

## **Multiscale Modeling in Mesoscale Materials**

George Crabtree

Argonne National Laboratory  
University of Illinois at Chicago

Mesoscale science embraces the bottom-up manipulation of interactions among atomic, molecular and nanoscale components to produce new behavior not found in the constituents, a rich opportunity not only for new materials and phenomena, but also for multiscale modeling at the descriptive and predictive levels. New features that emerge at the mesoscale include interacting degrees of freedom, statistical variation, defects and collective behavior. A general introduction to mesoscale science will be followed by materials challenges that are ripe for multiscale modeling solutions drawn from solvation in organic liquids, fractures and other defects in solid materials, and heterogeneous and amorphous materials.