The Shapes of Molecules Really Matter for Heat Conduction

September 24 2004

Too much heat can destroy a sturdy automobile engine or a miniature microchip. As scientists and engineers strive to make ever-smaller nanoscale devices, from molecular motors and switches to single-molecule transistors, the control of heat is becoming a burning issue.

The shapes of molecules really matter, say scientists from the University of Illinois at Urbana-Champaign and the University of Scranton who timed the flow of vibrational heat energy through a water-surfactant-organic solvent system. The rate at which heat energy moves through a molecule depends specifically on the molecule’s structure, they found. "The flow of vibrational energy across a molecule is dependent upon where and how the energy is deposited," said Dana Dlott, a professor of chemistry at Illinois and a co-author of a paper to appear in the journal Science, as part of the Science Express Web site, on Sept. 23. "Unlike normal heat conduction, different excitations may travel across the molecule along different paths and at different rates."

To monitor energy flow, Dlott and his colleagues - Scranton chemistry professor John Deak, Illinois postdoctoral research associate Zhaohui Wang and graduate student Yoonsoo Pang, and Scranton undergraduate student Timothy Sechler - used an ultrafast laser spectrometer technique with picosecond time resolution.

The system the scientists studied is called a reverse micelle, and consisted of a nanodroplet containing 35 water molecules enclosed in a sphere of surfactant (sodium dioctyl sulfosuccinate) one molecule thick that was suspended in carbon tetrachloride. The ultrafast laser technique, developed at Illinois, monitored vibrational energy flow as it moved from water, through the surfactant shell out to the organic solvent, atom by atom.

When the researchers deposited energy in the nanodroplet, the vibrations moved through the surfactant and into the carbon tetrachloride within 10 picoseconds. However, when the energy was deposited directly into the surfactant, the vibrations required 20 to 40 picoseconds to move into the carbon tetrachloride. Even though the distance was shorter, the energy transfer took significantly longer. "This is opposite of what you would think in terms of simple and ordinary heat conduction," Dlott said. "To explain this strange result, we have to analyze the energy transfer in terms of specific vibrational couplings that occur through a vibrational cascade."

There are hundreds of different vibrations in the water-surfactant-organic solvent system, Dlott said. "When energy moves through molecules, the detailed structure of the molecules and the way the vibrations interact are extremely important."

When the water was excited by a laser pulse, the scientists report, much of the energy was immediately moved to the surfactant, which then efficiently transferred the energy to the carbon tetrachloride. But when the surfactant was excited by the laser, the energy took a different path among the atoms, delaying the transfer to the carbon tetrachloride.

"The movement of vibrational energy within and between molecules is a fundamental process that plays a significant role in condensed matter physics and chemistry," Dlott said. "In designing nanoscale devices, the shapes of the molecules must be designed not only to be small and fast, but also to efficiently move heat."

Source: University of Illinois

Citation: The Shapes of Molecules Really Matter for Heat Conduction (2004, September 24) retrieved 11 May 2024 from https://phys.org/news/2004-09-molecules.html

This document is subject to copyright. Apart from any fair dealing for the purpose of private study or research, no part may be reproduced without the written permission. The content is provided for information purposes only.