

How will the growing use of plug-in electric vehicles affect the power grid?



A new model based on a bottom-up approach quantifies consumer energy-use behavior and real-world vehicle usage.

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KEY CONCEPTS

A new study suggests the increasing use of plug-in electric vehicles might negatively affect the power grid.

The overall effect of more plug-in electric vehicles on the aggregate power grid is limited.

If local clusters of consumers charge their plug-in electric vehicles at the same time, the study concludes that the power grid will be stressed.

Demand for plug-in electric vehicles (PEVs) is growing globally as regulations are motivating automotive OEMs and consumers to move away from cars powered by internal combustion engines. In 2016 the number of PEVs in use globally was greater than two million vehicles, an approximately 60% increase from 2015.¹

A challenge facing researchers is better understanding how electric vehicle performance can be optimized. In a previous TLT article, a reinforcement-learning energy management system model was developed that enables plug-in-hybrid electric vehicles to more efficiently operate by constantly learning about the environment in which the automobile is traveling.² A trial

conducted on a highway reduced fuel consumption by 12%.

As PEV use grows, one concern that must be addressed is: How will this affect the power grid? The nightmare scenario is consumers will all decide to plug in their PEVs at the same time to recharge their batteries. This growing demand may place too much demand on the power grid leading to its collapse in the worst-case scenario. Growth in the use of PEVs is adding further complexity for electric utilities in figuring out how to manage power generation, transmission and distribution.

Most past efforts to model the power demand originating from PEVs had limitations. Dr. Matteo Muratori, transportation and energy systems engineer at

the National Renewable Energy Laboratory in Golden, Colo., says, "Previous models assessing how PEVs affected the electric

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grid assumed that consumers charged their vehicles in a smart manner, which was convenient for the electric utility."

Muratori believes that there is another side to the story. He

says, "PEV owners may decide to charge their vehicles at a time and in a manner that is convenient for them and not for the electric utility. They are not paid to charge the vehicle in a particular manner."

To take into consideration that consumers will act in their own best interests, Muratori developed a new model that is based on a bottom-up approach quantifying consumer energy-use behavior and real-world vehicle use in a specific U.S. region.

Muratori's model evaluated how in-home PEV charging in an uncoordinated manner affects residential power demand (see Figure 1). The model was a simulation that included 200 residential households in the U.S. Midwest. Within this community, Muratori indicated that the Midwest was used because his modelling data is validated in this region as compared to other regions.

Muratori says, "An evaluation was done on demand for electricity from the aggregate and the local level perspectives. Due to the small number of PEVs and the large residential electricity consumption, the overall effect on the aggregate power grid is limited. But the challenge will be at the local level where there may be clusters of consumers who purchased PEVs and may charge them at the same time, placing a burden on the local power grid."

Muratori feels there is an important difference between gasoline consumption and electricity use when it comes to automobiles. He says, "When a consumer fills up the gas tank in the automobile, it makes very little difference as liquid fuels are easy to store. In the case of electricity, however, consumption occurs at the same time as



Figure 1. A new study showed that locations with clusters of plug-in electric vehicles might stress the power grid if all of the vehicles are charged at the same time. (Figure courtesy of the National Renewable Energy Laboratory.)

production. It is instantaneous. This means that time at which electricity is used impacts the power grid."

Further complicating the situation at the local level is the role of the transformer. Muratori says, "A cluster of PEVs can place a significant burden on the transformer that could potentially reduce its operating life."

Another factor is whether the consumer has the opportunity to use Level 1 charging or Level 2 charging. Muratori explains, "Level 1 charging is done with a normal plug at 120 volts in a similar manner to using an extension cord. This already exists for all consumers, but it takes longer to charge the PEV. Level 1 chargers operate at 1.92 kilowatts. Level 2 chargers are similar in appearance to a gas pump and operate at 240 volts. They have the capability to operate up to 19.2 kilowatts, but for the purpose of this modeling study they are assumed to

operate at 6.6 kilowatts, which is typical for residential use. Consumers can charge a vehicle three times faster than when using Level 1 charging."

This means that consumers should have a preference for using Level 2 charging due to convenience of charging their PEV faster, or maybe only needing to charge a PEV two to three times a week instead of seven days a week with a Level 1 charger. Muratori found that consumers in the same cluster who used Level 2 charging at the same time stressed the electric grid, requiring upgrades to the distribution infrastructure.

Muratori also pointed out that PEVs can help ease the burden by acting as electric storage devices that can relieve pressure by transmitting electricity back to the grid during periods of high demand. He says, "The technology is in place to do this, but it is a matter of whether utilities can coordinate this benefit

with consumers and create an effective business model."

This study showed that PEVs can negatively impact the electric grid. In the future, Muratori will be evaluating the value of flexibility in charging and assessing the impact of charging at public stations on the electric grid. Additional information is available in a recent Nature Energy article³ or by contacting Muratori at Matteo.Muratori@nrel.gov.

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Converting shale gas into hydrocarbon fuels



KEY CONCEPTS

A single atom alloy prepared by dispersion of platinum atoms in a copper metal surface catalyzed the conversion of light alkanes into their corresponding alkenes.

No coking and good durability were observed with the single atom alloy catalyst.

If higher concentration of platinum were added to the copper metal surface, then catalyst performance declined due to coking.

A new catalyst activates carbon-hydrogen bonds under viable operating conditions.

The rapid development of hydraulic fracturing over the past decade has led to the production of larger quantities of shale gas that mainly contain light alkanes such as ethane and propane. One of the challenges facing researchers is finding ways to activate the C-H bonds in these alkanes so that they can be used as precursors to derivatives such as hydrocarbon fuels.

A previous TLT article describes a new approach at activating carbon-hydrogen bonds by inserting an aromatic molecule to produce alkylated aromatic hydrocarbons.¹ This process occurs through the formation of a phenyl carbocation intermediate. Alkylated aromatic hydrocarbons are precursors to aromatic sulfonates utilized in the lubricant industry as detergents, corrosion inhibitors, emulsifiers and extreme-pressure additives.

The main industrial approach for activating carbon-

hydrogen bonds in alkanes is steam cracking, but this reaction is inefficient and energy intensive. One reaction with significant industrial interest is converting light alkanes to al-

'Single platinum atoms reduced the barrier to carbon-hydrogen activation without breaking any carbon-carbon bonds that would lead to coking.'

kenes such as ethylene, which is a precursor to an important base stock used in lubricants, polyalphaolefins (PAOs).

E. Charles H. Sykes, professor of chemistry at Tufts University in Medford, Mass., indicates that metal catalysts have been used in an effort to improve the

conversion of alkanes to alkenes, but yields are limited due to coking problems. He says, "Coking is a buildup of carbon that takes place as the carbon-hydrogen bonds are breaking. Current catalysts such as nickel and platinum are so reactive that they break carbon-hydrogen and carbon-carbon bonds leading to a buildup of carbon on the catalyst surface. This causes major difficulties because it literally blocks the catalyst sites shutting down the reaction."

Sykes continues, "Platinum has an additional disadvantage due to its high cost. One option is to work with copper, which is just as inexpensive as nickel but is much more resistant to coking. The problem with using copper is the high energy barrier making it difficult to activate carbon-hydrogen bonds."

If an approach can be found that combines the high reactivity of platinum with the ability of copper to minimize coking, then

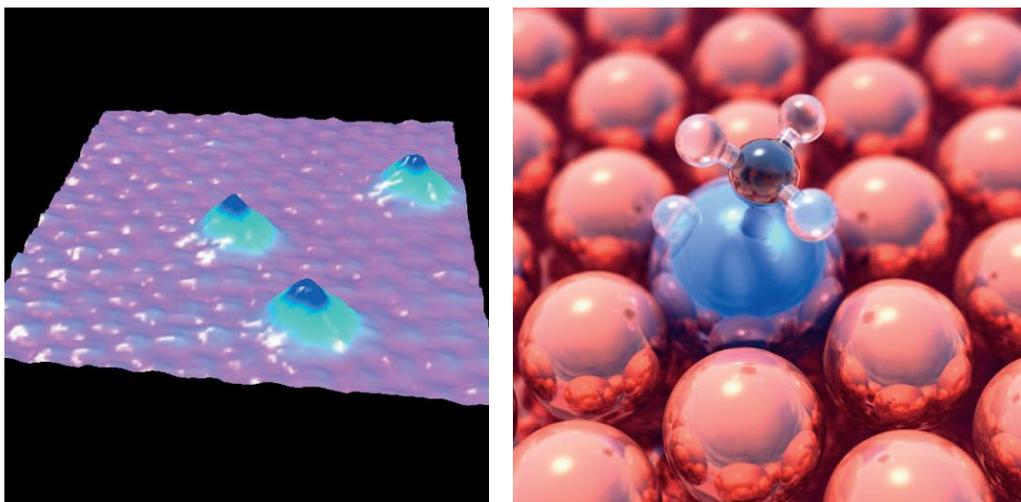


Figure 2. A scanning tunneling microscopy image on the left showed a model of the single atom alloy catalyst with three platinum atoms in a copper metal surface. The image on the right showed a simulation of how methane is activated on the surface of a single atom alloy catalyst. (Figure courtesy of Tufts University.)

a catalyst could be prepared that activates carbon-hydrogen bonds under viable operating conditions. Such a catalyst has now been developed.

Single atom alloys

Sykes and his colleagues from Tufts and University College London, UK, developed a new catalyst in which single platinum atoms are dispersed in a copper metal surface to produce a single atom alloy (SAA) that acts to convert light alkanes under realistic operating conditions. He says, "Based on our work using scanning tunneling microscopy (STM), we have achieved a higher magnification of a metal alloy surface than has been seen before. This enables us to see every single atom on the metal surface. We decided to produce a catalyst with the smallest amount of the precious metal platinum that can alloy in the copper."

One of the reasons the researchers selected this ap-

proach is that past work showed that platinum dispersed in a copper surface acted as a catalyst for selective hydrogenation reactions including the industrially relevant partial hydrogenation of butadiene. The SAA catalyst was prepared by reducing cupric nitrate in an aqueous solution with sodium borohydride followed by deposition on a silica support and calcination in air at 300 C to produce copper nanoparticles (0.2-0.3 micron average aggregate particle size). Platinum atoms were added to form the SAA catalyst through a galvanic replacement procedure.

Sykes says, "Dissolving platinum in copper is a thermodynamically favored process. We found that adding 1-4 atomic % platinum into copper produced the most desirable concentration of single platinum atoms in the copper (see the left STM image in Figure 2). When we added higher concentrations of platinum, dimers and trimers of platinum atoms started to form

and higher levels of coking were observed during reaction of light alkanes."

The researchers conducted catalyst studies under flow conditions evaluating C-H activation in butane and found that the SAA catalyst is effective at 250 C as compared to 550 C for copper. Platinum catalyzed the reaction at 100 C but catalytic activity quickly deteriorated due to coking. The researchers then showed that SAA catalyst were stale for over two days on stream converting butane to butene and hydrogen at 400 C.

Sykes says, "Based on quantum mechanical studies by our colleagues at University College London, we found that the single platinum atoms reduced the barrier to carbon-hydrogen activation without breaking any carbon-carbon bonds that would lead to coking."

The researchers also examined the addition of methyl groups to the SAA catalyst surface by using methyl iodide. Sykes says, "We used a

technique called temperature-programmed reaction combined with STM and initially placed the methyl iodide on the catalyst surface at 5 K. Then we heated the surface to whatever temperature activated the carbon-iodine bond and then cooled the reaction back down to gain an atomic-scale snapshot of the reaction by examining the active sites."

The right image in Figure 2 shows theoretically how a methane is activated on the surface of the SAA catalyst.

Sykes indicates that future work will include evaluation of metal catalysts in activating other bonds such as oxygen-hydrogen, nitrogen-hydrogen, carbon-oxygen and nitrogen-oxygen in addition to carbon-hydrogen using a combination of experiments under ultra-high vacuum conditions and theoretical studies. He adds, "We also are looking to design and then test catalysts that can be effective in accelerating many other reactions such as the conversion of ethanol to ethylene glycol. Our efforts will include identifying catalysts that will break one specific bond selectively."

Additional information can be found in a recently published paper² or by contacting Sykes at charles.sykes@tufts.edu.

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Hydrogen generation using a ruthenium-based catalyst



KEY CONCEPTS

A new graphene-carbon-nitride-ruthenium nanocomposite showed promise in splitting water into hydrogen and oxygen.

Favorable conditions for proton absorption and reduction were established through complexing between ruthenium metal ions and pyridinic nitrogens in carbon nitride.

The new catalyst also exhibited reduced charge-transfer resistance and an increased number of catalytic active sites.

Introduction of graphene into the ruthenium-carbon nitride nanocomposite produced a sandwich structure that facilitated the splitting of water.

While a good deal of attention is being paid to the development of battery technology, research is still continuing to find approaches for more effectively manufacturing hydrogen, which can be used in fuel cells to generate electricity. An example of how fuel cell technology is being commercialized is the recent announcement by Shell and ITM Power that the world's largest polymer electrolyte membrane hydrogen electrolysis plant will be built at Shell's Rheinland Refinery in Germany with a capacity of 10 megawatts.¹ The plant is due to become operational in 2020.

In a previous TLT article, a photoelectrochemical process was developed that can produce hydrogen at over 100% quantum efficiency.² The researchers used a technique called multiple excitation generation that enables the energy of one photon to be converted into multiple electrons.

Currently platinum-based catalysts on carbon supports are favored for splitting water into hydrogen and oxygen, but wide use of this catalyst type commercially will probably not occur due to the high cost and low supply of platinum. Shaowei Chen, faculty director for COSMOS and professor in the department of chemistry and biochemistry at the University of California at Santa Cruz in Santa Cruz, Calif., says, "Thermodynamically, protons can be reduced at the potential of 0 volt to produce hydrogen, but the kinetics of the process are slow. Catalysts are required to facilitate the reaction."

Chen indicates that an overpotential needs to be applied to enable catalysts to split water into hydrogen and oxygen. He says, "Platinum exhibits the best performance so far with an overpotential between -30 and -40 millivolts to reach the current density of 10.0 milli-

A current density of 10 milliamps per square centimeter was achieved at an overpotential of only -80 millivolts.

amps per square centimeter. Non-platinum-based catalysts exhibit overpotentials that are typically over -100 millivolts. To obtain a negative overpotential, < -100 millivolts would be remarkable."

In a recently published study, Chen and his colleagues found that embedding ruthenium ions in carbon nitride nanosheets led to the formation of a catalyst that was active in producing hydrogen.³ He says, "We took advantage of the fact that the nitrogen atoms present in carbon nitride act in a similar manner to pyridine, which

is a good coordination agent for metal ions. The ruthenium atoms form a nanocomposite with carbon nitride leading to enhanced catalytic activity. At an overpotential of -140 millivolts, the ruthenium-carbon nitride nanocomposite generated a current density of 10.0 milliamps per square centimeter."

Chen and his researchers have now modified the ruthenium-carbon nitride nanocomposite to further improve its performance in splitting water.

Graphene

Improved catalytic performance was realized by adding graphene to the ruthenium-carbon nitride complex. Chen says, "Electrochemical measurements of this new complex with graphene produced a current density of 10.0 milliamps per square centimeter at an overpotential of only -80 millivolts, which is an upgrade in performance."

Based on analysis by the researchers, the graphene-carbon nitride-ruthenium nanocomposite catalyst exhibited about 80% of the performance of the current platinum/carbon catalyst and was six times better than the ruthenium-carbon nitride nanocomposite.

The graphene-carbon nitride-ruthenium nanocomposite was prepared by blending carbon nitride nanosheets with reduced graphene oxide and reacting these two materials with ruthenium chloride in water. Atomic force microscopy analysis showed that the composite consists of sandwich-type structures with a thickness of 6.3 nanometers.

Chen says, "The sandwich structure was probably an indication of a strong π - π interaction between the carbon nitride and the graphene nanosheets inducing greater charge re-

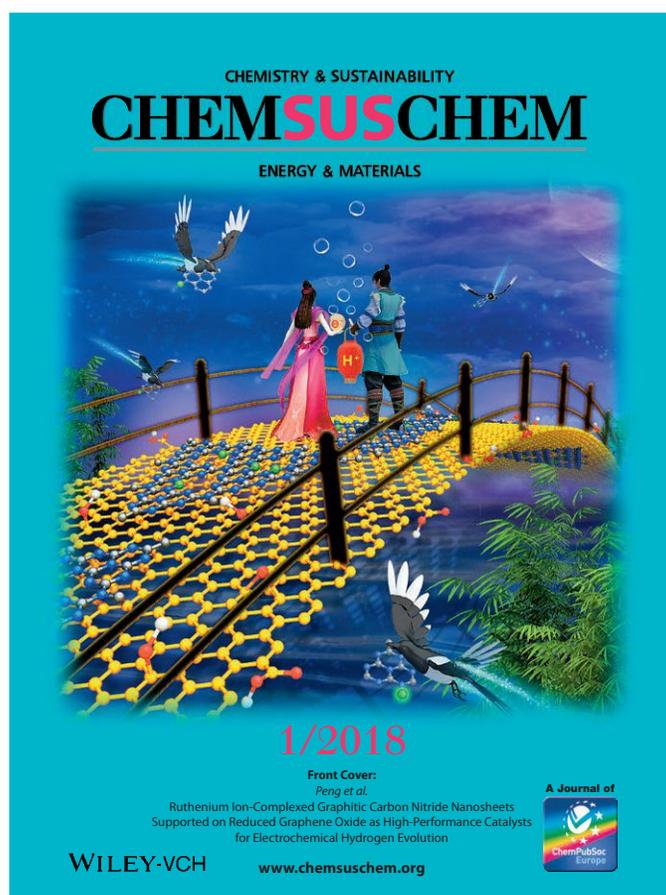


Figure 3. This cover image from the journal ChemSusChem is based on the ancient Chinese legend of Niulang and Zhinu and shows them meeting on a bridge consisting of the newly developed composite nanocatalyst that effectively splits water into hydrogen and oxygen. (Figure courtesy of the University of California at Santa Cruz.)

distribution that facilitated the splitting of water. Complexing between the ruthenium metal ions and the pyridinic nitrogens in carbon nitride established favorable conditions for proton absorption and reduction. Other favorable characteristics we attribute to this catalyst were reduced charge-transfer resistance and an increased number of catalytic active sites."

In running the experiments, the researchers loaded the catalyst on a glassy carbon electrode and negatively charged the potential to quantify hydrogen evolution. Chen says, "We

measured hydrogen generation as a function of the current detected. There is a direct relationship between current density and reaction rate."

Figure 3, which is taken from the cover of a journal that published the research, ChemSusChem, was designed by Chen's co-author, Yi Peng. The image was based on the ancient Chinese legend of Niulang and Zhinu. The two characters are shown meeting on a bridge consisting of the graphene-carbon nitride-ruthenium composite nanocatalyst and shows the formation of hydrogen.

Chen will be evaluating other low-carbon materials besides carbon nitride for their effectiveness in producing hydrogen in the future. He says, "We found that the conductivity of carbon nitride was not that good because this material is a semi-conductor. There are other low carbon materials that we intend to evaluate with metal ions such as cobalt, copper and nickel to determine if the resulting complexes are any more effective in splitting water."

Additional information on this research can be found in a recent article⁴ or by contacting Chen at shaowei@ucsc.edu.

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