

CABLE Big Idea RDD&D Workshop

Advanced Manufacturing Office

Workshop Summary Report

April 7–9, 2021

Within the U.S. Department of Energy (DOE) Office of Energy Efficiency and Renewable Energy (EERE), the Advanced Manufacturing Office (AMO) partners with industry, small business, academia, and other stakeholders to identify and invest in emerging technologies with the potential to significantly decarbonize industry, create high-quality domestic manufacturing jobs, and enhance the global competitiveness of the United States.

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Thanks are due to the panel moderators who worked hard to organize their panel discussions, recruit and confirm speakers, and develop questions for their sessions. Moderators included:

- Andre Pereira (DOE Office of Electricity) – Electricity Delivery System Applications Panel
- Isik Kizilyalli (Advanced Research Projects Agency–Energy) – Transportation Applications Panel
- Fredericka Brown (DOE Building Technologies Office) – Efficiency Applications Panel
- Jian Fu (DOE Wind Technologies Office) – Renewables Applications Panel
- Brian Valentine (DOE AMO) – Metal/Nanocarbon Conductor Panel
- Chris Hovanec (DOE AMO) – Metal Enhanced without Nanocarbon Panel
- Tony Bouza (DOE AMO) – Polymer and Other Non-metallic Enhanced Conductor Concepts Panel
- George Maracas (DOE Basic Energy Sciences Program) – Material Modeling and Computation Panels
- Santanu Chaudhuri (ANL) – Materials Modeling and Computation Panels
- Hal Stillman (Independent Consultant) – Supply Chain, Available Technical Resources, and Patenting Panels.

Special thanks to moderator Dr. Isik Kizilyalli for recruiting prominent speakers from NASA and two different U.S. Department of Defense agencies. The interagency discussions that occurred during his panel laid the groundwork for subsequent meetings. Isik also participated in valuable discussions following the workshop that are reflected in this report's conclusions.

Special thanks are also due to Dr. Maracas and Dr. Chaudhuri who drafted the chapter on the theory sessions which could not have been done without their help.

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List of Acronyms

3D	Three-dimensional
AAAC	All-aluminum-alloy conductor
ACCC	Aluminum conductor composite core
ACCR	Aluminum conductor composite-reinforced
ACSR	Aluminum conductor steel-reinforced
ACSS	Aluminum conductor steel-supported
AMO	Advanced Manufacturing Office (U.S. Department of Energy)
ANL	Argonne National Laboratory
ARPA-E	Advanced Research Projects Agency–Energy
BES	Basic Energy Sciences Program (U.S. Department of Energy)
BNL	Brookhaven National Laboratory
BTO	Building Technologies Office (U.S. Department of Energy)
CABLE	Conductivity-enhanced materials for Affordable, Breakthrough Leapfrog Electric and thermal applications
CNT	Carbon nanotube
CO ₂	Carbon dioxide
DFT	Density functional theory
DMMC	Deformed metal-metal composites
DOE	U.S. Department of Energy
EDS	Electricity delivery system
EERE	U.S. Department of Energy, Office of Energy Efficiency & Renewable Energy
ELECTRRON	Enabling eLEctrical Conductor Technologies for Resistance ReductiON
EV	Electric vehicle
FOA	Funding opportunity announcement
FY	Fiscal year
GTO	Geothermal Technologies Office (U.S. Department of Energy)
HEA	High-entropy alloys
HFTO	Hydrogen and Fuel Cell Technologies Office (U.S. Department of Energy)
HVAC	Heating, ventilation, and air conditioning
HVDC	High-voltage, direct current
IACS	International Annealed Copper Standard
ISO	International Standards Organization
LBNL	Lawrence Berkeley National Laboratory

ML	Machine learning
NASA	National Aeronautics and Space Administration
NETL	National Energy Technology Laboratory
NREL	National Renewable Energy Laboratory
ORNL	Oak Ridge National Laboratory
PNNL	Pacific Northwest National Laboratory
PV	Photovoltaic
Q&A	Question and answer
RDD&D	Research, development, demonstration, and deployment
rGO	Reduced graphene oxide
SBIR	Small Business Innovation Research
SC	Office of Science (U.S. Department of Energy)
SETO	Solar Energy Technologies Office (U.S. Department of Energy)
ShAPE	Shear Assisted Processing and Extrusion™
SLAC	Stanford Linear Accelerator Center
SNL	Sandia National Laboratories
STTR	Small Business Technology Transfer
SWCNT	Single-walled carbon nanotube
VTO	Vehicle Technologies Office (U.S. Department of Energy)
WETO	Wind Energy Technologies Office (U.S. Department of Energy)
WPTO	Water Power Technologies Office (U.S. Department of Energy)

Executive Summary

The U.S. Department of Energy's (DOE's) Advanced Manufacturing Office (AMO) held the *CABLE Big Idea RDD&D Workshop* April 7–9, 2021. The virtual workshop brought together approximately 250 leading scientific and technical experts to gather information on the state of the art in conductivity-enhanced materials and their applications. These stakeholders included scientists, engineers, manufacturers, materials experts, utility companies, and other entities within the conductor material and electrical product manufacturing supply chains. The two main goals of the workshop were to 1) start building and strengthening a research ecosystem around conductivity-enhanced materials and 2) inform AMO's future portfolio of research, development, demonstration, and deployment (RDD&D) investments and other program activities in the area of conductivity-enhanced materials.

CABLE—or Conductivity-enhanced materials for Affordable, Breakthrough Leapfrog Electric and thermal applications—was established as an Office of Energy Efficiency and Renewable Energy initiative as a result of a competitive internal process to identify and prioritize potentially high-impact research topics. Since then, conductivity-enhanced materials have been identified as an important element of the shift to an electrified and decarbonized industry sector, and CABLE remains a Big Idea. The CABLE effort is led by AMO and supported by eight other offices within DOE. The first major effort under CABLE was the development of several subtopics for DOE's Small Business Innovation Research/Small Business Technology Transfer (SBIR/STTR) programs in 2020. Another major activity was the launch of the CABLE Conductor Manufacturing Prize in March 2021.

Discussions at the workshop focused on potential applications for conductivity-enhanced materials and development status of different types of materials, including both metals and non-metallic materials. Participants also heard about the various resources available at the national laboratories for materials R&D, as well as issues related to intellectual property.

A preliminary finding from the workshop was that enhanced electrical conductivity seems to be observed only in metastable phases. If proven with additional research, this finding indicates a major direction for R&D on fabrication of conductivity-enhanced materials. Any fabrication technology (e.g., traditional melting/casting) that allows the composition to equilibrate may not yield microstructures demonstrating enhanced electrical conductivity. In addition, this finding explains why enhanced conductivity often appears in small-scale samples, in which achieving metastable microstructures is easier, but not in bulk material with equilibrium microstructures. This challenge is surmountable; several industrially produced products, including carbon steel, are in long-term metastable phases.

These findings, among others, led workshop organizers to conclude that adding modeling and simulation efforts to the CABLE innovation ecosystem should be a priority action. It is critical to understand the potential mechanisms for achieving conductivity enhancement in conductive materials. The urgency of this conclusion was supported by the fact that, despite the large number of presenters discussing different potential approaches to manufacturing conductivity-enhanced metals, no convincing, unequivocal peer-reviewed studies of materials showing significantly enhanced electrical conductivity at room temperature or elevated temperature were presented or referenced. However, there was convincing evidence of maintaining conductivity while improving strength, ampacity, temperature coefficient of resistance, and other attributes. In addition, strong evidence of enhancing thermal conductivity was presented.

During the workshop, attendees provided input and feedback on the CABLE program and its various aspects. Several common themes and high-priority needs emerged:

- The CABLE portfolio does not effectively balance key aspects of its research ecosystem. Throughout the workshop, multiple participants offered the perspective that there had previously been too much emphasis on fabrication and not enough on theory, modeling, and characterization. Any investment in

materials fabrication must be guided by an understanding of a plausible mechanism for enhanced conductivity. This work also needs to be supported by detailed characterization, including in operando analysis.

- The recommendation for additional characterization, theory, and modeling suggests that some basic science research is also necessary. Workshop organizers noted that the DOE Office of Science Basic Energy Sciences (BES) workshop report on [*Basic Research Needs for Transformative Manufacturing*](#), which was released around the time of the CABLE workshop, could serve as a guide for how to apply basic science capabilities to CABLE R&D problems—especially the sections on precision synthesis and multiscale modeling. AMO–BES coordination in this area is therefore crucial.
- The individual projects in different parts of DOE and other agencies need better coordination and comprehensive research management. CABLE should continue and expand sharing of information and common goals among the multiple federal agencies active in development of conductivity-enhanced materials. Specific areas where collaboration and coordination are needed include partnering with BES’s Nanoscale Science Research Centers; conducting materials characterization at user facilities with appropriate resources; and establishing and maintaining a user-friendly library to store high-quality fabrication and characterization data for the theory, modeling, and simulation community.
 - Shortly after the workshop ended, the Advanced Research Projects Agency–Energy (ARPA-E) released a [request for information on the potential for electrical conductivity enhancement](#) as part of the agency’s Enabling eLEctrical Conductor Technologies for Resistance ReductiON (ELECTRRON) effort. AMO is encouraged to exchange information with ARPA-E on respective results.
- Once AMO has preliminary results from its CABLE Conductor Manufacturing Prize and SBIR efforts and has enhanced information-sharing—particularly with BES and ARPA-E—AMO will be well positioned to develop a FOA for fiscal year (FY) 2023.
- AMO was encouraged to manage RDD&D of conductivity-enhanced materials as a multi-institutional collaboration with a single leadership organization, integrated strategy, and sustained funding.

Based on the feedback received at the workshop, the CABLE team updated its research ecosystem chart (see Figure ES.1 and Figure ES.2). The post-workshop CABLE research ecosystem reduces overall emphasis on applications and increases focus on materials development, including theory and characterization, and features the FY 2021 SBIR and the Pacific Northwest National Laboratory (PNNL) seedling awards.

This workshop report summarizes the presentations, panel discussions, and breakout group discussions that took place at this event. The results presented here are a snapshot of the viewpoints expressed by the experts who attended the workshop and do not necessarily reflect those of the broader conductivity-enhanced materials community.

Original CABLE Research Ecosystem

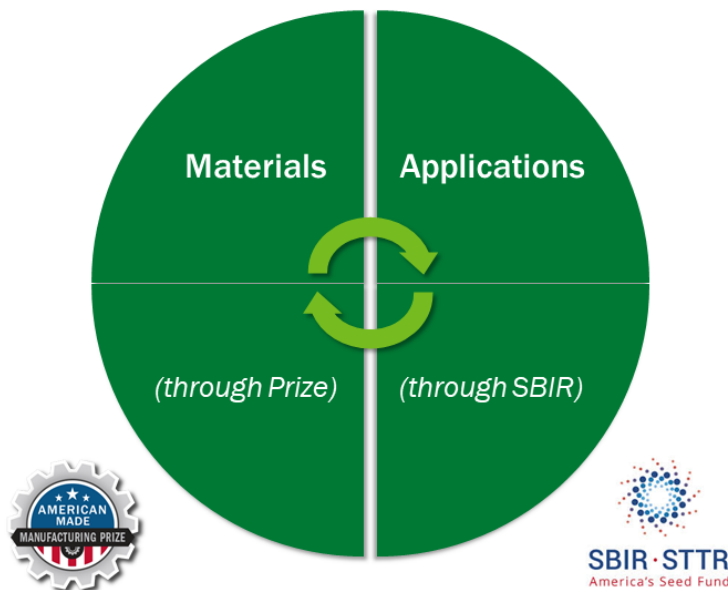


Figure ES.1. The original, pre-workshop CABLE research ecosystem. With this approach, multiple small independent efforts are undertaken to explore and fabricate samples of conductivity-enhanced materials.

New CABLE Research Ecosystem

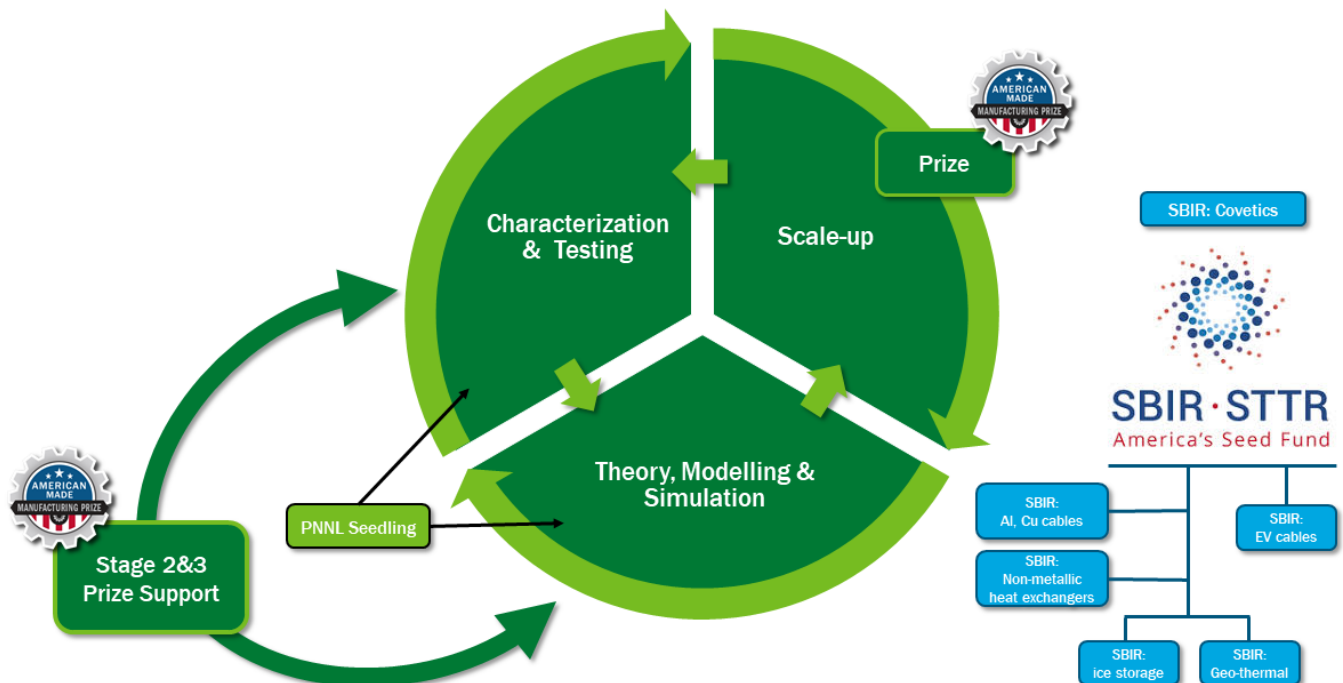


Figure ES.2. Updated CABLE research ecosystem, as envisioned based on feedback received at the workshop. The CABLE effort seeks to establish a technical basis for creating conductivity-enhanced materials. This will require theory, modeling and simulation, fabrication from small samples to scalable processes, and characterization and testing to confirm compositions, properties, performance, and scientific understanding. This iterative, cyclical development loop can apply to technical ideas from innovators throughout the ecosystem and across government agencies.

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Chapter 1: Background and Workshop Proceedings

On April 7–9, 2021, the U.S. Department of Energy (DOE) Advanced Manufacturing Office (AMO) held a workshop to better understand potential areas for future research, development, demonstration, and deployment (RDD&D) efforts and other program activities related to advanced electrical and thermal conductors. The *CABLE Big Idea RDD&D Workshop* featured an in-depth discussion of the CABLE (Conductivity-enhanced materials for Affordable, Breakthrough Leanfrog Electric and thermal applications) initiative and brought together materials scientists, application developers, manufacturers, and other interested stakeholders.



Materials with enhanced conductivity can help transition to a zero-carbon grid by 2035 through lowering cost and footprint of electricity delivery systems, increasing grid resilience to extreme temperatures and weather, and lowering cost and improving performance of all electrical equipment.

*– Mike McKittrick,
Acting Director, AMO*

1.1 CABLE Big Idea Overview and History

Conductive materials are fundamental to nearly all energy use applications. Developing manufacturing processes for conductivity-enhanced materials would enable product manufacturers to lower costs, improve performance, and allow their customers and the United States to substantially improve energy efficiency and reduce greenhouse gas emissions. As electrification grows worldwide in response to the climate crisis, so too will demand for conductivity-enhanced materials and applications. The International Energy Agency estimates that 10 million miles of new transmission cable—enough to reach to the moon and back 21 times—will be needed to connect renewables to the planet’s grids in the next decade.¹ In addition, the passage of the Infrastructure and Jobs Act provides the United States with a once-in-a-generation opportunity to replace aging electric and transportation infrastructure with new high-performance materials. There is an urgent need for conductivity-enhanced materials that can lower transmission cable costs and improve transmission cable performance—including resilience against extreme weather events. Furthermore, conductivity-enhanced materials support new transformational technologies ranging from electric cars, trains, and planes to smartphones, heat pumps, and other electrical and thermal technologies that improve people’s everyday lives.

To supercharge the effort to develop new conductors, AMO led development of this CABLE initiative which is now led by AMO and supported by the Office of Electricity and seven other offices within the Office of Energy Efficiency and Renewable Energy (EERE): Building Technologies Office (BTO), Geothermal Technologies Office (GTO), Hydrogen and Fuel Cells Technologies Office (HFTO), Solar Energy

¹ Wanner, Brent and Laura Cozzi. 2020. *Electricity security in tomorrow’s power systems: Insights from World Energy Outlook 2020*. Paris: International Energy Agency. Published October 23. [iea.org/articles/electricity-security-in-tomorrow-s-power-systems](https://www.iea.org/articles/electricity-security-in-tomorrow-s-power-systems).

Technologies Office (SETO), Vehicle Technologies Office (VTO), Water Power Technologies Office (WPTO), and Wind Energy Technologies Office (WETO).

Building a clean energy economy and addressing the climate crisis is a top priority of the Biden Administration. This will be achieved by national decarbonization through electrification and increasing infrastructure resilience, a key element supported by conductivity-enhanced materials. These actions will ultimately create new, high-paying jobs for Americans in the process. Additionally, CABLE's RDD&D can bolster the nation's ability to produce carbon-pollution-free electricity by 2035 and "deliver an equitable, clean energy future, and put the United States on a path to achieve net-zero (greenhouse gas) emissions, economy-wide, by no later than 2050,"² steps that will benefit all Americans.

The first major effort under CABLE was the development of a CABLE Topic through DOE's Small Business Innovation Research/Small Business Technology Transfer (SBIR/STTR) program, which seeks to increase private-sector commercialization of technology developed through DOE-supported R&D. SBIR/STTR stimulates technological innovation in the private sector, encourages participation by women-owned and minority-owned small businesses, and improves the return on investment from federally funded research for economic and social benefits to the nation. The FY 2021 Phase I SBIR/STTR FOA included the following CABLE-related subtopics:³

- 20a: Metal–Carbon Composition and Composites Manufacturing (a technology transfer opportunity)
- 20b: Electricity Delivery System (EDS) Applications
- 20c: Non-Metallic Heat Exchangers
- 20d: Ice Storage and Other Thermal Storage-Related Systems
- 20e: Electric Systems – Generators and Motors
- 20f: Photovoltaics (PV) Module and System Electrical Connections
- 20g: Geothermal: Direct Use and Electricity Generation Applications
- 20h: Enhanced-Conductivity Electric Vehicle (EV) Charging Cables and Couplers.

Subtopic 20a entailed further research on a conductivity-enhanced materials manufacturing technology developed at a national laboratory. All other subtopics support leapfrog applications in the design and use of conductivity-enhanced materials that will make the performance improvements and energy savings of the applications more affordable. In June 2021, ten CABLE SBIR/STTR proposals were awarded funding. There

Table 1.1 DOE Offices Involved in CABLE

Office of Electricity
Office of Science
Office of Energy Efficiency and Renewable Energy (EERE)

Table 1.2 EERE Suboffices Involved in CABLE

Advanced Manufacturing Office
Building Technologies Office
Geothermal Technologies Office
Hydrogen and Fuel Cells Technologies Office
Solar Energy Technologies Office
Vehicle Technologies Office
Water Power Technologies Office
Wind Energy Technologies Office

² The White House. 2021. "Executive Order on Tackling the Climate Crisis at Home and Abroad." Published January 17. [whitehouse.gov/briefing-room/presidential-actions/2021/01/27/executive-order-on-tackling-the-climate-crisis-at-home-and-abroad/](https://www.whitehouse.gov/briefing-room/presidential-actions/2021/01/27/executive-order-on-tackling-the-climate-crisis-at-home-and-abroad/).

³ DOE (U.S. Department of Energy). 2020. *Department of Energy (DOE) Small Business Innovation Research (SBIR) Small Business Technology Transfer (STTR) FY2021 Phase I Release 2 Funding Opportunity Announcement Number DE-FOA-0002360*. Washington D.C.: DOE. Released December 14. science.osti.gov/-/media/grants/pdf/foas/2021/DE-FOA-0002360.pdf?la=en&hash=BC1C1C808A07212CF2385A8328B57D4CF7385740.

were four proposals funded in subtopic 20c, two in subtopic 20b, and one each in subtopics 20a, 20d, 20g, and 20h.⁴

The second major activity was the launch of the CABLE Conductor Manufacturing Prize in March 2021. The \$4.5 million prize encourages researchers and inventors to develop and manufacture breakthrough conductivity-enhanced materials. Competitors must design affordable conductors that demonstrate significant enhancements in conductivity and enable U.S. manufacturers to leapfrog to next-generation materials. The prize includes three technical classes of conductivity-enhanced materials: 1) metal enhanced with nanocarbon, 2) metal enhanced without nanocarbon, and 3) non-metallic materials (e.g., polymer or nanocarbon) enhanced with metal. Up to four Grand Prize winners are selected in the three-stage, three-year contest. The submission deadline for Stage 1 of the competition was August 19, 2021. More information about the Conductor Manufacturing Prize can be found on the American-Made Challenges website at stage.americanmadechallenges.org/cable/.⁵

More information about the overall CABLE initiative is available on the CABLE website at cable-bigidea.anl.gov/.



Figure 1.1. March 2021 launch of the CABLE Conductor Manufacturing Prize.

1.2 Workshop Objectives

AMO hosted the *CABLE Big Idea RDD&D Workshop* to gather information from stakeholders on the state of the art in a wide variety of conductivity-enhanced materials and their applications—particularly applications that align with the Office of Electricity EDS efforts and the three EERE research



Figure 1.2. The CABLE Big Idea RDD&D Workshop, April 7–9, 2021.

sectors: energy efficiency, renewable power, and sustainable transportation. These stakeholders included scientists, engineers, manufacturers, materials experts, utility companies, and other entities within the conductor material and electrical product manufacturing supply chains.

The two main goals of the workshop were to 1) start building and strengthening a research ecosystem around conductivity-enhanced materials and 2) inform AMO and the broader CABLE research community's future portfolio of RDD&D investments and other program activities in the area of conductivity-enhanced materials.

⁴ DOE. 2021. "AMO Awards Nearly \$2.8 Million to Support American Small Businesses and Entrepreneurs." Published June 10.

energy.gov/eere/amo/articles/amo-awards-nearly-28-million-support-american-small-businesses-and-entrepreneurs.

DOE. 2021. "FY21 Phase I Release 2 Award Listing." Excel file last modified June 10. science.osti.gov/-/media/sbir/excel/2021/FY21_Phase-I-Release-2_Award-Listing_06-10-2021.xls?la=en&hash=880A9489445C59FC1E0E4A055921628DB5E4512F.

⁵ An informational webinar about the CABLE Conductor Manufacturing Prize was held on March 30, 2021. The webinar recording is available at youtube.com/watch?v=V1JK978qY6w. The latest updates on the Conductor Manufacturing Prize are available at herox.com/cable/updates, and resources can be found at herox.com/cable/resources.

1.3 Workshop Metrics

The *CABLE Big Idea RDD&D Workshop* took place virtually over three consecutive days, from April 7 to 9, 2021. The agenda for each day lasted approximately 5.5 hours, featuring 13 separate panel sessions and a total of 60 speakers and panel moderators (see Appendix A for the detailed agenda).

Nearly 300 individuals registered for the workshop. Of those registrants, approximately 250 participated in at least some part of the workshop. There was broad participation from various stakeholder sectors, including different federal agencies, national laboratories, academia, and private industry. The breakdown of registrants by sector is provided in Figure 1.3. A list of workshop attendees is in Appendix C.

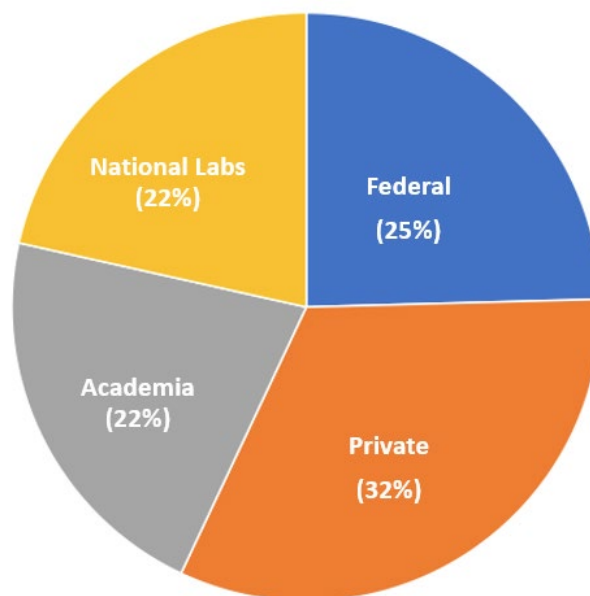


Figure 1.3. CABLE Workshop participant breakdown by sector.

Information was gathered through the registration process on participant interest in various panels to staff them adequately. The materials fabrication panel on metal enhanced with nanocarbon had the greatest advance signup and highest attendance. The wide array of stakeholders was able to benefit from the communications tailored to all audiences from theorists to manufacturers to modelers.

1.4 Workshop Overview

Dr. Mike McKittrick, Acting Director of AMO, opened the workshop, and Dr. Tina Kaarsberg, AMO lead for the overall CABLE effort, introduced the CABLE initiative. The bulk of the workshop consisted of panel sessions, as described below. The workshop concluded with a summary session in which panel moderators provided high-level summaries and initial conclusions from each panel.

Day 1

The focus of the first day's agenda was on potential applications of conductivity-enhanced materials. The application areas were divided into four separate panel sessions:

1.2.1 Electric Delivery System Applications

1.2.2 Transportations Applications

1.3.1 Efficiency Applications

1.3.2 Renewable Energy Applications

The four panels were followed by facilitated discussions to gather additional information from participants on high-potential application areas and priority research needs.

Day 2

The first part of Day 2 was focused on materials fabrication. This topic area was divided into three separate panels:

2.2.1 Metal/Nanocarbon Conductors

2.2.2 Metal Enhanced without Nanocarbon

2.2.3 Polymer and Other Non-Metallic Conductor Concepts

The latter part of Day 2 focused on materials theory modeling and computation. The three panels in this area covered the following topics:

2.3.1 Atomistic-Scale Simulation

2.3.2 Multiscale Simulation

2.3.3 Crosscutting Topics in Materials Simulation

All six panels were followed by facilitated question and answer (Q&A) sessions.

Day 3

The third day included three panels:

3.2.1 Supply Chain

3.2.2 Available Technical Resources (relevant national laboratory facilities)

3.2.3 Patenting

All three panels were followed by facilitated Q&A sessions.

More detailed discussion on the panels, presentations, and other workshop deliberations and conclusions are provided in the following chapters of this report. To put the workshop presentations and discussions in context, this report also includes additional background and other information that was not presented or discussed at the workshop. The full workshop agenda with links to all presentation slides is provided in Appendix A. Note that the structure of this workshop report does not follow the workshop agenda. Some parts of the agenda—including the sessions on the supply chain, available technical resources, and patenting—are covered in Appendix B. A [read-ahead document](#) providing relevant background information was shared with all registrants prior to the workshop.

Chapter 2: Applications

The first day of the CABLE workshop included four panel sessions on applications, as shown in Table 2.1. The detailed agendas for the different applications panels and links to presentations are included in Appendix A.

Table 2.1 Applications Panel Sessions

- Electricity Delivery Systems
- Transportation
- Energy Efficiency Applications
- Renewable Power (Solar, Geothermal, Wind, Water)

2.1 Electricity Delivery Systems

The EDS panel session began with a presentation by [Ben Shrager](#) of DOE's Office of Electricity, who explained that transmission and distribution lines, transformers, and power electronics could all benefit from conductors with lower electrical resistance, higher strength, and improved thermal conductivity. Additionally, the use of earth-abundant and recyclable materials is highly desirable. The first presentation was followed by a discussion from [Joe Hagerman](#) of Oak Ridge National Laboratory (ORNL) on the importance of CABLE materials for transformer and component resilience for the modern power grid. The EDS panel ended with a presentation by [Iver Anderson](#) of Ames Laboratory on current efforts to produce aluminum–calcium composite conductors for higher strength and conductivity in transmission cables. Key findings from the panel presentations are included in Table 2.2.

Table 2.2 Key Findings from EDS Applications Panel

Main Discussion Points	High-Level Takeaways	Technical Challenges Identified	Outstanding Research Needs
• EDS • Conductors in EDS • Transformers • Transmission and distribution lines • Power electronics • Solid-state power substations • Al/Ca composite conductors	• There are many R&D opportunities for conductors in EDS. • There is no right answer on the prioritization of CABLE EDS R&D; all applications are equally important for a carbon-free future.	• Key EDS conductor performance challenges are cost, resistivity, mechanical strength, and thermal conductivity. • High penetration of distributed energy resources, bi-directional power flows, and added control points will require the modernization of EDS.	• Efforts should continue in several application areas related to EDS. • Aggressive EDS R&D efforts will be needed to fully prepare the grid for, and move it toward, a carbon-free future.

Facilitated Discussion: EDS

The facilitated discussions following the EDS panel led to several observations:

- Strength, low cost, reduced weight, and corrosion resistance were among the most critical non-conductivity requirements for EDS applications.
- Offshore wind power and other undersea cables are among the niche applications that can afford higher costs for improved conductivity.

- Transmission cables require scale-up and cost reductions to integrate higher-conductivity materials.
- Utility operators and other EDS sector decision-makers seem to be the drivers for innovations in conductivity.

Table 2.3 Facilitated Discussion Input on EDS Applications

EDS Applications That Will Drive <u>Short-Term</u> Innovations in Conductivity	Niche EDS Applications That Can Afford <u>Higher Costs</u> in Exchange for Improved Conductivity	EDS Application Areas That Require <u>Scale-up</u> and <u>Cost Reductions</u> Before They Can Integrate Higher-Conductivity Products or Materials	<u>Non-Conductivity</u> Performance Requirements for Conductive Materials in EDS Applications
• Transformers • Storage and charging • Power electronics • Electric motors	• Undersea cables (e.g., for offshore wind) • Distribution in congested areas • Military	• Transmission lines • Microgrids • Renewable power	• Strength • Low cost • Reduced weight • Corrosion resistance • Creep resistance • Improved durability • Thermal conductivity • Properties of insulation materials • Low carbon dioxide (CO₂) footprint

Related SBIR Projects – EDS Applications

Mainstream Engineering Corporation, located in Rockledge, Florida, is leading the “Copper-Encapsulated Carbon Nanotubes to Enhance Copper Transmission Cable Properties” project. Copper-carbon nanotube (CNT) hybrid composites, which boast low coefficients of thermal expansion yet high conductivity, pose significant opportunity for applications in electric power cables. Typically, CNT mixing into metals results in particle aggregation and poor interfacial bonding which reduces material performance. This project will demonstrate the production and scalability of Cu-coated CNTs using Mainstream’s patent pending CNT treatment process which improves CNT loading, distribution, and interface between the CNT and copper cable. One possible use for this technology is as a high-performance electrical conductor that can improve the lifespan and function of undersea and underground power transfer cables. This innovation enables an increase in transmission capacity needed to support higher levels of renewable generation on the grid, such as undersea cable buildout required by increased offshore wind capacity, and reliable, high-capacity undergrounding of power lines.

QuesTek Innovations LLC, based in Evanston, Illinois, was awarded funding for the “Enhanced Aluminum Conductor for Overhead Electrical Transmission Application” project. The company is developing a high-strength, high-conductivity aluminum alloy for overhead transmission line applications in the EDS. The project’s success will enable a reduction in energy waste associated with transmitting electrical power over large distances. As increased renewable generation on the grid requires transmission capacity increases, innovations in this area are essential to a sustainable and reliable power grid and the future growth of the energy sector.

2.2 Transportation

The Transportation Panel session included presentations by [Timothy Haugan](#) of the U.S. Air Force Research Laboratory and [Lynn Petersen](#) of Office of Naval Research describing the pressing need for more efficient, lighter, and more reliable wire conductors for aerospace, naval transportation, and defense systems. [Maricela Lizcano](#) from NASA discussed the need for high-voltage conductors and insulation to prevent discharge arcing in aviation applications. [Burak Ozpineci](#) of ORNL shared current needs for improved electrical conductors for wireless power transfer applied to EVs. Finally, [Don Hillebrand](#) from Argonne National Laboratory (ANL)

discussed the role of conductor materials in EV charging and the importance of material cost. Key findings from the panel presentations are included in Table 2.4.

Table 2.4 Key Findings from Transportation Applications Panel

Applications Driving Innovation	Premium Markets	Medium-Term Applications	Non-Conductivity Requirements
- Aviation - Long-haul transport - Shipping	- Military - Aerospace	- Electric motor coils - Electric drive systems for vehicles - Signal cables for road vehicles requiring low weight - EV drive motors	- Review and potentially update electrical standards - Thermal management in power conversion devices

Facilitated Discussion: Transportation

The facilitated discussions following the Transportation panel led to several observations:

- Weight, strength, fatigue resistance, and recyclability are among the most important non-conductivity performance requirements for conductive materials in transportation applications.
- The niche applications in transportation that can afford higher costs in exchange for improved conductivity are high-end vehicles, aerospace, and military.
- The transportation applications that require scale-up and cost reductions before they can integrate higher-conductivity products or materials include passenger cars, trucks, and public transportation.

Table 2.5 Facilitated Discussion Input on Transportation Applications

Transportation Applications That Will Drive <u>Short-Term</u> Innovations in Conductivity	Niche Transportation Applications That Can Afford <u>Higher Costs</u> in Exchange for Improved Conductivity	Transportation Application Areas That Require <u>Scale-up</u> and <u>Cost Reductions</u> Before They Can Integrate Higher-Conductivity Products or Materials	Non-Conductivity Performance Requirements for Conductive Materials in Transportation Applications
- EV charging - Electric aviation - Space applications - Electric motor windings - Connectors	- Aerospace - Military - High-end vehicles	- Passenger cars and trucks - Electric public transportation	- Weight - Recyclability - Strength - Fatigue resistance, including ability to withstand vibrations - Manufacturability - Reliability - Cost

Related SBIR Project – Transportation Applications

NAECO, LLC, of Peachtree City, Georgia, was awarded funding for the “Fabrication and Evaluation of Electric Vehicle Charging System Subcomponents Made from Enhanced Conductivity Copper” project. Because of energy losses in EV charger components, improvements are needed in the cables and contacts that operate at up to 400 amps and 1,000 volts. Use of commercially demonstrated conductivity-enhanced materials in these components could improve EV charging efficiency. NAECO seeks to create charging cable assemblies using a novel copper–carbon nanocomposite and validate their performance for potential scale-up in commercial applications.

2.3 Energy Efficiency Applications

[Kashif Nawaz](#) of ORNL opened this panel with an overview of the lab's efforts to develop non-metallic heat exchangers for applications in buildings. [Jason Woods](#) from the National Renewable Energy Laboratory (NREL) shared his knowledge of thermal energy storage and how phase-change materials can match the performance characteristics of electrochemical batteries. [Matteo Pasquali](#) of Rice University discussed the different types of metrics that can be used to evaluate conductivity improvements, including metrics for CO₂ footprints. He also described recent improvements in CNT conductors and their potential applications. One of the main themes of this panel was that materials with higher thermal conductivity are necessary to improve heat transfer and eventually implement thermal energy storage. Other key findings from the panel presentations are included in Table 2.6.

Table 2.6 Key Findings from Energy Efficiency Applications Panel

Applications Driving Innovation	Premium Markets	Medium-Term Applications	Non-Conductivity Requirements
- Buildings (heating, ventilation, and air conditioning [HVAC], heat pumps) - Motor stator windings - Aircraft - EVs - Offshore technologies	- Aerospace, including electric aircraft - Computing, microelectronics cooling - Military	- Energy storage (grid-scale, automotive) - Solar panels - Appliances - HVAC fans - Pumps - Home wiring and other consumer applications	- Weight - Physical footprint - Thermal conductivity - Mechanical strength - Flexibility - Corrosion resistance - Wear resistance - Manufacturability - Energy and environmental impacts of making conductors

Facilitated Discussion: Energy Efficiency

The facilitated discussions following the Energy Efficiency Panel led to several observations:

- Heat exchangers, low-temperature waste heat recovery, and thermal storage are applications that will drive thermal conductivity innovations in the short term. Computing applications and energy storage can drive electrical conductivity innovation.
- Medical devices and military and aerospace applications are among the niche energy efficiency application areas that can afford higher costs in exchange for improved conductivity.
- Many consumer products (such as appliances) and industry facilities (including steel mills, heat treatment shops, and foundries) are among the energy efficiency applications that require scale-up and cost reductions before they can integrate higher-conductivity products or materials.
- Cost, strength, and durability are among the key non-conductivity performance requirements for conductive materials in energy efficiency applications.

Table 2.7 Facilitated Discussion Input on Energy Efficiency Applications

Energy Efficiency Applications That Will Drive Short-Term Innovations in Conductivity	Niche Energy Efficiency Applications That Can Afford Higher Costs in Exchange for Improved Conductivity	Energy Efficiency Application Areas That Require Scale-up and Cost Reductions Before They Can Integrate Higher-Conductivity Products or Materials	<u>Non-Conductivity</u> Performance Requirements for Conductive Materials in Energy Efficiency Applications
• Heat exchangers • Low-temperature waste heat recovery • Electric and thermal storage • Computing and microelectronics • Electric motors for vehicles	• Military • Aerospace • Medical devices	• HVAC • Household appliances and other consumer products • Energy storage • Industry, such as metal manufacturing and refining	• Manufacturability • Strength • Durability • Corrosion resistance • Cost • Weight

Related SBIR Projects – Energy Efficiency Applications

Energy Wall, located in Lancaster, Pennsylvania, is undertaking the “Non-Metallic Heat Exchangers – Ceramic Polymer Hybrid Microchannel” project. Although the technology is less conductive than traditional aluminum, its potential benefits related to light weight, manufacturability, corrosion resistance, and low cost make compact polymer heat exchangers a significant innovation. Ceramic polymer heat exchangers can even scrub pollutants from indoor environments while increasing heat pump efficiency by more than 60%, providing significant energy saving opportunities in both buildings and industrial processes.

T2M Global, LLC, of Danbury, Connecticut, is partnering with *Trevi Systems* for the “High-Performance, Lower-Cost Plastic Heat Exchangers” project. With extensive experience in extrusion, weaving, and assembly, T2M Global has the capability to package its products into tailorable shapes and sizes, depending on the application. The project seeks to increase the thermal conductivity of conventional polymer composites by over 500% by doping the materials with highly conductive “smart” additives and enhancing the shape of the material. If successful, the technology would be beneficial to multiple industries across the United States, owing to its ability to reduce energy use energy consumption.

Technology Assessment & Transfer, Inc., of Annapolis, Maryland, was awarded funding for the “High-Payoff 3D Printed Ceramic Heat Exchangers for HVAC” project. The company uses stereolithography to print highly efficient compact ceramic heat exchangers to lower energy costs associated with heating and cooling, thereby extending the life of heat pumps and air conditioning systems and reducing associated pollution. The innovation can also be applied to a host of waste heat recovery applications, further broadening the technology’s potential impacts.

Triton Systems, Inc., of Chelmsford, Massachusetts, was awarded funding for the “Plastic Heat Exchangers with High Conductance” project. The company is developing plastic heat exchangers that are half the size of conventional metal equivalents and offer 500% greater heat transfer rate. Currently, 20% of electricity used in buildings is for heating and cooling, relying on refrigerants that exacerbate global warming. Using a microscale geometry and manufacturing process, Triton seeks to improve efficiency, reduce cost (at least 40% lower than the traditional aluminum design), reduce refrigerant use, and bring cost-competitive manufacturing back to the United States.

Mainstream Engineering Corporation, located in Rockledge, Florida, was awarded funding for the “Residential-Scale HVAC Thermal Energy Storage Subcooler” project. Mainstream, in collaboration with researchers at NREL, will develop two low-cost thermal energy storage heat exchangers that use water as a phase-change

material, allowing customers to shift their electrical usage from periods of peak demand to off-peak periods with lower rates. One heat exchanger is a metal-coated polymer composite, and the other is alumina-based, using microfluidics. Both take advantage of the water-ice phase change. This process is particularly attractive for thermal energy storage because of its large heat of fusion, which results in high energy density, low cost, near-constant storage temperature (melt temperature), and minimal environmental impact. Mainstream intends to use advanced material and construction techniques to integrate thermal energy storage heat exchangers with existing air conditioning systems, resulting in seamless and affordable energy efficiency in residential and commercial HVAC systems with a 2–4-year return on investment.

2.4 Renewable Power

[Eduard Muljadi](#) of NREL began the renewable power panel by providing an overview of the role of electrical and thermal conductors in a grid powered by renewable sources. Generator design, mechanical properties, and reliability are limiting factors for CABLE materials. [Bill Vandermeer](#) of DOE GTO shared how materials with higher thermal conductivity can improve the heat transfer from subsurface geothermal reservoirs to the surface for direct use and for electricity production. [Nate McKenzie](#) of DOE WETO described the shift to higher-voltage transmission cables, in addition to the need for lighter cables with more efficient transmission. Finally, [Susan Huang](#) from DOE SETO shared that durability of cables, along with performance and reduced installation time, are crucial for solar applications. Key findings from the panel presentations are included in Table 2.8.

Table 2.8 Key Findings from Renewable Power Applications Panel

Applications Driving Innovation	Premium Markets	Medium-Term Applications	Non-Conductivity Requirements
• Solar panels • Generators for offshore and hydropower • Energy storage • Cables and wiring • Geothermal well casings	• Military • Aerospace • Isolated communities	• Offshore wind • Power electronics • High-voltage, direct current (HVDC) cables	• Weight • Size • Strength • Flexibility • High-voltage insulation • Power density • Manufacturing cost and scalability

Facilitated Discussion: Renewables

The facilitated discussions following the Renewables panel led to the following observations:

- Offshore energy applications and solar PV interconnects and metallization are among the applications that will drive short term innovations in conductivity.
- Military and aerospace PV applications are among the niche renewable power application areas that can afford higher costs in exchange for improved conductivity.
- Corrosion-resistance, high strength, and low weight are among the key non-conductivity performance requirements and associated metrics for conductive materials in renewables applications.

Table 2.9 Facilitated Discussion Input on Renewable Power Applications

Renewable Applications That Will Drive <u>Short-Term</u> Innovations in Conductivity	Niche Renewable Applications That Can Afford <u>Higher Costs</u> in Exchange for Improved Conductivity	Renewable Application Areas That Require <u>Scale-up</u> and <u>Cost Reductions</u> Before They Can Integrate Higher-Conductivity Products or Materials	<u>Non-Conductivity</u> Performance Requirements for Conductive Materials in Renewable Applications
• Solar PV interconnects and metallization (e.g., replacing silver with copper) • Large-scale wind generation • Undersea cables • Umbilical tethers for floating wind and marine energy	• Aerospace solar • Military	• Generators • Power electronics • Power cables and wiring • Smaller-scale wind and solar	• Corrosion resistance • Weight • Strength • Cost • Fatigue and creep • Manufacturability

Related SBIR Project – Renewable Power Applications

Greenpath Systems LLC, of Norman, Oklahoma, was awarded funding for the “Highly Conductive Nano-Engineered Geopolymer Cements for Geothermal Applications” project. By harnessing energy from natural heat sources within the earth, ground source heat pumps, also known as geothermal heat pumps, can provide heating and cooling for a significant number of buildings. With a critical need to lower heat pump installation costs and increase heat pump efficiency, the company offers a scalable solution: repurposing waste materials from other industrial streams to develop geopolymer grouts enhanced with nano-material fillers in the subsurface wells of geothermal heat pumps. This solution could help reduce the cost, improve the heat transfer efficiency, and ultimately reduce the carbon footprint for geothermal energy installations to benefit residential, commercial, and industrial buildings.

Chapter 3: Metals

The second day of the workshop focused on conductivity-enhanced metals, with panels on metals with and without nanocarbons. (A third panel, Polymer and Other Non-Metallic Conductor Concepts, is discussed in Chapter 4.) In addition, metals were discussed by presenters in the Applications, Theory and Modeling, and Available Technical Resources panels. The metals talks were the best-attended and most intensely interactive sessions, with participants openly questioning many results that were presented.⁶ In response to this level of interest, this chapter provides some general background information on metal conductors in general, conductivity-enhanced metal with nanocarbon, and metal with its conductivity enhanced without nanocarbon. The two metal related panels are then summarized in a Q&A section.

3.1 Metal Conductor Background

Metals and metal alloys, such as those listed in Table 3.1, are currently used for nearly all electrical conductors. The two base-metals that dominate most applications are copper and aluminum.

Copper: Historically, the most-used conductor metal has been copper, as it offers the benefit of having the highest electrical conductivity and corrosion resistance for its price. While silver has the highest absolute conductivity and gold has the best corrosion resistance, both are substantially more expensive than copper. Copper-based conductor wires are used in nearly all electrical equipment, such as motors, generators, and electrical appliances for which weight is not a critical factor but efficiency and size (cross-sectional area or footprint) are. Historically, copper was also used for transmission lines, but now copper cables are used only in medium- to low-voltage line applications because of their higher conductivity and flexibility (the wires can bend in a tight radius). Copper is also used for underground and underwater applications because of its relatively low corrosivity (compared to aluminum). In subsea applications, copper also has the benefit of a smaller cross-section than an aluminum conductor with the same capacity. The result is that cable laying ships can carry longer conductors, requiring fewer splices, which are a significant source of failure.

Aluminum: Because it has about half the weight and a lower cost than a copper cable of comparable resistance, aluminum is now preferred for overhead transmission lines. The most common aluminum-based power line conductor is aluminum conductor steel-reinforced (ACSR). Other market options include all-aluminum-alloy conductor (AAAC), aluminum conductor composite core (ACCC), aluminum conductor composite-reinforced (ACCR), and aluminum conductor steel-supported (ACSS). Aluminum does, however, require a larger diameter than copper because of its lower conductivity. If conductivity-enhanced aluminum can be manufactured cost-effectively, resulting in a conductor with a smaller cross-sectional footprint, it could become a notable contender for transportation applications in which both light weight and small footprint are desired.

Table 3.1 Most Commonly Used Metallic Conductors and Their Properties

Material	IACS (%)	Notes
Silver (Ag)	108	• Used for premium applications 1/3 the strength of Cu
Copper (Cu), pure	103	• Less expensive (<10x) than silver
Copper (Cu)*, annealed	100	• More flexible and corrosion resistant than Al • Low static strength (in the pure form)
Gold (Au)	71	• Highest cost • Most corrosion-resistant • Lowest thermal coefficient of resistance

⁶ Detailed questions asked during metals talks included several on how conductivity measurements were made, other requesting updates on low performance test results of several years ago. One questioner asked why low quality non-electric (impure) copper was used as a measurement baseline; another asked about sufficient availability of single layer graphene to enable commercial-scale production.

Aluminum (Al) alloy 1350 (Used in ASCR for power line applications)	~62	• Half the weight per length compared to copper • Less expensive than copper
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*International Annealed Copper Standard (IACS) is the standard of conductivity.

3.2 Nanocarbon and Metal–Nanocarbon Background

In this report, “nanocarbon” refers to new carbon allotropes: CNTs, single- or few-layer graphene, doped or undoped, and other carbon allotropes. The excitement surrounding the new carbon allotropes discovered in recent decades (see Table 3.2) led the CABLE Big Idea team and others to consider them first in developing the CABLE concept. While several groups have observed conductivities of >120% IACS in metal nanocarbon combinations, all of these values are for nanoscale samples, none are for microscale and larger (macroscale) samples. Before the workshop, a paper was circulated to attendees: “Advanced Electrical Conductors: An Overview and Prospects of Metal Nanocomposite and Nanocarbon Based Conductors,” by [Mehran Tehrani](#) of the University of Texas at Austin.⁷ This paper summarizes many of the nanocarbon and metal-nanocarbons being explored for their potential as enhanced conductors.

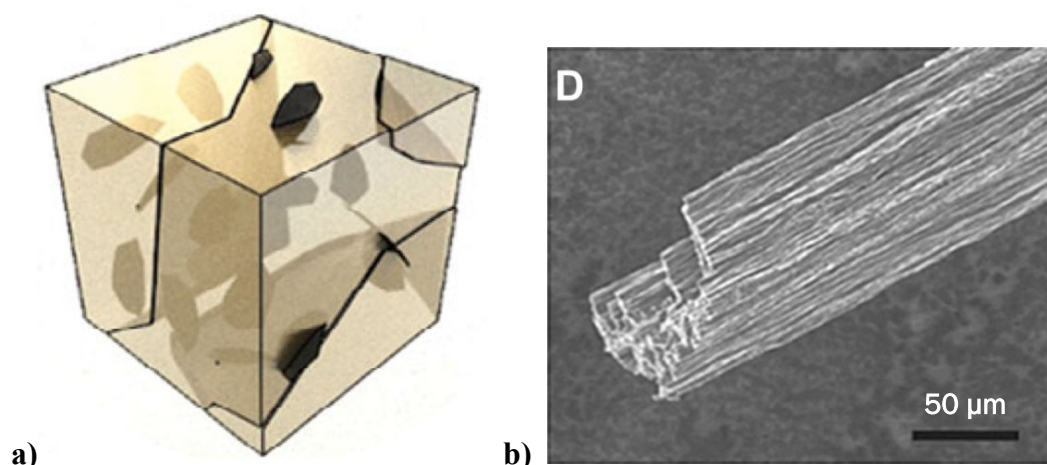


Figure 3.1 a) Schematic of a metal enhanced with nanocarbon⁷;
b) SEM image of doped graphene for application in electrical conductors⁸

Table 3.2 Conductivity and Other Properties of Various Forms of Carbon

Carbon Allotrope	IACS (%)	Notes
Diamond	10^{-17} – 10^{-24}	• Hardest and highest thermal conductivity • Natural diamond: 2,200 W/m.K (5X>Ag) • Synthetic: 3320 W/m.K
Graphite	0.3 – 0.5 along plane	• Softest form of carbon
Single-walled CNTs (SWCNTs) in armchair carbon arrangement	17.2 – 50 along axis ~ 10^{-16} perpendicular	• Varies according to manufacturing and post-processing techniques

⁷ Tehrani, Mehran. 2021. “Advanced Electrical Conductors: An Overview and Prospects of Metal Nanocomposite and Nanocarbon Based Conductors.” *Physica Status Solidi A* 218: 2000704. doi.org/10.1002/pssa.202000704.

⁸ Liu, Yingjun, Zhen Xu, Jianming Zhan, Peigang Li, and Chao Gao. 2016. “Superb Electrically Conductive Graphene Fibers via Doping Strategy.” *Advanced Materials* 28(36): 7941-7947. doi.org/10.1002/adma.201602444.

Graphene	<172	• Theoretical maximum for monolayer defect-free graphene
Copper–CNT nanocomposite ⁹	47*	• Density 5.2 g/cm ³
Ultraconductive copper ¹⁰	117	• Density 8.9 g/cm ³

* Exhibits a better electrical conductivity than copper above 80 °C.⁹

There have been some measurements of graphene's and SWCNTs' electric and thermal conductivities as a function of the unintentional impurities present and their crystalline structures.¹¹ Still, these conductive properties appear to depend on the material's processing approach. In addition, because there is no standard (e.g., grading) of the widely varying qualities of graphene, proper comparison is challenging and tedious. From a quantum physics perspective, graphene is a monolayer of sp² carbon rings. However, according to the International Standards Organization (ISO), materials comprising as many as 10 such sp² carbon monolayers are also referred to as graphene. But even a couple additional monolayers of graphene disrupt the graphene pi-cloud structure and lower the conductivity and other performance metrics compared to monolayer graphene. For conductivity in particular, the presence of defects in graphene structure, such as hepta-rings, penta-rings, or grain boundaries, can lead to lower electron velocities.¹² The defect density of monolayer graphene can be measured using Raman spectroscopy and can become a tangible method for defining graphene quality. The arrangement of the carbon atoms at the edges of graphene monolayers is also a major contributor to the electronic properties of graphene. The CNT arrangement—armchair or zigzag—affects the conductivity of the monolayers, especially at heterogeneous interfaces.

In addition to structural defects and numbers of layers, graphene performance also depends on impurities present in its structure. For example, reduced graphene oxide (rGO),¹³ while casually referred to as graphene, is one of the more impure forms of few-layer graphene. Occurring as a “black” powder, this substance is few-layer or many-layer graphene that is typically manufactured from delamination of graphite using Hummers' method or super-acid synthesis (among other methods), followed by pyrolyzation. This pyrolyzed graphene oxide has a physical structure similar to few-layer graphene; the key difference is that the pi-cloud electrons are used to form chemical reactions to leave functional groups along the surface of the graphene layers, which induces several physical structural defects along the layers, as well as in between the layers. The pyrolyzation process is not 100% efficient, which leads to reduction in some of the functional groups and produces several impurities on the few-layer rGO particle surfaces and in between the layers as well. While rGO is inexpensive and available in large quantities commercially, it typically demonstrates very low electronic properties. On the other hand, high-purity, low-defect density monolayer graphene, manufactured via methods such as chemical vapor deposition, molecular beam epitaxy, physical vapor deposition, or arc deposition, is >97% transparent and demonstrates ultra-high electron velocities, which are even greater than those of CNTs.

⁹ Subramaniam, Chandramouli, Takeo Yamada, Kazufumi Kobashi, Atsuko Sekiguchi, Don N. Futaba, Motoo Yumura, and Kenji Hata. 2013. “One hundred fold increase in current carrying capacity in a carbon nanotube–copper composite.” *Nature Communications* 4(2013): 2202. doi.org/10.1038/ncomms3202.

¹⁰ Cao, Mu, Ding-Bang Xiong, Li Yang, Shuaishuai Li, Yiqun Xie, Qiang Guo, Zhiqiang Li, et al. 2019. “Ultrahigh Electrical Conductivity of Graphene Embedded in Metals.” *Advanced Functional Materials* 29(17): 1806792. doi.org/10.1002/adfm.201806792.

¹¹ Graphene is the focus here because some metal–nanocarbon results have been tied to potential graphene nanoribbons. CNT is also mentioned because of a CNT paper that features an Al composite with a network structure of MWCNTs with electrical conductivity of $3.316 \times 10^7 \text{ Sm}^{-1}$ (half aluminum) and thermal conductivity of 172 W/m K. This paper has been cited in recent metal nanocarbon publications (Ma et al, PRL) as support for enhanced conductivity of composites:

Shin, S.E., H.J. Choi, and D.H. Bae. 2012. “Electrical and thermal conductivities of aluminum-based composites containing multi-walled carbon nanotubes.” *Journal of Composite Materials* 47(18): 2249–2256. doi.org/10.1177/02F0021998312456891.

¹² Liu, Lili, Miaoqing Qing, Yibo Wang, and Shimou Chen. 2015. “Defects in Graphene: Generation, Healing, and Their Effects on the Properties of Graphene: A Review.” *Journal of Materials Science & Technology* 31 (6): 599–606. doi.org/10.1016/j.jmst.2014.11.019.

¹³ Wang, Lidong and Weidong Fei. 2014. “Preparation method of graphene powder.” CN102838110B. Patent Filed September 17, 2012. Issued April 2.

3.3 Metals without Nanocarbon Background

This category includes any metal-based conductivity enhancement approach that does not rely on the addition of nano-carbons. Within this category, there are two broad metal types: metals with additives (other than nano-carbons) such as rare earth elements (see Sec. 3.4 summary of John Hryn's presentation); and metals with nano-process innovations (with minimal or no additives) (See Sec. 3.4 summaries of talks by Nhon Vo, Iver Anderson and Duane Johnson). Because we have very little information on the first category, section 3.3.1 below focuses on the second category—specifically metal-metal composites.

3.3.1 Metal-Metal Composite (Dual-Metals without Nanocarbon) Background

Metal-metal composites are a composite family that is made by extreme levels of deformation processing (typically either drawing or rolling) without alloying of metals. To date, the best performing prototype for such composites comprises a ductile metal matrix reinforced with nano-metric ductile metal filaments. Unlike metals enhanced with nanocarbon, such deformed metal-metal composites (DMMC) come from research initially aimed at maintaining conductivity while increasing other properties—such as strength—normally known to be anticorrelated with conductivity. The success of these approaches may bode well for the converse—increasing conductivity without decreasing strength.

Some of the best DMMC options for maintaining high conductivity while increasing strength come with Al- or Cu-based combinations that have pure metal reinforcement filaments. Prime examples of these are Al/Ti, Al/Sn, or most recently Al/Ca, along with Cu/Nb, Cu/Cr, and Cu/Fe.¹⁴ All of these metal-metal composite systems are formed by co-extrusion at very high levels of true strain and are characterized by extremely low equilibrium solubility of the minor part of the composite. The systems are heavily dependent for anomalous gains in strength on extreme reduction in spacing of the secondary pure metal reinforcement filaments and reduction in the filament diameter. Generally speaking, the conductivity is set by the highly conductive matrix phase, either the Al or Cu, where the reinforcement metal is not a good conductor. But recently, the Al/Ca system, has a very lightweight, highly ductile Ca reinforcement metal that does have reasonably good conductivity in its initial metal-metal composite state.

The [Al/Ca system readily deforms and also can contribute to the total conductivity](#). After annealing at temperatures of about 200°C, the Ca filaments transform into an intermetallic phase which results in strengthening, and effectively transfers the full conductivity task to the remaining Al matrix. Another example would be the Al/Ti DMMC, which forms refractory Al₃Ti when heated to 400°C. Al₃Ti has a much higher melting temperature and elastic modulus than Al, and this approach could be used to produce another nano-scale Al/Al₃Ti composite with high strength and high conductivity. Numerous other potential systems exist that could use ductile, non-equilibrium metals to achieve nano-scale phase structure, and that deformation processed material could then be annealed to form ultra-fine filamentary or lamellar intermetallic phases.

3.4 Metal-Related Enhanced Conductivity Research Pathways Described During Workshop

Several speakers at the workshop discussed various approaches to manufacturing conductivity-enhanced metals:

- [Mehran Tehrani](#) of the University of Texas at Austin presented an overview of research in the field of electrical conductivity enhancement. The presentation is based on a recently published paper, "[Advanced Electrical Conductors: An Overview and Prospects of Metal Nanocomposite and Nanocarbon-Based](#)

¹⁴ Xu, Kai. 2003. "Microstructure and strength of a deformation processed Al-20%Sn metal-metal composite." PhD diss., Iowa State University. doi:10.31274/rtd-180813-9840.

[Conductors](#),” describing theories about conductivity enhancement, various methods of fabrication, and conductivity measurement methods.

- [Ben Gould](#) of ANL demonstrated the ability to detect changes at the metal–nanocarbon interface using the Advanced Photon Source and the potential effects on electrical conductivity. This work examined a multilayer copper–graphene–copper sample with a claimed IACS of 115% and also investigated the interface effects of nanocarbon deposition on single-crystal copper.
- NASA’s [Maricela Lizcano](#) described how copper electroplated onto CNT yarn demonstrated proof of concept for a durable, lightweight composite conductor with approximately 25% to 30% reduction in weight, increase in strength over copper, and the promise of matching or exceeding the conductive performance of copper.
- ANL’s [Jeff Elam](#) discussed CNTs coated by atomic layer deposition to achieve a conformal coating with uniform thickness; the CNTs were then cold-pressed and sintered. The results showed 4× the conductivity of copper powder processed in the same way. The concept being pursued is to achieve control of the copper–CNT interface.
- ANL’s [Balu Balachandran](#) described a potential industrial-scale process for infusing nanocarbon into molten metals called Covetics. The process uses a graphite electrode to add carbon to copper to form high-conductivity nanocarbon structures enabling conductivity-enhanced metal conductors. Recently, Dr. Balachandran’s intellectual property was used for an SBIR Technology Transfer Opportunity topic; the award selection was announced on May 17 (see the Nanocarbon-Enhanced Metals callout box below).
- [Hal Stillman’s patent presentation](#) mentioned Chinese patent application CN112410606, a “Method for continuous casting of nano carbon copper-based composite material through rapid solidification,” which discloses a process produces a material that is in a metastable condition.¹⁵
- [Keerti Kappagantula](#) of PNNL described a method of combining metals with graphene to achieve an enhanced conductivity condition. The Shear Assisted Processing and Extrusion™ (SHAPE) process has been shown to achieve a 5% increase in the conductivity of copper and a change in the temperature coefficient of resistance that allows lower resistance at elevated temperature.
- [John Hryn](#) of ANL reported on research conducted in China indicating that the addition of cerium or lanthanum to copper can form nanoprecipitates at copper alloy grain boundaries. This strategy increases conductivity by up to 139% IACS, as well as increasing strength. Workshop participants were skeptical about the claimed improvements.
- [Nhon Vo](#) of NanoAl discussed his company’s method of alloy strengthening via tailored nanoprecipitation technology and its applicability to aluminum conductors.
- Ames Laboratory’s [Iver Anderson](#) reported on research into an aluminum–calcium composite that enhances the strength of aluminum cable for overhead transmission lines. Results indicate that conductivity is decreased by only a few percent.
- [Duane Johnson](#) of Iowa State University described the design and processing of complex solid solution alloys for lightweight aluminum alloys for overhead transmission lines and noted that density functional theory (DFT) can be used to calculate resistance in disordered alloys.

¹⁵ University of Shanghai for Science and Technology. 2020. “Method for preparing long-size nano carbon copper-based composite material through rapid solidification, application and device thereof.” CN112410606A. Patent Filed October 28.

- ORNL's [Alex Plotkowski](#) spoke about the fabrication of metals enhanced without nanocarbon using additive manufacturing. The potential opportunities for utilizing the Manufacturing Demonstration Facility at ORNL to generate complex structures with potentially higher conductivity and/or strength were presented along with past successes in the manufacturing of other metals and alloys.
- [Jonathan McCrea](#) of Integran spoke about tradeoffs between conductivity and strength in conductors and relevant design strategies. Electroforming was one manufacturing method highlighted for its ability to produce unique nanomaterials that have good combinations of strength and conductivity.

Despite the large number of presenters discussing different potential approaches to manufacturing conductivity-enhanced metals, there were no convincing peer-reviewed studies of materials showing significantly enhanced electrical conductivity at room temperature or elevated temperature. However, there was convincing evidence of approaches that maintain conductivity while improving strength, ampacity, temperature coefficient of resistance, and other attributes. Other key discussion points and findings from the presentations in the two metals panels are included in Table 3.3 and Table 3.4.

Table 3.3 Key Findings from Metal Enhanced with Nanocarbon Panel

Discussed Materials/Approaches	Important Factors
• CNT wire • Doped CNT wire • CNT-Cu wire • Gr-Cu composite • Cu-Gr film • Solid phase processing (e.g., ShAPE) • Covetics	• Impacts of processing on materials' properties • Conductivity measurements prone to error and often difficult to compare to each other • More foundational work required to understand interaction between metal and carbon material • Need for deeper evaluation and understanding of results, despite extensive research and existing results • Many potential applications for metal enhanced with nanocarbon

Related SBIR Project – Nanocarbon-Enhanced Metals

Directed Vapor Technologies International of Charlottesville, Virginia, was awarded an SBIR for metal carbon composite manufacturing. The company will use its existing industrial-scale equipment to scale and commercialize manufacturing advances developed at ANL. The ability to manufacture these substances in significant quantities will enable enhancements to the company's existing product line of lightweight wiring. In addition, the emerging technology would augment electromagnetic interference shielding materials and benefit additional energy-related products, including advanced electrodes for renewable energy devices.

Table 3.4 Key Findings from Metal Composites (No Nanocarbon) Panel

Tradeoffs/Performance Metrics	New Approaches	Important Factors
• Market value (\$) of improved combinations of electrical and mechanical performance • Application-specific performance requirements • Complex and diverse performance tradeoffs (e.g., conductivity/resistance, strength, weight, ductility, creep resistance, fatigue performance, corrosion resistance)	• Stable nanocrystalline microstructure features • Processing-microstructure-property relationships to optimize application-specific material performance • Design of new/modified material compositions • Hybrid microstructures for optimized performance • Abundant and lighter rare earth elements	• Transitioning material and realizing the benefits of improved importance • Understanding and control of the spatial distribution microstructure features • Communicating application-specific property/performance requirements • Industry and end-user engagement early in development • Strategic importance of developing a market for abundant rare earth elements

Questions and Answers on Metal Conductors

This Q&A is intended to illustrate why there is both great excitement and significant skepticism about the potential to increase the conductivity of metals, whether through nanocarbon or other means.

Question 1: Why are physicists generally skeptical about the potential for enhancing bulk metal conductivity by adding nanocarbons or any other material?

Answer: The enormous success of the so-called “free electron model” for bulk metals at room temperature¹⁶ for nearly a century accounts for physicists’ skepticism of enhanced conductivity. Physicists have long used the free electron model to explain the behavior related to metal conductivity. The classical free electron theory, first posited in 1900, assumes that all metals contain large numbers of electrons that move freely, like a gas, through the positive ionic core of the metals. The electrons cause conduction in metal under the application of an electrical field, and resistance is caused by scattering of the electrons. This classical model predicted—accurately, by all early century measurements—that adding any material to a pure conductor only increases scattering centers for electrons and hence increases resistance and reduces conductivity. However, this classical theory has failed to predict other properties (e.g., the electronic heat capacity of a metal at room temperature seems to come from 100× fewer electrons than were in the electric current). As a result, the classical theory was updated in 1926 with quantum mechanical Fermi–Dirac statistics that account for the $\frac{1}{2}$ integer quantum mechanical spin of the electron. *This* model successfully predicted not only the electron heat capacity of metal at room temperature but also its temperature dependence and many other experimental phenomena.¹⁷ This updated model also explains why copper, aluminum, silver, and gold have the highest conductivity, as they all have the same sp^3 orbital electronic structure.

Question 2: Why is there so much excitement about metal nanocarbon materials?

Answer: In recent decades, the Nobel Prize-winning discoveries of carbon allotropes such as buckyballs, CNTs,¹⁸ and graphene¹⁹ led to an explosion of research into their properties such as conductivity, strength, and low density (see Table 4.2), as well as other remarkable electronic properties, such as electron mobility.²⁰ Note that the free electron theory also accounts for the possibility of very high conductivity at the atomic scale where the mean free path for scattering is relatively large compared with the crystal dimension. Nanoscale [imaging technologies for conductive materials](#) have now improved to the point where monolayers of atoms could begin to be visualized. Ordered structures detected in mixtures of carbon and metal have been hypothesized to be graphene nanoribbons that might increase electrical conductivity.

Question 3: Why is there skepticism about conductivity-enhanced metal nanocarbon materials?

Answer: First, as noted in Question 1, it goes against more than a century of physics theory and experiment to posit that bulk conductivity can be increased by adding any material. Second, carbon allotropes such as CNTs and graphene do not exist in pure form, and neither the resistivity nor its temperature dependence are well-characterized all the way from the nano to the bulk scales. Hence, no bulk nanocarbon measurement that does not specify chemical purity and defect density is reproducible. Claims of metal nanocarbon bulk

¹⁶ It is important to specify the temperature at which conductivity occurs. At very low temperatures near absolute zero temperature (-273°C) an entirely different type of conductivity—so called traditional superconductivity—can occur. Such “traditional” superconductivity can be explained by the Bardeen Cooper-pair theory. But “high-temperature superconductivity” is not yet explained by any theory. Note that while “high temperature” superconductivity occurs at relatively higher temperatures (e.g. Liquid Nitrogen temperature of 77K)—it still is at hundreds of degrees below room temperature and hence has not been practical for most applications—MRI machines being a notable premium exception.

¹⁷ In particular, the revised model successfully predicted the Wiedemann–Franz law, which relates electrical conductivity and thermal conductivity, the shape of the electronic density of states, the range of binding energy values, and the Seebeck coefficient of the thermoelectric effect.

¹⁸ Iijima, Sumio. 1991. “Helical microtubules of graphitic carbon.” *Nature* 354 (1991): 56-58. doi.org/10.1038/354056a0.

¹⁹ Geim, Andre K. and K. Novoselov. 2007. “The rise of graphene.” *Nature Materials* 6(3): 183-191. doi.org/10.1038/nmat1849.

²⁰ Dürkop, T., A. Getty, Enrique Cobas, and M.S. Fuhrer. 2004. “Extraordinary Mobility in Semiconducting Carbon Nanotubes.” *Nano Letters* 4 (1): 35-39. doi.org/10.1021/nl034841q.

conductivity greater than copper lack such information on the nanocarbon purity, and claimed conductivity enhancements have been difficult to verify.

Question 4: Why are metallurgists skeptical about claims that both strength and conductivity can be increased?

Answer: Metallurgists have known for centuries that a metal's strength can be greatly increased by adding other substances and/or through certain types of processing. For example, the addition of defects like grain boundaries (i.e., Hall-Petch strengthening) and dislocations (i.e., Taylor strengthening) increases the energy cost for nucleation and movement of defects that accommodate plastic deformation, but these defects also typically increase the probability of electron scattering. These mechanisms have been repeatedly verified by showing the correlation between strength and the number and size of "grains" that can be seen in microstructure of the metal, as has the role of defects in the crystal lattice of metals on electrical conductivity. Historically, the same mechanisms that produce higher strength also tends to lead to an increase in electron scattering and thus lower electrical conductivity.²¹ As a result, most metallurgists believe that any method of processing metal to increase its strength will also decrease its conductivity.

Question 5: Why are measurement and metrology experts so concerned about measurement error in claims of enhanced conductivity?

Answer: Measuring electrical conductivity of small samples is difficult and prone to errors that scale quadratically. As was explained at the workshop, [accurate measurement of electrical conductivity requires relatively large, pure, and uniform samples](#). The usual technique for electric conductivity measurement involves a four-point bridge that measures voltage differences and requires a precise knowledge of sample dimensions. Errors arise from, among other things, non-uniform physical properties, non-uniform dispersion or alignment of nanocarbons in the sample, undetected porosity, limited accuracy of very small voltage measurements, non-uniform dimensions, and deformation from the application of probes. Workshop participants also learned of similar difficulties in measuring thermal conductivity and that [none of the standard techniques are optimal](#). It was suggested that [designated facilities](#) may be the best way to measure conductivity.

Question 6: Why should we have hope that metals with nanocarbons can get around these known barriers?

Answer: First, the "known barriers" are not absolute laws of physics that apply universally. For example, the free electron theory of conductivity fails to explain important bulk physics phenomena, such as the Hall effect, or why the conductivity of some metals and nanocarbons can depend on the orientation of the crystal with respect to the electric field. Nor does the free electron theory offer any explanation for why silver, copper, gold, and aluminum have electrical conductivity in that order (Silver having the highest conductivity and gold the third highest). Second, the past decade has seen great progress being made in purifying CNTs and graphene at the bulk scale, as well as a [dramatic increase in their bulk conductivity](#). If bulk CNT and graphene can be made more conductive than the sp^3 metals, then the conductivity of a composite comprising pure metal and pure nanocarbon might follow the rule of mixtures for their properties (i.e., the overall composite property—in this case, conductivity—is the sum of the conductivities of the matrix and each added component, with the matrix and each additional component weighted by their respective volume fractions). Third, great progress has been made in the past decade in creating carefully controlled metal matrix composites in which the strength is increased greatly without decreasing conductivity substantially. As detailed in Section 3.3.1, Metal Composite (Metal without Nanocarbon) Background, DMMC, use of oxide particles that are incoherent with the matrix and thus avoid lattice distortion, use of incoherent intermetallic compounds, and cold working are all proven techniques to strengthen metal cables without decreasing conductivity. Fourth, preliminary theory and

²¹ Mayadas, A.F. and M. Shatzkes. 1970. "Electrical-Resistivity Model for Polycrystalline Films: the Case of Arbitrary Reflection at External Surfaces." *Physical Review B* 1(4): 1382-1389. doi.org/10.1103/PhysRevB.1.1382.

modeling appears to show enhanced conductivity in metastable states, and metallurgists have a long history of processing methods that enable metals to remain long-term in such metastable states.

The hope is that composite manufacturing and nanocarbon purification and manufacturing improve to the point at which conductivity can be increased without decreasing strength or other mechanical properties. Ideally, adding highly conductive forms of nanocarbon to a metal matrix has the potential to result in a composite with higher conductivity than the matrix. There are multiple factors that need to be pursued to achieve such conductivity-enhanced materials: availability of nanocarbon material without defects or impurities, nanocarbon that is well-dispersed and aligned in a preferred direction, nanocarbon materials available in bulk quantities at a reasonable cost, and excellent conductive interfaces between nanocarbon and the matrix metal. Hence, advanced manufacturing research is needed to achieve conductivity-enhanced materials.

Chapter 4: Non-Metals

In addition to Polymer and Other Non-Metallic Conductor Concepts Panel on Day 2, which looked at non-metals, one of the application panels on Day 1 discussed non-metallic conductors, including both electrical and thermal conductivity of such materials (see Section 2.3 on energy efficiency). In addition, heat exchangers and their thermal conductivity were discussed during a facilitated session that followed the energy efficiency panel and materials thermal conductivity was discussed during the solar part of the renewable panel. All of these inputs are reflected in this chapter.

4.1 Non-Metallic Material Background and Potential Applications

Electrical conductivity performance: According to the free electron theory, by definition, non-metals do not conduct electricity. But as noted above, in Chapter 3 and in Table 4.1, there are a few exceptions, such as nano-carbons, graphite and doped silicon semiconductors. In addition, we learned during the non-metal panel that materials that are non-metal in bulk (e.g. plastics), but that have coatings containing metal (e.g. silver nanoparticles) also can be fair electrical conductors.

Thermal conductivity performance: In real-world applications, thermal conductivity performance is more than just a single material property. It is an enabling factor for new technologies that requires an innovative design to leverage enhancements. These design improvements cannot be an exercise in simple material substitution/exchange. Thermal conductivity performance enhancements will be driven by additional system design constraints that are specific to the application (e.g., operating temperatures, material compatibility, geometric design constraints, volume, mass requirement, etc.). Table 4.1 includes thermal conductivities of several non-metallic materials that are not new nanocarbons, as well as plastics that may become electrically conductive with nanometallic coating. Table 4.2, by contrast, shows thermal conductivities of exciting new carbon allotropes also discussed as additives (in the prior chapter—see Table 3.2) but discussed here as non-metals (involving no bulk metal).

Table 4.1 Conductivity and Other Properties of Select Non-Metal Materials

	Electrical Conductivity (MS/m)	Thermal Conductivity (W/m-K)	Strength (GPa)	Density (g/cm ³)
Graphite ^{22,23}	0.2–0.3 on plane	25–470	0.031–0.345	1.3–1.95
Doped silicon (semiconductor) ^{24,25}	2.5–3.33 x10 ⁻³	130–148	3.2–3.5	2.3
Silicon carbide ^{22,25}	1x10 ⁻⁸ – 10 ⁻⁴	3.8–120	0.13–1.3	4.36–4.84
Silica (quartz, e.g. fiber optic) ^{25,26}	1x10 ⁻²³ – 10 ⁻²¹	1.4–3.0	1.5–1.7	2.2
Polyethylene high-density ^{22,23}	1x10 ⁻²¹ – 10 ⁻⁹	0.29–0.52	2.8 x 10 ⁻⁴ –1.9 x 10 ⁻³ (tensile)	0.924–0.995
Polyurethane (PUR) ²³	1x10 ⁻²⁰ – 1.25x10 ⁻¹⁷	0.14–0.39	0.14 x 10 ⁻³ –6.3 x 10 ⁻² (tensile)	0.21–1.5

The Day 2 panel showed that increasing the electrical and thermal conductivity of non-metallic materials is possible and has been done. Non-metallic conductors with enhanced electrical conductivity may have

²² Engineering Toolbox. 2003. “Solids, Liquids and Gases – Thermal Conductivities.” [engineeringtoolbox.com/thermal-conductivity-d_429.html](https://www.engineeringtoolbox.com/thermal-conductivity-d_429.html).

²³ Matweb. 2021. “Material Property Database.” Accessed August 12. [matweb.com/](https://www.matweb.com/).

²⁴ EL-CAT Inc. 2021. “Properties of Silicon and Silicon Wafers.” Accessed August 12. el-cat.com/silicon-properties.htm.

²⁵ Matmatch GmbH. 2021. “Matmatch.” Accessed December 28. matmatch.com/.

²⁶ Technical Glass Products, Inc. 2021. “Properties of Fused Quartz.” Accessed August 12. technicalglass.com/technical_properties/.

application as high thermally conductive materials. This would be the case in applications that require low electrical resistance, as well as low thermal resistance to dissipate heat. In pure heat transfer applications, non-metallic conductivity-enhanced materials are advantageous in heat exchangers for condensers or evaporators in air conditioners, heating-only heat pumps, and heat exchangers suitable for both condensing and evaporating reversible heat pumps. Non-metallic materials may also be lighter weight, offering benefits in vehicles, power stations, and aerospace applications. In addition, new shapes and geometries moving beyond “round tubes” can be created without expensive and complex additive manufacturing. This offers exciting new design possibilities. Currently, most heat exchangers use materials that have isotropic properties. In the future, heat exchanger design could take advantage of anisotropic materials,²⁷ leading to opportunities for new shapes and innovative product designs.

There are opportunities for enhanced thermal conductivity for heat exchange devices to make devices smaller, lighter, and more cost-effective. For air conditioning, heat pumps, and manufacturing processes, there are operational temperature ranges that vary, depending on the application. For water heating, residential and commercial heat pumps, and air conditioning applications, materials should typically be able to withstand temperatures of up to 75°C. For metals processing, temperatures in the range of 160°C to 200°C are expected. In the paper, pulp, and chemical industries, an operational temperature range of 120°C to 200°C is typically encountered. For the food processing industry, a wide temperature range from 40°C to 200°C could be encountered, depending on the application.²⁸

Prior R&D investments by DOE have funded explorations of high-performance compact heat exchangers, low-charge heat exchanger designs, and rotating designs. The development of polymer or non-metal heat exchanger designs is ideal because of their light weight, manufacturing potential, wide range of geometric design possibilities, corrosion resistance, and potential to be low-cost. Despite their advantages, polymer heat exchangers have entered the market slowly (compared to other energy recovery devices), as they have relatively low thermal conductivity in the direction of fluid flow.²⁹

4.2 Non-Metal Workshop Presentations and Findings

Three presentations were given during the Polymer and Other Non-metallic Enhanced Conductor Concepts Panel. [Dan Gianola](#) of the University of California, Santa Barbara, showed that using an acoustic focusing field (pressure) in manufacturing could increase conductivity, with the ability to independently control (performance-tune) anisotropic and isotropic thermal conductivity while maintaining good strain resistance. [Chuck Booten](#) of NREL summarized an infrared fiber optic concept with the potential for localized personal cooling. This new approach could allow targeted heating and cooling in applications such as chips and other electronic devices. In the last presentation, [Michael Ohadi](#) of the University of Maryland discussed highly conductive polymers for advanced heat exchanger designs. In addition, in the Session on Metal/Nanocarbon Conductors, [Saniya LeBlanc](#) of George Washington University gave a presentation summarizing the methods to measure thermal conductivity and discussed challenges related to such measurements. Finally, in the paper by [Mehran Tehrani](#) circulated to attendees before the meeting, a small portion was devoted to thermal conductivity.³⁰ The technologies discussed in the panel presentations are summarized in Table 4.1 and Table 4.2.

²⁷ Anisotropic materials have good thermal conductivity in one direction and poor thermal conductivity perpendicular to the first. Such properties preserve the temperature wavefronts in the device.

²⁸ Arpagaus, Cordin, Frédéric Bless, Michael Uhlmann, Jürg Schiffmann, and Stefan S. Bertsch. 2018. “High Temperature Heat Pumps: Market Overview, State of the Art, Research Status, Refrigerants, and Application Potential.” *International Refrigeration and Air-conditioning Conference*. Paper 1876. docs.lib.purdue.edu/iracc/1876/.

²⁹ For examples of innovative HVAC system designs in the market, see <https://www.airxchange.com/>.

³⁰ Tehrani, Mehran. 2021. “Advanced Electrical Conductors: An Overview and Prospects of Metal Nanocomposite and Nanocarbon Based Conductors.” *Physica Status Solidi A* 218: 2000704. doi.org/10.1002/pssa.202000704.

An upper bound (see Table 4.1) for the thermal conductivity of metal–carbon composites can be calculated. The high thermal conductivity of CNT and graphene ($3000\text{--}6000\text{ W m}^{-1}\text{ K}^{-1}$) can be exploited to improve the conductivity of Cu, Al, and Ag (390 , 200 , and $400\text{ W m}^{-1}\text{ K}^{-1}$, respectively). Engineering nanocarbon–metal interfaces requires minimizing their thermal resistance.³⁰ As the three presentations in Polymer and Other Non-Metallic Conductor Concepts Panel indicated, there is a large gap between the projected thermal conductivity, as reported by Tehrani, and actual measurements that have been achieved. For example, Tehrani’s projections and the carbon fiber thermal conductivity data from Dan Gianola’s presentation, show a 10-fold difference in thermal conductivity. Careful and comprehensive measurements are needed to reconcile these apparent disparities.

Table 4.2 Properties (Ambient Condition) for Nanocarbon-Based Materials³⁰

	IACS (%)	Thermal Conductivity (W/m-K)	Strength (GPa)	Density (g/cm ³)
Individual CNT or graphene ^{31,32}	33–72	>3,000	20–100	1.4
Doped CNT fiber ³³	15	625	3	1.5
Doped graphene fiber ³⁴	2 ³⁵	1,575	2	-
Doped carbon fiber ³⁶	24	>1,000	1	2.5

It has previously been reported that SWCNTs with an armchair arrangement have a good thermal conductivity in one direction and very low conductivity perpendicular to the nanotube axis. However, it should be highlighted that the temperature dependence of electric and thermal conductivity in new carbon allotropes has not been clearly established and measured, and the identification of the most accurate method of measurement is not straightforward. These measurement challenges were discussed by Saniya LeBlanc at the workshop. For the development of new anisotropic materials, the ability to conduct high quality thermal conductivity measurements will be critical to evaluate new materials that are being developed.

Table 4.3 Discussed New Approaches in Polymer and Other Non-Metallic Enhanced Conductor Concepts Panel

- Acoustophoresis, or acoustic focusing, to make pattern composites
 - Conductivity can be changed with different patterns of microstructure
 - Material-agnostic (usable with many different materials)
- Infrared fiber optics for heat transfer
 - Transfer of infrared radiation in a controlled fashion
 - Potential for very localized heat transfer, such as cooling for microelectronics
- High-conductivity polymer composite conductors for thermal management applications
 - Use of additive manufacturing methods
 - Bio-inspired electrically controlled conductors for active thermal management

³¹ Balandin, Alexander A. 2020. “Phononics of Graphene and Related Materials.” *ACS Nano* 14(5): 5170–5178. doi.org/10.1021/acsnano.0c02718.

³² Nika, Denis L. and Alexander A. Balandin. 2017. “Phonons and thermal transport in graphene and graphene-based materials.” *Reports on Progress in Physics* 80: 036502. doi.org/10.1088/1361-6633/80/3/036502.

³³ Tsentalovich, Dmitri E., Robert J Headrick, Francesca Mirri, Junli Hao, Natnael Behabtu, Colin C. Young, and Matteo Pasquali. 2017. “Influence of Carbon Nanotube Characteristics on Macroscopic Fiber Properties.” *ACS Applied Materials and Interfaces* 9(41): 36189–36198. doi.org/10.1021/acsaami.7b10968

³⁴ Xin, Guoqing, Weiguang Zhu, Yanxiang Deng, Jie Cheng, Lucy T. Zhang, Aram J. Chung, Suvranu De, and Jie Lian. 2019. “Microfluidics-enabled orientation and microstructure control of macroscopic graphene fibres.” *Nature Nanotechnology* 14: 168–175. doi.org/10.1038/s41565-018-0330-9.

³⁵ An electrical conductivity of 38% IACS has been reported for a potassium-doped (measured in an inert atmosphere) graphene fiber. Reference: Liu, Yingjun, Zhen Xu, Jianming Zhan, Peigang Li, and Chao Gao. 2016. “Superb Electrically Conductive Graphene Fibers via Doping Strategy.” *Advanced Materials* 28(36): 7941–7947. doi.org/10.1002/adma.201602444.

³⁶ Oshima, Hisashi, John A. Woollam, Andre Yavrouian, and Michael B. Dowell. 1983. “Electrical and mechanical properties of copper chloride-intercalated pitch-based carbon fibers,” *Synthetic Metals* 5(2): 113–123. [doi.org/10.1016/0379-6779\(83\)90125-X](https://doi.org/10.1016/0379-6779(83)90125-X).

Chapter 5: Theory and Modeling

This chapter provides (1) background on past assessments of modeling needs, (2) a session overview, (3) brief summaries of each of the three modeling panels, including discussion questions, and (4) session conclusions and recommendations. Speakers in this Day 2 session covered key theoretical concepts and computational methods and tools for design and optimization of conductivity-enhanced materials. The goal of the session was to assess the state of the art in theoretical methods, explore their predictive power, and discuss gaps needing further investments. The theory and modeling session consisted of three separate panels: (1) Atomistic-Scale Simulation, (2) Multiscale Simulation Approaches, and (3) Crosscutting Topics in Materials Simulation.

5.1 Theory and Modeling Background

In the past, enhanced electrically conductive materials were found through experimental trial and error. A theoretical first principles approach was not possible because of the extreme computing demands for complex mixtures of hybrid and homogenous materials.³⁷ Successful first principles modeling was thought to enable a complete understanding of the physics involved in enhanced conductivity. This physics understanding, once verified, was thought to permit the prediction of the material's characteristics, with a large span of parameters verifying candidate material combinations, and even lead to insights on nano- and micro-manufacturing methods.³⁸ Unfortunately, as was revealed in the workshop, first principles models alone are insufficient to predict macroscale “bulk” conductivity because bulk conductivity is affected by both the material's (atomistic) composition and the microstructure formed as a result of the manufacturing processes. Without additional “mesoscale” modeling, what is modeled at the atomic scale may not translate into behavior at the macroscale. This modeling gap can be filled only by detailed characterization of material samples for discovery and validation of the fundamental relationships between composition and microstructure.³⁹ The atomistic and mesoscale modeling can be combined in “multiscale” or “multiphysics” models.

5.2 Modeling, Characterization, and Their Implications for Conductor Manufacturing

Starting at the extreme low end of length scales (sub-nanometer) is modeling that requires quantum mechanical calculations of interfaces at the atomic level and identification of atomic configurations that can positively or negatively impact conduction processes. The next level is mesoscale modeling. This intermediate scale of modeling is required because bulk conductivity is partially dependent on microstructure (micron scale) formed in the manufacturing process. Expanding the understanding and modeling of a conductor from atomic scale to a realistic prediction at macroscopic scale requires both atomic- and meso-scale modeling. This is challenging because bulk conductivity is affected by both the material's atomic composition and the microstructure formed in the manufacturing processes.

In addition to requiring models at different length scales, successful modeling of enhanced conductivity requires experimental data collected at these different length scales. This modeling gap can be filled only by detailed atomic and bulk characterization of material samples, which is required for discovery and validation of the fundamental relationships between composition and microstructure. It is for this reason that the session participants concluded that effective theory and modeling require close linkage with existing and emerging characterization of samples that are fabricated with the intent to include the desired conductivity-enhanced characteristics.

³⁷ Lee, Dominic F., Malcolm Burwell, and Hal Stillman. 2015. *Priority Research Areas to Accelerate the Development of Practical Ultra-Conductive Copper Conductors*. Oak Ridge, TN: Oak Ridge National Laboratory (ORNL). Published September. info.ornl.gov/sites/publications/files/Pub58011.pdf.

³⁸ Kasap, Safa, Cyril Koughia, and Harry Ruda. 2017. “Electrical Conduction in Metals and Semiconductors.” In *Springer Handbook of Electronic and Photonic Materials*, 1-1. Cham: Springer. doi.org/10.1007/978-3-319-48933-9_2.

³⁹ DOE SC (DOE Office of Science). 2012. *From Quanta to the Continuum: Opportunities for Mesoscale Science*. Washington D.C.: DOE. Published September. science.osti.gov/-/media/bes/besac/pdf/12_Mesoscale_Report_full_v8.pdf.

The sessions revealed that a coordinated effort in this domain will require large computational resources and teams of experts working toward a consensus on a strategy for the scale-bridging. The predictions and explorations of variabilities need to be validated by measurements relating to the underlying phenomena, as discussed in other sessions in this workshop. In addition, the processes of manufacturing wire from composites need precise control of microstructure. Many metastable compositions can provide an increase in conductivity in small-scale samples but can degrade to more thermodynamically stable forms with lower conductance once made into practical conductors. Therefore, theory and simulations can play a pivotal role in guiding understanding and the strategy for materials processing. Maintaining required strength, ductility, domain distributions, and macroscopic electrical conductance will require an interdisciplinary team effort.

5.3 Panel Presentations and Discussion Points

In the panel on atomistic-scale simulation, [Subramanian Sankaranarayanan](#) of ANL described the laboratory's efforts to use artificial-intelligence-guided inverse design of metal–carbon composites with high thermal and electrical conductivity. [David Drabold](#) of Ohio University presented on the use of the Kubo–Greenwood formula to compute the electrical conductivity in new materials that are being developed. In the third presentation, [Panchapakesan Ganesh](#) of ORNL described a collaborative research effort to develop a modeling approach to studying what material characteristics govern metal-to-insulator transitions and their impact on electrical and thermal conductivity.

In the second panel on multiscale simulation, [Pallab Barai](#) of ANL presented his research team's efforts to develop a multiscale computational model to estimate properties, including thermal and electrical conductivity for metal–nanocarbon composites. [Duane Johnson](#) of Iowa State University and Ames Laboratory discussed his team's use of modeling techniques for the development of strong, lightweight complex solid-solution alloys for transmission lines. [Rajeev Kumar](#) of ORNL concluded the panel with his presentation on modeling the structure and ionic transport in polymer electrolytes.

In the crosscutting panel, [Maria Chan](#) of ANL reported her team's efforts to develop a model for thermal conductivity in C-in-Cu structures, with the ultimate goal of enabling design of new materials with improved conductivity. [Angel Yanguas-Gil](#) of ANL discussed how the significant high-performance computing resources at the national laboratories can be leveraged to create better models for the analysis of conductivity-enhanced materials. [Bobby Sumpter](#) of ORNL presented on the laboratory's work on molecular modeling and simulation of hybrid materials, polymers, and polymer nanocomposites. He explained how such models can help optimize materials research by narrowing the scope of experiments and identifying highest-viability routes.

Validating atomistic-scale models requires high-quality and repeatable values for bulk conductivity, thermal resistance, and mechanical properties. Many well-established measurement techniques are available to do this at bulk scale, and even at the nanoscale. There is emerging activity in trying to measure properties of atoms, from a single atom to a few atoms, and to develop sub-nanometer measurement techniques.

Regarding theoretical models for predicting conductivity, first principles DFT used for electronics structure calculations is reliable for predictions when the number of atoms is small. In the conductivity domain, the reliability needs to be extended to much larger system sizes. Tight-binding models proposed by ANL are promising but may still fall short of grain-level conductivity predictions, owing to the heavy computational expense needed to calculate properties of structures consisting of many millions of atoms.

The Multiscale Simulation Approaches panel highlighted the lack of systematic samples with well-known composition and distribution of nanotubes or graphene in well-defined microstructure. With the lack of measurable bulk sample environments, the multiscale coupling needs to rely on lower-length-scale (nanoscale) measurements, interfacial resistance calculations, and mesoscale empirical model calculations. Sample preparation and guidance on observed distribution and orientations of nanocarbon domains remain important for connecting the dots.

For multiscale modeling, accurate experimental information is needed at the atomic scale to build the models for bulk conductivity. Homogeneous bulk materials with millions of atoms can be efficiently modeled because simplifying assumptions significantly reduce the computation expense. Heterojunctions of dissimilar materials, grain boundaries, defects, and nanostructures are very computationally intensive because simplifying assumptions are generally not available. An example of a complex system is a metal alloy that contains randomly distributed CNTs where simplifying assumptions for computation are not available.

Workshop speakers and attendees agreed on the need for a validated multiscale framework. However, a consensus still needs to emerge on how to validate across the length scales and provide a measure for uncertainty in theory and measurement. There could be a role for national laboratories to provide standards for theory and experiments in collaboration with leaders from industry and academia.

Researchers are working intensively on multiphysics and multiscale modeling to successfully inform material and manufacturing research in conductivity-enhanced materials (see example box below). Achieving such modeling will require different types of scientific, modeling, analytic, and computation expertise. The workshop panelists recommended this combined-expertise approach, as necessary, to increase the likelihood of creating enhanced conductors at scale.

Connecting Experimental Researchers with Theorists and Computation Researchers – An Example

ANL's Center for Nanoscale Materials explored nanotribology in which the materials researchers worked with the theorists and co-designed (iterating experiment – theory – experiment – theory) to create a product. Theorists came up with a theory, or theories, to explain what the experimentalists observed. Ultimately, theory guided the materials design, resulting in a near-zero-friction dry lubricant (superlubricity).⁴⁰ Currently, work is under way to scale up the coating process and license the ANL-developed technology to encourage commercialization and widescale adoption.

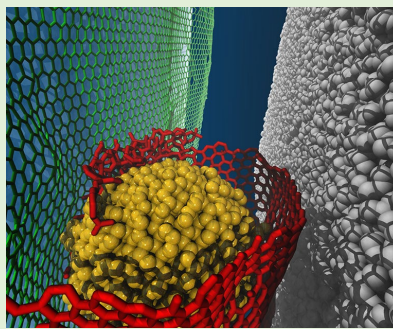


Figure 5.1. Visualized model of a superlubricity system.

Image courtesy of ANL

For atomic-scale researchers, enhanced conductivity is explored in the electronic structure as a result of different chemical bonding possibilities between metals and nanocarbon-based domains. For materials scientists, these are inter- and intragranular phenomena that can be highly dependent on processing. A systematic approach for better atomic-scale understanding and ability to make measurements on same samples across length scales using DOE user facilities could constitute a viable approach to achieving breakthroughs in understanding the mechanisms to manufacture conductivity-enhanced materials.

After a strong analytic foundation for enhanced conductivity is built, high-performance computing capabilities must also be strengthened to enable actual physical materials manufacturing advancements. As the number of models and their predictive accuracy increase, comprehensive understanding of the structure–property–processing relationships must be developed. The role of processing in changing conductivity is also large but poorly understood. Although the need for better in situ measurements was discussed by workshop panelists, there was no clear consensus on how to use computation to improve manufacturing processes. Among potential goals for models, the use of multiphysics in modeling the manufacturing process is an interesting and

⁴⁰ Berman, Diana, Sanket A. Deshmukh, Subramanian K. R. S. Sankaranarayanan, Ali Erdemir, and Anirudha V. Sumant. 2015. "Macroscale superlubricity enabled by graphene nano-scroll formation." *Science* 348(6239): 1118-1122. doi.org/10.1126/science.1262024.

important subtopic for research. For example, workshop presenters described the ShAPE process, or the so-called Covetic process, involving high current in metal–carbon melts, but neither of these processes pursued at national laboratories has been realistically modeled, and both have process optimization challenges ahead.

5.4 Key Findings

A surprising preliminary finding of this session was that enhanced conductivity seemed to be observed only in metastable compositions. If proven with additional research, this finding has enormous implications for the successful fabrication of conductivity-enhanced materials. Any fabrication technology (e.g., traditional melting/casting) that allows the composition to equilibrate may not yield microstructures demonstrating enhanced conductivity.

The session participants were in agreement that effective theory and modeling require a close linkage with existing and emerging characterization of samples that are fabricated with the intent to include the desired conductivity-enhanced characteristics. Relevant data and theories must be coupled to form an integrated and validated research program in this domain. The panels also concluded that theorists and modelers should work with materials researchers to co-design conductivity-enhanced materials through iterations of experiment and characterizations. Theory should be developed to explain what the experimentalists observe using advanced characterization methods across different length scales, feedback should be provided for design of experiments and characterization, and those results should be used to refine the theory. Ultimately, theory could guide materials design and processing.

The sessions highlighted that a coordinated effort in this domain will require large computational resources and teams of experts working toward a consensus on a strategy for the scale-bridging. The predictions and explorations of variabilities must be validated by measurements relating to the underlying phenomena, as was also discussed in other sessions of the workshop. In addition, the processes of manufacturing conductivity-enhanced forms (e.g., wire) ultimately used in applications from precursor materials need precise control of microstructure. Many metastable compositions can provide an increase in conductivity in small-scale samples but fail to maintain enhanced conductivity in more thermodynamically stable forms once manufactured in bulk. Therefore, theory and simulations can play a pivotal role in guiding understanding and the strategy for materials processing. Maintaining required strength, ductility, domain distributions, and macroscopic electrical conductance will require an interdisciplinary team effort.

Theory and multiscale modeling can be improved, and capabilities from other domains can enrich the discovery and development process. Modeling coupled with detailed characterization of material samples, and discovery and validation of the fundamental relationships between composition and microstructure, can identify potential pathways toward success. Speakers highlighted possible pathways toward an integrative approach for developing enhanced conductivity by increasing charge carrier densities and mobility in metal–carbon, alloys, and polymer composite formulations. The presenters indicated that searches for new and promising candidate conductivity-enhanced materials could be undertaken by closely coupling modern computational tools with experiment:

- In computational models for transport, traditional Kubo–Greenwood models using DFT showed convincing evidence of anisotropic conduction in aluminum alloys. Other speakers discussed multiple levels of theory, including some emerging models using a tight-binding approach that can reduce computational power needed to allow investigation of realistic, larger grain sizes and metal–carbon interfaces. Finally, multiscale computational methods were discussed, along with empirical numerical models for connecting the mesoscopic detail to macroscale performance of conduction for coarse-to-finer-scale understanding of enhanced conductivity. An emphasis was placed on conductivity and distribution of nanocarbon domains.
- Machine learning (ML) can open up a range of unexplored composition space. Monte Carlo Tree Search and related classical atomic-scale methods are used to rank metastable to stable configurations of metals

and nanocarbon domains. The challenge will be driving the power of ML toward guiding the exploration of metastable metal–nanocarbon composites where researchers can only begin to imagine the possibilities: from going beyond traditional crystallographic thinking and design experiments to determining the experimental viability of achieving such qualities in bulk samples. Additionally, ML and DFT methods can be combined to build more robust force field models for representing thermodynamic stability and local bonding for metal–nanocarbon domains using classical force field, trained using DFT calculated data and ML models for grain-level calculations.

Less discussed during the session was modeling of materials processing, mechanics, creep, and corrosion. Measurements need to be included across relevant voltage–temperature ranges for microstructures produced by different materials processing techniques. Training sets for validating theory and experiments must be built. Empirical and physics-guided multiscale theories can play a strong role in providing guidance and generate synthetic data for training ML models. These are other coupled dimensions of the problem in theory and modeling that need to be kept in mind. It is promising that researchers are pursuing approaches that can grow in maturity and predictive accuracy by combining experiments and measurements across different length scales to enhance our understanding of enhanced conductivity and realign current plans for investment in this area.

Key findings from the three panels are included in Table 5.1, Table 5.2, and Table 5.3.

Table 5.1 Key Findings from Atomistic-scale Simulation Panel

Main Discussion Points	High-Level Takeaways	Technical Challenges Identified	Outstanding Research Needs
- Atomic-scale theories and their effectiveness in screening the composition and grain orientations in highly conductive nanocarbon composites - State of theory and ability to use past progress to form a core theory group from DFT to tight-binding methods to show the aggregated set of tools for conductivity calculations	- Metastable states appear more likely to exhibit enhanced conductivity. - ML can point to metastable states of matter using thermodynamics simulations. - Fundamental building blocks of theory can provide conductivity and their real-space projections on crystalline materials, including Al and Cu-graphene. - Theory of metal–insulator transitions of oxides for rapid switching can be extrapolated successfully.	- The throughput of conductivity calculations needs to match ML output. New codes and scalable methods are under construction. - Theory is often hard to extrapolate to amorphous or highly defected interfaces formed by nanocarbon systems in complex metal alloys. - Oxides are poor mechanical representatives for conductors. More thinking is needed on how to fully build targets for materials processing.	- Taxonomy to categorize and quantify ML-identified structures and their conductivity probabilities - Measurements of conductivity and flow back to train ML prediction - Advanced materials synthesis with control of atomic-level structure and domain structure - Understanding of how interfacial structure, properties, and interactions, combined with mesoscale confinement, affect molecular motions and macroscopic properties in intrinsically heterogeneous materials

Table 5.2 Key Findings from Multiscale Simulation Approaches Panel

Main Discussion Points	High-Level Takeaways	Technical Challenges Identified	Outstanding Research Needs
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- Nanocarbon whiskers in metal alloys and their distribution can be important variables for both conductivity and mechanical performance. - State of theory on high-entropy alloys (HEAs) is highly accurate at predicting mechanical properties. - Conductivity in a large space is less well understood and can unleash the potential.	- Nanocarbon metal composites in mesoscale and conductivity calculations are promising. - HEAs are a well-understood and open space for innovation in enhanced conductivity. - Polymer electrolyte is of interest as a possible system for high conductivity and a large space for effective characterization.	- Work shows promise and needs a closer look at volume ratios and maximum achievable performance. - HEAs or multi-principal element alloys are very good in mechanical and creep resistance alloy design. A comparison is needed with the current state of the art and identification of cost-performance advantages of HEAs, if any. - Most examples come from the lithium-ion domain. It was not clear whether it can compete and provide the current density needed.	- Better alignment between multiscale theory and data from materials processing to evaluate performance of the models - Conductivity measurements for HEAs and polymers to compare the possible conductivity values and to demonstrate whether they are in the ballpark of cost and performance to emerge as an alternative - More work on microstructural models, with prediction of grain refinement from nanocarbon
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Table 5.3 Key Findings from Crosscutting Topics in Materials Simulation Panel

Main Discussion Points	High-Level Takeaways	Technical Challenges Identified	Outstanding Research Needs
- Theory from atomistic to mesoscale, with the addition of empirical and ML approaches, can crosscut the various size domains. - Empirical theories on conductivity and multiscale approaches can provide an ecosystem for experimental researchers.	- Thermal conductivity in Cu-C as starting point with a Green-Kubo approach with DFT and force-field-derived insights - Multiscale empirical models and use of ML to solve the challenge - Using theory to address the complexity of the metal-polymer-nanocarbon composite space using a systematic approach from molecular-level theories	- Connecting the overall better understanding of thermal conductivity to Kubo-Greenwood-type models for conductivity using tight-binding - Establishing a better definition of data sources for ML, avoiding an otherwise arduous path to training models - Providing better uncertainty quantification methods between the techniques and scales to provide confidence across theory/experimental communities	- Demonstrations confirming that ML in this domain can use empirical relationships and mesoscale data to form a predictive framework - Improved ways to extract structure and dynamical evolution of materials in operando - Integration of artificial intelligence and ML into the workflow for prediction and design of materials and manufacturing processes

Chapter 6: Conclusions

Feedback provided during the workshop and in the follow-up survey indicated that attendees were very pleased with the workshop. One long-time federal researcher noted it was “the best workshop I ever attended.” In addition, the CABLE team immediately used information shared at the workshop. For example, metrics for the CABLE Manufacturing Prize were modified based on information provided by one of the workshop presenters.⁴¹

During the workshop, attendees provided input and feedback on the CABLE program and its various aspects. Following the workshop, this feedback was distilled into this report. Creating this workshop report led the CABLE team to several key conclusions:

- The team had insufficiently emphasized several key parts of the research ecosystem in the initial development of the CABLE idea—most importantly, theoretical research, including especially research on thermal conductivity of non-metal and more careful measurements.
- Numerous detailed proposals and ideas were put forward for where the research focus should be in the different parts of the ecosystem.
- The individual projects in different parts of DOE and other agencies could greatly benefit from better coordination and comprehensive research management.

6.1 Research Ecosystem

Throughout the workshop, and particularly on its last day, multiple participants offered the perspective that there had previously been too much emphasis on fabrication and not enough on theory, modeling, and characterization. Participants noted that materials science, especially theory, modeling, and simulation, must be a major part of a successful CABLE effort (see “Why Theory, Modeling and Simulation is Urgently Needed – An Example” in Section 6.2).

During the last day of the workshop, the CABLE team started to revise the research ecosystem map for the overall effort. After the event, the revision was further simplified based on all inputs from the workshop. Figure 6.1 shows key details of the ecosystem entering the workshop. After the workshop, the organizers proposed a third major thrust in theory and modeling. In addition, characterization work was added to the materials fabrication thrust, and fabrication scale-up was added to the applications area. Figure 6.2 shows how existing elements of CABLE SBIR and the CABLE Conductor Manufacturing Prize could fit into the expanded ecosystem. The post-workshop CABLE research ecosystem has less emphasis on overall applications and much greater focus on materials development, including theory and characterization, and on the FY 2021 SBIR and seedling awards.

⁴¹ Pasquali, Matteo. 2021. “Rethinking the conductor challenge: we must leap-frog metals by 2030.” PowerPoint Presentation, Virtual DOE/AMO CABLE Workshop, April 7. chptap.lbl.gov/profile/381/CABLE_1-3-1_03_Pasquali.pdf.

Original CABLE Research Ecosystem

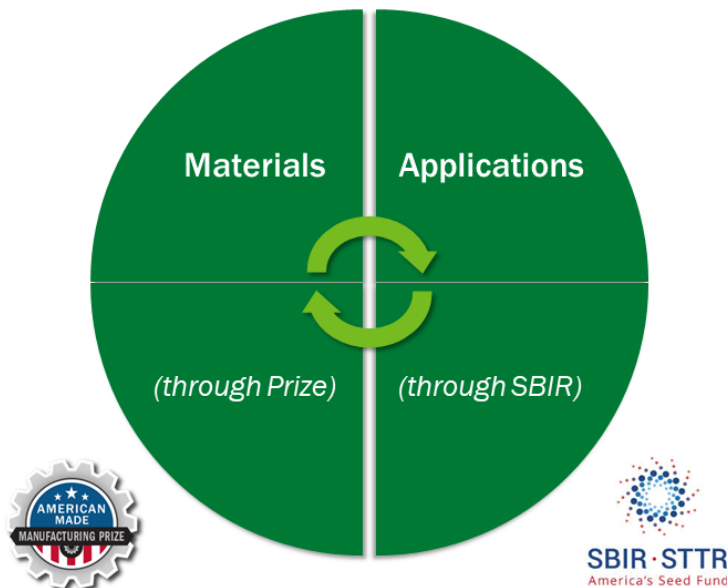


Figure 6.1 CABLE research ecosystem before the workshop. With this approach, multiple small independent efforts are undertaken to explore and fabricate samples of conductivity-enhanced materials.

New CABLE Research Ecosystem

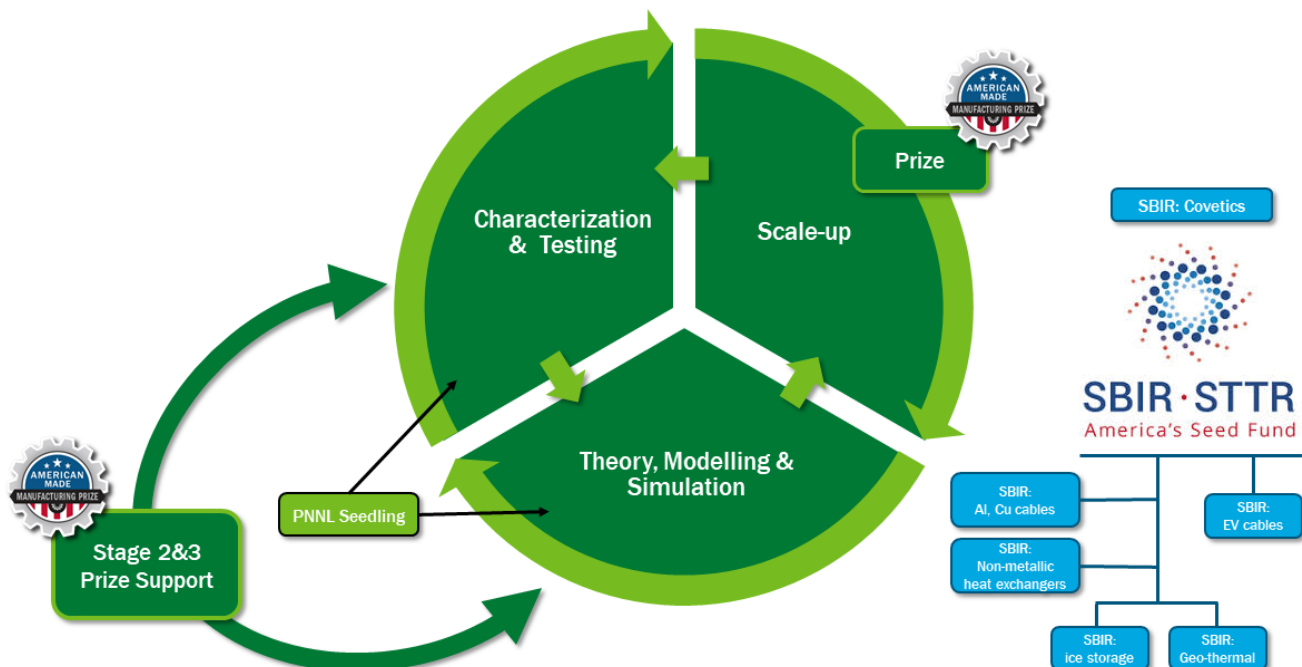


Figure 6.2 Updated CABLE research ecosystem, with linkages to Conductor Manufacturing Prize and SBIR components. The CABLE effort seeks to establish a technical basis for creating conductivity-enhanced materials. This will require theory, modeling, and simulation, fabrication from small samples to scalable processes, and characterization and testing to confirm compositions, properties, performance, and scientific understanding. This iterative, cyclical development loop can apply to technical ideas from innovators throughout the ecosystem and across government agencies.

6.2 Research Directions

The workshop participants extensively discussed priority scientific directions. Each of the research ecosystem elements below, and recommendations for their respective focus areas, were discussed in detail.

Theory, Modeling, and Simulation

While expanding the understanding and modeling of a conductor from atomic scale to a realistic prediction at macroscopic scale is challenging, exponential improvements in theory, modeling, simulation, and computation make it now within reach—at the cost of applying computational science expertise and intensive computing power. CABLE participants noted that any investment in materials fabrication must be guided by an understanding of a plausible mechanism for enhanced conductivity, which in turn is supported by detailed characterization. While the theory and modeling presentations were intriguing, they all were quite preliminary, and more resources are needed (see “Why Theory, Modeling and Simulation is Urgently Needed – An Example” below).

Conducting research on the theoretical underpinnings of conductivity starts at the atomic level, with understanding the new types of bonding modalities that can increase electron density and electron mobility. Improved modeling at the mid-length scale—or “mesoscale”—also is greatly improved, especially with the advent of ML approaches fed by increasing experimental and simulated data. For enhanced conductivity, resources are becoming available for “atomistic” or “first principles” quantum mechanical calculations of interfaces at the atomic level, as well as mesoscale calculations that identify grain size and other micron-scale configurations that can have positive or negative impacts on conduction processes. DOE is about to launch exascale (billion billion floating point operations per second) speed computing and has the computational science experts to utilize those resources. Thus, the computing power to understand conductivity mixtures of materials from first principles is now available. In addition to computing and data-intensive “brute force” approaches, smaller-scale efforts with scalable and validated approaches to reduce the cost of first principles and ML also are needed. Workshop participants had specific suggestions:

- AMO should consider partnering with the Office of Science (SC) and its Basic Energy Sciences program (BES) on materials theory, modeling, and simulation, especially with the Nanoscale Science Research Centers. Rigorous modeling and characterization activities require sustained funding. Investors (federal or private) are reluctant to invest in the risky area of electrical conductivity-enhanced materials until a scientific understanding promising economically attractive and scalable production has been achieved. The workshop organizers noted that the BES workshop report on [*Basic Research Needs on Transformative Manufacturing*](#), which was released around the time of the CABLE workshop, could serve as a guide for how to apply basic science capabilities to CABLE R&D problems—especially the sections on precision synthesis and multiscale modeling. AMO–BES coordination in this area is crucial.
- CABLE Conductor Manufacturing Prize applicants whose materials demonstrate enhanced conductivity should be awarded vouchers to work with a DOE national laboratory to help understand the fundamental scientific basis for the enhancement, particularly from a theory, modeling, and simulation standpoint. To this end, AMO should consider partnering with EERE’s NREL, the Office of Fossil Energy’s National Energy Technology Laboratory (NETL), SC’s ten laboratories, and National Nuclear Security Administration’s three laboratories to ensure this option is made available.

Why Theory, Modeling and Simulation is Urgently Needed – An Example

The workshop showed that there is a lack of definitive/scientific proof that enhanced electric conductivity is achievable in a bulk material at room temperature. The workshop also showed a historical lack of comprehensive rigorous experiments or methods of testing that are grounded in theory. The modelers’ preliminary finding that enhanced electrical conductivity seemed to be observed only in metastable compositions has enormous implications for both the materials fabrication and the scale-up portions of the CABLE initiative. If confirmed with additional research, this finding could lead to the successful fabrication of

conductivity-enhanced materials at the bulk scale. The finding implies that any scaled-up fabrication technology (e.g., traditional melting/casting) that allows the composition to equilibrate may reduce conductivity. The scale-up processes typically used allow the conductivity-enhanced material to attain more thermodynamically stable forms without the microstructural features typically associated with enhanced conductivity. In addition, this finding provides a key focus for both microfabrication and scale-up. With some additional validation, compositions and processes that do not create and/or maintain metastable microstructures might be eliminated from consideration, thus enabling a more focused R&D effort.

Nanofabrication, Characterization, and Testing

Specific research suggestions related to enhancing and measuring electric and thermal conductivity are grouped into four categories: (1) nanofabrication, (2) characterization, (3) testing, and (4) a library to link them.

Nanofabrication: There is a need for plausible scientific explanations describing the physical mechanism(s) for enhanced electric and thermal conductivity for given materials combinations/processing. AMO might partner with SC, BES, or the National Science Foundation on accelerated fundamental materials science for conductor fabrication as an initial target for future CABLE research. From this, first principles as well as thermodynamic modeling should give insights into potentially promising compositions for conductivity-enhanced materials. In turn, high-throughput fabrication of small (nanoscale) samples with varying composition can be combined with characterization to create data to develop model parameters or perform ML.

Characterization: High-priority theory work requires a steady stream of reliable information from a robust characterization effort. Large amounts of data are needed—including from in operando characterization—for both phenomenological analytic and ML models. These, as well as first principles models that have predictive power to reveal a plausible mechanism for enhanced conductivity, would greatly increase investor confidence and point researchers in the best directions to enhance conductivity. Specifically, AMO might consider working with SC, including BES, to enable participants in the CABLE initiative to access user facilities with resources such as x-ray light sources (e.g., ANL's Advanced Photon Source) and their characterization tools, such as ultra-small-angle x-ray scattering (see Appendix B for more examples).

Testing: Given all the uncertainties and difficulties identified at the workshop regarding accurate measurement of both electrical and thermal conductivity, it is vital to develop and standardize procedures that are more reliable and less prone to error for the measurement of conductivity of small-area samples. This would enable an accurate evaluation of research progress. For Stage 2 of the CABLE Conductor Manufacturing Prize, appropriate protocols need to be developed for testing conductivity-enhanced materials, and at least three testing sites should be certified for these protocols. In parallel with electrical conductivity, standard methods for measuring thermal conductivity should be developed and available at three different sites. In addition, CABLE prize competitors and other participants in CABLE activities should have access to user facilities and other resources (see Appendix B) for conductivity measurement that are staffed with personnel familiar with the multiple methods available and the preferred method(s) for a given type and size of material. Standardized procedures should also be developed for needed material measurements and testing for other key properties, such as density and specific heat.

Library: In addition to systematic high-throughput fabrication of various compositions, there should be an effort in systematic characterization and uniform conductivity testing of all known nanoscale conductivity-enhanced materials. One interim goal of the CABLE prize is to begin to establish a virtual library of such characterization and conductivity testing results that includes curation of the materials. Other CABLE initiative efforts, such as the SBIR projects, should also contribute to this library. Establishment of a user-friendly library that stores high-quality fabrication and characterization data for the theory, modeling, and simulation communities could be critical to the success of CABLE and enable ecosystem participants to have access to

fundamental pre-competitive knowledge. The library should distinguish between the properties of materials and the use and implications of such materials in applications.

Interrelationships between Electric and Thermal Conductivity

Because electrical conductivity is a measure of how well electrical current (electrons in motion) can pass through a material under the influence of an applied voltage/electric field, most good electrical conductors—and, by definition, metals—should also conduct heat well (where the quantum of thermal energy is called a phonon). Table 4.2 shows that there are very few non-metals (e.g., nanocarbons and semiconductors) with both high thermal and electrical conductivity. There are also metal-based “thermoelectrics” that have high electric and low thermal conductivity. Finally, as shown in Table 4.1 and Table 4.2, the converse—that most good thermal conductors are good electric conductors—is generally not true for non-metals. For example, graphite and doped silicon (in Table 4.1) and doped graphene fiber (in Table 4.2) are excellent thermal conductors, but their electrical conductivity is so low that they can be classified as electrical insulators. Other materials in this class include those used for insulating transistors from their heat sinks and some exotic materials, such as superconductors and vanadium dioxide, under some circumstances. Recently, scientists have probed these exceptions and discovered that dynamic behaviors of electrons and phonons in metals have been misunderstood.⁴² Specifically, it has been discovered that while models of electron heat transfer at ordinary temperatures suggest electrons and phonons are correlated, femtosecond spectroscopy of metals has recently shown that their electrons and phonons re-equilibrate nearly independently. In addition, while these electronic transfer models agree with thermal conductivity data, they fail to predict thermal diffusivity data. To understand these discrepancies, researchers separately measured electronic and phononic components and discovered that (nearly) free electrons absorb and transmit only a small fraction of the incoming heat, whereas phonons absorb and transmit the majority. These new discoveries suggest that enhancement of thermal and electrical conductivity can be explored separately.

Scale-up of Fabrication and Applications

As noted throughout, scale-up of enhanced electrical conductivity materials from the nano to the bulk scale has been challenging and not yet documented in a peer-reviewed publication. Preliminary modeling results suggest why this has been the case. In particular, the preliminary indication is that nanocarbon metals must be in a metastable state to exhibit enhanced conductivity; if this finding is proven to be more generally true in both experimental and theoretical efforts, it will guide more detailed modeling work that, in turn, will guide scale-up efforts. Although electric and thermal conductivity are often correlated and desired in similar applications (see Applications for Electric Conductivity and Applications for Thermal Conductivity, below), for application research, having separate tracks would likely be beneficial. For all applications, desirable properties and temperature ranges should be developed and regularly updated. New tools could be developed to enable additive manufacturing processes to manufacture smart composite materials that can be used in both enhanced electric and thermal systems.

Applications for Electric Conductivity

Conference organizers noted that there were no private-sector speakers on any of the applications panels. Until material with enhanced electrical conductivity can be scaled up to bulk form, application-directed R&D for electrical applications is probably premature, and it should be de-emphasized until theory and modeling can provide further guidance on scaling up fabrication. Nanoscale thin film applications may be an exception.

Applications for Thermal Conductivity

Unlike the case with enhanced electrical conductivity, enhancement of thermal conductivity at the bulk scale has been shown—at least in non-metals. Hence, application-directed R&D for some non-metal thermal applications is promising. Thermal conductivity has many different applications, and (as was pointed out in the workshop) its anisotropic nature can result in advantages in energy systems. Thermal conductivity-enhanced

⁴² Criss, Everett M. and Anne M. Hofmeister. 2017. “Isolating lattice from electronic contributions in thermal transport measurements of metals and alloys above ambient temperature and an adiabatic model.” *International Journal of Modern Physics B* 31(14): 1750205. doi.org/10.1142/S0217979217502058.

applications that are close to commercialization, such as the non-metallic SBIR heat exchanger awards, should continue and possibly be expanded.

6.3 CABLE Research Management and Coordination

Workshop participants made multiple suggestions for improving the management and coordination of government-sponsored CABLE-related research. Overall, the workshop revealed that, to date, there had been very little coordination and sharing of information and common goals among the multiple federal agencies and programs doing conductivity-related research. While this and any future CABLE workshops were a good beginning point for such sharing, participants concluded that there is an urgent need for a more sustained mechanism to coordinate efforts by various agencies working on conductivity-enhanced materials. At the project level, past efforts showed a history of multiple short-lived and uncoordinated projects that failed to develop conductivity-enhanced materials at the bulk scale. All this suggests the need for coordination at three levels—agency, program, and project—with an integrated strategy and sustained funding. Workshop participants had specific suggestions:

- A fabrication-oriented entity, such as AMO, should take the lead in coordinating efforts among agencies and programs aimed at conductivity-enhanced materials.
- AMO might revise its Conductor Manufacturing Prize Stage 2 and 3 rules to include elements of theory and characterization, including items suggested under Section 6.2.
- Other CABLE-funded efforts, such as DOE SBIR projects, or efforts at other agencies should be connected to expert modelers who can assist in determining pathways to successful conductivity enhancement as part of a system-focused co-design effort, as detailed under Section 6.2.
- AMO and SC BES might coordinate efforts on topics recommended under Section 6.2.
- AMO is encouraged to establish linkages through the CABLE community to all the potential partners listed in Table 6.1 and explore efforts to manage RDD&D of conductivity-enhanced materials as a multi-institutional collaboration, with a single leadership organization, integrated strategy, and sustained funding.

Table 6.1 Potential AMO Partners for Recommended Future Activities

Major Conclusion	Potential Partners
Theory, modeling, and characterization efforts	SC\BES\Nanoscale Science Research Centers, SC's Advanced Scientific Computing Research Program, National Nanotechnology Initiative, National Science Foundation
Research on fabrication and scale-up, including testing	DOE laboratories, private partners
Comprehensive research management and coordination	Across EERE, SC, ARPA-E, NASA, Office of Electricity, U.S. Department of Defense

Appendix A. Agenda

All presentations from the Workshop are linked within the agenda below, hosted on the CABLE initiative website: cable-bigidea.anl.gov/workshop/.

Day 1 – Wednesday, April 7			
Time (ET)	Segment	Speaker/Panelist	Presentation Link
11:30 AM – 12:00 PM	Opening Plenary	• Tina Kaarsberg (DOE-AMO) • Mike McKittrick (DOE-AMO)	Welcome from Organizers Welcome from the DOE Overview of CABLE
12:00 – 12:35 PM	Applications Panel Session 1	Moderator: Andre Pereira (DOE Office of Electricity) Speakers: • Benjamin Shrager (DOE Office of Electricity) • Joe Hagerman (ORNL) • Iver Anderson (Ames Laboratory)	Electric Delivery Systems • Electricity Delivery System Overview • Transformer Resilience and Advanced Components • Al/Ca Composite Conductor Characterization
12:35 – 1:30 PM	Applications Panel 2	Moderator: Isik Kizilyalli (ARPA-E) Speakers: • Timothy Haugan (U.S. Air Force Research Laboratory) • Maricela Lizcano (NASA) • Lynn Petersen (Office of Naval Research) • Burak Ozpineci (ORNL) • Don Hillebrand (ANL)	Transportation • Advanced Electric Conductors for Aerospace Transportation • Materials Research Activities for High Voltage Power Transmission Cables in Electric Aircraft Propulsion • Risk Reduction Research: DC Cables for Electric Ships • Enhanced Conductors for EVs • Ground Transportation Considerations
1:30 – 2:15 PM	Facilitated Session	• All speakers and attendees • Moderators: Emmanuel Taylor and Ridah Sabouni (Energetics)	Facilitated discussion on energy delivery systems and transportation applications

2:15 – 2:45 PM	Break		
2:45 – 3:15 PM	Applications Panel 3	Moderator: Fredericka Brown (DOE BTO) Speakers: • Kashif Nawaz (ORNL) • Jason Woods (NREL) • Matteo Pasquali (Rice University)	Efficiency • Non-metallic heat exchangers for energy conversion systems in buildings and beyond • Rate Capability and Ragone Plots for Phase Change Thermal Energy Storage • Carbon Hub: Rethinking the conductor challenge: we must leap-frog metals by 2030
3:15 – 4:00 PM	Applications Panel 4	Moderator: Jian Fu (DOE WETO) • Eduard Muljadi (NREL) • Nate McKenzie (DOE WETO) • Bill Vandermeer (DOE GTO) • Susan Huang (DOE SETO)	Renewables • Renewables Applications • Wind Energy • Geothermal Applications for Enhanced-Conductivity Materials • Metallization and Cables in Photovoltaics
4:00 – 4:45 PM	Facilitated Discussion	• All speakers and attendees • Moderators: Emmanuel Taylor and Ridah Sabouni (Energetics)	Facilitated discussion on efficiency and renewables applications
4:45 – 5:00 PM	Day 1 Close	Tina Kaarsberg (AMO)	Closing remarks for Day 1 and preview of Day 2

Day 2 – Thursday, April 8

Time (ET)	Segment	Speaker/Panelist	Presentation Link
11:30 – 11:40 AM	Welcome	• Emily Evans (NREL)	CABLE Conductor Manufacturing Prize

11:40 AM – 12:20 PM	Materials Fabrication Panel 1	Moderator: Brian Valentine (DOE AMO) Speakers: • Saniya LeBlanc (George Washington University) • Mehran Tehrani (University of Texas at Austin) • Keerti Kappagantula (PNNL) • Balu Balachandran (ANL)	Metal/Nanocarbon Conductors • Thermal Metrology to Measure Thermal Conductivity • Advanced Electrical Conductors: An Overview and Prospects • Enhanced Conductivity Composites using Solid Phase Processing • Fabrication of CABLE Materials by Industrially Viable Process (aka 'Covetics')
12:20 – 1:00 PM	Materials Fabrication Panel 2	Moderator: Chris Hovanec (DOE AMO) Speakers: • Nhon Vo (NanoAL, LLC) • Alex Plotkowski (ORNL) • Jon McCrea (Integran) • John Hryn (ANL)	Metal Enhanced without Nanocarbons • NanoAl Technologies for Wire and Cable Applications • Microstructure Control using Additive Manufacturing • Nanostructure Enabled High Strength Electrical Conductors • Copper-Rare Earth Alloys from China
1:00 – 1:30 PM	Materials Fabrication Panel 3	Moderator: Tony Bouza (DOE AMO) Speakers: • Dan Gianola (University of California, Santa Barbara) • Chuck Booten (NREL) • Michael Ohadi (University of Maryland)	Polymers and Other Non-metallic • Flexible Composites with Programmable Electrical (and Thermal) Anisotropy Using Acoustophoresis • Far Infrared Fiber Optics for Heat Transfer • High-conductivity Polymer Composite Conductors for Thermal Management– Case Examples
1:30 – 2:30 PM	Facilitated Session	• All speakers and attendees • Moderators: Emmanuel Taylor and Ridah Sabouni (Energetics)	Facilitated discussion on materials fabrication
2:30 – 2:45 PM	Break		

2:45 – 3:20 PM	Materials Modeling and Computation Panel 1	Moderators: George Maracas (BES) and Santanu Chaudhuri (ANL) Speakers: • Subramanian Sankaranarayanan (ANL) • David Drabold (Ohio University) • Panchapakesan Ganesh (ORNL)	Atomistic-Scale Simulation • Exploring Metastable Metal-nanocarbon Composites for Enhanced Electrical and Thermal Conductivity • Conduction in Aluminum and Copper: Defects and Impurities • Understanding Metal-Insulator Transitions in Correlated Oxides for Rapid Electrical Switching
3:20 – 3:50 PM	Materials Modeling and Computation Panel 2	Moderators: George Maracas (BES) and Santanu Chaudhuri (ANL) Speakers: • Pallab Barai (ANL) • Duane D. Johnson (Iowa State University/Ames Laboratory) • Rajeev Kumar (ORNL)	Multiscale Simulation • Multiscale Computational Model to Estimate Effective Properties for Metal/Carbon Nano Composites • Strong, lightweight “Mary Shelley” alloys for transmission lines • Modeling Structure and Ionic Transport in Polymer Electrolytes
3:50 – 4:20 PM	Materials Modeling and Computation Panel 3	Moderators: George Maracas (BES) and Santanu Chaudhuri (ANL) Speakers: • Maria Chan (ANL) • Angel Yanguas-Gil (ANL) • Bobby Sumpter (ORNL)	Crosscutting topics • Thermal Transport Modeling of C-in-Cu Nanoscale Inclusions • Why Cu-C Composites Underperform? • Molecular Modeling and Simulation of Hybrid Materials, Polymers and Polymer Nanocomposites
4:20 – 4:50 PM	Facilitated Discussion	• All speakers and attendees • Moderators: Emmanuel Taylor and Ridah Sabouni (Energetics)	Facilitated discussion on materials modeling and computation
4:50 – 5:00 PM	Day 2 Close	Tina Kaarsberg (AMO)	Closing remarks for Day 2 and preview of Day 3

Day 3 - Friday, April 9			
Time (ET)	Segment	Speaker/Panelist	Presentation Link
11:30 – 11:40 AM	Welcome	Tina Kaarsberg (AMO)	Opening remarks
11:40 AM – 12:30 PM	Plenary Talk 1	Moderator: Hal Stillman (Independent Consultant) Speakers: • Richard Collins (IDTechEx) • Joseph Saleh (former Fiske Alloy Wire) • Srini Siripurapu (Prysmian Group) • Terrence Barkan (The Graphene Council)	Supply Chain Outlook and Requirements for Enhanced Conductivity • Nanocarbons: Supply Chain Analysis and Market Outlook • Perspective on High Conductivity Copper Conductors • Supply Chain: Key Industry and Innovation Trends • The Graphene Council Overview
11:20 – 11:40 AM	Plenary Talk 2	Moderator: Hal Stillman (Independent Consultant) Speakers: • Keerti Kappagantula (PNNL) • Paul Jablonski (NETL) • Ben Gould (ANL) • Jeff Elam (ANL) • Michael Kirka (ORNL) • M. Parans Paranthaman (ORNL)	Available Technical Resources and Processing Capabilities • Available Technical Resources for Enhanced Conductivity Material Development • Melt Processing of Covetic Materials • Using the Advanced Photon Source to Investigating the Interface of Metal Nanocarbon Composites • Controlling the Carbon-metal Interface through Chemical Vapor Functionalization • ORNL/MDF Metal AM Capabilities • ORNL/MDF – Nonmetallic Capabilities
1:30 – 2:00 PM	Plenary Talk 3	Moderator: Hal Stillman (Independent Consultant)	Intellectual Property

		Speakers: • Hal Stillman (independent consultant) • Glen Drysdale (DOE)	• Global Overview: Patents Related to Conductivity-enhanced Materials • Patent Rights under Government Awards: Bayh-Dole
2:00 – 2:30 PM	Break		
2:30 – 3:30 PM	Facilitated Session	All speakers and attendees	Priority research directions
3:30 – 4:00 PM	Closing Remarks	Tina Kaarsberg (AMO)	Conclusions and next steps

Appendix B: Technical Resources: Facilities, Networks, and Intellectual Property

The speaker and participant input from Day 3 for Supply Chain, Topical/Facility Combined Talks, Facility Overviews, and Introductions are summarized in the tables below.

Table B.1 Facilities

National Laboratory Resources	User Facilities
• Manufacturing Demonstration Facility Additive manufacturing, and roll-to-roll processing @ ORNL • Carbon Fiber Technology Facility @ ORNL • ShAPE Solid phase processing and conductivity measurements @ PNNL • Covetecs Vacuum induction melting and direct current @ NETL • Chemical vapor and atomic layer deposition @ ANL • NASA laboratories • U.S. Department of Defense laboratories: Air Force Research Lab, Naval Research Lab, among others	• Advanced Photon Source @ ANL • Other light and neutron sources @ Brookhaven National Laboratory (BNL), Lawrence Berkeley National Laboratory (LBNL), ORNL, and Stanford Linear Accelerator Center (SLAC) • Nanoscale Science Research Centers: Center for Functional Nanomaterials @ BNL, Center for Integrated Nanotechnologies @ LANL and Sandia National Laboratories (SNL), Center for Nanophase Materials Sciences @ ORNL, Center for Nanoscale Materials @ ANL, The Molecular Foundry @ LBNL

Table B.2 Supply Chain and Relevant Resources

Supply Chain Presentations – See Day 3, Plenary Talk 1	Other Relevant Resources – See Day 3, Plenary Talk 2
• IDTechEx: Nanocarbon supply chain analysis and outlook • Fiske Alloy Wire: Copper alloy market • Prysmian Group (General Cable): Enhanced-conductivity requirements for advanced cable applications • The Graphene Council: Neutral representor of graphene users and producers	• Workshop read-ahead document • Advanced Electrical Conductors: An Overview and Prospects of Metal Nanocomposite and Nanocarbon Based Conductors • American-Made Network

Table B.3 Intellectual Property

See Day 3, Plenary Talk 3: • Global overview of patents related to conductivity-enhanced materials (Hal Stillman) • Patent rights under government awards (Glen Drysdale)	• Bayh–Dole Act allows universities and non-profit organizations to keep intellectual property ownership under a government contract; it does not apply to large businesses, foreign entities, or state/local governments. • iEdison helps many government agencies, including DOE, comply with the Bayh–Dole regulations and securely report inventions.
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