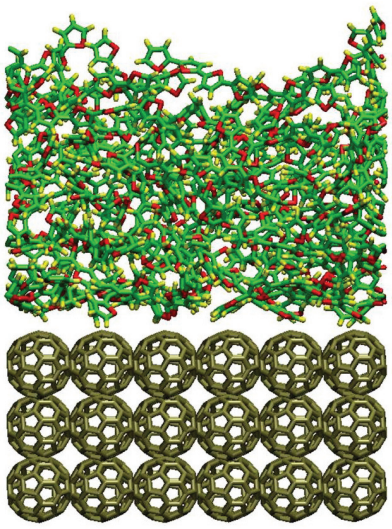
Evaluating organic materials for solar energy



above: Researchers like University of Cincinnati's Vikram Kuppa are studying the potential of combining oligothiophene and fullerene to produce viable solar cell systems.

Organic photovoltaic systems (OPVs) have generated considerable interest from researchers in recent years as materials relevant to harnessing renewable and sustainable sources of solar energy. OPVs are called "organic" because the substances are carbon-based, like the molecules of living things. The great potential of organic materials lies in their lower production costs, greater flexibility and higher optical absorption coefficients than their traditional, inorganic counterparts, such as copper or silicon.

Vikram Kuppa, Ph.D., an assistant professor of chemical and materials engineering at the University of Cincinnati, is conducting molecular dynamics simulations at the Ohio Supercomputer Center to evaluate the behavior of the carbon-based material oligothiophene when applied to a carbon-based substrate of fullerene.

"We seek to probe the effect of the surface, as well as process variables such as temperature, on the behavior of the oligothiophene," said Kuppa. "The goal is to enable a fundamental understanding of the factors that influence the properties of these hybrid systems, and their role in the transport of electrical charges that are generated in the conjugated polymers upon exposure to sunlight."

To generate these detailed simulations, Kuppa uses the classical molecular dynamics code LAMMPS, an acronym for Large-scale Atomic/Molecular Massively Parallel Simulator, and OSC's flagship Glenn Cluster, a 9,500-node IBM 1350 Opteron system.

"The ultimate goal of this research," Kuppa said, "is to employ molecular dynamics simulations in conjunction with experimental tools to develop cost-effective and efficient materials for energy conversion." ■

Project lead: Vikram Kuppa, University of Cincinnati
Research title: Simulation of organic photovoltaic materials
Funding sources: University of Cincinnati

Exploring EM wave behavior in metamaterials

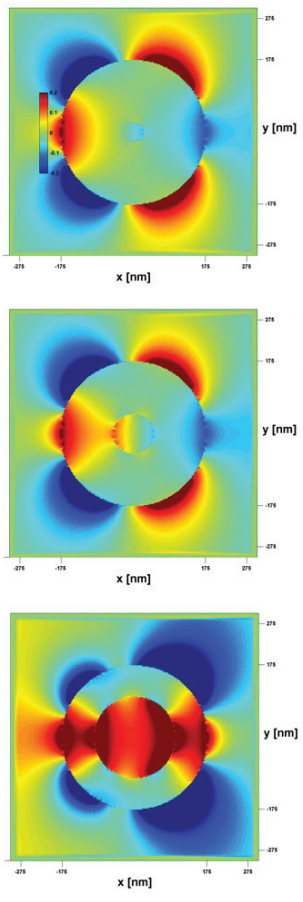
Various materials can be used to control the path of light or any other type of electromagnetic (EM) wave. For example, the lenses in a pair of eyeglasses are shaped to achieve a desired optical function. While nature and chemistry have provided many such materials, it is only in more recent years that scientists have been working at the nanoscale to create a range of "metamaterials" with novel and promising EM properties.

"Metamaterials increase the degrees of freedom for controlling EM wave behavior," according to Fernando L. Teixeira, associate professor of Electrical and Computer Engineering at The Ohio State University and a faculty member of OSU's ElectroScience Laboratory. "For example, it might be possible to create metamaterials to provide super-resolution lenses, negative refraction and electromagnetic cloaks."

The fabrication-associated design process of new metamaterial-based EM devices is expensive, time-consuming and sometimes very difficult. Manufacturers often turn to modeling and simulation to limit trial-and-error before the actual fabrication and prototyping process begins.

Teixeira and his research team have found that existing commercial codes do not have the capability of analyzing complex metamaterials with a sufficient degree of accuracy. Therefore, they are using the large parallel systems of the Ohio Supercomputer Center to develop faster, more accurate computer algorithms to investigate EM wave behavior in metamaterials, focusing especially on three types:

- photonic crystals (for slow pulse propagation)
- nanoscale metallic structures (for compact optical devices)
- isoimpedance metamaterials (for reflectionless waveguide bands) ■



Project lead: Fernando Teixeira, The Ohio State University
Research title: Large-scale time-domain simulations for electromagnetic wave propagation and scattering in metamaterials
Funding sources: National Science Foundation, Air Force Office of Scientific Research