

The Interplay of Theory and Experiment in Nanoscience

Peter T. Cummings
Department of Chemical and Biomolecular Engineering
Vanderbilt University
Nashville, TN 37235-1604
and
Center for Nanophase Materials Sciences
Oak Ridge National Laboratory
Oak Ridge, TN 37831-6496

Theory and simulation have played, and continue to play, a central role in nanoscience. In fact, it can be argued that theory and simulation play a greater role in nanoscience than in macroscopic materials and chemical sciences for at least three reasons: first, many experiments performed at the nanoscale can only be interpreted through theory; second, theory and simulation can provide a convenient framework to isolate effects and phenomena in a way that may be difficult or impossible to achieve in an experiment (i.e., in theory and/or simulation, the boundary and initial conditions are under complete control, which may be impossible to achieve in an experiment), thus making theory and simulation a crucial tool in understanding emergent phenomena in nanoscale systems; and, finally, theory and simulation can be used to design new nanostructured materials, as well as systems based on nanoscale phenomena.

In this presentation, these roles of theory and simulation will be illustrated through examples from the published literature, from the speaker's own research program, from user research projects at the Center for Nanophase Materials Sciences (CNMS), and from the CNMS internal scientific research program. The latter has three major themes: imaging nanoscale functionality, synthesis and dynamics of nanostructured polymeric and hybrid materials, and emergent behavior in nanoscale systems. Theory and simulation play prominent roles in all three themes, in addition to leading the emergent behavior theme.

In conclusion, the prospects for the future role of theory and simulation in nanoscience will be assessed, in light of continuing advances in theory, computational methods and computing hardware.