Computational Nanoscience and the Interplay Between Experiment and Theory

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ABSTRACT

Theory, modeling and simulation (TMS) tools constitute key enabling technologies for making fundamental advances in nanoscience and for making nanotechnology a practical reality. Many of the problems encountered in this emerging field of computational nanoscience are inherently multiscale. In this talk, we provide an overview of the role of TMS in nanoscience, as well as an overview of applications of many-scale and multi-scale TMS methods to several outstanding problems in nanoscience.