Awardee: **Graeme Henkelman, Professor, Chemistry**

Research Award Title: From Complex Potential Energy Surfaces to Material Function and Design

Research Summary

The opportunity provided to me through the Grand Challenge Faculty Award was extremely valuable for my research program. With the freedom to focus on research, I published seventeen papers,[i-xvi] gave four invited talks, and perhaps most importantly, established new research directions for the future. I was able to spend an extended period of time at the Institute for Pure and Applied Mathematics (IPAM) on the campus of UCLA during my leave in the Fall. Here, I will briefly describe a few of the research highlights from the award period and the opportunities that it has allowed.

The focus of my research has been the computational design of materials, with application to the development of new energy sources. The research involves development of the computational methods required to model the function of materials, as well as strategies to invert the problem and predict new materials with a desired function.

A good model system for these studies is that of nanoparticle catalysts. Catalysts are important whenever energy is converted to or from a chemical form. A grand challenge, for example, is to find a catalytic system which will allow the production of fuel from sunlight; another is to replace platinum for the efficient electrochemical burning of fuel in a fuel cell. Nanoparticles are attractive because they can have properties which are different from bulk materials, and with on the order of 100 atoms, the problem of searching the composition space and predicting catalytic activity is tractable.

We made several advances in this area in the Fall of 2017. In the area of catalysts for water purification, we have worked with the group of Charlie Werth to design PdAu nanoparticle catalysts for nitrite reduction, which is a common pollutant from excess fertilizer in water sources.[xii] For CO oxidation, we have screened bimetallic catalysts which will not be poisoned by CO.[xiii] On Pd/Au and Rh/Au surfaces, we have done comprehensive studies of ethanol dehydrogenation to obtain more valuable chemical fuels.[iiiii] Perhaps the most scientifically interesting aspect of our work was to determine the conditions under which a bimetallic catalyst would have properties that are tunable as a function of composition. Remarkably, very similar alloys, Au/Pt and Au/Pd have completely different tunability properties as a function of composition for hydrogenation reactions. The underlying chemistry was understood in a theoretical and experimental study.[xi]

In the area of battery materials, the degradation process of lithium-rich cathode materials were studies computational in terms of the phase transformation that can occur from an active to an insert phase, as well as ways to prevent this deactivation.[vi] Interestingly, we also found that a structural transformation in Li_2MnSiO_4: is actually reversible, even threw a disordered phase – a phenomena that has not been understood in the literature. In the area of Li-S batteries, we helped to design Cu-Sn-S nanotubes with high lithiation and delithiation performance.[v]

The Moncrief Award allowed me to organize a three-month long program at IPAM entitled “Complex High-Dimensional Energy Landscapes”. This program included four week-long workshops focusing