The terms nanostructure, nanoscience, and nanotechnology are currently quite popular in both the scientific and the general press. These intermediate-length structures are intriguing because generally in the nanometer region, almost all physical and chemical properties of systems become size-dependent. For example, although the color of a piece of gold remains golden as it reduces from inches to millimeters to microns, the color changes substantially in the regime of nanometers. Similarly, the melting points of such particles change as they enter the nanoscale, where the surface energies become comparable to the bulk energies. Because properties at the nanoscale are size-dependent, nanoscale science and engineering offer an entirely new design motif for developing advanced materials and their applications.

From the point of view of computation, nanostructures are of interest in two quite different directions. As a computational challenge, they are quite striking: ordinarily, we define nanosstructures as having characteristic dimensions between one and 100 nm. Given that atoms have characteristic sizes between 0.1 and 0.3 nm, this suggests that nanoscale structures will contain between $10^3$ and $10^{10}$ atoms. Modeling the behavior of such structures is then a substantial computational undertaking.

The second reason that nanostructures are of interest to the computational community is that the tools with which we compute will almost certainly involve nanoscale structures. As Moore’s law is extended beyond the next 10 years, functional devices will certainly operate below 100 nm. Design rules for transport based on simple Ohmic behavior and digital off/on field-effect transistor function will then become dubious, and we will need entirely new design schemes to deal with the idiosyncrasies of nanoscale structures. Such components as molecular switches, nanotube connectors, crossbar arrays, magnetic nanodot memories, and electronic paper embody the challenge and promise of nanomaterials in computing.

This issue of CiSE contains three articles that pinpoint particular important avenues in the modeling of nanostructures. All three point out the difficulty that scaling imposes as we move from the characteristic size of small molecules (containing a few atoms) to true nanostructures containing more than $10^5$ atoms. Modeling methods thus require a judicious integration of high-accuracy quantum-mechanical treatments for small structures ranging from approximate quantum dynamics for medium-length-scale materials, to classical molecular electronics for large-scale materials, through a form of continuum mechanics for macroscopic structures. Be-
cause continuum mechanics and continuum electrodynamics work so well for materials larger than the micron scale, the correspondence principle requires the computations using quantum or atomistic methods to eventually reproduce the correct predictions of continuum analysis.

Deepak Srivastava, Madhu Menon, and Kyeongjae Cho focus on one of the most striking families of nanomaterials: carbon. The authors use several levels of theory, ranging from quantum conductance and quantum structure calculations for small particles through tight-binding molecular dynamics, Car-Parrinello-type dynamics for medium-size structures, and classical electrodynamics for larger particles. They discuss the mechanical, activator, and transport structures associated with these new carbon materials, which are fascinating in their own right because they are unique in their mechanical and transport properties.

The contribution from Aiichiro Nakano, Martina E. Bachlechner, Rajiv K. Kalia, Elefterios Lidorikis, Priya Vashishta, George Z. Voyiadjis, Timothy J. Campbell, Shuji Ogata, and Fuyuki Shimojo deals directly with the challenge of multiscale simulation. The emphasis here is on methodology, although cases from such challenging problems as oxidation of the silicon (100) surface and the impact of projectiles on a silicon surface are given as examples. Here the methodologies range from the use of density-functional quantum mechanics for the smaller systems to classical molecular dynamics for medium-scale to finite-element dynamics in the continuum limit. An important issue here is the embedding of the more accurate method for smaller systems within more coarse-grained methods for larger systems. All of this requires both high-performance computational environments and a reasonable interaction environment between the computational resource and the scientist using that resource; visualization is stressed as perhaps the key to such successful interfacing.

The article by K. Lance Kelly, Anne A. Lazarides, and George C. Schatz begins from the macroscopic and works down toward the nanostructure. Using the critical insights Mie developed a century ago, these researchers show that the optical properties of gold and silver nanoparticles can be treated well by using computational electromagnetics. It is indeed true that all properties are size-dependent in the nano regime, but it is also true that well-chosen extensions of classical methods can give strikingly accurate predictions for such complex features as optical properties and their shape and environment dependence.

Although modeling of nanoscale systems is a dominant theme in contemporary chemical engineering, chemistry, condensed-matter sciences, electrical engineering, and materials science, the three articles in this issue demonstrate that there are many approaches to the challenging issues of nanoscale behavior. They do not attempt to review any aspects of the field, but they illustrate some of the important and valuable approaches to the issue of nanoscale modeling and computation.

James R. Chelikowsky is the Institute of Technology Distinguished Professor in the Department of Chemical Engineering and Materials Science and a fellow of the Minnesota Supercomputing Institute at the University of Minnesota. Contact him at jrc@msi.umn.edu.

Mark A. Ratner is a professor in the Department of Chemistry and Materials Research Center and a director of the Center for Nanofabrication and Molecular Self-Assembly at Northwestern University. Contact him at ratner@chem.nwu.edu.