對外合作組織與機構 動態報導

2018/2/9

STUDY OF SALTS IN WATER CAUSING STIR

鹽在水中引起的騷動

February 1, 2018

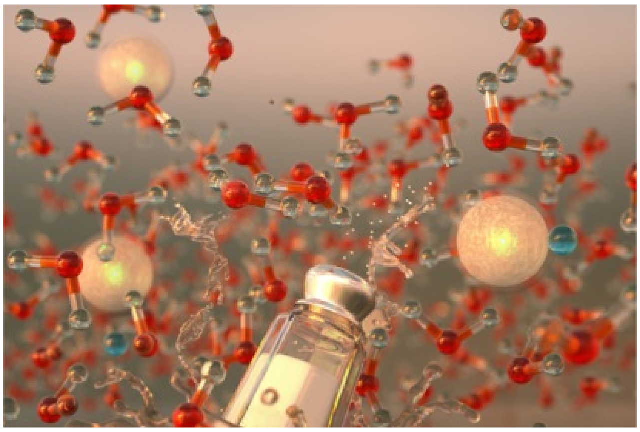
New insight into science that seems, on its surface, exceedingly simple — what happens when you add salt to water — could ultimately lead to a better understanding of biochemical processes in cells and perhaps advance sources of clean energy.

An article published in the *Journal of Physical Chemistry Letters* on that topic earlier in 2017 has generated considerable interest, according

報告摘要(KEY INFORMATION)

1. 有些科學洞見看似簡單，卻能帶領我們深入瞭解細胞中的生化反應，進而開發新藥物，或者推動乾淨能源的研究。這樣的洞見只發源自一個問題：當在水中加入鹽會發生什麼，鹽水中的離子能影響水體中多大範圍的結構？
2. 阿岡國家實驗室 ReCell 計畫負責人表示，阿岡現已拓展長久以來在電池研發方面的專長，深入檢視製造至回收的一系列環節，未來將為該產業注入活力，以期有一日能精確控制電池生命週期所產生的成本，使對環境與經濟造成的影響降到最低。
3. 2018 年，要完善電力收購制度尚須許多建議及調整，包含如何改善競價系統、如何回應電網連接限制，以及如何保持生質能發電的永續性。
4. 依國際協商，巴黎協定之執行規則手冊(the rulebook for implementing the Paris Agreement)原預期於締約方第 24 屆會議 (COP24)前完成。然而，待討論的重要議題不少，包含開發中國家在財政適應與減少碳排之間如何取得平衡，以及 2020 年前後的行動目標，目前看來要於 COP24 前完成巴黎協定執行手冊顯有難度。
5. 全世界許多私人公司、政府單位和機構組織，都漸漸改以 AI 取代人類決策。一般認為，演算法的決策比人類更有效率且客觀公平，但它真的能藉已知資訊做出最佳化決策嗎？確實，人會受到許多偏誤影響，但人腦的決策可以考量眾多複雜因素，而 AI 只能依照已知事件的資料進行運算。

to the journal's editors. The article was written by Giulia Galli, a Liew Family Professor in Molecular Engineering at the University of Chicago who has a joint appointment at the U.S. Department of Energy's (DOE) Argonne National Laboratory, and Alex Gaiduk, a Natural Sciences and Engineering Research Council of Canada postdoctoral fellow at the University of Chicago.



"One of the questions that has puzzled researchers for decades is how far ions affect the structure of saline water, the same kind of solutions that are present in our bodies," said Gaiduk, a chemist and theorist. One popular view is that ions have a local effect on the structure of water, causing hydrogen bonds to form or break only close to the ion. But it seems that isn't always the case.

"The reason this problem was still open is that experiments do not provide direct detailed information about the structure of the liquid at the molecular level," Gaiduk said. "Instead, they provide averaged information coming from the entire molecular system, which is often hard to interpret."

Meanwhile, molecular simulations provide first-hand information about the molecular structure of the liquid and can shed light on the ions' influence on the water structure. Determined to answer these questions, Gaiduk and Galli turned to the Argonne Leadership Computing Facility (ALCF), a DOE Office of Science User Facility capable of carrying out simulations that require massive computational capabilities — 10 to 100 times more powerful than those of systems typically used for scientific research.

Gaiduk and Galli used the ALCF to simulate sodium chloride in water, and gathered extensive amounts of data. They analyzed the results and discovered that the sodium ion indeed has only a local effect on water structure, while the chlorine ion has a farther-reaching effect, modifying the water structure at least up to a nanometer away from the ion. (A nanometer is one-billionth of a meter.)

"We have provided important information about the structure of water in the presence of dissolved salts — namely that some ions, including chloride, have a long-range effect while others, such as sodium, do not," Gaiduk said. "We used non-empirical simulation methods and a rather sophisticated choice of molecular signatures of the water structure."

The research provides a new fundamental understanding of sodium chloride in water. This is one of the aqueous systems used in photoelectrochemical cells. These cells are used to split water into hydrogen and oxygen, a technology that has long-term potential as a clean energy source. Additional research will be required to determine how this new understanding might be used to improve the technology, Galli said.

Their finding could also prove valuable for biochemistry on a number of fronts.

"Processes like protein folding, crystallization and solubility are at the core of all biological and biochemical processes that essentially define life," said Gaiduk, adding that this finding may contribute to explaining the solubility of proteins. "Scientists can now perhaps develop new computational models to describe biochemical processes in cells, and this could lead to the development of new drugs."

However, the authors concluded that the subtle modifications of the structure of water by the ions — even chlorine — are probably insufficient to explain the different solubility of biomolecules in pure and salty water. Clearly researchers have more work to do before they can fully understand and model interactions of ions with the functional groups of proteins. However, this technique for analyzing the hydrogen bond network of water is a first step to help scientists understand how the structure of water changes with the addition of salt.

Using the results obtained by Gaiduk and Galli, another research group has developed a new model that correctly describes the effect of ions on the structure of water. Their findings are detailed in the Aug. 31, 2017 issue of the *Journal of Physical Chemistry B*.

Funding for the work by Gaiduk and Galli was provided by DOE's Office of Science, Basic Energy Sciences, through the Midwest Integrated Center for Computational Materials and the Natural Sciences and Engineering Research Council of Canada. Computer time was provided by the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program.

CLOSING THE LOOP ON BATTERY RECYCLING

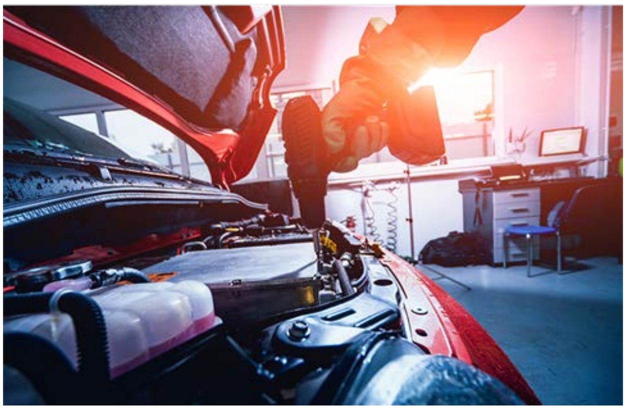
電池回收終結者

January 25, 2018

A novel model developed at the U.S. Department of Energy's (DOE) Argonne National Laboratory allows industry, the Department and others to gauge the impact of recycling batteries in electric vehicles. It could further energize this market.

"Argonne has a long track record of expertise in battery research and development, and now we have added the ability to examine every step along the way, from manufacturing to recycling," said Argonne's Jeff Spangenberger, the project leader.

From cathodes to anodes and electrolytes, Argonne's understanding of batteries, combined with ReCell, a closed-loop battery recycling model, offers preliminary estimates of total costs as well as environmental impacts such as carbon dioxide emissions. The model breaks down each process from when a battery leaves the factory to when it is recycled.



Argonne's ReCell model can provide information to manufacturers up front, so those manufacturers can determine life cycle costs with precision and provide batteries to consumers with minimal environmental and economic impacts. Argonne's researchers have designed ReCell to be versatile and adapt to the challenges that recycling of lithium ion batteries present, such as differing battery chemistries and formats.

"ReCell helps determine where we need to focus our efforts. This results in more efficient research and expedites the process of reaching our life cycle, or circular, goal," said Spangenberger, who is also a recent recipient of a DOE Technology Commercialization Fund award.

The model includes three basic recycling technologies:

- Extracting metals with heat (pyrometallurgical)
- Extracting metals with liquids (hydrometallurgical)
- Direct recycling

Preliminary findings estimate that a cell with a recycled cathode could cost 5 percent, 20 percent and 30 percent less than a new cell using pyrometallurgy, hydrometallurgy and direct recycling routes, respectively, according to estimates from Argonne's Greenhouse gases, Regulated Emissions and Energy use in Transportation (GREET) model recycling parameters. That same cell could consume 10 percent, 20 percent and 30 percent less energy, respectively.

Additionally, the model considers transportation-related cost and environmental factors, which can help steer the development of a recycling infrastructure. For instance, is it more effective to have one large central recycling center or several smaller centers located throughout the country? Preliminary results from the ReCell model show how a simple change in shipping classification for end-of-life batteries could potentially change a recycled cathode's cost from 30 percent less than a new cathode to one that only breaks even.

Information provided by ReCell will become increasingly important as thousands of batteries from vehicles sold over the last decade reach their end of life, according to Spangenberger, who added that plug-in electric vehicle (PEV) sales in the U.S. more than doubled in the last four years. Currently, PEVs comprise only 1 percent of new vehicle sales. But by 2025, annual sales of PEVs will exceed 1.2 million vehicles, reaching more than 7 percent of annual vehicle sales.

The model, developed by Spangenberger and Qiang Dai, an Argonne postdoctoral fellow, also incorporates the work of Linda Gaines, a transportation systems analyst and battery recycling expert. This work, Gaines noted, could also help extend limited supplies of lithium, cobalt and other valuable elements. Ultimately, it could also reduce U.S. dependence on foreign resources and enhance national security.

ReCell leverages Argonne's patented GREET life-cycle model and Battery Performance and Cost, or BatPaC, a lithium-ion battery performance and cost model for electric-drive vehicles.

GREET, developed by Michael Wang and his team, is a free program that allows users to analyze technologies over an entire life cycle — from well to wheels — and from raw material mining to vehicle disposal.

BatPaC, developed by Paul Nelson, is also a free program that captures the interplay between design and cost of lithium-ion batteries for transportation applications.

ReCell initially received support from Argonne's Laboratory Directed Research and Development program. The DOE Office of Energy Efficiency and Renewable Energy's (EERE) Vehicle Technologies Office is funding the current work.

RENEWABLE ENERGIES

可再生能源近況

By Yoshiaki Shibata

2017 was the first year of the FIT system reform. Several measures were implemented to control the increasing burden of the surcharge, including introducing a bid system for mega solar PV and setting a multi-year schedule for lowering the purchase price of other renewable energies. Still, problems remain.

First, regarding the bidding system, the first feed-in-tariff bidding was held in Japan in November for solar PV capacities of 2 MW and more. However, there was no real competition as only 141 MW of capacity was offered for bidding against a total bidding amount of 500 MW, and all offered capacities were sold. The lowest successful bidding price was 17.2 yen/kWh but the highest was 21 yen/kWh, which is the upper price limit. The lack of competition was inevitable because the shortage of offered capacities was due to the "experimental" nature of the bid and insufficient preparation period for this first attempt. These issues will need to be resolved in the second bid in FY 2018.

However, some fundamental issues of the system were also revealed. The main issue is that the deposit to participate in the bidding will be confiscated unless a grid connection contract is signed for the purchased capacity within three months, and also that there is no spare space in the power grid for connections. Such uncertainty in grid connection is a risk for operators and deters them from participating in the bidding. In Japan, renewable generation equipment is connected to the grid, within the then-available capacity, on a first-come-first-served basis, and this is becoming a barrier. Consequently, the bid highlighted the need for "Connect & Manage," a mechanism introduced in Europe and the US in which a renewable energy operator is allowed to connect to the grid only if it accepts output restrictions when the grid is congested.

Second, regarding biomass power, its licensed capacity has soared to 14 GW as of September 2017 due to last-minute demand triggered by a fall in the purchase price for general wood and crop residue. This is an enormous leap from 4 GW in March 2016.

Many of these projects are yet to secure sources for fuel and funds, and some estimate that only around 20% of licensed projects that have not yet started, will actually do so. An increase in nonperforming projects also occurred with mega solar PV a few years ago, and measures such as license cancellation had to be taken. A government council is set to meet shortly to discuss countermeasures such as revising already decided purchase prices and introducing a bid system. Other issues have been pointed out for biomass power since last year, such as its high dependence on imports and uncertainty in continuing business after the purchase period ends. In addition to the actions recently implemented, further institutional revisions are required for biomass power.

In 2018, adjustment and revision of the FIT system will continue to be required, including improving the bid system, responding to grid connection constraints, and the sustainability of biomass power.

UPDATE ON POLICIES RELATED TO CLIMATE CHANGE

氣候變遷相關政策近況

By Takahiko Tagami

Regarding international negotiations, the rulebook for implementing the Paris Agreement is scheduled to be completed by the twenty-fourth session of the Conference of the Parties to the UNFCCC (COP24). However, with so many outstanding issues, including developing countries’ insistence on a balance between finance/adaptation and mitigation (reduction) and between pre- and post-2020 actions, it appears difficult to complete the work in time for COP24 scheduled for 2018.

In the United States, the procedure for repealing the Obama administration's Clean Power Plan (a regulation to reduce emissions from existing power plants) has begun. The repeal, however, is not expected to have a significant impact on the emission situation in 2018, as several states are preparing to file lawsuits, and state-level policies on renewables and energy conservation will continue to be implemented. The US has submitted a communication to the UN to withdraw from the Paris Agreement, but has also stated that the country will continue to participate in international climate change negotiations and meetings to protect its interests and ensure that all future policy options remain open to the administration, and has participated in COP23. The impact of the US's withdrawal announcement on international climate change negotiations should be limited in the near term.

China's National Emissions Trading Scheme was scheduled to start in 2017 but an official announcement had been delayed due to doubts about the credibility of statistical data. On December 19, 2017, the emissions trading scheme for only the power sector was announced, without specifying a date. The shape of the scheme leading up to 2020 should be monitored. Further, the government has required automobile manufacturers to ensure that a certain percentage of their production are new energy vehicles (electric vehicles (EVs), fuel cell vehicles, plug-in hybrids, etc.), and has announced a credit trading system to maintain compliance. Attention must be paid to the future of China's strategy to develop its green low-carbon industry, such as EVs.

The EU's targets for 2030 appear difficult to meet, unlike those for 2020. Under such circumstances, in 2018, full-scale coordination is expected to start with the European Parliament and the Council over the revised Emissions Trading Scheme (ETS) Directive , Effort Sharing Regulation regarding non-ETS sectors, and revised Energy Efficiency Directive.

While the US and the EU are revising their car fuel economy standards, it is noteworthy that China and India have embarked on schemes and support measures for EVs. With France and the UK announcing plans to eventually prohibit the sale of internal combustion engine vehicles, the moves of various countries concerning the promotion and expansion of EVs and other advanced vehicles must be watched.

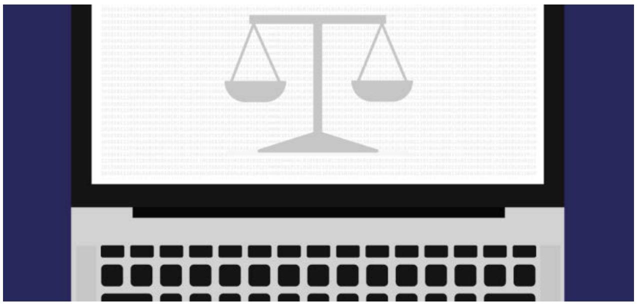
In Japan, government councils are discussing such topics as the challenges in achieving the FY2030 emissions reduction target, designing a non-fossil-value trading market to achieve the target non-fossil power ratio of at least 44%, the progress in achieving the thermal power efficiency indices under the Energy Conservation Act, the long-term strategy toward 2050, and the policy on carbon pricing (carbon tax, etc.). Developments in these discussions must be closely monitored.

WHICH IS MORE FAIR: A HUMAN OR A MACHINE?

AI 和人類相比，誰較公正？

January 31 By Tom Abate and Marina Krakovsky

Companies, governments and organizations all over the world use artificial intelligence to help make decisions that were formerly left to human judgment.



Their expectation: that the algorithms underpinning AI are more efficient and more fair than is humanly possible.

But how do humans and machines compare in terms of fairness; that is, making the optimal decision given the available information? Turns out science can't say for sure. Humans are prone to all sorts of biases, but algorithms have their own challenges.

These begin with how algorithms are trained, by feeding them "labeled" data. To train a computer to spot the difference between cats and dogs, for instance, the system is fed pictures labeled "cat" or "dog" until the algorithm is able to make that distinction on unlabeled pictures. It's trickier, however, to train computational systems to perform tasks that require human judgment.

Machine learning specialists can find examples of past decisions made by humans and feed these to an algorithm, but we can only feed computers information about known outcomes.

We can't know what would have happened if the decision had gone the other way. Computer scientists call this the problem of "selective labeling."

There is a second challenge to training computational systems to make judgments: There may be no way to know all the factors that influenced the human decision makers whose past actions were presented to the algorithm. Computer scientists call this the problem of "unobserved information."

Computer scientists have known of these two related challenges and tried to take them into account. But in a new paper, Jure Leskovec, associate professor of computer science, and collaborators propose a new approach to this training conundrum: Study the track records of the human decision makers whose past examples will be part of the training mix, and choose those whose past decisions seem to have the desired, if fuzzy, outcome, such as fairness

Hima Lakkaraju, a PhD student in computer science at Stanford, worked with Leskovec on this new approach, which they devised during the course of co-authoring a scientific paper about a situation where selective labeling and unobserved information occurs: the process of granting or denying bail to a defendant charged with a crime and awaiting trial.

Such decisions have historically been made by judges, but in recent years also by algorithms, with the goal of helping to make the system fairer and thus better better and thus fairer. By law, defendants are presumed innocent until proven guilty, and bail is generally granted unless the defendant is deemed a flight risk or a danger to the public.

But deciding whether to grant bail is more complicated than distinguishing between cats and dogs. The training system still has to show the algorithm past decisions made by humans. Trainers can label whether the defendants granted bail by a human judge appeared in court or skipped town. But there is no label to identify the defendants who were denied bail and put in jail but would have broken bail had they been set free. Put another way, labeled outcomes are selective: more likely to exist for some defendants than for others.

Likewise, human judges may be influenced by variables that seem reasonable but can't be recorded by the training materials. Leskovec offered the example of a judge who makes a mental note of whether the defendant's family appears in court to show support. But the training system may not capture this unobserved information that played a critical part in the judge's decision. Algorithms will never record all the "soft" information available to judges, so how could algorithms perform better/fairer decisions?

Leskovec and collaborators propose to take what seems like a problem—the variability and opaqueness of human judgment—and make it an input of the training system. Their method harnesses the natural variability between human judges to train systems using the judgments from the most lenient humans, and then challenging algorithms to do better. By learning from the most lenient judges, who release the most defendants, the algorithms are able to discover rules that lead to better/fairer decisions.

In addition to bail-setting, the researchers believe this methodology could be applied in other judgment-based scenarios; for example:

- **Banking.** Here, increasing the level of fairness might involve efforts to train AI to prevent redlining poor neighborhoods. That's the term for the illegal but prevalent practice of avoiding low-income areas because of a real or perceived elevated risk of default. Applying the Stanford fix, AI trainers might search out successful examples of profitable lending in low-income areas and use this to train algorithms.

- **Medicine.** Patients visit doctors complaining of wheezing and coughing. Doctors must decide whether the symptoms are mild enough to send the patient home without prescribing a powerful and costly asthma drug. The labeled outcome is whether the patient gets better after the mild treatment—or comes back with an asthma attack within two weeks. But information about outcomes is not available for people for whom the doctor made the choice to prescribe the powerful drug. In this instance, increasing the level of fairness might include new ways of looking into the record to find doctors with great track records in this regard.
- **Education.** In some school districts, teachers can decide whether to assign a struggling student to a remedial program or other educational intervention. Although we can see the outcome of a student assigned to the intervention, we can't see whether other students, who were not candidates for interventions, would have done better with the extra assist—a problem of selective labeling. Again, making this fairer would mean looking more carefully at the training examples to make sure that the algorithm is being fed the best examples.

The common denominator in these examples is that the decision makers' deliberate choices determine which outcomes are known.

Jure Leskovec, associate professor of computer science.

"Let's devise ways to give proven decision makers additional weight in teaching machines," Leskovec said. "It's a way to bake best practices into the AI systems."