**Nanoscience and Nanotechnology: the Role of Computation at the Atomic Level**

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Nanoscience and nanotechnology has advanced remarkably over the last 30 years. Over the same period, computational molecular and materials science has become central to many research programs. This is due to recent advances in algorithms, availability of software and greatly enhanced computer hardware. It has also been due to successful outcomes from integration of atomic level computational studies into research programs. Nanoscale systems are of particular interest because their feature size is often accessible for such a treatment and because it can be difficult to probe these systems using experiment. However, limitations on timescales and length-scales remain problematic. Furthermore, for some systems including nonequilibrium systems, the fundamental theory is not fully developed. Improving knowledge of these systems opens opportunities to develop new fundamental relations and new algorithms. This would also further expand capabilities for modelling.

We will discuss some advances nanoscience and nanotechnology that have been facilitated by computation molecular and materials science, current work in the area and challenges that remain. We will focus on the application of computational molecular science to the study of materials and processes for sustainable energy technologies. I will also present some examples of our work where we have used conventional methods to study materials for sustainable energy and another when we have applied relatively new nonequilibrium approaches for these studies..