

**Title:** “Nanoscale simulations and large data”

**Abstract:**

Over the past decade, with advances in high-performance computing, new algorithms, and data science, theory, simulation, and computation continue to partner with experiment in discovery and innovation in nanoscience and nanotechnology. The next decade promises extraordinary breakthroughs as new algorithms, tools as well as a new generation of computational and data scientists appear on the scene. I will provide a brief overview of the field, with examples that include material design and discovery, and the use of neural networks analyses.