對外合作組織與機構動態報導

2018/1/26

ELECTRONS IN THE WATER

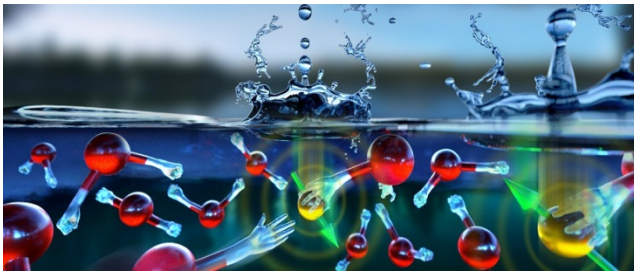
水中的電子

January 19, 2018

It's a popular tradition to throw coins into fountains in the hopes of having wishes granted. But what would happen if you could “throw” electrons into the water instead? That is, what happens shortly after an electron is injected into water?

報告摘要(KEY INFORMATION)

1. 若將電子丟入水中，會產生什麼變化？要模擬電子在固體、液體中轉移的過程，關鍵是瞭解電子對水的親和性。芝加哥大學與美國國家能源部的研究人員合力探討「液體是否會立即與電子鍵結」的問題，發現在水體及水面的親合度有所不同。該結果可能影響水性質相關研究與水溶液之氧還反應研究等領域。
2. 阿岡國家實驗室率領的研究團隊藉中子的特性探測金屬中的電子，對材料有了新的瞭解。研究者表示：我們認為，許多金屬中負責導電的移動電子，其獨立運動幾乎不受電子與電子間的斥力影響。然而有一類型的材料，其電子與電子間的作用力強到不可忽略，在高溫時，這類材料中的電子作用力會產生隨機變動，並妨礙導電。
3. 隨著可再生能源發電之新興，一直以來作為尖峰發電供應的石油火力發電，佔比正逐漸下降。目前日本電力現價大部分的價格波動都由石油火力發電決定；然而，在 2018 會計年度中，液化石油氣和碳火力發電對價格的影響將逐漸增幅。
4. 2018 年國際石油局勢的關鍵，在於美國頁岩石油氣產量提升的程度，OPEC 與非 OPEC 國家於六月聯合減產的情況，以及中東、委內瑞拉的情勢變化。預計 2018 年國際平均油價（以 Brent 原油而言）將落在每桶 65 美元左右。
5. 對於科學家和一般熱愛自然的人來說，生物體的發育是一個直觀且迷人的問題。在 19 世紀時曾有一些精巧的實驗，但原理始終撲朔迷離，一直到近五十年基因體學與分子生物學才給出接近的答案。今日，機械生物學結合新的儀器與構想，將使我們進一步瞭解生物體的構成，並期待有朝一日能重塑軀體。



This decades-old question now has an answer, thanks to an article published in Nature Communications on January 16. The study is the result of collaboration among researchers at the University of Chicago, the U.S. Department of Energy's (DOE) Argonne and Lawrence Livermore National Laboratories, and the University of California — San Diego.

"Knowing the electron affinity of liquid water is crucial to understanding and modeling processes involving electron transfer between solids and the liquid, ... " — Alex Gaiduk, postdoctoral fellow at the University of Chicago.

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Until now, scientists faced technical challenges when they wanted to experimentally measure the electron affinity of water, said Professor Giulia Galli, Liew Family Professor at the Institute for Molecular Engineering at the University of Chicago and senior scientist at Argonne.

"Most of the results quoted in the literature as experimental numbers are actually values obtained by combining some measured quantities with crude theoretical estimates," she said.

Accurate theoretical measurements, on the other hand, have been out of reach for some time due to the difficulty and high computational cost of simulating the interactions directly, said University of California-San Diego professor Francesco Paesani, a co-author of the study who has spent years developing an accurate potential for the modeling of liquid water.

The interaction potential between water molecules developed by Paesani was used to model the structure of both liquid water and the water's surface. Once the structure was obtained, highly accurate theoretical methods and software to study excited states of matter, developed by Galli's team, were used to understand what happens when an electron is injected into water.

Fundamentally, the researchers sought to understand whether the electron resides in the liquid and eventually participates in chemical reactions. The central question was, "Does the liquid bond with the electron right away?"

The researchers found that the electron binds with the water; however, its binding energy is much smaller than previously thought. This prompted the researchers to revisit a number of well-accepted data and models for the electron affinity of water.

Galli and her co-workers developed the methods for excited states used in this study

over the years, in collaborations with T. A. Pham, from Lawrence Livermore, and Marco Govoni, from Argonne, both of whom are co-authors of this study.

"Using the software developed to study excited state phenomena in realistic systems (named Without Empty STates, or WEST) and the Argonne Leadership Computing Facility (ALCF), we were finally able to generate data for samples both large enough and on sufficiently long timescales to study the electron affinity of liquid water," Govoni said.

"We found large differences between the affinity at the surface and in the bulk liquid. We also found values that were different from those accepted in the literature, which prompted us to revisit the full energy diagram of an electron in water," Pham added.

This finding has important consequences, both for scientists who seek to fundamentally understand the properties of water and for those who want to describe reduction/oxidation reactions in aqueous solutions, which are widespread in chemistry and biology.

In particular, scientists often use information about the energy levels of water when they screen materials for photo-electrochemical cells. A reliable estimate of the water electron affinity (which the researchers of the study provided for both bulk water and its surface) will help scientists establish computational protocols that are more robust and more reliable, and improve computational screening of materials.

Funding for the work by Gaiduk and co-workers was provided by the DOE Office of Science through the Midwest Integrated Center for Computational Materials. Additional support was provided by the Natural Sciences and Engineering Research Council of Canada, the National Science Foundation and the Lawrence Fellowship. The researchers used the ALCF, a DOE Office of Science User Facility, for the study. Computer time was provided by the Innovative and Novel Computational Impact on Theory and Experiment (INCITE), Extreme Science and Engineering Discovery Environment (XSEDE) and Lawrence Livermore National Laboratory Grand Challenge programs.

BREAKING BAD METALS WITH NEUTRONS

用中子破解壞金屬

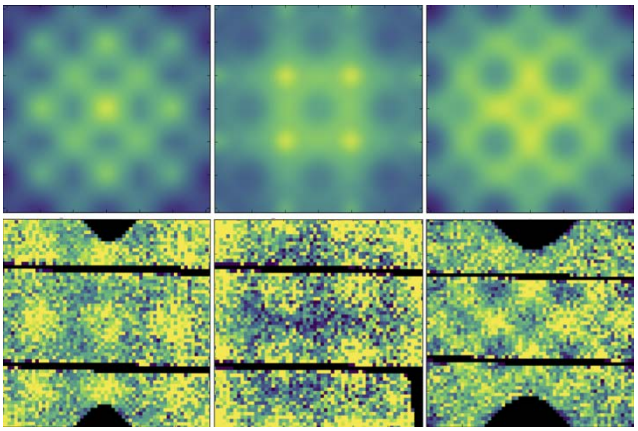
By Ron Walli • January 11, 2018

By exploiting the properties of neutrons to probe electrons in a metal, a team of researchers led by the U.S. Department of Energy's (DOE) Argonne National Laboratory has gained new insight into the behavior of correlated electron systems, which are materials that have useful properties such as magnetism or superconductivity.

The research, to be published in *Science*, shows how well scientists can predict the properties and functionality of materials

allowing us to explore their potential to be used in novel ways.

"How do you get to a stage where the models are reliable? This paper shows that we can now theoretically model even extremely complex systems. These techniques could accelerate our discovery of new materials." — Ray Osborn, Argonne senior scientist



"Our mission from the Department of Energy is to discover and then understand novel materials that could form the basis for completely new applications," said lead author Ray Osborn, a senior scientist in Argonne's Neutron and X-ray Scattering Group.

Osborn and his colleagues studied a strongly correlated electron system ($CePd_3$) using neutron scattering to overcome the limitations of other techniques and reveal how the compound's electrical properties change at high and low temperatures. Osborn expects the results to inspire similar research.

"Being able to predict with confidence the behavior of electrons as temperatures change should encourage a much more ambitious coupling of experimental results and models than has been previously attempted," Osborn said.

"In many metals, we consider the mobile electrons responsible for electrical conduction as moving independently of each other, only weakly affected by electron-electron repulsion," he said. "However, there is an important class of materials in which electron-electron interactions are so strong they cannot be ignored."

Scientists have studied these strongly correlated electron systems for more than five decades, and one of the most important theoretical predictions is that at high temperatures the electron interactions cause random fluctuations that impede their mobility.

"They become 'bad' metals," Osborn said. However, at low temperatures, the electronic excitations start to resemble those of normal metals, but with much-reduced electron velocities.

The existence of this crossover from incoherent random fluctuations at high temperature to coherent electronic states at low temperature had been postulated in 1985 by one of the co-authors, Jon Lawrence, a professor at the University of California, Irvine. Although there is some evidence for it in photoemission experiments, Argonne co-author Stephan Rosenkranz noted that it is very difficult to compare these measurements with realistic theoretical calculations because

there are too many uncertainties in modeling the experimental intensities.

The team, based mainly at Argonne and other DOE laboratories, showed that neutrons probe the electrons in a different way that overcomes the limitations of photoemission spectroscopy and other techniques.

Making this work possible are advances in neutron spectroscopy at DOE's Spallation Neutron Source (SNS) at Oak Ridge National Laboratory, a DOE Office of Science User Facility, and the United Kingdom's ISIS Pulsed Neutron Source, which allow comprehensive measurements over a wide range of energies and momentum transfers. Both played critical roles in this study.

"Neutrons are absolutely essential for this research," Osborn said. "Neutron scattering is the only technique that is sensitive to the whole spectrum of electronic fluctuations in four dimensions of momentum and energy, and the only technique that can be reliably compared to realistic theoretical calculations on an absolute intensity scale."

With this study, these four-dimensional measurements have now been directly compared to calculations using new computational techniques specially developed for strongly correlated electron systems. The technique, known as Dynamical Mean Field Theory, defines a way of calculating electronic properties that include strong electron-electron interactions.

Osborn acknowledged the contributions of Eugene Goremychkin, a former Argonne scientist who led the data analysis, and Argonne theorist Hyowon Park, who performed the calculations. The agreement between theory and experiments was "truly remarkable," Osborn said.

Looking ahead, researchers are optimistic about closing the gap between the results of condensed matter physics experiments and theoretical models.

"How do you get to a stage where the models are reliable?" Osborn said. "This paper shows that we can now theoretically model even extremely complex systems. These techniques could accelerate our discovery of new materials."

Other Argonne authors of the paper, titled "Coherent Band Excitations in $CePd_3$: A Comparison of Neutron Scattering and *ab initio* Theory," are Park and John-Paul Castellan of the Materials Science Division. Also contributing to this work were researchers at the Joint Institute for Nuclear Research in Russia; the University of Illinois at Chicago; Karlsruhe Institute of Technology in Germany; Oak Ridge National Laboratory; Los Alamos National Laboratory and the University of California at Irvine.

Research at Argonne and Los Alamos was funded by DOE's Materials Sciences and Engineering Division of the Office of Basic Energy Sciences. Research at Oak Ridge's SNS was supported by the Scientific User

Facilities Division of the Office of Basic Energy Sciences. Neutron experiments were performed at the SNS and the ISIS Pulsed Neutron Source, Rutherford Appleton Laboratory in the UK. Blues, a high-performance computing cluster operated by the Laboratory Computing Resource Center at Argonne, also contributed to this research

CHALLENGES FOR THE ELECTRIC POWER BUSINESS

電力産業的挑戰

By Junichi Ogasawara

With the expansion of renewable power capacities, the ratio of oil-fired thermal power, which has so far served as peak supply capacity, is decreasing. The day-ahead spot price of the Japan Electric Power Exchange, which is determined by the marginal supply capacity, has been determined by oil-fired thermal power, which is the peak supply capacity, in most time slots. However, in FY2018, LNG thermal and coal thermal will be increasingly responsible for these time slots.

In terms of retail competition, the day-ahead spot price was around 8 yen/kWh in many months in 2017. In 2018, that price is likely to remain unchanged as the marginal supply capacity will gradually shift to LNG and coal thermal power even though oil prices are expected to rise. As more PPSs procure supplies in the day-ahead spot market, the unchanged spot price will help PPSs become competitive, although the benefit may be offset by the shrinking margin of electricity tariffs, particularly for high voltage users.

In Europe and the US, as renewable power capacities expand, there is a debate on how the wholesale electricity market price should be formed and how to pass it on to retail tariffs, and on the direction of power distribution charges. In these countries, revisions of wholesale price formation are underway, reflecting a supply-demand crunch in price formation and incorporating supply capacities that cannot meet load-dispatch instructions, such as must-run power (power sources operating irrespective of profitability to meet grid constraints), into wholesale pricing, as renewable power capacities expand and make it difficult to recoup the fixed costs of thermal power. As power suppliers grow inflexible with the increase in renewable electricity, there is a growing need for a mechanism to ensure that power consumption responds to the supply-demand situation, and hence growing

calls to strengthen the link between retail tariffs and the wholesale spot price. For leased transmission fees, the focus is on how to set incentives to avoid enhancements to the distribution system that result in higher electricity tariffs, even as more dispersed supply capacities connect to the distribution system.

Regarding system reforms, the trading of use of inter-regional connection lines at the power exchange and the sale of non-fossil-fuel-value certificates for the FIT portion are scheduled to start in FY2018. With the planned launch of the base load electricity market, which provides PPSs access to nuclear and hydropower generation sources, and indirect transmission rights, which hedge inter-regional price differences, and the sale of non-fossil-fuel-value certificates for the FIT portion in FY 2019, it will also be necessary to draw up the detailed design of these schemes and develop necessary systems. The detailed design must make progress in FY2018 in order for the capacity market to start trading in FY2020. With a fundamental review of conventional electric power systems underway in Europe and the US as described above, Japan must conduct such reforms after determining the future direction of the electric power system. The discussion on system reforms in FY2018 must be firmly based on such vision of the future.

INTERNATIONAL OIL SITUATION

2018 國際石油局勢

By Tetsuo Morikawa

The key issues for the international oil situation in 2018 are the scale of increase in US shale oil production, the review of the OPEC/non-OPEC joint production cut in June, and the situation in the Middle East and Venezuela.

US oil output recovered to as much as 9.48 million barrels per day (mb/d) in September 2017, with shale oil accounting for half the amount (4.76 mb/d). Since the summer of 2017, the number of operating rigs and the productivity of shale oil has begun to flatten out. However, the number of drilled but uncompleted (DUC) wells in shale oil fields reached a record 7,342 wells as of October 2017. Active hedging by producers in the WTI futures market is also a sign of their intention to increase output. Shale oil will undoubtedly remain the driver of rising oil production in 2018, and the US output could grow by around 1 mb/d from 2017 levels. Depending on the

growth in the US production, inventory might rise again, putting downward pressure on prices.

On November 30, 2017, the parties to the OPEC/non-OPEC joint production cut decided to extend the joint reduction of approx. 1.8 mb/day to the end of 2018. Nigeria and Libya, which were excluded from the production cut agreement, will also set a production cap of 2.8 mb/day or lower. Meanwhile, a review of the progress of the joint production cut was set for June 2018, presumably reflecting wariness by Russia, which itself is participating. Nonetheless, the extension has made it more likely for supply and demand to remain roughly in equilibrium. However, the compliance rate may fall as the production cut continues. The decision to be made in June 2018 by those participating in the production cut must be monitored.

Even though IS has been defeated, the Middle East is becoming more unstable. There is no end in sight to the confrontation between Saudi Arabia and Iran, and in November and December 2017, Yemeni Houthis launched ballistic missiles at Riyadh and Abu Dhabi. Saudi Arabia also saw a mass arrest and detainment of its royals and ministers. Further, President Trump's official acknowledgement of Jerusalem as the capital of Israel has infuriated Middle Eastern countries. The market is once again recognizing the risks in the Middle East as a factor for higher prices. Facing chaos in society and imminent default, Venezuelan oil production dropped by as much as 7% (0.14 mb/d) between January and October 2017. The sanctions by the US that began in August 2017 have put further strain on the finances of PDVSA, the state oil company. If the debt problem cannot be resolved and PDVSA's assets are confiscated, Venezuelan oil output could plummet.

There are various uncertainties, but assuming that the supply-demand balance remains even or tightens slightly, and that no major disruptions occur in producer countries, average international oil prices are estimated at around $65/bbl in 2018 for Brent.

HOW DO TREES KNOW WHERE TO PUT THEIR BRANCHES?

樹木怎麼知道它的樹枝要長在哪裡？

January 17 by Nathan Collins

When he was a boy, Alex Dunn, an associate professor of chemical engineering, looked at trees and wondered how they knew where to put their branches.

It's the sort of question biologists and laypeople have been asking for hundreds

or even hundreds of thousands of years, Dunn said, but for much of that time, researchers didn't have the tools they needed to find answers.

"There were some beautiful experiments in the 19th century trying to think about how living things came to adapt the form they have," said Dunn, a member of Stanford Bio-X and a faculty fellow of Stanford ChEM-H. "That's an obvious question to anyone who is interested in the natural world would happen upon."

But answers remained elusive until the last 50 years or so with advances in genetics and molecular biology. Now, a new set of tools and ideas aimed at understanding how mechanical forces affect cells, genes and other biological systems—a field dubbed "mechanobiology"—is poised to further improve how we understand our bodies and one day, perhaps, how we rebuild them.

Tools and questions converge

Although the name mechanobiology is relatively new, the basic idea is not, said Beth Pruitt, a professor of bioengineering and of mechanical engineering who directs ChEM-H's Interdisciplinary Postdoctoral Training Program in Quantitative Mechanobiology. More than a century ago, biologists observed that transplanting cells onto hard glass slides for observation under a microscope radically changed some of those cells' basic properties, while others hypothesized that mechanical forces were responsible for guiding bone formation.

But, Pruitt said, researchers of the day really had no way of exploring those ideas in a particularly rigorous way.

Today, Pruitt said, "I think there's a convergence of tools and technologies that allow us to observe things and quantify biology in unprecedented manners."

Her own lab, for example, has developed microscopic probes that make controlled movements over distances less than the width of a human hair and exert forces comparable to the weight of fruit fly. In collaboration with Miriam Goodman, a professor of molecular and cellular physiology, Pruitt's lab is using those tools to study the sense of touch, but others at Stanford are using related tools to study everything from brain folding to heart disease.

A molecular front and back

Dunn has been exploring even older questions about the physical structure of living things—for example, why we have fronts and backs that look different from each other. "You started from a single cell," Dunn said, yet somehow grow into

something with a front and back and top and bottom. How?

In a recent paper published in the journal Science, Dunn; William Weis, a professor of structural biology and of molecular and cellular physiology; and their lab members Derek Huang and Nick Bax and postdoc Craig Buckley provide a hint in the form of a special protein that binds to the molecular scaffold that gives a cell physical structure. That protein, the team showed, actually attached more tightly when pulled from one direction than another, like a person pulling harder backward than forward. What's more, the effect could potentially build up across the entire cell, giving it an asymmetry it would not otherwise have.

Understanding to engineering

Although part of the goal of Dunn's research is to understand the rules, so to speak, for building animals, there is a more practical side to this as well: regenerative medicine, or engineering human stem cells to form tissues and organs to replace what's been lost to accident or disease. Engineers can do a little bit of that now—for example, they've been able to build skin to help burn victims—"but our ability to build other really useful things is really primitive," Dunn said.

Building other things—say, one day building a human heart in the lab—is an extremely tall order and one that will take decades, if not longer, to fill, but beginning to understand the basics of how animals build themselves up from single cells and the genes within, Dunn said, will bring scientists closer to that goal.

"What I'm told is that for subsonic flight, computer simulation is pretty much good enough now that you can design the plane, simulate it and it will behave pretty much the way you expect," Dunn said. "That's what I would like to see for tissue engineering by the time I retire."