

Multiscale modeling for nanomedicine: Challenges and Opportunities
Deepak Singh, Accelrys, Inc, San Diego, CA, USA

Nanotechnology has been widely recognized as having the potential to make a significant impact on the future of healthcare and medicine. Nanoscale materials, devices and technologies are being researched and developed for molecular diagnostics, drug delivery, therapeutics, imaging, and regenerative medicine. It is estimated that within the next decade, many of these technologies will be available as products, driving forward the systems medicine revolution. Computational tools will play a key role in the design and analysis of nanoscale materials and systems for nanomedicine. Successful design and analysis of nanoscale materials and architectures requires the development of algorithms and methods that can span multiple length and time scales and the ability to model complex systems consisting of inorganic, organic and biomolecular components. This presentation will discuss some existing technologies that are available to study nanoscale systems, the current state-of-the-art and discuss some future developments necessary for the successful application of computational technologies for nanomedicine.