Exploiting the Properties of Very Small Objects

Posted By Jason On March 9, 2012 @ 7:10 pm In Features | No Comments

By Robin Herron

[1]

Estela Blaisten-Barojas

From the soles of your sneakers to the shingles on your roof, nanoscience is at work in your daily life.

Nanoscience, or nanotechnology, looks at and manipulates objects at the atomic and molecular level. One nanometer is one-billionth of a meter, and nanoscale objects range in size from about 1 to 100 nanometers.

Amazingly, manipulating particles of minerals or metals at the nanoscale can make sneakers more resilient and roofs more energy efficient.

And for some, such as Mason computational physicist Estela Blaisten-Barojas [2], determining the nanoscale properties of, say, the porous network of zeolite minerals, is fascinating.

Zeolites are used in a variety of industries because of their absorbent and catalytic properties. Gasoline, for example, is produced using zeolite as a catalyst. Several of Blaisten-Barojas's recent papers analyze networks of atoms that form within zeolite crystals.

"Depending on the internal structure of these zeolites, they may be good or bad catalysts," explains Blaisten-Barojas, who directs the Computational Materials Science Center [3] at Mason.

Because zeolites can have so many useful characteristics, Blaisten-Barojas and her research team created an automated way to classify zeolites according to their internal nanostructure network. This classification of more than 1,400 zeolites will be a basic reference and standard for future work in chemistry, materials science, and applied mathematics. The model and data will be available in the cloud computing Microsoft Azure platform.

The interdisciplinary nanoscience field is relatively new and still growing rapidly. "Nanoscience and nanotech have found a way to exploit the peculiar characteristics of very small objects and bring them to the technological arena," Blaisten-Barojas says. "They have applications that go from health to electronics, and everything in between."

In 2000, the federal government established the National Nanotechnology Initiative [4] (NNI) to coordinate federal research and development. The NNI website notes, "Nanotechnology research is estimated to have impacted $251 billion across the global economy in 2009. This is estimated to grow to $2.4 trillion by 2015."

The National Science Foundation has been a major funder of nanoscience research, and Blaisten-Barojas has had NSF support for her work, including support to use the high-performance computing resources of the TeraGrid (recently succeeded by XSEDE). She has also received grants from the Office of Naval Research, the National Institute for Standards and Technology (NIST), the Naval Research Laboratory, and the U.S. Army.

Over the course of her career, Blaisten-Barojas has published more than 100 scientific papers, many of them dealing with atomic clusters. "I have approached the clusters from many perspectives," Blaisten-Barojas says. "Computational approaches are similar to experiments that allow one to obtain structural, chemical, and thermodynamic properties based on models; I would call 'simulation' the methodology in between the model and the results. I like this approach very much.

"For these simulations and modeling, one needs to develop better algorithms for the computations, so we have some in-house algorithms that are very effective."

Among the clusters and the properties Blaisten-Barojas has studied are

- Metallic clusters, such as alkali and alkaline earth atoms, that "do not behave as a small chunk of metal"
- The thermal management properties of silicon carbide nanotubes, a material often used in electronics
- Structural changes in rhodium clusters that can be used as magnetic switches if triggered externally
- Clusters of organic molecules that absorb light and then emit light in a different wavelength if excited for use in markers
- Polymers or organic metals that bundle together like a fiber and have the potential to make artificial muscles

In 2003, Mason established the Nanotechnology Initiative, a virtual association of faculty researchers in chemistry, computational sciences, engineering, mathematics, molecular biology and medicine, operations research, and physics. Blaisten-Barojas coordinates this initiative, which is a resource for Mason researchers looking for scientific, as well as for industrial, collaborators. For example, Blaisten-Barojas recently met with an entrepreneur to discuss certain properties of nanoparticles for absorbing and reflecting light.

Blaisten-Barojas is collaborating with Mason colleagues Iosif Vaisman [5], associate director of the School of Systems Biology; Dmitri Klimov [6], professor of bioinformatics and computational biology; and Igor Griva [7], professor of mathematics and computational and data sciences, on research involving small objects with unprecedented strength formed from biomolecules, such as silk .

Originally from Argentina, Blaisten-Barojas earned a bachelor's degree in physics from Universidad Nacional Autónoma de México (UNAM) and then went on to complete a a doctorate degree at the Université Pierre et Marie Curie (Paris VI) in France. There she studied theoretical atomic and molecular physics and had the opportunity to meet such physicists as Nobel Prize winners Alfred Kastler, who sat in on her doctoral defense; Claude Cohen-Tannoudji, who was one of her professors; and Louis de Broglie, who founded the laboratory where she did her research.

Blaisten-Barojas returned to Mexico and built her career in the Institute of Physics at UNAM over the next 17 years. After moving to the United States, she held positions at NIST and Johns Hopkins University before joining Mason in 1992.

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