From Complex Potential Energy Surfaces to Material Function and Design

Graeme Henkelman, Professor, Chemistry

Abstract: The focus of this Grand Challenge project is to develop computational methods for exploring high-dimensional potential energy landscapes of increasing complexity with application to materials for renewable energy. This Grand Challenge is important because the ability to navigate and control potential energy surfaces is critical to a theoretical understanding of how materials function at the atomic scale. Sometimes described as the materials genome, the fundamental parameters which govern the function of materials, such as the voltage of a battery material or the efficiency of a catalyst, can then be used for the rational design of new materials.

As part of this Grand Challenge award, I am co-organizing a three-month program at the Institute for Pure and Applied Mathematics on the campus of the University of California at Los Angeles. This program, entitled "Complex High-Dimensional Energy Landscapes," will bring together applied mathematicians, physicists, material scientists, computer scientists, chemists, and engineers to work collaboratively on this complex problem.