



Materials Research Society celebrates 40th anniversary with more cutting-edge research at the 2013 MRS Fall Meeting

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While celebrating its 40th anniversary in Boston, the Materials Research Society forged ahead in exploration of the latest frontiers of materials research. At its 2013 MRS Fall Meeting, the Society speedily assembled a Rump Session on organo-metal halide perovskites, the hottest topic in photovoltaics due to recent reports demonstrating that these materials could yield high-efficiency solar cells. “Big data” as it relates to materials science was also a topic of major importance. As always, the special talks delivered by the Society’s award recipients attracted large crowds and were well received.

The Meeting Chairs, **Charles T. Black** (Brookhaven National Laboratory, USA), **Elisabetta Comini** (Università di Brescia, Italy), **Gitti Frey** (Technion–Israel Institute of Technology, Israel), **Kristi L. Kiick** (University of Delaware, USA), and **Loucas Tsakalacos** (General Electric–Global Research Center, USA) convened the

Meeting on December 1–5, 2013 in Boston, Mass. Close to 6000 attendees were treated to 51 technical symposia in the six broad categories of Biomaterials and Soft Matter, Electronics and Photonics, Energy and Sustainability, General Materials and Methods, Materials and Society, and Nanomaterials. The Meeting also hosted an international equipment exhibit, tutorials, a Science as Art competition, and sessions on government funding opportunities, technology innovations, and professional development and public outreach opportunities.

In order to further the research on organo-metal halide perovskites, Dave Ginley of the National Renewable Energy Laboratory and David Cahen of the Weizmann Institute of Science in Israel quickly organized a rump session within Symposium Y: Physics of Organic and Hybrid Organic–Inorganic Solar Cells. With a 10-minute limit per talk, 15 speakers presented their work, capturing


the excitement of this early period in the investigation of these materials. The most common formulation of the organo-metal halide perovskite material is methyl-ammonium lead iodide (MAPbI_3), $\text{CH}_3\text{NH}_3\text{PbI}_3$. The halide chlorine is often substituted for some of the iodide, resulting in $\text{CH}_3\text{NH}_3\text{PbI}_{3-x}\text{Cl}_x$. Bromine is also being investigated as the halide by at least one group giving a presentation at this session. Tin and copper were mentioned as substitutes for lead by two different speakers.


As might be expected at such an early stage of the research, scientists are meeting the challenge from numerous angles. O. Yaffe from Columbia University is pursuing an understanding of the fundamental electronic properties of organic–inorganic perovskite crystals (OIPCs), including bandgap, trap states, work function, charge mobility, and the transport mechanism. His group is studying monolayers of OIPCs, which they synthesize by substituting butylammonium for methylammonium in the MAPbI_3 structure. They reported an absorption of 25% at 2.5 eV for one monolayer of this OIPC.

David T. Moore of Cornell University identified three distinct phases during processing: precursor, perovskite, and a decomposition phase. Full crystallization of the perovskite can take from 10 minutes to 3 hours, but decomposition can be fast—a matter of minutes, Moore said.

Eran Edri of the Weizmann Institute is using electron-beam-induced current (EBIC) to directly measure the location of charge separation in a device. He reports two peaks of charge separation in an $\text{MAPbI}_{3-x}\text{Cl}_x$ perovskite, and concludes that I_3 and $\text{I}_{3-x}\text{Cl}_x$ perovskites are basically *p-i-n* solar cells.

Philip Schultz of Princeton University and the Weizmann Institute is studying the interface energetics of these perovskites by direct and indirect photoemission spectroscopy. His team has found that the work function is equal for all perovskites on TiO_2 , and that there are similar band offsets for both I and ICl compounds. His group also reports a large bandgap in a Br perovskite (substituting Br for Cl).





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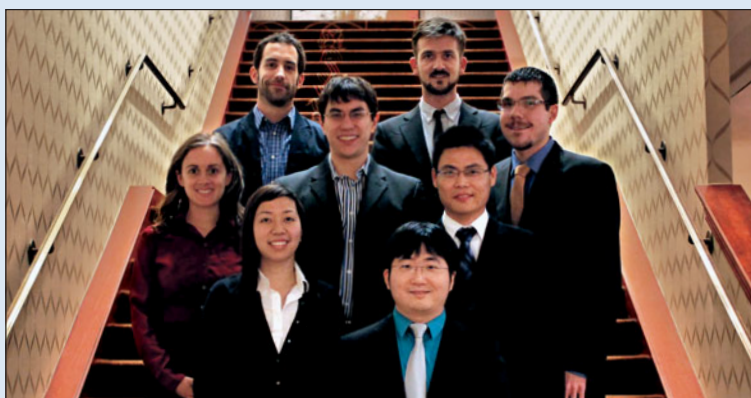
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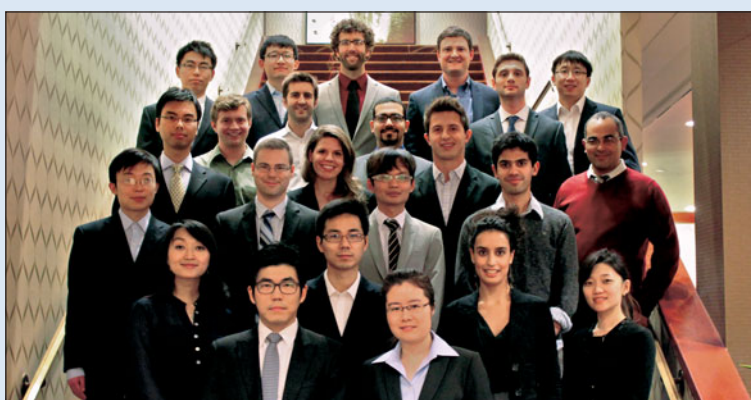
Members of MRS and other scientific societies are increasingly interested in the opportunities and challenges presented by government initiatives on big data and open data. A Symposium X panel discussion was held to follow up on the Big Data Survey conducted last year* by MRS and The Minerals, Metals and Materials Society, and to gain some enlightenment from experts in this area in academia, government, and industry. Tia Benson Tolle of The Boeing Company—now serving MRS as the 2014 President—moderated the panel discussion.

Panelist Jim Pinkelman of Microsoft Research said that researchers are heading into a data-intensive research cycle that is going to change the scientific method. He said materials science in general is lagging behind other research fields, such as astronomy and particle physics, which are already immersed in big data that is collected around the clock by radio telescopes and satellites (astronomy) and in quick bursts of activity (particle physics), such as at CERN's Large Hadron Collider. Rick Barto of Lockheed said that within the next

Graduate Students Receive Gold and Silver Awards



Gold Graduate Student Awards (front row): Chunjie Zhang; (second row, left to right): Evelyn Auyeung, Bin Yang; (third row, left to right): Julia Mundy, Reid Van Lehn, Steven Spurgeon; (fourth row, left to right): Lance Wheeler, Deniz Bozyigit; (not pictured): James Pikul



Silver Graduate Student Awards (front row, left to right): Gibum Kwon, Limei Tian; (second row, left to right): Yi Ke, Zhibin Yang, Aristi Christofi, Dahyun Oh; (third row, left to right): Desheng Kong, Richard Baumer, Su-Wen Hsu, Nisarg Shah; (fourth row, left to right): Ziliang (Carter) Lin, Melissa Johnson, Phillip Barton, Sina Najmaei; (fifth row, left to right): Nicholas Schneider, Mostafa Bedewy; (sixth row, left to right): Adam Paxson, Tuncay Ozel; (seventh row, left to right): Long Lin, Fei Meng, Daniel Bufford, David Yancey, Shuai Wei; (not pictured): Chi Hwan Lee

*For more information on the survey, see the September 2013 (p. 751) and October 2013 (p. 766) issues of *MRS Bulletin*, www.mrs.org/bulletin.



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decade he believes the materials community will deal with real instances of big data. (Barto stated on the record that he was speaking for himself and not as a representative of Lockheed or its views.)

Putting the scale of information in perspective, J. Michael Simonson of Oak Ridge National Laboratory said that he used to be able to do an experiment and record results on a single sheet of graph paper, but that recently he was given a terabyte of disk space and filled it in one night.

Nicola Marzari of École Polytechnique Fédérale de Lausanne, Switzerland, said that big data is one of the pillars of materials science, though not the only one. Big data is already very important for computational materials scientists, but in the rest of materials science its role is not yet as clear. He recommends that the materials community focus on tools, most importantly computer codes, that will be able to break through the big data bottleneck. Also, how the data is generated is important, he said.

One of the reasons Marzari said he had always been a fan of open data is that he believes it increases the quality of data. In response to this comment, panelist Mary Galvin of the US National Science Foundation—Division of Materials Research said she was unsure whether open data protocols will increase data accuracy because researchers have always had the ability to reproduce experiments and data from the literature; she questions how much open data will change this. She also said that the cultural aspect of integrating computation, experiment, and data mining is an equal or greater challenge than the technical challenges involved.

The panelists explored questions of reciprocity internationally, and whether open data is an opportunity or a threat to progressing materials research.

Various advances in materials research were recognized in awards presented at the Meeting, followed by lectures from the award recipients. A superstar in the materials research field, Von Hippel Award recipient Mildred S. Dresselhaus of the Massachusetts Institute of Technology received a long and

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loud ovation from the audience in the packed hall before delivering her award talk. Having been directly mentored by Arthur von Hippel, Dresselhaus said, “This is a particularly lovely award for me because of my long working relationship and friendship” with von Hippel. Dresselhaus said that von Hippel was intrigued by complicated materials, such as perovskites, which seemed complex at that time, and he also liked to explore simple, fundamental systems, like carbon. At his suggestion, she embarked on the study of graphite, which launched her into preeminence as a renowned researcher in carbon science. “[Von Hippel] worked every day in the lab until

he was 90,” Dresselhaus said, “and after that he still came in but mostly listened. He was always interested in new things.” He lived to be 103, passing away in 2003. Dresselhaus said that von Hippel never got to see the excitement caused by graphene in 2004, but that he would have enjoyed it.

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