Improving computer memory, solar cells goal of UH chemist

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Vas Lubchenko, a theoretical physical chemist at UH, takes raw data from researchers in the lab and crunches formulas and numbers to solve the puzzle of electrical phenomena in amorphous materials. Lubchenko was one of 16 recipients to win the Beckman Young Investigator Award in 2008, receiving a three-year $300,000 grant with which he will hire a postdoctoral researcher and two graduate students to assist him. Credit: Thomas Shea

A high-tech breakthrough in solar cells and flash drives may just come down to good old-fashioned pencil and paper calculations, says an award-winning young chemist at the University of Houston.

Amorphous materials, such as glass, expensive porcelain and plastics, may be at the very root of advances in solar batteries and computer memory, according to Vassiliy Lubchenko, an assistant professor of chemistry at UH who researches the electronic structure of these

materials.

The underlying physics and chemistry of electrical properties of amorphous materials is one the most fascinating and difficult problems in chemistry and physics. Direct computer modeling and existing theoretical approaches that have worked well for regular crystals and small molecules have not provided satisfactory insight into these disordered systems.

"The molecular structure of an amorphous solid is similar to that of a liquid," Lubchenko said. "Their atoms are not arranged in a periodic fashion, and chemists do not understand precisely how they conduct electrical charge. The inability to control and predict the materials' optical and electrical properties limits their use in photovoltaic devices such as solar cells and in information processing and storage."

Cracking the mystery of amorphous and disordered materials would pave the way for their use in affordable solar batteries. Amorphous materials, similar to those used in rewritable CDs, also have potential to greatly expand the speed and capacity of computer memory.

To solve this puzzle of electrical phenomena in amorphous materials, Lubchenko will rely heavily on what he calls "old-fashioned" math because the molecular events underlying the formation of these materials are so rare they would take too many computer cycles to simulate even on the most powerful present-day computer. For example, these rare events are responsible for the sluggishness of melted glass that gives glassblowers enough time to work their melts into various shapes. Conversely, such events are not necessary for water to flow, which is why water doesn't hold its shape.

"To adequately simulate a molecular system on a computer we, in a sense, need to produce an action movie with snapshots frequent enough

to capture individual molecular vibrations – at least two snapshots per full vibration," Lubchenko said. "To make a comparison, a regular movie with sufficiently many snapshots to reliably detect one of those rare events would take as long as a century to watch in a movie theater. Imagine how long it would take to make that movie."

'Paper and pencil' calculations offer a way out of this impasse, Lubchenko explains, because it is always possible to convey the plot of any movie – no matter how long – in just a few sentences, upon identifying the key characters and sources of tension. Analogously, a scientist uses his imagination to find a reduced description that uses a small number of parameters and laws of interaction. A theoretician can encode these laws in the form of equations and use his mathematical skills to find arbitrarily long-term solutions of these equations thus capturing even the rarest events.

As a theoretical physical chemist, Lubchenko does not spend much time in a lab. Instead, he takes the raw data from researchers in a lab and crunches formulas and numbers so that he can explain existing measurements and predict what will occur in future experiments and other systems.

Providing support in his efforts to tackle these mysteries, Lubchenko was recently awarded the coveted Beckman Young Investigator Award that carries with it a three-year, $300,000 grant. The award money will allow him to hire a postdoctoral researcher and two graduate students to assist him with his work.

"We are very proud to have Vas as a colleague," said David Hoffman, professor and chair of the chemistry department in the College of Natural Sciences and Mathematics at UH. "His award is an indication that our faculty competes very well for national awards and recognition."

One of only 16 recipients, Lubchenko is among a select group of 2008 winners – all within the first three years of a tenure-track appointment – including scientists from Columbia University, the University of California at Berkeley, The Salk Institute and other top-tier institutions. Lubchenko is currently at the end of that third year.

Bestowed by the Arnold and Mabel Beckman Foundation, the award is given to young faculty in chemistry and the life sciences at non-profit research institutions engaged in the most innovative research – those with the potential to achieve major advances in their fields. With its goals of promoting research and fostering new methods, instruments and materials in the chemical and life sciences, the foundation's grants open much-needed new avenues of research in science.

Lubchenko, a Ukrainian native, received his Ph.D. from the University of Illinois at Urbana-Champaign and was a postdoctoral research fellow at the Massachusetts Institute of Technology before coming to UH in 2005.

Source: University of Houston