Executive Summary

The performance of materials in extreme environments is central to a number of national security challenges, including especially the need for sustainable energy solutions. From fission & fusion energy to nuclear weapons to a broad suite of renewable challenges, a science-based approach to certifying materials performance for extended lifetimes is needed. The need to develop materials that perform in new and more extreme environments is also acute. Put simply, we lack sufficient confidence in the materials we have to reliably predict or extend their lifetime. Materials often fail at one tenth or less of their intrinsic limit and we do not know why.

There is great potential to change this reality. Materials research is on the brink of a new era of science in which the traditional approach of observation and validation of materials performance is replaced by prediction and control of materials functionality. Progress in this endeavor will enable a new generation of materials solutions from a more reliable nuclear stockpile to paths to higher efficiency clean energy technologies. The urgency of the challenge extends beyond the benefits from the envisioned end uses: the next generation of materials qualification facilities is presently being contemplated and designed with known materials. Near-term progress can yield smarter, more effective facility designs as well as higher performing materials.

Against this backdrop of urgent mission need and high scientific potential, a workshop of approximately 100 international leaders in materials research was convened in Santa Fe, New Mexico in December, 2009, to explore "Decadal Challenges in Predicting and Controlling Materials Performance in Extremes." While a number of recent workshops have recognized the challenge of materials in extremes, far fewer have focused on the means to meet this challenge. Therefore, the present workshop emphasized specifically needed capabilities and tools to seize the opportunity.

To achieve the vision of prediction and control of materials functionality, workshop participants recognized that a key grand challenge is the ability to predictively manipulate microstructures to achieve desired macroscopic performance. Central to this challenge is the potency of defects, either to be exploited intentionally for enhanced performance or to suffer their deleterious effects. The role of defects is a microcosm of the broader impact of rare events and fluctuations that are a key stumbling block in achieving prediction and control: the extremes of heterogeneity in a material dominate performance at the expense of the homogenous bulk. Considering only the time- and space-averaged properties of an "ideal" material is inadequate; the complexity of "real" materials must be embraced.

Further, while the era of 'cook and look' Edisonian materials discovery is largely behind us and 'directed serendipity' is a potent engine of materials discovery, there is a key difference between 'prediction and control' and 'more cooking' and 'more looking' or even 'looking while cooking.' The seamless integration of theory, observation, and synthesis is required to achieve desired functionality and accelerate materials discovery by design.

The vision of prediction and control will only be achieved through the development of in-situ, real-time, multi-probe “tools” (including advanced theories and information science and technology methods, high performance computing, advanced measurement capabilities, and controlled environments) to enable dynamic, in-situ measurements of real materials in real environments.

A final element of the challenge relates to the workforce required to achieve success. Predictive control of materials functionality lies at the boundary between ‘science’ and ‘engineering’ and requires the integration of multi-disciplinary teams that span traditional ‘chemists’, ‘materials scientists’, ‘physicists’, etc. This approach necessitates broader education and training for materials researchers in which the focus is not structure→ property relationships, but rather property→ structure relationships.

In the end, workshop attendees enthusiastically concluded that achieving the grand challenge of prediction and control of materials performance in extremes was within our reach. The workshop helped to identify a roadmap of capability gaps that need to be addressed. This report documents the fruits of those efforts.