Breakout Report on Electronic and Photonic Materials

Identification of Grand Challenges

Breakout Electronic and Photonic Materials

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Meeting Timeline

- 6/25 Breakout plenaries
- 6/25 Brainstorming on Grand Challenges, keeping in mind the following three questions
  - *“If materials scientists could ________, then new pathways of ________ materials discovery would be possible.”*
  - *“If materials scientists could ________, materials/product engineers would be able to ________.”*
  - *"Materials/product engineers need to be able to ________, which materials scientists could enable by _________."*
- 6/26 AM Brainstorming—Sort ideas into categories, refine
- 6/26 AM Brainstorming—Priorities

Background of the Challenge

- The Electronics (photonics) Industry is exceptionally large and, in many crucial respects, a mature field of technology.
- The sophistication of the technology is without peer in modern commerce—the manufacturing processes provide the most complex objects constructed by human beings at vast scales and extremely low cost.
- It is by its nature capital intensive and difficult to effect paths of nearer-term progress.

Still, Challenging Opportunities Abound

(an incomplete list)

- Provide a Useful Design and Scalable Technology Path for a Post CMOS Electronic Switch
    - To go beyond the performance capabilities of the 5nm feature width world with less requirements for power consumption than has been possible to date?
- Provide a Useful Design and Scalable Technology Path for PV with Module Performance at the Shockley–Queisser Limit
    - Single pn-junction Silicon PV with a module level performance reaching 33.7%?
- EE (ubiquitous deployment of electronics everywhere)
- …

Challenges for MGI in this Space

- Establish transformational synergies between advances in Theory/Computational Modeling and Experiment to accelerate useful outcomes in technology.
- Define features of materials and modes for their their functional integration—where properties often emerge from the nature of forms of integration—that most beneficially promote desired requirements for performance.

An Essential Need for Advances in Theory Meshed with Experiment

- A database of calculations on relevant materials for electronic and photonic applications can be of substantial value, particularly for surfaces and interfaces. Further advances in first principles theory are needed to provide guidance on many crucial properties, including excited state energies and lifetimes, defects and traps, barriers to diffusion and reaction, surface states, nonradiative electron-hole recombination, electron transfer and quantum confinement. It is essential that the development of next generation theory goes hand-in-hand with experiments designed to provide challenging quantitative tests of theory.

An Essential Need for Advances in Modeling Meshed with Engineering Development

- There exists a need for significantly better models at all scales, and property-based data to support them, that can treat important forms of complexity that will be important in next generation technology in ways that accelerate development and reduce cost. These include models treating: nonlinear properties, anisotropy, inhomogeneity, non-equilibrium states/organizations, synthesis/growth, …

Grand Challenges

(in no special order…)

1) Predict excited states, transport, and non-equilibrium structures in electronic materials

2) Demonstrate highly accurate theories and methods for modeling electrical/optical properties of materials in structures below 10nm.

3) Establish models for prediction of the full-device/emergent/system properties using inputs from materials properties, modes of integration, processing history, structural/defect attributes, and spatial/geometric features.

4) Implement means that progressively validate, and render transparent, materials-centric databases—facilitating understandings rather than providing data.

Other challenges, less grand

- Establish a database of material properties including various aspect of performance
- Modes of experiment and modeling conjoined research to facilitate transition from a function directed design to an optimized full system prototype
- Facilities that enable the above.
- Models for the prediction of the part-to-part variability of production devices as a function of material features and processing.
- Models for the prediction of the properties of a devices/circuits/electronic systems at production scale using only information obtained at research scale.

Breakout XYZ

"If materials scientists could ________, then new pathways of ________ materials discovery would be possible."

If materials scientists could ________	Then new pathways of _____materials discovery would be possible
Develop accurate physical descriptions and models for interfaces	Electronic and photonic
Establish a database of topological insulators	Design new, smaller devices
Establish a facility for rapid prototyping and/or "filling in the blanks" in the existing databases of materials properties	Assessing an increasing range of options in

Use as many slides as needed

Breakout XYZ

"If materials scientists could ________, materials/product engineers would be able to

If ~~materials scientists~~ could ________	Materials/product engineers would be able to _____
Predict interfacial properties	Design advanced electronic devices in half the time
Predict device structure and properties based on synthesis	Optimize devices more quickly
Develop integrated simulation/data-based tools that predicts synthesis to performance	Design advanced electronic devices in half the time
Model and measure recombination losses at extended defects	Predict real-life manufacturing and performance

Breakout XYZ

"If materials scientists could ________, materials/product engineers would be able to ________."

If materials scientists could ________	Materials/product engineers would be able to _____
Predict processing/fabrication paths to produce desired devices	Could shorten the design cycle
Identify material processes and model synthesis and processing pathways in device geometries	Shorten device design an optimization
Predict the effects of defects on performance	Accelerate design and manufacturing
Conduct research with industrial participation	Better narrow down selections suitable for production with shorter time to market
Solution processable materials that mimic evaporative materials	Low cost, large scale printable, flexible electronics

Breakout XYZ

"Materials/product engineers need to be able to ________, which materials scientists could enable by __________."

Materials/product engineers need to be able to ______	Which materials scientists could enable by ______
Accelerate both computational and experimental materials discovery	Developing a searchable database of interface and thin film properties

Some Specific Challenges

- 1) Predictive and accurate theories for excited states and non-equilibrium structures in electronic materials
- 2) Highly accurate theories and methods for modeling electrical/optical properties of materials in structures below 10nm.
- 3) Models for prediction of the full-device/circuit/system properties using inputs from materials properties, modes of integration, processing history, structural/defect attributes, and spatial/geometric features.
- 4) Models for the prediction of the part-to-part variability of production devices as a function of material features and processing.
- 5) Models for the prediction of the properties of a devices/circuits/electronic systems at production scale using only information obtained at research scale.
- 6) Means that progressively validate and render transparent materials-centric databases—facilitating understandings rather than providing data
- 7) Modes of experiment and modeling conjoined research to facilitate transition from a function directed design to an optimized full system prototype
- 8) Facilities that enable the above. (more a need?)