Joint Industry Research Needs[1] and
A Proposed Framework for Collaborative Research
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Abstract

In 2003, the US Chemical Industry Vision2020 published a nanotechnology research needs roadmap[1], and in 2004 the US Semiconductor Industry independently published a nanotechnology research needs document. While many of the research needs identified in these roadmaps were very different, both industry groups identified the need for fundamental understanding and modeling of synthesis and material properties that can integrate from the atomic scale through the macroscale and over multiple timescales. In 2005, a work group between the Chemical and Semiconductor Industries was formed to identify common research needs.

On May 24-25, 2006, the Chemical Industry Vision 2020, and Semiconductor Research Corporation held a meeting at the National Institute of Standards and Technology (NIST) with university, national laboratory and industrial researchers to identify the critical needs for developing improved nanomaterial models for predicting structure, composition and properties.

High-performance materials applications require simultaneous optimization of multiple properties such as electronic, mechanical, surface chemical reactivity, and others. Some nanomaterials possess unique properties that make them candidates to enhance or replace conventional materials and approaches, but the need for optimization of multiple properties requires models that correlate nanostructure to properties.

Examples of these joint needs to optimize multiple properties include low dielectric constant materials for chip level interconnect isolation, chemicals and polymers with improved control of purity and properties, and controlling chemical reactivity of carbon nanotubes. Our industries are seeking an ultra low dielectric constant material with high mechanical strength, no water absorption, and excellent adhesion to multiple surfaces. Similarly, the semiconductor industry needs organic molecules and polymers with tighter control of properties and the chemical industry uses nanostructured catalyst to control the molecular weight of polymers and the purity of organic chemicals. While these examples represent a few of the common nanomaterial needs, the modeling capabilities identified in this document could be used for many joint nanomaterials, and for optimizing nanomaterials for many other applications in each industry.

Both industries agree that predictive models are needed for: optimization of the *synthesis of nanoparticles, surface chemical reactivity, electronic and transport properties, nanomechanical properties, and properties of self-assembled materials*. These modeling needs include:
Cross Cutting Modeling Needs: Several common themes cross all model areas:
1. Innovative algorithms to model over multiple length and timescales for realistic system sizes
   -More foundational long term algorithm development is needed
2. Close collaboration between modelers and experimentalists to design experiments and validate models
3. Systematic experiments that develop fundamental understanding
   -Experiments that are on a scale that models can duplicate
   -Metrology to characterize structure and properties of materials at the nanometer scale with analysis to decouple probe-sample interactions
4. Modelers need increased access to high speed computing capabilities
5. Guidelines to improve portability of models on existing operating systems and hardware platforms

Since these needs were identified, other industries have identified that these capabilities are needed. This presentation will summarize a joint set of strategic modeling and characterization needs that are shared by multiple industries, and propose a framework for collaboratively engaging industrial, academic, and government research communities.

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[1] D. Anthony, M. Garner, D. Herr, Joint Chemical & Semiconductor Industry Research Needs for Modeling of Nanomaterials: Chemical Industry Vision 2020 & Semiconductor Research Corporation/SNB Consultative Working Group 2, September, 2006.