The Waterloo Institute for Nanotechnology & The faculty of Mathematics

Presents

The Role of Mathematical Modeling and Computer Simulation in Nanotechnology

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The ability to understand, design and control structural, electronic, and optical properties at the nanoscale has led to a plethora of exciting potential applications of nanotechnology research. To fully exploit these opportunities requires a positive interplay between theory, simulation, and experiment. This may be achieved through theory and simulation (1) corroborating experimental measurements, (2) providing an understanding of the underlying mechanisms, (3) predicting the properties of new materials, and (4) computationally designing nanomaterials with specifically tailored properties. With the advent of teraflop computing, density functional theory based methods have arisen as the computational workhorses for simulations of quantum phenomena at the nanoscale. After providing a general introduction to the basic concepts behind density functional theory, we will analyze the role played by simulation and theory in catalysis, nanoelectronics, nanosensing, photocatalysis, and photovoltaics using specific examples from my research at the density functional theory, non-equilibrium Green's function methods, random phase approximation, quasiparticle, and Bethe-Salpeter levels of theory.

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3:30-4:30pm
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