New Materials for Tomorrows Energy Industry

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1. Introduction

Many of my posts start with a new material that accelerates an application. This is one of those posts. However, this post started by an Editorial in the May 17 issue of Science pointing out the need for new materials, so that is where we will start.

The decreasing cost of electricity worldwide from wind and solar energy, as well as that of end-use technologies such as electric vehicles, reflect substantial progress made toward replacing fossil fuels with alternative energy sources. But a full transition to clean energy can only be realized if numerous challenges are overcome. Many problems can be addressed through the discovery of new materials that improve the efficiency of energy production and consumption; reduce the need for scarce mineral resources; and support the production of green hydrogen, clean ammonia, and carbon-neutral hydrocarbon fuels. However, research and development of new energy-materials are not as aggressive as they should be to meet the demands of climate change.[1]

There are two major obstacles to the clean energy transition. Parts of the world's energy system can't be electrified, such as aviation, heavy freight transport, and shipping. Alternatives include hydrogen, ammonia, biofuels, or synthetic fuels, but current costs are far too high. As well, the growth of renewables—whose availability varies both daily and seasonally—demands changes in energy storage where global adoption is driven by cost savings rather than regulation and policy.

In the United States, a strategy is needed that integrates applied research, policy, financing, and infrastructure development to address these challenges. For example, despite progress in hydrogen production through electrolysis, there are commercialization obstacles. Iridium is a catalyst for the oxygen evolution reaction that is used to make hydrogen from water. However, iridium is rare and expensive, and is primarily sourced from South Africa and Russia, which poses geopolitical challenges. Any alternatives to iridium must not only match its performance and reliability but also be globally accessible and adopt more environmentally friendly mineral extraction practices. Speeding the discovery of new materials to replace iridium—as well as other elements used in catalysts, cathodes, electrolytes, and additives—requires increased investment across federal funding agencies.

Author's comment: We will start by addressing the challenge pointed out in the above paragraph in section 2 of this paper, but first let's finish the editorial (Reference 1).

[1] Chad A. Mirkin & Edward H. Sargent, Northwestern University and Daniel P. Schrag, Harvard University, Published in Science, May 17, 2024 Issue, "Energy transition needs new materials," https://www.science.org/doi/10.1126/science.adq3799

To expedite discovery, accelerating the synthesis and testing of candidate materials is vital. One approach involves creating "mega-libraries," microchips designed to simultaneously test millions of positionally encoded materials, generating vast amounts of data on material properties. These data should guide the identification of new technology-enabling materials. By learning from these datasets, artificial intelligence should predict promising material compositions faster than human researchers could through traditional experimentation.

Another component of a materials revolution is talent. Scientists, from students to researchers, must become sufficiently familiar with physics, chemistry, materials science, engineering, and computer science. This will require a new approach to education. One way forward is to develop graduate curricula in which students identify their own paths to acquire the skills and knowledge needed for their specific interests and innovative projects. Nations also need to ensure that scientists can relocate to collaborate on clean technologies. This may mean moving among the sites of R&D and discovery, commercialization, and manufacturing.

To achieve this acceleration in materials discovery, investment from industry is vital. Government support will continue to play a role, but private sector involvement is necessary to scale breakthroughs from the lab to commercialization. Establishing new kinds of partnerships between academia, industry, and government should be created that drive both innovation and deployment. Mission-oriented research, such as the design of new batteries and alternative liquid fuels, would be ideal training grounds for a new breed of scientist-engineer-entrepreneur. "Accelerator grants" from the public and private sectors that foster such activities will be essential.

Last year, global clean energy investments reached US$1.7 trillion, surpassing fossil energy investments by 70%. Yet this falls short of what is needed to mitigate the impacts of climate change. Governments must reimagine the innovation ecosystem for material discovery. As the world saw during the pandemic, lowering barriers for translating discoveries to products transformed vaccine development for the benefit of billions of people. Doing the same for clean energy materials will protect the planet, serving billions now and into the future.

2. Reducing the Demand for Iridium

As of today (early June) the market price of iridium is $171.51 per gram (about $78,000 per pound). Thus, using it as a major component in electrolysis systems that convert water to hydrogen and oxygen is a non-starter. There are two potential fixes for this: (1) replace the iridium with another material or (2) greatly reduce the amount of iridium that is used in the electrolyzer while maintaining the performance advantage that iridium brings. In other-words, effectively use the iridium as a catalyst for the catalyst while using much less expensive materials for a large majority of the latter.

The paper referenced below takes the second approach, and extracts from this paper explain this approach below.

Abstract: *Designing active and stable electrocatalysts with economic efficiency for acidic oxygen evolution reaction is essential for developing proton exchange membrane water electrolyzers. Herein, we report on a cobalt oxide incorporated with iridium single atoms (Ir-Co_3O_4), prepared by a mechanochemical approach… Theoretical calculations disclose the isolated Ir atoms can effectively boost the electronic conductivity and optimize the energy barrier. As a result, Ir-Co_3O_4 exhibits significantly higher mass activity and turnover frequency than those of benchmark IrO_2 in acidic conditions. Moreover, the catalyst preparation can be easily scaled up to gram-level per batch. The present approach highlights the concept of constructing single noble metal atoms incorporated cost-effective metal oxides catalysts for practical applications.*[2]

Author's comment: for the record, the market price of Cobalt (Co) is &12.44 per pound vs. about $78,000 per pound for iridium). Note that I have deleted the references for the paper below. Go through the link in reference 2 below to see the original paper with references.

2.1. Introduction

Centuries of industrialization and human activities have consumed enormous amounts of fossil fuels, which has inevitably led to the current energy crisis and global warming. Hydrogen (H_2) is considered a promising alternative energy carrier of the future owing to its high energy density and potential for carbon-free emission. Among many H_2 production methods, water electrolysis has received much attention as a feasible technology for practical applications. Nevertheless, due to the sluggish kinetics of the complex four-electron transfer process, the oxygen evolution reaction (OER) at the anode side of the water electrolyzer demonstrates high overpotentials, which severely limit the overall operation efficiency and impede the large commercialization of water electrolyzers. Therefore, tremendous effort has been devoted to the rational design of robust electrocatalysts which improve the OER activity and energy conversion efficiency.

Over the past few decades, the noble metal oxides based on iridium (Ir) and ruthenium (Ru) are considered the state-of-the-art OER electrocatalysts. However, their widespread applications are limited by the cost and scarcity of Ir and Ru. As a result, the first row 3d transition metal oxides and their derivatives, with merits of high abundance and low cost have received much attention as alternative OER candidates. Among all 3d transition metal oxides, cobalt-based oxides such as spinel Co_3O_4 have been widely used to activate OER activity, as demonstrated by both experimental data and theoretical calculations. Nevertheless, Co_3O_4 still suffers from an overpotential of more than 400 mV for the OER at a current density of 10 mA/cm^2, which is far from meeting the requirements for practical applications. Moreover, Co_3O_4 is unstable under the harsh OER conditions at the high oxidizing potential in corrosive media such as an acidic electrolyte. It is well known that the 4d/5d noble elements possess a large d-electronic wave-function spatial extent, generating versatile electronic structures via the interaction between 3d and 4d/5d orbitals, which is beneficial for enhancing OER activity.

[2] Yiming Zhu, Jiaao Wang, Toshinari Koketsu, Matthias Kroschel, Jin-Ming Chen, Su-Yang Hsu, Graeme Henkelman, Zhiwei Hu, Peter Strasser & Jiwei Ma; note that author's affiliations can be found through the link in this reference, This paper was published in Nature Communications on Dec 14, 2022, "Iridium single atoms incorporated in Co_3O_4 efficiently catalyze the oxygen evolution in acidic conditions," https://www.nature.com/articles/s41467-022-35426-8

One available method that has been frequently used is incorporating bulk amounts of noble metals with Co or its derivatives to obtain hybrid 3d/4d or 3d/5d nanomaterials as OER electrocatalysts. In this regard, Li et al. reported that the Sr_2CoIrO_6-δ, which benefits from a synergy between Co and Ir active sites, exhibits a low overpotential toward OER. Pi and co-workers also demonstrated that IrCo bimetallic nanoclusters can be employed as efficient OER electrocatalysts. In addition, Shah et al. developed a catalyst with single Co atoms doped on RuO_2 sphere, yielding remarkable catalytic performances for water splitting. Notwithstanding these efforts to modify Co-based nanomaterials as alternative OER catalysts, it remains difficult to tip the balance between low cost and high performance. Recently, the strategy of constructing highly dispersed single-sites catalysts has attracted significantly attentions for a range of electrocatalytic reactions. Downsizing the materials into isolated atoms is beneficial for reducing the amount of bulk metal, which can greatly maximize the atom-utilization efficiency, leading to remarkable catalytic mass activity. Additionally, the unique electronic structure of uniformly dispersed active sites usually results in a strong interaction with the host material, effectively adjusting the electrochemical microenvironment over catalysts and potentially boosting the electrocatalytic activity. Motivated by the abovementioned guidelines, the integration of spinel Co-based oxide with noble metal single atoms as the prospective OER electrocatalyst, possesses advantages of minimized noble metal usage and optimized catalytic performances. Nevertheless, the large lattice discrepancy between the diverse atoms and strong binding energy between the same atoms, are great challenges to disperse homogeneous noble metal single sites in the transition metal oxide host. And the production of traditional methods to prepare the single-atom materials such as impregnation are usually limited to milligram level, it is extremely urgent to explore a mass-production method to meet the requirements for practical applications.

In this work, we deploy a simple and economical strategy to prepare atomically dispersed Ir atoms doped in spinel Co_3O_4 (Ir-Co_3O_4) via a mechanochemical method. By introducing a trace amount of Ir (~1.05%), Ir-Co_3O_4 displays a remarkable OER overpotential of 236 mV in an acid medium at the current density of 10 mA/cm^2, which is significantly lower than that of as-prepared Co_3O_4 (412 mV). Significantly, the normalized mass activity of Ir-Co_3O_4 can reach almost two order magnitudes higher than that of commercial IrO_2 at an overpotential of 300 mV, respectively. Meanwhile, the stability can also be extended much longer after incorporating Ir single atoms within the lattice of Co_3O_4…

2.2. Results

In conclusion, the active Ir-Co_3O_4 OER catalyst was successfully synthesized via a facile and economical mechanochemical method. It was confirmed that isolated Ir single atoms are homogeneously dispersed in the Co_3O_4 host material. Consequently, OER measurement in acidic medium reveals that the overpotential of as-prepared Co_3O_4 (412 mV) sharply decreases to 236 mV by doping a trace amount of Ir atoms, and its long-term stability is prolonged. Notably, the normalized mass activity and TOF of Ir-Co_3O_4 are higher than those of commercial IrO_2. We recognize that the Ir single atoms are partially activated to higher valence under anodic voltages, simultaneously both Co and Ir atoms with their electrophilic O ligands served as active sites are synergistically responsible for charge transferring during OER process. The improved electronic conductivity and lower energy barrier towards OER by the electrophilic characters of oxygen ligands induced by high-valence Ir, boosting OER activity.

Additionally, in contrast to most traditional synthesis methods for single-atom catalysts, which are limited to milligram-level production, the Ir-Co_3O_4 preparation can be easily scaled up to gram-level production with negligible activity loss. This study highlights the rational design of a promising, cost-effective and energy-efficient catalyst for boosting oxygen evolution in the acidic medium, and this prototype would potentially stimulate industrial interest in a larger scale for practical applications.

Author's comment: The above text required heavy editing to reach a form that I could reasonably understand it. I'm sure that (at least) some readers will still have difficulty with it, but this is an important enough development, and will enable much more efficient hydrogen production, so I felt it was worth including in this paper.

3. New Methods for Material Discovery

This content also came from in the May 17 issue of Science. The excerpts from this article below are not about a specific material per se, but rather a process to produce a massive number of new materials that are designed to meet a specific application. In this case new materials for lasers.

Who needs scientists anyway? A global consortium of six automated laboratories, overseen by artificial intelligence (AI), set out to produce new laser materials, dividing the labor from synthesis to testing. The effort yielded a compound that emits laser light with record-setting efficiency. Along with other recent results, the feat suggests that, in some areas, self-driving labs can surpass the best scientists, making discoveries missed by humans.[3]

"Automated labs are going beyond proof-of-concept demonstrations," says Milad Abolhasani, a chemical engineer at North Carolina State University who developed a self-driving lab unaffiliated with the new work. "They have started to push the edge of science to the next level."

The allure of AI-driven labs for developing new drugs, industrial catalysts, and energy and emission-reduction technologies is clear. Creating new molecules and materials is normally slow and tedious. Researchers must explore not only myriad recipes for making molecules, but also different reaction conditions. They have to test new compounds at every step and evaluate schemes for scaling up production and assembling materials into devices.

Over the past decade, robots have begun to automate many of these repetitive steps. In 2015, for example, Martin Burke, a chemist at the University of Illinois Urbana-Champaign, unveiled an automated system for synthesizing small molecules (Science, 13 March 2015, p. 1190). Later, by incorporating AI, researchers added feedback loops, so data from newly characterized compounds could guide decisions on what to synthesize next (Science, 21 April 2023, p. 230). But discovering new materials and assembling them into devices requires robots to work in concert across even more steps, Burke says. "Nobody has all those tools and perspectives in one lab."

[3] Robert F. Service, Science Magazine, "AI-driven robots discover record-setting laser compound," May 17, 2024 Issue, https://www.science.org/content/article/no-humans-needed-ai-robots-discover-new-laser-materials-on-their-own Note that the title of the article linked is different than the title in this reference, but the content appears to be the same.

Author's comment: Note that I covered the subject of this section in an earlier post, summarized and linked below, which describes the techniques used in this section.

Betty Crocker It Is Not: *I just started a paper with the following words: "Many of my papers start with a chemists identifying a material that performs a particular function much more effectively than the incumbent material."*

I completed the first draft of the above-mentioned paper, and started reading my latest issue of Science Magazine, and encountered a new technology that will substantially accelerate the development of these new compounds.

Imagine a cookbook with 150,000 tempting dishes—but few recipes for making them. That's the challenge facing an effort at the Lawrence Berkeley National Laboratory (LBNL) known as the Materials Project. It has used computers to predict some 150,000 new materials that could improve devices such as battery electrodes and catalysts. But the database's users around the globe have managed to make just a fraction of these for testing, leaving thousands untried.

Now, LBNL has married artificial intelligence (AI) and robotics to eliminate that bottleneck. The AI system makes a best guess at a recipe for a desired material and then iterates the reaction conditions as robots try to create physical samples. The new setup, known as the A-Lab, is already synthesizing about 100 times more new materials per day than humans in the lab can manage…

https://energycentral.com/c/ec/betty-crocker-it-not

Back to reference 3.

Burke and Alán Aspuru-Guzik, a theoretical chemist at the University of Toronto, thought they could unite these disparate functions, hosted in different labs. "We thought, let's make a self-driving lab made of self-driving labs," Aspuru-Guzik says.

So, the duo teamed up with labs at the Institute for Basic Science in South Korea, the University of Glasgow, the University of British Columbia (UBC), and Kyushu University to focus on a specific goal: discovering organic compounds that can emit highly pure laser light. Such materials could power advanced displays and telecommunications devices because they can be made into thin, flexible, light-emitting films. But despite more than a decade of work in the field, only about a dozen candidate organic laser emitters have been discovered.

To start, the Glasgow and UBC labs made sugar cube–size quantities of building blocks for the materials. These colored powders were packaged up and sent to Burke's and Aspuru-Guzik's groups, where robots knitted them in different combinations into candidate emitters. All of those were passed to Toronto, where other robots characterized their light-emitting properties in solution. For the best ones, the UBC lab determined how to synthesize and purify the larger quantities needed for making devices. In batches of a few grams, the materials were then shipped to Japan, where the Kyushu lab incorporated them into working lasers and tested their properties.

The whole operation was overseen by a cloud-based AI platform designed primarily by the teams in Toronto and South Korea to learn from each experiment and incorporate feedback into subsequent iterations. "It was almost like a symphony," says Lee Cronin, who leads the lab in Glasgow. The main hurdle became shipping compounds around the world in time. "FedEx became the bottleneck," Burke says.

The collaboration paid off. The effort produced 621 new compounds, including 21 that rivaled state-of-the-art laser emitters and one that emits blue laser light more efficiently than any other organic material. "It's really impressive to make all of these different components work together," says Philippe Schwaller, an expert in self-driving labs at the Swiss Federal Institute of Technology. And the pace of discoveries was "fantastic," says Donna Blackmond, a chemical engineer at Scripps Research. "Their methods got them to the good candidates much faster than usual," she says.

It's not the only recent success. Last year, for example, Abolhasani's lab reported creating nanoparticles of so-called perovskite minerals that showed record-setting photoluminescence, a property that can identify materials likely to work well in solar cells. And in a preprint posted last year on ChemRxiv, Burke's team reported an AI setup that not only synthesized a bevy of new light-harvesting compounds, but also revealed what made them stable rather than prone to rapid breakdown, offering a rare glimpse of how an AI—normally a black box—made its decisions.

Burke hopes that advances in automation and AI will allow more and more labs to join forces. "That's something we desperately need," he says. It might ultimately allow scientists to stop pursuing robotic tasks and become robot overlords.

4. Other Examples of Material Breakthroughs

The following earlier three posts and referenced sections contain other examples of recent material advances using innovative methods. All from mobility industries.

4.1. NREL's Battery Breakthroughs

See section 3 of the following paper:

Transportation Decarbonization & NREL's Battery Breakthroughs: Our modern transportation systems are both a benefit and a hindrance for today's civilizations. They are a benefit in that they enable many more activities that would be impossible in the past. During my career, I traveled all over the world helping electric utilities automate their processes and collaborating with peers. Without modern international air travel this would not be possible.

The hinderance for the world's economies is, the transportation systems are the single largest emitter of greenhouse gas, and thus a primary driver of climate change. The world's economies need to decorbamize these systems ASAP.

https://energycentral.com/c/cp/transportation-decarbonization-nrel%E2%80%99s-battery-breakthroughs

4.2. Niron Iron-Nitride Permanent Magnets

Any vehicle (road, marine, air, tracked) that uses electricity as its energy source, regardless whether it's from batteries fuel-cells, etc., probably uses electric motors to convert the electricity into motion. The earlier paper below, subsection 2.5 describes a highly efficient electric motor that doesn't use rare-earth materials and thus is much less expensive than motors that use rare earth metals.

EV Motors without Rare Earth Metals? A large majority of current road-going electric vehicles use two new technologies. One is Lithium-Ion Batteries, and the other is electric traction motors. I've written about the former extensively, and my recent major paper on these is described and linked in this paper.

I have also written about EV motors, but not recently. This post will fix this tardiness.

Like Lithium-Ion Batteries, traction motors have a materials problem, rare-earth metals. There is no question that the lightest, most efficient, most long-lived motors use rare-earth metals, mainly by using neodymium-iron-boron permanent-magnets. Neodymium is the rare earth element here, but boron is also increasing in price. However, the post linked below has some potential solutions to the rare-earth metal problem.

https://energycentral.com/c/rm/ev-motors-without-rare-earth-metals

4.3. Sustainable Aviation Fuel

The most rapid method of converting existing (or future) vehicles to sustainable operation is to use zero-carbon fuel. However, as described in section 3 of the earlier post summarized and linked below, this is a really tough road, even when the road is in the air.

Fast and Sustainable: I write about all types of mobility. That includes aviation and even space-travel. This post is about two parts of the aviation industry, and I've written about one previously, but not about the other. The latter is what may be the first supersonic airliner to enter service in the U.S.

…Boom Supersonic, a private company based in Colorado, aims to bring commercial supersonic flights back to US airlines by 2029. When completed, its passenger aircraft, Overture, is expected to fly at speeds up to Mach 1.7, which is about 1,300 miles per hour—or twice as fast as today's passenger planes.

The former part of the aviation industry is Sustainable Aviation-Fuels (hereafter SAF). I wrote about this most recently (Aug. 2023) in a post referenced in the paper linked below.

https://energycentral.com/c/ec/fast-and-sustainable