Extended Final Report:

Challenges in Photovoltaic Science, Technology, and Manufacturing:

A workshop on the role of theory, modeling, and simulation

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An NSF-sponsored workshop organized by

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Executive Summary

The development of computer simulations for electronic materials and devices began in earnest in the late 1970's, and until the mid-1980's, the state of the art for simulation in microelectronics and photovoltaics was similar. Since then, however, simulation has transformed microelectronics, but the impact on photovoltaics has been modest. Today PV is challenged to significantly reduce costs to compete with traditional power sources on an unsubsidized basis. To do so, the performance of existing technologies must improve, and new technologies must be identified, demonstrated, and developed. Theory, modeling, and simulation (TMS) currently play important roles in photovoltaic research and development, but to achieve PV's ambitious goals, TMS must play a larger role.

The workshop objectives were to: 1) Identify key successes and future technical challenges, 2) Discuss the current status of TMS in photovoltaics, 3) Identify critical challenges and key opportunities for TMS, 4) Discuss models for multi-disciplinary research, software development and dissemination, and industry-university cooperation, and 5) Identify key opportunities for TMS to advance PV research and development. The unique aspect of this workshop was its breadth. It was not directed at the modeling community or at a specific technology, but, rather, engaged the broad PV community. Participants came from academia, national laboratories, and industry and represented a wide range of expertise, disciplines and technologies. The workshop provided a forum for lively discussions about how TMS can more effectively address the challenges and opportunities in photovoltaics.

Key PV successes and challenges. Ambitious programs in China and Germany along with continued advances in c-Si and CdTe cell performance have played important roles in expanding the PV market. Notable advances in other PV technologies have also occurred, but alternative technologies may find it increasingly challenging to compete with the cumulative learning curve advantage of c-Si and CdTe for utility-scale deployment. Strategies for advancing PV must recognize the rapidly increasing size and scope of the PV industry.

Current status of simulation in photovoltaics. <u>Developing a model is a process of understanding a problem</u> ("modeling = understanding") and is valuable itself while also providing a vehicle for educating those new to PV. Simulation is commonly used in PV research and by several companies for process and device optimization. Online tools from NREL are widely used by PV system designers and analysts, and NREL increasingly couples simulation with characterization. Universities also provide PV simulation tools to the research community.

Key challenges for TMS. Compared to microelectronics, PV is challenged by the breadth and complexity of materials, which leads some to conclude that PV is "too technology specific" and "too complex to model". The wide range of technologies makes it difficult to develop standard simulation platforms. Existing tools have several limitations, such as treating complex, nanostructured materials and interfaces and treating photons and electrons on an equal footing. First principles-based models have a long history of treating bulk materials, but until recently, the complexities of interfaces have not be considered. Most importantly, connections from first principles to device-level models and then to compact circuit models are not well established. Physics-based compact models are lacking, and models to treat reliability and statistical variations are needed.

Models for research, software tool dissemination, and industry-university cooperation. NSF programs to support multidisciplinary research in centers and small groups provide successful models for the kind of research needed for PV. Platforms such as nanoHUB have proved effective in providing problem solvers with "finger-tip" access to simulations. The Semiconductor Research Corporation and the DOE's new Bay Area PV Consortium provide a set of best practices for industry-university research.

Opportunities for TMS. In research, the development of first-principles treatments of interfaces is needed as is the development of multiscale approaches to link first principles simulations to device level simulation. New tools that treat photon and electron management on an equal footing could also have great impact, and there is a pressing need to couple simulation more tightly with characterization. In manufacturing, the development of an end-to-end capability that comprehends statistical variations and reliability and relates material properties and device performance to PV system performance could have significant impact in PV manufacturing. Achieving these goals in a technology agnostic way that engages the entire PV community and leads to the creation of common platforms for community development should be an objective.

As the history of microelectronics shows, simulation-driven research, development, and manufacturing can have enormous impact. With the right programs that engage the entire community TMS can contribute make significant contributions to the advance of PV technology.

Table of Contents

1. Project Overview

Computational modeling is a well-established field of research with a broad range of applications in research and industry. Theory, modeling, and simulation play important roles in photovoltaic research and development, but today photovoltaics is challenged to significantly reduce the cost. To do so, efficiencies of existing technologies must be substantially improved, and new technologies identified, demonstrated, and developed. To achieve these ambitious goals, theory, modeling, and simulation must play a larger role. The objectives of this workshop are to: 1) Identify the key technical challenges in photovoltaics, 2) Identify the current state-of-the-art and state-of-practice of theory, modeling, and simulation in photovoltaics. 3) Identify successful models for multi-disciplinary research, software development and dissemination, and industry-university cooperation, 4) Identify key intellectual and computational challenges in multi-scale, multi-physics, and multi-disciplinary materials to modules PV simulation, 5) Discuss opportunities and approaches to increase the effectiveness of TMS in photovoltaics. The unique aspect of this workshop is its breadth. It is not directed at the modeling community or at a specific photovoltaic technology, but, rather, at engaging the broader PV community of theorists and computational experts, academic and industrial research, across a range of disciplines and technologies in a discussion about how theory, modeling, and simulation can more effectively address the challenges and opportunities in photovoltaics.

This project provides funding to support a workshop on "Challenges in Photovoltaic Science, Technology, and Manufacturing: A workshop on the role of theory, modeling, and simulation." The 1.5-day workshop was held on August 2-3 at Purdue University in West Lafayette, IN. The workshop was co-chaired by Mark Lundstrom, Purdue and by Robert H. Havemann Energy Research Initiative, Semiconductor Research Corporation). The co-chairs were assisted by a steering committee. The expected outcome of the workshop was a clearly articulated strategy programs to address the challenges and opportunities of theory, modeling, and simulation in photovoltaics.

2. Workshop Description:

2.1 Plans for the workshop

Over the 2011 – 2012 academic year, plans for the workshop were developed and finalized in collaboration with an organizing committee consisting of:

Mark Lundstrom, Ashraful Alam, Peter Bermel, and Pankaj Sharma -
Network for Photovoltaic Technology, Purdue University
Bob Havemann, Energy Research Initiative - Semiconductor Research Corporation
Michel Frei, Applied Materials
Jeff Neaton, Lawrence Berkeley National Laboratory
Ali Javey and John Benner, Bay Area Photovoltaic Consortium
Bill Tumas, National Renewable Energy Laboratory

The workshop was designed to be focused, informal, and to address the following questions:

- How can theory, modeling, and simulation (TMS) accelerate progress in photovoltaics?
- What are the specific opportunities?
- What should the PV community do to address them?

The meeting was designed to be small (about 50 people) with equal representation from the TMS and experimental communities and strong representation from industry and government as well as academia. NSF funds were used to support the travel of a limited number of participants from academia – participants from industry and national labs covered their own travel costs.

The meeting consisted of short presentations, lively discussions, a breakout session and report of overall conclusions. The workshop dinner highlighted the nanoHUB's success in disseminating and sharing simulations globally. Individual talks (15 minutes + 5 for Q and A) set the stage for discussion. Speakers discussed broad trends, key challenges, and identified opportunities – rather than reporting on their latest research. A 40-minute panel discussion followed each session and engaged the speakers and audience as well. A 90 min. breakout session on the morning of day 2 drew conclusions from each of the panel discussions, made connections between panels, and formulated overall recommendations. The workshop wrapped up with a 60-minute discussion to identify key challenges, opportunities, and strategies. The desired outcome of the workshop was a clear and compelling report that identifies key opportunities, challenges, and strategies for addressing critical issues in PV through TMS.

2.2. Workshop Format and Agenda

The workshop drew a strong set of participants and resulted in much sharing of wisdom and experience. Attendance was 83 with 34 of the participants being faculty members from 14 different universities, 10 being representatives from the photovoltaic industry, and 11 representing national laboratories. Several (28) students from Purdue also attended and assisted in conducting the workshop. The discussions both during the presentation part of the program and during the breakout sessions were lively and interesting. Most of the workshop presentations are available at the workshop website: https://nanohub.org/groups/PVWorkshop

The agenda for the workshop is listed below, and a list of attendees is attached as an Appendix.

Thursday, August 2
Opening Session: Neil Armstrong Hall of Engineering, Room 1010

7:30-8:00AM Breakfast and Registration
8:00-8:20AM Mark Lundstrom (Purdue) Opening Remarks
8:20-8:40AM Dick Swanson (SunPower)
8:40-9:00AM Larry Kazmerski (NREL)
9:00-9:20AM Eli Yablonovitch (Berkeley)
9:20-10:00AM Panel Discussion – Steve Hillenius (SRC)

Fig. 1 Dr. Larry Kazmerski, Director of Photovoltaics at the National Renewable Energy Laboratory. Dr. Kazmerski shared his thoughts on the role of theory, modeling, and simulation in photovoltaics based on his 40 years of experience in PV. As shown here, Dr. Kazmerski is illustrating one of the earliest applications of solar cells – as a power source for the Explorer I satellite.

10:00-10:30AM BREAK

Technical Session 1:
Crystalline PV – Bill Tumas (NREL)
10:30-10:50AM Richard Schwartz (Purdue)
10:50-11:10AM Tonio Buonassisi (MIT)
11:10-11:30AM Dick Swanson (SunPower)
11:30-11:50AM Scott Dunham (U Wash)
11:50-12:30PM Panel Discussion – Bill Tumas (NREL)

12:30-1:30PM WORKING LUNCH
SERIIUS by Larry Kazmerski
SRC ERI by Steve Hillenius
BAPVC by John Benner

Technical Session 2:
Thin-Film PV – Rakesh Agrawal (Purdue)

1:30-1:50PM Vladan Stevanovic (NREL)
1:50-2:10PM Vikram Dalal (Iowa)
2:10-2:30PM Supratik Guha (IBM)
2:30-2:50PM Marcus Gloeckler (First Solar)
2:50-3:30PM Panel Discussion - Rakesh Agrawal (Purdue)

3:30-3:50PM BREAK

Technical Session 3:
Organic PV – Jeff Neaton (LBNL)

3:50-4:10PM Sean Shaheen (U. Denver)
4:10-4:30PM Gang Li (UCLA)
4:30-4:50PM M. Ashraf Alam (Purdue)
4:50-5:10PM Seth B. Darling (Argonne)
5:10-5:50PM Panel Discussion – Jeff Neaton (LBL)

6:00PM RECEPTION – Armstrong Atrium
7:00PM DINNER
Followed by Demonstration of nanoHUB and PVhub
By Gerhard Klimeck

Friday, August 3, 2012
Technical Session 4
Characterization, Modeling and Simulation – John Benner (Bay Area PV Consortium)

7:30-8:00AM Breakfast
8:00-8:20AM Dean Levi (NREL)
8:20-8:40AM Angus Rockett (UIUC)
8:40-9:00AM Jim Sites (Colorado State)
9:00-9:20AM Christina Honsberg (ASU)
9:20-10:00AM Panel Discussion – John Benner

10:00-11:30AM – BREAK and BREAKOUT DISCUSSIONS

Breakout 0: Broad Issues (ARMS 1021 Room) – B.J. Stanbery
Breakout 1: Crystalline PV (ARMS Room 1028) – Bob Havemann
Breakout 2: Thin-Film (ARMS Room1103) – Oki Guanwan
Breakout 3: OPV (ARMS Room 3109) – Jim Yardley
Breakout 4: Characterization (ARMS Room 3115) – David Ginley

11:30-12:30PM WRAP-UP
Breakout discussion leaders summarize their two slides and the audience responds.
(10 min per topic)

12:30PM – BOX LUNCHES – WORKSHOP ADJOURNS

1:30PM – Tour of the Birck Facilities – Ali Shakouri, Director

3. Workshop Report

3.1 General Approach

The workshop as a whole was organized around five themes: broad issues, crystalline silicon, thin films, organic photovoltaics, and characterization. After several plenary talks were given on each theme, panel discussions were held on the issues raised by the speakers. Afterwards, breakout sessions were used to gather and amplify key points discussed in the presentations and question and answer session, as well as to collect further information from other interested participants. Instructions to the breakout sessions were as follows:

- There was one breakout session for each of the 5 sessions (#'s 0-4).
- Speakers in each session, the panel discussion that follows each session, and the breakout session itself addressed the questions that follow – each from their perspective.
- A breakout leader (moderator), the panel discussion leader, and the session recorder conducted each breakout.
- Breakout sessions lasted 90 minutes– to refine the thoughts, impressions, recommendations from the relevant session and panel discussion.
- The final wrap-up was a short 10 minute summary by the breakout leader, presented to the entire workshop.

The questions for each breakout session are listed below.

1) Identify key PV Successes during the last 10 years
2) Identify challenges and opportunities for the next 10 years
3) Discuss how can TMS address these challenges / realize the opportunities?
4) Describe the status of TMS in PV in your organization
5) Is end-to-end TMS simulation possible?
6) Is TMS a "pre-competitive activity"?
7) Clarify roles of academia, industry, and national labs
8) Identify emerging topics and priorities
9) List goals for the next 10 years
10) Describe R&D strategies
11) List needed infrastructure

The discussion that took place in each of the five themes is summarized below.

3.2. Opening Session, Panel, and Breakout Session (Moderator: Dr. BJ Stanbery; Reporter: Prof. Ali Shakouri)

Major Accomplishments over the Last Decade (Question 1): Innovative German feed-in tariffs have greatly facilitated market growth, from 2.2 GW globally (373 MW EU) in 2002, up to an estimated 28.5 GW installed globally in 2012. Also, the last few years marked the arrival of low-cost manufacturing from China, with average selling prices of multicrystalline silicon dropping from \$3.55/Wp in 2006 to \$0.88/Wp in 2012. At the same time, the efficiency of PV modules improved in most market segments, including cadmium telluride (CdTe), monocrystalline silicon, and multicrystalline silicon. Also, promising new technologies showed enhanced commercial viability, including gallium arsenide (GaAs), copper indium gallium diselenide (CIGS), and organic heterojunctions, as discussed in more detail in Sections 3.3-3.5.

Opportunities for the Next Decade (Questions 2, 8, and 9): It is an open question whether any technologies have the potential to leapfrog the learning curve and economies of scale already achieved by crystalline silicon and cadmium telluride-based PV cells. Furthermore, it must be considered whether any incumbent or novel solar PV technology can compete with emerging fossil fuel options, such as shale-based natural gas. It must be considered whether cost-effective storage is needed and can be developed for deep on-grid penetration, or alternatively, how widely solar PV can be deployed in its absence. A more scientific question with cross-cutting implications is the exploration of suppression of nonradiative recombination mechanisms, which can be broadly referred to as defect engineering. Finally, predictive physics-based reliability models are needed to capture both intrinsic and extrinsic failure modes.

How can TMS Address These Opportunities (Questions 3, 4): TMS can help with basic scientific understanding, as well as the optimization of existing device and system designs. Specific scientific areas of interest include carrier-selective current extraction contact materials; intrinsic and extrinsic reliability of new materials and modules in outdoor environments; reliability of balance-of-systems components (e.g., power conditioners); and characterization modeling unique to PV. Specific areas in which optimization is desirable include maximizing process yield and throughput, as well as minimizing the overall dollar-per-watt cost and the total cost of ownership over the lifetime of a PV system (including factors such as maintenance, replacement of parts, performance degradation over time, *etc*.).

Is TMS a Pre-Competitive Activity; What Role for Academia, National Labs, Industry (Questions 6,7): Yes, TMS is a pre-competitive activity - particularly for less mature PV technology. Academia and national labs can play similar roles in terms of developing basic theoretical understanding; new characterization and metrology techniques and capabilities; and fabricating and early testing of advanced materials (CIGS is a good example).

What R&D Infrastructure Strategies are Needed (Questions 10, 11): First, an R&D consortium of academic institutions, national labs, and industry focusing on all stages of characterization and reliability could accelerate progress in this area. Second, developing an expanded PVhub simulation resource, which can consolidate and catalog different PV simulation tools relevant to current research, would provide access for the whole community to best practices.

3.3. Crystalline Photovoltaics (Moderator: Dr. Bob Havemann; Reporter: Prof. Jeff Gray)

Major Accomplishments Over the Last Decade (Question 1): Improved cell design, efficiency, and affordability were achieved for both single and multijunction photovoltaic devices in the last decade.

In single junction cells, new records approaching the Shockley-Queisser limit were set. Keys to this achievement include improved management of recombination as well as photon management. Theory, modeling, and simulation allowed for the prediction and optimization of performance, particularly in monocrystalline silicon devices. However, the introduction of heterojunctions (HITs), as well as unusual surface or bulk recombination mechanisms, has posed some challenges requiring significant further investigation.

For multijunction cells, novel material platforms were developed, particularly the dilute III-nitride platform enabling the epitaxial growth of multiple III-V materials with distinct bandgaps. Accurate simulations allowed for improved design and optimization, in analogy with the earlier case of monocrystalline silicon PV. Furthermore, concentrated PV system designs were greatly improved, by focusing on both enhancing performance of individual components (e.g., lenses, mirrors, spectral splitters such as dichroic filters), as well as optimizing yearly electrical energy generation, as validated by field tests.

Opportunities for the Next Decade (Questions 2, 8, and 9): Research opportunities include new materials, device, system designs, and end-to-end models (incorporating processes, devices, modules, systems, and reliability). TMS already play a critical role in the design and manufacturing of cells. It identifies problem areas and speeds the development process by reducing the number of experimental runs needed, because modeling *is* understanding. TMS has proven to be critical in system development as well, particularly concentrator systems using complex optics. It allows for the rapid evaluation of system trade-offs, filter designs, dichroic mirror cutoff wavelengths and sharpness, the impact of tracking errors, and annual energy production under realistic conditions.

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How can TMS Address These Opportunities (Questions 3, 4):

To help address key materials challenges, there is a need to develop processing and deposition models specifically relevant to PV, as well as a quantitative understanding of the connection between process, carrier lifetime, and reliability. Specifically, low temperature front passivation with $J_o < 2x10^{-15}$ A/cm^2 is a goal of the industry, which may be enabled by low-oxygen deposition and charge passivation. Additionally, models for new wide bandgap materials such as GaN (which are piezoelectric) must be developed, as they will be an important component of multijunction cells with 5 or more junctions. Furthermore, a better understanding of the degradation physics of encapsulant materials would be helpful, particularly under exposure to moisture, heat, or UV. Finally, strategies for creating large-area patterns at the nanoscale could be quite useful.

From the device perspective, 2D/3D models are needed to address the following problems: monolithic multi-junction cells under non-uniform high insolation; the physics and technology of both heterojunction contacts and tunnel junctions; advanced photon management techniques (both ray tracing and Maxwell's Equations solvers).

As for modules, improvements in packaging are greatly needed. Simulating lamination technology, taken from back-plane microelectronic circuits, could help with this goal. An improved understanding of encapsulants would enable more reliable package design.

Finally, fielded PV systems, while already having experienced significant improvements, could benefit from practical models to reduce installed costs. Creating a set of parameterized simple (compact) models that are accurate over a wide range of concentrations and temperatures, including local weather data could help with rapid, site-specific optimization. These should include optical, electronic, and thermal transport mechanisms.

Is TMS a Pre-Competitive Activity; What Role for Academia, National Labs, Industry (Questions 6,7): TMS is pre-competitive, especially for generalized models, and is well-suited for work with industrial consortia. The fundamental difference from the electronics industry is the greater number of material platforms still under consideration. Academia can lead in the following areas: research in TMS, fabrication of proof-of-concept devices, and development of novel characterization techniques. Industry can provide data and packaged devices for model verification relevant in the real world. National labs can contribute to all of the above efforts, particularly in the context of multi-institutional collaborations.

What R&D Infrastructure Strategies are Needed (Questions 10, 11): Federal government should support fundamental, broad-based research rather than picking winners and losers. In such a context, effective use of modeling and simulation requires a close, transparent, and trusting collaboration between modelers, cell and system designers, fabricators, and testers.

TMS tools targeted toward PV audiences are needed to offer a combination of the latest research capabilities with user-friendly interfaces. Enhanced sharing of data between theorists and experimentalists is needed to help validate modeling results. While there an examples of individual groups achieving such close collaboration, platforms can help facilitate this process. One platform that has seen recent success is web-accessible modeling (e.g., nanoHUB/PVhub and NREL's SAM and CREST models).

3.4. Thin Film Photovoltaics (Moderator: Dr. Oki Gunawan; Reporter: Prof. Peter Bermel)
Major Accomplishments Over the Last Decade (Question 1): Major developments in the area of thin-films in the last decade include the achievement of dramatically lower PV module manufacturing costs at large scale (e.g., $0.72/W with 6 GW cumulative production as of Q2 2012 at First Solar); record efficiencies for single junction cells (28.8% for Alta Devices); and demonstrated feasibility of earth-abundant thin-films (11% efficient solution-processed copper zinc tin sulfide).

Opportunities for the Next Decade (Questions 2, 8, and 9): Key research opportunities include the development of 20% efficient commercial thin-film PV modules, ideally with earth-abundant components for scalability; development of earth-abundant alternatives to CdTe or CIGS, like CZTS, to a commercially viable level; as well as development of greater material and device understanding for higher overall performance and reliability.

How can TMS Address These Opportunities (Questions 3, 4): TMS can help develop comprehensive, end-to-end models of deposition processes, characterization, and reliability assessment; there is an opportunity to use first-principles calculations to perform initial screening of novel materials, based on multiple criteria for effective PV absorber materials; TMS can help optimize cells with novel optical, electronic, and thermal designs for higher performance; and create a modeling framework for assessment of manufacturing techniques, throughput, yields, and costs.

Is TMS a Pre-Competitive Activity; What Role for Academia, National Labs, Industry (Questions 6,7): TMS definitely is a pre-competitive activity. Academia and national labs should explore high-risk, high-reward investigations, and build multi-disciplinary teams to address all aspects of TMS, including characterization; creating central data repositories for PV material parameters; and educating and inspiring the next generation of scientists. Industry should adopt good models in order to perform better R&D, particularly improved characterization, modeling, and metrology; redesign processes and devices as appropriate to achieve sustainable profit margins.

What R&D Infrastructure Strategies are Needed (Questions 10, 11): A community-wide simulation and characterization infrastructure is needed to calculate and store important material properties for thin films as a whole, plus each class of materials, particularly including thin-film Si, CdTe, and CIGS. NSF Engineering Research Centers (ERCs) can be used as a model.

3.5. Organic Photovoltaics (Moderator: Prof. Jim Yardley; Reporter: Prof. Bryan Boudouris)
Major Accomplishments Over the Last Decade (Question 1): Over the last decade, organic PV cell efficiencies have increased from 2-3% to recent values of 10-11%, thanks to impressive efforts by the research community. A number of different approaches have been shown to work well, including small molecules, polymer-based, and dye-sensitized solar cells, over a range of materials, device architectures, and processing techniques. Tandem devices have allowed operating voltages to increase significantly with little current loss. Driven in part by the International Summit on Organic Photovoltaic Stability (ISOS), the estimated lifetime of the devices has also increased greatly in recent years (up to 15 years on flexible substrates and 30 years with Heliatek's glass encapsulation). Furthermore, high-performance materials costs have been driven down to below $0.50/watt, which could enable low-cost, large-scale manufacturing. As a result, multiple commercial ventures have recently been initiated.

Opportunities for the Next Decade (Questions 2, 8, and 9): Opportunities for OPV over the next decade lie in three broad, related areas: developing high-performance materials, connecting the molecular/nano scale with exciton/charge dynamics and transport, and combining these two areas of research to predict overall module performance, manufacturability, and reliability.

Needs still exist for several types of high-performance materials: specifically, active layers (including "transparent" OPV materials for building-integrated PV), interface layers, and transparent electrodes (e.g., graphene). To date, there have been many Edisonian experiments, but a comparative lack of fundamental understanding. TMS can address this issue in several ways. First, it can help by developing conceptual models that capture the key quantum interactions between the atoms of each individual material. Second, developing new algorithms with substantially greater accuracy than naive density functional theory approaches could greatly enhance the predictive and explanatory power of the simulations. Third, creating design rules that heuristically point out areas of likely success could accelerate research efforts. Finally, developing suitable semiclassical approximations of individual material properties could enable rapid modeling and performance prediction for larger devices.

It is also clear that understanding the structure of materials on a small scale, whether it be molecular scale, nanoscale, or mesoscale, is not sufficient in itself. This miniature structure, even if completely accurate, must still be connected to the electronic properties of the material. Of particular interest are the exciton dynamics governing electron/hole binding energies, as well as the charge dynamics governing their separation and collection. Work is still needed in two areas: first, in building theoretical models that can accurately predict these properties for a given structure; and second, in creating experimental characterization techniques that can probe the larger areas needed for PV cells.

Third, and most importantly from the perspective of photovoltaics, basic materials properties (structure and excitonic transport) must be connected with specific predictions of performance for both single junction, tandem cells, and other high-efficiency device concepts. Design and optimization work should then help OPV cells approach modified Shockley-Queisser limits. Alternative high-efficiency concepts include multijunction designs, consisting of three or more separate active absorbers; multiple exciton generation, exciton fission, and quantum coherence; novel light-trapping strategies for ultra-thin layers, including but not limited to plasmonics; and upconversion of long-wavelength photons that may otherwise go unused. Manufacturability is required, of course, and must combine high-throughput synthesis with relatively inexpensive purification of precursors and processing techniques, preferably at atmospheric pressures. Reliability is also a crucial consideration, and expectations must be raised from the current typical values of 3-5 years (with 15 years in the best cases) to 25 years or more. Enabling innovations may include the creation of functional materials to extend device lifetimes (e.g., self-healing materials).

How can TMS Address These Opportunities (Questions 3, 4): TMS can help create the design rules needed for an “end-to-end,” “molecule-to-module” approach. At the basic level, it will encompass molecular-scale behavior both quantum mechanically and semiclassically (using molecular dynamics). This will in turn help predict basic optical, mechanical, and electronic materials properties, including the effects of impurities. As such, it can be used to explore the design of new packing motifs and chromophores, needed to help improve exciton generation and charge separation. At a higher level, the overall desired device morphology and performance will be important to model. Making accurate predictions will require appropriate semiclassical 3D models for photon management and electronic transport. Successfully packaging these devices into a module with high performance is a challenging but crucial follow-up task. Creating a simulation tool accounting for the heterogeneous and variable nature of the module sub-components will be helpful -- e.g., an extended SPICE-like model framework. Finally, manufacturing high-quality devices in an affordable, reliable and scalable fashion is critical. Prediction of mesoscale morphology under high-throughput deposition and aging would represent an important contribution to this goal.

Is TMS a Pre-Competitive Activity; What Role for Academia, National Labs, Industry (Questions 6,7): TMS is a generally pre-competitive activity, which is highly multidisciplinary in the case of PV. It will be important to combine the physics- and chemistry-based models discussed previously with downstream considerations of manufacturability, reliability, cost, and environmental impact at the terawatt scale. Experts will be needed within academia and the national labs from chemistry, physics, chemical, electrical, mechanical, industrial, and environmental engineering, as well as experts on environmental and policy analysis. Cross-campus centers and multi-institutional partnerships can help bring together the needed experts in each area. Partnership with industry will be necessary to analyze the market, life cycle, and environmental impact, which will enable a transition of OPV technology from laboratories to large-scale deployment.

What R&D Infrastructure Strategies are Needed (Questions 10, 11): A community-wide database is needed to calculate and store important organic PV material properties. Creating networks of web-enabled, openly accessible TMS tools from leading research groups should facilitate further advances in OPV performance.

3.6. Characterization (Moderator: Dr. Souvik Mahapatra; Reporter: Prof. Rakesh Agrawal)
Major Accomplishments (Question 1): There has been significant advances and refinement in various characterization techniques over the years. This include broad availability of high precision and multi-functional characterization equipment, an increasing realization that the parameters extracted from the experiments are often model dependent, and an increasing role of TMS in deconvolving the complex interaction probed by a characterization technique.

Opportunities for the Next Decade (Questions 2, 8, and 9): There is a critical need for a fundamental understanding of the properties of the interfaces, because many of the most critical issues of PV device performance and reliability occur at interfaces such as p-n junctions, back and front contacts, between various additional functional layers (e.g., light and carrier reflectors, tunnel junctions, passivation and buffer layers), as well as at the grain boundaries in polycrystalline semiconductors. Examples of needed research include: prediction and evaluation of interface intermixing; improvement of contact resistance to high work-function high resistance materials such as CdTe; better understanding of the physics, chemistry, and stability of grain boundaries in polycrystalline semiconductors; improvement of the adherence and lifetime of semiconductor (metal) /encapsulant interfaces. Considering the issues above, there is a strong need for fundamental insights into the basic properties of interfaces relevant to PV cells and modules.

In addition, an improved understanding of degradation mechanisms in devices and protective materials could help improve module lifetimes and further lower the cost of PV electricity. The PV community realizes that they have only a limited grasp of photochemical degradation, dielectric breakdown, and leakage current in the presence of water and oxygen. Similarly, the industry must increase the understanding of impurity diffusion processes in semiconductors and through interfaces, especially in large-area devices (which have inevitable compositional variations in all dimensions). In addition, there is a significant need to develop well-designed stress tests to define and test potential degradation mechanisms, as well as parallel accelerated lifetime models that correlate these new tests with actual outdoor performance over many decades.

How can TMS Address These Opportunities (Questions 3, 4): Better computational models and tools can assist in correlating processing parameters with fundamental device physics to accelerate research and commercial product development. One such opportunity is with existing silicon and thin film based modules: one would develop a set of standardized material metrics to facilitate optimization of electronic and optical performance. There is another opportunity to develop and employ *in situ* process controls and in-line diagnostics for improved manufacturing yield. These challenges require adoption of sophisticated modeling tools as well as the advanced and insightful analysis only available through the best characterization of modern PV materials in order to provide input parameters and understand results. For example, while most work to date on interface characterization has been empirical, there is an opportunity to use more sophisticated R&D tools and expertise to better understand the optical, electrical, mechanical, and chemical properties of these interfaces, as well as to predict their dependence on time and environmental conditions.

Is TMS a Pre-Competitive Activity; What Role for Academia, National Labs, Industry (Questions 6,7): TMS is a generally pre-competitive activity, which is highly multidisciplinary in the case of PV. Bringing together TMS capabilities in academia with strong lab capabilities both in national labs and industry should be helpful in further leveraging the capabilities of each individual research group.

What R&D Infrastructure Strategies are Needed (Questions 10, 11): A community-wide database is needed to calculate and store important material properties for characterizing thin films, particularly including but not limited to thin-film Si, CdTe, and CIGS. Creating networks of web-enabled, openly accessible TMS characterization tools from leading research groups should facilitate use of reproducible, best practices in characterizing materials.

4. Summary and Recommendations

This workshop was executed as planned and concluded successfully from a scientific standpoint, addressing within the various areas of photovoltaics both recent accomplishments, emerging opportunities, and the importance and role of theory, modeling and simulation.

Looking back at the last decade of photovoltaics, many significant achievements were noted. They include in particular subsidy programs seeding the growth of the solar industry such as the German feed-in tariff; the subsequent, dramatic decrease in the costs of photovoltaic cells and modules enabled by the entry of low-cost producers in China; and substantial improvements in champion and manufactured cell performance. On the commercial side, continued improvements in c-Si and CdTe had significant impacts. Scientifically, notable advances in CIGS, GaAs, organic PV, and multijunction cells occurred, including 28.8% single-junction unconcentrated performance, as well as 44% triple-junction cells under concentration. However, alternative technologies may find it increasingly challenging to compete with the cumulative subsidized learning curve advantage of c-Si and CdTe.

Emerging opportunities highlighted by multiple participants include the development of new material platform systems (particularly CIGS, CZTS, and OPV) as alternatives to crystalline silicon and cadmium telluride; improving overall device and module efficiencies through various strategies, particularly suppressing non-radiative recombination at grain boundaries and for advanced low-combination contacts to absorbers; decreasing the levelized cost of energy for PV to compete with fossil fuels on an unsubsidized basis; developing strategies for cost-effective integration of large amounts of PV generation into the electric grid, which may include innovative storage; and improving lifetime and reliability prediction for PV materials, devices, and systems.

Already, a number of solar cell companies make extensive use of simulation in process and device optimization. PV system designers and analysts make extensive use of online tools from NREL like Solar Advisor Model (SAM). NREL also has begun to couple characterization techniques more closely with simulations. Although several universities already provide PV simulation tools to the community, current tools do not adequately address cutting-edge research problems, such as photon recycling in PV cells near the Shockley-Queisser limit, enhanced open-circuit voltage for restricted spectral angles of incidence, multiple exciton generation, etc.

Key challenges for TMS.

TMS can help create the design rules needed for an "end-to-end," "materials-to-modules" approach for all major PV technologies. At the basic level, it will encompass atomic-scale behavior both quantum mechanically and semiclassically (using molecular dynamics). This will in turn help predict basic optical, mechanical, and electronic materials properties, including the effects of impurities. As such, it can be used to explore the design of suitable materials. At a higher level, the overall desired device morphology and performance will be important. Making accurate predictions will require appropriate semiclassical 3D models for photon management and electronic transport. High efficiency cell designs will also need to account for additional physical phenomena such as photon recycling and heterojunction interfaces. Successfully packaging these devices into high-performance modules is a challenging but crucial follow-up task. Creating a simulation tool accounting for the heterogeneous and variable nature of the module sub-components will be helpful -- e.g., an extended SPICE-like model framework. Finally, manufacturing high-quality devices in an affordable, reliable and scalable fashion is critical. Prediction of mesoscale morphology under high-throughput deposition and aging would represent an important contribution to this goal.

The participants all agreed that TMS can be effective only if it is treated as a pre-competitive activity by the industry. And, as a pre-competitive activity, theory, modeling and simulation should be explored by multi-disciplinary team from academia and national labs in high-risk, high-reward investigations. Areas of interest will include characterization; creating central data repositories for PV material parameters; and educating and inspiring the next generation of scientists. Industry should adopt good models in order to perform better R&D, particularly improved characterization, modeling, and metrology; redesign processes and devices as appropriate to achieve sustainable profit margins.

Models for multi-disciplinary research, software development and dissemination, and industry-university cooperation.

The participants came to a consensus that TMS is a pre-competitive activity, well-suited for support through federally-funded multi-university projects and industrial consortia, in collaboration with national labs. NSF Engineering Research Centers (ERCs) can be used as a model for this style of collaboration. Another important model for pre-competitive efforts that bring together the broad community is the web-accessible modeling. Recent examples include nanoHUB, which has over 250,000 unique users per year, and includes PVhub as working group specifically targeted toward the PV community; PVCDROM as an educational and training resource with some basic simulations built in as Java applications; as well as the NREL solar advisor model (SAM) and cost of renewable energy model (CREST).

Going forward, a community-wide simulation and characterization infrastructure is needed to facilitate "materials-to-modules" end-to-end modeling efforts. It will need to combine the latest research modeling capabilities as well as highly-accessible, user-friendly interfaces. These tools should be consolidated, cataloged, and made accessible in a logical and straightforward fashion. It should also facilitate sharing of data between theorists and experimentalists to help validate modeling results. Finally, it should serve as an educational resource that can help bring new and continuing PV researchers up to speed on the latest developments in the field.

Increasing the effectiveness of TMS in photovoltaics

Theory, modeling and simulation (TMS) will play an integral role in addressing many emerging challenges. In general, a consensus emerged that problems that can be modeled are also well-understood; avoiding this step could cause unanticipated problems, particularly in new device or module designs. More specifically in the area of emerging PV materials, TMS drawn from first principles, as well as semi-classical electronic and optical transport, allow for the best candidates to be selected before entering the lab, and for down-selection upon model refinement. In order to improve performance of fabricated devices and modules, modeling that incorporates variability between regions in a realistic fashion will also be needed – particularly for thin films. The intrinsic reliability of modules may also be amenable to significant improvement if novel predictive, physics-based intrinsic reliability models can be created. Further challenges such as spectral, temporal, and temperature variations may be amenable to solution via multiphysics models. Finally, there is room for both economic and physics-based process flow models to help predict and optimize overall manufacturing costs and yields.

Appendix 1: List of participants

LIST OF PARTICIPANTS

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Appendix 2: List of Recommended experts and area of expertise:

- Alex Zunger, UC Boulder: first-principles (ab initio) theory & simulation
- Harry Atwater, Caltech: optics of novel thin-film designs, theory & simulation
- Rob W. Collins, U. Toledo: optical analysis of CdTe, CIGS
- Clemens Heske, UNLV: X-ray electron based surface interface probes
- Jeff Grossman, MIT: first-principles computational tools for many problems
- Elif Ertekin, UIUC: first-principles computational tools for many problems