Mechanical Engineering

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Nicole Benedek Receives Grant to Study Low-Temperature Fuel Cell Material

Assistant Professor Nicole Benedek with research group members: (L-R) Xinyu Li, Aqyan Bhatti and Alex Miller.

AUSTIN, TEXAS—June 16, 2014

Assistant Professor Nicole Benedek, a theoretical/computational materials scientist in the Mechanical Engineering Department at The University of Texas at Austin, has been awarded the **Ralph E. Powe Junior Faculty Enhancement Award**. Benedek is one of 35 recipients (two from UT Austin) from 134 applicants submitted from 114 institutions. These awards seed research funds by junior faculty at Oak Ridge Associated Universities (ORAU) member institutions. The one-year grant for $5,000 requires a match from the university for at least an additional $5,000.

Lower Temperature Cathode Materials

Nicole Benedek is working on understanding how to make atoms move faster at lower temperatures in cathode material found in solid oxide fuel cells (SOFC). Though solid oxide fuel cells are not a new technology, one reason widespread commercial adoption has continued to elude engineers for over a century is because they require heat at ~800-1000° C (1500 to 1800° F) to work efficiently.

She is studying the movement of **negatively charged oxygen atoms (a charged atom is an ion)** from the cathode to the anode, the electrodes that make contact with a circuit. As in a rechargeable battery, electrodes in a fuel cell are reversible.

At these high temperatures, SOFCs can quickly degrade parts, meaning very expensive components must be used to withstand the extremely high operating temperatures, rendering them not very practical. With more advanced technology, SOFCs could have a bright future in clean energy, as their by-product materials are water, electricity and heat, making the incentive to lower their operating temperature extremely high.

Related Links

- Dr. Nicole Benedek's Faculty Bio
- Ralph E. Powe Junior Faculty Enhancement Award
- Dr. Benedek's Research Group Website
- Introductory ME news story
- Interactive Periodic Table
- Solid Oxide Fuel Cells (SOFCs)
- Perovskites
- Ions
- Anions and Cations
- Electrodes, Anodes and Cathodes

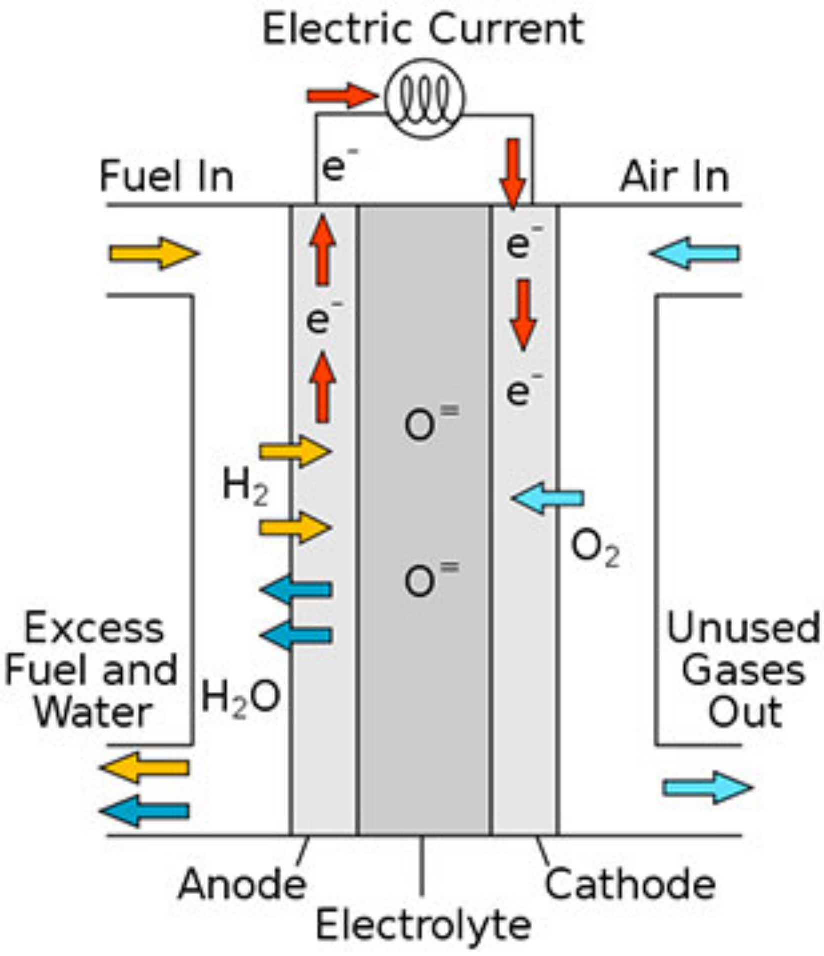
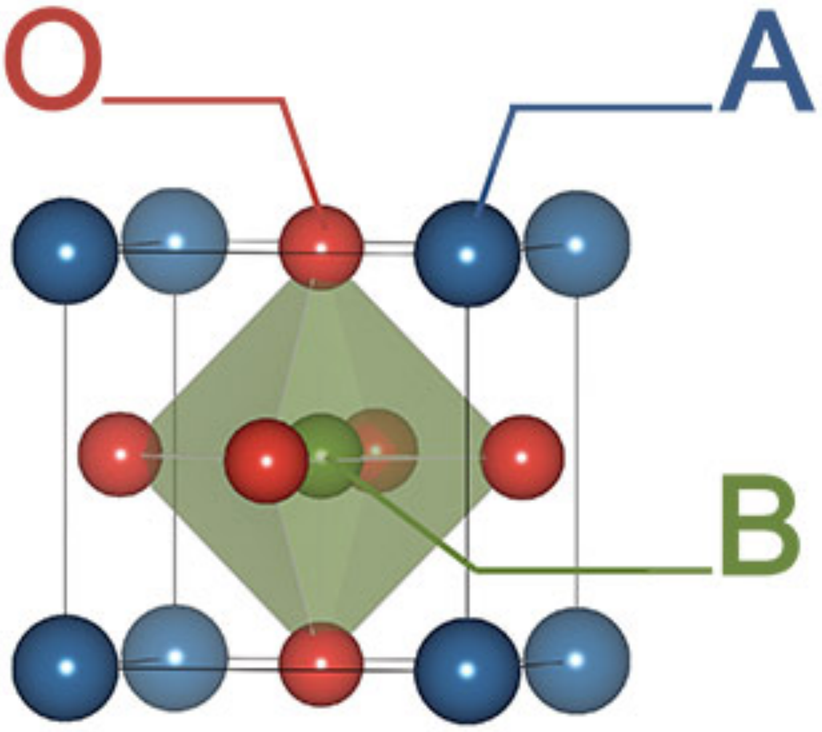


Diagram of a solid oxide fuel cell. Wikipedia Commons License, by Sakurambo.

How Solid Oxide Fuel Cells Work

A fuel cell produces energy from electrochemical reactions, similar to a battery, and will keep producing power as long as fuel is supplied, like an engine. The hydrogen (H_2) fuel enters the fuel cell at the anode side, where it reacts with oxygen to form water. Some electrons are released during this reaction, which travel through an external circuit to the cathode side. At the cathode, these electrons combine with oxygen molecules to make O^{2-} ions. These ions travel through the electrolyte to the anode, where they combine with H_2 in the reaction that produces water and electrons.



This is a diagram of the atomic-scale crystal structure of a perovskite that the team is studying. Perovskites have the chemical formula ABO_3, where A and B are different cations. These are marked on the image.

How solid oxide fuel cells differ from lithium-ion batteries

Solid oxide fuel cells, like lithium ion batteries, produce electricity through an electrochemical conversion by oxidizing a fuel. The way this works, though, is different from a traditional battery, as they require hydrogen and oxygen to function. Unlike batteries, fuel cells will only run as long as there is a continuous supply of fuel. There are different types of fuel cells, but Benedek's team is only studying SOFCs. They are the only type of fuel cell that can use hydrocarbons directly. The other types of fuel cells require pure hydrogen, which is not readily available. Hydrogen fuel cells, the type used in electric cars, run at lower temperatures, but are much more expensive to manufacture. SOFCs c an run on the same type of gasoline or diesel fuel as an engine.

Benedek's group is studying the materials used to make cathodes, where oxygen molecules pick up electrons and are converted to negatively charged oxygen atoms. These oxygen atoms then travel through the electrolyte to the anode. The actual materials needed for manufacturing the cathodes are not expensive, so if it proves possible to get them to work at lower temperatures, widespread adoption of the technology would be one step closer.

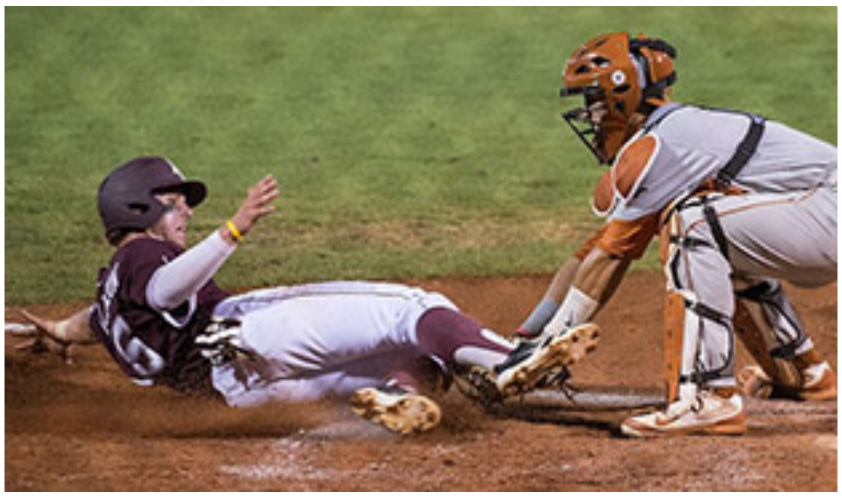
Perovskites for cathode material

Benedek and her researchers are studying a class of crystalline materials called **perovskites** that can have different chemical and physical makeup, but still maintain a crystal structure, some of which are highly conductive. Perovskites are extremely versatile: nearly every element of the periodic table is present in the perovskite family. This leads to a wide range of different properties, including ionic conduction.

Raw perovskite, a crystalline material being researched for cathode production.

The Benedek Group is not inventing another material, but studying the transport mechanisms through various perovskites to understand how they work, as well as predict which type of materials would likely be the best candidates for making lower temperature cathode material. Currently, the mechanism by which atoms travel through the material (and how this depends on the material itself) is not well understood. The team aims to identify and predict which materials and properties could work well at lower temperatures (~500-700°C), while still maintaining fast movement of the negatively charged oxygen atoms and longevity of the fuel cell.

Ion transport—much like baseball

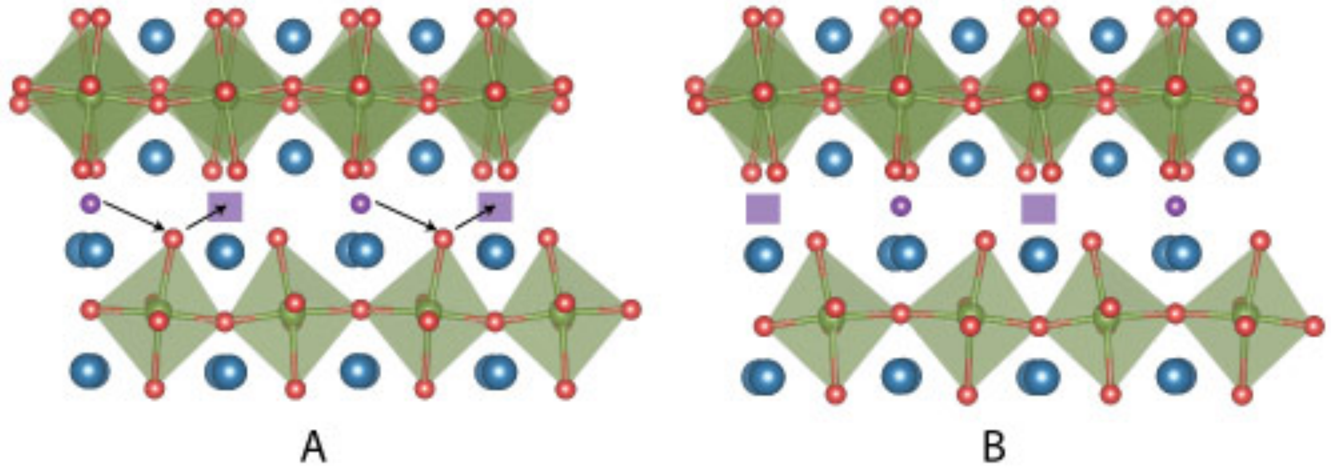


Interstitialcy ion transport can be compared to baseball when the hitter makes a run to base, and the player currently on that base moves to the next one.
Photo courtesy UT Athletics.

The group is studying a **tilting property** exhibited in some perovskites when negatively charged oxygen atoms travel through the cathode material using a low energy (low heat) transport method known as **interstitialcy transport**. To make them run at lower temperatures, a low-energy transport method is needed. To understand this, think of a baseball player who has just hit the ball and is running to first base. He can't move to first base unless he displaces the current team member already on first base, who must move to second base. That is how interstitialcy ion transport works. Oxygen atoms must displace each other to cross the cathode material. They can't just hit a home run with no one on base and run all the bases, or just hit the ball and run to third base, or run to first base and share it with someone else. Interstitialcy ion transport is a bit like baseball.

Atomic tilting makes ion transport at lower temperatures with less energy

When oxygen atoms move through certain perovskite materials, the individual atoms tilt,



This is a computational simulation of ***oxygen interstitialcy migration through a perovskite.*** *In the diagram, the migrating oxygen atoms are shown as purple spheres. The vacant interstitial sites where they are going are shown as purple boxes. In baseball, those would be the bases.*
In A, the octahedral structures of perovskite are tilting away from the traveling purple atom.
In B, using the baseball analogy again, the process is repeated as the oxygen atom has now moved to the next base, leaving its previous base (or interstitial spot) vacant for the next atom to move onto.

allowing the ions to travel through the material with less energy. The team knows why they tilt, but is now trying to find or design a material that does it well. If the atoms tilt too much or too little, it slows down the atomic transport. This is the research work that the Powe Award funding will support.

For more information on the Benedek Group

Please see our 2012 introductory news story and Dr. Benedek's research group web site for more information on her research and background.

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