Summary of Panel Discussions

The panel was chaired by John Prater and Eliot Fang with participation from all available invitees of the workshop. The Panel discussed both short-term mission-oriented and long-term basic science needs. The consensus was that a balanced focus on basic research with relevance to mission is the way to go. The Panel Discussions have led to the identification of two grand challenges and suggested solutions.

The first challenge is represented by the lack of knowledge in non-ideal defect structures of ionic solids such as ferroelectrics. Defects - including interfaces, dislocations and point defects - are of particular importance in affecting or even dictating performance of ferroelectrics systems. In most quantum mechanics calculations, and atomistic simulations in general, ideal structures of interfaces and other defects are the prototype. However, actual and experimentally verifiable structures (instead of the ideal ones) are largely unknown. A possible solution is to bring in the growth and mechanics expertise to study how the defect structures form from synthesis. The non-idealized defect structures further serve as the basis for studies of their effects on performance.

The second challenge is the lack of mechanism to integrate expertise across multiple scales, and between experimentalists and modelers. It is recognized that modelers often pick the experiments that support a particular model, even without knowing the details of experimental conditions or artifacts. A team or network that truly encourages experimentalist-modeler collaboration will be very beneficial. Further, the modeling element can benefit from integration of expertise across multiple time and length scales. The Panel considers the DoE/BES Computational Materials Science Network as a good example. There is a general agreement among the panel members, including scientists and program managers, that a similar Network within Army Research Office would be desirable.