SunShot
U.S. Department of Energy

SunShot Energy Materials Network (EMN) Workshop

Break Out Summaries

Crystal City Marriott
Arlington, VA

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Break Out 1

Break Out 1 Questions

- What research challenges for the development of durable PV modules can be addressed using “materials genome” approaches?
- What are the specific strengths and weaknesses in applying MGI techniques to applied technology development, with a goal of market impact in the near term (5-10 years)?
- What are the metrics that are required in order to understand how to design materials solutions?

Question 1

- What research challenges for the development of durable PV modules can be addressed using “materials genome” approaches?
  - Potential problems – PID, yellowing, adhesion, cell cracking, wire fatigue, solder bond failure
  - AR coatings on glass and cell - durability
  - Up-converters and Down-converters
    - More similar to the successes in organic absorber work
    - On glass coatings or in encapsulant
  - High throughput, automated measurements of properties and degradation
  - Impurity sensitivity of encapsulants, fluxes, glass surfaces
    - Yellowing, PID
  - IR rejection (reflection, conduction, emissivity) to lower temperature
  - Conductive adhesives with stable contact resistivity
  - Moisture barriers and solubility of moisture
  - Materials changes to allow higher voltage operation
  - Materials and designs to allow lighter panels
  - Recyclability (re-usability) of panels after end of life

Question 1

- What research challenges for the development of durable PV modules can be addressed using “materials genome” approaches?
  - More digital data (DB) related to existing experimental data (e.g. encapsulant degradation, solder bond degradation)
  - Computational tools on panel, interface, and degradation level, including the 4 stressors (e.g. impact additives on EVA degradation)
  - Integration from materials to application modeling (ICME) and creating DB allowing all disciplines to interact and use these DB
  - High-Throughput experimental tools on panel, interface, and degradation level, including the 4 stressors
  - Materials by design (e.g. solder phase diagrams, encapsulants structure-property relationship)
  - Models need to include climate specific panel design and parameters relevant to the materials (yellowing, WVTR, etc.)

Question 1

- What research challenges for the development of durable PV modules can be addressed using "materials genome" approaches?
  - Multi-material system analysis is challenge. How can we predict performance of the system? It is easy to design one material, but designing a binary of surface system is harder. Predicting ageing of that system is even harder. Example: acid development under EVA. That means they did not predict correct operating conditions and did not understand;
  - Defining the functional requirements are a start point. A lot of times, for material, we just use "standard" material (for example, conductive = metal) – but there could be other material systems. So, if we provide functional specs (even including costs) to researchers. Then they can use MGI to define a fitting set of material.
  - Accelerated testing methods still need validation. Different types of fatigue. Not only for solder joints but for wind as well. We'll have intermediate, mild and strong wind gusts. Can we bring this analysis into NGI ? Can we learn that from analysis from MGI or other industries.
  - About 50 years lifetime: do we need to come with a completely new set of requirements? Can this be defined through MGI ? How do you figure out materials that can support that?
  - Bottleneck is learning what exists in other industries and assembling the data. Some of our functional requirements may be close to other industries. There's enormous amount of glass fracture collected by NASA – does anyone in PV use that data. It's not only the material – but HOW you processes and compositional variations , that general and generic properties may be not applicable.

Question 1

- What research **challenges** for the development of **durable PV modules** can be addressed using “materials genome” approaches?
  - Context questions/challenges:
    - Need to identify most important specific target specs/properties, not only of individual materials, but interfaces, cross-couplings, and correlations – might use data collection, aggregation, and statistical sampling to discover these
    - Possible critical parts (module-related): interconnect, encapsulant, ARC, TCO, etc. (of course not necessarily in isolation)
    - Data generation and mining is one approach and can be challenging, probably without having complete coverage over search space (DoE, importance sampling, etc.)
    - System vs component requirements (e.g., module efficiency or lifetime vs ARC reflection over time)
    - Agnostic to absorber (but module issues are sometimes is absorber-dependent or cell-dependent) → broaden DOE emphasis to new absorber materials; perhaps allow for cell-dependence of proposed work
  - Specific challenges:
    - Electrical, optical, thermal, etc.: Module lifetime is the main goal, but do we know enough fundamentally to understand long-term degradation?
    - Flexibility of topic to optimize module materials for possible new absorber platforms, etc. (methodology and open to new ideas within generic “module” paradigm) → let’s explicitly not focus mostly/only on Silicon
    - Essential to collaborate with industry to remain relevant to real-world & enable validation, etc.
    - Short-term vs long-term goals

Question 1

- What research challenges for the development of durable PV modules can be addressed using "materials genome" approaches?
  - Separate intrinsic from extrinsic (engineering) properties & look for synergy and input from industries
  - Articulation of "design principles or descriptor" or what is needed based on performance needs/wants : translating durability into MGI language; How to translate durability into MGI language
  - How to incorporate synthesis into MGI
  - Multiscale. Using atomistic into device level
  - Development of accurate validated accelerated testing experiments and computations that is validated and accepted by industry, how to incorporate / determine relevant mechanisms
  - Develop/determine the mechanisms that cause actual degradations, eg. Cracks, snail tracks, …
  - Getting data from mfgs re cell manufacturering details on module conditions and relation to long/short term failures

Question 1

- What research challenges for the development of durable PV modules can be addressed using “materials genome” approaches?
  - Development of models that can take materials inputs / module architecture and determine module lifetimes.
  - Lack of knowledge of **interfaces** plus materials
  - How does MGI quickly develop experience with PV relevant materials?
  - Can we use knowledge of degradation mechanisms to develop improved materials
  - How can we use knowledge from other fields to inform relevant models
  - Development of approaches to account for interactions of materials
  - Can we take lots of data -> specific (limited) degradation models and broaden
  - Modelling and validating crack formation at low & high levels
  - Mining existing reliability data

Question 2

- What are the specific strengths and weaknesses in applying MGI techniques to applied technology development, with a goal of market impact in the near term (5-10 years)?
  - Limitations – incorporation defect & impurity effects
    - e.g. – chlorine contamination in EVA resin
  - Simulation vs modeling – Modeling is more relevant to properties that we are interested in than simulating
  - IP issues. How work on a precompetitive basis with shared resources that are too expensive for each company to purchase.
  - Process and recipe (reaction pathways) is critical to any material properties
  - Many properties are required and larger scales (microns) than can be easily modeling
  - Data sets used for modeling are “dirty”
  - Encapsulant degradation has so many interactive effects that MGI may not be appropriate
  - Chemical simulation and modeling doesn’t capture the mechanical issues in the modules. Expand MGI to include large scale structural stress-strain analysis? Optimize material properties for a particular module design. Systems level analysis methods are needed. Comsol example.
  - Difficulty in capturing cost. E.g. – could keep pushing back toward silicone

Question 2

- What are the specific strengths and weaknesses in applying MGI techniques to applied technology development, with a goal of market impact in the near term (5-10 years)?
- Weaknesses:
  - 1. Only basic properties are accessed right now. . A lot of points of interest are intrinsic properties at the beginning of life. Durability and/or lifetime performance is not one of the functional parameters to be studied or identified by MGI as of now. That is extremely needed if we are to access durability and/or lifetime
  - 2. Proprietary of confidential information is not shared or there are significant barriers for sharing. A LOT of outcomes are VERY dependent on process and formulation variation.
    - => Opportunity from this weakness: Can there be a mechanism to "carefully share" confidential and proprietary data. Processor manufacturers set up something similar for "co-design" for future chipsets. May be a similar framework. This can be exactly the job for national labs. So DOE may need to step in and standardize.
  - 3. "Information overload". One of our goals should be to draw a "boundary" around a set of functional requirements and material properties that *may* be relevant to PV industry (without, accidentally, throwing away any that might be of interest). Therefore, information overload again.
- Strength:
  - 1. A vast variety of materials and material systems available for analysis.
  - 2. DOE and national labs need to define a set of requirements for MGI to define a search space – and to define a realistic search space without information overload. Can we break down a set of questions for MGI that can be classified as "generic" search spaces. And some data may already exist – National Labs may need to compile all the relevant data
- One of the research challenges is mapping out criteria or specifications? All Sunshot goals are centered around LCOE. We need to translate relevant LCOE metrics into relevant properties ? For example: Glass properties: adhesion, transmission, etc.
- How can we look at original manufacturing flaws that can percolate through lifetime and manifest themselves in various issues. Industries are afraid of high tech technologies. How would you use this techniques to reduce LCOE? And who should do this analysis?

- **What can MGI of “Materials by Design” try to address?**
  - Try not to miss candidate materials
  - Accelerate their adoption

Question 2

- What are the specific strengths and weaknesses in applying MGI techniques to applied technology development, with a goal of **market impact in the near term** (5-10 years)?
  - Strengths:
    - Methodology is very widely applicable
    - Can address both inorganic and organic components, as well as the coupling between them, but…
  - Weaknesses:
    - Possible need to generate new “forward models” or descriptors as proxies for the important properties, which may be unknown presently → maturity of technology provides a spectrum of existing knowledge on the key problems & target specs
    - Method development needed for some of the novel challenges in pertinent module-level
    - MGI terminology may be misinterpreted by many people, so that a FOA should be explicit about breadth of approach

Question 2

- What are the specific strengths and weaknesses in applying MGI techniques to applied technology development, with a goal of market impact in the near term (5-10 years)?
  - Incorporate Multiscale, multiphysics, interfaces; is this tractable?
  - Development of validated model of degradation, with known mechanisms
  - Focused so far on low level (atomic) and thermodynamics; how to incorporate kinetics
  - how do you quantify uncertainty in models (DFT, …)
  - Lack of knowledge of failure mechanisms in modules & how these change in time/environment
  - Top-down vs bottom-up or middle-out relevant to degradation
  - Lack of accuracy at DFT level + others for some properties
  - Accounting for chemistry, reactions beyond two molecules
  - (+) MGI can allow simplification
  - (+) brings interdisciplinary , coupled researchers to address problems
  - (+) data mining fro existing data
  - What questions can MGI answer?

Question 3

- What are the metrics that are required in order to understand how to design materials solutions?
  - Encapsulation discoloration vs UV exposure
  - Solder bond breakage vs dynamic loading
  - How likely to crack cells vs module load
  - Power losses vs various stresses
  - How likely is it for moisture to enter
  - AR optical properities and durability vs chemical and abrasive forces
  - Module operating temperature
  - Lowest cost

Question 3

- What are the metrics that are required in order to understand how to design materials solutions?
  - Durability, (before and after stresses)
  - Adhesion,
  - Interaction with other materials and material systems.
  - Surface properties and surface chemical dynamics
  - Interaction processes and characteristic with unexpected material systems (such as salt brine, etc)
  - Which material(s) may lead to “set-and-forget” operation – i.e. requiring lowest or no maintenance.
    - Example: which materials can be intrinsically soiling-resistant?
  - A separate metric: timeliness of the analysis (results should not take longer to achieve than our current experimental approaches or waiting 5-10 years. As we generate more data, analysis will start taking longer and longer….),
  - And finally, will our environment will change in 50 years due to global warming? And should we worry about that?

Question 3

- What are the metrics that are required in order to understand how to design materials solutions?
  - Heterogeneous materials systems → an important core concept
  - Metrics
    - Degradation rate, lifetime metrics
      - How to predict lifetime? How to improve predictive ability of accelerated testing?
    - Some other examples: dielectric breakdown, corrosion, cracking, dust/obscuring defects, shadowing tolerance, etc.
  - Let PI's define some of the metrics (can be hypotheses)
  - Cell may need to be an intimate part of the module discussion, not explicitly separated out
  - Better power transmission: May be important to consider the whole power plant, which is a level above even the module
  - Improved LCOE should be evident in proposed solutions

Question 3

- What are the metrics that are required in order to understand how to design relevant solutions?
  - Be specific to some problem/mode – eg. Interface stability, transport through barrier,
  - Hard to state b/c market dependence, environment,
  - Really LCOE, but EMN not measure
  - Define standard conditions for durability

Break Out 2

Break Out 2 Question

- Are there gaps in the current U.S. capabilities that need to be addressed in order to develop new durable PV module materials that reduce the cost of PV energy?

Question 1

- Are there gaps in the current U.S. capabilities that need to be addressed in order to develop new durable PV module materials that reduce the cost of PV energy?
    - Gaps are not just MGI
    - Independent source that test finished product wrt durability / reliability
        - outdoor testing, need for multiple test centers, 2 years +,
    - Models connecting tech changes to LCOE changes projected to production
    - Models connecting in-module functionality to designable material property spec
    - Access to high-qualility bidirectional models connecting module design and materials properties
    - Facile access to relevant testing not available in-house at PV companies
    - Too few people working on hard relevant but not high-profile materials (eg. solder bond stability)
    - Lack of effecting Matchmaking the between the people with the technical issue and the problem solvers
    - Much more effort on glass replacement
    - Rapid effective degradation testing that maps to long term durability
    - Lack of easy access to relevant existing data for relevant issues

Question 1

- Are there gaps in the current U.S. capabilities that need to be addressed in order to develop new durable PV module materials that reduce the cost of PV energy?
  - **Computational Technique improvements to study defects and impurities in modules**
  - Environmental conditions data
  - Big scale gaps: Missing secondary components of modules (solar cells)
    - Optical coating for many DFT people
  - Mechanistically tied durability tests (real word examples moisture etc.)
  - **Understanding the temporal evolution from single property to understanding degradation pathways**
  - **Ability to model whole devices**
    - Exoscale computing resources high-performance computational

Question 1

- **Are there gaps in the current U.S. capabilities that need to be addressed in order to develop new durable PV module materials that reduce the cost of PV energy?**
  - Knowledge gap:
    - packaging/interfaces not treated scientifically
    - extrapolation of time scales for degradation
    - exact structure and components of multi-component complex materials (e.g. EVA)
    - history of modules
  - Research capability gaps:
    - accelerated testing
      - standardized facility/protocols
      - environment-dependent standards
      - active-material dependent standards

Question 1

- **Are there gaps in the current U.S. capabilities that need to be addressed in order to develop new durable PV module materials that reduce the cost of PV energy?**
  - Research capability gaps (cont'd):
    - combinatorial interface studies
    - in-situ monitoring/characterization of degradation mechanisms
    - "digital-twins"
    - module architectures and component integration
  - Manufacturing capability gap:
    - on-boarding new absorbers: scale up & commercialization (avoid "chasm")
    - in-situ monitoring/characterization of synthesis

Question 1

- Are there gaps in the current U.S. capabilities that need to be addressed in order to develop new durable PV module materials that reduce the cost of PV energy? What unique capabilities could be built
  - **Strong computing capabilities, to correlate properties and materials, to process the vast quantities of data that can be collected.**
  - **Model development: that can interconnect length and time scales.**
  - Develop a methodological concept that will help close the loop, experiment to computation, across scales, etc.
  - Broaden applicability of computations to varied scales, couple DFT to monte carlo, etc. Develop accepted ways to combine models. So that they can talk to each other.
  - **Database building, integration, maintenance of materials properties, and physical, electrical, mechanical properties, optical properties. Figure out the data sharing aspect of proprietary data. Quality assurance. Integrate globally.**
  - Common approach to predict failures with ranking, with probabilities.
  - Technology roadmap – prioritize questions. Compare to the International Technology Roadmap for Semiconductor.

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Break Out 3

Break Out 3 Questions

- What unique capabilities could be built as part of a consortium focused on module materials, and how could these be leveraged to encourage innovation in the PV module and system space?
- What relevant data sets already exist and how could a consortium leverage other research centers to develop durable module materials that reduce the cost of PV energy?

Question 1

- What unique capabilities could be built as part of a consortium focused on module materials, and how could these be leveraged to encourage innovation in the PV module and system space?
  - Ability to demonstrate improvements in new module materials. Prof of concept scalabilty
  - Link of field system properties, processes to accelerated testing.
  - Manufacturing capabilities, sharing resources across natl labs, academia, industry.
  - A route to validate new materials: for upsteam suppliers, downstream users
  - A manufacturing proving ground, full scale – gets you across the trough of despair in development pathway

Question 1

- What unique capabilities could be built as part of a consortium focused on module materials, and how could these be leveraged to encourage innovation in the PV module and system space?
  - Connecting issues to solvers
  - Create ModuleMaterials.org
  - Timely techno-economic modeling – online tools ?
  - No cost to customer consulting
  - Access to relevant experimental capabilities

Question 1

- **What unique capabilities could be built as part of a consortium focused on module materials, and how could these be leveraged to encourage innovation in the PV module and system space?**
  - Roadmap on packaging and complete PV system
  - Module fabrication & scale up facility
  - Failure testing capabilities industry does not have
  - Industry & research community agreed-upon metrics
  - Long-term databases with built-in security features (see Critical Materials Institute) & selective access
  - Cross-platform student training (see Semiconductor Research Corporation)
  - Streamlined usage of facilities and expertise with pre-negotiated IP agreements

Question 1

- What unique capabilities could be built as part of a consortium focused on module materials, and how could these be leveraged to encourage innovation in the PV module and system space?
  - **Create a database of recorded experimental and theoretical information that currently exists**
  - **Grand challenge to predict module stability to 50 years: GB to GWatts.**
  - Connection through European sources for access to durability data

Question 2

- What relevant data sets already exist and how could a consortium leverage other research centers to develop durable module materials that reduce the cost of PV energy?
  - NIST on polymer degradation
  - Adhesion
  - Granta Design (metal alloy database)
  - materials.nrel.gov, materialsproject.org, alfowlib
  - citrine.io
  - nist ?

Question 2: What relevant datasets exists

- Regional Testing Centers
- EPRI – module reliability data
- PV Quality Assurance Taskforce
- Norskov – template for data submissions to create database
- Historical weather database
- Cost of electricity dataset
- Proprietary datasets, industry-formed roadmap
- Utility scale datasets
- LED initiative

Question 2

- **What relevant data sets already exist and how could a consortium leverage other research centers to develop durable module materials that reduce the cost of PV energy?**

  (important: establishing mechanism and trust for data sharing between industry and research communities)
  - MGI computational data
  - critical material data
  - manufacturing data -- materials, cells, modules
  - accelerated testing data
  - multiple-property characterization and modeling data
  - historical performance of power plants/panels/cells
    - correlate with weather data

Question 2

- What relevant data sets already exist and how could a consortium leverage other research centers to develop durable module materials that reduce the cost of PV energy?
  - **DOE could provide information about existing facilities to PIs to reduce redundancy and wasted efforts**
  - **Materials Project, NREL, Clean Energy Project**
  - **Datasets from DOE-funded projects**
  - Standard data sets to validate new models/methods for degradation mechanism computation
  - Future ties to BES facilities data

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Break Out 4

Break Out 4 Questions

- How can a national lab-led consortia best integrate academic and industry activities and participants?

- What consortia management structure might allow for a nimble organization that can address the rapidly evolving PV industry?

Question 1

- How can a national lab-led consortia best integrate academic and industry activities and participants?
  - Industry directly input into proposals funded and shaping and materials studied.
  - How do you sustain this interest?
  - Role for academia: understanding of problems -> innovative solutions.
  - Workforce training: internships, PhD training to go to industry,
  - How do you engage industry?
  - Leveraging resources at labs to be shared with industry & labs; concierge to direct
  - Documentation for best practices.

Question 1

- How can a national lab-led consortia best integrate academic and industry?
  - Industry brings relevance +National lab- expensive expertise + capabilities. Balance science and applied target.
  - Communicate value of research
  - Need high level of trust. Honest disclosure (both industry and science)
  - Solve possible IP issues (joint or proprietary)
  - DOE EERE Hydrogen project , Critical materials interests, SSL interesting examples of successful consortia.
  - Bring the value chain/interest holders
  - Leverage with existing user facilities

Question 1

- How can a national lab-led consortia best integrate academic and industry activities and participants?
  - National Lab (one) as leader and other Nat. Labs, universities, and industry as partners.
  - Special project funding to be provided by industry members through DOE funding mechanisms
  - Benefits for Industry is access to new technologies on special arrangements and recruit well trained graduates.
  - Nat. Labs provide depth of expertise, special user facilities, data and project management.
  - Universities to provide research participants and ideas and produce future workforce members from graduates of program.

Question 1

How can a national lab-led consortia best integrate academic and industry activities and participants?

- Best way to integrate: Energy materials consortium (DuraMAT): An example - LightMAT FOA released (light weight metal alloys - a national-lab led consortium) – Entities outside consortium can compete to become a partner in the consortium – Entities will receive funding from the national lab, not DOE.
- Best way to integrate: Do we want to propose the LightMAT approach for EnerMAT as well?
  - Challenge: **IP matter** maybe stuck at the national lab. How can we address it?
  - Challenge: Consortium should be **ahead of the industry curve** to make an impact
  - Success: How can we measure the **success of the consortium**? It cannot be, for example, 20% efficiency.

Question 1

- *How can a national lab-led consortia best integrate academic and industry activities and participants?*
  - Emphasis on lowering the barrier to communication over substantial time
  - Industry wants greater access to people, not just equipment
    - Consider donation of time from both sides
    - 20% of time to lab staff, 20% of company staff (with half cost shared)
    - Consortia would get redirection to commercial relevance
  - Challenge to bring graduate students in on longer time scale, consortia may serve to string shorter projects together into a thesis project
  - Labs can take leadership on data management, where companies don't have motivation and academics don't have long time scale
  - Issue in hub is that industry has nothing to do, same issue here?
  - Just impetus to bring everyone together on a regular basis

Question 2

- What consortia management structure might allow for a nimble organization that can address the rapidly evolving PV industry?
  - Consulting service, everything under NDA
  - How to handle proprietary work?
  - How to handle FOA? Selection developed from roadmap
  - Multi structured: short-term, FOAs for mid term, longer term (3-5 yrs) FOAs, seedlings (SPRINT).
  - Selection:: industry review, who selects.
  - Industry provide input into longer term projects (yearly).
  - How to evaluate success? Ask industry members?
  - Biyearly mtgd with
  - WFO at higher TRL

Question 2

- What consortia management structure might allow for a nimble organization that can address the rapidly evolving PV industry?
  - Consortia should be flexible
  - Possibility to have user proposal + Core research.
  - Mechanism: Hub, virtual center or centrally located.
  - Management-director, sub leaders
  - Science board review every year Go/no Go decision points
  - Need a mechanism to bring new members to team

Question 2

- What consortia management structure might allow for a nimble organization that can address the rapidly evolving PV industry?
  - Industry members to provide relevant problems.
  - Solicit proposals from all partners from list of relevant topics.
  - Need to make progress toward goals in appropriate timeline (5 yrs.?)

Question 2

What consortia management structure might allow for a nimble organization that can address the rapidly evolving PV industry?

- Structure: How can we organize it?
  - What do you want the objective be? Industry input is needed to identify the specific problems – it is up to us to **develop the modeling tools** and we need to push/market the tool to the industry.
  - There should be a common goal for the industry but also specific-industry need may also be addressed; **IP-neutral capabilities** which can be used by the industrywide entities, **not for any specific entities**
  - What is the roadmap? Should it be **long-term based goals** or short-term based goals?
  - **Industry advisory committee** maybe needed to support the consortium.

Question 2

- What consortia management structure might allow for a nimble organization that can address the rapidly evolving PV industry?
  - List of national lab resources (people and equipment) available to industry
  - Works better when lab coordinator/concierge selects the project, more nimble
  - Companies cost share but don’t have to cover lab’s cost share
  - Fraunhofer model, graduate student dedicated to an instrument interacting with all parts
  - Perhaps consortium can be used to move standards forward by getting input from lab, academia, and industry.
    - Not just standards for module but each component/material