Jaguar Calculations Help Turn Vehicle Exhaust into Power

Researchers simulate materials that turn heat into electricity

Materials researchers are using ORNL's Cray XT4 Jaguar system to help recover the energy that flows out your car's tailpipe.

A team led by Jihui Yang of General Motors is performing first-principles calculations of thermoelectric materials capable of turning waste heat into electricity. The team's efforts will take us a step toward capturing and using the 60 percent of the energy generated by an automobile's engine that is lost through waste heat.

Yang has been working with Changfeng Chen of the University of Nevada–Las Vegas to examine an especially promising lead-tellurium-based material for use as a thermoelectric converter. The team has been able to simulate various properties of the material in a more than 1,000-atom supercell, several times larger than previous simulations of its type.

Yang noted that the calculations would have been impossible had the team not had access to leadership computing facilities.

"Quantum mechanical ab initio calculations are usually done with 200 to 300 atoms," Yang explained. "We're doing calculations with a unit cell of more than 1,000 atoms. People would not be able to dream of doing these calculations without a large computing facility."

Yang's simulations are part of a $13 million, 5-year Department of Energy (DOE)-sponsored program entitled "Developing Thermoelectric Technology for Automotive Waste Heat Recovery." While he would not predict when the materials he simulates might appear in vehicles, he did note that DOE's goal is to have a demonstration of the technology—which promises to improve fuel economy and reduce fuel consumption—in the next 3 to 5 years.

Yang said he is very pleased with the help he has received from the NCCS, especially in using massively parallel computers. He said User Assistance and Outreach Group leader Julia White has been especially supportive.

He also noted that the simulations being performed on Jaguar are important beyond the properties of a single material, no matter how promising. He said the methodology being developed by the team will pave the way for researchers to simulate materials that have not yet been created, dramatically reducing the time to and cost of innovative materials advancements.

"The general approach can be designated as material by design," he explained.

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