. However, with an appropriate materials representation even standard AI models can point the way to new exciting discoveries and provide correlations that spur scientists to identify new causal relationships. AI and so-called high-throughput experimentation (computation) have been demonstrated to synergize well together, in essence reducing the time spent for discovering new materials by more than 100x. More recently, there has been a move to place an AI-agent directly in control of automated experimental platforms for the autonomous discovery of new materials.<sup>45</sup>

It is easy to predict that methods of machine learning will increasingly be useful for mining the complex data resulting from our ambition to watch and direct electrochemistry in real time, at high spatial resolution or high throughput, thus processing and interpreting signals to identify compounds that have been detected or extract kinetic parameters. A special challenge is multianalyte detection, which may require algorithms to deconvolute signals from multiple chemicals. Beyond data analysis, machine learning might also advance new methodologies of analysis or prediction that are not possible today, such as to detect ambient levels of chemicals of interest and not just fast changes, as normally measured using fast-scan cyclic voltammetry, or to collect multidimensional images in real time.

### **Summary and Future Outlook**

Electrochemical science continues its expansion into a vast array of applications with potential for high societal impact. Over the past five years, NGenE has contributed to this expansion by providing budding researchers with a deep dive into the most pressing research questions and challenges. In 2021, our program showcased the pervasiveness of electrochemistry, but emphasized that the challenges have only increased in complexity because of our aspirations to control and monitor reactivity along chemical, temporal and spatial dimensions, across changes in scale of multiple orders of magnitude. By fostering a dialog across disciplines, electrochemists from different walks of life delineated common questions of interest, tackled through different approaches. Above all, the discussions highlighted that electrochemical science is ripe for cross-pollination, and that technological solutions depend on the vigorous exchange of information between disciplines. NGenE will continue to facilitate the exchange between generations, preserving interdisciplinary knowledge to leap forward to exciting outcomes. It is worth highlighting the deep interest NGenE participants expressed to learn how they can have an impact beyond simply generating knowledge in a vacuum. Impact on a worldwide issue such as energy requires multiple skills coming together, and the students fully embraced this responsibility for a broader impact. Our program highlights that educating the next generations demands more than what one can find in textbooks as well as recognizing that research today is more than what each of us knows by ourselves.

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#### Notes

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