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Gordon Research Conferences, Inc. 512 Liberty Lane West Kingston, RI 02892 -1502	

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Approved for public release; distribution is unlimited.

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The views, opinions and/or findings contained in this report are those of the author(s) and should not contrued as an official Department of the Army position, policy or decision, unless so designated by other documentation.

14. ABSTRACT

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a. REPORT	b. ABSTRACT	c. THIS PAGE			Rampi Ramprasad
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Agency Code: 21XD

Proposal Number: 79847SMCF   **Agreement Number: W911NF-22-1-0008**
INVESTIGATOR(S):

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Organization: **Gordon Research Conferences, Inc.**
Address: 512 Liberty Lane, West Kingston, RI 028921502
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DUNS Number: 075712877   EIN: 050300482
Report Date: 28-Feb-2023   Date Received: 19-Dec-2022
Final Report for Period Beginning 01-Feb-2022 and Ending 30-Nov-2022
Title: 2022 Computational Materials Science and Engineering Gordon Research Conference
Begin Performance Period: 01-Feb-2022   **End Performance Period:** 30-Nov-2022
Report Term: 0-Other
Submitted By: Ph.D. Nancy Gray   Email: grants@grc.org
                                        Phone: (401) 742-8826
Distribution Statement: 1-Approved for public release; distribution is unlimited.

STEM Degrees: 0   **STEM Participants:**

Major Goals: Within Materials Science and Engineering, there exist semi-isolated programs; ceramists infrequently interact with metallurgists and both of those communities rarely interact with polymer scientists. In terms of Computational Materials Science and Engineering (CMSE), we also find the underpinning theories, algorithms and computational protocols evolved independently to address science questions and engineering needs for their own communities. This situation is untenable for the agile and fast-paced development of theories and algorithms needed by the materials science and engineering community. The scientific objectives of this conference are: (1) to cross-pollinate ideas between disparate communities agglomerated within CMSE and to better connect engineers with scientists, (2) to promote the creation of testable scientific theories, algorithmic developments and data-centric platforms/methodologies, (3) to accelerate the growth of computational tools needed for materials simulations over multiple time and length scales covering both extant and emerging classes of materials, and (4) to provide graduate students and post-doctoral fellows, with nascent careers in a given scientific domain, the networking opportunities to interact with and learn from seasoned professionals from another discipline that is otherwise hard to achieve in standard discipline-based or society-driven conferences. The method used to accomplish these objectives is to bring together leading researchers in the different sub-disciplines of MSE to compare, contrast and share extant theories, algorithms and computational protocols. The ambiance afforded by a traditional Gordon Research Conference is perfect for accomplishing this; it is a safe and intimate environment where dialog, debate and argument can take place about what can and what cannot be done across disciplines. This proposal seeks ARO support for the 2022 Computational Materials Science and Engineering Gordon Research Conference, to be held at the GRC site Grand Summit Hotel in Newry, Maine, USA on July 31 – August 5, 2022.

Accomplishments: Within Materials Science and Engineering (MS&E), there exist semi-segregated programs; ceramists infrequently interact with metallurgists and both of those communities rarely interact with polymer scientists. In terms of Computational Materials Science and Engineering (CMSE), the underpinning theories, algorithms and computing protocols evolved independently to address science questions and engineering needs for their own communities. Each discipline brings different perspectives and computational strategies, which are bound to have value for the other sub-disciplines. The purpose of this GRC was to see what we can learn from one another by comparing and contrasting development of theory, algorithms and best practices across sub-disciplines of MS&E.

Training Opportunities: Speakers, discussion leaders, poster presenters and attendees simultaneously contributed to and benefited from the collective skills and experience shared throughout the conference.

Results Dissemination: The final program has been posted on the GRC website.

Honors and Awards: Nothing to Report

Protocol Activity Status:

Technology Transfer: Nothing to Report

Partners

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I certify that the information in the report is complete and accurate:
Signature: Darlene Armstrong
Signature Date: 12/19/22 12:08PM

GORDON RESEARCH CONFERENCES
FINAL REPORT
Army Research Office
Computational Materials Science and Engineering
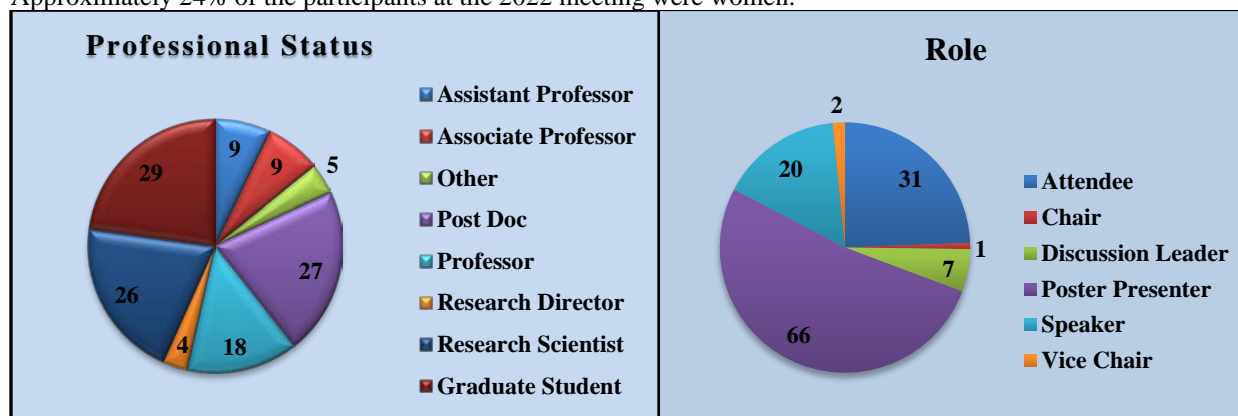**Grant Number W911NF2210008**

Operational Summary

The Gordon Research Conference (GRC) Computational Materials Science and Engineering was held at the Grand Summit Hotel at Sunday River in Newry, Maine from July 31-August 5, 2022. The meeting covered a variety of scientific topics and the content presented was highly rated by participants.

Conference Participants

The Conference was well-attended with 127 participants. Scientists from academia represented 66% of the participants while attendees from government accounted for 22% and those from industry totaled 12%. The meeting also attracted a strong mix of young investigators and senior scientists. Students and post-docs accounted for 44% of all attendees. Approximately 24% of the participants at the 2022 meeting were women.

Conference Program

Within Materials Science and Engineering (MS&E), there exist semi-segregated programs; ceramists infrequently interact with metallurgists and both of those communities rarely interact with polymer scientists. In terms of Computational Materials Science and Engineering (CMSE), the underpinning theories, algorithms and computing protocols evolved independently to address science questions and engineering needs for their own communities. Each discipline brings different perspectives and computational strategies, which are bound to have value for the other sub-disciplines. The purpose of this GRC was to see what we can learn from one another by comparing and contrasting development of theory, algorithms and best practices across sub-disciplines of MS&E.

Conference Budget

Funding provided by the Army Research Office supported partial registration for 1 graduate student, 3 professors, 1 assistant professor, 1 post doc and 2 associate professors at the GRC.

Conference Feedback

Participants had an opportunity to provide feedback at the end of the Conference. The feedback collected from the meeting was extremely positive. Evaluations included numerous positive remarks regarding the interactions at the poster sessions, selection of topics and the great speakers.

GRC would like to thank the Office of Naval Research for its continued support of the meetings. The contributions received have been critical to the success of the conferences and are having a measurable impact in advancing the frontiers of science worldwide.

Dr. Rampi Ramprasad, GRC Chair
Georgia Institute of Technology

Dr. Heather Kulik, GRC Vice Chair
Massachusetts Institute of technology

Dr. Katsuyo Thornton, GRC Vice Chair
University of Michigan

Dr. Nancy Ryan Gray
President and Chief Executive Officer
Gordon Research Conferences

Computational Materials Science and Engineering

Gordon Research Conference

Comparing Theories, Algorithms and Computation Protocols in Materials Science and Engineering

July 31 - August 5, 2022

Chair Rampi Ramprasad

Vice Chairs Katsuyo S. Thornton and Heather J. Kulik

Grand Summit Hotel at Sunday River

97 Summit Road

Newry, ME, United States

Conference Program

Sunday

2:00 pm - 9:00 pm	Arrival and Check-in
6:00 pm - 7:00 pm	Dinner
7:30 pm - 7:40 pm	Introductory Comments by GRC Site Staff / Welcome from the GRC Chair
7:40 pm - 9:30 pm	Synthesis Planning Algorithms Discussion Leaders: Victor Fung (Georgia Institute of Technology, United States)
7:40 pm - 8:20 pm	Daniel Schwalbe-Koda (Lawrence Livermore National Laboratory, United States) "Data and Algorithms for Planning Inorganic Syntheses"
8:20 pm - 8:35 pm	Discussion
8:35 pm - 9:15 pm	Connor Coley (Massachusetts Institute of Technology, United States) "Data-Driven Synthesis Planning for Organic Chemistry"
9:15 pm - 9:30 pm	Discussion

Monday

7:30 am - 8:30 am	Breakfast
9:00 am - 12:30 pm	Machine Learning Discussion Leader: Christopher Kuenneth (Georgia Institute of Technology, United States)
9:00 am - 9:40 am	Wenhao Sun (University of Michigan, Ann Arbor, United States) "Unsupervised Knowledge Discovery in 'Big' Materials Data"
9:40 am - 10:00 am	Discussion
10:00 am - 10:30 am	Coffee Break
10:30 am - 11:10 am	Stefan Chmiela (Technische Universität Berlin, Germany) "Machine Learning Meets Quantum Chemistry"
11:10 am - 11:30 am	Discussion

11:30 am - 12:10 pm	Rama Vasudevan (Oak Ridge National Laboratory, United States) "Machine Learning for Materials Characterization and Visualization"
12:10 pm - 12:30 pm	Discussion
12:30 pm - 1:30 pm	Lunch
1:30 pm - 4:00 pm	Free Time
3:00 pm - 4:00 pm	The GRC Power Hour™ *The GRC Power Hour™ is designed to address diversity and inclusion in the scientific workplace by providing a safe environment for informal and meaningful conversations amongst colleagues of all career stages. The program supports the professional growth of all members of our communities, including ethnicity, race and/or gender identity by providing an open forum for discussion and mentoring.* Organizers: Jennifer Carter (Case Western Reserve University, United States) and Aeriel Leonard (The Ohio State University, United States)
4:00 pm - 6:00 pm	Poster Session
6:00 pm - 7:00 pm	Dinner
7:30 pm - 9:30 pm	Coarse Graining Discussion Leaders: Katsuyo Thornton (University of Michigan, United States)
7:30 pm - 8:10 pm	Nikolas Provatas (McGill University, Canada) "Advances in Quantitative Phase Field Crystal Models for Metals and Alloys"
8:10 pm - 8:30 pm	Discussion
8:30 pm - 9:10 pm	Meenakshi Dutt (Rutgers, The State University of New Jersey, United States) "Coarse-Grained Methods for Soft and Biological Materials"
9:10 pm - 9:30 pm	Discussion
Tuesday	
7:30 am - 8:30 am	Breakfast
8:30 am - 9:00 am	Group Photo
9:00 am - 12:30 pm	Concurrent and Hierarchical Multiscale Modeling Discussion Leader: Yan Wang (Georgia Institute of Technology, United States)
9:00 am - 9:40 am	David McDowell (Georgia Institute of Technology, United States) "Computational Support for Design of Hierarchical Materials and Structures"
9:40 am - 10:00 am	Discussion
10:00 am - 10:30 am	Coffee Break
10:30 am - 11:10 am	Martin Steinhauser (Frankfurt University of Applied Sciences, Germany)

	"Destruction of Tumor Cells by Laser-Induced Shock Wave Generation: Experiments and Multiscale Computer Simulations"
11:10 am - 11:30 am	Discussion
11:30 am - 12:10 pm	Ellad Tadmor (University of Minnesota, United States) "Accelerated Quasicontinuum Methods"
12:10 pm - 12:30 pm	Discussion
12:30 pm - 1:30 pm	Lunch
1:30 pm - 4:00 pm	Free Time
4:00 pm - 6:00 pm	Poster Session
6:00 pm - 7:00 pm	Dinner
7:30 pm - 9:30 pm	Non-Adiabatic Quantum Mechanics Discussion Leader: Claudia Draxl (Humboldt University of Berlin, Germany)
7:30 pm - 8:10 pm	André Schleife (University of Illinois at Urbana-Champaign, United States) "A First Principles Model of Hot-Electron-Mediated Diffusion in Ceramics and Alloys"
8:10 pm - 8:30 pm	Discussion
8:30 pm - 9:10 pm	Priya Vashishta (University of Southern California, United States) "Exascale Quantum Dynamics, Machine Learning and Ultrafast Experiments"
9:10 pm - 9:30 pm	Discussion
Wednesday	
7:30 am - 8:30 am	Breakfast
9:00 am - 12:30 pm	Autonomous Robotic Systems Discussion Leader: Christoph Kreisbeck (Kebotix, United States)
9:00 am - 9:40 am	Andy Cooper (University of Liverpool, United Kingdom) "Autonomous Discovery of Functional Materials Using a Mobile Robotic Scientist"
9:40 am - 10:00 am	Discussion
10:00 am - 10:30 am	Coffee Break
10:30 am - 11:10 am	A. Gilad Kusne (National Institute of Standards and Technology, United States) "Informatics Tools for Accelerating Experimentation"
11:10 am - 11:30 am	Discussion
11:30 am - 12:10 pm	Loïc Roch (Atinary Technologies, Switzerland)

	"Atinary SDLabs: ML Software Solutions and Self-Driving Labs to Accelerate R&D Today"
12:10 pm - 12:30 pm	Discussion
12:30 pm - 1:30 pm	Lunch
1:30 pm - 4:00 pm	Free Time
4:00 pm - 6:00 pm	Poster Session
6:00 pm - 7:00 pm	Dinner
7:30 pm - 9:30 pm	Calculation of Phase Diagrams (CALPHAD) Discussion Leader: Raymundo Arroyave (Texas A&M University, United States)
7:30 pm - 8:10 pm	Ursula Kattner (National Institute of Standards and Technology, United States) "Recent Advances in CALPHAD Modeling"
8:10 pm - 8:30 pm	Discussion
8:30 pm - 9:10 pm	Maryam Ghazisaeidi (Ohio State University, United States) "Multi-Cell Monte Carlo Method for Phase Prediction"
9:10 pm - 9:30 pm	Discussion
Thursday	
7:30 am - 8:30 am	Breakfast
8:30 am - 9:00 am	Business Meeting *Nominations for the Next Vice Chair(s); Complete the GRC Evaluation Forms; Discuss Future Dates and Venue; Election of the Next Vice Chair(s)*
9:00 am - 12:30 pm	Materials by Design Discussion Leader: Alejandro Strachan (Purdue University, United States)
9:00 am - 9:40 am	Ghanshyam Pilania (Los Alamos National Laboratory, United States) "Polymer Informatics for Sustainability"
9:40 am - 10:00 am	Discussion
10:00 am - 10:30 am	Coffee Break
10:30 am - 11:10 am	Arun Kumar Mannodi Kanakkithodi (Purdue University, United States) "Driving Perovskite Discovery using Multi-Fidelity DFT-ML"
11:10 am - 11:30 am	Discussion
11:30 am - 12:10 pm	James Warren (National Institute of Standards and Technology, United States) "Computational Materials Science and Engineering and the MGI: Reflections and Opportunities"

12:10 pm - 12:30 pm	Discussion
12:30 pm - 1:30 pm	Lunch
1:30 pm - 4:00 pm	Free Time
4:00 pm - 5:30 pm	Poster Session
5:30 pm - 7:30 pm	Quantum Computing Discussion Leaders: Heather Kulik (Massachusetts Institute of Technology, United States)
5:30 pm - 6:10 pm	Mario Motta (IBM Quantum, IBM Research Almaden, United States) "Emerging Quantum Computing Algorithms for Electronic Structure"
6:10 pm - 6:30 pm	Discussion
6:30 pm - 7:10 pm	Veera Sundararaghavan (University of Michigan, United States) "Quantum Annealers for Variational Problems in Materials Science"
7:10 pm - 7:30 pm	Discussion
8:00 pm - 9:00 pm	Dinner
Friday	
7:30 am - 8:30 am	Breakfast
9:00 am	Departure

Contributors

GRC Attendee List

The list of attendees appears below, sorted by the role recorded in their registration record.

Name	Affiliation	Participation	Gender
Ramprasad, Rampi	Georgia Institute of Technology	Chair	Male
Kulik, Heather J	Massachusetts Institute of Technology	Vice Chair	Female
Thornton, Katsuyo S	University of Michigan	Vice Chair	Female
Chmiela, Stefan	Technische Universität Berlin	Speaker	Male
Coley, Connor W	Massachusetts Institute of Technology	Speaker	Male
Cooper, Andy	University of Liverpool	Speaker	Male
Dutt, Meenakshi	Rutgers, The State University of New Jersey	Speaker	Female
Ghazisaeidi, Maryam	Ohio State University	Speaker	Female
Kattner, Ursula R	National Institute of Standards and Technology	Speaker	Female
Kusne, A. Gilad	National Institute of Standards and Technology	Speaker	Male
Mannodi Kanakkithodi, Arun Kumar	Purdue University	Speaker	Male
McDowell, David L	Georgia Institute of Technology	Speaker	Male
Motta, Mario	IBM Quantum, IBM Research Almaden	Speaker	Male
Pilania, Ghanshyam	Los Alamos National Laboratory	Speaker	Male
Provatas, Nikolas	McGill University	Speaker	Male
Roch, Loïc M	Atinary Technologies	Speaker	Male
Schleife, André	University of Illinois at Urbana-Champaign	Speaker	Male
Schwalbe-Koda, Daniel	Lawrence Livermore National Laboratory	Speaker	Male
Steinhauser, Martin O.	Frankfurt University of Applied Sciences	Speaker	Male
Sun, Wenhao	University of Michigan, Ann Arbor	Speaker	Male
Sundararaghavan, Veera	University of Michigan	Speaker	Male
Tadmor, Ellad B	University of Minnesota	Speaker	Male
Vashishta, Priya	University of Southern California	Speaker	Male
Vasudevan, Rama K	Oak Ridge National Laboratory	Speaker	Male
Warren, James A	National Institute of Standards and Technology	Speaker	Male
Arroyave, Raymundo	Texas A&M University	Discussion Leader	Male
Draxl, Claudia	Humboldt University of Berlin	Discussion Leader	Female
Fung, Victor	Georgia Institute of Technology	Discussion Leader	Male
Kreisbeck, Christoph	Kebotix	Discussion Leader	Male
Kuenneth, Christopher B	Georgia Institute of Technology	Discussion Leader	Male
Strachan, Alejandro	Purdue University	Discussion Leader	Male
Wang, Yan	Georgia Institute of Technology	Discussion Leader	Male
Born, Daniel	Institute for Theoretical Chemistry, University Stuttgart	Poster Presenter	Male
Carter, Jennifer L	Case Western Reserve University	Poster Presenter	Female

Name	Affiliation	Participation	Gender
Chandra, Anirban	University of Illinois Chicago	Poster Presenter	Male
Chen, Jiadong	University of Michigan	Poster Presenter	Male
Christiansen, Mads-Peter V.	Aarhus University	Poster Presenter	Male
Elder, Kate LM	Lawrence Livermore National Laboratory	Poster Presenter	Female
Fey, Lauren	University of California, Santa Barbara	Poster Presenter	Female
Gissinger, Jacob R.	NASA Langley Research Center	Poster Presenter	Male
Goff, James M	Sandia National Laboratories	Poster Presenter	Male
Gulyuk, Alexey	NCSU	Poster Presenter	Male
Han, Ming	the University of Chicago	Poster Presenter	Male
He, Tanjin	University of California, Berkeley	Poster Presenter	Male
Ji, Kaihua	Northeastern University	Poster Presenter	Male
Jung, Gwan-Yeong	Washington University in St. Louis	Poster Presenter	Male
Kurlin, Vitaliy	University of Liverpool	Poster Presenter	Male
Lam, Stephen	University of Massachusetts Lowell	Poster Presenter	Male
Lany, Stephan	National Renewable Energy Laboratory	Poster Presenter	Male
Law, Jeffrey	National Renewable Energy Lab	Poster Presenter	Male
LEE, BYUNGJU	Korea Institute of Science and Technology	Poster Presenter	Male
Lee, Kwang-Ryeol	Korea Inst Sci & Tech	Poster Presenter	Male
Lei, Xiangyun	Toyota Research Institute	Poster Presenter	Male
Limbu, Dil	New Jersey Institute of Technology	Poster Presenter	Male
Limmer, Krista	DEVCOM Army Research Laboratory	Poster Presenter	Female
Liu, Guangchen	Worcester Polytechnic Institute	Poster Presenter	Male
Liu, Yifan	Georgia Institute of Technology	Poster Presenter	Female
Lu, Gang	California State University Northridge	Poster Presenter	Male
Mahmood, Akhlak	NC State University	Poster Presenter	Male
Mandal, Nila	University of Connecticut	Poster Presenter	Female
McCarthy, Megan J	Sandia National Laboratories	Poster Presenter	Female
Mishra, Rohan	Washington University in St. Louis	Poster Presenter	Male
Mukherjee, Arnab	Northwestern University	Poster Presenter	Male
Muy, Sokseiha	Ecole Polytechnique Federale de Lausanne	Poster Presenter	Male
Nguyen, Nuong	The University of Kansas	Poster Presenter	Female
Nistane, Janhavi	Georgia Institute of Technology	Poster Presenter	Female
Oates, William S	Florida A&M-Florida State University	Poster Presenter	Male
Oliphant, Emily	University of Michigan	Poster Presenter	Female
Otis, Richard	Jet Propulsion Laboratory	Poster Presenter	Male
Ou, Pengfei	University of Toronto	Poster Presenter	Male
Pal, Koushik	Northwestern University	Poster Presenter	Male
Prince, Gollapalli	Indian Institute of Technology Madras	Poster Presenter	Male
Purcell, Thomas A. R.	NOMAD Laboratory at the Fritz Haber Institute	Poster Presenter	Male
Reynolds, Colleen	University of California, Santa Barbara	Poster Presenter	Female

Name	Affiliation	Participation	Gender
Rinderspacher, Christopher	US DEVCOM Army Research Laboratory	Poster Presenter	Male
Rohskopf, Drew	Sandia National Laboratories	Poster Presenter	Male
Saathoff, Jonathan D	ExxonMobil Technology and Engineering Company	Poster Presenter	Male
Saber, Muna	University of California- Santa Barbara	Poster Presenter	Female
Sadhukhan, Tumpa	Northwestern University	Poster Presenter	Female
Schiller, Ulf D	Clemson University	Poster Presenter	Male
Sharma, Abhiraj	Lawrence Livermore National Lab	Poster Presenter	Male
Shukla, Shivank	Georgia Institute of Technology	Poster Presenter	Male
Sikorski, Ember	Sandia National Laboratories	Poster Presenter	Female
St. John, Peter C	National Renewable Energy Lab	Poster Presenter	Male
Staublin, Philip	Northwestern University	Poster Presenter	Male
Suryanarayana, Phanish	Georgia Institute of Technology	Poster Presenter	Male
Tao, Peng	Southern Methodist University	Poster Presenter	Male
Toland, Aubrey	Georgia Institute of Technology	Poster Presenter	Male
Vaddi, Kiran	University of Washington	Poster Presenter	Male
Vargas-Lara, Fernando	ExxonMobil	Poster Presenter	Male
Vazquez Mayagoitia, Alvaro	Argonne National Laboratory	Poster Presenter	Male
Wilson, Steven	Arizona State University	Poster Presenter	Male
Wilson, Nolan N	National Renewable Energy Laboratory	Poster Presenter	Male
Xiong, Liming	Associate Professor	Poster Presenter	Male
Yang, Quanpeng	University of California - Merced	Poster Presenter	Male
Yang, Yuhan	Georgia Institute of Technology	Poster Presenter	Female
Ye, Weike	Toyota Research Institute	Poster Presenter	Female
Yingling, Yaroslava G	North Carolina State University	Poster Presenter	Female
Zhang, Jize	WPI	Poster Presenter	Male
Zhang, Lei	Carnegie Mellon University	Poster Presenter	Male
Allan, Douglas C	Corning Incorporated	Attendee	Male
Barhoum, Moussa	Covestro Deutschland AG	Attendee	Male
Bishop, Seann	Naval Nuclear Laboratory	Attendee	Male
Botu, Venkatesh	Corning Inc.	Attendee	Male
Curtin, William A	EPFL - Swiss Federale Institute of Technology	Attendee	Male
Ebna Hai, Bhuiyan Shameem Mahmood	BlueSc.AI - FEHRMANN Materials, Hamburg	Attendee	Male
Gorai, Prashun	Colorado School of Mines, NREL	Attendee	Male
Kamal, Deepak	Solvay	Attendee	Male
Leonard, Aeriel	The Ohio State University	Attendee	Female
Liu, Liping	Rutgers University	Attendee	Male
Maria, Eymana	University of Michigan	Attendee	Female
McCardle, Kaitlin	Springer Nature	Attendee	Female

Name	Affiliation	Participation	Gender
Meng, Zhaoxu	Clemson University	Attendee	Male
Peprah, David Kofi	University of L' Aquila	Attendee	Male
Provost, Bianca	Royal Society of Chemistry	Attendee	Female
Ransom, Brandi	Stanford University, Materials Engineering	Attendee	Female
Saidi, Wissam	National Energy Technology Laboratory, NETL	Attendee	Male
Shi, Lingxia	University of Michigan, Ann Arbor	Attendee	Female
Small, Yolanda	York College, City University of New York	Attendee	Female
Tepesch, Patrick D	Corning Incorporated	Attendee	Male
Wen, Youhai	US DOE - NETL	Attendee	Male
Westbrook, Maria	Naval Nuclear Laboratory - Knolls Atomic Power Laboratory	Attendee	Female
Windl, Wolfgang	The Ohio State University	Attendee	Male
Yu, Zhenzi	Georgia Tech	Attendee	Male
Zhao, Ji-Cheng (JC)	University of Maryland	Attendee	Male
Zhong, Yu	Worcester Polytechnic Institute	Attendee	Male
Ziebarth, Benedikt	Schott AG	Attendee	Male