'Walking Molecule' Research in AIP's Top 25

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It wasn't the biggest story of the year. But Kansas State University distinguished professor of physics Talat Rahman's work on "walking molecules" was big: So big that it has been named by the American Institute of Physics as one of the Top 25 Physics stories for 2005.

Rahman is a condensed matter theorist who investigates the physics of nano-materials and solid surfaces and interfaces. This work is important for solving technological issues such as thin film growth, new materials development, tailoring of properties of nanomaterials, controlling characteristics of catalysis and corrosion. It also is important for the fundamental questions it raises about the nature of the bonding between atoms at surfaces and interfaces and in other regions of low coordination like those on nanocrystals.

In her research, Rahman was able to male a single molecule "walk" on two legs. Ludwig Bartels and his colleagues at the University of California at Riverside, guided by Rahman and Sergey Stolbov, a K-State assistant professor of physics, created a molecule -- called 9,10-dithioanthracene -- or DTA -- with two "feet" configured in such a way that only one foot at a time can rest on the substrate.

Activated by heat or the nudge of a scanning tunneling microscope tip, DTA will pull up one foot, put down the other, and thus walk in a straight line across a flat surface. The planted foot not only supplies support but also keeps the body of the molecule from veering or stumbling off course.

In tests on a standard copper surface, such as the kind used to manufacture microchips, the molecule has taken 10,000 steps without faltering. According to Bartels, possible uses of an atomic-sized walker include guidance of molecular motion for molecule-based information storage or even computation.

"I find this work to be an excellent example of how theory, experiment and computer simulations can go hand-in-hand in developing functional materials for a variety of applications in nanotechnology such as nanomaterials for drug delivery," Rahman said.

Rahman is a pioneer in delineating the impact of atomic vibrations on the characteristics of materials. She is recognized worldwide for her contributions in the area of surface dynamics. One area of recent focus is establishing the theoretical framework for multiscale modeling of materials which allow an understanding of the macroscopic properties of materials from information obtained at the microscopic level.

Her efforts to model and visualize complex phenomena prompted her to seek funding from the National Science Foundation to expand the scientific and technical computing capability at K-State. The NSF grant and matching funds from the university established K-State's Center for Scientific Supercomputing, a facility that served the need for faculty across campus for a number of years.

Rahman's research programs have been continuously funded by national funding sources throughout her tenure at K-State, beginning in 1983. Rahman's work on the walking molecule is funded by a collaborative grant of $1.5 million from the Department of Energy under its special initiative "Catalysis Science Future."

Rahman has been an invited scientist at many of the world's most important research labs. Her awards include the UNDP Fellowship and

the CNR-Italy Research Fellowship and Alexander von Humboldt Fellowship and research prize. Rahman is a Fellow of the American Physical Society. In 2002 she received the $10,000 Higuchi/Olin Petefish Award for research achievement in the basic sciences from the University of Kansas.

She also has received K-State's University Distinguished Graduate Faculty Member Award and was named University Distinguished Professor in 2001.

She has published hundreds of research articles, many of which have been accepted by Physical Review Letters, one of the most prestigious of the peer-reviewed publications in the physical sciences. Rahman received K-State's William L. Stamey Teaching Award in 1992. A faculty senator for several years, she is a former president of Faculty Senate. She was instrumental in establishing the K-State Developing Scholars' Program, which aims to enhance the retention and graduation rates of students from historically under-privileged groups. For the past several years Rahman has been funded by the National Science Foundation to organize scientific activities at the international summer college in Nathiagali, Pakistan, on "Frontiers in Physics and Contemporary Needs of Developing Countries." Currently Rahman is serving a three-year term on the executive committee of the Division of Materials Physics, American Physical Society.

According to Dean Zollman, head of the department of physics, Rahman's research is "an excellent example of the collaboration of an outstanding group of K-State faculty and students with researchers elsewhere."

"Dr. Rahman and her colleagues at K-State provided the theoretical foundation so that Dr. Bartels at University of California-Riverside could create molecules that moved in a walking pattern," Zollman said.

"This type of collaboration enhances the reputation of K-State and provides unique opportunities for our students."

The complete list of the Top 25 stories can be found on the institute's Web site at: www.aip.org/pnu/2005/split/757-1.html

Source: Kansas State University