Nanoscale Modeling and Simulation

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This talk provides an overview into the use of theory and simulation in nanoscience research. Five different topic areas will be considered, and for each I will show where simulation has provided important insights into a problem, sometimes setting the framework for further work in a given subdiscipline. The five areas are:

1. Structures of disordered soft nanomaterials. We show how peptide amphiphile fibers and their functions that can now be modeled and predicted with simulations.
2. Interfaces of carbon-based nanomaterials. Chemical functionalization plays a big role in optical and electrical measurements but characterizing complex surfaces is challenging. However it is now possible to model this functionalization.
3. Nonequilibrium in molecular machines and pumps. Bioinspiration tells that we should be able to synthesize interesting machines, but the results have been disappointing. Simulation can be used to provide a quantitative picture.
4. Optical properties: The convergence of top-down and bottom-up models of optical properties promises a new generation of plasmonic materials.
5. Linking nanoscale to mesoscale properties. Simulation provides key predictions for the development of mesoscale materials based on DNA-linked nanostructures.

George C. Schatz is Charles E. and Emma H. Morrison Professor of Chemistry and of Chemical and Biological Engineering at Northwestern University. He received his undergraduate degree in chemistry at Clarkson University and a Ph. D at Caltech. He was a postdoc at MIT, and has been at Northwestern since 1976. Schatz is a theoretician who studies the optical, structural and thermal properties of nanomaterials, including plasmonic nanoparticles, DNA and peptide nanostructures, and carbon-based materials, with applications in chemical and biological sensing, electronic and biological materials, high performance fibers, and solar energy.